



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 11:42 AM EDT

PDB ID : 7TNT
EMDB ID : EMD-26020
Title : The tubulin-based conoid from detergent-extract *Toxoplasma gondii* cells
Authors : Sun, S.Y.; Pintilie, G.D.; Chen, M.; Chiu, W.
Deposited on : 2022-01-21
Resolution : 9.30 Å (reported)
Based on initial model : 7MIZ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

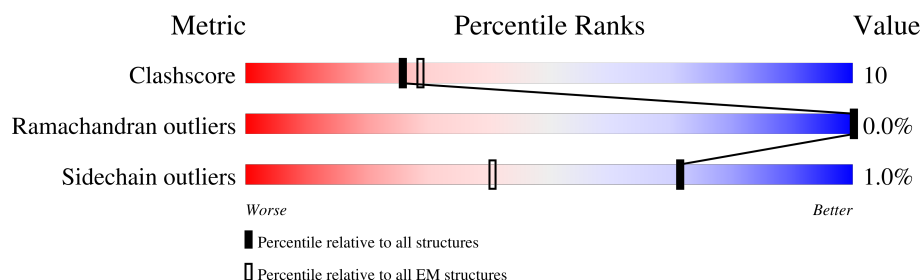
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2A	437	<div> <div>22%</div> <div>71%</div> <div>23%</div> <div>..</div> </div>
1	2B	437	<div> <div>27%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	2C	437	<div> <div>27%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	2D	437	<div> <div>33%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
1	2E	437	<div> <div>33%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>
1	2F	437	<div> <div>31%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	2G	437	<div> <div>30%</div> <div>67%</div> <div>27%</div> <div>...</div> </div>
1	2H	437	<div> <div>35%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	2I	437	
1	4A	437	
1	4B	437	
1	4C	437	
1	4D	437	
1	4E	437	
1	4F	437	
1	4G	437	
1	4H	437	
1	4I	437	
2	3A	426	
2	3B	426	
2	3C	426	
2	3D	426	
2	3E	426	
2	3F	426	
2	3G	426	
2	3H	426	
2	3I	426	
2	5A	426	
2	5B	426	
2	5C	426	
2	5D	426	
2	5E	426	
2	5F	426	

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Mol	Chain	Length	Quality of chain
2	5G	426	<div><div></div><div>38%</div><div>69%</div><div>26%</div><div></div></div>
2	5H	426	<div><div></div><div>38%</div><div>72%</div><div>25%</div><div></div></div>
2	5I	426	<div><div></div><div>23%</div><div>79%</div><div>19%</div><div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 119808 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2A	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2B	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2C	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2D	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2E	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2F	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2G	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2H	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	2I	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4A	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4B	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4C	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4D	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4E	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4F	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4G	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
1	4H	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4I	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

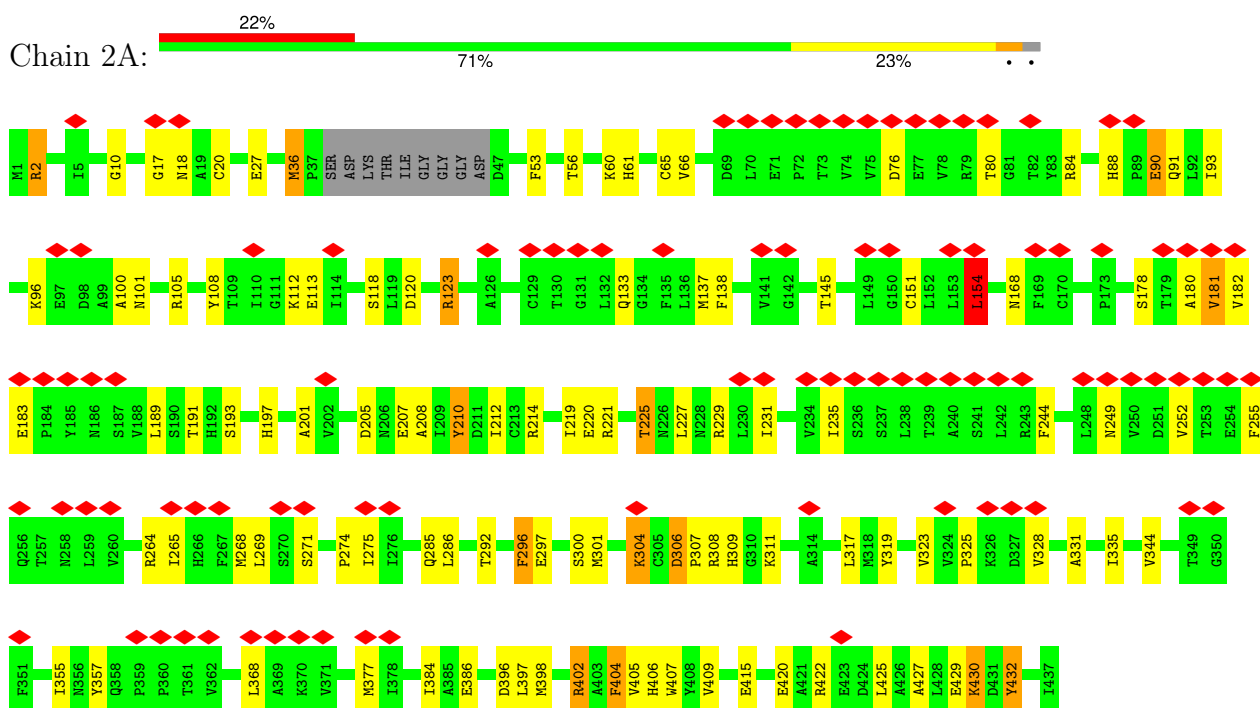
- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3A	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3B	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3C	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3D	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3E	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3F	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3G	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3H	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	3I	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5A	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5B	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5C	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5D	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5E	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5F	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5G	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5H	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
2	5I	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

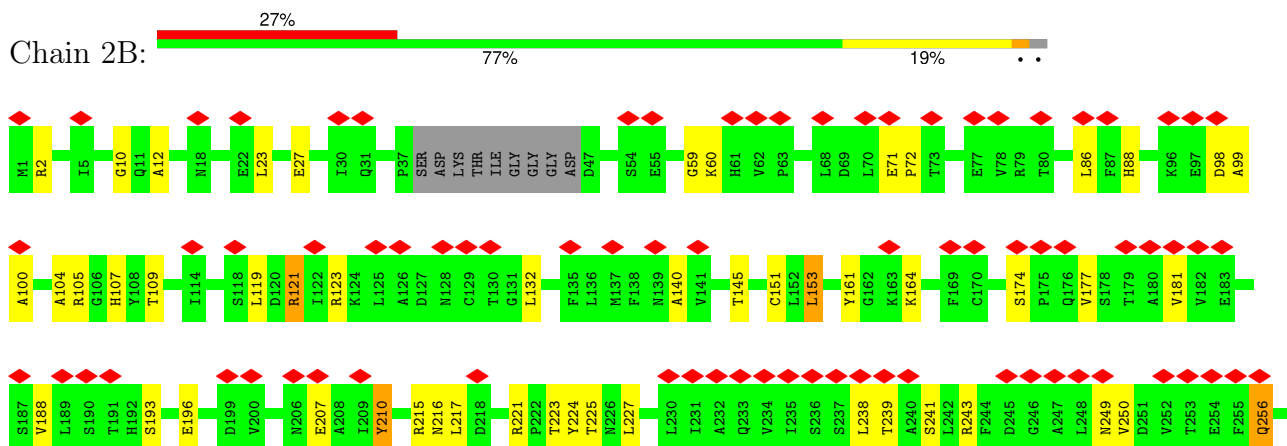
3 Residue-property plots

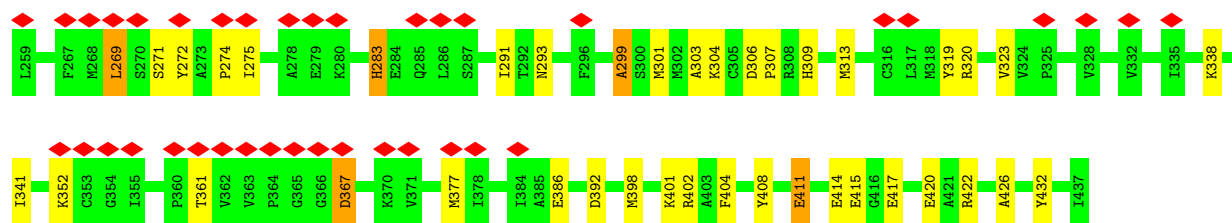
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha chain

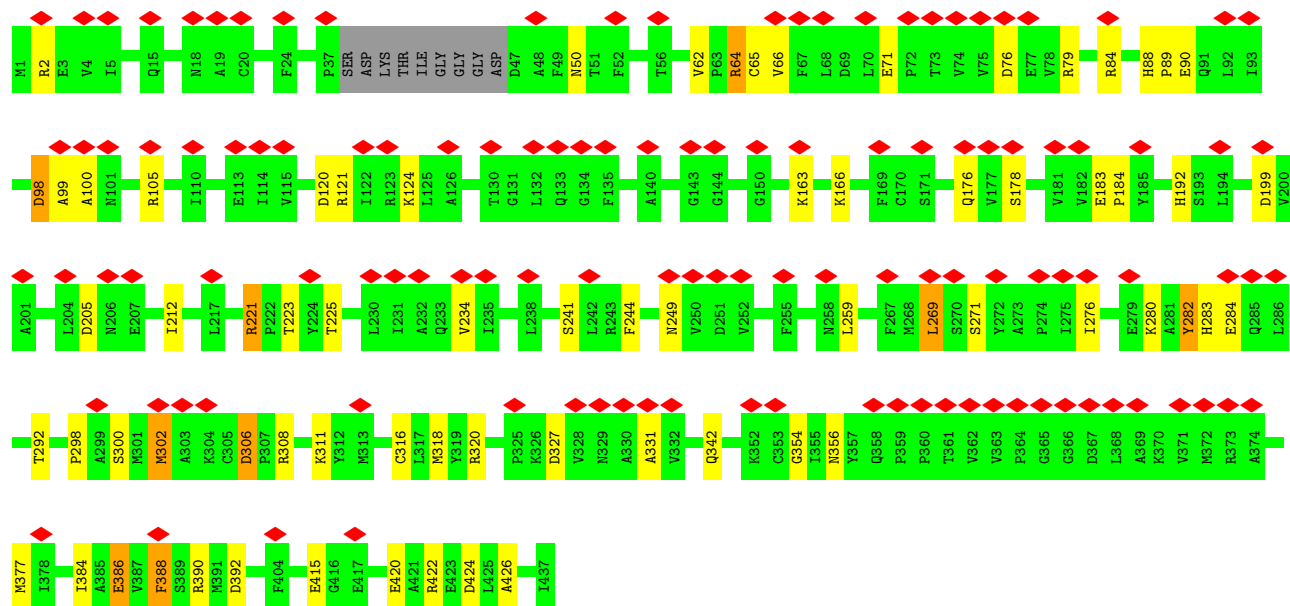
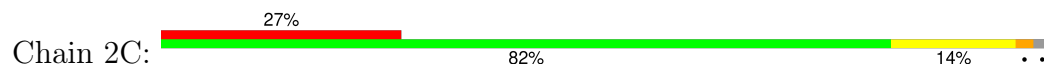


• Molecule 1: Tubulin alpha chain

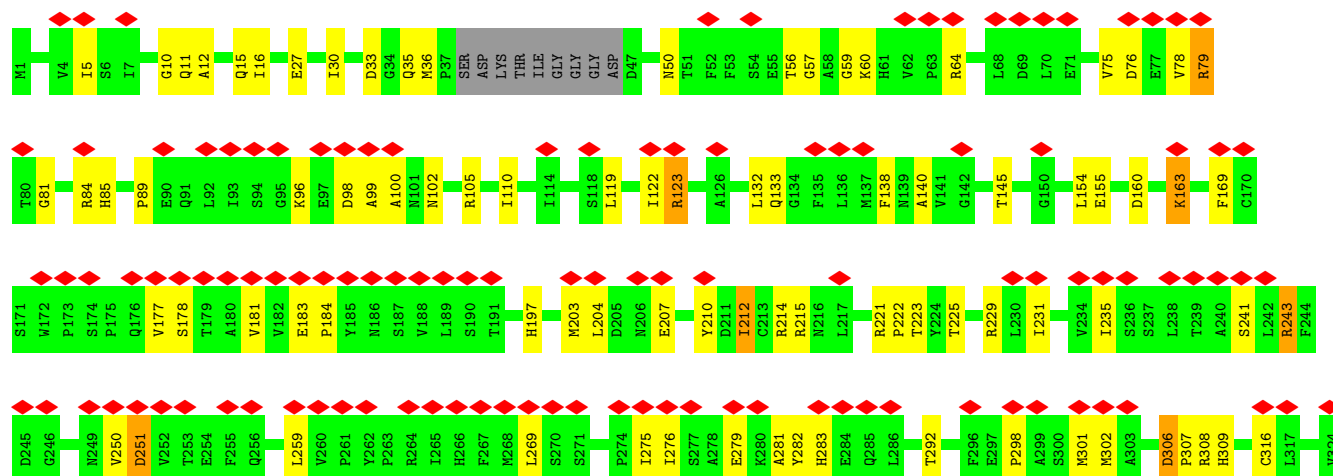
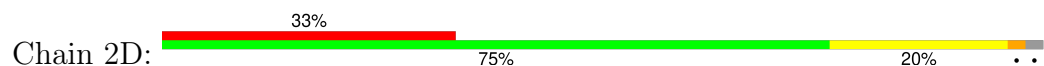


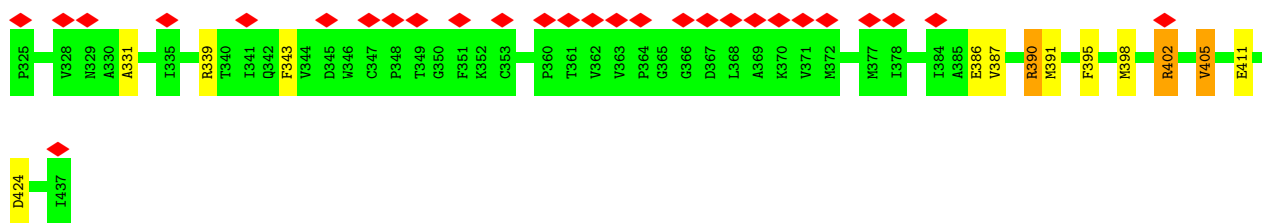


• Molecule 1: Tubulin alpha chain

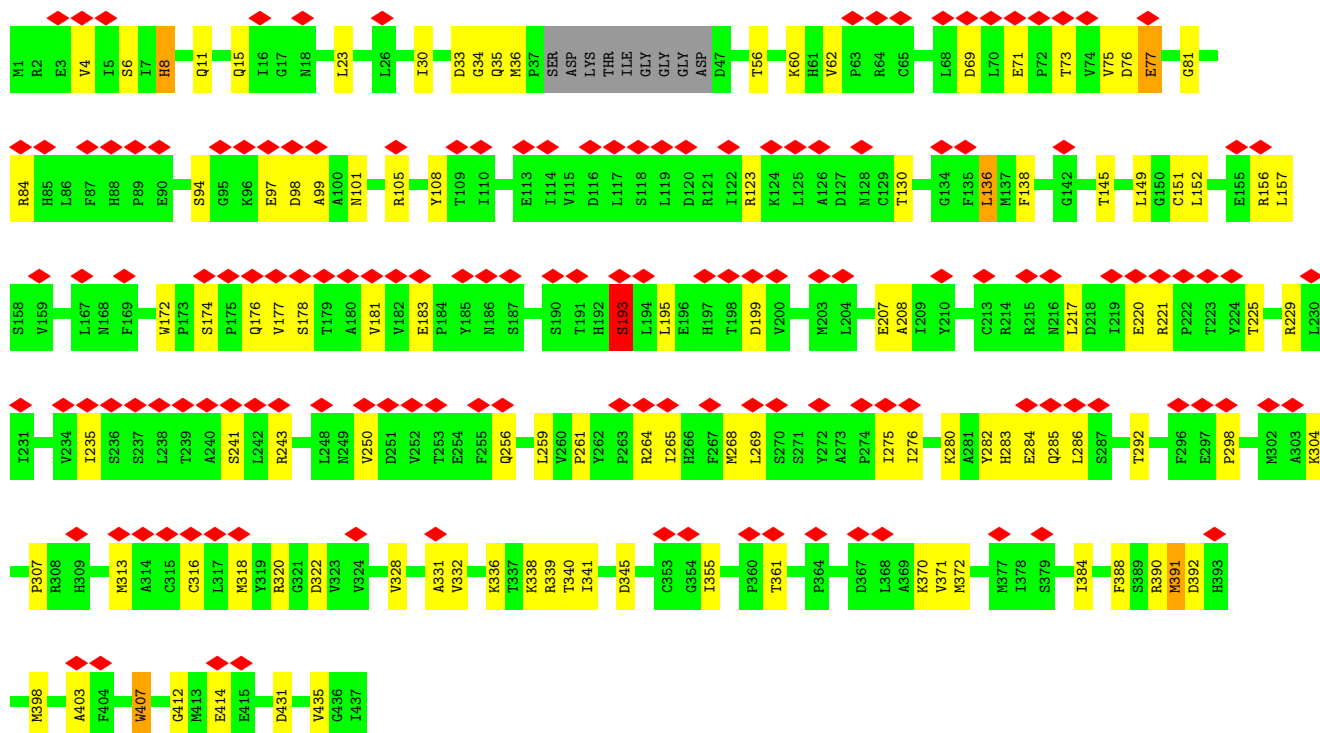
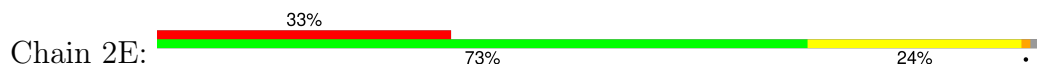


• Molecule 1: Tubulin alpha chain

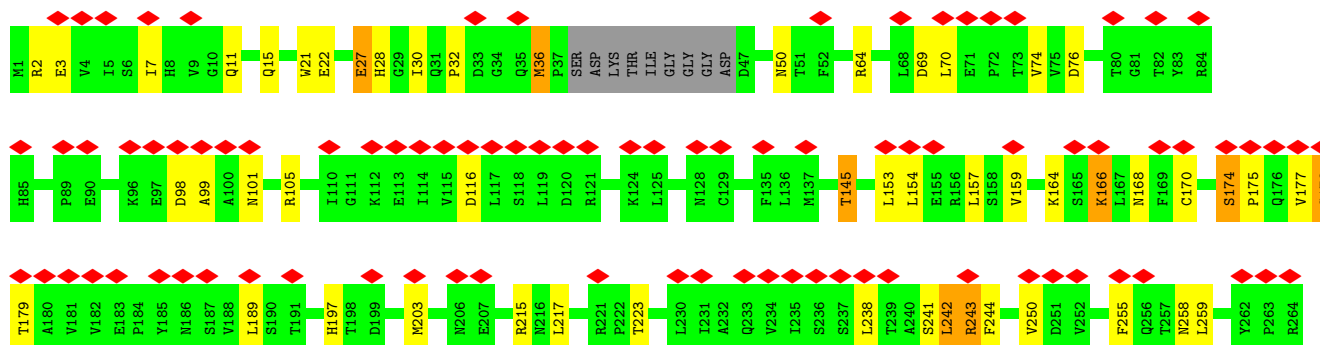
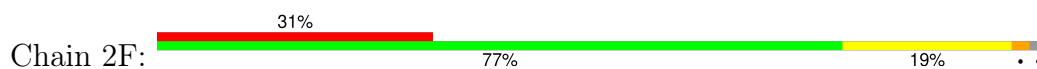


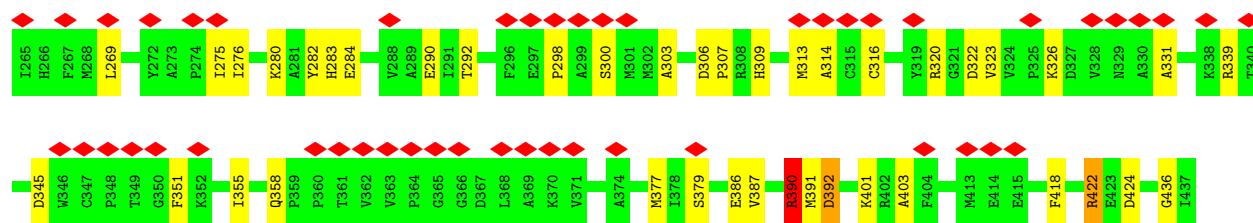


• Molecule 1: Tubulin alpha chain

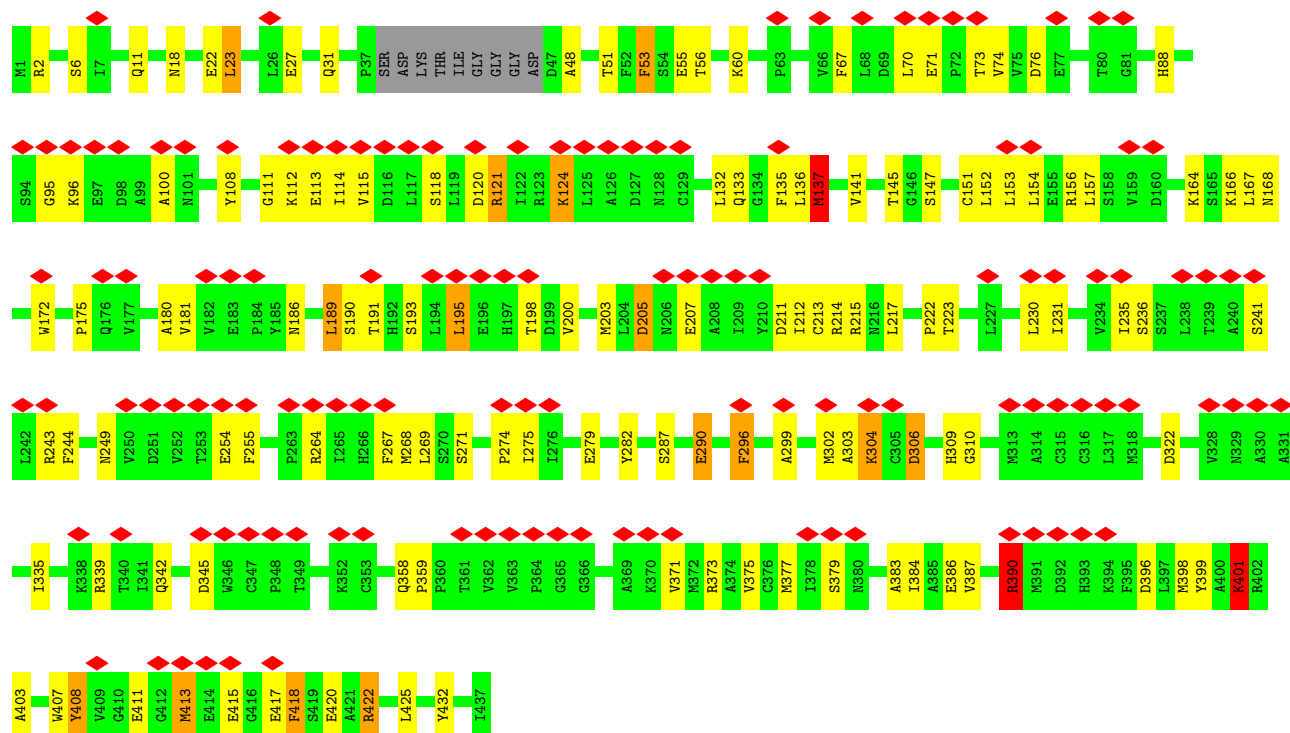


• Molecule 1: Tubulin alpha chain

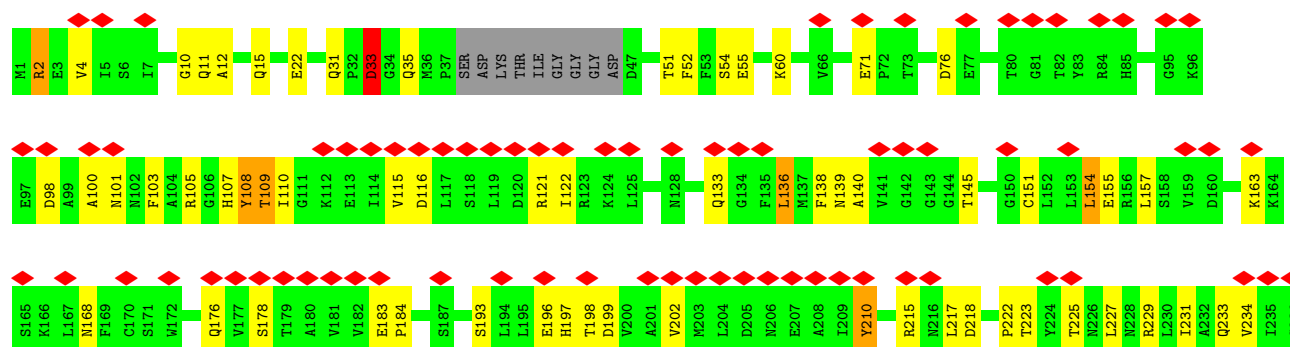
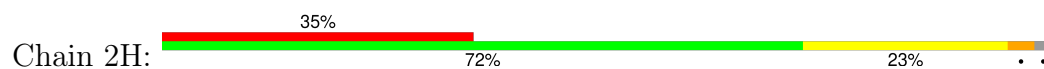


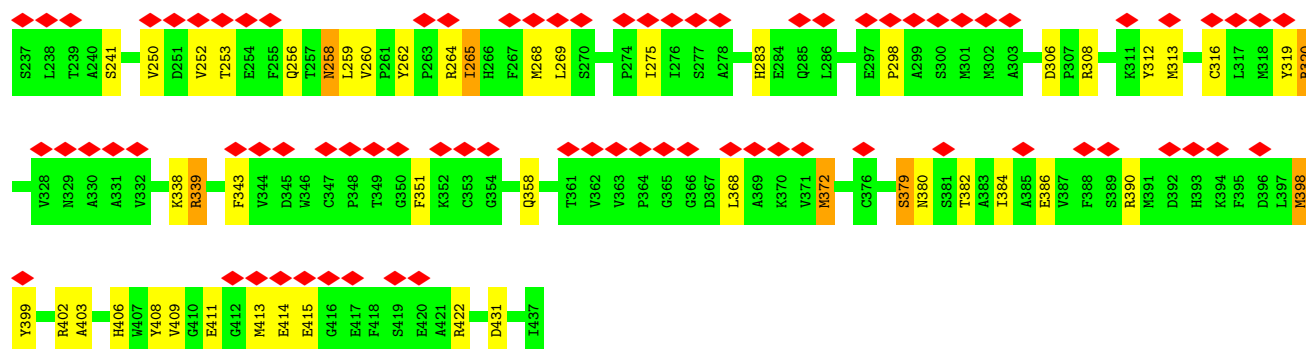


• Molecule 1: Tubulin alpha chain

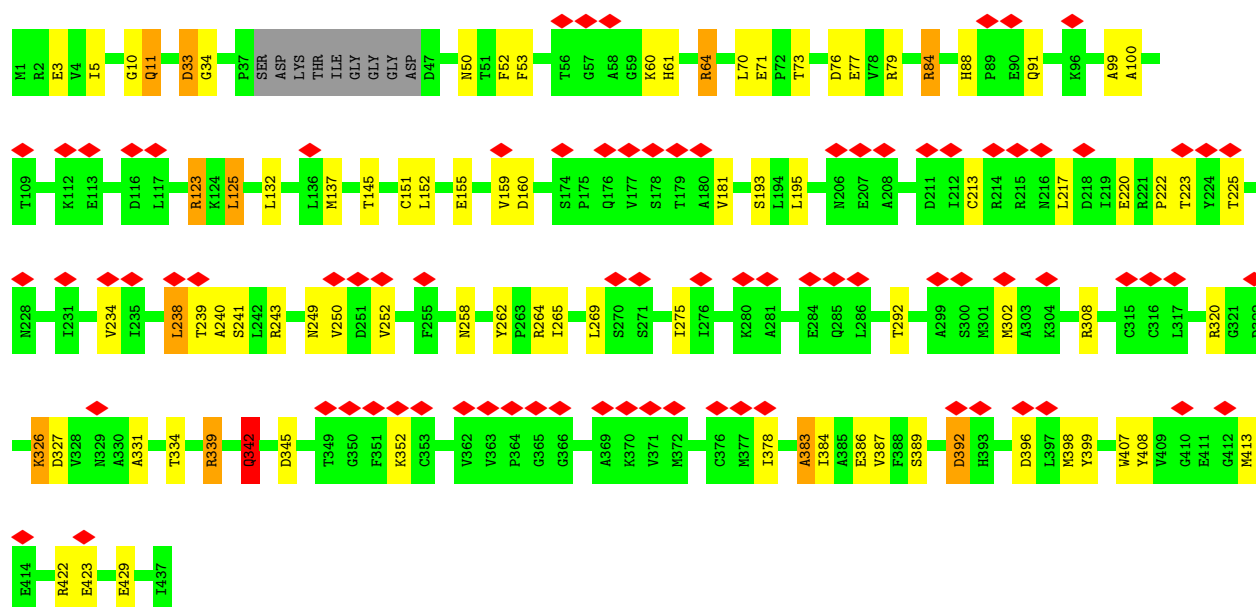
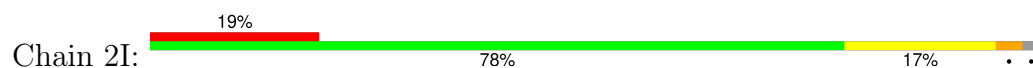


• Molecule 1: Tubulin alpha chain

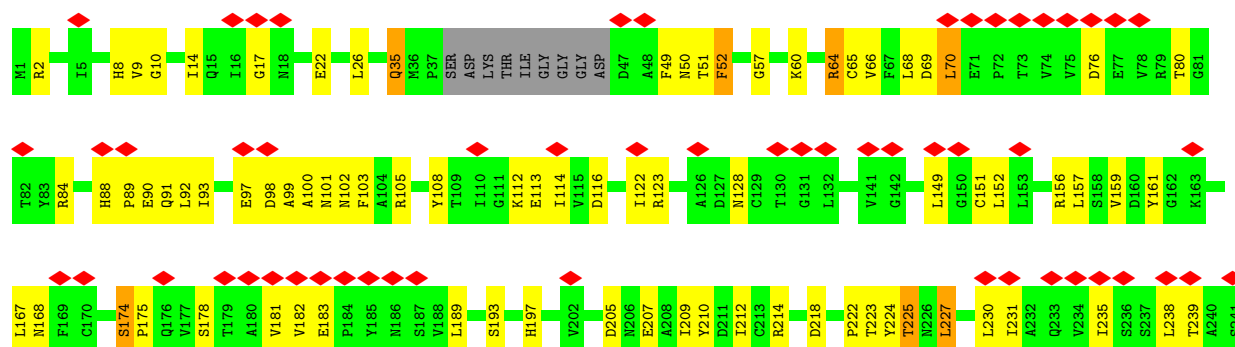


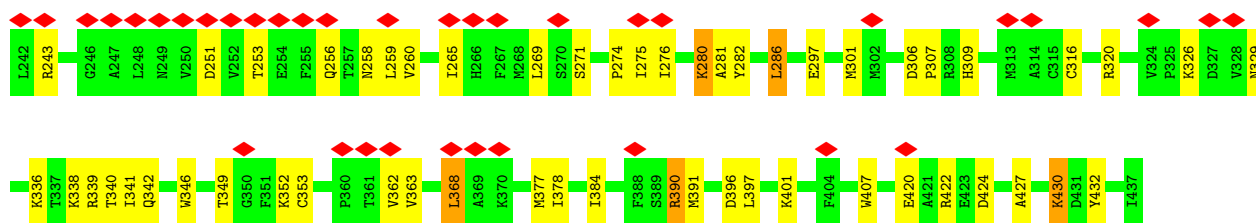


• Molecule 1: Tubulin alpha chain

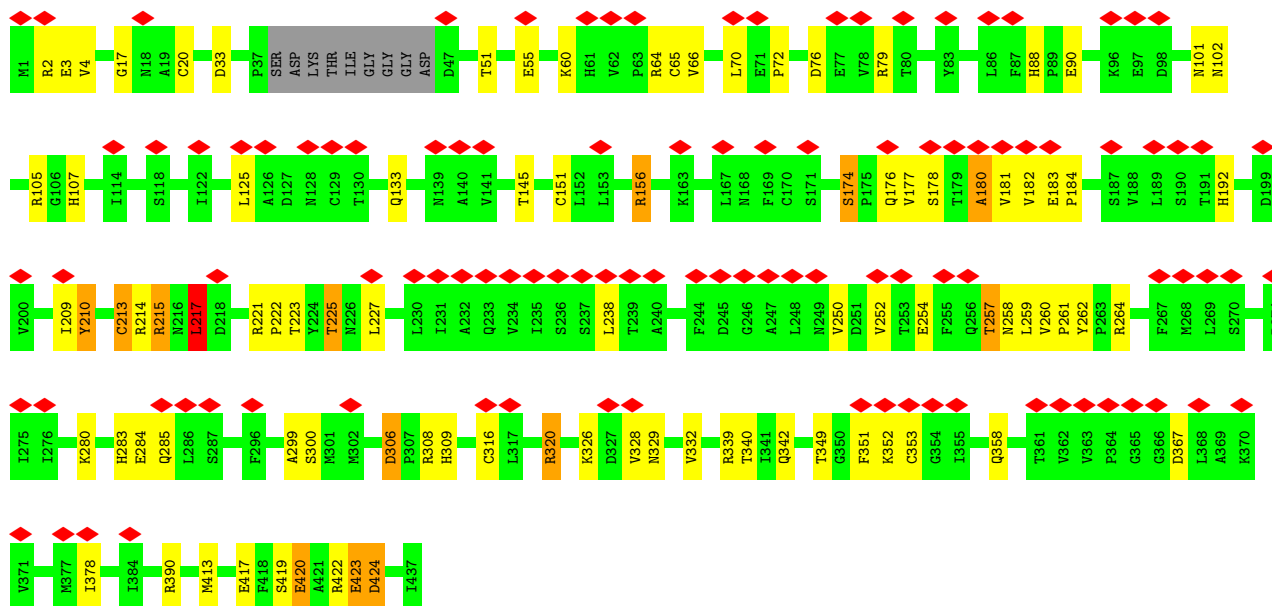
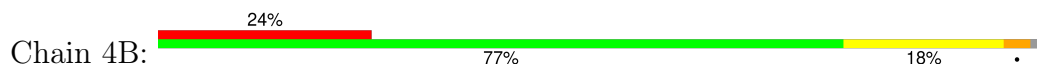


• Molecule 1: Tubulin alpha chain

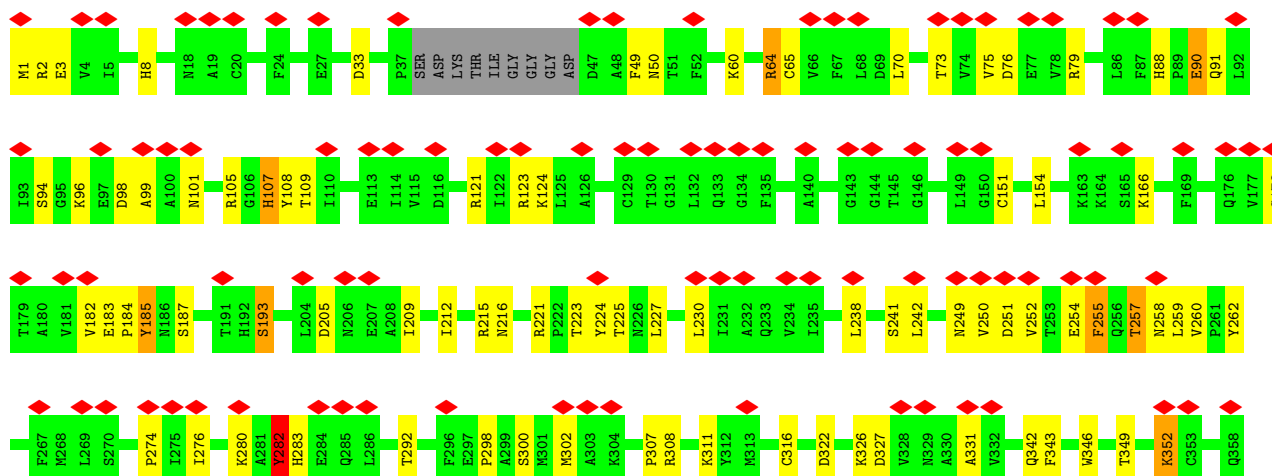
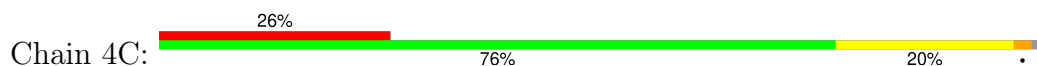


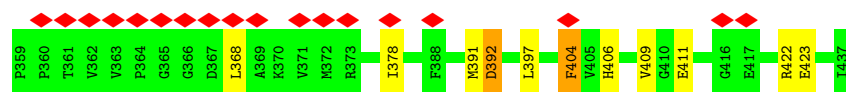


• Molecule 1: Tubulin alpha chain

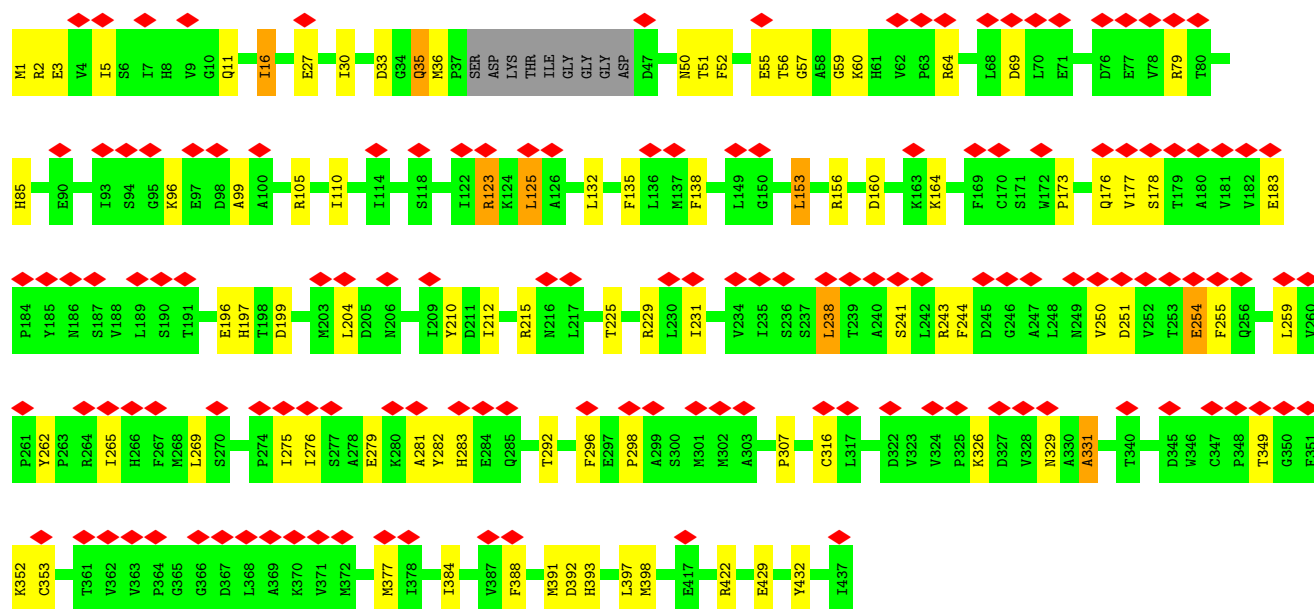
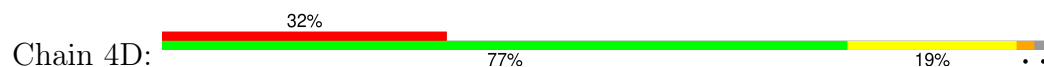


• Molecule 1: Tubulin alpha chain

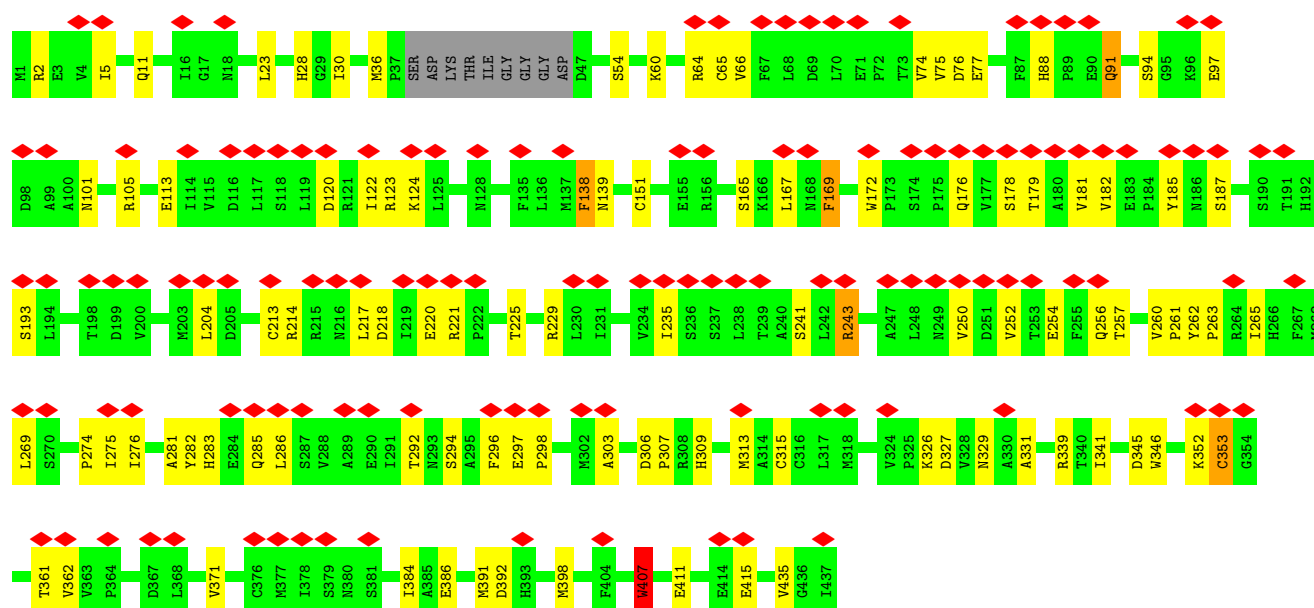




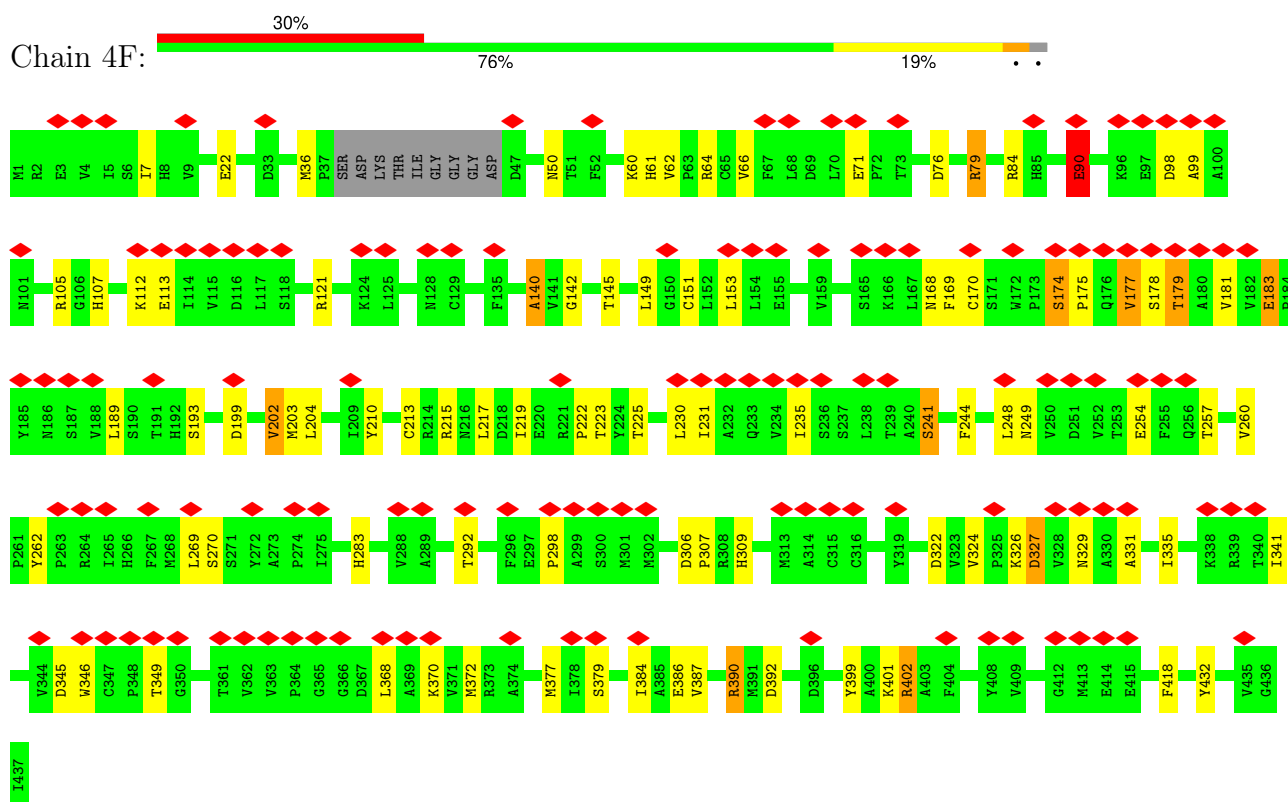
• Molecule 1: Tubulin alpha chain



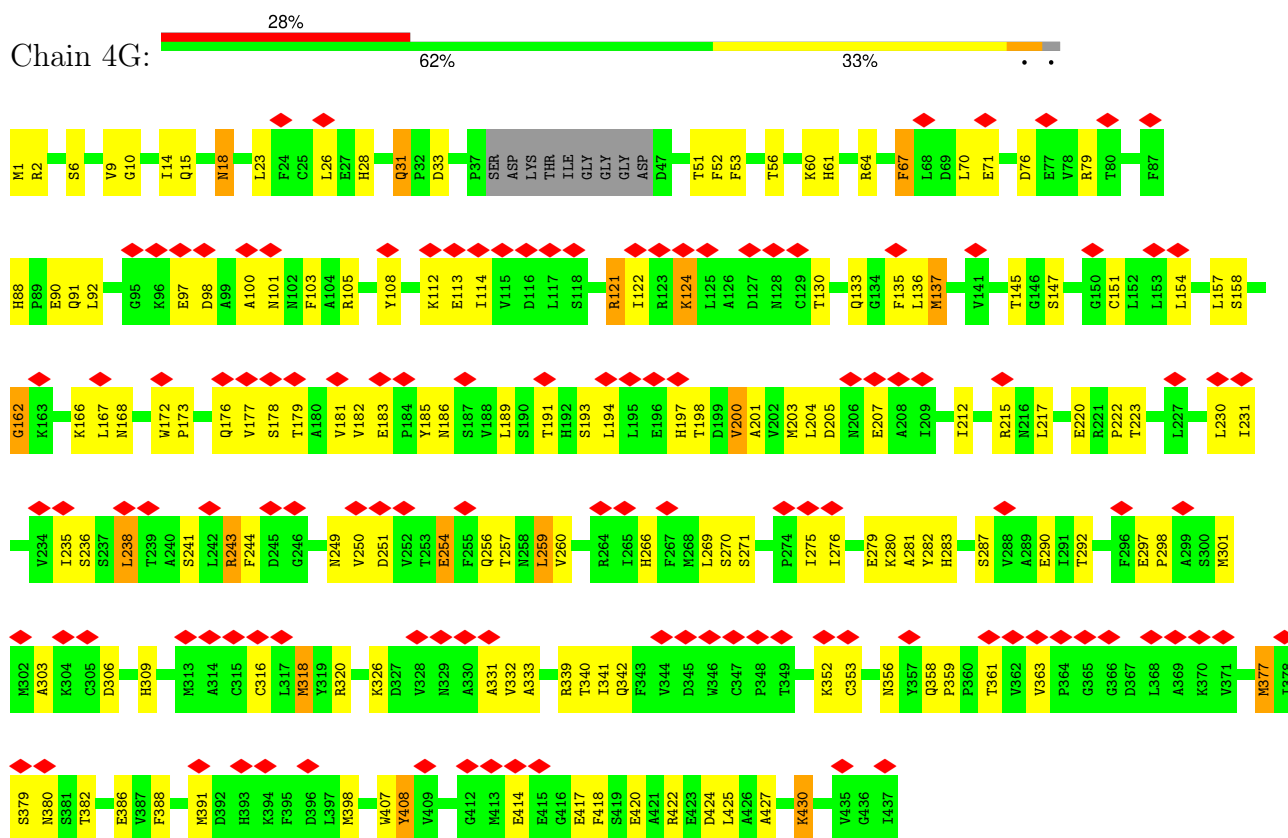
• Molecule 1: Tubulin alpha chain



• Molecule 1: Tubulin alpha chain

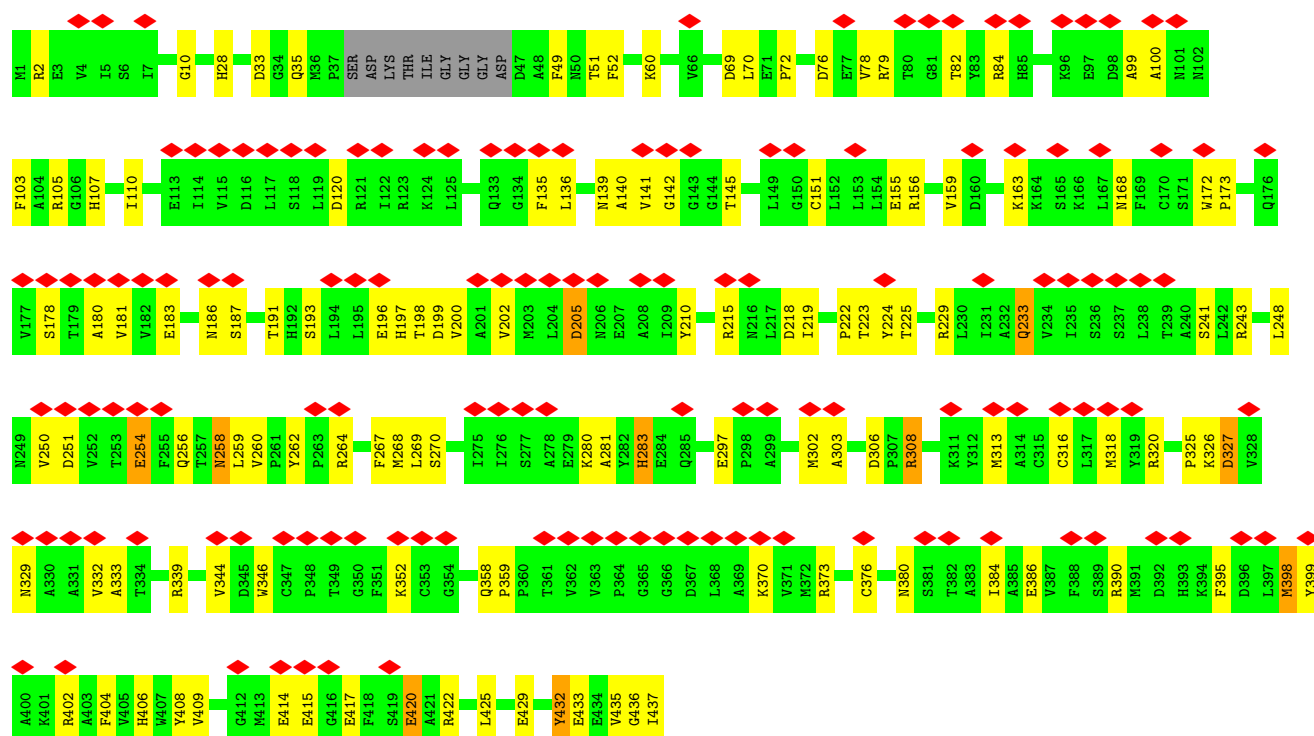


• Molecule 1: Tubulin alpha chain




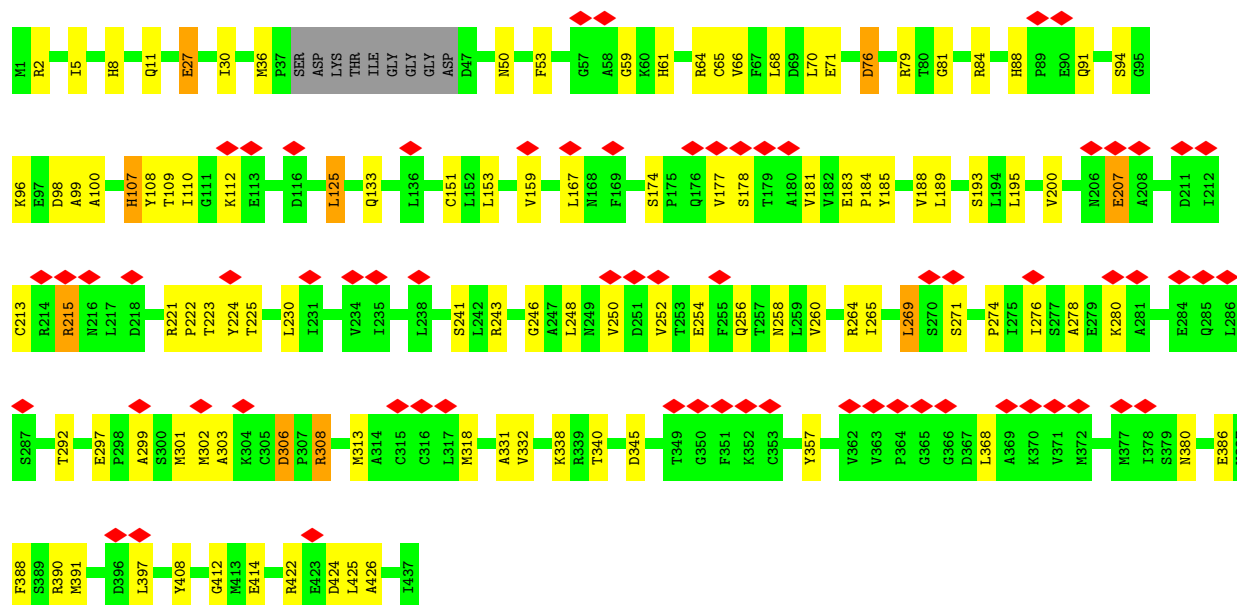
• Molecule 1: Tubulin alpha chain

Chain 4H: 




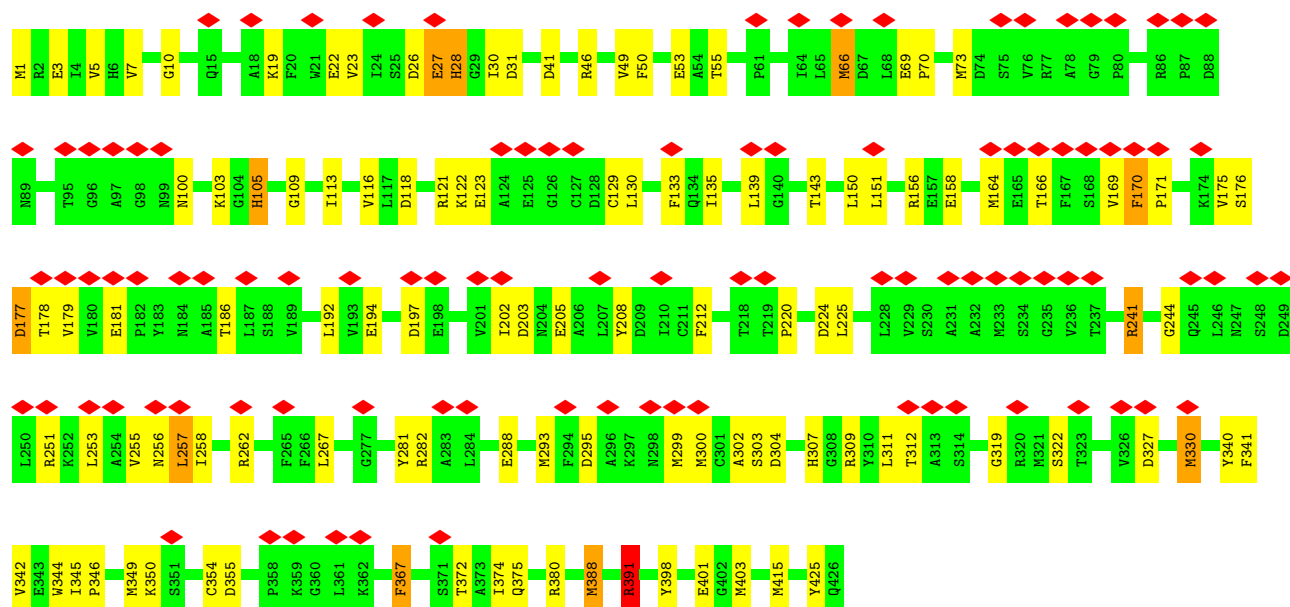
• Molecule 1: Tubulin alpha chain

Chain 4I: 

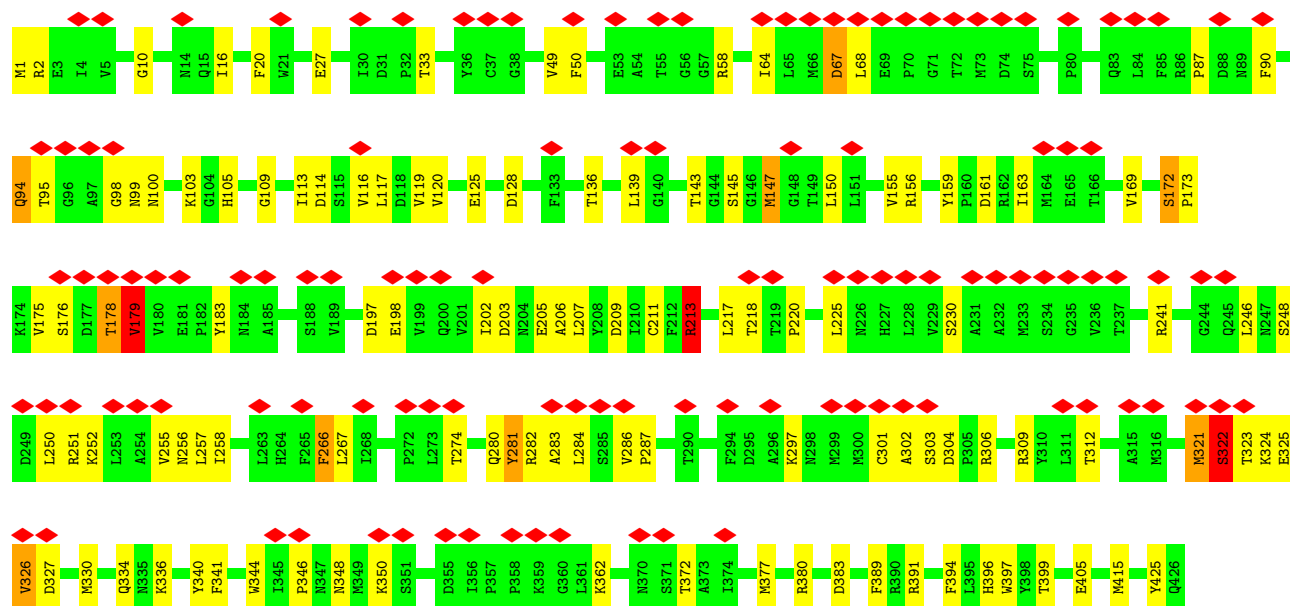


• Molecule 2: Tubulin beta chain

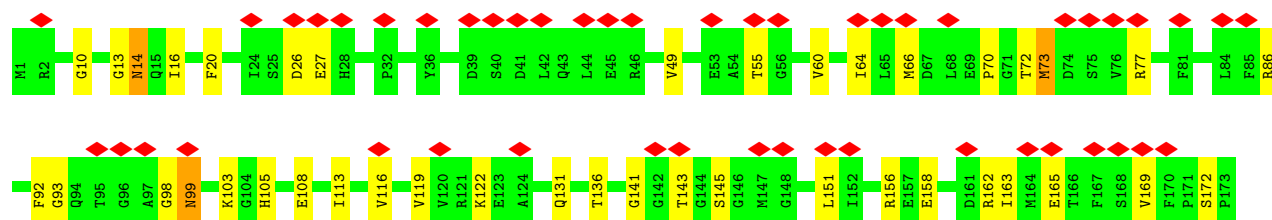
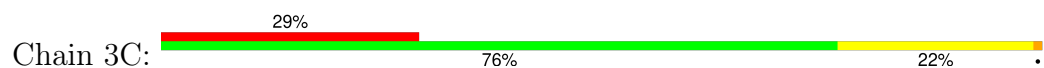
Chain 3A: 

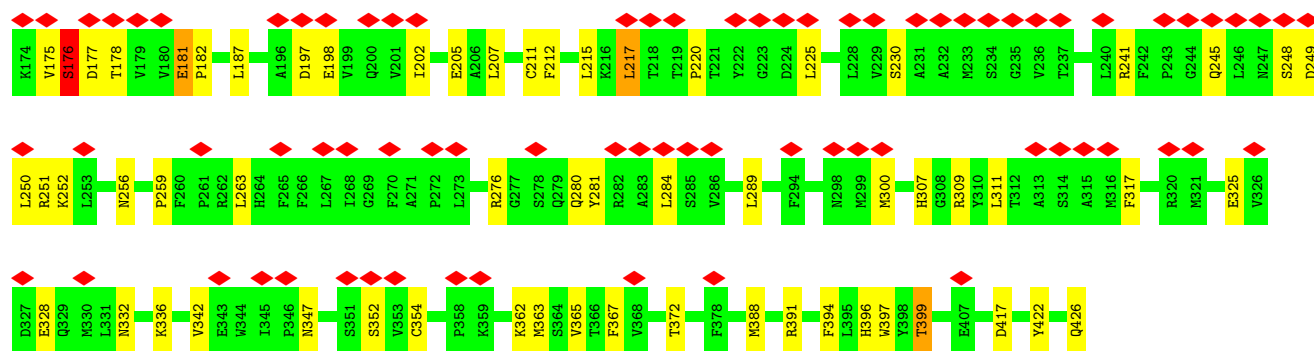


• Molecule 2: Tubulin beta chain

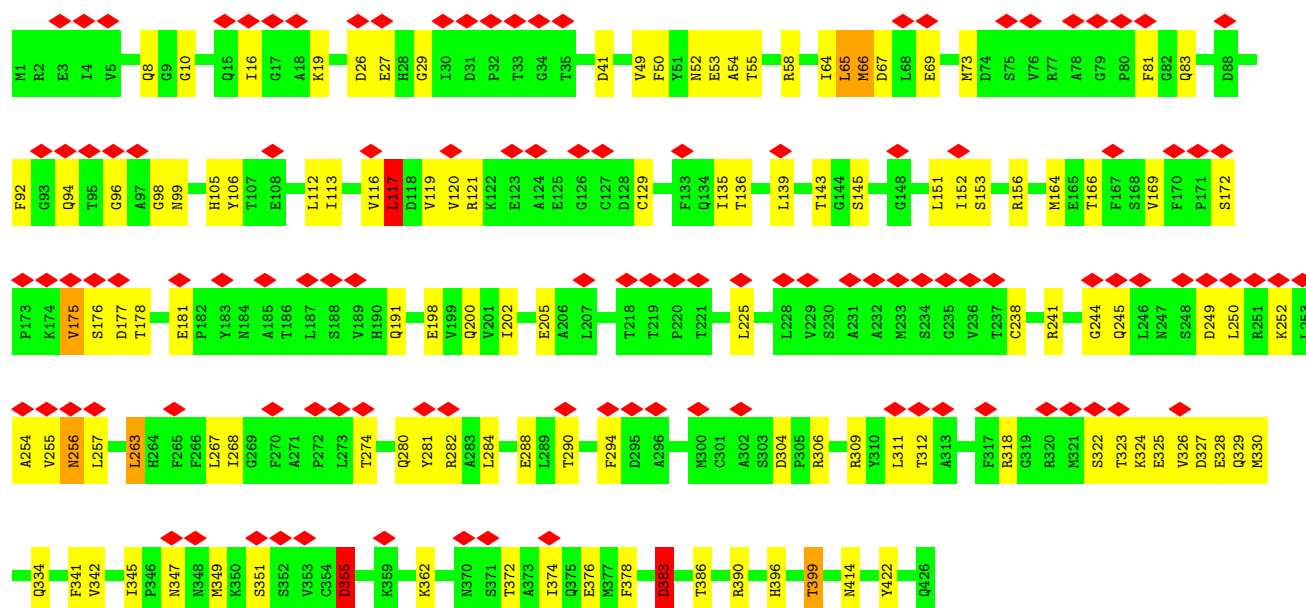


• Molecule 2: Tubulin beta chain

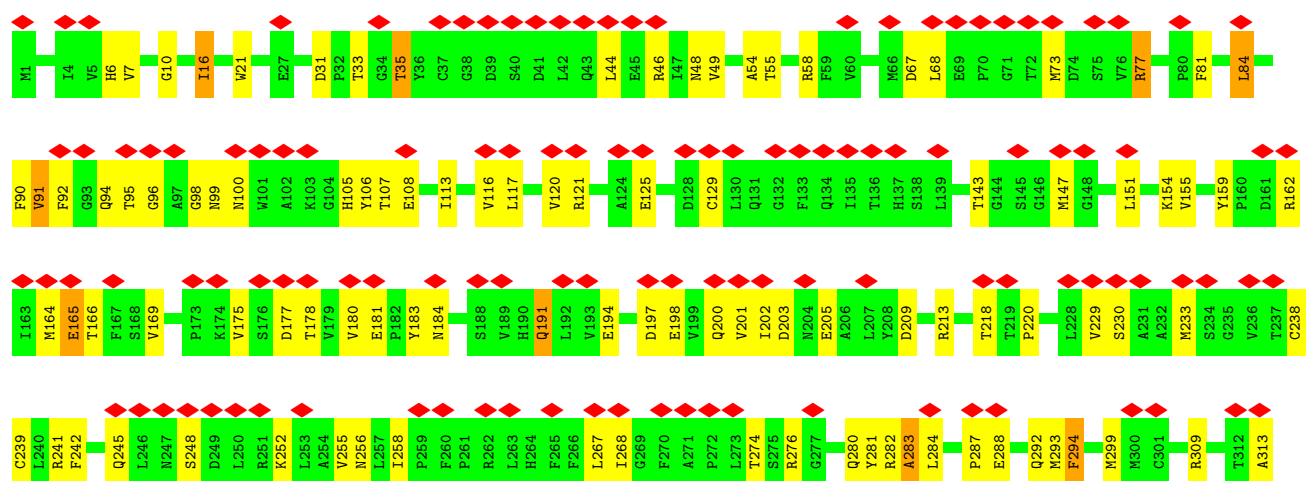


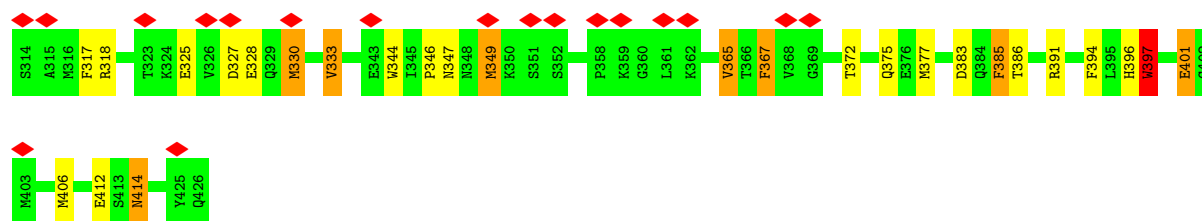


• Molecule 2: Tubulin beta chain

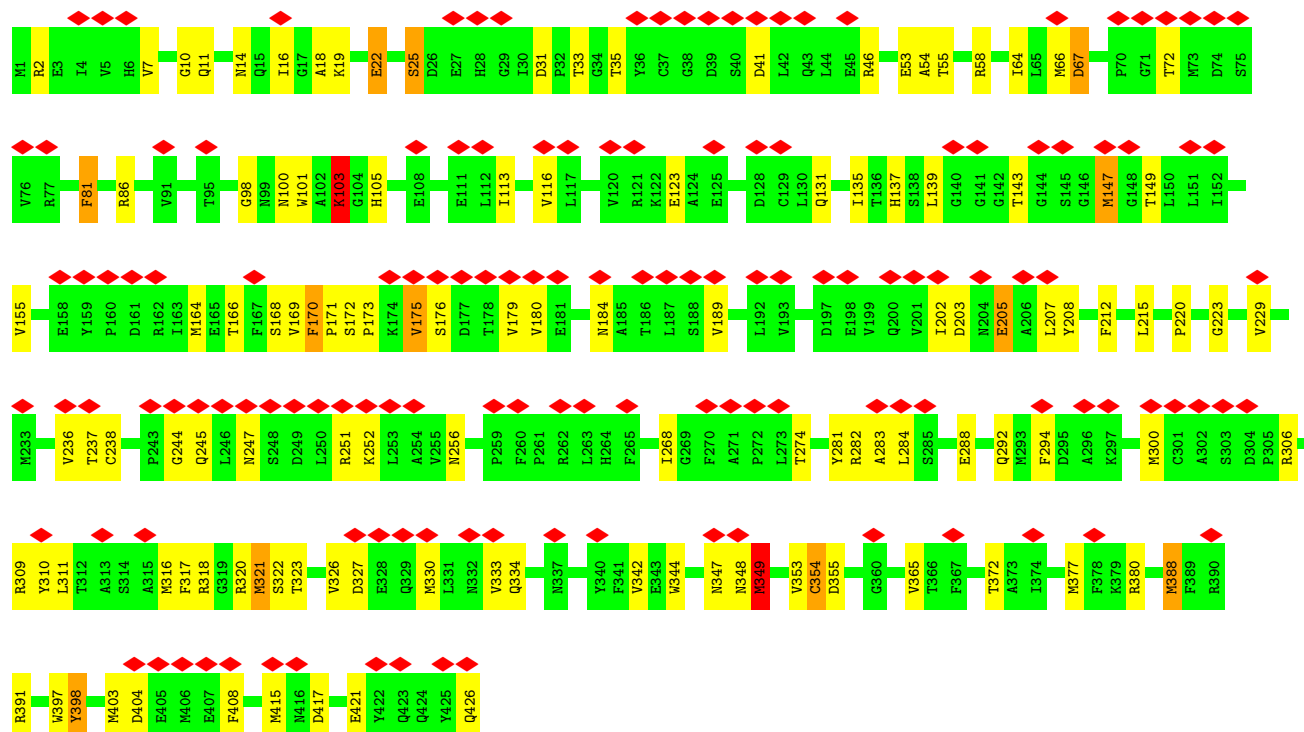


• Molecule 2: Tubulin beta chain

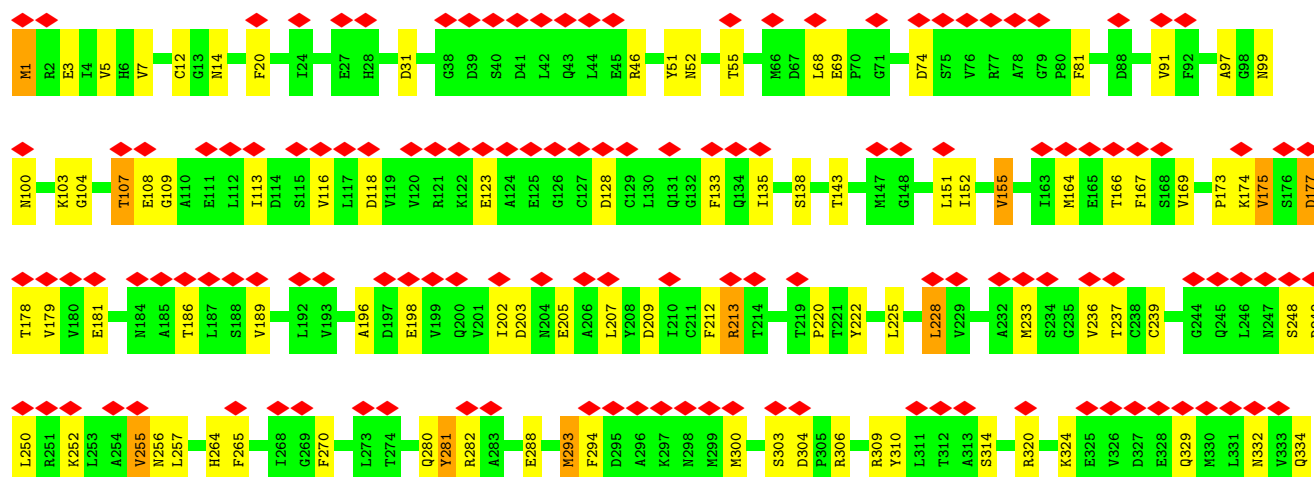
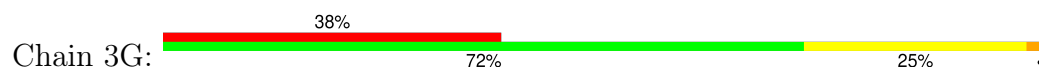




• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain

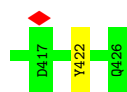




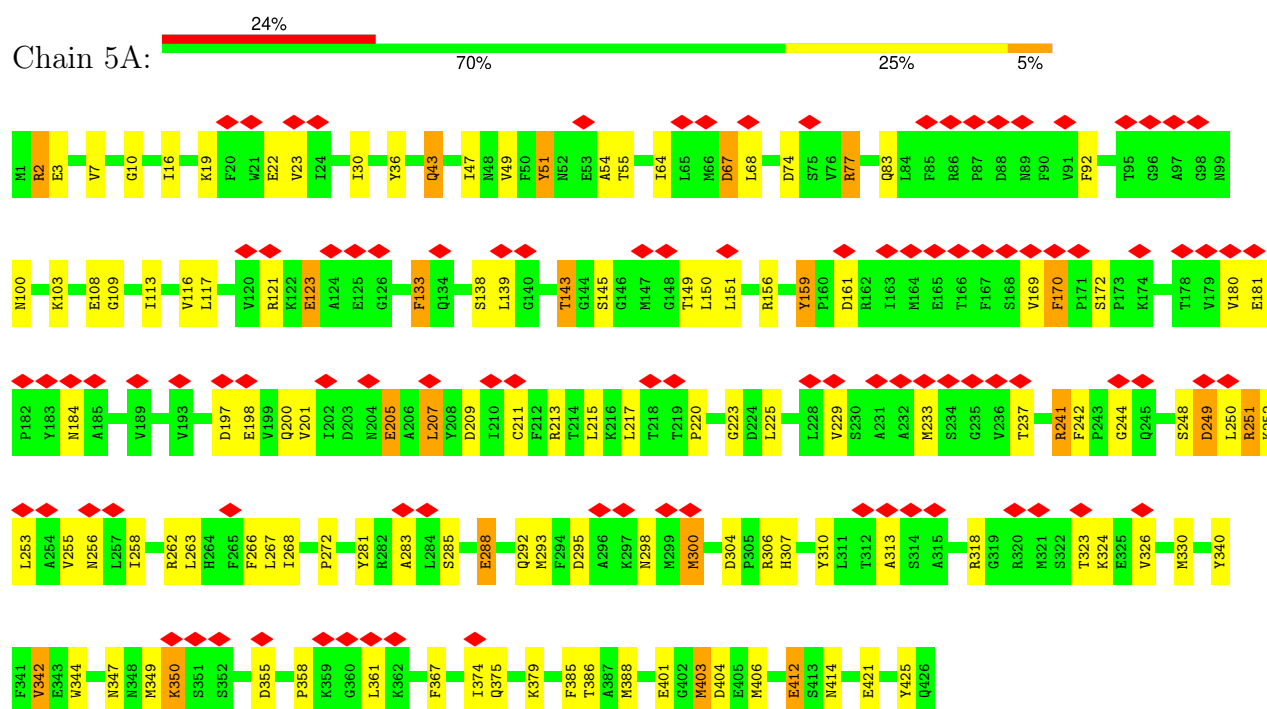
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						L250	R251	K252	L253	A254	V255	N256	L257	I258	P259	F260	P261	L262	L263	H264	F265	F266	L267	L268	P272	L273	T274	G277	Y281	R282	A283	L284	S285	E288	Q292	M293	F294	D295	A296	K297	N298	M299	M300	D304	P305	R306	R309	Y310	L311	T312	A313	S314	R318	T323	K324	E325			
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						M1	R2	E3	I4	V5	H6	V7		C12	G13	N14	O15	I16	F20		S25		I30	T35	C36	G37	G38	D39	S40	D41	L42	Q43	L44	E45	R46	V49	T55	L64	L65	H66	D67	L68		D74	S75	V76	R77	G79	P80	F81		D88	V91	F92	G93	Q94	N99		

- Molecule 2: Tubulin beta chain

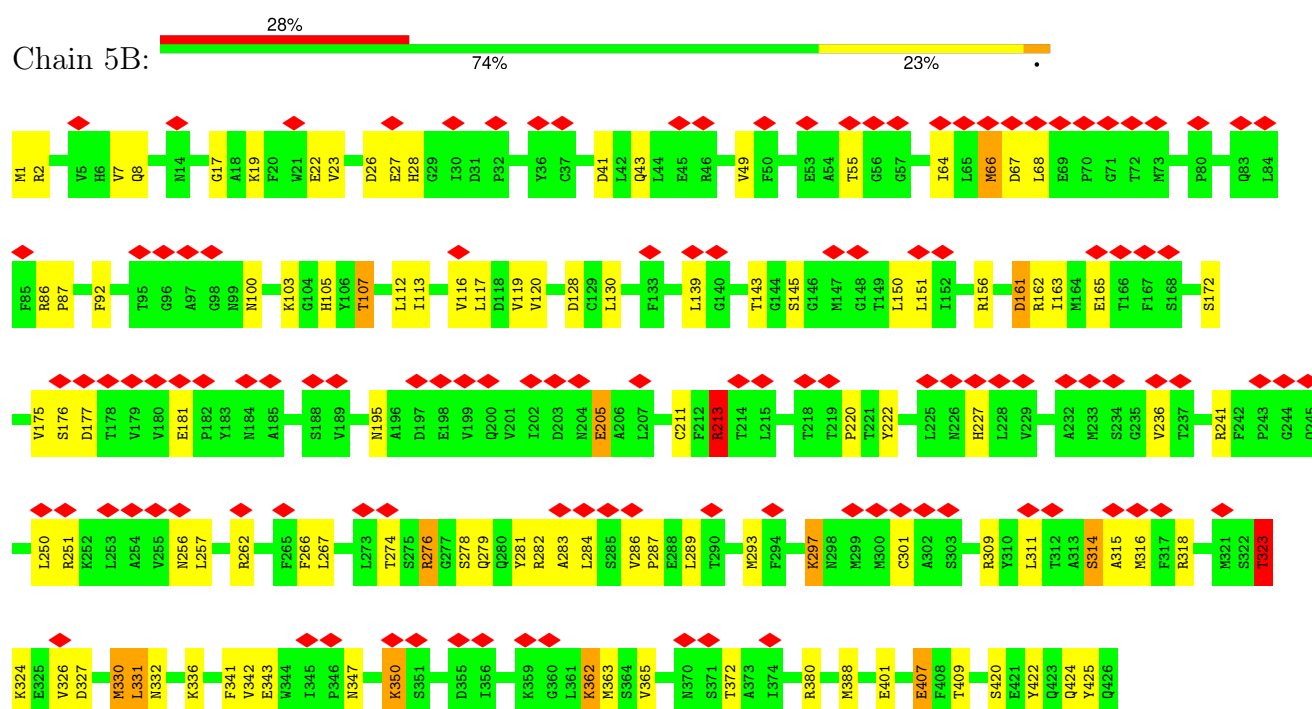
M298	M299	M300	C301	A302	S303	D304	L311	R318	G319	R320	M321	S322	T323	K324	E325	V326	D327	E328	L331	F341	V342	E343	W344	I345	P346	N347	M348	M349	C354	D355	T356	P357	P358	K362	M363	T372	Q375	D383	T386	H386	W387	Y388	T399	G400	E401	D404	E405				
T218	Y222	G223	D224	L225	V229	G235	V236	T237	T238	C239	L240	R241	F242	P243	G244	Q245	L246	N247	D248	S249	L250	I345	K252	V255	N256	L257	L258	R262	L267	L268	L273	T274	S275	S278	Q279	Q280	T281	R282	A283	L284	E288	L289	T290	Q291	Q292	N293	F294	D295	A296		
S138	L139	G140	G141	G142	T143	G144	S145	G146	M147	G148	T149	R156	E158	Y159	P160	D161	R162	E165	T166	F167	Q168	V169	F170	P171	S172	P173	K174	V175	S176	L177	T178	V179	L192	N195	E198	V199	Q200	I202	D203	N204	E205	A206	L207	Y208	D209	L210	R213	T214	L215	K216	L217
M1	R2	Q8	G9	G10	Q11	N14	Q15	Q16	V23	E27	Y36	C37	Q38	D39	S40	D41	L42	L44	E45	R46	V49	T55	M66	D74	S75	A78	D88	F92	T95	N99	K103	T107	E108	V120	E125	D128	T136	H137													



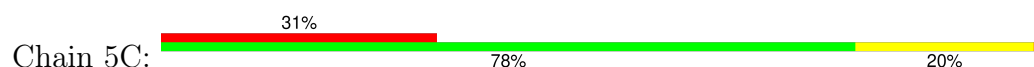
- Molecule 2: Tubulin beta chain

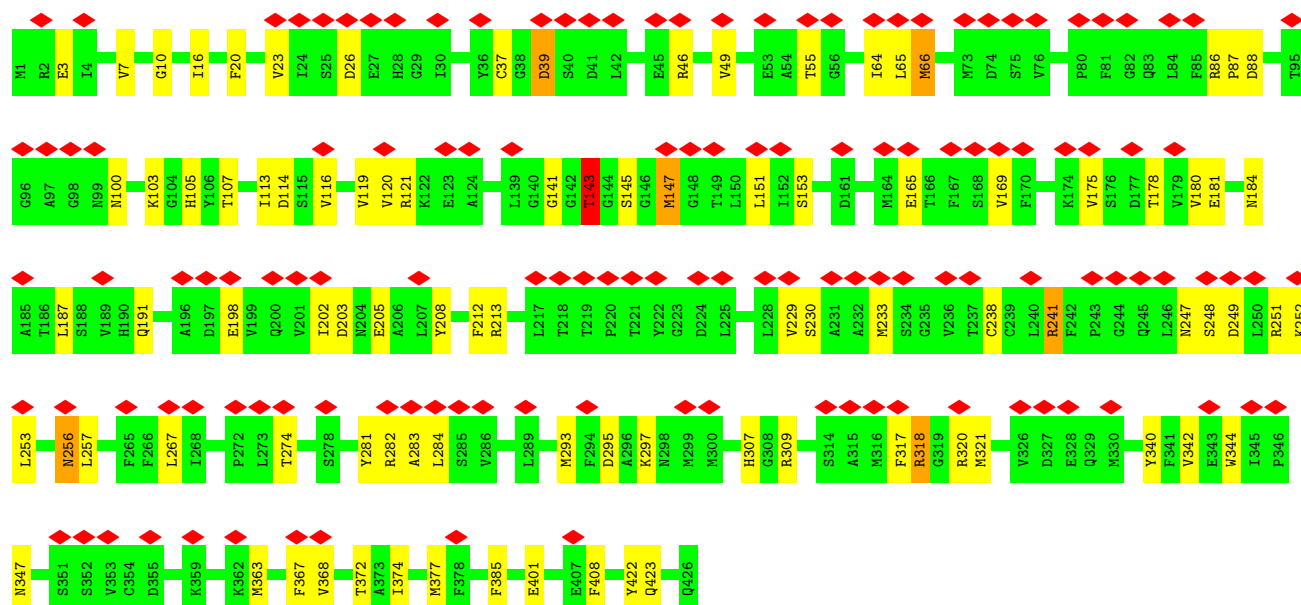


- Molecule 2: Tubulin beta chain

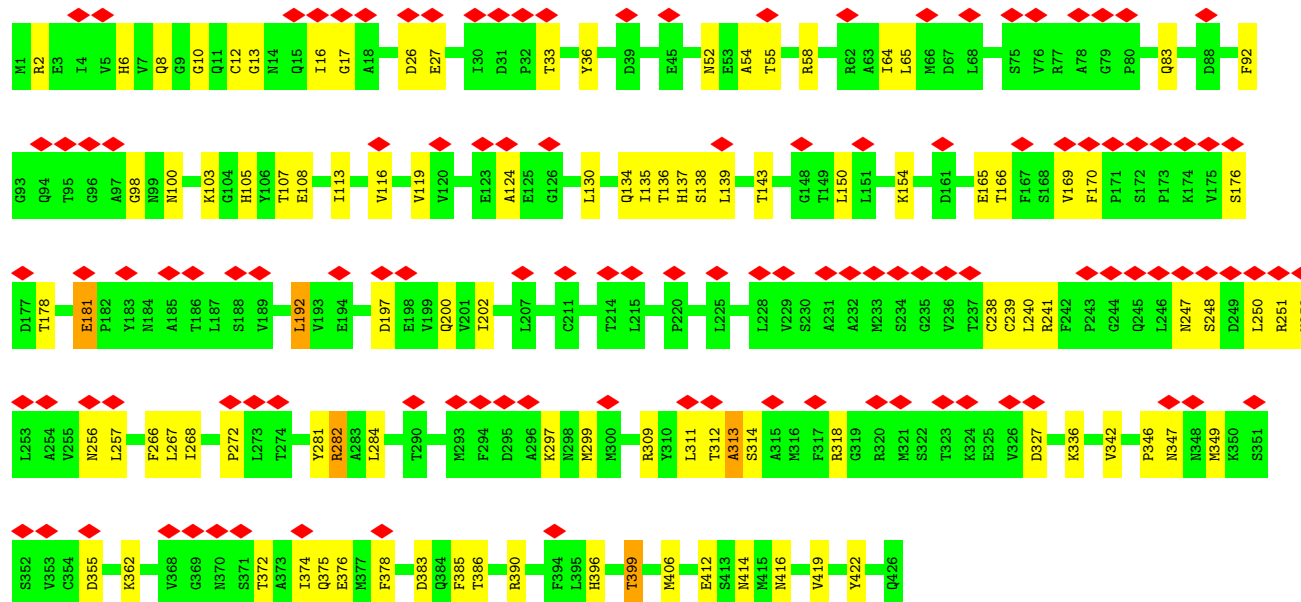
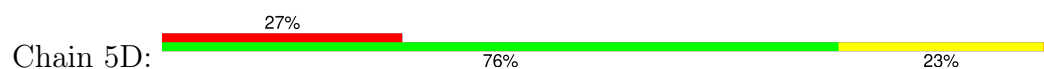


- Molecule 2: Tubulin beta chain

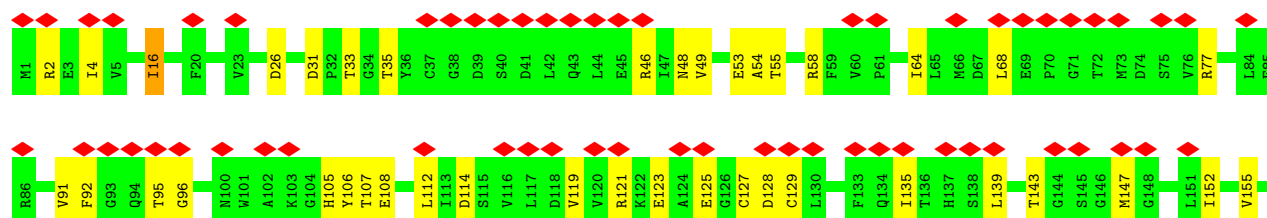
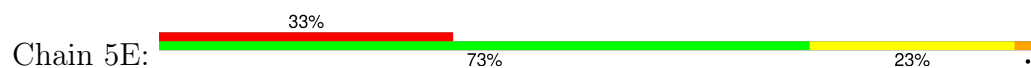


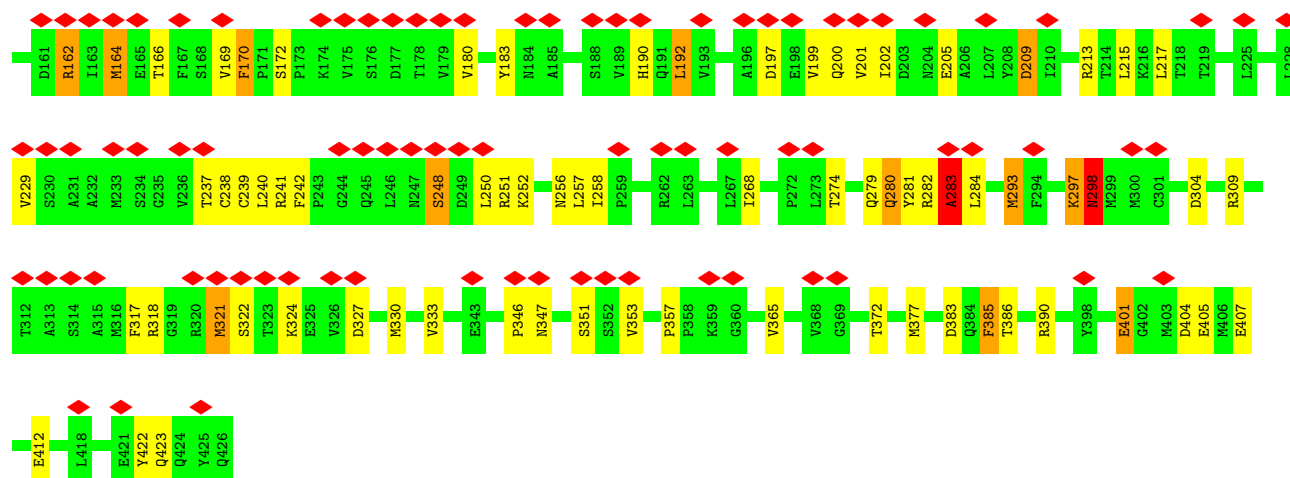


• Molecule 2: Tubulin beta chain

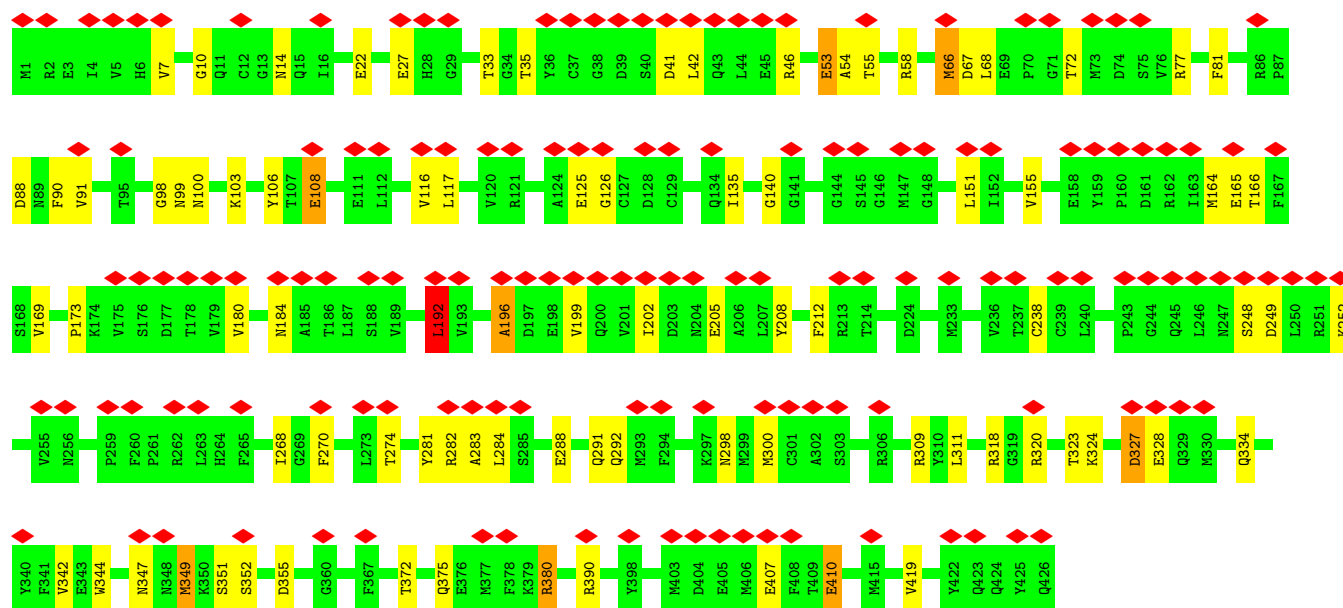
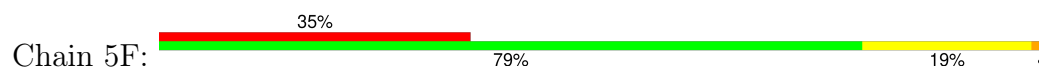


• Molecule 2: Tubulin beta chain

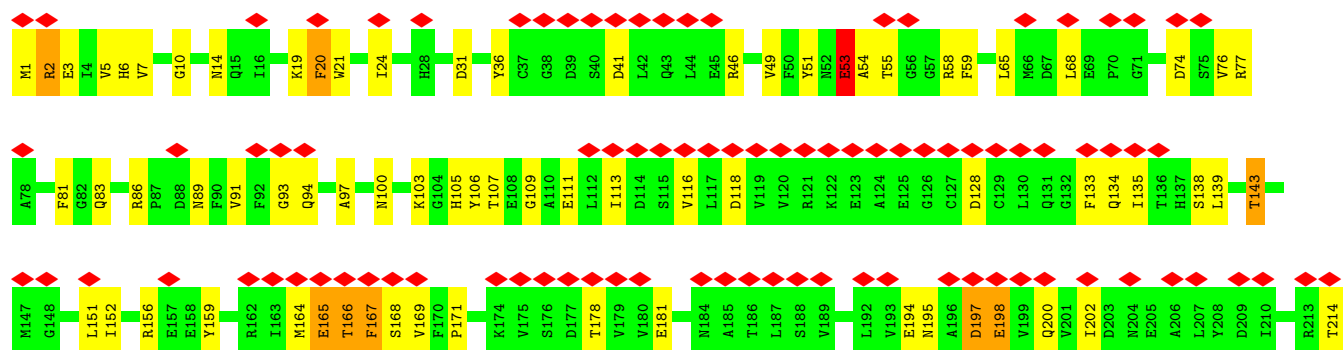
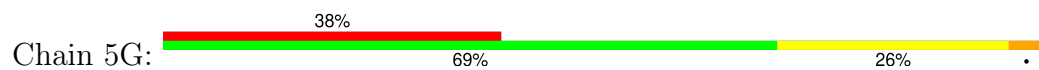


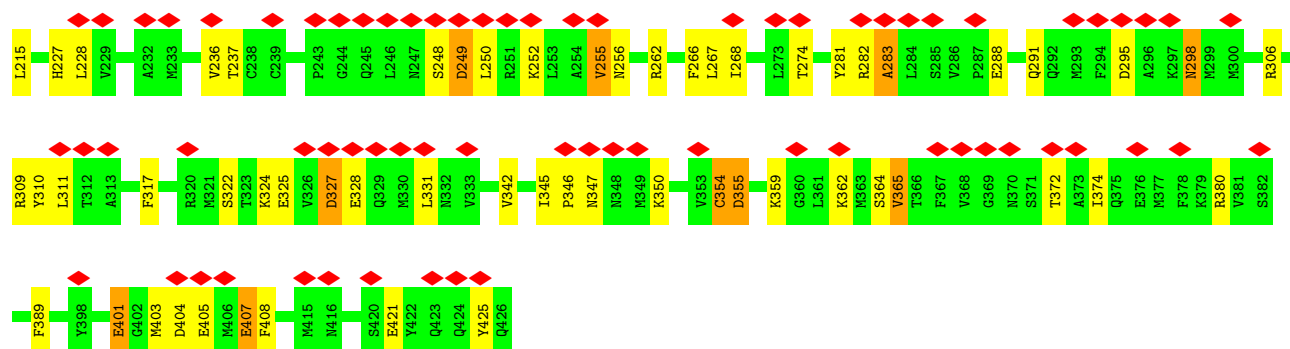


• Molecule 2: Tubulin beta chain

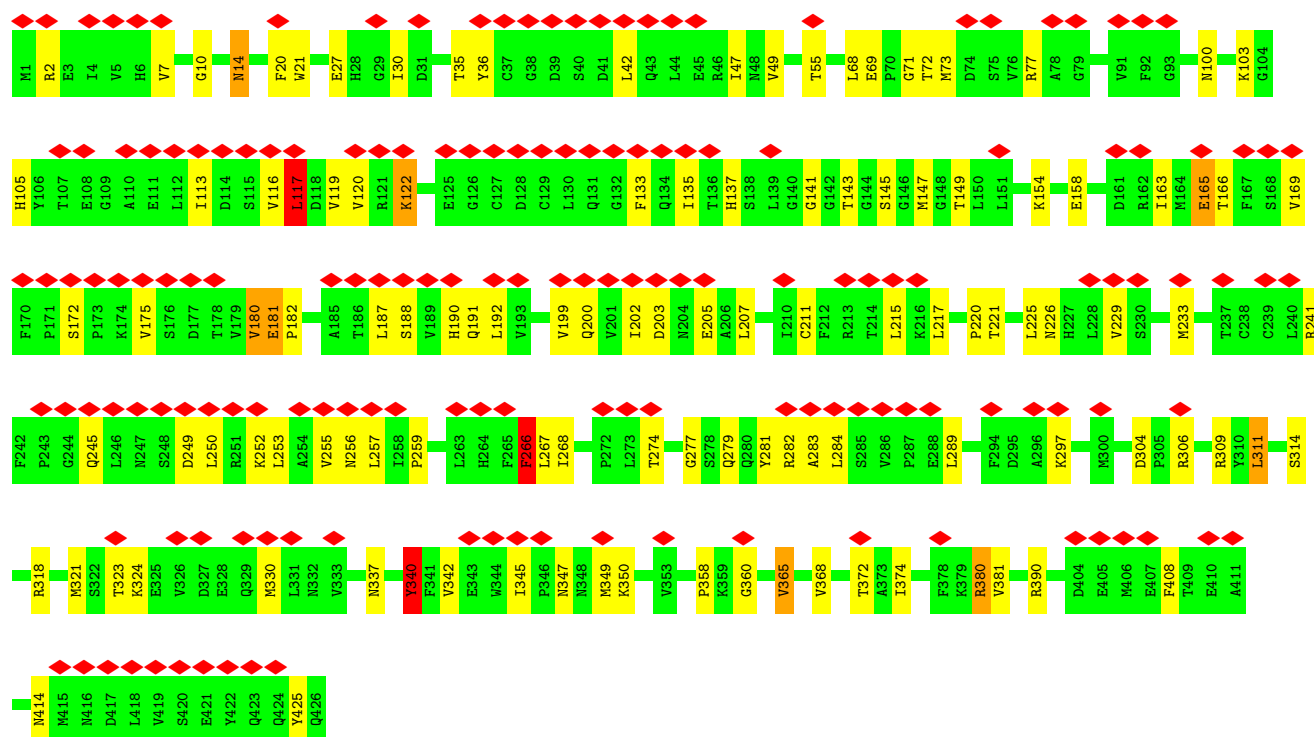
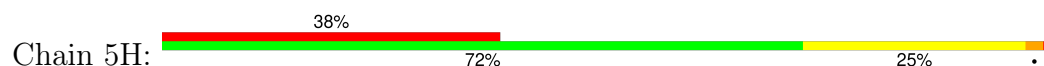


• Molecule 2: Tubulin beta chain

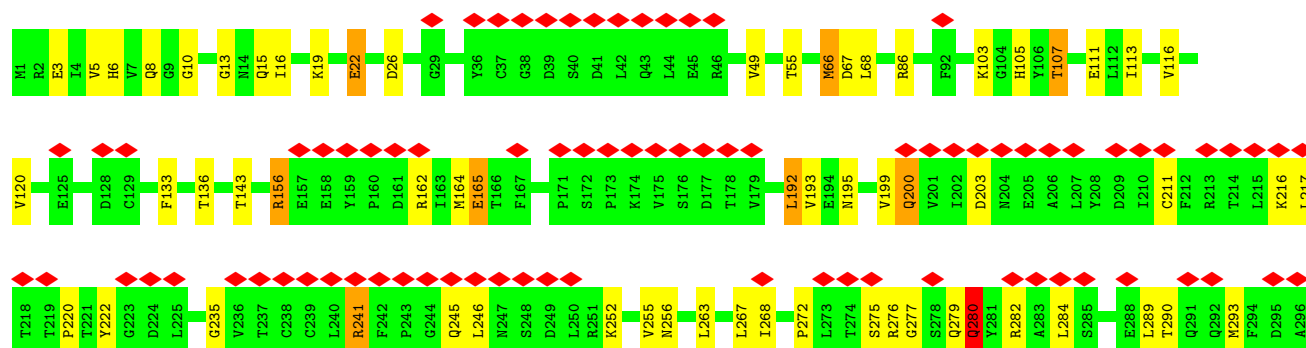
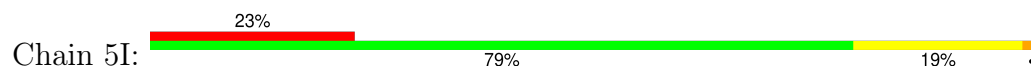


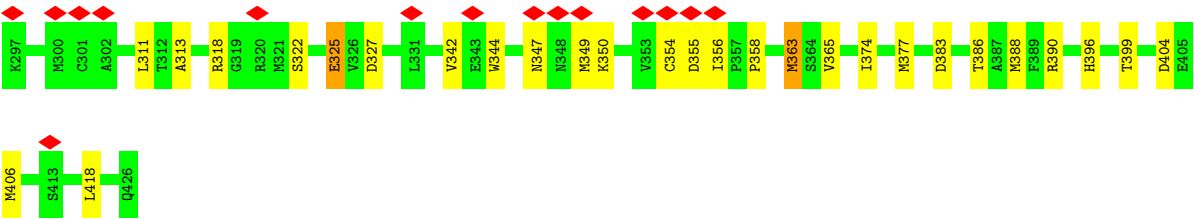


• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	29524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	96	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.463	Depositor
Minimum map value	-3.203	Depositor
Average map value	0.053	Depositor
Map value standard deviation	0.287	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	452.352, 452.352, 452.352	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	3.534, 3.534, 3.534	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2A	0.92	9/3398 (0.3%)	1.27	33/4606 (0.7%)
1	2B	0.86	5/3398 (0.1%)	1.14	21/4606 (0.5%)
1	2C	0.80	3/3398 (0.1%)	1.07	14/4606 (0.3%)
1	2D	0.77	1/3398 (0.0%)	1.12	23/4606 (0.5%)
1	2E	0.87	8/3398 (0.2%)	1.20	23/4606 (0.5%)
1	2F	0.89	6/3398 (0.2%)	1.26	27/4606 (0.6%)
1	2G	0.96	8/3398 (0.2%)	1.28	36/4606 (0.8%)
1	2H	0.90	3/3398 (0.1%)	1.26	29/4606 (0.6%)
1	2I	0.84	7/3398 (0.2%)	1.14	17/4606 (0.4%)
1	4A	0.95	5/3398 (0.1%)	1.28	32/4606 (0.7%)
1	4B	0.90	9/3398 (0.3%)	1.16	24/4606 (0.5%)
1	4C	0.85	4/3398 (0.1%)	1.20	21/4606 (0.5%)
1	4D	0.82	4/3398 (0.1%)	1.19	27/4606 (0.6%)
1	4E	0.83	4/3398 (0.1%)	1.15	18/4606 (0.4%)
1	4F	0.92	8/3398 (0.2%)	1.19	27/4606 (0.6%)
1	4G	0.96	7/3398 (0.2%)	1.30	34/4606 (0.7%)
1	4H	0.94	3/3398 (0.1%)	1.30	31/4606 (0.7%)
1	4I	0.88	5/3398 (0.1%)	1.15	18/4606 (0.4%)
2	3A	0.91	7/3404 (0.2%)	1.28	35/4606 (0.8%)
2	3B	0.87	7/3404 (0.2%)	1.28	38/4606 (0.8%)
2	3C	0.85	7/3404 (0.2%)	1.12	19/4606 (0.4%)
2	3D	0.88	3/3404 (0.1%)	1.18	24/4606 (0.5%)
2	3E	0.84	6/3404 (0.2%)	1.23	44/4606 (1.0%)
2	3F	0.88	4/3404 (0.1%)	1.23	35/4606 (0.8%)
2	3G	0.98	11/3404 (0.3%)	1.29	31/4606 (0.7%)
2	3H	0.90	4/3404 (0.1%)	1.28	33/4606 (0.7%)
2	3I	0.82	3/3404 (0.1%)	1.13	21/4606 (0.5%)
2	5A	0.92	9/3404 (0.3%)	1.33	46/4606 (1.0%)
2	5B	0.86	5/3404 (0.1%)	1.21	31/4606 (0.7%)
2	5C	0.81	3/3404 (0.1%)	1.19	33/4606 (0.7%)
2	5D	0.85	3/3404 (0.1%)	1.17	20/4606 (0.4%)
2	5E	0.86	5/3404 (0.1%)	1.22	31/4606 (0.7%)
2	5F	0.89	7/3404 (0.2%)	1.16	24/4606 (0.5%)
2	5G	0.97	7/3404 (0.2%)	1.34	40/4606 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	5H	0.90	4/3404 (0.1%)	1.26	21/4606 (0.5%)
2	5I	0.83	2/3404 (0.1%)	1.14	21/4606 (0.5%)
All	All	0.88	196/122436 (0.2%)	1.22	1002/165816 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2A	0	7
1	2B	0	5
1	2C	0	6
1	2D	0	3
1	2E	0	7
1	2F	0	7
1	2G	0	12
1	2H	0	8
1	2I	0	6
1	4A	0	10
1	4B	0	5
1	4C	0	6
1	4D	0	5
1	4E	0	8
1	4F	0	7
1	4G	0	7
1	4H	0	9
1	4I	0	5
2	3A	0	11
2	3B	0	7
2	3C	0	8
2	3D	0	8
2	3E	0	8
2	3F	0	8
2	3G	0	5
2	3H	0	9
2	3I	0	4
2	5A	0	14
2	5B	0	4
2	5C	0	6
2	5D	0	6
2	5E	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	5F	0	4
2	5G	0	12
2	5H	0	8
2	5I	0	5
All	All	0	259

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4F	183	GLU	CD-OE2	-14.74	1.09	1.25
1	2E	77	GLU	CD-OE2	10.97	1.37	1.25
2	3A	288	GLU	CD-OE2	10.82	1.37	1.25
2	5G	401	GLU	CD-OE1	-9.34	1.15	1.25
1	4H	420	GLU	CD-OE1	-9.26	1.15	1.25
1	4F	174	SER	CB-OG	-9.16	1.30	1.42
1	2G	290	GLU	CD-OE1	9.15	1.35	1.25
2	5G	288	GLU	CD-OE1	9.02	1.35	1.25
2	5A	401	GLU	CD-OE1	8.98	1.35	1.25
2	5D	181	GLU	CD-OE1	-8.96	1.15	1.25
2	5F	410	GLU	CD-OE1	-8.93	1.15	1.25
2	5I	3	GLU	CD-OE2	-8.81	1.16	1.25
1	2E	71	GLU	CD-OE1	-8.63	1.16	1.25
1	4B	284	GLU	CD-OE2	8.61	1.35	1.25
1	4I	27	GLU	CD-OE1	8.46	1.34	1.25
2	5G	3	GLU	CD-OE2	-8.24	1.16	1.25
1	2A	27	GLU	CD-OE1	-8.22	1.16	1.25
2	5F	53	GLU	CD-OE1	-8.18	1.16	1.25
1	4A	183	GLU	CD-OE2	8.03	1.34	1.25
2	3C	198	GLU	CD-OE1	-7.97	1.16	1.25
2	5H	165	GLU	CD-OE2	-7.96	1.16	1.25
1	2C	71	GLU	CD-OE1	-7.67	1.17	1.25
2	5G	165	GLU	CD-OE2	-7.55	1.17	1.25
2	3G	3	GLU	CD-OE2	-7.37	1.17	1.25
2	3A	194	GLU	CD-OE2	7.33	1.33	1.25
2	3E	288	GLU	CD-OE1	-7.32	1.17	1.25
1	2G	190	SER	CB-OG	-7.29	1.32	1.42
2	3G	410	GLU	CD-OE1	7.24	1.33	1.25
1	2B	392	ASP	CG-OD1	-7.21	1.08	1.25
1	2A	118	SER	CB-OG	-7.17	1.32	1.42
1	2I	3	GLU	CD-OE2	-7.15	1.17	1.25
2	3H	285	SER	CB-OG	7.08	1.51	1.42
1	4C	423	GLU	CD-OE2	7.05	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2E	414	GLU	CD-OE2	-7.04	1.18	1.25
1	2I	3	GLU	CD-OE1	-7.03	1.18	1.25
2	5C	401	GLU	CD-OE1	-7.03	1.18	1.25
1	4I	297	GLU	CD-OE2	-7.02	1.18	1.25
2	3B	172	SER	CB-OG	-6.95	1.33	1.42
1	4G	297	GLU	CD-OE1	-6.86	1.18	1.25
1	2I	386	GLU	CD-OE2	6.85	1.33	1.25
1	2G	207	GLU	CD-OE1	-6.79	1.18	1.25
2	5E	401	GLU	CD-OE1	6.76	1.33	1.25
2	3I	165	GLU	CD-OE2	6.73	1.33	1.25
1	4F	392	ASP	CG-OD1	-6.72	1.09	1.25
1	4A	113	GLU	CD-OE2	6.65	1.32	1.25
1	2F	3	GLU	CD-OE1	-6.63	1.18	1.25
2	3D	181	GLU	CD-OE2	6.62	1.32	1.25
2	3B	198	GLU	CD-OE1	-6.60	1.18	1.25
1	4B	55	GLU	CD-OE1	6.60	1.32	1.25
1	4E	187	SER	CB-OG	6.59	1.50	1.42
1	2A	90	GLU	CD-OE1	-6.56	1.18	1.25
1	4H	433	GLU	CD-OE1	6.53	1.32	1.25
2	3F	205	GLU	CD-OE2	6.52	1.32	1.25
1	4G	414	GLU	CD-OE2	6.51	1.32	1.25
1	4B	90	GLU	CD-OE1	6.44	1.32	1.25
1	4C	423	GLU	CD-OE1	-6.44	1.18	1.25
1	2F	386	GLU	CD-OE1	-6.41	1.18	1.25
1	2B	411	GLU	CD-OE1	-6.37	1.18	1.25
1	2F	290	GLU	CD-OE1	-6.36	1.18	1.25
2	5G	407	GLU	CD-OE2	6.35	1.32	1.25
1	2A	415	GLU	CD-OE2	-6.34	1.18	1.25
1	2E	193	SER	CA-CB	-6.33	1.43	1.52
1	2E	183	GLU	CD-OE2	-6.30	1.18	1.25
2	5G	53	GLU	CD-OE1	-6.29	1.18	1.25
2	5F	352	SER	CB-OG	-6.29	1.34	1.42
2	3A	3	GLU	CD-OE1	-6.25	1.18	1.25
1	4B	178	SER	CB-OG	-6.24	1.34	1.42
2	5F	22	GLU	CD-OE1	-6.21	1.18	1.25
2	5A	3	GLU	CD-OE2	6.21	1.32	1.25
1	2E	391	MET	CG-SD	-6.19	1.65	1.81
1	2G	411	GLU	CD-OE2	-6.14	1.18	1.25
2	5F	249	ASP	CG-OD1	-6.09	1.11	1.25
2	5A	288	GLU	CD-OE1	6.07	1.32	1.25
2	3E	165	GLU	CD-OE2	-6.05	1.19	1.25
1	4B	420	GLU	CD-OE1	-6.05	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5B	278	SER	CB-OG	-6.04	1.34	1.42
2	5B	165	GLU	CD-OE1	6.01	1.32	1.25
2	3B	27	GLU	CD-OE2	-5.97	1.19	1.25
1	4H	429	GLU	CD-OE1	-5.97	1.19	1.25
2	5A	181	GLU	CD-OE2	5.97	1.32	1.25
2	5C	205	GLU	CD-OE1	5.94	1.32	1.25
1	4I	207	GLU	CD-OE2	-5.94	1.19	1.25
1	4G	306	ASP	CG-OD1	-5.94	1.11	1.25
2	5H	27	GLU	CD-OE1	5.93	1.32	1.25
2	5C	3	GLU	CD-OE1	-5.93	1.19	1.25
1	2I	423	GLU	CD-OE1	5.93	1.32	1.25
1	2D	155	GLU	CD-OE1	5.92	1.32	1.25
2	3G	104	GLY	C-O	-5.92	1.14	1.23
2	5E	53	GLU	CD-OE2	5.90	1.32	1.25
1	4G	254	GLU	CD-OE2	5.89	1.32	1.25
1	4E	77	GLU	CD-OE2	5.89	1.32	1.25
1	2I	389	SER	CB-OG	-5.88	1.34	1.42
2	5B	205	GLU	CD-OE1	5.87	1.32	1.25
1	2I	429	GLU	CD-OE2	-5.86	1.19	1.25
2	3C	165	GLU	CD-OE1	-5.84	1.19	1.25
2	5H	229	VAL	CB-CG1	-5.83	1.40	1.52
1	2G	113	GLU	CD-OE1	-5.82	1.19	1.25
2	3C	158	GLU	CD-OE2	-5.81	1.19	1.25
1	4F	71	GLU	CD-OE2	-5.81	1.19	1.25
2	3C	181	GLU	CD-OE1	5.80	1.32	1.25
2	3H	123	GLU	CD-OE2	-5.80	1.19	1.25
1	2H	415	GLU	CD-OE2	-5.78	1.19	1.25
2	3F	25	SER	CB-OG	-5.76	1.34	1.42
2	3H	288	GLU	CD-OE2	-5.76	1.19	1.25
1	4B	174	SER	CB-OG	-5.76	1.34	1.42
2	3C	352	SER	CB-OG	-5.75	1.34	1.42
1	2A	264	ARG	NE-CZ	-5.75	1.25	1.33
1	2A	297	GLU	CD-OE1	-5.73	1.19	1.25
2	5A	3	GLU	CD-OE1	-5.69	1.19	1.25
2	3G	303	SER	CA-CB	-5.66	1.44	1.52
2	5A	74	ASP	CG-OD1	-5.65	1.12	1.25
2	3A	3	GLU	CD-OE2	-5.64	1.19	1.25
1	2F	22	GLU	CD-OE2	5.62	1.31	1.25
2	3F	22	GLU	CD-OE2	-5.62	1.19	1.25
1	4I	71	GLU	CD-OE1	5.62	1.31	1.25
1	4C	90	GLU	CD-OE1	5.62	1.31	1.25
2	3I	157	GLU	CD-OE2	5.61	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4F	90	GLU	CD-OE2	5.59	1.31	1.25
2	5A	108	GLU	CD-OE2	-5.57	1.19	1.25
1	2A	27	GLU	CD-OE2	-5.57	1.19	1.25
2	3D	181	GLU	CB-CG	-5.55	1.41	1.52
1	2A	113	GLU	CD-OE2	5.54	1.31	1.25
1	4I	414	GLU	CD-OE2	-5.54	1.19	1.25
2	3G	198	GLU	CD-OE2	5.52	1.31	1.25
1	2G	55	GLU	CD-OE2	-5.52	1.19	1.25
2	3E	230	SER	CB-OG	5.50	1.49	1.42
2	3A	303	SER	CA-CB	-5.46	1.44	1.52
1	2C	71	GLU	CD-OE2	-5.46	1.19	1.25
2	3B	405	GLU	CD-OE1	-5.46	1.19	1.25
2	3G	304	ASP	CG-OD1	-5.45	1.12	1.25
1	2F	174	SER	CB-OG	-5.45	1.35	1.42
1	4C	193	SER	CA-CB	-5.43	1.44	1.52
2	3A	288	GLU	CD-OE1	5.43	1.31	1.25
1	2F	27	GLU	CD-OE2	-5.43	1.19	1.25
1	4B	284	GLU	CD-OE1	-5.42	1.19	1.25
1	4A	22	GLU	CD-OE1	-5.42	1.19	1.25
1	4F	113	GLU	CD-OE1	-5.41	1.19	1.25
2	5A	22	GLU	CD-OE2	-5.40	1.19	1.25
2	3D	29	GLY	C-O	-5.40	1.15	1.23
2	3C	176	SER	CA-CB	-5.39	1.44	1.52
2	5E	407	GLU	CD-OE2	5.38	1.31	1.25
1	4E	113	GLU	CD-OE1	5.38	1.31	1.25
1	4D	27	GLU	CD-OE2	5.37	1.31	1.25
1	4F	22	GLU	CD-OE2	-5.35	1.19	1.25
1	2A	420	GLU	CD-OE1	5.34	1.31	1.25
1	4F	183	GLU	CD-OE1	-5.33	1.19	1.25
1	2B	196	GLU	CD-OE1	5.31	1.31	1.25
1	4E	415	GLU	CD-OE2	5.31	1.31	1.25
2	3E	181	GLU	CD-OE2	-5.30	1.19	1.25
2	5D	165	GLU	CD-OE2	-5.30	1.19	1.25
1	4A	98	ASP	CG-OD1	-5.28	1.13	1.25
2	3C	426	GLN	C-O	5.27	1.33	1.23
2	3G	407	GLU	CD-OE2	5.27	1.31	1.25
2	3F	288	GLU	CD-OE1	-5.26	1.19	1.25
1	2B	415	GLU	CD-OE1	-5.25	1.19	1.25
2	3G	181	GLU	CB-CG	5.24	1.62	1.52
1	2C	415	GLU	CD-OE1	-5.23	1.19	1.25
1	2H	22	GLU	CD-OE1	-5.22	1.20	1.25
1	2B	414	GLU	CD-OE2	-5.22	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3A	53	GLU	CD-OE1	-5.21	1.20	1.25
2	3H	108	GLU	CD-OE1	-5.20	1.20	1.25
1	4B	423	GLU	CG-CD	-5.20	1.44	1.51
2	3E	31	ASP	CG-OD1	-5.20	1.13	1.25
2	5I	165	GLU	CD-OE2	5.19	1.31	1.25
1	4B	300	SER	CA-CB	-5.18	1.45	1.52
2	5A	412	GLU	CD-OE2	5.18	1.31	1.25
2	5F	165	GLU	CD-OE2	-5.18	1.20	1.25
1	2H	116	ASP	CG-OD2	5.17	1.37	1.25
2	3B	322	SER	CA-CB	-5.17	1.45	1.52
1	4G	113	GLU	CD-OE1	-5.17	1.20	1.25
1	4D	69	ASP	CG-OD2	-5.17	1.13	1.25
1	4A	297	GLU	CD-OE1	-5.15	1.20	1.25
2	5B	314	SER	CB-OG	-5.15	1.35	1.42
2	5G	111	GLU	CD-OE1	5.14	1.31	1.25
1	4G	147	SER	CA-CB	-5.13	1.45	1.52
2	5B	27	GLU	CD-OE1	-5.12	1.20	1.25
2	5H	380	ARG	NE-CZ	-5.12	1.26	1.33
2	5E	158	GLU	CD-OE1	-5.12	1.20	1.25
1	2I	327	ASP	CG-OD1	5.11	1.37	1.25
1	2G	147	SER	CA-CB	-5.11	1.45	1.52
2	5D	376	GLU	CD-OE2	5.11	1.31	1.25
2	5F	328	GLU	CD-OE1	-5.09	1.20	1.25
2	3I	108	GLU	CD-OE2	-5.08	1.20	1.25
1	4D	254	GLU	CD-OE1	-5.08	1.20	1.25
2	3G	31	ASP	CG-OD1	-5.07	1.13	1.25
2	5E	248	SER	CA-CB	-5.05	1.45	1.52
1	2E	220	GLU	CD-OE1	5.05	1.31	1.25
2	3B	198	GLU	CD-OE2	5.05	1.31	1.25
2	3E	125	GLU	CD-OE2	-5.05	1.20	1.25
1	4D	392	ASP	CG-OD1	-5.04	1.13	1.25
1	2E	8	HIS	CE1-NE2	-5.03	1.21	1.32
2	3G	1	MET	N-CA	-5.02	1.36	1.46
1	2G	118	SER	CB-OG	-5.01	1.35	1.42
2	3G	108	GLU	CD-OE2	5.01	1.31	1.25
2	3B	125	GLU	CD-OE2	-5.00	1.20	1.25
1	4G	377	MET	CG-SD	-5.00	1.68	1.81

All (1002) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5C	208	TYR	CB-CG-CD1	-15.71	111.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2F	244	PHE	CB-CG-CD2	-14.95	110.33	120.80
1	2E	138	PHE	CB-CG-CD1	14.53	130.97	120.80
1	2F	244	PHE	CB-CG-CD1	14.36	130.85	120.80
1	2E	138	PHE	CB-CG-CD2	-13.54	111.32	120.80
1	2A	108	TYR	CB-CG-CD1	13.19	128.91	121.00
2	3B	425	TYR	CB-CG-CD1	12.93	128.76	121.00
2	5G	197	ASP	CB-CG-OD1	-12.84	106.74	118.30
1	4C	282	TYR	CB-CG-CD2	-12.57	113.46	121.00
2	5C	208	TYR	CB-CG-CD2	12.56	128.54	121.00
1	4D	244	PHE	CB-CG-CD1	12.42	129.49	120.80
1	2H	108	TYR	CB-CG-CD2	-12.27	113.64	121.00
1	4C	108	TYR	CB-CG-CD2	-12.11	113.74	121.00
2	5A	340	TYR	CB-CG-CD2	-11.87	113.88	121.00
2	3B	50	PHE	CB-CG-CD1	11.81	129.06	120.80
2	5D	266	PHE	CB-CG-CD1	11.40	128.78	120.80
2	3G	51	TYR	CB-CG-CD2	-11.34	114.20	121.00
2	3A	425	TYR	CB-CG-CD1	11.32	127.79	121.00
1	2A	108	TYR	CB-CG-CD2	-11.27	114.24	121.00
2	3B	50	PHE	CB-CG-CD2	-11.26	112.92	120.80
1	4D	244	PHE	CB-CG-CD2	-11.02	113.09	120.80
2	3D	383	ASP	CB-CG-OD2	10.97	128.17	118.30
2	3B	425	TYR	CB-CG-CD2	-10.96	114.42	121.00
2	3G	51	TYR	CB-CG-CD1	10.91	127.54	121.00
1	4G	320	ARG	NE-CZ-NH1	-10.86	114.87	120.30
2	5A	266	PHE	CB-CG-CD2	-10.83	113.22	120.80
2	3A	425	TYR	CB-CG-CD2	-10.80	114.52	121.00
2	3B	340	TYR	CB-CG-CD2	-10.69	114.59	121.00
2	5A	266	PHE	CB-CG-CD1	10.61	128.23	120.80
1	4D	215	ARG	CG-CD-NE	10.49	133.82	111.80
2	5A	207	LEU	CB-CG-CD2	-10.45	93.23	111.00
1	4H	327	ASP	CB-CG-OD1	-10.41	108.93	118.30
2	5A	77	ARG	NE-CZ-NH1	-10.25	115.17	120.30
2	5A	340	TYR	CB-CG-CD1	10.17	127.10	121.00
1	2A	181	VAL	CA-CB-CG2	10.16	126.14	110.90
2	5A	159	TYR	CB-CG-CD1	10.13	127.08	121.00
2	3H	265	PHE	CB-CG-CD2	-10.09	113.73	120.80
2	3B	147	MET	CG-SD-CE	-10.05	84.12	100.20
1	2A	123	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	4A	214	ARG	NE-CZ-NH2	-9.88	115.36	120.30
2	5H	408	PHE	CB-CG-CD2	-9.82	113.92	120.80
2	5C	249	ASP	CB-CG-OD1	-9.67	109.59	118.30
1	2F	390	ARG	CG-CD-NE	9.65	132.06	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2F	422	ARG	NE-CZ-NH2	9.63	125.11	120.30
2	5A	295	ASP	CB-CG-OD1	-9.62	109.64	118.30
2	5D	266	PHE	CB-CG-CD2	-9.61	114.08	120.80
1	2I	64	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	2D	215	ARG	CG-CD-NE	9.59	131.93	111.80
2	5G	51	TYR	CB-CG-CD2	-9.54	115.27	121.00
1	4B	308	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	2A	154	LEU	CB-CG-CD2	-9.47	94.89	111.00
1	4F	169	PHE	CB-CG-CD1	9.44	127.41	120.80
2	5C	39	ASP	CB-CG-OD1	-9.43	109.82	118.30
2	5H	408	PHE	CB-CG-CD1	9.40	127.38	120.80
2	3E	242	PHE	CB-CG-CD1	-9.40	114.22	120.80
1	2H	108	TYR	CB-CG-CD1	9.38	126.62	121.00
2	3E	385	PHE	CB-CG-CD2	-9.12	114.41	120.80
2	5E	385	PHE	CB-CG-CD2	-8.98	114.51	120.80
2	5F	106	TYR	CB-CG-CD1	8.98	126.39	121.00
1	4H	432	TYR	CB-CG-CD2	-8.94	115.64	121.00
2	3H	304	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	2E	372	MET	CG-SD-CE	8.89	114.42	100.20
1	2B	402	ARG	CG-CD-NE	8.88	130.46	111.80
1	2H	105	ARG	NE-CZ-NH2	8.88	124.74	120.30
2	5G	77	ARG	NE-CZ-NH2	-8.88	115.86	120.30
2	5A	425	TYR	CB-CG-CD1	8.87	126.32	121.00
1	4D	392	ASP	CB-CG-OD2	8.86	126.27	118.30
1	4H	120	ASP	CB-CG-OD1	-8.85	110.34	118.30
1	4H	432	TYR	CB-CG-CD1	8.84	126.31	121.00
2	5G	77	ARG	NE-CZ-NH1	-8.81	115.89	120.30
2	3H	425	TYR	CB-CG-CD1	8.80	126.28	121.00
2	3B	340	TYR	CB-CG-CD1	8.75	126.25	121.00
2	5B	425	TYR	CB-CG-CD2	-8.75	115.75	121.00
2	5A	241	ARG	CG-CD-NE	8.66	129.98	111.80
2	5E	121	ARG	CA-CB-CG	8.64	132.42	113.40
2	5E	304	ASP	CB-CG-OD2	8.64	126.08	118.30
1	4I	391	MET	CB-CG-SD	-8.60	86.61	112.40
2	5I	325	GLU	N-CA-CB	8.56	126.00	110.60
2	3A	391	ARG	CB-CG-CD	8.51	133.73	111.60
2	3B	183	TYR	CB-CG-CD2	-8.51	115.89	121.00
2	5E	192	LEU	CB-CG-CD2	-8.50	96.56	111.00
2	3I	375	GLN	CB-CG-CD	-8.49	89.52	111.60
2	3B	304	ASP	CB-CG-OD1	-8.47	110.68	118.30
2	5F	106	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	4D	52	PHE	CB-CG-CD1	8.45	126.71	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5E	77	ARG	NE-CZ-NH1	-8.40	116.10	120.30
1	4B	33	ASP	CB-CG-OD1	-8.35	110.79	118.30
1	2G	418	PHE	CB-CG-CD1	8.34	126.64	120.80
2	3H	265	PHE	CB-CG-CD1	8.33	126.63	120.80
2	3E	242	PHE	CB-CG-CD2	8.30	126.61	120.80
1	4D	238	LEU	CB-CG-CD1	-8.30	96.89	111.00
2	5E	321	MET	CG-SD-CE	-8.30	86.92	100.20
2	5H	133	PHE	CB-CG-CD2	-8.30	114.99	120.80
2	3E	77	ARG	CG-CD-NE	8.28	129.19	111.80
2	3E	209	ASP	CB-CG-OD1	-8.27	110.86	118.30
1	2C	205	ASP	CB-CG-OD1	-8.27	110.86	118.30
1	4C	423	GLU	CG-CD-OE1	-8.23	101.85	118.30
1	2F	358	GLN	CB-CA-C	8.22	126.84	110.40
1	4A	76	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	2B	123	ARG	CG-CD-NE	8.18	128.98	111.80
2	3B	179	VAL	CA-CB-CG1	8.18	123.17	110.90
1	4H	218	ASP	CB-CG-OD1	-8.17	110.95	118.30
2	3H	377	MET	CG-SD-CE	-8.14	87.17	100.20
1	2A	319	TYR	CB-CG-CD2	-8.11	116.13	121.00
1	4G	243	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	2A	402	ARG	CG-CD-NE	8.10	128.80	111.80
2	5E	121	ARG	CB-CA-C	-8.09	94.21	110.40
2	3F	310	TYR	CB-CG-CD2	8.09	125.85	121.00
1	4C	108	TYR	CB-CG-CD1	8.07	125.84	121.00
1	4F	66	VAL	CG1-CB-CG2	8.04	123.76	110.90
2	5G	365	VAL	CA-CB-CG2	8.01	122.92	110.90
2	5E	385	PHE	CB-CG-CD1	8.01	126.41	120.80
1	4C	392	ASP	CB-CG-OD1	-8.01	111.09	118.30
2	5H	117	LEU	CB-CG-CD1	8.00	124.60	111.00
2	3F	365	VAL	CA-CB-CG2	8.00	122.89	110.90
1	4H	156	ARG	CG-CD-NE	-7.97	95.07	111.80
2	3B	281	TYR	CB-CG-CD2	-7.92	116.25	121.00
2	3E	183	TYR	CB-CG-CD1	-7.92	116.25	121.00
2	3H	425	TYR	CB-CG-CD2	-7.90	116.26	121.00
1	4A	282	TYR	CB-CG-CD1	7.90	125.74	121.00
2	3F	147	MET	CG-SD-CE	-7.90	87.56	100.20
2	5B	425	TYR	CB-CG-CD1	7.90	125.74	121.00
1	2I	33	ASP	CB-CG-OD1	-7.88	111.21	118.30
2	3E	385	PHE	CB-CG-CD1	7.87	126.31	120.80
1	2B	121	ARG	CG-CD-NE	7.86	128.31	111.80
2	5A	425	TYR	CB-CG-CD2	-7.82	116.31	121.00
2	5G	51	TYR	CB-CG-CD1	7.81	125.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2H	339	ARG	CG-CD-NE	7.80	128.17	111.80
2	3A	241	ARG	CG-CD-NE	7.80	128.17	111.80
1	4G	130	THR	OG1-CB-CG2	7.78	127.88	110.00
1	4E	296	PHE	CB-CG-CD1	-7.77	115.36	120.80
1	2D	424	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	4G	408	TYR	CB-CG-CD1	-7.76	116.34	121.00
2	3H	81	PHE	CB-CG-CD2	-7.74	115.38	120.80
2	3F	404	ASP	CB-CG-OD1	-7.72	111.35	118.30
2	3C	300	MET	CG-SD-CE	-7.71	87.86	100.20
2	5E	209	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	2I	11	GLN	CB-CA-C	7.69	125.77	110.40
2	3I	304	ASP	CB-CG-OD2	-7.67	111.40	118.30
2	3B	281	TYR	CB-CG-CD1	7.67	125.60	121.00
1	4A	420	GLU	N-CA-CB	7.67	124.40	110.60
2	3A	340	TYR	CB-CG-CD2	-7.63	116.42	121.00
2	3E	159	TYR	CB-CG-CD2	7.63	125.58	121.00
2	5E	365	VAL	CA-CB-CG2	7.63	122.35	110.90
2	3B	183	TYR	CB-CG-CD1	7.58	125.55	121.00
2	5G	197	ASP	CB-CG-OD2	7.57	125.12	118.30
2	3E	159	TYR	CB-CG-CD1	-7.57	116.46	121.00
1	4I	215	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	4B	215	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	4D	296	PHE	CB-CG-CD1	7.55	126.09	120.80
2	3B	383	ASP	CB-CG-OD1	-7.54	111.51	118.30
2	5B	350	LYS	CD-CE-NZ	-7.54	94.36	111.70
2	3F	310	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	2E	390	ARG	CG-CD-NE	7.52	127.59	111.80
1	2I	392	ASP	CB-CG-OD1	7.50	125.05	118.30
1	4F	244	PHE	CB-CG-CD1	-7.50	115.55	120.80
2	3D	50	PHE	CB-CG-CD1	7.50	126.05	120.80
1	4A	282	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	2D	251	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	4C	205	ASP	CB-CG-OD1	-7.45	111.60	118.30
2	3D	117	LEU	CB-CG-CD1	7.43	123.63	111.00
1	4C	343	PHE	CB-CG-CD1	7.42	125.99	120.80
1	4F	79	ARG	CG-CD-NE	7.41	127.36	111.80
1	4G	320	ARG	NH1-CZ-NH2	7.41	127.55	119.40
1	2F	22	GLU	N-CA-CB	7.41	123.94	110.60
2	5E	197	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	2A	404	PHE	CB-CG-CD1	7.39	125.98	120.80
1	2B	119	LEU	CB-CG-CD2	7.39	123.57	111.00
1	2H	351	PHE	CB-CG-CD1	-7.38	115.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5B	66	MET	CA-CB-CG	7.38	125.84	113.30
1	2G	418	PHE	CB-CG-CD2	-7.37	115.64	120.80
1	4H	84	ARG	NE-CZ-NH1	-7.36	116.62	120.30
2	3B	197	ASP	CB-CG-OD1	-7.35	111.68	118.30
1	2D	390	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	2G	255	PHE	CB-CG-CD1	7.32	125.92	120.80
1	4H	339	ARG	CG-CD-NE	7.32	127.17	111.80
1	2A	319	TYR	CB-CG-CD1	7.31	125.39	121.00
1	4A	49	PHE	CB-CG-CD2	-7.30	115.69	120.80
1	4F	66	VAL	CA-CB-CG1	7.29	121.83	110.90
1	4G	64	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	4C	33	ASP	CB-CG-OD1	-7.27	111.76	118.30
2	3B	159	TYR	CB-CG-CD1	7.26	125.36	121.00
1	2I	383	ALA	O-C-N	-7.24	111.11	122.70
1	2E	322	ASP	CB-CG-OD1	-7.24	111.79	118.30
1	4A	210	TYR	CB-CG-CD1	-7.24	116.66	121.00
1	2A	210	TYR	CB-CG-CD2	-7.24	116.66	121.00
2	3F	164	MET	CG-SD-CE	7.24	111.78	100.20
2	5C	340	TYR	CB-CG-CD1	-7.19	116.69	121.00
2	3C	217	LEU	CB-CG-CD1	7.18	123.21	111.00
2	3D	225	LEU	CB-CA-C	7.17	123.82	110.20
2	3A	341	PHE	CB-CG-CD1	-7.17	115.78	120.80
2	3H	81	PHE	CB-CG-CD1	7.16	125.81	120.80
2	5D	197	ASP	CB-CG-OD2	-7.14	111.87	118.30
2	3G	304	ASP	CB-CG-OD1	-7.14	111.87	118.30
2	5E	209	ASP	CB-CG-OD2	7.13	124.72	118.30
2	3B	90	PHE	CB-CG-CD1	7.13	125.79	120.80
1	4B	320	ARG	NE-CZ-NH2	7.13	123.86	120.30
2	5G	77	ARG	NH1-CZ-NH2	7.12	127.23	119.40
2	5B	26	ASP	CB-CG-OD1	-7.12	111.89	118.30
2	5C	340	TYR	CB-CG-CD2	7.11	125.27	121.00
2	5B	107	THR	OG1-CB-CG2	-7.11	93.64	110.00
1	2G	120	ASP	CB-CG-OD1	7.08	124.68	118.30
1	2G	223	THR	CA-CB-CG2	7.08	122.31	112.40
2	5F	81	PHE	CB-CG-CD2	-7.08	115.84	120.80
1	4C	250	VAL	CA-CB-CG1	7.08	121.52	110.90
2	5B	222	TYR	CB-CG-CD1	-7.07	116.75	121.00
2	5G	41	ASP	CB-CG-OD1	-7.06	111.95	118.30
1	2G	255	PHE	CB-CG-CD2	-7.05	115.86	120.80
2	5C	321	MET	CG-SD-CE	7.04	111.47	100.20
1	2H	339	ARG	O-C-N	-7.03	111.45	122.70
1	4A	49	PHE	CB-CG-CD1	7.02	125.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3G	118	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	2E	339	ARG	CG-CD-NE	7.02	126.54	111.80
2	3I	147	MET	CG-SD-CE	-7.02	88.97	100.20
2	3I	14	ASN	CB-CG-OD1	-7.00	107.59	121.60
1	4C	327	ASP	CB-CG-OD1	7.00	124.60	118.30
2	3E	367	PHE	CB-CG-CD2	-6.99	115.90	120.80
2	5B	318	ARG	NE-CZ-NH2	-6.99	116.81	120.30
2	3D	383	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	4D	156	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	4H	69	ASP	CB-CG-OD2	-6.96	112.03	118.30
2	3F	398	TYR	CB-CG-CD2	6.96	125.18	121.00
1	2D	123	ARG	CG-CD-NE	6.96	126.41	111.80
1	4F	402	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	3A	118	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	4A	116	ASP	CB-CG-OD1	6.95	124.55	118.30
2	3D	50	PHE	CB-CG-CD2	-6.94	115.94	120.80
1	2G	53	PHE	CB-CG-CD2	-6.94	115.94	120.80
1	4E	353	CYS	N-CA-CB	6.94	123.09	110.60
2	5C	422	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	2B	153	LEU	CB-CG-CD1	-6.92	99.23	111.00
2	5D	36	TYR	CB-CG-CD1	6.92	125.15	121.00
1	4I	391	MET	CA-CB-CG	6.91	125.05	113.30
2	3A	170	PHE	CB-CG-CD2	-6.91	115.96	120.80
2	3G	425	TYR	CB-CG-CD1	6.91	125.15	121.00
2	3A	380	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	2E	136	LEU	CB-CG-CD1	6.89	122.72	111.00
2	3E	197	ASP	CB-CG-OD1	-6.89	112.10	118.30
2	5G	159	TYR	CB-CG-CD1	6.89	125.13	121.00
1	4B	422	ARG	NE-CZ-NH1	-6.88	116.86	120.30
2	5C	65	LEU	CB-CG-CD2	6.88	122.69	111.00
2	3E	213	ARG	CG-CD-NE	6.87	126.24	111.80
2	3B	159	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	4A	161	TYR	CB-CG-CD1	6.87	125.12	121.00
2	3E	377	MET	CG-SD-CE	-6.86	89.23	100.20
2	3H	262	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	4B	214	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	2E	388	PHE	CB-CG-CD1	-6.84	116.01	120.80
1	4G	70	LEU	CB-CG-CD2	-6.83	99.38	111.00
2	5G	118	ASP	CB-CG-OD1	-6.83	112.15	118.30
2	5G	365	VAL	CA-CB-CG1	6.83	121.14	110.90
2	5A	159	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	2H	351	PHE	CB-CG-CD2	6.83	125.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5F	81	PHE	CB-CG-CD1	6.83	125.58	120.80
1	4D	392	ASP	CB-CG-OD1	-6.82	112.16	118.30
2	5E	170	PHE	CB-CG-CD1	6.82	125.58	120.80
1	2G	53	PHE	CB-CG-CD1	6.82	125.57	120.80
2	5E	170	PHE	CB-CG-CD2	-6.82	116.03	120.80
2	5G	255	VAL	CG1-CB-CG2	6.81	121.79	110.90
1	2A	123	ARG	NH1-CZ-NH2	6.79	126.87	119.40
2	3A	41	ASP	CB-CG-OD1	-6.77	112.20	118.30
1	2C	320	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	2D	402	ARG	NE-CZ-NH1	6.77	123.68	120.30
2	5A	241	ARG	NE-CZ-NH1	-6.77	116.92	120.30
2	3E	365	VAL	CA-CB-CG2	6.76	121.05	110.90
1	4A	161	TYR	CB-CG-CD2	-6.76	116.94	121.00
2	5D	26	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	4B	390	ARG	CG-CD-NE	6.75	125.98	111.80
2	5A	23	VAL	CA-CB-CG1	6.75	121.02	110.90
2	5H	321	MET	N-CA-CB	6.75	122.74	110.60
1	4A	52	PHE	CB-CG-CD1	6.74	125.52	120.80
1	2G	322	ASP	CB-CG-OD1	-6.74	112.23	118.30
2	3F	388	MET	CG-SD-CE	-6.73	89.43	100.20
2	3F	333	VAL	CA-CB-CG1	6.73	120.99	110.90
2	5D	282	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	5D	378	PHE	CB-CG-CD1	-6.72	116.09	120.80
2	5H	340	TYR	CB-CG-CD1	-6.72	116.97	121.00
2	3A	26	ASP	CB-CG-OD1	-6.72	112.25	118.30
2	3I	327	ASP	CB-CG-OD1	-6.72	112.25	118.30
2	5C	203	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	5D	250	LEU	CB-CG-CD1	6.72	122.42	111.00
2	3F	41	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	4F	84	ARG	CG-CD-NE	6.71	125.90	111.80
2	5G	36	TYR	CB-CG-CD1	-6.71	116.97	121.00
2	3A	330	MET	CG-SD-CE	6.70	110.92	100.20
1	4F	322	ASP	CB-CG-OD1	-6.70	112.27	118.30
2	5I	200	GLN	CB-CA-C	6.70	123.80	110.40
2	3A	31	ASP	CB-CG-OD2	6.70	124.33	118.30
2	3D	41	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	4A	70	LEU	CB-CG-CD2	6.69	122.37	111.00
1	2G	282	TYR	CB-CG-CD1	-6.68	116.99	121.00
2	5C	187	LEU	CB-CG-CD1	6.67	122.35	111.00
2	5D	92	PHE	CB-CG-CD1	-6.65	116.14	120.80
1	2E	123	ARG	CG-CD-NE	-6.65	97.84	111.80
1	4C	343	PHE	CB-CG-CD2	-6.65	116.15	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2G	244	PHE	CB-CG-CD1	6.64	125.45	120.80
1	4G	279	GLU	CB-CA-C	-6.64	97.11	110.40
2	5B	41	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	4F	345	ASP	CB-CG-OD1	-6.63	112.33	118.30
2	3A	341	PHE	CB-CG-CD2	6.63	125.44	120.80
2	5F	327	ASP	CB-CG-OD1	-6.62	112.34	118.30
2	5H	342	VAL	CA-CB-CG2	6.62	120.83	110.90
2	5H	221	THR	CA-CB-CG2	-6.60	103.16	112.40
2	5D	192	LEU	CB-CG-CD2	-6.60	99.78	111.00
2	3A	31	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	4H	373	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	2D	343	PHE	CB-CG-CD1	6.58	125.41	120.80
1	4G	200	VAL	CG1-CB-CG2	6.58	121.44	110.90
1	4A	98	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	2G	390	ARG	CG-CD-NE	-6.58	97.99	111.80
2	5C	212	PHE	CB-CG-CD1	6.57	125.40	120.80
1	4G	424	ASP	CB-CG-OD1	-6.55	112.40	118.30
2	5F	90	PHE	CB-CG-CD2	-6.55	116.22	120.80
2	3E	377	MET	CA-CB-CG	-6.54	102.17	113.30
2	5C	385	PHE	CB-CG-CD2	-6.54	116.22	120.80
2	3B	90	PHE	CB-CG-CD2	-6.53	116.23	120.80
2	3E	183	TYR	CB-CG-CD2	6.53	124.92	121.00
2	3F	81	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	2I	326	LYS	CB-CA-C	6.53	123.46	110.40
2	3D	67	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	4D	123	ARG	CG-CD-NE	6.52	125.50	111.80
2	5G	214	THR	CA-CB-OG1	6.51	122.68	109.00
2	5A	310	TYR	CB-CG-CD1	6.51	124.91	121.00
2	5G	380	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	5B	92	PHE	CB-CG-CD1	6.49	125.35	120.80
1	2I	392	ASP	CB-CG-OD2	-6.49	112.46	118.30
2	3G	281	TYR	CB-CG-CD1	6.49	124.89	121.00
2	3G	213	ARG	CG-CD-NE	6.48	125.41	111.80
2	3G	177	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	2A	432	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	4E	169	PHE	CB-CG-CD2	-6.47	116.27	120.80
2	5A	169	VAL	CG1-CB-CG2	6.47	121.25	110.90
2	3F	22	GLU	N-CA-CB	6.47	122.24	110.60
1	4F	90	GLU	CG-CD-OE1	-6.47	105.37	118.30
2	3F	274	THR	OG1-CB-CG2	-6.46	95.13	110.00
2	5F	164	MET	CG-SD-CE	6.46	110.54	100.20
1	4A	123	ARG	NE-CZ-NH1	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5F	320	ARG	CG-CD-NE	6.46	125.36	111.80
2	5G	20	PHE	CB-CG-CD1	-6.45	116.28	120.80
2	3F	398	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	4D	153	LEU	CB-CG-CD2	-6.45	100.04	111.00
2	3A	295	ASP	CB-CG-OD1	-6.45	112.50	118.30
2	5E	242	PHE	CB-CG-CD1	-6.44	116.29	120.80
1	4B	320	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	4H	281	ALA	N-CA-CB	6.43	119.11	110.10
2	5A	253	LEU	CB-CA-C	6.43	122.41	110.20
1	4F	179	THR	CA-CB-CG2	6.42	121.39	112.40
1	4D	52	PHE	CB-CG-CD2	-6.42	116.30	120.80
2	3A	170	PHE	CB-CG-CD1	6.41	125.29	120.80
1	2A	210	TYR	CB-CG-CD1	6.41	124.84	121.00
2	5G	228	LEU	CB-CA-C	6.41	122.37	110.20
2	3E	81	PHE	CB-CG-CD2	-6.40	116.32	120.80
2	5H	311	LEU	CB-CG-CD2	-6.39	100.13	111.00
2	3G	310	TYR	CB-CG-CD1	6.39	124.83	121.00
2	5B	409	THR	OG1-CB-CG2	-6.39	95.30	110.00
2	5B	177	ASP	CB-CG-OD2	6.39	124.05	118.30
1	4C	98	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	2F	314	ALA	N-CA-CB	-6.38	101.17	110.10
1	2H	431	ASP	CB-CG-OD1	-6.38	112.56	118.30
2	5B	293	MET	N-CA-CB	6.38	122.08	110.60
1	2G	345	ASP	CB-CG-OD1	-6.37	112.56	118.30
2	5A	310	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	3C	187	LEU	CB-CG-CD1	6.37	121.83	111.00
1	4F	169	PHE	CB-CG-CD2	-6.37	116.34	120.80
2	5E	333	VAL	CA-CB-CG1	6.37	120.45	110.90
1	4H	49	PHE	CB-CG-CD2	-6.36	116.35	120.80
2	3H	367	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	4D	35	GLN	CA-CB-CG	6.35	127.38	113.40
1	2G	408	TYR	CB-CG-CD1	-6.34	117.19	121.00
1	2G	282	TYR	CB-CG-CD2	6.34	124.81	121.00
2	3C	73	MET	CG-SD-CE	-6.34	90.06	100.20
2	3H	281	TYR	CB-CG-CD1	6.34	124.80	121.00
2	5I	280	GLN	CA-CB-CG	6.33	127.33	113.40
1	2A	357	TYR	CB-CG-CD1	6.33	124.80	121.00
2	5F	88	ASP	CB-CG-OD1	6.33	124.00	118.30
1	2I	339	ARG	CG-CD-NE	6.33	125.09	111.80
1	4I	185	TYR	CB-CG-CD2	-6.32	117.21	121.00
2	5G	58	ARG	CG-CD-NE	-6.32	98.52	111.80
1	2F	345	ASP	CB-CG-OD1	-6.32	112.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3B	213	ARG	NE-CZ-NH1	-6.31	117.14	120.30
2	5D	385	PHE	CB-CG-CD1	-6.31	116.38	120.80
1	2H	109	THR	OG1-CB-CG2	-6.31	95.49	110.00
2	5B	331	LEU	CB-CG-CD2	6.30	121.72	111.00
2	3F	321	MET	CA-CB-CG	6.30	124.01	113.30
1	2F	339	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	2E	123	ARG	CB-CG-CD	6.29	127.95	111.60
1	2C	388	PHE	CB-CG-CD1	-6.29	116.40	120.80
1	4A	390	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	5C	143	THR	O-C-N	-6.28	112.52	123.20
1	4E	392	ASP	CB-CG-OD2	-6.27	112.65	118.30
2	5G	36	TYR	CB-CG-CD2	6.27	124.76	121.00
1	2C	320	ARG	CG-CD-NE	6.27	124.96	111.80
2	5H	425	TYR	CB-CG-CD1	6.25	124.75	121.00
1	2H	215	ARG	NE-CZ-NH1	-6.25	117.17	120.30
2	3E	203	ASP	CB-CG-OD2	-6.25	112.68	118.30
2	5E	242	PHE	CB-CG-CD2	6.25	125.17	120.80
1	2F	386	GLU	CB-CG-CD	6.24	131.06	114.20
1	4H	283	HIS	N-CA-CB	-6.24	99.37	110.60
2	3G	422	TYR	CB-CG-CD1	-6.24	117.26	121.00
2	3I	203	ASP	CB-CG-OD1	-6.23	112.69	118.30
2	5F	192	LEU	CB-CG-CD2	-6.23	100.41	111.00
1	4D	296	PHE	CB-CG-CD2	-6.23	116.44	120.80
2	5I	241	ARG	NE-CZ-NH2	6.23	123.42	120.30
2	5C	249	ASP	CB-CG-OD2	6.23	123.91	118.30
1	2C	327	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	4C	187	SER	CB-CA-C	6.22	121.92	110.10
2	3G	270	PHE	CB-CG-CD2	-6.22	116.45	120.80
2	5F	155	VAL	CA-CB-CG1	6.21	120.22	110.90
2	5C	121	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	5E	293	MET	CA-CB-CG	6.21	123.85	113.30
1	2D	79	ARG	CB-CA-C	6.21	122.81	110.40
2	5F	90	PHE	CB-CG-CD1	6.20	125.14	120.80
1	2F	424	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	4I	278	ALA	N-CA-CB	6.20	118.78	110.10
1	2I	399	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	4A	396	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	2B	320	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	2I	238	LEU	CB-CG-CD1	-6.18	100.50	111.00
2	3D	355	ASP	N-CA-CB	6.18	121.72	110.60
2	3G	107	THR	CA-CB-OG1	6.18	121.97	109.00
2	3B	197	ASP	CB-CG-OD2	6.17	123.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3E	367	PHE	CB-CG-CD1	6.17	125.12	120.80
1	2A	2	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	2E	69	ASP	CB-CG-OD1	6.16	123.84	118.30
1	4B	340	THR	OG1-CB-CG2	6.16	124.16	110.00
2	3H	367	PHE	CB-CG-CD1	6.15	125.11	120.80
2	3E	330	MET	CG-SD-CE	-6.15	90.36	100.20
1	4G	250	VAL	CA-CB-CG1	6.13	120.10	110.90
1	4H	205	ASP	CB-CG-OD2	6.13	123.82	118.30
2	3G	155	VAL	CA-CB-CG1	6.13	120.10	110.90
1	4A	92	LEU	CB-CG-CD2	6.13	121.43	111.00
1	2G	432	TYR	CB-CG-CD2	-6.13	117.32	121.00
2	3G	392	LYS	CB-CG-CD	6.13	127.54	111.60
1	2B	161	TYR	CB-CG-CD2	-6.13	117.32	121.00
2	3F	81	PHE	CB-CG-CD1	6.13	125.09	120.80
1	2E	345	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	4E	345	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	4G	250	VAL	CA-CB-CG2	6.12	120.08	110.90
1	4F	204	LEU	CB-CG-CD2	6.12	121.41	111.00
1	4C	33	ASP	CB-CG-OD2	6.11	123.80	118.30
1	4F	199	ASP	CB-CG-OD2	-6.11	112.80	118.30
2	3F	316	MET	CA-CB-CG	6.11	123.68	113.30
1	4H	248	LEU	CB-CG-CD2	6.10	121.38	111.00
1	2B	119	LEU	CB-CA-C	6.10	121.79	110.20
1	4C	49	PHE	CB-CG-CD1	6.10	125.07	120.80
2	3H	77	ARG	NE-CZ-NH1	-6.09	117.25	120.30
2	5E	298	ASN	O-C-N	-6.09	112.95	122.70
2	5H	181	GLU	CA-CB-CG	6.08	126.78	113.40
1	4A	227	LEU	CA-CB-CG	6.08	129.27	115.30
1	4I	2	ARG	NE-CZ-NH1	-6.07	117.26	120.30
2	5A	170	PHE	CB-CG-CD2	-6.07	116.55	120.80
2	3G	425	TYR	CB-CG-CD2	-6.07	117.36	121.00
2	5G	167	PHE	CB-CG-CD1	-6.07	116.55	120.80
2	5F	390	ARG	CG-CD-NE	6.06	124.53	111.80
1	2E	320	ARG	NE-CZ-NH1	-6.06	117.27	120.30
2	5H	365	VAL	CG1-CB-CG2	6.05	120.59	110.90
1	2D	243	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	2D	391	MET	CB-CG-SD	-6.05	94.25	112.40
1	4E	371	VAL	CG1-CB-CG2	6.05	120.58	110.90
2	5H	425	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	2D	402	ARG	CG-CD-NE	6.05	124.50	111.80
1	4B	306	ASP	CB-CG-OD2	-6.04	112.86	118.30
2	5F	41	ASP	CB-CG-OD1	6.04	123.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	207	GLU	OE1-CD-OE2	6.04	130.54	123.30
2	5H	120	VAL	CA-CB-CG1	6.03	119.95	110.90
1	2A	225	THR	CA-CB-CG2	6.03	120.84	112.40
1	2D	210	TYR	CB-CG-CD2	-6.03	117.38	121.00
2	3I	27	GLU	N-CA-CB	6.03	121.45	110.60
1	4F	392	ASP	CB-CG-OD1	6.03	123.72	118.30
1	4G	121	ARG	CG-CD-NE	6.02	124.45	111.80
2	3F	300	MET	CG-SD-CE	-6.02	90.57	100.20
1	2E	268	MET	CA-CB-CG	6.02	123.53	113.30
2	3E	209	ASP	CB-CG-OD2	6.02	123.71	118.30
1	4E	353	CYS	CA-CB-SG	-6.01	103.17	114.00
1	2H	398	MET	CG-SD-CE	-6.01	90.58	100.20
2	3F	169	VAL	CG1-CB-CG2	-6.00	101.29	110.90
2	5B	222	TYR	CB-CG-CD2	6.00	124.60	121.00
2	3C	422	TYR	CB-CG-CD2	-6.00	117.40	121.00
2	3I	422	TYR	CB-CG-CD2	-5.99	117.41	121.00
2	5C	66	MET	CG-SD-CE	5.99	109.78	100.20
1	2A	168	ASN	CB-CA-C	5.98	122.36	110.40
1	2H	199	ASP	CB-CG-OD2	-5.98	112.92	118.30
2	3F	155	VAL	CA-CB-CG1	5.98	119.86	110.90
2	5A	133	PHE	CB-CG-CD2	-5.98	116.62	120.80
1	4D	79	ARG	NE-CZ-NH1	-5.97	117.32	120.30
2	3H	267	LEU	CB-CG-CD1	5.96	121.14	111.00
1	2I	345	ASP	CB-CG-OD1	5.96	123.67	118.30
2	5H	42	LEU	CB-CG-CD2	-5.96	100.87	111.00
2	3H	304	ASP	CB-CG-OD1	5.96	123.66	118.30
1	4E	339	ARG	CG-CD-NE	5.95	124.30	111.80
2	3C	276	ARG	CG-CD-NE	5.95	124.30	111.80
1	2A	120	ASP	CB-CG-OD1	-5.95	112.94	118.30
2	3A	50	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	2F	322	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	2I	399	TYR	CB-CG-CD2	5.93	124.56	121.00
1	2C	64	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	4A	64	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	2H	398	MET	CA-CB-CG	5.92	123.36	113.30
2	3G	179	VAL	CA-CB-CG2	5.91	119.77	110.90
1	2A	404	PHE	CB-CG-CD2	-5.91	116.66	120.80
2	3C	354	CYS	CA-CB-SG	5.91	124.64	114.00
2	5B	177	ASP	CB-CG-OD1	-5.91	112.98	118.30
2	5G	327	ASP	CB-CG-OD1	5.91	123.62	118.30
2	5I	22	GLU	CA-CB-CG	5.91	126.41	113.40
2	5C	377	MET	CG-SD-CE	5.91	109.65	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3I	23	VAL	CA-CB-CG1	5.91	119.76	110.90
2	5B	23	VAL	CA-CB-CG1	5.90	119.76	110.90
2	5I	363	MET	CA-CB-CG	5.90	123.34	113.30
2	3A	66	MET	CG-SD-CE	5.90	109.64	100.20
1	4C	64	ARG	NE-CZ-NH1	-5.90	117.35	120.30
2	3E	406	MET	CG-SD-CE	5.89	109.63	100.20
2	3D	355	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	2A	357	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	2D	251	ASP	CB-CG-OD2	5.88	123.60	118.30
1	4F	432	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	4D	16	ILE	CB-CA-C	5.88	123.35	111.60
2	3E	147	MET	CA-CB-CG	5.88	123.29	113.30
1	2C	84	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	2H	218	ASP	CB-CG-OD1	-5.87	113.02	118.30
2	5A	385	PHE	CB-CG-CD1	5.87	124.91	120.80
1	2E	108	TYR	CB-CG-CD1	5.87	124.52	121.00
2	5G	317	PHE	CB-CG-CD2	-5.87	116.69	120.80
2	5A	149	THR	OG1-CB-CG2	-5.86	96.52	110.00
2	3G	222	TYR	CB-CG-CD1	5.86	124.52	121.00
1	4B	413	MET	CG-SD-CE	5.86	109.57	100.20
1	4D	135	PHE	CB-CG-CD1	-5.85	116.70	120.80
2	5B	175	VAL	CA-CB-CG1	5.85	119.67	110.90
1	2E	391	MET	CA-CB-CG	-5.84	103.36	113.30
2	3B	415	MET	CB-CG-SD	5.84	129.93	112.40
1	2G	205	ASP	CB-CG-OD2	-5.84	113.05	118.30
2	3C	99	ASN	N-CA-CB	5.84	121.11	110.60
1	4D	391	MET	CB-CG-SD	-5.83	94.91	112.40
2	5G	31	ASP	CB-CG-OD1	5.83	123.55	118.30
1	2F	351	PHE	CB-CG-CD2	-5.83	116.72	120.80
2	5H	203	ASP	CB-CG-OD2	5.83	123.54	118.30
1	2D	169	PHE	CB-CG-CD2	-5.82	116.72	120.80
2	5A	295	ASP	CB-CG-OD2	5.82	123.54	118.30
1	4G	133	GLN	N-CA-CB	5.82	121.07	110.60
2	3I	209	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	4F	387	VAL	CA-CB-CG1	5.81	119.61	110.90
1	4G	418	PHE	CB-CG-CD2	-5.81	116.73	120.80
2	3H	281	TYR	CB-CG-CD2	-5.81	117.52	121.00
1	2F	159	VAL	CA-CB-CG1	5.80	119.61	110.90
2	5C	23	VAL	CA-CB-CG1	5.80	119.61	110.90
1	2D	343	PHE	CB-CG-CD2	-5.80	116.74	120.80
2	3B	251	ARG	CG-CD-NE	-5.79	99.63	111.80
2	5A	201	VAL	CG1-CB-CG2	-5.79	101.64	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5H	133	PHE	CB-CG-CD1	5.79	124.85	120.80
1	4B	262	TYR	CB-CG-CD2	-5.78	117.53	121.00
2	5D	390	ARG	CG-CD-NE	5.78	123.95	111.80
1	2B	408	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	4B	3	GLU	N-CA-CB	5.78	121.00	110.60
2	3D	121	ARG	CG-CD-NE	5.78	123.93	111.80
2	3G	255	VAL	CA-CB-CG1	5.78	119.56	110.90
1	4E	339	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	4A	210	TYR	CB-CG-CD2	5.77	124.46	121.00
1	4D	135	PHE	CB-CG-CD2	5.77	124.84	120.80
2	5B	330	MET	CB-CG-SD	5.76	129.68	112.40
1	2E	108	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	2G	306	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	2D	207	GLU	CA-CB-CG	5.75	126.04	113.40
1	4C	262	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	4G	203	MET	CA-CB-CG	5.75	123.07	113.30
2	3D	304	ASP	CB-CG-OD1	5.74	123.47	118.30
2	3H	77	ARG	CB-CA-C	5.74	121.88	110.40
2	3A	391	ARG	N-CA-CB	5.74	120.93	110.60
1	4G	179	THR	CA-CB-CG2	5.74	120.43	112.40
2	5G	159	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	3C	181	GLU	CA-CB-CG	5.73	126.02	113.40
2	5B	213	ARG	CG-CD-NE	5.73	123.84	111.80
2	3E	255	VAL	CA-CB-CG1	5.73	119.50	110.90
1	4H	78	VAL	CA-CB-CG1	-5.73	102.30	110.90
2	3G	81	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	4F	399	TYR	CB-CG-CD1	-5.72	117.56	121.00
2	3A	367	PHE	CB-CG-CD1	-5.72	116.80	120.80
2	3G	20	PHE	CB-CG-CD1	-5.72	116.80	120.80
2	5B	323	THR	CA-CB-OG1	5.72	121.01	109.00
2	5I	282	ARG	CG-CD-NE	5.72	123.81	111.80
2	5A	342	VAL	CA-CB-CG2	-5.71	102.33	110.90
2	5G	167	PHE	CB-CG-CD2	5.71	124.80	120.80
2	5I	86	ARG	NE-CZ-NH1	-5.71	117.44	120.30
2	3B	218	THR	CA-CB-OG1	5.71	120.98	109.00
2	5C	422	TYR	CB-CG-CD1	5.71	124.42	121.00
1	4G	18	ASN	CB-CA-C	5.71	121.81	110.40
2	3D	106	TYR	CB-CG-CD1	5.70	124.42	121.00
1	4E	138	PHE	CB-CG-CD1	5.70	124.79	120.80
2	5C	342	VAL	CG1-CB-CG2	5.70	120.03	110.90
2	5I	66	MET	CA-CB-CG	5.70	123.00	113.30
2	5A	138	SER	N-CA-CB	5.70	119.05	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3A	253	LEU	CB-CA-C	5.70	121.03	110.20
2	3A	300	MET	CA-CB-CG	5.70	122.99	113.30
2	5F	212	PHE	CB-CG-CD1	5.69	124.78	120.80
2	5E	390	ARG	CG-CD-NE	5.69	123.75	111.80
1	2A	304	LYS	N-CA-CB	-5.69	100.36	110.60
1	4B	306	ASP	CB-CG-OD1	5.69	123.42	118.30
2	3G	91	VAL	CG1-CB-CG2	-5.69	101.80	110.90
2	5F	77	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	2G	290	GLU	OE1-CD-OE2	5.68	130.11	123.30
2	3B	389	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	5B	380	ARG	CG-CD-NE	-5.67	99.89	111.80
1	2C	269	LEU	CB-CG-CD2	5.67	120.64	111.00
2	3E	394	PHE	CB-CG-CD2	-5.66	116.83	120.80
1	4H	422	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	4E	214	ARG	CB-CG-CD	5.66	126.32	111.60
1	4H	187	SER	CB-CA-C	5.66	120.86	110.10
1	2A	429	GLU	CB-CA-C	5.66	121.72	110.40
1	4E	218	ASP	CB-CG-OD1	5.66	123.39	118.30
1	4H	302	MET	CG-SD-CE	-5.65	91.15	100.20
1	2C	120	ASP	CB-CG-OD2	-5.65	113.21	118.30
2	3H	164	MET	CA-CB-CG	5.65	122.91	113.30
2	3I	176	SER	N-CA-CB	5.65	118.97	110.50
1	2F	179	THR	CA-CB-CG2	5.65	120.31	112.40
1	4C	123	ARG	CG-CD-NE	5.64	123.65	111.80
2	3B	203	ASP	CB-CG-OD1	5.64	123.38	118.30
2	3A	304	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	5E	164	MET	CG-SD-CE	5.64	109.22	100.20
2	5E	330	MET	CG-SD-CE	-5.64	91.18	100.20
2	3B	94	GLN	N-CA-CB	-5.63	100.46	110.60
2	3H	293	MET	CG-SD-CE	-5.63	91.19	100.20
1	2B	188	VAL	CG1-CB-CG2	5.62	119.90	110.90
2	3D	81	PHE	CB-CG-CD1	-5.62	116.86	120.80
1	2I	159	VAL	CA-CB-CG1	5.62	119.33	110.90
1	4I	345	ASP	CB-CG-OD1	5.62	123.36	118.30
1	4B	262	TYR	CB-CG-CD1	5.62	124.37	121.00
2	5G	58	ARG	CB-CG-CD	-5.61	97.00	111.60
2	3E	166	THR	OG1-CB-CG2	-5.61	97.10	110.00
2	3H	309	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	4G	9	VAL	CG1-CB-CG2	5.61	119.88	110.90
1	4G	270	SER	N-CA-CB	-5.61	102.08	110.50
2	5D	313	ALA	N-CA-CB	-5.61	102.25	110.10
2	5E	147	MET	CA-CB-CG	5.60	122.83	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2H	33	ASP	CB-CA-C	5.60	121.60	110.40
1	4D	197	HIS	N-CA-CB	5.60	120.69	110.60
2	3G	408	PHE	CB-CG-CD2	-5.60	116.88	120.80
2	5E	31	ASP	CB-CG-OD2	5.60	123.34	118.30
2	5B	22	GLU	CA-CB-CG	5.60	125.71	113.40
1	2H	319	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	4H	270	SER	N-CA-CB	-5.59	102.11	110.50
2	3I	66	MET	CG-SD-CE	5.59	109.14	100.20
1	2F	178	SER	N-CA-CB	5.59	118.88	110.50
1	2G	432	TYR	CB-CG-CD1	5.58	124.34	121.00
2	5B	363	MET	CG-SD-CE	-5.58	91.28	100.20
2	5C	120	VAL	CA-CB-CG1	5.57	119.26	110.90
2	3E	349	MET	CG-SD-CE	5.57	109.11	100.20
2	3A	354	CYS	O-C-N	-5.57	113.79	122.70
2	3A	401	GLU	CG-CD-OE1	-5.57	107.16	118.30
1	2C	306	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	2G	244	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	4A	108	TYR	CB-CG-CD2	-5.56	117.67	121.00
2	3C	151	LEU	CB-CG-CD2	5.55	120.44	111.00
1	2G	31	GLN	CA-CB-CG	5.55	125.61	113.40
1	4G	320	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	3G	228	LEU	CB-CA-C	5.55	120.75	110.20
2	3E	414	ASN	O-C-N	-5.54	113.84	122.70
2	3F	103	LYS	O-C-N	-5.54	113.79	123.20
2	3D	390	ARG	CG-CD-NE	5.53	123.42	111.80
2	3H	294	PHE	CB-CG-CD1	5.53	124.67	120.80
2	3G	422	TYR	CB-CG-CD2	5.53	124.32	121.00
2	3H	213	ARG	CG-CD-NE	5.53	123.42	111.80
2	3D	81	PHE	CB-CG-CD2	5.53	124.67	120.80
1	4G	318	MET	CG-SD-CE	-5.52	91.37	100.20
2	3A	304	ASP	CB-CG-OD1	5.52	123.27	118.30
1	4G	137	MET	O-C-N	-5.52	113.87	122.70
2	3G	293	MET	CB-CA-C	-5.52	99.37	110.40
2	3H	120	VAL	CA-CB-CG1	5.51	119.17	110.90
2	5I	120	VAL	CA-CB-CG1	5.51	119.17	110.90
2	5I	192	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	4H	320	ARG	NE-CZ-NH1	-5.51	117.55	120.30
2	5I	222	TYR	CB-CG-CD1	-5.51	117.70	121.00
1	4H	218	ASP	CB-CG-OD2	5.50	123.25	118.30
2	5A	51	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	4B	422	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	3F	170	PHE	CB-CG-CD1	-5.50	116.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3B	257	LEU	CB-CG-CD2	5.49	120.33	111.00
2	3D	26	ASP	CB-CG-OD1	5.49	123.24	118.30
2	3I	179	VAL	CA-CB-CG2	5.48	119.12	110.90
1	2H	154	LEU	CB-CG-CD2	5.48	120.32	111.00
1	4I	408	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	4A	52	PHE	CB-CG-CD2	-5.47	116.97	120.80
2	3A	388	MET	O-C-N	-5.47	113.95	122.70
1	4H	398	MET	N-CA-CB	-5.46	100.77	110.60
2	5G	407	GLU	CB-CG-CD	-5.46	99.45	114.20
1	2D	212	ILE	CB-CA-C	5.46	122.52	111.60
2	5B	330	MET	CG-SD-CE	-5.46	91.47	100.20
2	5C	317	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	4H	49	PHE	CB-CG-CD1	5.46	124.62	120.80
2	5E	423	GLN	CG-CD-OE1	5.45	132.50	121.60
2	3F	215	LEU	CB-CG-CD1	-5.45	101.73	111.00
2	5F	208	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	5B	276	ARG	CG-CD-NE	5.45	123.24	111.80
1	2G	121	ARG	CG-CD-NE	5.45	123.23	111.80
1	2C	424	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	2E	431	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	2B	283	HIS	N-CA-CB	-5.44	100.81	110.60
1	2F	392	ASP	CB-CG-OD1	5.44	123.20	118.30
2	3I	363	MET	CA-CB-CG	5.44	122.55	113.30
2	5F	323	THR	CA-CB-OG1	5.44	120.42	109.00
2	5A	241	ARG	NH1-CZ-NH2	5.44	125.38	119.40
1	2H	101	ASN	CB-CG-OD1	-5.43	110.73	121.60
2	5G	310	TYR	CB-CG-CD1	5.43	124.26	121.00
2	3F	306	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	5A	51	TYR	CB-CG-CD1	5.43	124.26	121.00
2	3A	225	LEU	CB-CG-CD2	5.43	120.23	111.00
1	2G	195	LEU	CB-CG-CD1	-5.42	101.78	111.00
2	5E	31	ASP	CB-CG-OD1	-5.42	113.42	118.30
2	3F	147	MET	CB-CG-SD	5.42	128.67	112.40
1	4F	177	VAL	CA-CB-CG1	-5.42	102.77	110.90
1	2H	210	TYR	CB-CG-CD1	5.42	124.25	121.00
2	3E	201	VAL	CA-CB-CG2	5.42	119.02	110.90
1	2F	145	THR	OG1-CB-CG2	-5.41	97.55	110.00
2	5A	304	ASP	CB-CG-OD1	5.41	123.17	118.30
2	3B	391	ARG	CB-CG-CD	5.41	125.67	111.60
2	5H	340	TYR	N-CA-CB	-5.41	100.87	110.60
2	3H	251	ARG	NE-CZ-NH1	-5.41	117.60	120.30
2	3D	263	LEU	CA-CB-CG	5.40	127.73	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3G	341	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	4B	51	THR	OG1-CB-CG2	-5.40	97.58	110.00
1	2G	115	VAL	CA-CB-CG1	5.40	119.00	110.90
2	3E	106	TYR	CB-CG-CD1	5.40	124.24	121.00
2	5A	169	VAL	CA-CB-CG1	5.40	119.00	110.90
2	3H	177	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	4B	180	ALA	CB-CA-C	5.40	118.20	110.10
1	4A	251	ASP	N-CA-CB	5.40	120.31	110.60
1	2I	345	ASP	CB-CG-OD2	-5.39	113.44	118.30
2	3E	233	MET	CG-SD-CE	5.39	108.83	100.20
2	5F	196	ALA	N-CA-CB	-5.39	102.55	110.10
1	2B	313	MET	CG-SD-CE	-5.39	91.57	100.20
2	3E	81	PHE	CB-CG-CD1	5.39	124.58	120.80
2	5H	390	ARG	CG-CD-NE	5.39	123.13	111.80
1	2H	264	ARG	CA-CB-CG	5.39	125.26	113.40
1	4I	424	ASP	CB-CG-OD1	5.39	123.15	118.30
1	2B	161	TYR	CB-CG-CD1	5.39	124.23	121.00
2	3C	417	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	4B	424	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	2B	217	LEU	CB-CG-CD2	-5.38	101.85	111.00
2	3E	397	TRP	O-C-N	-5.38	114.09	122.70
2	3I	120	VAL	CA-CB-CG1	5.38	118.98	110.90
1	4G	408	TYR	CB-CG-CD2	5.38	124.23	121.00
1	2G	215	ARG	CG-CD-NE	5.38	123.10	111.80
1	4B	156	ARG	CB-CA-C	5.38	121.16	110.40
1	2C	2	ARG	CB-CG-CD	-5.38	97.62	111.60
1	2E	392	ASP	CB-CG-OD2	5.38	123.14	118.30
2	3C	317	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	4G	382	THR	OG1-CB-CG2	-5.38	97.63	110.00
2	5I	377	MET	CG-SD-CE	-5.38	91.59	100.20
1	2F	242	LEU	CB-CA-C	5.37	120.41	110.20
2	3D	156	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	3B	67	ASP	CB-CG-OD2	5.37	123.13	118.30
2	3B	321	MET	O-C-N	-5.37	114.11	122.70
1	4I	386	GLU	OE1-CD-OE2	5.37	129.75	123.30
2	5C	408	PHE	CB-CG-CD1	-5.37	117.04	120.80
2	5G	198	GLU	N-CA-CB	5.37	120.27	110.60
2	3C	354	CYS	O-C-N	-5.37	114.11	122.70
1	2A	138	PHE	CB-CG-CD2	5.37	124.56	120.80
1	2B	367	ASP	CB-CA-C	5.37	121.14	110.40
2	5F	33	THR	O-C-N	-5.36	114.08	123.20
2	5F	66	MET	CA-CB-CG	5.36	122.42	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2I	84	ARG	CB-CA-C	5.36	121.12	110.40
2	5G	49	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	2B	269	LEU	CB-CG-CD2	5.36	120.11	111.00
1	4C	352	LYS	CA-CB-CG	-5.35	101.63	113.40
1	4E	77	GLU	N-CA-CB	5.35	120.23	110.60
2	3G	340	TYR	CB-CG-CD1	5.35	124.21	121.00
2	3H	199	VAL	CG1-CB-CG2	-5.34	102.35	110.90
2	5A	233	MET	CB-CA-C	5.34	121.09	110.40
1	2A	18	ASN	CB-CA-C	5.34	121.08	110.40
2	3E	276	ARG	CB-CG-CD	5.34	125.48	111.60
2	5A	251	ARG	CB-CG-CD	5.34	125.48	111.60
2	5D	282	ARG	NH1-CZ-NH2	5.34	125.27	119.40
2	3F	349	MET	N-CA-CB	-5.34	101.00	110.60
2	5C	318	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	4G	282	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	4D	210	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	3H	208	TYR	CB-CG-CD1	5.32	124.19	121.00
2	5A	123	GLU	CB-CG-CD	5.32	128.56	114.20
2	3H	167	PHE	CB-CG-CD1	5.32	124.52	120.80
1	2B	210	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	3E	401	GLU	N-CA-CB	5.31	120.16	110.60
2	3B	178	THR	OG1-CB-CG2	-5.31	97.79	110.00
1	4H	135	PHE	CB-CG-CD2	5.31	124.52	120.80
1	2A	56	THR	N-CA-CB	-5.31	100.22	110.30
1	2G	88	HIS	CA-CB-CG	5.31	122.62	113.60
2	3B	114	ASP	CB-CG-OD1	-5.30	113.53	118.30
2	5G	249	ASP	CB-CG-OD1	5.30	123.07	118.30
1	2F	387	VAL	CA-CB-CG1	5.30	118.85	110.90
2	3I	166	THR	OG1-CB-CG2	5.30	122.20	110.00
1	4G	418	PHE	CB-CG-CD1	5.30	124.51	120.80
2	5C	317	PHE	CB-CG-CD2	5.30	124.51	120.80
2	5G	355	ASP	CB-CA-C	5.30	121.00	110.40
1	2G	137	MET	CB-CA-C	-5.30	99.80	110.40
2	5E	26	ASP	CB-CG-OD1	5.30	123.07	118.30
1	2A	244	PHE	CB-CG-CD1	5.30	124.51	120.80
2	5A	318	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	2B	408	TYR	CB-CG-CD1	5.29	124.17	121.00
1	2D	405	VAL	CG1-CB-CG2	5.29	119.37	110.90
2	3I	222	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	2F	358	GLN	N-CA-CB	5.28	120.11	110.60
1	2G	396	ASP	CB-CG-OD1	-5.28	113.55	118.30
2	3I	341	PHE	CB-CG-CD1	-5.28	117.10	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4E	123	ARG	CB-CG-CD	5.28	125.33	111.60
2	5A	241	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	5E	283	ALA	N-CA-CB	-5.28	102.72	110.10
2	5B	407	GLU	CB-CG-CD	-5.27	99.96	114.20
1	2I	342	GLN	CB-CG-CD	5.27	125.30	111.60
1	2F	243	ARG	CG-CD-NE	5.27	122.86	111.80
2	3H	14	ASN	CB-CG-ND2	5.27	129.34	116.70
1	2H	265	ILE	CA-CB-CG2	5.26	121.43	110.90
2	3E	84	LEU	CB-CG-CD1	5.26	119.95	111.00
1	4I	107	HIS	CB-CA-C	-5.26	99.87	110.40
1	4B	351	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	4C	255	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	4I	159	VAL	CA-CB-CG1	5.26	118.79	110.90
2	3E	147	MET	N-CA-CB	5.26	120.06	110.60
2	5A	403	MET	CB-CG-SD	5.26	128.17	112.40
2	3F	103	LYS	CB-CA-C	5.25	120.91	110.40
2	3G	222	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	5I	325	GLU	CB-CA-C	-5.25	99.89	110.40
1	4A	391	MET	CG-SD-CE	-5.25	91.80	100.20
1	4D	377	MET	CG-SD-CE	5.25	108.60	100.20
2	3G	270	PHE	CB-CG-CD1	5.25	124.47	120.80
1	4A	108	TYR	CB-CG-CD1	5.25	124.15	121.00
2	5C	175	VAL	CA-CB-CG1	5.24	118.76	110.90
1	2H	372	MET	CB-CG-SD	5.24	128.11	112.40
1	2E	157	LEU	CB-CG-CD2	5.23	119.90	111.00
1	2I	137	MET	CG-SD-CE	-5.23	91.83	100.20
1	2F	69	ASP	CB-CG-OD2	-5.23	113.59	118.30
2	3A	27	GLU	CA-CB-CG	5.23	124.91	113.40
2	3C	175	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	4F	270	SER	N-CA-CB	5.23	118.35	110.50
1	2H	138	PHE	CB-CG-CD1	-5.23	117.14	120.80
2	3C	177	ASP	N-CA-CB	5.23	120.01	110.60
1	4E	407	TRP	CA-CB-CG	-5.23	103.76	113.70
2	5G	389	PHE	CB-CG-CD1	-5.23	117.14	120.80
2	3C	367	PHE	CB-CG-CD1	-5.23	117.14	120.80
2	5A	181	GLU	CA-CB-CG	5.22	124.89	113.40
2	5A	249	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	3H	183	TYR	O-C-N	-5.22	114.34	122.70
2	3A	130	LEU	CB-CG-CD1	-5.22	102.13	111.00
2	3H	260	PHE	CB-CG-CD1	5.22	124.45	120.80
2	5D	166	THR	CA-CB-OG1	-5.22	98.04	109.00
1	4D	422	ARG	NE-CZ-NH2	-5.22	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4G	162	GLY	CA-C-O	-5.22	111.21	120.60
2	5B	213	ARG	N-CA-CB	5.21	119.99	110.60
1	2H	233	GLN	CG-CD-OE1	-5.21	111.17	121.60
2	5A	300	MET	CG-SD-CE	5.21	108.54	100.20
2	5G	359	LYS	CA-CB-CG	5.21	124.87	113.40
1	2D	16	ILE	CB-CA-C	5.21	122.02	111.60
1	4I	302	MET	CA-CB-CG	5.21	122.15	113.30
2	5I	15	GLN	N-CA-CB	5.21	119.98	110.60
1	4F	327	ASP	O-C-N	-5.20	114.38	122.70
2	5I	66	MET	N-CA-CB	-5.20	101.23	110.60
1	4E	362	VAL	CA-CB-CG1	-5.20	103.10	110.90
2	5C	114	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	5B	161	ASP	CB-CG-OD1	5.20	122.98	118.30
1	2G	413	MET	CA-CB-CG	5.20	122.13	113.30
1	2G	422	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	5G	166	THR	OG1-CB-CG2	5.20	121.95	110.00
1	4A	214	ARG	NH1-CZ-NH2	5.19	125.11	119.40
2	5A	342	VAL	CG1-CB-CG2	5.19	119.20	110.90
1	2A	189	LEU	CB-CG-CD2	5.19	119.82	111.00
1	2B	320	ARG	NH1-CZ-NH2	-5.19	113.70	119.40
1	2D	395	PHE	CB-CG-CD2	-5.18	117.17	120.80
2	5A	67	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	3D	414	ASN	CB-CA-C	5.18	120.75	110.40
2	3F	404	ASP	CB-CG-OD2	5.18	122.96	118.30
1	2H	320	ARG	CA-CB-CG	5.17	124.78	113.40
2	3G	341	PHE	CB-CG-CD1	5.17	124.42	120.80
2	5A	350	LYS	CB-CG-CD	5.17	125.05	111.60
2	3C	363	MET	CA-CB-CG	5.17	122.09	113.30
1	4F	202	VAL	CA-CB-CG1	5.17	118.66	110.90
1	4F	203	MET	CG-SD-CE	-5.17	91.93	100.20
2	5B	422	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	4A	424	ASP	CB-CG-OD2	-5.17	113.65	118.30
2	5E	162	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	4I	390	ARG	CG-CD-NE	-5.17	100.95	111.80
2	3F	175	VAL	CG1-CB-CG2	5.16	119.16	110.90
1	4B	280	LYS	CA-CB-CG	5.16	124.75	113.40
1	4H	339	ARG	O-C-N	-5.16	114.45	122.70
1	2D	35	GLN	CA-CB-CG	5.15	124.73	113.40
1	4I	306	ASP	CB-CG-OD2	-5.15	113.67	118.30
2	5C	241	ARG	NE-CZ-NH2	5.15	122.87	120.30
2	3D	66	MET	CA-CB-CG	5.14	122.04	113.30
1	4H	308	ARG	CA-CB-CG	5.14	124.72	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2F	116	ASP	CB-CG-OD1	5.14	122.93	118.30
2	3A	262	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	5I	203	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	2G	279	GLU	CB-CA-C	-5.14	100.12	110.40
1	4G	388	PHE	CB-CG-CD2	-5.14	117.20	120.80
2	5E	106	TYR	CB-CG-CD1	5.14	124.08	121.00
1	4A	35	GLN	CA-CB-CG	5.13	124.69	113.40
1	4H	82	THR	OG1-CB-CG2	5.13	121.81	110.00
1	2E	35	GLN	CA-CB-CG	5.13	124.69	113.40
1	2G	375	VAL	CG1-CB-CG2	-5.13	102.69	110.90
2	3H	380	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	4F	390	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	2D	214	ARG	CB-CG-CD	5.13	124.94	111.60
2	5F	108	GLU	CB-CA-C	5.13	120.66	110.40
1	4C	49	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	4I	76	ASP	CB-CG-OD1	-5.13	113.69	118.30
2	3F	294	PHE	CB-CG-CD2	-5.12	117.21	120.80
1	4D	243	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	5D	251	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	3G	281	TYR	CB-CG-CD2	-5.12	117.93	121.00
2	3B	326	VAL	CG1-CB-CG2	-5.12	102.72	110.90
2	5D	65	LEU	N-CA-CB	-5.12	100.17	110.40
2	3E	91	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	4D	199	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	4F	324	VAL	CA-CB-CG2	-5.11	103.23	110.90
1	4G	90	GLU	CB-CA-C	5.11	120.63	110.40
2	5C	37	CYS	CA-CB-SG	5.11	123.20	114.00
1	2E	371	VAL	CG1-CB-CG2	5.11	119.08	110.90
2	3A	192	LEU	CB-CG-CD1	-5.11	102.31	111.00
2	3F	149	THR	OG1-CB-CG2	-5.11	98.25	110.00
2	5B	251	ARG	CG-CD-NE	-5.11	101.08	111.80
1	2H	210	TYR	CB-CG-CD2	-5.11	117.94	121.00
2	3A	391	ARG	CB-CA-C	5.11	120.61	110.40
2	5D	406	MET	CB-CG-SD	5.10	127.71	112.40
2	3B	251	ARG	NE-CZ-NH1	-5.10	117.75	120.30
2	3B	415	MET	CG-SD-CE	-5.10	92.04	100.20
1	2B	392	ASP	CB-CG-OD1	5.09	122.89	118.30
2	3A	73	MET	CB-CG-SD	-5.09	97.11	112.40
2	3B	155	VAL	CG1-CB-CG2	5.09	119.05	110.90
2	3F	403	MET	CG-SD-CE	-5.09	92.05	100.20
1	2F	36	MET	CA-CB-CG	5.09	121.95	113.30
1	4I	388	PHE	CB-CG-CD2	-5.08	117.24	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2G	137	MET	O-C-N	-5.08	114.57	122.70
1	4E	91	GLN	CA-CB-CG	5.08	124.58	113.40
1	4G	185	TYR	CB-CG-CD1	-5.08	117.95	121.00
2	5G	143	THR	OG1-CB-CG2	-5.08	98.31	110.00
1	2G	23	LEU	CB-CG-CD2	5.08	119.63	111.00
2	3I	341	PHE	CB-CG-CD2	5.08	124.36	120.80
1	4B	210	TYR	CB-CG-CD1	-5.08	117.95	121.00
2	5I	111	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	2A	432	TYR	CB-CG-CD1	5.08	124.05	121.00
1	4B	217	LEU	CB-CG-CD2	-5.08	102.37	111.00
2	5I	390	ARG	CB-CG-CD	5.08	124.80	111.60
1	2H	105	ARG	CG-CD-NE	-5.07	101.14	111.80
2	3D	294	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	4D	391	MET	CA-CB-CG	5.07	121.92	113.30
1	4E	120	ASP	CB-CG-OD2	-5.07	113.73	118.30
2	3E	77	ARG	NE-CZ-NH1	-5.07	117.77	120.30
2	3I	241	ARG	NE-CZ-NH1	-5.07	117.77	120.30
2	5G	274	THR	OG1-CB-CG2	-5.07	98.34	110.00
2	5H	266	PHE	CB-CG-CD2	-5.07	117.25	120.80
2	5I	26	ASP	CB-CG-OD1	5.07	122.86	118.30
1	2C	98	ASP	CB-CG-OD1	5.07	122.86	118.30
2	3B	147	MET	CB-CG-SD	5.07	127.60	112.40
2	3E	121	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	4A	422	ARG	NE-CZ-NH1	-5.07	117.77	120.30
2	3E	333	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	4F	432	TYR	CB-CG-CD2	5.07	124.04	121.00
2	5H	304	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	2A	36	MET	CG-SD-CE	-5.06	92.10	100.20
1	2F	391	MET	CG-SD-CE	5.06	108.30	100.20
2	3E	92	PHE	CB-CG-CD1	5.06	124.34	120.80
2	5E	317	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	2A	402	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	2A	123	ARG	NE-CZ-NH1	-5.05	117.77	120.30
2	3F	212	PHE	CB-CG-CD1	5.05	124.34	120.80
2	5F	380	ARG	CG-CD-NE	-5.05	101.19	111.80
2	3D	175	VAL	CA-CB-CG1	5.05	118.48	110.90
2	3F	408	PHE	CB-CG-CD1	-5.05	117.26	120.80
2	5D	282	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	4G	179	THR	CA-CB-OG1	-5.05	98.40	109.00
2	5C	342	VAL	CA-CB-CG1	5.05	118.47	110.90
2	3D	65	LEU	N-CA-CB	-5.05	100.31	110.40
1	2H	115	VAL	CA-CB-CG1	5.04	118.47	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4H	233	GLN	CG-CD-OE1	-5.04	111.51	121.60
2	5A	306	ARG	CB-CG-CD	5.04	124.70	111.60
2	3F	31	ASP	CB-CG-OD1	5.04	122.83	118.30
2	3H	159	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	4G	121	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	4H	199	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	2A	308	ARG	CB-CG-CD	5.03	124.68	111.60
1	2G	267	PHE	CB-CG-CD2	-5.03	117.28	120.80
2	3C	197	ASP	CB-CG-OD1	-5.03	113.77	118.30
2	5D	36	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	5F	208	TYR	CB-CG-CD1	5.03	124.02	121.00
1	4A	362	VAL	CA-CB-CG1	-5.03	103.36	110.90
1	4G	137	MET	CB-CA-C	-5.03	100.35	110.40
1	2C	320	ARG	CB-CG-CD	-5.02	98.54	111.60
1	4A	159	VAL	CA-CB-CG1	5.02	118.44	110.90
1	4F	140	ALA	CB-CA-C	5.02	117.64	110.10
2	3I	157	GLU	CG-CD-OE1	-5.02	108.25	118.30
2	5I	263	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	2H	351	PHE	N-CA-CB	5.02	119.63	110.60
2	3C	212	PHE	CB-CA-C	-5.02	100.36	110.40
2	5G	215	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	4D	432	TYR	CB-CG-CD2	-5.02	117.99	121.00
2	3E	375	GLN	N-CA-CB	5.01	119.62	110.60
2	5A	161	ASP	O-C-N	-5.01	114.68	122.70
2	5C	212	PHE	CB-CG-CD2	-5.01	117.29	120.80
2	3E	35	THR	OG1-CB-CG2	-5.01	98.48	110.00
1	4I	94	SER	N-CA-CB	5.01	118.02	110.50
1	2F	313	MET	N-CA-CB	5.01	119.61	110.60
2	5A	318	ARG	CG-CD-NE	5.01	122.31	111.80
1	2B	432	TYR	CB-CG-CD1	-5.00	118.00	121.00
1	2D	306	ASP	CB-CG-OD1	5.00	122.80	118.30
1	2E	62	VAL	CG1-CB-CG2	5.00	118.91	110.90
1	4H	159	VAL	CA-CB-CG1	5.00	118.41	110.90
2	5G	74	ASP	CB-CG-OD1	5.00	122.80	118.30
2	5C	26	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (259) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2A	201	ALA	Mainchain
1	2A	205	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	2A	208	ALA	Mainchain
1	2A	249	ASN	Sidechain
1	2A	285	GLN	Mainchain
1	2A	296	PHE	Sidechain
1	2A	306	ASP	Sidechain
1	2B	2	ARG	Mainchain
1	2B	293	ASN	Sidechain
1	2B	299	ALA	Mainchain
1	2B	367	ASP	Sidechain
1	2B	59	GLY	Mainchain
1	2C	163	LYS	Mainchain
1	2C	176	GLN	Mainchain
1	2C	282	TYR	Peptide
1	2C	284	GLU	Peptide
1	2C	388	PHE	Sidechain
1	2C	392	ASP	Sidechain
1	2D	163	LYS	Mainchain
1	2D	279	GLU	Mainchain
1	2D	59	GLY	Mainchain
1	2E	130	THR	Mainchain
1	2E	176	GLN	Mainchain
1	2E	193	SER	Mainchain
1	2E	284	GLU	Peptide
1	2E	341	ILE	Mainchain
1	2E	407	TRP	Mainchain
1	2E	412	GLY	Mainchain
1	2F	2	ARG	Mainchain
1	2F	21	TRP	Mainchain
1	2F	242	LEU	Mainchain
1	2F	258	ASN	Mainchain
1	2F	284	GLU	Peptide
1	2F	326	LYS	Mainchain
1	2F	436	GLY	Mainchain
1	2G	111	GLY	Peptide
1	2G	137	MET	Mainchain
1	2G	145	THR	Mainchain
1	2G	189	LEU	Mainchain
1	2G	203	MET	Mainchain
1	2G	296	PHE	Sidechain
1	2G	299	ALA	Mainchain
1	2G	304	LYS	Peptide
1	2G	401	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	2G	413	MET	Mainchain
1	2G	53	PHE	Mainchain
1	2G	67	PHE	Sidechain
1	2H	136	LEU	Mainchain
1	2H	139	ASN	Sidechain
1	2H	163	LYS	Mainchain
1	2H	2	ARG	Mainchain
1	2H	33	ASP	Mainchain
1	2H	343	PHE	Mainchain
1	2H	379	SER	Peptide
1	2H	422	ARG	Sidechain
1	2I	11	GLN	Mainchain
1	2I	225	THR	Mainchain
1	2I	326	LYS	Mainchain
1	2I	383	ALA	Mainchain
1	2I	387	VAL	Mainchain
1	2I	84	ARG	Mainchain
2	3A	105	HIS	Mainchain
2	3A	175	VAL	Mainchain
2	3A	177	ASP	Peptide
2	3A	257	LEU	Mainchain
2	3A	28	HIS	Sidechain
2	3A	281	TYR	Mainchain
2	3A	282	ARG	Mainchain
2	3A	302	ALA	Mainchain
2	3A	307	HIS	Mainchain
2	3A	319	GLY	Mainchain
2	3A	388	MET	Mainchain
2	3B	161	ASP	Mainchain
2	3B	213	ARG	Mainchain
2	3B	266	PHE	Mainchain
2	3B	321	MET	Peptide
2	3B	322	SER	Peptide
2	3B	323	THR	Mainchain
2	3B	33	THR	Mainchain
2	3C	105	HIS	Mainchain
2	3C	14	ASN	Sidechain
2	3C	176	SER	Mainchain
2	3C	256	ASN	Mainchain
2	3C	26	ASP	Sidechain
2	3C	307	HIS	Mainchain
2	3C	399	THR	Mainchain

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Mol	Chain	Res	Type	Group
2	3C	93	GLY	Mainchain
2	3D	105	HIS	Mainchain
2	3D	256	ASN	Mainchain
2	3D	263	LEU	Mainchain
2	3D	355	ASP	Mainchain
2	3D	376	GLU	Mainchain
2	3D	378	PHE	Sidechain
2	3D	383	ASP	Sidechain
2	3D	399	THR	Mainchain
2	3E	105	HIS	Mainchain
2	3E	16	ILE	Mainchain
2	3E	283	ALA	Mainchain
2	3E	294	PHE	Sidechain
2	3E	33	THR	Mainchain
2	3E	35	THR	Mainchain
2	3E	397	TRP	Mainchain
2	3E	414	ASN	Mainchain
2	3F	103	LYS	Mainchain
2	3F	105	HIS	Mainchain
2	3F	223	GLY	Mainchain
2	3F	33	THR	Mainchain
2	3F	349	MET	Mainchain
2	3F	35	THR	Mainchain
2	3F	354	CYS	Mainchain
2	3F	67	ASP	Mainchain
2	3G	14	ASN	Sidechain
2	3G	175	VAL	Mainchain
2	3G	300	MET	Mainchain
2	3G	389	PHE	Sidechain
2	3G	74	ASP	Sidechain
2	3H	105	HIS	Mainchain
2	3H	118	ASP	Sidechain
2	3H	140	GLY	Mainchain
2	3H	183	TYR	Mainchain
2	3H	277	GLY	Mainchain
2	3H	30	ILE	Mainchain
2	3H	304	ASP	Sidechain
2	3H	388	MET	Mainchain
2	3H	421	GLU	Mainchain
2	3I	149	THR	Mainchain
2	3I	156	ARG	Mainchain
2	3I	262	ARG	Mainchain

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Mol	Chain	Res	Type	Group
2	3I	372	THR	Mainchain
1	4A	168	ASN	Mainchain
1	4A	197	HIS	Mainchain
1	4A	205	ASP	Mainchain
1	4A	225	THR	Mainchain
1	4A	253	THR	Mainchain
1	4A	286	LEU	Mainchain
1	4A	35	GLN	Mainchain
1	4A	368	LEU	Mainchain
1	4A	69	ASP	Sidechain
1	4A	89	PRO	Mainchain
1	4B	156	ARG	Mainchain
1	4B	213	CYS	Mainchain
1	4B	225	THR	Mainchain
1	4B	257	THR	Mainchain
1	4B	264	ARG	Mainchain
1	4C	185	TYR	Sidechain
1	4C	257	THR	Mainchain
1	4C	282	TYR	Sidechain
1	4C	322	ASP	Mainchain
1	4C	404	PHE	Mainchain
1	4C	411	GLU	Mainchain
1	4D	176	GLN	Mainchain
1	4D	196	GLU	Mainchain
1	4D	279	GLU	Mainchain
1	4D	331	ALA	Mainchain
1	4D	59	GLY	Mainchain
1	4E	139	ASN	Sidechain
1	4E	165	SER	Mainchain
1	4E	169	PHE	Sidechain
1	4E	176	GLN	Mainchain
1	4E	243	ARG	Mainchain
1	4E	341	ILE	Mainchain
1	4E	411	GLU	Mainchain
1	4E	54	SER	Mainchain
1	4F	140	ALA	Mainchain
1	4F	202	VAL	Mainchain
1	4F	215	ARG	Mainchain
1	4F	217	LEU	Mainchain
1	4F	241	SER	Mainchain
1	4F	327	ASP	Mainchain
1	4F	90	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	4G	1	MET	Mainchain
1	4G	137	MET	Mainchain
1	4G	162	GLY	Mainchain
1	4G	217	LEU	Mainchain
1	4G	259	LEU	Mainchain
1	4G	380	ASN	Mainchain
1	4G	67	PHE	Sidechain
1	4H	136	LEU	Mainchain
1	4H	139	ASN	Sidechain
1	4H	140	ALA	Mainchain
1	4H	163	LYS	Mainchain
1	4H	233	GLN	Sidechain
1	4H	254	GLU	Mainchain
1	4H	258	ASN	Mainchain
1	4H	264	ARG	Mainchain
1	4H	327	ASP	Sidechain
1	4I	225	THR	Mainchain
1	4I	269	LEU	Mainchain
1	4I	412	GLY	Mainchain
1	4I	59	GLY	Mainchain
1	4I	96	LYS	Mainchain
2	5A	143	THR	Mainchain
2	5A	170	PHE	Sidechain
2	5A	205	GLU	Mainchain
2	5A	281	TYR	Sidechain
2	5A	283	ALA	Mainchain
2	5A	293	MET	Mainchain
2	5A	307	HIS	Mainchain
2	5A	342	VAL	Mainchain
2	5A	349	MET	Mainchain
2	5A	36	TYR	Sidechain
2	5A	388	MET	Mainchain
2	5A	414	ASN	Mainchain
2	5A	43	GLN	Mainchain
2	5A	83	GLN	Sidechain
2	5B	195	ASN	Mainchain
2	5B	266	PHE	Mainchain
2	5B	341	PHE	Mainchain
2	5B	388	MET	Mainchain
2	5C	105	HIS	Mainchain
2	5C	143	THR	Mainchain
2	5C	256	ASN	Mainchain

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Mol	Chain	Res	Type	Group
2	5C	283	ALA	Mainchain
2	5C	307	HIS	Mainchain
2	5C	423	GLN	Sidechain
2	5D	105	HIS	Mainchain
2	5D	297	LYS	Mainchain
2	5D	33	THR	Mainchain
2	5D	355	ASP	Mainchain
2	5D	399	THR	Mainchain
2	5D	414	ASN	Mainchain
2	5E	105	HIS	Mainchain
2	5E	16	ILE	Mainchain
2	5E	257	LEU	Mainchain
2	5E	280	GLN	Mainchain
2	5E	283	ALA	Mainchain
2	5E	293	MET	Mainchain
2	5E	298	ASN	Mainchain
2	5E	33	THR	Mainchain
2	5E	35	THR	Mainchain
2	5F	126	GLY	Mainchain
2	5F	196	ALA	Mainchain
2	5F	349	MET	Mainchain
2	5F	35	THR	Mainchain
2	5G	105	HIS	Mainchain
2	5G	106	TYR	Mainchain
2	5G	14	ASN	Sidechain
2	5G	194	GLU	Mainchain
2	5G	283	ALA	Mainchain
2	5G	298	ASN	Mainchain
2	5G	354	CYS	Mainchain
2	5G	425	TYR	Mainchain
2	5G	53	GLU	Sidechain
2	5G	59	PHE	Mainchain
2	5G	81	PHE	Sidechain
2	5G	94	GLN	Mainchain
2	5H	14	ASN	Sidechain
2	5H	180	VAL	Mainchain
2	5H	21	TRP	Mainchain
2	5H	226	ASN	Sidechain
2	5H	266	PHE	Mainchain
2	5H	277	GLY	Mainchain
2	5H	340	TYR	Mainchain
2	5H	360	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	5I	105	HIS	Mainchain
2	5I	107	THR	Mainchain
2	5I	156	ARG	Mainchain
2	5I	277	GLY	Mainchain
2	5I	388	MET	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	3325	0	3252	80	0
1	2B	3325	0	3252	73	0
1	2C	3325	0	3252	60	0
1	2D	3325	0	3252	104	0
1	2E	3325	0	3252	95	0
1	2F	3325	0	3252	60	0
1	2G	3325	0	3252	93	0
1	2H	3325	0	3252	84	0
1	2I	3325	0	3252	56	0
1	4A	3325	0	3252	89	0
1	4B	3325	0	3252	93	0
1	4C	3325	0	3252	79	0
1	4D	3325	0	3251	82	0
1	4E	3325	0	3252	120	0
1	4F	3325	0	3252	79	0
1	4G	3325	0	3252	105	0
1	4H	3325	0	3252	92	0
1	4I	3325	0	3252	71	0
2	3A	3331	0	3207	94	0
2	3B	3331	0	3207	108	0
2	3C	3331	0	3207	73	0
2	3D	3331	0	3207	104	0
2	3E	3331	0	3207	132	0
2	3F	3331	0	3209	112	0
2	3G	3331	0	3209	97	0
2	3H	3331	0	3209	93	0
2	3I	3331	0	3209	56	0
2	5A	3331	0	3207	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5B	3331	0	3207	80	0
2	5C	3331	0	3208	62	0
2	5D	3331	0	3206	111	0
2	5E	3331	0	3207	118	0
2	5F	3331	0	3209	72	0
2	5G	3331	0	3209	98	0
2	5H	3331	0	3209	77	0
2	5I	3331	0	3209	57	0
All	All	119808	0	116277	2367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (2367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4E:60:LYS:HZ2	1:4F:283:HIS:CD2	1.13	1.63
2:3E:58:ARG:NH1	2:3F:281:TYR:HE1	0.98	1.44
1:4C:121:ARG:HH12	1:4D:283:HIS:CE1	1.35	1.40
1:4E:60:LYS:NZ	1:4F:283:HIS:HD2	0.94	1.40
2:3E:58:ARG:NH1	2:3F:281:TYR:CE1	1.89	1.39
2:5C:88:ASP:N	2:5D:281:TYR:OH	1.56	1.34
2:3A:220:PRO:HD2	1:4A:326:LYS:CE	1.58	1.33
1:2C:121:ARG:HH12	1:2D:283:HIS:CE1	1.51	1.25
2:5D:55:THR:OG1	2:5E:284:LEU:N	1.71	1.23
2:3D:55:THR:OG1	2:3E:284:LEU:N	1.72	1.23
1:4G:178:SER:OG	2:5G:347:ASN:ND2	1.70	1.21
1:2E:60:LYS:NZ	1:2F:282:TYR:CE2	2.12	1.18
2:5E:55:THR:HB	2:5F:283:ALA:HA	1.22	1.17
2:3G:55:THR:HG21	2:3H:283:ALA:HA	1.22	1.16
2:3D:58:ARG:HD3	2:3E:281:TYR:CA	1.76	1.16
2:3D:58:ARG:CD	2:3E:281:TYR:HA	1.75	1.16
1:4B:181:VAL:HG13	2:5B:350:LYS:NZ	1.60	1.16
1:2H:210:TYR:CD1	2:3H:324:LYS:HE3	1.81	1.15
1:2F:178:SER:HB2	2:3F:347:ASN:ND2	1.60	1.15
2:5A:55:THR:HG21	2:5B:283:ALA:HA	1.26	1.15
1:4E:60:LYS:NZ	1:4F:283:HIS:CD2	1.83	1.14
2:5G:55:THR:HG21	2:5H:283:ALA:HA	1.30	1.14
2:5D:54:ALA:O	2:5E:283:ALA:HA	1.46	1.12
1:4C:121:ARG:NH1	1:4D:283:HIS:CE1	2.17	1.11
2:3E:58:ARG:HD3	2:3F:281:TYR:HD1	1.14	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5D:58:ARG:HD3	2:5E:281:TYR:CA	1.79	1.11
1:4F:178:SER:HB2	2:5F:347:ASN:ND2	1.65	1.11
2:3A:220:PRO:CD	1:4A:326:LYS:HE2	1.79	1.11
2:5D:58:ARG:CD	2:5E:281:TYR:HA	1.81	1.11
1:4D:57:GLY:H	1:4E:285:GLN:HB3	1.14	1.09
2:5E:55:THR:HG22	2:5F:282:ARG:O	1.51	1.09
2:5E:54:ALA:HB1	2:5F:281:TYR:O	1.54	1.07
1:2D:60:LYS:HD3	1:2E:282:TYR:O	1.52	1.06
1:4B:181:VAL:HG13	2:5B:350:LYS:HZ2	1.05	1.06
1:4D:60:LYS:HD3	1:4E:282:TYR:O	1.53	1.06
2:5D:58:ARG:NH2	2:5E:281:TYR:CE1	2.24	1.06
2:3B:179:VAL:H	1:4B:352:LYS:NZ	1.54	1.05
1:2E:60:LYS:HE2	1:2F:283:HIS:HD2	1.22	1.05
2:5D:54:ALA:C	2:5E:283:ALA:HA	1.74	1.04
1:4E:221:ARG:HG2	2:5E:322:SER:CB	1.87	1.04
1:2C:62:VAL:HG12	1:2D:282:TYR:OH	1.59	1.02
2:3E:397:TRP:CH2	1:4E:260:VAL:HG23	1.93	1.02
2:3E:55:THR:HG22	2:3F:282:ARG:O	1.60	1.01
2:5E:55:THR:CB	2:5F:283:ALA:HA	1.91	1.01
2:3A:55:THR:HG21	2:3B:283:ALA:CB	1.89	1.01
2:3B:175:VAL:HG11	1:4B:332:VAL:HG13	1.40	1.01
1:2C:121:ARG:NH1	1:2D:283:HIS:CE1	2.27	1.01
1:2C:88:HIS:HA	1:2D:282:TYR:HE2	1.22	1.00
1:4I:181:VAL:HG22	2:5I:256:ASN:OD1	1.59	1.00
1:4D:55:GLU:O	1:4E:285:GLN:HG2	1.61	1.00
2:3D:54:ALA:O	2:3E:283:ALA:HA	1.60	1.00
2:5A:267:LEU:HD21	2:5A:374:ILE:HD11	1.44	1.00
2:3A:55:THR:CG2	2:3B:283:ALA:HB2	1.92	0.99
1:4D:60:LYS:CE	1:4E:283:HIS:CD2	2.46	0.99
1:4E:151:CYS:HG	1:4E:193:SER:HG	1.04	0.99
1:2H:259:LEU:O	1:2H:380:ASN:ND2	1.96	0.98
1:2D:60:LYS:CE	1:2E:283:HIS:CD2	2.46	0.98
2:3H:99:ASN:HD22	1:4H:254:GLU:CD	1.66	0.98
2:3C:86:ARG:HD3	2:3D:281:TYR:HD1	1.26	0.98
2:5F:125:GLU:OE1	2:5G:291:GLN:NE2	1.95	0.97
2:5F:54:ALA:HB1	2:5G:281:TYR:O	1.62	0.97
2:3E:58:ARG:CD	2:3F:281:TYR:HD1	1.77	0.97
1:2C:88:HIS:HA	1:2D:282:TYR:CE2	1.98	0.97
2:5A:55:THR:CG2	2:5B:283:ALA:HA	1.93	0.97
1:2C:62:VAL:CG1	1:2D:282:TYR:OH	2.12	0.97
1:2A:181:VAL:HG22	2:3A:350:LYS:HZ1	1.27	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3D:55:THR:HG1	2:3E:283:ALA:HA	1.28	0.96
1:2E:60:LYS:HE2	1:2F:283:HIS:CD2	2.00	0.96
2:3C:60:VAL:HG11	2:3D:280:GLN:HE22	1.25	0.96
2:3F:208:TYR:HD1	1:4F:326:LYS:HE2	1.27	0.95
1:2H:222:PRO:HG2	2:3H:324:LYS:NZ	1.82	0.95
1:4B:60:LYS:NZ	1:4C:282:TYR:CE2	2.35	0.95
2:5H:259:PRO:HG2	2:5H:311:LEU:HD21	1.49	0.95
1:4D:60:LYS:NZ	1:4E:283:HIS:CD2	2.35	0.94
1:4F:213:CYS:SG	1:4F:219:ILE:HD11	2.08	0.94
2:5F:54:ALA:HB1	2:5G:281:TYR:C	1.88	0.94
1:4A:151:CYS:HG	1:4A:193:SER:HG	1.12	0.93
1:4B:60:LYS:HE3	1:4C:282:TYR:CZ	2.02	0.93
2:5D:55:THR:HG1	2:5E:284:LEU:H	0.99	0.93
2:3E:54:ALA:HB1	2:3F:281:TYR:O	1.66	0.93
2:3I:175:VAL:HG21	1:4I:332:VAL:HG13	1.49	0.93
1:2D:56:THR:CB	1:2E:283:HIS:O	2.17	0.92
1:2G:60:LYS:CD	1:2H:283:HIS:HD2	1.82	0.92
2:3C:60:VAL:HG11	2:3D:280:GLN:NE2	1.84	0.92
2:3C:220:PRO:HD2	1:4C:326:LYS:HD2	1.48	0.92
2:3E:58:ARG:HD3	2:3F:281:TYR:CD1	2.04	0.92
2:3A:267:LEU:HD21	2:3A:374:ILE:HD11	1.51	0.92
2:3F:208:TYR:CD1	1:4F:326:LYS:HE2	2.04	0.92
1:4C:151:CYS:HG	1:4C:193:SER:HG	0.95	0.92
2:3E:55:THR:CG2	2:3F:283:ALA:HA	1.97	0.92
2:5G:55:THR:CG2	2:5H:283:ALA:HA	2.00	0.92
1:2B:151:CYS:HG	1:2B:193:SER:HG	1.13	0.91
1:2C:124:LYS:HD2	1:2D:283:HIS:NE2	1.84	0.91
1:4H:151:CYS:HG	1:4H:193:SER:HG	0.92	0.91
1:2D:222:PRO:O	2:3D:324:LYS:NZ	2.03	0.91
1:4A:222:PRO:HD2	2:5A:324:LYS:NZ	1.85	0.91
2:3A:212:PHE:HE1	1:4A:326:LYS:HZ2	0.91	0.90
1:2D:60:LYS:HE3	1:2E:283:HIS:CD2	2.06	0.90
1:4F:222:PRO:HD2	2:5F:324:LYS:HD3	1.52	0.90
2:5D:54:ALA:O	2:5E:283:ALA:CA	2.17	0.90
2:3E:58:ARG:HH11	2:3F:281:TYR:HE1	0.98	0.90
1:4A:57:GLY:H	1:4B:285:GLN:HG2	1.35	0.90
1:2D:85:HIS:O	1:2E:283:HIS:NE2	2.04	0.90
2:5B:87:PRO:HD2	2:5C:281:TYR:CE2	2.06	0.90
2:5D:58:ARG:HD2	2:5E:280:GLN:O	1.70	0.90
2:5G:54:ALA:HB1	2:5H:281:TYR:O	1.70	0.90
1:2A:407:TRP:HZ2	2:3A:258:ILE:HD11	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3D:153:SER:HB2	2:3D:191:GLN:HE22	1.36	0.89
2:5D:58:ARG:CD	2:5E:280:GLN:O	2.20	0.89
2:3A:55:THR:HG23	2:3B:283:ALA:HB2	1.53	0.89
1:2D:56:THR:HA	1:2E:285:GLN:HB3	1.54	0.89
2:5C:88:ASP:HB2	2:5D:281:TYR:CE1	2.07	0.89
1:4F:178:SER:HB2	2:5F:347:ASN:HD22	1.26	0.89
2:3E:55:THR:HB	2:3F:283:ALA:HA	1.55	0.88
2:3G:55:THR:CG2	2:3H:283:ALA:HA	2.01	0.88
1:2D:33:ASP:HB3	1:2E:282:TYR:OH	1.71	0.88
1:2A:96:LYS:HE3	2:3A:129:CYS:SG	2.14	0.88
2:3D:54:ALA:C	2:3E:283:ALA:HA	1.94	0.88
1:4G:168:ASN:HD21	1:4G:194:LEU:HD11	1.38	0.88
1:4D:33:ASP:OD1	1:4E:282:TYR:CE2	2.26	0.87
2:3E:58:ARG:CZ	2:3F:281:TYR:CE1	2.57	0.87
2:3D:54:ALA:O	2:3E:283:ALA:CA	2.23	0.86
2:3E:218:THR:O	1:4E:326:LYS:HE2	1.74	0.86
2:5F:54:ALA:CB	2:5G:281:TYR:O	2.24	0.86
2:5H:200:GLN:HB3	2:5H:266:PHE:HB2	1.58	0.86
1:4D:85:HIS:O	1:4E:283:HIS:NE2	2.08	0.85
1:4H:222:PRO:HD2	2:5H:324:LYS:NZ	1.91	0.85
1:2F:178:SER:HB2	2:3F:347:ASN:HD22	1.37	0.85
1:2A:407:TRP:CZ2	2:3A:258:ILE:HD11	2.11	0.85
2:3A:220:PRO:HD2	1:4A:326:LYS:HE2	0.88	0.85
2:3A:212:PHE:HE1	1:4A:326:LYS:NZ	1.75	0.85
2:5A:55:THR:HG21	2:5B:283:ALA:CA	2.05	0.85
2:3E:202:ILE:HD11	2:3E:268:ILE:HD12	1.60	0.84
1:4B:258:ASN:HB3	1:4B:352:LYS:HE3	1.57	0.84
2:3I:99:ASN:ND2	1:4I:254:GLU:OE1	2.09	0.84
2:5E:135:ILE:HG13	2:5E:152:ILE:HD11	1.59	0.84
1:2G:60:LYS:NZ	1:2H:283:HIS:CD2	2.45	0.84
2:3F:220:PRO:HG2	1:4F:326:LYS:HE3	1.57	0.84
2:5E:55:THR:HB	2:5F:283:ALA:CA	2.08	0.84
1:4D:85:HIS:O	1:4E:283:HIS:CD2	2.31	0.84
2:5A:207:LEU:HD21	2:5A:225:LEU:HB3	1.57	0.84
1:4C:121:ARG:HH12	1:4D:283:HIS:HE1	1.24	0.84
2:3C:176:SER:HB2	1:4C:349:THR:OG1	1.78	0.83
1:4D:57:GLY:H	1:4E:285:GLN:CB	1.89	0.83
2:3B:98:GLY:O	1:4B:257:THR:HG21	1.79	0.83
2:3B:286:VAL:HG23	2:3B:287:PRO:HD3	1.61	0.83
1:4B:60:LYS:HE3	1:4C:282:TYR:OH	1.79	0.82
1:2A:96:LYS:NZ	2:3A:1:MET:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4D:60:LYS:HE3	1:4E:283:HIS:HA	1.61	0.82
1:4E:60:LYS:HZ1	1:4F:283:HIS:HD2	1.23	0.82
2:3F:139:LEU:HD13	2:3F:168:SER:HB2	1.59	0.82
2:5B:87:PRO:CD	2:5C:281:TYR:CE2	2.62	0.82
2:5F:58:ARG:HD3	2:5G:281:TYR:CD1	2.14	0.82
2:3A:55:THR:HG21	2:3B:283:ALA:HA	1.61	0.82
2:3D:55:THR:OG1	2:3E:283:ALA:HA	1.79	0.82
2:5F:54:ALA:HB1	2:5G:281:TYR:CA	2.09	0.82
1:4D:57:GLY:N	1:4E:285:GLN:HB3	1.94	0.81
2:3A:55:THR:CG2	2:3B:283:ALA:CB	2.54	0.81
2:3E:55:THR:CB	2:3F:283:ALA:HA	2.09	0.81
2:3E:58:ARG:CD	2:3F:281:TYR:CD1	2.61	0.81
1:2C:124:LYS:HD2	1:2D:283:HIS:CE1	2.16	0.81
1:4D:60:LYS:HE3	1:4E:283:HIS:CD2	2.15	0.81
2:5F:55:THR:CG2	2:5G:283:ALA:HA	2.11	0.81
1:4A:212:ILE:HG23	1:4A:275:ILE:HD12	1.61	0.81
2:3A:55:THR:HG21	2:3B:283:ALA:CA	2.11	0.81
1:2E:60:LYS:NZ	1:2F:282:TYR:HE2	1.72	0.81
1:2I:292:THR:HG21	1:2I:331:ALA:HB1	1.63	0.81
1:2H:222:PRO:HG2	2:3H:324:LYS:HZ3	1.42	0.80
2:3H:99:ASN:ND2	1:4H:254:GLU:OE1	2.13	0.80
2:5E:55:THR:CG2	2:5F:283:ALA:HA	2.11	0.80
1:2G:407:TRP:CE3	2:3G:255:VAL:HG22	2.15	0.80
1:4D:178:SER:HB2	2:5D:347:ASN:ND2	1.96	0.80
1:2D:221:ARG:HA	2:3D:324:LYS:HE3	1.63	0.80
2:5D:54:ALA:C	2:5E:283:ALA:CA	2.50	0.80
2:5D:58:ARG:CZ	2:5E:281:TYR:CD1	2.64	0.80
2:5D:54:ALA:HA	2:5E:283:ALA:HB2	1.64	0.79
1:2C:100:ALA:HA	2:3C:252:LYS:HD2	1.63	0.79
1:4H:191:THR:HG21	1:4H:425:LEU:HD21	1.65	0.79
2:3F:179:VAL:HG23	1:4F:349:THR:O	1.82	0.79
1:4G:407:TRP:HE3	2:5G:255:VAL:HG12	1.47	0.79
1:2F:177:VAL:HG13	2:3F:327:ASP:OD2	1.83	0.79
2:3B:179:VAL:H	1:4B:352:LYS:HZ1	1.24	0.79
1:4D:178:SER:HB2	2:5D:347:ASN:HD22	1.46	0.79
2:5B:286:VAL:HG23	2:5B:287:PRO:HD3	1.62	0.79
1:2B:338:LYS:HZ1	1:2B:341:ILE:HG12	1.48	0.79
1:2G:2:ARG:HB3	1:2G:133:GLN:HE21	1.48	0.79
1:2G:181:VAL:HG12	2:3G:256:ASN:HB2	1.65	0.78
2:3D:54:ALA:O	2:3E:283:ALA:N	2.16	0.78
1:4E:221:ARG:HG2	2:5E:322:SER:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3C:176:SER:CB	1:4C:349:THR:OG1	2.30	0.78
1:4F:213:CYS:SG	1:4F:219:ILE:CG1	2.71	0.78
1:2F:178:SER:HB2	2:3F:347:ASN:HD21	1.41	0.78
2:5E:202:ILE:HD11	2:5E:268:ILE:HD12	1.63	0.78
1:2G:287:SER:OG	1:2G:290:GLU:OE1	2.00	0.78
1:2E:181:VAL:HG22	2:3E:256:ASN:HD22	1.46	0.78
2:5C:87:PRO:N	2:5D:281:TYR:OH	2.16	0.78
1:2B:221:ARG:CZ	2:3B:325:GLU:H	1.96	0.78
2:3D:178:THR:HG22	1:4D:352:LYS:HZ3	1.48	0.78
1:4G:108:TYR:O	1:4G:112:LYS:NZ	2.16	0.78
1:2C:292:THR:HG21	1:2C:331:ALA:HB1	1.64	0.78
1:2E:60:LYS:CE	1:2F:283:HIS:CD2	2.67	0.78
1:4E:221:ARG:HG2	2:5E:322:SER:HB3	1.66	0.78
2:3C:98:GLY:O	1:4C:257:THR:HG21	1.83	0.78
1:2E:60:LYS:CE	1:2F:283:HIS:HD2	1.95	0.77
1:2H:399:TYR:O	1:2H:402:ARG:NH2	2.17	0.77
2:5C:88:ASP:HB2	2:5D:281:TYR:CZ	2.19	0.77
2:5C:86:ARG:HG2	2:5D:281:TYR:OH	1.55	0.77
1:2G:60:LYS:HZ2	1:2H:283:HIS:CD2	2.03	0.77
1:2G:387:VAL:HA	1:2G:390:ARG:HH21	1.48	0.77
1:2D:89:PRO:HG2	1:2E:280:LYS:HE3	1.66	0.77
2:3H:391:ARG:O	1:4H:262:TYR:OH	2.03	0.77
1:4F:213:CYS:SG	1:4F:219:ILE:CD1	2.73	0.77
2:5C:49:VAL:HG21	2:5C:241:ARG:HG2	1.66	0.77
2:3A:178:THR:HA	1:4A:352:LYS:HE3	1.66	0.77
1:2G:60:LYS:HD3	1:2H:283:HIS:HD2	1.47	0.77
1:4G:151:CYS:SG	1:4G:193:SER:OG	2.42	0.77
1:2I:238:LEU:HD11	1:2I:378:ILE:HD11	1.67	0.76
1:4H:399:TYR:O	1:4H:402:ARG:NH2	2.18	0.76
2:5E:49:VAL:HG21	2:5E:241:ARG:HG2	1.67	0.76
1:4C:121:ARG:NH1	1:4D:283:HIS:HE1	1.79	0.76
1:2D:27:GLU:OE1	1:2D:243:ARG:NH1	2.18	0.76
2:5A:49:VAL:HG11	2:5A:241:ARG:HG2	1.65	0.76
1:4C:60:LYS:HE2	1:4D:282:TYR:OH	1.86	0.76
2:5C:88:ASP:N	2:5D:281:TYR:CZ	2.53	0.76
2:3B:178:THR:HA	1:4B:352:LYS:NZ	2.00	0.76
2:3B:175:VAL:CG1	1:4B:332:VAL:HG13	2.16	0.76
1:4H:202:VAL:HG22	1:4H:268:MET:HG3	1.68	0.76
1:2E:407:TRP:HZ2	2:3E:258:ILE:HD11	1.51	0.76
2:3D:49:VAL:HG21	2:3D:241:ARG:HG2	1.67	0.76
1:4H:222:PRO:HD2	2:5H:324:LYS:HZ3	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4I:292:THR:HG21	1:4I:331:ALA:HB1	1.68	0.76
2:3C:49:VAL:HG21	2:3C:241:ARG:HG2	1.69	0.75
2:3C:86:ARG:HD3	2:3D:281:TYR:CD1	2.17	0.75
1:4G:181:VAL:HG22	2:5G:347:ASN:O	1.86	0.75
2:3B:179:VAL:N	1:4B:352:LYS:NZ	2.32	0.75
1:4D:35:GLN:OE1	1:4E:282:TYR:OH	2.00	0.75
1:2G:151:CYS:SG	1:2G:193:SER:OG	2.41	0.75
1:2E:56:THR:CB	1:2F:283:HIS:O	2.35	0.75
2:3H:179:VAL:HG12	1:4H:258:ASN:OD1	1.87	0.74
2:3G:55:THR:HG21	2:3H:283:ALA:CA	2.11	0.74
2:3A:49:VAL:HG21	2:3A:241:ARG:HG2	1.68	0.74
1:4A:57:GLY:N	1:4B:285:GLN:HG2	2.03	0.74
1:4F:292:THR:HG21	1:4F:331:ALA:HB1	1.69	0.74
2:5B:332:ASN:OD1	2:5B:336:LYS:NZ	2.20	0.74
2:3B:205:GLU:OE1	1:4B:329:ASN:ND2	2.19	0.74
2:3E:49:VAL:HG21	2:3E:241:ARG:HG2	1.67	0.74
2:3H:7:VAL:HB	2:3H:135:ILE:HD13	1.69	0.74
1:4G:407:TRP:CE3	2:5G:255:VAL:HG12	2.23	0.74
1:2A:151:CYS:SG	1:2A:193:SER:OG	2.41	0.74
1:4B:88:HIS:ND1	1:4C:283:HIS:CG	2.55	0.74
1:4G:6:SER:HA	1:4G:136:LEU:HB2	1.69	0.74
2:3E:391:ARG:O	1:4E:262:TYR:OH	2.05	0.74
2:3E:313:ALA:HB1	2:3E:367:PHE:HE1	1.53	0.74
1:4D:33:ASP:OD1	1:4E:282:TYR:HE2	1.67	0.74
2:5A:55:THR:HG23	2:5B:283:ALA:HB2	1.70	0.74
2:3C:66:MET:HE2	2:3C:116:VAL:HG21	1.70	0.73
2:3E:248:SER:HA	2:3E:252:LYS:HD3	1.68	0.73
1:4F:189:LEU:HD11	1:4F:418:PHE:HD1	1.53	0.73
2:3B:205:GLU:CD	1:4B:329:ASN:HD21	1.91	0.73
1:2E:217:LEU:HD11	1:2E:275:ILE:HG22	1.68	0.73
2:3H:221:THR:HG22	2:3H:223:GLY:H	1.52	0.73
1:4G:121:ARG:HH12	1:4G:124:LYS:HE3	1.53	0.73
1:4H:223:THR:OG1	2:5H:245:GLN:OE1	2.04	0.73
2:5F:55:THR:HG21	2:5G:283:ALA:HA	1.70	0.73
1:4I:11:GLN:NE2	2:5I:245:GLN:O	2.21	0.73
1:2G:212:ILE:HG23	1:2G:275:ILE:HD12	1.70	0.73
1:4D:212:ILE:CG2	1:4D:275:ILE:HD11	2.19	0.73
1:4E:60:LYS:HZ1	1:4F:283:HIS:CD2	1.96	0.73
2:5D:58:ARG:HD3	2:5E:281:TYR:HA	0.87	0.73
1:2E:398:MET:CE	2:3E:346:PRO:HD2	2.18	0.73
1:2B:221:ARG:NH2	2:3B:322:SER:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2H:176:GLN:HB3	2:3H:331:LEU:HD11	1.69	0.73
2:3A:256:ASN:HD21	2:3A:350:LYS:HG2	1.52	0.73
1:4D:60:LYS:HE3	1:4E:283:HIS:CG	2.23	0.73
1:4F:213:CYS:SG	1:4F:219:ILE:HG13	2.28	0.73
2:5I:318:ARG:HD2	2:5I:358:PRO:HD3	1.69	0.73
1:2H:151:CYS:SG	1:2H:193:SER:OG	2.47	0.73
2:3D:58:ARG:NH1	2:3E:280:GLN:HG3	2.03	0.73
1:4B:176:GLN:HB3	2:5B:331:LEU:HD11	1.70	0.73
2:5D:58:ARG:CZ	2:5E:281:TYR:CE1	2.72	0.73
2:5H:55:THR:OG1	2:5I:280:GLN:O	2.06	0.73
2:3A:176:SER:OG	1:4A:349:THR:OG1	2.04	0.73
1:4F:174:SER:OG	1:4F:177:VAL:O	2.06	0.73
2:5B:274:THR:HG21	2:5B:282:ARG:HD2	1.71	0.73
2:3D:58:ARG:HD2	2:3E:280:GLN:O	1.89	0.72
2:3E:397:TRP:CZ3	1:4E:260:VAL:O	2.42	0.72
2:5F:54:ALA:HB1	2:5G:281:TYR:HA	1.69	0.72
1:4C:292:THR:HG21	1:4C:331:ALA:HB1	1.71	0.72
1:2B:221:ARG:NH1	2:3B:325:GLU:H	1.86	0.72
2:3H:49:VAL:HG11	2:3H:241:ARG:HG2	1.71	0.72
1:4A:222:PRO:HD2	2:5A:324:LYS:HZ3	1.54	0.72
1:4B:60:LYS:CE	1:4C:282:TYR:CZ	2.73	0.72
1:4D:388:PHE:HB2	1:4D:429:GLU:OE2	1.90	0.72
1:2B:72:PRO:HD2	2:3B:2:ARG:HH22	1.54	0.72
1:2D:212:ILE:HG12	1:2D:275:ILE:HD11	1.72	0.72
2:5E:200:GLN:HB3	2:5E:268:ILE:HD11	1.72	0.72
2:3B:267:LEU:HD12	2:3B:301:CYS:HB3	1.71	0.72
1:4G:76:ASP:OD2	2:5G:46:ARG:NH1	2.23	0.72
1:4G:151:CYS:HG	1:4G:193:SER:HG	1.29	0.72
1:2G:56:THR:CB	1:2H:283:HIS:O	2.37	0.72
1:4C:88:HIS:HB3	1:4C:91:GLN:HG2	1.70	0.72
2:3E:55:THR:CG2	2:3F:282:ARG:O	2.37	0.72
1:4E:398:MET:HE2	2:5E:346:PRO:HD2	1.71	0.72
1:2D:56:THR:HA	1:2E:285:GLN:H	1.55	0.71
2:3G:135:ILE:HD11	2:3G:152:ILE:HD11	1.72	0.71
2:5E:55:THR:HG21	2:5F:284:LEU:H	1.55	0.71
2:5A:7:VAL:HG22	2:5A:64:ILE:CG2	2.18	0.71
1:2E:60:LYS:NZ	1:2F:282:TYR:CD2	2.58	0.71
1:2A:191:THR:HG23	1:2A:425:LEU:HD21	1.71	0.71
1:2B:88:HIS:CD2	1:2C:283:HIS:HB3	2.26	0.71
1:4E:292:THR:HG21	1:4E:331:ALA:HB1	1.70	0.71
1:2G:6:SER:HA	1:2G:136:LEU:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3D:177:ASP:CG	1:4D:353:CYS:SG	2.69	0.71
2:5F:55:THR:HG23	2:5G:283:ALA:CB	2.21	0.71
1:2A:96:LYS:CE	2:3A:129:CYS:SG	2.78	0.71
1:4A:222:PRO:HD2	2:5A:324:LYS:HZ1	1.55	0.71
2:3E:129:CYS:SG	2:3E:162:ARG:NH2	2.64	0.71
2:5G:91:VAL:HG21	2:5G:116:VAL:HG12	1.73	0.71
1:4H:181:VAL:HG22	2:5H:256:ASN:OD1	1.89	0.71
1:4G:292:THR:HG21	1:4G:331:ALA:HB1	1.72	0.71
2:3B:220:PRO:HD2	1:4B:326:LYS:HD2	1.73	0.70
1:2B:60:LYS:HE2	1:2C:282:TYR:CD2	2.26	0.70
1:2F:223:THR:HG22	2:3F:322:SER:HA	1.72	0.70
1:2H:76:ASP:OD2	2:3H:46:ARG:NH1	2.24	0.70
2:5H:306:ARG:HA	2:5H:340:TYR:HE1	1.55	0.70
2:3B:49:VAL:HG11	2:3B:241:ARG:HG2	1.72	0.70
2:3E:220:PRO:HD2	1:4E:326:LYS:HD3	1.72	0.70
2:5B:163:ILE:HD13	2:5B:250:LEU:HB3	1.73	0.70
2:5F:55:THR:HG23	2:5G:283:ALA:HB2	1.72	0.70
2:3B:179:VAL:H	1:4B:352:LYS:HZ3	1.37	0.70
2:3B:87:PRO:HD2	2:3C:281:TYR:CE2	2.26	0.70
2:3B:172:SER:OG	2:3B:175:VAL:O	2.10	0.70
1:4I:27:GLU:OE2	1:4I:243:ARG:NH1	2.24	0.70
2:5A:55:THR:CG2	2:5B:283:ALA:CA	2.67	0.70
2:3D:396:HIS:HA	2:3D:399:THR:HG22	1.71	0.70
2:5F:274:THR:HG21	2:5F:282:ARG:HD2	1.71	0.70
2:3F:208:TYR:HD1	1:4F:326:LYS:CE	2.04	0.70
1:4A:397:LEU:HD21	2:5A:344:TRP:HA	1.73	0.69
1:4C:182:VAL:HG12	2:5C:256:ASN:HD21	1.56	0.69
1:2E:221:ARG:HD3	2:3E:325:GLU:OE2	1.92	0.69
1:4C:184:PRO:HA	1:4C:391:MET:HE1	1.72	0.69
1:4E:407:TRP:HH2	2:5E:258:ILE:HB	1.57	0.69
2:5B:49:VAL:HG11	2:5B:241:ARG:HG2	1.73	0.69
1:4B:181:VAL:H	2:5B:350:LYS:HE3	1.56	0.69
1:4C:209:ILE:HD11	1:4C:302:MET:HG3	1.74	0.69
2:5H:49:VAL:HG11	2:5H:241:ARG:HG2	1.75	0.69
2:5A:55:THR:CG2	2:5B:283:ALA:CB	2.70	0.69
1:2C:88:HIS:CA	1:2D:282:TYR:HE2	2.00	0.69
1:2D:269:LEU:HD23	1:2D:301:MET:HG2	1.73	0.69
1:2H:298:PRO:HG3	1:2H:308:ARG:HH12	1.58	0.69
2:5I:49:VAL:HG11	2:5I:241:ARG:HG2	1.75	0.69
2:5B:213:ARG:HH22	2:5B:297:LYS:HB2	1.58	0.69
2:5G:55:THR:CG2	2:5H:283:ALA:CA	2.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2H:217:LEU:HD21	1:2H:275:ILE:HG13	1.74	0.68
1:2B:151:CYS:SG	1:2B:193:SER:OG	2.40	0.68
1:2C:62:VAL:HG11	1:2D:282:TYR:CZ	2.29	0.68
1:2C:62:VAL:HG11	1:2D:282:TYR:OH	1.93	0.68
1:2G:60:LYS:CD	1:2H:283:HIS:CD2	2.73	0.68
1:4G:56:THR:CB	1:4H:283:HIS:O	2.42	0.68
2:3C:176:SER:OG	1:4C:349:THR:OG1	2.11	0.68
1:4I:397:LEU:HD21	2:5I:344:TRP:HA	1.75	0.68
1:4B:133:GLN:HG3	1:4B:252:VAL:HG22	1.75	0.68
1:2D:57:GLY:H	1:2E:285:GLN:CB	2.07	0.68
2:3D:54:ALA:HB1	2:3E:281:TYR:O	1.94	0.68
1:2F:292:THR:HG21	1:2F:331:ALA:HB1	1.73	0.68
2:3D:55:THR:OG1	2:3E:283:ALA:C	2.31	0.68
2:3H:397:TRP:HH2	1:4H:260:VAL:O	1.77	0.68
2:5A:113:ILE:HG13	2:5A:150:LEU:HD22	1.76	0.67
1:4A:212:ILE:CG2	1:4A:275:ILE:HD12	2.24	0.67
2:5A:374:ILE:O	2:5A:374:ILE:HG22	1.94	0.67
2:3B:274:THR:HG21	2:3B:282:ARG:HD2	1.77	0.67
2:3B:396:HIS:HA	2:3B:399:THR:HG22	1.77	0.67
2:3F:220:PRO:HG2	1:4F:326:LYS:CE	2.24	0.67
1:4D:60:LYS:CD	1:4E:282:TYR:O	2.36	0.67
2:3A:113:ILE:HG13	2:3A:150:LEU:HD22	1.76	0.67
1:4G:60:LYS:HD2	1:4H:283:HIS:CD2	2.30	0.67
2:3B:175:VAL:HG11	1:4B:332:VAL:CG1	2.20	0.67
2:3F:208:TYR:CD1	1:4F:326:LYS:CE	2.78	0.67
2:3H:208:TYR:HE2	1:4H:329:ASN:HD22	1.42	0.67
1:2H:151:CYS:HG	1:2H:193:SER:HG	1.28	0.67
1:2A:181:VAL:HG22	2:3A:350:LYS:NZ	2.07	0.67
2:3I:175:VAL:HG21	1:4I:332:VAL:CG1	2.24	0.67
1:4F:151:CYS:SG	1:4F:193:SER:OG	2.47	0.67
1:2A:268:MET:N	1:2A:268:MET:SD	2.67	0.67
1:4G:398:MET:CE	2:5G:345:ILE:HG23	2.25	0.67
1:4I:5:ILE:HD12	1:4I:125:LEU:CD2	2.24	0.67
1:4B:181:VAL:CG1	2:5B:350:LYS:NZ	2.49	0.66
2:5D:396:HIS:HA	2:5D:399:THR:HG22	1.77	0.66
2:3D:58:ARG:HD3	2:3E:281:TYR:HA	0.82	0.66
2:5E:55:THR:CG2	2:5F:282:ARG:O	2.37	0.66
1:4E:181:VAL:HG22	2:5E:256:ASN:HD22	1.60	0.66
1:2D:60:LYS:CD	1:2E:282:TYR:O	2.36	0.66
1:4C:397:LEU:HD21	2:5C:344:TRP:HA	1.78	0.66
1:4F:179:THR:OG1	2:5F:351:SER:OG	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4G:97:GLU:OE2	1:4G:105:ARG:NH2	2.25	0.66
2:5H:117:LEU:HD13	2:5H:154:LYS:HG3	1.77	0.66
2:5G:178:THR:OG1	2:5G:181:GLU:OE2	2.13	0.66
1:2D:138:PHE:HZ	1:2D:235:ILE:HD12	1.60	0.66
2:3I:49:VAL:HG11	2:3I:241:ARG:HG2	1.77	0.66
2:5I:289:LEU:HD12	2:5I:365:VAL:HG12	1.77	0.66
1:2D:292:THR:HG21	1:2D:331:ALA:HB1	1.78	0.66
2:5D:55:THR:HG1	2:5E:284:LEU:N	1.67	0.66
2:3A:212:PHE:CE1	1:4A:326:LYS:NZ	2.58	0.66
2:3F:54:ALA:HB1	2:3G:281:TYR:HA	1.77	0.66
1:2A:2:ARG:HE	1:2A:133:GLN:HE21	1.44	0.66
1:2D:33:ASP:O	1:2D:60:LYS:NZ	2.28	0.66
1:2E:151:CYS:SG	1:2E:193:SER:OG	2.46	0.66
1:4G:31:GLN:NE2	1:4G:33:ASP:OD2	2.29	0.66
1:2H:133:GLN:HG3	1:2H:252:VAL:HG22	1.76	0.65
2:3D:54:ALA:C	2:3E:283:ALA:CA	2.63	0.65
2:3D:55:THR:OG1	2:3E:283:ALA:CA	2.44	0.65
2:3F:330:MET:HB3	2:3F:349:MET:SD	2.35	0.65
1:4I:8:HIS:HD2	1:4I:65:CYS:SG	2.18	0.65
2:5G:139:LEU:HD13	2:5G:168:SER:HB2	1.79	0.65
2:3F:377:MET:HG3	2:3F:380:ARG:NH1	2.11	0.65
1:4D:33:ASP:OD2	1:4E:282:TYR:OH	2.14	0.65
1:4G:177:VAL:HG13	2:5G:327:ASP:OD2	1.96	0.65
1:2A:178:SER:HB3	1:2A:183:GLU:HG3	1.79	0.65
1:4H:254:GLU:HG2	1:4H:352:LYS:HZ2	1.61	0.65
2:3D:274:THR:HG21	2:3D:282:ARG:HD2	1.78	0.65
2:5D:412:GLU:O	2:5D:416:ASN:ND2	2.29	0.65
1:4E:407:TRP:CH2	2:5E:258:ILE:HB	2.32	0.65
1:4G:122:ILE:HD13	1:4G:157:LEU:HD11	1.78	0.65
2:3B:178:THR:CA	1:4B:352:LYS:HZ3	2.10	0.65
2:3F:98:GLY:O	1:4F:257:THR:HG21	1.97	0.65
2:3F:220:PRO:HG2	1:4F:326:LYS:HG3	1.78	0.65
2:5A:207:LEU:HD23	2:5A:225:LEU:HD22	1.79	0.65
2:5E:129:CYS:SG	2:5E:162:ARG:NH2	2.70	0.65
2:3E:396:HIS:CE1	1:4E:263:PRO:HD3	2.32	0.65
2:3H:391:ARG:HD2	1:4H:346:TRP:CE2	2.32	0.65
1:4B:181:VAL:CG1	2:5B:350:LYS:HZ2	1.96	0.65
2:5C:88:ASP:OD2	2:5D:281:TYR:CD2	2.50	0.65
1:2D:60:LYS:NZ	1:2E:283:HIS:CD2	2.65	0.65
1:4G:88:HIS:CE1	1:4H:280:LYS:HD2	2.32	0.65
2:5H:163:ILE:HD13	2:5H:250:LEU:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5I:396:HIS:HA	2:5I:399:THR:HG22	1.78	0.64
1:2C:178:SER:HB2	2:3C:347:ASN:ND2	2.12	0.64
2:3D:249:ASP:OD1	2:3D:250:LEU:N	2.30	0.64
1:4A:60:LYS:CE	1:4B:283:HIS:HD2	2.10	0.64
1:4D:60:LYS:CE	1:4E:283:HIS:CG	2.79	0.64
2:5C:88:ASP:CB	2:5D:281:TYR:CZ	2.80	0.64
2:5E:95:THR:OG1	2:5E:108:GLU:OE2	2.14	0.64
1:2B:23:LEU:HD11	1:2B:361:THR:HG23	1.78	0.64
1:2B:221:ARG:NH2	2:3B:325:GLU:H	1.95	0.64
1:2C:298:PRO:HG3	1:2C:308:ARG:HH22	1.62	0.64
1:2G:401:LYS:HD2	2:3G:344:TRP:CH2	2.33	0.64
1:4D:30:ILE:HG22	1:4D:36:MET:HB3	1.78	0.64
2:5A:55:THR:HG23	2:5B:283:ALA:CB	2.27	0.64
2:5A:248:SER:OG	2:5A:350:LYS:NZ	2.31	0.64
1:2A:101:ASN:HB3	1:2A:182:VAL:HG21	1.78	0.64
1:2I:5:ILE:HD12	1:2I:125:LEU:CD2	2.26	0.64
2:3G:257:LEU:HD11	2:3G:314:SER:HB3	1.80	0.64
1:2H:210:TYR:HD1	2:3H:324:LYS:HE3	1.56	0.64
1:4G:339:ARG:O	1:4G:342:GLN:NE2	2.30	0.64
2:5B:87:PRO:HD3	2:5C:281:TYR:CZ	2.32	0.64
1:2A:311:LYS:HE2	1:2A:344:VAL:HA	1.80	0.64
1:2D:100:ALA:HA	2:3D:252:LYS:HG3	1.77	0.64
1:2E:292:THR:HG21	1:2E:331:ALA:HB1	1.80	0.64
2:3H:166:THR:HB	2:3H:199:VAL:HG12	1.80	0.64
2:3E:175:VAL:HG23	1:4E:329:ASN:OD1	1.97	0.63
1:4D:55:GLU:O	1:4E:285:GLN:CG	2.43	0.63
2:5D:54:ALA:O	2:5E:283:ALA:N	2.30	0.63
1:2A:96:LYS:HG2	2:3A:129:CYS:SG	2.38	0.63
1:2E:73:THR:HA	2:3E:46:ARG:HH11	1.64	0.63
2:5G:165:GLU:OE2	2:5G:200:GLN:NE2	2.30	0.63
1:2B:398:MET:SD	2:3B:346:PRO:HD2	2.38	0.63
1:2E:328:VAL:HG21	1:2E:355:ILE:HD11	1.80	0.63
2:3B:179:VAL:N	1:4B:352:LYS:HZ3	1.96	0.63
2:3D:54:ALA:O	2:3E:282:ARG:C	2.37	0.63
2:3E:313:ALA:HB1	2:3E:367:PHE:CE1	2.33	0.63
2:3E:397:TRP:CH2	1:4E:260:VAL:CG2	2.77	0.63
1:2A:191:THR:CG2	1:2A:425:LEU:HD21	2.28	0.63
1:4I:5:ILE:HD12	1:4I:125:LEU:HD23	1.79	0.63
1:2E:101:ASN:ND2	2:3E:252:LYS:HZ2	1.97	0.63
2:5D:83:GLN:O	2:5E:281:TYR:OH	2.14	0.62
2:5D:83:GLN:O	2:5E:281:TYR:CE1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:301:MET:HE3	1:2A:307:PRO:HG3	1.80	0.62
1:2E:208:ALA:HB2	1:2E:304:LYS:HG2	1.81	0.62
1:2E:398:MET:HE2	2:3E:346:PRO:HD2	1.81	0.62
1:2G:407:TRP:HE3	2:3G:255:VAL:HG22	1.60	0.62
2:3F:208:TYR:CD1	1:4F:326:LYS:HD3	2.34	0.62
2:5E:58:ARG:HD3	2:5F:281:TYR:CD1	2.34	0.62
1:2B:181:VAL:HG12	2:3B:256:ASN:OD1	1.99	0.62
2:3B:87:PRO:CD	2:3C:281:TYR:CE2	2.83	0.62
1:2E:407:TRP:CZ2	2:3E:258:ILE:HD11	2.34	0.62
2:3H:175:VAL:HG11	1:4H:332:VAL:HG13	1.81	0.62
2:5A:249:ASP:OD1	2:5A:250:LEU:N	2.32	0.62
2:3I:318:ARG:HD3	2:3I:358:PRO:HD3	1.81	0.62
2:5A:7:VAL:HG22	2:5A:64:ILE:HG22	1.82	0.62
1:2D:56:THR:HA	1:2E:285:GLN:N	2.15	0.62
1:2G:151:CYS:HG	1:2G:193:SER:HG	1.35	0.62
2:3A:391:ARG:NH2	1:4A:346:TRP:CD1	2.68	0.62
2:3D:54:ALA:HA	2:3E:283:ALA:HB2	1.80	0.62
2:3D:55:THR:HG1	2:3E:284:LEU:H	1.43	0.62
2:3F:180:VAL:O	2:3F:184:ASN:ND2	2.32	0.62
2:3I:95:THR:OG1	2:3I:108:GLU:OE2	2.09	0.62
1:4I:109:THR:HG22	1:4I:110:ILE:HG23	1.82	0.62
2:5H:68:LEU:HD12	2:5H:143:THR:HG22	1.81	0.62
1:2A:105:ARG:HH12	2:3A:251:ARG:HD2	1.65	0.62
1:2G:212:ILE:CG2	1:2G:275:ILE:HD12	2.29	0.62
1:2H:176:GLN:HB3	2:3H:331:LEU:CD1	2.28	0.62
1:4A:66:VAL:HG12	1:4A:91:GLN:HB2	1.81	0.62
1:4E:221:ARG:CG	2:5E:322:SER:HB3	2.29	0.62
1:2C:221:ARG:HG3	2:3C:325:GLU:CD	2.20	0.61
2:3B:334:GLN:OE1	2:3B:348:ASN:ND2	2.32	0.61
2:3C:64:ILE:HD12	2:3C:119:VAL:HG12	1.82	0.61
1:2I:100:ALA:HA	2:3I:252:LYS:HE3	1.82	0.61
1:2I:392:ASP:OD1	1:2I:422:ARG:NH2	2.20	0.61
1:2G:417:GLU:HA	1:2G:420:GLU:HG3	1.81	0.61
2:3F:54:ALA:HB1	2:3G:281:TYR:CA	2.30	0.61
1:4E:167:LEU:HD21	1:4E:252:VAL:HG13	1.80	0.61
1:4G:178:SER:CB	2:5G:347:ASN:ND2	2.62	0.61
1:4I:68:LEU:CD1	1:4I:153:LEU:HD11	2.30	0.61
1:4I:241:SER:OG	1:4I:250:VAL:O	2.17	0.61
2:5B:161:ASP:OD1	2:5B:162:ARG:NH1	2.32	0.61
2:5I:211:CYS:SG	2:5I:217:LEU:HB2	2.40	0.61
2:5I:404:ASP:HB3	2:5I:406:MET:SD	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2G:200:VAL:HG23	1:2G:268:MET:CE	2.30	0.61
2:3B:99:ASN:OD1	1:4B:254:GLU:OE1	2.18	0.61
1:4B:316:CYS:HA	1:4B:352:LYS:HB2	1.81	0.61
2:5D:267:LEU:HB3	2:5D:299:MET:HE2	1.81	0.61
2:3E:99:ASN:ND2	1:4E:254:GLU:OE1	2.33	0.61
1:4I:195:LEU:HD21	1:4I:264:ARG:HE	1.65	0.61
1:2D:85:HIS:O	1:2E:283:HIS:CD2	2.52	0.61
2:3E:58:ARG:HH12	2:3F:281:TYR:HE1	1.33	0.61
2:5F:55:THR:CG2	2:5G:283:ALA:CB	2.79	0.61
1:2A:60:LYS:HE2	1:2B:283:HIS:HD2	1.66	0.61
1:2D:30:ILE:HG22	1:2D:36:MET:HB3	1.83	0.61
2:3B:220:PRO:CD	1:4B:326:LYS:HD2	2.30	0.61
2:3C:70:PRO:HD2	1:4C:2:ARG:HH22	1.65	0.61
1:2B:221:ARG:HH12	2:3B:324:LYS:HB3	1.66	0.61
2:3F:391:ARG:O	1:4F:262:TYR:OH	2.14	0.61
1:4E:23:LEU:HD11	1:4E:361:THR:HG23	1.82	0.61
1:4E:274:PRO:HG3	1:4E:286:LEU:HD23	1.83	0.61
2:3E:294:PHE:CD2	2:3E:333:VAL:HG21	2.36	0.61
1:2B:27:GLU:HB3	1:2B:361:THR:HG21	1.82	0.61
1:4D:292:THR:HG21	1:4D:331:ALA:HB1	1.81	0.61
1:4E:88:HIS:HB3	1:4E:91:GLN:HG2	1.83	0.61
1:4H:223:THR:HG23	1:4H:225:THR:HG22	1.83	0.61
1:4I:8:HIS:CD2	1:4I:65:CYS:SG	2.94	0.61
2:3G:69:GLU:HG2	1:4G:2:ARG:HH22	1.65	0.60
2:3H:175:VAL:HG21	1:4H:333:ALA:HA	1.82	0.60
1:4B:328:VAL:CG1	1:4B:353:CYS:SG	2.89	0.60
1:4D:177:VAL:HG11	2:5D:327:ASP:HB3	1.83	0.60
1:4E:407:TRP:HZ3	2:5E:258:ILE:O	1.84	0.60
1:4H:33:ASP:O	1:4H:60:LYS:NZ	2.25	0.60
2:5B:8:GLN:OE1	2:5B:17:GLY:HA3	2.01	0.60
2:5H:68:LEU:HD21	2:5H:147:MET:SD	2.41	0.60
2:3C:122:LYS:HE2	2:3D:281:TYR:OH	2.02	0.60
1:4C:154:LEU:HD13	1:4C:166:LYS:HE3	1.82	0.60
1:4H:202:VAL:HA	1:4H:268:MET:HB2	1.82	0.60
1:2D:56:THR:CA	1:2E:285:GLN:HB3	2.28	0.60
2:3G:249:ASP:OD1	2:3G:250:LEU:N	2.34	0.60
1:4B:223:THR:HG23	1:4B:225:THR:HG22	1.82	0.60
1:4E:398:MET:CE	2:5E:346:PRO:HD2	2.31	0.60
1:4H:51:THR:HG23	1:4H:52:PHE:HD1	1.66	0.60
1:2E:177:VAL:HG11	2:3E:327:ASP:HB3	1.83	0.60
2:3G:55:THR:HG23	2:3H:283:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4F:178:SER:HB2	2:5F:347:ASN:HD21	1.63	0.60
2:5B:87:PRO:HD3	2:5C:281:TYR:OH	2.02	0.60
1:2H:262:TYR:HB2	1:2H:265:ILE:HG22	1.84	0.60
2:3I:325:GLU:HA	2:3I:328:GLU:HG3	1.82	0.60
2:5C:64:ILE:HD12	2:5C:119:VAL:HG12	1.83	0.60
2:5F:58:ARG:HD3	2:5G:281:TYR:CE1	2.37	0.60
2:5H:105:HIS:HE1	2:5H:191:GLN:HE22	1.49	0.60
2:3C:396:HIS:HA	2:3C:399:THR:HG22	1.84	0.60
1:4A:178:SER:HB2	2:5A:347:ASN:CG	2.22	0.60
1:4A:390:ARG:NH2	1:4A:390:ARG:HB3	2.17	0.60
2:5D:6:HIS:HD2	2:5D:134:GLN:HE21	1.48	0.60
2:5H:166:THR:HB	2:5H:199:VAL:HG22	1.84	0.60
1:2I:238:LEU:CD1	1:2I:378:ILE:HD11	2.31	0.60
2:5A:54:ALA:HB1	2:5B:281:TYR:O	2.02	0.60
2:3C:178:THR:HA	1:4C:352:LYS:HD3	1.83	0.60
1:2B:239:THR:OG1	1:2B:243:ARG:NH1	2.34	0.60
1:2G:230:LEU:CD2	1:2G:302:MET:HE2	2.32	0.60
2:5A:2:ARG:NH2	2:5A:249:ASP:OD2	2.35	0.60
1:4D:57:GLY:N	1:4E:285:GLN:HA	2.17	0.59
1:4H:168:ASN:HD22	1:4H:198:THR:HG21	1.67	0.59
1:4D:60:LYS:HE3	1:4E:283:HIS:CA	2.30	0.59
1:4I:178:SER:HB3	2:5I:347:ASN:ND2	2.16	0.59
1:2G:18:ASN:O	1:2G:22:GLU:HG2	2.01	0.59
2:3F:16:ILE:HD11	2:3F:229:VAL:HG21	1.84	0.59
1:4G:222:PRO:HD2	2:5G:324:LYS:HG2	1.82	0.59
1:2F:276:ILE:HG23	1:2F:280:LYS:HB2	1.84	0.59
1:2G:339:ARG:O	1:2G:342:GLN:NE2	2.34	0.59
1:2G:403:ALA:HB2	2:3G:344:TRP:CZ3	2.38	0.59
1:4H:215:ARG:NH2	1:4H:297:GLU:OE2	2.34	0.59
1:2A:60:LYS:CE	1:2B:283:HIS:HD2	2.14	0.59
1:2D:105:ARG:HG2	1:2D:110:ILE:HG12	1.84	0.59
1:4G:178:SER:CB	2:5G:347:ASN:HD21	2.10	0.59
2:5A:10:GLY:HA2	2:5A:143:THR:HG23	1.85	0.59
2:5B:87:PRO:HD3	2:5C:281:TYR:CE2	2.38	0.59
2:5E:91:VAL:HG12	2:5E:112:LEU:HD21	1.83	0.59
1:2C:241:SER:OG	1:2C:249:ASN:HB2	2.02	0.59
2:3A:267:LEU:HB3	2:3A:299:MET:SD	2.43	0.59
2:3F:176:SER:OG	1:4F:349:THR:HB	2.03	0.59
1:4D:60:LYS:HZ1	1:4E:283:HIS:CD2	2.11	0.59
2:5D:64:ILE:HD12	2:5D:119:VAL:HG12	1.84	0.59
1:2D:60:LYS:HE3	1:2E:283:HIS:CG	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4D:259:LEU:HD11	1:4D:316:CYS:HB2	1.84	0.59
1:4E:105:ARG:HH12	2:5E:251:ARG:HD3	1.68	0.59
1:4G:51:THR:HG23	1:4G:52:PHE:HD1	1.66	0.59
2:3D:83:GLN:O	2:3E:281:TYR:HE2	1.86	0.59
1:4C:124:LYS:HD2	1:4D:283:HIS:CE1	2.38	0.59
1:4I:177:VAL:HB	2:5I:327:ASP:OD2	2.02	0.59
1:2I:5:ILE:HD12	1:2I:125:LEU:HD23	1.83	0.59
2:3I:175:VAL:CG2	1:4I:332:VAL:HG13	2.30	0.59
2:5B:172:SER:HB3	2:5B:205:GLU:OE1	2.03	0.59
2:3I:235:GLY:HA2	2:3I:238:CYS:SG	2.42	0.58
1:4D:241:SER:OG	1:4D:250:VAL:O	2.19	0.58
1:4G:191:THR:OG1	1:4G:425:LEU:HD21	2.03	0.58
2:5I:103:LYS:HA	2:5I:107:THR:HG22	1.84	0.58
2:5I:267:LEU:CD2	2:5I:374:ILE:HD11	2.33	0.58
2:3D:172:SER:HB3	2:3D:205:GLU:OE1	2.03	0.58
2:3G:100:ASN:HB2	1:4G:257:THR:HG21	1.86	0.58
2:3H:397:TRP:CH2	1:4H:260:VAL:O	2.55	0.58
1:4B:60:LYS:CE	1:4C:282:TYR:CE2	2.86	0.58
1:4F:142:GLY:HA3	1:4F:183:GLU:HG2	1.85	0.58
1:4F:189:LEU:HD11	1:4F:418:PHE:CD1	2.37	0.58
2:3E:55:THR:HG21	2:3F:283:ALA:HA	1.84	0.58
1:2C:276:ILE:HG23	1:2C:280:LYS:HB2	1.85	0.58
1:2F:323:VAL:HG13	1:2F:355:ILE:HG23	1.84	0.58
2:3D:322:SER:OG	2:3D:325:GLU:OE2	2.22	0.58
1:4H:241:SER:OG	1:4H:250:VAL:O	2.18	0.58
1:2B:401:LYS:HE2	2:3B:344:TRP:CD2	2.39	0.58
2:3B:176:SER:HB2	1:4B:349:THR:HB	1.84	0.58
2:3E:165:GLU:OE2	2:3E:200:GLN:NE2	2.36	0.58
2:3E:178:THR:HA	1:4E:352:LYS:HD2	1.84	0.58
2:3H:55:THR:OG1	2:3I:280:GLN:O	2.21	0.58
1:4A:390:ARG:HB3	1:4A:390:ARG:HH21	1.67	0.58
1:4E:217:LEU:HD11	1:4E:275:ILE:HG22	1.85	0.58
2:5F:91:VAL:HG11	2:5F:116:VAL:HG22	1.86	0.58
1:2E:23:LEU:HD11	1:2E:361:THR:HG23	1.84	0.58
2:3A:220:PRO:HB3	2:3A:224:ASP:OD2	2.04	0.58
2:5G:237:THR:HG22	2:5G:250:LEU:HD11	1.86	0.58
2:5H:72:THR:HG23	2:5H:73:MET:HE2	1.86	0.58
1:2F:174:SER:OG	1:2F:177:VAL:O	2.19	0.58
2:3B:256:ASN:HD21	2:3B:350:LYS:HD3	1.68	0.58
2:3D:58:ARG:HH11	2:3E:280:GLN:HG3	1.67	0.58
1:4E:65:CYS:O	1:4E:91:GLN:NE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2B:60:LYS:HE2	1:2C:282:TYR:HD2	1.65	0.58
1:2F:175:PRO:HB3	1:2F:390:ARG:HD3	1.84	0.58
2:5G:156:ARG:HG2	2:5G:195:ASN:HB2	1.85	0.58
2:5H:165:GLU:OE2	2:5H:200:GLN:NE2	2.35	0.58
1:2C:89:PRO:HD2	1:2D:282:TYR:HD2	1.69	0.58
2:3H:179:VAL:CG1	1:4H:258:ASN:OD1	2.50	0.58
2:5E:248:SER:HA	2:5E:252:LYS:HG2	1.85	0.58
2:5I:267:LEU:HD21	2:5I:374:ILE:HD11	1.86	0.58
1:2D:57:GLY:H	1:2E:285:GLN:HB3	1.68	0.58
2:3D:98:GLY:HA2	1:4D:254:GLU:OE2	2.04	0.58
1:4A:60:LYS:HE2	1:4B:283:HIS:HD2	1.69	0.58
1:4C:76:ASP:HA	1:4C:79:ARG:HD2	1.85	0.58
1:4I:221:ARG:HG2	2:5I:325:GLU:OE1	2.04	0.58
2:5C:257:LEU:HD11	2:5C:368:VAL:HG23	1.85	0.58
2:3A:139:LEU:HD12	2:3A:170:PHE:HE1	1.68	0.57
2:3G:167:PHE:CD2	2:3G:233:MET:HG2	2.39	0.57
1:4F:309:HIS:NE2	1:4F:386:GLU:OE1	2.29	0.57
1:4H:417:GLU:HA	1:4H:420:GLU:HG3	1.86	0.57
1:2A:181:VAL:HG11	1:2A:404:PHE:CE1	2.39	0.57
2:3C:248:SER:HA	2:3C:252:LYS:HG3	1.86	0.57
1:4G:60:LYS:HD2	1:4H:283:HIS:HD2	1.68	0.57
2:5A:285:SER:N	2:5A:288:GLU:OE2	2.34	0.57
1:2D:96:LYS:HE2	2:3D:129:CYS:HB2	1.87	0.57
1:2F:101:ASN:HD22	2:3F:256:ASN:HD21	1.52	0.57
2:3B:286:VAL:CG2	2:3B:287:PRO:HD3	2.34	0.57
2:5H:149:THR:HG21	2:5H:188:SER:OG	2.04	0.57
1:2B:274:PRO:HD3	1:2B:291:ILE:HD11	1.87	0.57
2:3E:397:TRP:CZ2	1:4E:260:VAL:HG23	2.39	0.57
2:5D:12:CYS:SG	2:5D:138:SER:HB2	2.44	0.57
2:5D:54:ALA:O	2:5E:282:ARG:O	2.22	0.57
2:5D:54:ALA:HA	2:5E:283:ALA:CB	2.34	0.57
2:3H:165:GLU:OE2	2:3H:200:GLN:NE2	2.38	0.57
1:4A:57:GLY:H	1:4B:285:GLN:CG	2.13	0.57
2:5D:58:ARG:NE	2:5E:281:TYR:CD1	2.72	0.57
2:3A:66:MET:HG3	2:3A:116:VAL:HG21	1.87	0.57
1:4H:318:MET:HB2	1:4H:376:CYS:SG	2.45	0.57
2:5C:253:LEU:HD11	2:5C:368:VAL:HG21	1.85	0.57
1:2H:256:GLN:O	1:2H:260:VAL:HG22	2.04	0.57
1:4B:101:ASN:HB3	1:4B:182:VAL:HG11	1.85	0.57
1:2B:422:ARG:HH12	1:2B:426:ALA:HB2	1.70	0.57
1:2F:70:LEU:HD12	1:2F:145:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:178:SER:HB2	2:5A:347:ASN:OD1	2.05	0.57
2:5H:172:SER:OG	2:5H:205:GLU:OE2	2.23	0.57
2:3E:117:LEU:HD11	2:3E:154:LYS:HD3	1.86	0.57
1:4A:174:SER:HB2	1:4A:207:GLU:OE1	2.04	0.57
1:4A:223:THR:HG23	1:4A:225:THR:HG22	1.86	0.57
1:2D:178:SER:HB3	2:3D:347:ASN:ND2	2.20	0.56
1:2H:403:ALA:HA	2:3H:260:PHE:CE1	2.40	0.56
2:3F:175:VAL:HB	1:4F:329:ASN:OD1	2.04	0.56
1:4B:88:HIS:CE1	1:4C:283:HIS:HB2	2.39	0.56
2:5D:27:GLU:OE2	2:5D:241:ARG:NH1	2.35	0.56
2:3C:70:PRO:HD2	1:4C:2:ARG:NH2	2.19	0.56
2:3D:55:THR:HG1	2:3E:283:ALA:CA	2.07	0.56
1:4B:176:GLN:HB3	2:5B:331:LEU:CD1	2.35	0.56
1:4D:212:ILE:HG21	1:4D:275:ILE:HD11	1.87	0.56
1:4G:352:LYS:NZ	1:4G:353:CYS:O	2.37	0.56
2:5F:55:THR:HG23	2:5G:283:ALA:HA	1.87	0.56
1:2I:53:PHE:HB3	1:2I:61:HIS:HB3	1.87	0.56
1:2I:269:LEU:HD21	1:2I:384:ILE:HD11	1.87	0.56
2:3A:105:HIS:HD2	2:3A:150:LEU:HD12	1.69	0.56
2:3A:220:PRO:CD	1:4A:326:LYS:CE	2.55	0.56
2:3D:374:ILE:HD11	2:3D:422:TYR:CZ	2.39	0.56
2:3E:391:ARG:HD2	1:4E:346:TRP:CD1	2.40	0.56
1:4B:60:LYS:NZ	1:4C:282:TYR:HE2	1.96	0.56
1:4B:417:GLU:HA	1:4B:420:GLU:HG3	1.86	0.56
1:4C:184:PRO:HA	1:4C:391:MET:CE	2.35	0.56
1:4D:398:MET:HE2	2:5D:346:PRO:HD2	1.87	0.56
1:4E:30:ILE:HG22	1:4E:36:MET:HB3	1.86	0.56
1:4G:220:GLU:O	2:5G:324:LYS:HD3	2.04	0.56
1:4G:309:HIS:NE2	1:4G:386:GLU:OE1	2.39	0.56
1:4G:407:TRP:CE3	2:5G:255:VAL:HA	2.41	0.56
2:5C:66:MET:HG2	2:5C:147:MET:HE1	1.86	0.56
2:5C:248:SER:HA	2:5C:252:LYS:HG2	1.87	0.56
2:5I:276:ARG:NH2	2:5I:279:GLN:OE1	2.38	0.56
1:2H:33:ASP:O	1:2H:60:LYS:NZ	2.37	0.56
2:3B:284:LEU:HD23	2:3B:362:LYS:HG2	1.88	0.56
2:3D:54:ALA:O	2:3E:282:ARG:O	2.22	0.56
2:3D:54:ALA:CB	2:3E:281:TYR:O	2.53	0.56
2:3G:282:ARG:NH1	2:3G:288:GLU:OE2	2.38	0.56
1:4D:56:THR:CB	1:4E:283:HIS:O	2.53	0.56
1:4I:68:LEU:HD12	1:4I:153:LEU:HD11	1.88	0.56
2:5C:153:SER:HB2	2:5C:191:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5D:55:THR:OG1	2:5E:283:ALA:HA	2.05	0.56
2:5D:169:VAL:HG12	2:5D:202:ILE:HB	1.88	0.56
2:5H:380:ARG:HH11	2:5H:381:VAL:HG23	1.70	0.56
1:4E:298:PRO:HB3	1:4E:307:PRO:HD2	1.86	0.56
1:4H:210:TYR:CE1	2:5H:324:LYS:HG2	2.40	0.56
2:5I:383:ASP:HA	2:5I:386:THR:HG22	1.88	0.56
1:2H:202:VAL:HA	1:2H:268:MET:HB2	1.88	0.56
2:3H:200:GLN:HB3	2:3H:266:PHE:HB2	1.86	0.56
1:2G:287:SER:HA	1:2G:373:ARG:HH21	1.70	0.56
2:3H:397:TRP:HH2	1:4H:260:VAL:HG23	1.71	0.56
1:2E:207:GLU:HG3	1:2E:304:LYS:HG3	1.88	0.56
1:2I:33:ASP:O	1:2I:60:LYS:NZ	2.39	0.56
2:3B:397:TRP:HZ2	1:4B:260:VAL:CG2	2.19	0.56
2:3C:86:ARG:CD	2:3D:281:TYR:HD1	2.09	0.56
1:4A:60:LYS:HD2	1:4B:283:HIS:CD2	2.40	0.56
1:4B:180:ALA:HA	2:5B:350:LYS:HE3	1.86	0.56
1:4G:158:SER:OG	1:4G:166:LYS:NZ	2.39	0.56
2:5B:236:VAL:O	2:5B:316:MET:HE1	2.06	0.56
2:3G:220:PRO:HD2	1:4G:326:LYS:HD3	1.87	0.56
2:3H:391:ARG:HD2	1:4H:346:TRP:CD2	2.40	0.56
1:4H:103:PHE:H	1:4H:408:TYR:HE1	1.54	0.56
2:5B:1:MET:N	2:5B:128:ASP:OD2	2.36	0.56
2:5F:14:ASN:ND2	2:5F:67:ASP:OD1	2.39	0.56
1:2C:212:ILE:HD11	1:2C:300:SER:HA	1.88	0.56
1:2G:309:HIS:NE2	1:2G:386:GLU:OE1	2.39	0.56
2:3B:64:ILE:HD12	2:3B:119:VAL:HG12	1.88	0.56
2:3G:1:MET:N	2:3G:128:ASP:OD2	2.38	0.56
1:4C:1:MET:N	1:4C:3:GLU:OE2	2.34	0.56
2:5C:213:ARG:HA	2:5C:213:ARG:HE	1.71	0.56
1:2C:269:LEU:HD22	1:2C:384:ILE:HD11	1.87	0.55
2:3D:83:GLN:O	2:3E:281:TYR:CE2	2.59	0.55
1:2B:215:ARG:NH1	1:2B:216:ASN:OD1	2.39	0.55
1:2H:10:GLY:HA2	1:2H:145:THR:HG23	1.87	0.55
2:3G:177:ASP:OD2	2:3G:178:THR:HG23	2.06	0.55
1:4H:10:GLY:HA2	1:4H:145:THR:HG23	1.87	0.55
2:5D:267:LEU:HD11	2:5D:374:ILE:HG23	1.89	0.55
2:5G:256:ASN:HD21	2:5G:350:LYS:HD3	1.71	0.55
1:2E:241:SER:OG	1:2E:250:VAL:O	2.17	0.55
2:3E:55:THR:HB	2:3F:283:ALA:CA	2.32	0.55
1:4B:258:ASN:CB	1:4B:352:LYS:HE3	2.34	0.55
1:4D:298:PRO:HB3	1:4D:307:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5C:284:LEU:HD21	2:5C:363:MET:HB2	1.88	0.55
2:5G:55:THR:HG23	2:5H:283:ALA:HB2	1.89	0.55
1:2A:181:VAL:CG2	2:3A:350:LYS:HZ1	2.10	0.55
1:2B:417:GLU:HA	1:2B:420:GLU:HG3	1.87	0.55
1:2D:222:PRO:HD2	2:3D:324:LYS:CE	2.37	0.55
1:2H:2:ARG:NH2	1:2H:133:GLN:OE1	2.40	0.55
2:3H:208:TYR:HE2	1:4H:329:ASN:ND2	2.03	0.55
1:4A:151:CYS:SG	1:4A:193:SER:OG	2.44	0.55
1:4A:209:ILE:HB	1:4A:227:LEU:HD13	1.89	0.55
1:4A:339:ARG:O	1:4A:342:GLN:NE2	2.39	0.55
2:5C:267:LEU:HD21	2:5C:374:ILE:HG12	1.88	0.55
2:5D:55:THR:OG1	2:5E:283:ALA:C	2.42	0.55
1:2B:221:ARG:NE	2:3B:322:SER:OG	2.40	0.55
1:2C:121:ARG:HH22	1:2D:283:HIS:CE1	2.24	0.55
1:2G:230:LEU:CD2	1:2G:302:MET:CE	2.85	0.55
1:2H:103:PHE:H	1:2H:408:TYR:HE1	1.55	0.55
1:2I:73:THR:HG22	2:3I:46:ARG:HE	1.70	0.55
2:5H:282:ARG:NH2	2:5H:284:LEU:HD13	2.21	0.55
1:2A:80:THR:HA	1:2A:84:ARG:HE	1.71	0.55
1:2D:60:LYS:CE	1:2E:283:HIS:CG	2.90	0.55
1:2E:276:ILE:HD11	1:2E:286:LEU:HD11	1.89	0.55
2:3D:169:VAL:HG12	2:3D:202:ILE:HB	1.88	0.55
1:4G:186:ASN:OD1	1:4G:408:TYR:OH	2.23	0.55
1:4H:398:MET:HE2	2:5H:345:ILE:HD13	1.89	0.55
2:5G:249:ASP:H	2:5G:252:LYS:HG2	1.70	0.55
1:2H:222:PRO:HG2	2:3H:324:LYS:HZ1	1.70	0.55
1:4H:51:THR:HG21	1:4H:243:ARG:HG2	1.88	0.55
1:4H:219:ILE:HG22	1:4H:222:PRO:HD3	1.88	0.55
1:2B:221:ARG:NH1	2:3B:324:LYS:HB3	2.21	0.55
1:2D:223:THR:HG23	1:2D:225:THR:HG22	1.88	0.55
1:2G:398:MET:HE1	2:3G:345:ILE:HG23	1.89	0.55
2:3A:100:ASN:HB3	2:3A:103:LYS:HG2	1.88	0.55
2:3C:215:LEU:HB3	2:3C:217:LEU:HD13	1.89	0.55
2:3I:11:GLN:NE2	1:4I:248:LEU:HD12	2.21	0.55
1:2B:223:THR:HG23	1:2B:225:THR:HG22	1.88	0.55
1:2C:88:HIS:CE1	1:2D:283:HIS:HB2	2.42	0.55
1:2D:402:ARG:HG3	1:2D:405:VAL:HG21	1.88	0.55
1:2H:231:ILE:O	1:2H:234:VAL:HG12	2.07	0.55
2:3G:55:THR:CG2	2:3H:283:ALA:CA	2.78	0.55
2:5E:372:THR:HA	2:5E:422:TYR:CD2	2.42	0.55
1:2D:298:PRO:HB3	1:2D:307:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2G:60:LYS:HD3	1:2H:283:HIS:CD2	2.35	0.55
2:3A:293:MET:SD	2:3A:367:PHE:HB2	2.47	0.55
2:3A:349:MET:C	2:3A:350:LYS:HD2	2.27	0.55
2:3B:172:SER:HB2	2:3B:205:GLU:HG2	1.89	0.55
1:4C:73:THR:HA	2:5C:46:ARG:NH1	2.22	0.55
1:4C:242:LEU:HD11	1:4C:252:VAL:HG23	1.89	0.55
1:2C:259:LEU:HD21	1:2C:316:CYS:HB2	1.90	0.54
2:3D:58:ARG:CD	2:3E:280:GLN:O	2.56	0.54
1:4B:339:ARG:NH2	1:4B:342:GLN:OE1	2.40	0.54
1:2I:213:CYS:SG	1:2I:222:PRO:HG3	2.48	0.54
1:4A:8:HIS:CD2	1:4A:17:GLY:HA3	2.42	0.54
1:4I:250:VAL:HG11	1:4I:318:MET:CE	2.38	0.54
2:5H:207:LEU:HB3	2:5H:225:LEU:HD12	1.89	0.54
1:2B:174:SER:OG	1:2B:177:VAL:O	2.21	0.54
1:2E:101:ASN:OD1	2:3E:252:LYS:NZ	2.40	0.54
1:2E:199:ASP:OD2	1:2E:256:GLN:NE2	2.40	0.54
1:2H:386:GLU:O	1:2H:390:ARG:HG2	2.07	0.54
2:3A:374:ILE:O	2:3A:374:ILE:HG22	2.07	0.54
2:5D:12:CYS:SG	2:5D:13:GLY:N	2.80	0.54
2:3E:107:THR:HG21	2:3E:401:GLU:HB2	1.89	0.54
2:3F:172:SER:HB3	2:3F:205:GLU:OE1	2.07	0.54
1:4C:311:LYS:NZ	1:4C:342:GLN:OE1	2.41	0.54
1:4D:60:LYS:HZ2	1:4E:283:HIS:CD2	2.24	0.54
1:4D:105:ARG:O	1:4D:110:ILE:HG22	2.07	0.54
1:4I:422:ARG:HH12	1:4I:426:ALA:HB2	1.72	0.54
2:5E:372:THR:HA	2:5E:422:TYR:HD2	1.72	0.54
2:5H:256:ASN:HD22	2:5H:350:LYS:HD2	1.73	0.54
1:2B:241:SER:HB2	1:2B:249:ASN:HB2	1.89	0.54
2:3D:244:GLY:HA2	2:3D:355:ASP:OD1	2.08	0.54
2:3F:55:THR:CG2	2:3G:282:ARG:O	2.56	0.54
2:3I:383:ASP:HA	2:3I:386:THR:HG22	1.90	0.54
1:4C:178:SER:OG	2:5C:347:ASN:ND2	2.40	0.54
1:4B:181:VAL:H	2:5B:350:LYS:CE	2.19	0.54
2:5A:262:ARG:NH2	2:5A:421:GLU:OE1	2.40	0.54
1:2A:96:LYS:NZ	2:3A:129:CYS:SG	2.80	0.54
1:2A:221:ARG:HB2	2:3A:322:SER:CB	2.37	0.54
1:2C:89:PRO:HD2	1:2D:282:TYR:CD2	2.43	0.54
2:3B:179:VAL:N	1:4B:352:LYS:HZ1	1.96	0.54
2:3D:66:MET:HE1	2:3D:151:LEU:HD22	1.88	0.54
2:3G:135:ILE:HG12	2:3G:166:THR:HG22	1.89	0.54
2:5H:192:LEU:HD21	2:5H:199:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2G:141:VAL:HG11	1:2G:172:TRP:CE3	2.42	0.54
2:3E:91:VAL:HG21	2:3E:116:VAL:HG22	1.90	0.54
1:4I:271:SER:HB2	1:4I:301:MET:HE1	1.90	0.54
2:5A:43:GLN:HA	2:5A:242:PHE:HE1	1.73	0.54
2:3B:1:MET:N	2:3B:128:ASP:OD2	2.38	0.54
2:3F:67:ASP:OD2	2:3F:72:THR:OG1	2.26	0.54
1:4E:220:GLU:O	2:5E:324:LYS:HE2	2.08	0.54
1:2H:338:LYS:HZ3	1:2H:339:ARG:H	1.56	0.54
2:3A:156:ARG:HH22	2:3A:197:ASP:HB2	1.73	0.54
2:3B:209:ASP:CG	2:3B:213:ARG:HH21	2.10	0.54
2:3F:11:GLN:HE22	1:4F:248:LEU:HA	1.73	0.54
2:5D:107:THR:OG1	2:5D:108:GLU:OE1	2.26	0.54
1:2I:50:ASN:O	1:2I:64:ARG:NH2	2.41	0.53
2:3B:178:THR:CA	1:4B:352:LYS:NZ	2.67	0.53
2:5F:282:ARG:NH1	2:5F:288:GLU:OE2	2.41	0.53
1:2A:301:MET:CE	1:2A:307:PRO:HG3	2.38	0.53
1:2E:178:SER:OG	2:3E:347:ASN:ND2	2.32	0.53
1:4D:85:HIS:HB3	1:4E:283:HIS:NE2	2.22	0.53
1:2A:252:VAL:HA	1:2A:255:PHE:HD2	1.72	0.53
1:2C:318:MET:HE1	1:2C:354:GLY:HA3	1.89	0.53
1:2G:181:VAL:CG1	2:3G:256:ASN:HB2	2.38	0.53
2:3F:282:ARG:NH1	2:3F:292:GLN:OE1	2.41	0.53
1:4B:60:LYS:HZ2	1:4C:282:TYR:HE2	1.46	0.53
1:4C:223:THR:HG23	1:4C:225:THR:HG22	1.90	0.53
1:2B:177:VAL:HG13	2:3B:327:ASP:OD1	2.08	0.53
1:2C:121:ARG:CZ	1:2D:283:HIS:CE1	2.91	0.53
1:2E:217:LEU:HD11	1:2E:275:ILE:CG2	2.38	0.53
1:2G:200:VAL:HG23	1:2G:268:MET:HE1	1.89	0.53
2:3B:87:PRO:HD3	2:3C:281:TYR:OH	2.09	0.53
1:4G:101:ASN:HB3	1:4G:182:VAL:HG21	1.90	0.53
2:5C:87:PRO:C	2:5D:281:TYR:OH	2.42	0.53
1:2I:258:ASN:HB3	1:2I:352:LYS:HG3	1.91	0.53
1:4C:259:LEU:HD21	1:4C:316:CYS:HB2	1.90	0.53
2:5D:8:GLN:NE2	2:5D:17:GLY:HA3	2.24	0.53
1:2D:177:VAL:HG13	2:3D:327:ASP:HB2	1.91	0.53
2:3I:284:LEU:HD23	2:3I:362:LYS:HG2	1.91	0.53
1:4F:178:SER:CB	2:5F:347:ASN:ND2	2.57	0.53
1:4G:398:MET:HE1	2:5G:345:ILE:HG23	1.89	0.53
2:5F:67:ASP:OD2	2:5F:72:THR:OG1	2.27	0.53
2:5F:282:ARG:NH1	2:5F:292:GLN:OE1	2.41	0.53
1:2G:76:ASP:OD2	2:3G:46:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3A:244:GLY:HA2	2:3A:355:ASP:HB2	1.90	0.53
2:5E:127:CYS:SG	2:5E:128:ASP:N	2.75	0.53
2:5G:135:ILE:HB	2:5G:166:THR:HG22	1.89	0.53
1:2C:178:SER:HB2	2:3C:347:ASN:HD22	1.74	0.53
1:2D:241:SER:OG	1:2D:250:VAL:O	2.20	0.53
2:3A:10:GLY:HA2	2:3A:143:THR:HG23	1.91	0.53
2:3G:248:SER:HA	2:3G:252:LYS:HE3	1.91	0.53
2:3H:1:MET:N	2:3H:128:ASP:OD2	2.40	0.53
2:3H:253:LEU:HD11	2:3H:368:VAL:HG21	1.91	0.53
2:3I:396:HIS:HA	2:3I:399:THR:HG22	1.91	0.53
1:4I:178:SER:HB3	2:5I:347:ASN:HD22	1.74	0.53
2:5A:113:ILE:HA	2:5A:116:VAL:HG12	1.91	0.53
2:5A:326:VAL:O	2:5A:330:MET:HE1	2.09	0.53
1:2C:89:PRO:CD	1:2D:282:TYR:CD2	2.92	0.53
2:3A:113:ILE:HA	2:3A:116:VAL:HG12	1.91	0.53
1:4A:181:VAL:HG22	2:5A:347:ASN:O	2.09	0.53
1:4A:276:ILE:HD12	1:4A:281:ALA:HA	1.89	0.53
2:5B:100:ASN:HB3	2:5B:103:LYS:HG2	1.89	0.53
2:5D:12:CYS:SG	2:5D:138:SER:CB	2.97	0.53
1:2H:241:SER:OG	1:2H:250:VAL:O	2.18	0.53
1:2I:234:VAL:HG21	1:2I:302:MET:HE1	1.90	0.53
1:4B:177:VAL:HG11	2:5B:327:ASP:HB3	1.91	0.53
1:4D:5:ILE:HD12	1:4D:125:LEU:HG	1.91	0.53
2:5B:286:VAL:CG2	2:5B:287:PRO:HD3	2.35	0.53
2:5D:313:ALA:HB3	2:5D:349:MET:HG2	1.90	0.53
1:2A:396:ASP:OD1	1:2A:422:ARG:NH1	2.42	0.52
1:2H:258:ASN:O	1:2H:258:ASN:ND2	2.36	0.52
2:3G:7:VAL:HB	2:3G:135:ILE:HG22	1.89	0.52
2:3I:267:LEU:HB3	2:3I:299:MET:CE	2.39	0.52
1:4B:181:VAL:HG13	2:5B:350:LYS:HZ1	1.67	0.52
2:5E:274:THR:OG1	2:5E:279:GLN:OE1	2.27	0.52
2:5F:238:CYS:SG	2:5F:318:ARG:NE	2.82	0.52
1:2A:180:ALA:HB3	1:2A:183:GLU:HG2	1.90	0.52
1:2B:207:GLU:OE1	1:2B:304:LYS:HG2	2.09	0.52
1:2G:23:LEU:HD23	1:2G:27:GLU:HG3	1.89	0.52
1:2G:152:LEU:O	1:2G:156:ARG:HG2	2.10	0.52
2:3A:330:MET:SD	2:3A:349:MET:HG3	2.49	0.52
2:3B:113:ILE:HA	2:3B:116:VAL:HG12	1.91	0.52
2:3D:334:GLN:HE21	2:3D:349:MET:HG2	1.74	0.52
2:3G:55:THR:CG2	2:3H:283:ALA:CB	2.87	0.52
1:4A:65:CYS:O	1:4A:91:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:102:ASN:OD1	2:5A:255:VAL:HG21	2.09	0.52
1:4D:57:GLY:N	1:4E:285:GLN:CA	2.73	0.52
1:4E:97:GLU:OE2	2:5E:2:ARG:HG2	2.09	0.52
2:5I:66:MET:SD	2:5I:116:VAL:HG11	2.49	0.52
1:2G:407:TRP:CZ3	2:3G:255:VAL:HG22	2.44	0.52
2:3F:139:LEU:CD1	2:3F:168:SER:HB2	2.36	0.52
1:4B:328:VAL:HG11	1:4B:353:CYS:SG	2.49	0.52
1:4F:168:ASN:ND2	1:4F:170:CYS:SG	2.82	0.52
1:4G:23:LEU:HD11	1:4G:361:THR:HG23	1.90	0.52
2:5D:10:GLY:HA2	2:5D:143:THR:HG23	1.90	0.52
2:5D:257:LEU:HD21	2:5D:314:SER:HB2	1.90	0.52
2:5D:311:LEU:HD12	2:5D:342:VAL:HG11	1.92	0.52
2:5F:248:SER:HA	2:5F:252:LYS:HG3	1.91	0.52
2:5I:10:GLY:HA2	2:5I:143:THR:HG23	1.91	0.52
1:2B:88:HIS:CD2	1:2C:283:HIS:CB	2.92	0.52
1:2B:422:ARG:NH1	1:2B:426:ALA:HB2	2.24	0.52
1:2E:75:VAL:HG11	1:2E:94:SER:HB3	1.92	0.52
1:2I:407:TRP:CZ2	2:3I:258:ILE:HD11	2.45	0.52
2:3B:207:LEU:HB3	2:3B:225:LEU:HD22	1.91	0.52
2:3G:354:CYS:SG	2:3G:355:ASP:N	2.83	0.52
2:3H:211:CYS:SG	2:3H:220:PRO:HB3	2.50	0.52
1:4I:100:ALA:HA	2:5I:252:LYS:HE3	1.92	0.52
1:2C:223:THR:HG23	1:2C:225:THR:HG22	1.90	0.52
1:2D:56:THR:HA	1:2E:285:GLN:CB	2.35	0.52
1:2G:60:LYS:CE	1:2H:283:HIS:HD2	2.23	0.52
2:3E:55:THR:HG23	2:3E:55:THR:O	2.10	0.52
2:3I:311:LEU:HD12	2:3I:342:VAL:HG11	1.91	0.52
1:4A:101:ASN:HB3	1:4A:182:VAL:HG21	1.92	0.52
2:5D:98:GLY:H	2:5D:103:LYS:HE2	1.73	0.52
2:5I:165:GLU:OE2	2:5I:200:GLN:NE2	2.41	0.52
2:5I:311:LEU:HD12	2:5I:342:VAL:HG11	1.92	0.52
1:2F:392:ASP:OD1	1:2F:422:ARG:NE	2.43	0.52
1:2G:241:SER:HB2	1:2G:249:ASN:HB2	1.92	0.52
2:3A:55:THR:OG1	2:3B:282:ARG:O	2.28	0.52
2:3G:12:CYS:HB3	2:3G:138:SER:HB3	1.92	0.52
1:4B:76:ASP:OD1	1:4B:79:ARG:NH2	2.42	0.52
1:4G:204:LEU:HD13	1:4G:231:ILE:HD12	1.91	0.52
1:4H:370:LYS:HG3	1:4H:370:LYS:O	2.10	0.52
1:4I:250:VAL:HG11	1:4I:318:MET:HE3	1.91	0.52
2:5A:207:LEU:CD2	2:5A:225:LEU:HD22	2.39	0.52
2:5D:58:ARG:NH2	2:5E:281:TYR:HE1	2.00	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2E:30:ILE:HG22	1:2E:36:MET:HB3	1.92	0.52
2:3A:257:LEU:O	2:3A:312:THR:HG21	2.09	0.52
2:3H:248:SER:HA	2:3H:252:LYS:HG3	1.92	0.52
2:3H:249:ASP:H	2:3H:252:LYS:HB2	1.75	0.52
2:3I:397:TRP:CZ2	1:4I:256:GLN:HB2	2.44	0.52
1:4B:209:ILE:HG22	1:4B:227:LEU:HD22	1.92	0.52
1:4B:217:LEU:HD23	1:4B:217:LEU:O	2.08	0.52
1:4E:138:PHE:CZ	1:4E:235:ILE:HD13	2.44	0.52
2:5H:181:GLU:HG3	2:5H:182:PRO:HD3	1.91	0.52
2:5I:313:ALA:HB3	2:5I:349:MET:HE1	1.92	0.52
1:2B:132:LEU:O	1:2B:164:LYS:NZ	2.43	0.52
1:2D:85:HIS:HB3	1:2E:283:HIS:HE2	1.74	0.52
1:4B:192:HIS:ND1	1:4B:424:ASP:OD2	2.43	0.52
1:4E:221:ARG:CG	2:5E:322:SER:CB	2.75	0.52
1:4G:238:LEU:HD13	1:4G:318:MET:HE1	1.91	0.52
2:5A:16:ILE:HD11	2:5A:229:VAL:HG11	1.92	0.52
1:2E:298:PRO:HB3	1:2E:307:PRO:HD2	1.90	0.52
2:3A:203:ASP:OD2	2:3A:205:GLU:HG3	2.10	0.52
1:4F:223:THR:HG23	1:4F:225:THR:HG22	1.90	0.52
2:5D:374:ILE:HD11	2:5D:422:TYR:CZ	2.45	0.52
2:5E:125:GLU:OE1	2:5F:291:GLN:NE2	2.42	0.52
1:2D:309:HIS:NE2	1:2D:386:GLU:OE1	2.43	0.52
1:2E:11:GLN:NE2	2:3E:245:GLN:O	2.42	0.52
1:2E:98:ASP:O	1:2E:105:ARG:NH2	2.32	0.52
1:2G:236:SER:O	1:2G:243:ARG:NH2	2.42	0.52
1:2H:398:MET:CE	2:3H:346:PRO:HD2	2.40	0.52
2:3E:397:TRP:CH2	1:4E:260:VAL:O	2.63	0.52
2:3F:354:CYS:SG	2:3F:355:ASP:N	2.83	0.52
2:3H:222:TYR:HD1	2:3H:225:LEU:HD12	1.74	0.52
1:4H:306:ASP:OD1	1:4H:308:ARG:NH1	2.43	0.52
2:5C:88:ASP:CG	2:5D:281:TYR:CE2	2.83	0.52
2:5E:16:ILE:HD11	2:5E:229:VAL:HG11	1.92	0.52
2:5G:55:THR:HG23	2:5H:283:ALA:CA	2.40	0.52
2:3D:200:GLN:HG2	2:3D:268:ILE:HD11	1.93	0.51
2:5B:309:ARG:H	2:5B:372:THR:HG22	1.75	0.51
1:2I:73:THR:HG22	2:3I:46:ARG:NE	2.26	0.51
1:4A:260:VAL:HG23	1:4A:260:VAL:O	2.10	0.51
2:5B:267:LEU:CD1	2:5B:301:CYS:HB3	2.40	0.51
2:5G:109:GLY:O	2:5G:113:ILE:HG12	2.09	0.51
2:5H:158:GLU:N	2:5H:158:GLU:OE1	2.43	0.51
1:2C:269:LEU:CD2	1:2C:384:ILE:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2H:223:THR:HG23	1:2H:225:THR:HG22	1.92	0.51
2:3B:109:GLY:O	2:3B:113:ILE:HG12	2.09	0.51
2:3H:16:ILE:CG2	2:3H:136:THR:HG21	2.41	0.51
2:5A:258:ILE:O	2:5A:258:ILE:HG13	2.10	0.51
2:5D:54:ALA:O	2:5E:282:ARG:C	2.48	0.51
2:5D:135:ILE:HG22	2:5D:137:HIS:HD2	1.74	0.51
2:5G:354:CYS:SG	2:5G:355:ASP:N	2.84	0.51
2:5I:284:LEU:CD2	2:5I:363:MET:HG2	2.40	0.51
1:2F:98:ASP:O	1:2F:105:ARG:NH2	2.43	0.51
1:4A:407:TRP:HZ2	2:5A:258:ILE:HD11	1.74	0.51
2:5B:66:MET:HG2	2:5B:116:VAL:HG21	1.92	0.51
2:5B:276:ARG:NH2	2:5B:279:GLN:OE1	2.35	0.51
2:5C:309:ARG:H	2:5C:372:THR:HG22	1.76	0.51
1:2F:28:HIS:HE1	1:2F:243:ARG:HH11	1.58	0.51
1:2G:60:LYS:HZ3	1:2H:283:HIS:CD2	2.27	0.51
1:2I:76:ASP:HA	1:2I:79:ARG:HD2	1.92	0.51
2:3C:289:LEU:HD12	2:3C:365:VAL:HG12	1.92	0.51
2:3G:350:LYS:NZ	2:3G:352:SER:OG	2.43	0.51
1:4F:177:VAL:HB	2:5F:327:ASP:OD2	2.11	0.51
2:5D:83:GLN:O	2:5E:281:TYR:CZ	2.63	0.51
2:5F:100:ASN:HB3	2:5F:103:LYS:HG2	1.92	0.51
2:5G:164:MET:N	2:5G:197:ASP:OD2	2.39	0.51
1:2G:254:GLU:N	1:2G:254:GLU:OE2	2.44	0.51
2:3D:135:ILE:HB	2:3D:166:THR:HG22	1.91	0.51
1:4F:107:HIS:HE2	1:4F:151:CYS:HG	1.58	0.51
1:4H:222:PRO:HD2	2:5H:324:LYS:HZ1	1.75	0.51
2:5A:100:ASN:HB3	2:5A:103:LYS:HG2	1.92	0.51
1:2F:76:ASP:OD2	2:3F:46:ARG:NH2	2.44	0.51
1:2G:70:LEU:HD13	1:2G:95:GLY:HA3	1.92	0.51
2:3B:336:LYS:HE2	2:3B:336:LYS:HA	1.93	0.51
2:3C:72:THR:HG23	2:3C:73:MET:HE2	1.93	0.51
2:3I:404:ASP:OD1	2:3I:405:GLU:N	2.43	0.51
1:4E:105:ARG:HH12	2:5E:251:ARG:CD	2.23	0.51
1:4I:178:SER:CB	2:5I:347:ASN:ND2	2.73	0.51
2:5A:262:ARG:HH21	2:5A:421:GLU:CD	2.14	0.51
2:5A:313:ALA:HB1	2:5A:367:PHE:CE1	2.46	0.51
2:5B:55:THR:O	2:5B:55:THR:HG23	2.10	0.51
2:5E:96:GLY:N	2:5E:108:GLU:OE2	2.44	0.51
2:5H:100:ASN:HB3	2:5H:103:LYS:HG2	1.91	0.51
2:5I:55:THR:HG23	2:5I:55:THR:O	2.11	0.51
1:2A:275:ILE:HD12	1:2A:275:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2G:71:GLU:HG2	1:2G:73:THR:HG22	1.93	0.51
1:2G:230:LEU:HD23	1:2G:302:MET:CE	2.40	0.51
2:3A:55:THR:CG2	2:3B:283:ALA:HA	2.38	0.51
2:3C:55:THR:HG23	2:3C:55:THR:O	2.11	0.51
2:3I:55:THR:HG23	2:3I:55:THR:O	2.11	0.51
1:4A:239:THR:OG1	1:4A:243:ARG:NH1	2.44	0.51
1:4E:309:HIS:NE2	1:4E:386:GLU:OE1	2.44	0.51
2:5B:28:HIS:HA	2:5B:43:GLN:HG2	1.91	0.51
2:5C:87:PRO:HG2	2:5D:281:TYR:HE2	1.76	0.51
2:5H:211:CYS:SG	2:5H:220:PRO:HB3	2.51	0.51
1:2C:100:ALA:HA	2:3C:252:LYS:CD	2.39	0.51
1:2H:260:VAL:HG23	1:2H:260:VAL:O	2.09	0.51
2:3E:95:THR:OG1	2:3E:108:GLU:OE1	2.28	0.51
2:3F:208:TYR:CD1	1:4F:326:LYS:CD	2.93	0.51
1:4F:241:SER:HB2	1:4F:249:ASN:HB2	1.92	0.51
1:4G:236:SER:O	1:4G:243:ARG:NH2	2.44	0.51
1:4H:173:PRO:HG3	1:4H:183:GLU:OE2	2.11	0.51
2:5G:6:HIS:HD1	2:5G:21:TRP:HE1	1.59	0.51
2:5G:248:SER:HA	2:5G:252:LYS:HD3	1.92	0.51
1:2A:105:ARG:HH12	2:3A:251:ARG:CD	2.24	0.51
1:2H:176:GLN:CB	2:3H:331:LEU:HD11	2.37	0.51
2:3A:208:TYR:CE1	1:4A:326:LYS:HB3	2.46	0.51
2:3C:10:GLY:O	2:3C:14:ASN:ND2	2.44	0.51
2:5A:55:THR:OG1	2:5B:282:ARG:O	2.29	0.51
2:5F:53:GLU:OE2	2:5F:54:ALA:N	2.43	0.51
1:2D:181:VAL:H	2:3D:256:ASN:ND2	2.09	0.50
1:2E:4:VAL:HG21	1:2E:136:LEU:HD13	1.93	0.50
2:3A:55:THR:CG2	2:3B:283:ALA:CA	2.87	0.50
1:4A:93:ILE:HG21	1:4A:114:ILE:HG23	1.93	0.50
1:4E:265:ILE:HD11	1:4E:435:VAL:HG21	1.93	0.50
2:5A:19:LYS:NZ	2:5A:223:GLY:O	2.44	0.50
2:5H:253:LEU:HD11	2:5H:368:VAL:HG21	1.92	0.50
1:2A:181:VAL:HG11	1:2A:404:PHE:CZ	2.47	0.50
2:3C:122:LYS:HG2	2:3D:281:TYR:OH	2.11	0.50
2:3G:207:LEU:HB3	2:3G:225:LEU:HD12	1.93	0.50
2:3H:329:GLN:OE1	2:3H:332:ASN:ND2	2.43	0.50
1:4D:173:PRO:HB3	1:4D:183:GLU:OE2	2.11	0.50
2:5A:180:VAL:O	2:5A:184:ASN:ND2	2.45	0.50
2:5E:55:THR:O	2:5E:55:THR:HG23	2.11	0.50
2:5F:311:LEU:HD12	2:5F:342:VAL:HG11	1.93	0.50
1:2B:221:ARG:HH12	2:3B:324:LYS:H	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3D:198:GLU:OE1	2:3D:254:ALA:HB2	2.12	0.50
2:3H:135:ILE:HG22	2:3H:137:HIS:HD2	1.76	0.50
1:4B:174:SER:OG	1:4B:177:VAL:O	2.23	0.50
1:4C:241:SER:OG	1:4C:249:ASN:HB2	2.11	0.50
2:5A:55:THR:HG21	2:5B:283:ALA:CB	2.35	0.50
2:5C:87:PRO:HG2	2:5D:281:TYR:CE2	2.46	0.50
2:5D:248:SER:HA	2:5D:252:LYS:HD2	1.93	0.50
2:5E:64:ILE:HD12	2:5E:119:VAL:HG12	1.92	0.50
1:2A:53:PHE:HB3	1:2A:61:HIS:HB3	1.92	0.50
1:2B:100:ALA:O	2:3B:255:VAL:HG11	2.12	0.50
1:2B:338:LYS:NZ	1:2B:341:ILE:HG12	2.25	0.50
1:2C:105:ARG:HH12	2:3C:251:ARG:HD3	1.77	0.50
1:2I:222:PRO:HD2	2:3I:324:LYS:HG2	1.92	0.50
1:2I:408:TYR:HB3	1:2I:413:MET:HE2	1.93	0.50
2:3C:172:SER:HB3	2:3C:205:GLU:HG2	1.93	0.50
2:3D:255:VAL:HG23	2:3D:256:ASN:OD1	2.11	0.50
2:3E:6:HIS:HD1	2:3E:21:TRP:HE1	1.59	0.50
2:3E:175:VAL:CG2	1:4E:329:ASN:OD1	2.58	0.50
2:3G:207:LEU:HG	2:3G:228:LEU:HD11	1.92	0.50
1:4D:56:THR:HA	1:4E:285:GLN:N	2.26	0.50
1:4F:370:LYS:NZ	1:4F:372:MET:CE	2.74	0.50
1:4G:53:PHE:HB3	1:4G:61:HIS:HB3	1.94	0.50
2:5D:383:ASP:HA	2:5D:386:THR:HG22	1.92	0.50
2:5H:175:VAL:HG12	2:5H:205:GLU:OE2	2.11	0.50
1:2E:101:ASN:CG	2:3E:252:LYS:NZ	2.65	0.50
1:2G:401:LYS:HD2	2:3G:344:TRP:CZ3	2.47	0.50
2:3F:100:ASN:HB3	2:3F:103:LYS:HG2	1.93	0.50
2:3G:109:GLY:O	2:3G:113:ILE:HG12	2.11	0.50
1:4B:320:ARG:HG3	1:4B:358:GLN:O	2.11	0.50
1:4I:177:VAL:HB	2:5I:327:ASP:CG	2.32	0.50
2:5B:86:ARG:HA	2:5C:281:TYR:CZ	2.46	0.50
2:5C:55:THR:HG23	2:5C:55:THR:O	2.10	0.50
2:5F:334:GLN:OE1	2:5F:349:MET:HB3	2.12	0.50
2:5H:337:ASN:HB3	2:5H:340:TYR:HB2	1.93	0.50
1:2G:175:PRO:HG3	1:2G:304:LYS:HG2	1.93	0.50
2:5C:374:ILE:O	2:5C:374:ILE:HG22	2.11	0.50
2:5G:262:ARG:NH1	2:5G:421:GLU:OE2	2.45	0.50
1:2A:275:ILE:HG23	1:2A:368:LEU:HD21	1.93	0.50
1:2D:123:ARG:NH1	1:2D:160:ASP:OD2	2.32	0.50
1:2E:250:VAL:HG11	1:2E:318:MET:HE1	1.94	0.50
1:2G:377:MET:SD	1:2G:379:SER:HB3	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2H:313:MET:HE3	1:2H:382:THR:HG23	1.92	0.50
1:2I:151:CYS:SG	1:2I:193:SER:OG	2.46	0.50
1:4B:17:GLY:HA2	1:4B:20:CYS:SG	2.52	0.50
1:4G:10:GLY:HA2	1:4G:145:THR:HG23	1.93	0.50
1:4G:223:THR:HG22	2:5G:322:SER:HA	1.93	0.50
2:5A:244:GLY:HA2	2:5A:355:ASP:HB2	1.94	0.50
2:5B:257:LEU:HD21	2:5B:314:SER:HB3	1.94	0.50
1:2A:325:PRO:HA	1:2A:328:VAL:HG12	1.94	0.50
1:2B:88:HIS:CD2	1:2C:283:HIS:CG	2.99	0.50
2:3D:66:MET:HE2	2:3D:116:VAL:HG21	1.92	0.50
1:4A:271:SER:HB2	1:4A:377:MET:HB3	1.94	0.50
1:4C:8:HIS:HD2	1:4C:65:CYS:SG	2.35	0.50
1:4F:7:ILE:HD13	1:4F:153:LEU:HD21	1.94	0.50
1:2G:230:LEU:HD23	1:2G:302:MET:HE1	1.94	0.50
1:2I:71:GLU:OE2	2:3I:2:ARG:NH2	2.44	0.50
2:3B:87:PRO:HD3	2:3C:281:TYR:CZ	2.47	0.50
2:3H:404:ASP:OD1	2:3H:407:GLU:HG3	2.11	0.50
1:4I:100:ALA:O	2:5I:255:VAL:HG11	2.11	0.50
1:4I:151:CYS:SG	1:4I:193:SER:OG	2.45	0.50
2:5I:216:LYS:HE2	2:5I:275:SER:HB3	1.93	0.50
1:2B:319:TYR:HB3	1:2B:323:VAL:HG21	1.94	0.49
1:2C:121:ARG:NH2	1:2D:283:HIS:CE1	2.80	0.49
1:2G:274:PRO:HG2	1:2G:371:VAL:HG11	1.94	0.49
2:3F:220:PRO:HG2	1:4F:326:LYS:CG	2.41	0.49
2:3F:334:GLN:HE22	2:3F:348:ASN:N	2.10	0.49
1:4B:260:VAL:O	1:4B:260:VAL:HG23	2.11	0.49
1:4H:224:TYR:HD1	2:5H:323:THR:HG1	1.55	0.49
2:5E:135:ILE:HB	2:5E:166:THR:HG22	1.93	0.49
2:5H:30:ILE:HD11	2:5H:47:ILE:HD11	1.94	0.49
2:5H:257:LEU:HD21	2:5H:314:SER:HB2	1.94	0.49
2:5I:235:GLY:HA2	2:5I:318:ARG:HH21	1.77	0.49
1:2I:76:ASP:OD2	2:3I:46:ARG:NH1	2.40	0.49
1:2I:217:LEU:HD11	1:2I:275:ILE:HG22	1.93	0.49
2:3D:152:ILE:HA	2:3D:164:MET:HE1	1.93	0.49
2:3E:55:THR:HG22	2:3F:282:ARG:C	2.29	0.49
2:3E:330:MET:HE3	2:3E:349:MET:HB3	1.93	0.49
2:3G:167:PHE:HZ	2:3G:236:VAL:HG11	1.77	0.49
1:2B:107:HIS:NE2	1:2B:151:CYS:SG	2.84	0.49
2:3C:169:VAL:HG12	2:3C:202:ILE:HB	1.93	0.49
2:3E:267:LEU:HB3	2:3E:299:MET:HE2	1.94	0.49
1:4I:50:ASN:O	1:4I:64:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:139:LEU:HA	2:5A:145:SER:HB2	1.93	0.49
1:2A:105:ARG:HH22	2:3A:251:ARG:NE	2.10	0.49
1:2E:60:LYS:HZ3	1:2F:282:TYR:HE2	1.35	0.49
1:2G:180:ALA:HA	2:3G:350:LYS:HD3	1.94	0.49
2:3C:27:GLU:OE2	2:3C:241:ARG:NH1	2.42	0.49
2:3G:397:TRP:CH2	1:4G:260:VAL:HB	2.47	0.49
1:4C:60:LYS:HE2	1:4D:282:TYR:CZ	2.47	0.49
1:4C:251:ASP:OD1	1:4C:254:GLU:HG2	2.12	0.49
1:4H:76:ASP:HA	1:4H:79:ARG:HD2	1.94	0.49
1:4I:30:ILE:HG22	1:4I:36:MET:HB3	1.94	0.49
1:2A:407:TRP:HE1	2:3A:258:ILE:HG13	1.76	0.49
1:2D:56:THR:CA	1:2E:285:GLN:N	2.76	0.49
1:2G:121:ARG:HH22	1:2G:124:LYS:HE3	1.77	0.49
2:3F:55:THR:HG23	2:3F:55:THR:O	2.12	0.49
2:3H:100:ASN:HB3	2:3H:103:LYS:HG2	1.94	0.49
1:4B:4:VAL:HG12	1:4B:133:GLN:HB3	1.93	0.49
1:4F:90:GLU:HG3	1:4F:121:ARG:HD3	1.94	0.49
1:4G:377:MET:SD	1:4G:379:SER:HB3	2.52	0.49
2:5C:238:CYS:SG	2:5C:318:ARG:NE	2.85	0.49
2:5G:407:GLU:N	2:5G:407:GLU:OE2	2.44	0.49
2:5H:73:MET:HB3	2:5H:77:ARG:HH22	1.78	0.49
1:2G:11:GLN:HB2	1:2G:74:VAL:HG21	1.93	0.49
1:2G:358:GLN:OE1	1:2G:359:PRO:HD2	2.13	0.49
1:2I:217:LEU:HD11	1:2I:275:ILE:CG2	2.42	0.49
2:3B:94:GLN:O	1:4B:2:ARG:NH2	2.46	0.49
2:3D:175:VAL:HG11	1:4D:329:ASN:HA	1.93	0.49
2:3D:311:LEU:HD12	2:3D:342:VAL:HG11	1.93	0.49
2:3F:55:THR:HG21	2:3G:282:ARG:O	2.12	0.49
2:3F:220:PRO:HD2	1:4F:326:LYS:HG3	1.95	0.49
1:4C:105:ARG:HD2	1:4C:109:THR:HB	1.93	0.49
1:4E:60:LYS:HZ2	1:4F:283:HIS:CG	2.03	0.49
2:5C:20:PHE:CD1	2:5C:233:MET:HG3	2.47	0.49
2:5D:256:ASN:O	2:5D:312:THR:HG21	2.11	0.49
2:5G:2:ARG:NH1	2:5G:249:ASP:OD2	2.46	0.49
1:2F:250:VAL:HG13	1:2F:255:PHE:HE1	1.77	0.49
1:2F:323:VAL:CG1	1:2F:355:ILE:HG23	2.43	0.49
1:2I:398:MET:HG2	2:3I:345:ILE:HD13	1.94	0.49
2:3A:19:LYS:HD2	2:3A:22:GLU:HG3	1.94	0.49
2:3B:58:ARG:NH1	2:3C:280:GLN:OE1	2.46	0.49
2:3E:287:PRO:HD3	2:3E:325:GLU:OE1	2.12	0.49
2:3F:252:LYS:O	2:3F:256:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4B:215:ARG:NH2	1:4B:299:ALA:O	2.43	0.49
1:4G:417:GLU:HA	1:4G:420:GLU:HG3	1.94	0.49
1:4H:267:PHE:O	1:4H:380:ASN:ND2	2.46	0.49
2:5A:211:CYS:SG	2:5A:220:PRO:HG3	2.53	0.49
2:5C:100:ASN:HB3	2:5C:103:LYS:HG2	1.94	0.49
1:2A:66:VAL:HG12	1:2A:91:GLN:HB2	1.93	0.49
1:2I:392:ASP:CG	1:2I:422:ARG:HH22	2.12	0.49
2:3B:10:GLY:HA2	2:3B:143:THR:HG23	1.93	0.49
1:4A:122:ILE:HG21	1:4A:157:LEU:HD21	1.95	0.49
1:4C:73:THR:HA	2:5C:46:ARG:HH12	1.76	0.49
1:4E:179:THR:HB	2:5E:351:SER:OG	2.12	0.49
1:4I:260:VAL:HG23	1:4I:260:VAL:O	2.13	0.49
2:5A:198:GLU:OE2	2:5A:200:GLN:NE2	2.44	0.49
2:5F:55:THR:OG1	2:5G:282:ARG:O	2.29	0.49
2:5H:137:HIS:HE1	2:5H:166:THR:HG21	1.77	0.49
1:2G:271:SER:HB3	1:2G:377:MET:HB3	1.95	0.49
2:3C:397:TRP:CH2	1:4C:260:VAL:O	2.66	0.49
1:4C:76:ASP:OD1	1:4C:79:ARG:NH2	2.41	0.49
1:4H:404:PHE:CD1	2:5H:259:PRO:HA	2.48	0.49
1:4I:276:ILE:HG23	1:4I:280:LYS:HG3	1.94	0.49
1:4I:422:ARG:NH1	1:4I:426:ALA:HB2	2.28	0.49
2:5E:180:VAL:HG22	2:5E:183:TYR:HB2	1.93	0.49
2:5F:180:VAL:O	2:5F:184:ASN:ND2	2.45	0.49
1:2D:60:LYS:HE3	1:2E:283:HIS:HA	1.95	0.49
1:2H:320:ARG:NH2	1:2H:358:GLN:OE1	2.46	0.49
1:2I:262:TYR:HB2	1:2I:265:ILE:HD12	1.95	0.49
2:3A:7:VAL:HG11	2:3A:151:LEU:HD23	1.95	0.49
2:3A:23:VAL:O	2:3A:27:GLU:HG2	2.13	0.49
1:4E:213:CYS:HA	1:4E:217:LEU:HD13	1.95	0.49
2:5B:64:ILE:HD13	2:5B:119:VAL:HG13	1.95	0.49
2:5B:256:ASN:HB3	2:5B:350:LYS:HE2	1.94	0.49
2:5C:180:VAL:O	2:5C:184:ASN:ND2	2.46	0.49
1:2A:80:THR:HG22	1:2A:84:ARG:HH21	1.78	0.48
1:2E:73:THR:O	1:2E:77:GLU:OE1	2.31	0.48
2:3A:70:PRO:HD2	1:4A:2:ARG:HH11	1.77	0.48
2:3G:220:PRO:HB2	2:3G:225:LEU:CD2	2.42	0.48
2:3H:179:VAL:HG12	1:4H:258:ASN:CG	2.32	0.48
1:4E:101:ASN:HB3	1:4E:182:VAL:HG21	1.95	0.48
1:4E:204:LEU:N	1:4E:204:LEU:HD12	2.28	0.48
1:4G:398:MET:HE3	2:5G:345:ILE:HG23	1.95	0.48
1:4H:186:ASN:OD1	1:4H:408:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4I:174:SER:HB3	1:4I:207:GLU:HG2	1.94	0.48
2:5B:68:LEU:HD12	2:5B:143:THR:HG22	1.95	0.48
2:5H:190:HIS:HB2	2:5H:414:ASN:HD21	1.78	0.48
1:2B:104:ALA:HB1	1:2B:411:GLU:OE2	2.13	0.48
1:2F:269:LEU:HD23	1:2F:303:ALA:HB3	1.95	0.48
2:3H:292:GLN:HG2	2:3H:298:ASN:HD22	1.78	0.48
1:4I:76:ASP:HA	1:4I:79:ARG:HD2	1.95	0.48
2:5B:282:ARG:HB2	2:5B:282:ARG:NH2	2.28	0.48
2:5E:107:THR:HG21	2:5E:401:GLU:HB2	1.93	0.48
2:5G:404:ASP:OD1	2:5G:405:GLU:N	2.45	0.48
1:2A:269:LEU:HD21	1:2A:384:ILE:HD11	1.96	0.48
1:2H:306:ASP:N	1:2H:386:GLU:OE2	2.45	0.48
1:2H:414:GLU:N	1:2H:414:GLU:OE2	2.46	0.48
1:2I:240:ALA:HB2	1:2I:320:ARG:HH11	1.78	0.48
2:3H:207:LEU:HB3	2:3H:225:LEU:HD22	1.95	0.48
1:4B:217:LEU:HD21	1:4B:367:ASP:HB3	1.95	0.48
1:4C:209:ILE:HB	1:4C:227:LEU:HD22	1.95	0.48
1:4G:271:SER:HB3	1:4G:377:MET:HB3	1.95	0.48
1:4H:28:HIS:CE1	1:4H:243:ARG:HE	2.31	0.48
2:5C:165:GLU:HG2	2:5C:198:GLU:HG3	1.93	0.48
2:5D:100:ASN:HB3	2:5D:103:LYS:HG2	1.95	0.48
2:5G:202:ILE:CD1	2:5G:268:ILE:HG21	2.42	0.48
1:2A:427:ALA:O	1:2A:430:LYS:HG3	2.12	0.48
1:2D:221:ARG:HA	2:3D:324:LYS:CE	2.40	0.48
1:2F:238:LEU:HD11	1:2F:255:PHE:HE2	1.79	0.48
1:2G:407:TRP:CZ3	2:3G:255:VAL:CG2	2.96	0.48
2:3B:100:ASN:HB3	2:3B:103:LYS:HG2	1.94	0.48
2:3G:237:THR:HG22	2:3G:237:THR:O	2.14	0.48
2:3I:103:LYS:HA	2:3I:107:THR:HG22	1.94	0.48
2:3I:258:ILE:O	2:3I:258:ILE:HG13	2.12	0.48
1:4C:230:LEU:HD21	1:4C:368:LEU:HD21	1.95	0.48
1:4D:123:ARG:NH1	1:4D:160:ASP:OD2	2.40	0.48
1:4D:398:MET:CE	2:5D:346:PRO:HD2	2.44	0.48
1:4E:76:ASP:OD2	2:5E:46:ARG:NH1	2.31	0.48
1:4G:269:LEU:HD23	1:4G:303:ALA:HB3	1.95	0.48
2:5C:230:SER:HA	2:5C:233:MET:HG2	1.95	0.48
2:5E:209:ASP:OD1	2:5E:213:ARG:NH1	2.46	0.48
2:5E:309:ARG:H	2:5E:372:THR:HG22	1.78	0.48
2:5H:330:MET:SD	2:5H:349:MET:HG2	2.53	0.48
1:2G:167:LEU:HA	1:2G:200:VAL:HG13	1.95	0.48
1:2G:387:VAL:HA	1:2G:390:ARG:NH2	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:211:CYS:SG	2:3B:217:LEU:HB2	2.53	0.48
2:5A:375:GLN:HE21	2:5A:379:LYS:HD3	1.78	0.48
1:2B:271:SER:HB2	1:2B:377:MET:HB3	1.94	0.48
1:2E:136:LEU:HD23	1:2E:235:ILE:HD11	1.94	0.48
1:2E:152:LEU:O	1:2E:156:ARG:HG2	2.14	0.48
2:3C:309:ARG:H	2:3C:372:THR:HG22	1.79	0.48
2:3E:200:GLN:HB3	2:3E:268:ILE:HD11	1.94	0.48
2:3E:293:MET:HG3	2:3E:367:PHE:HB2	1.94	0.48
2:3F:58:ARG:HD3	2:3G:281:TYR:CE1	2.48	0.48
2:3H:5:VAL:HB	2:3H:133:PHE:CD1	2.48	0.48
1:4E:274:PRO:HG3	1:4E:286:LEU:CD2	2.43	0.48
1:4G:177:VAL:HG13	2:5G:327:ASP:HB3	1.96	0.48
1:4I:215:ARG:NH2	1:4I:299:ALA:O	2.46	0.48
2:5D:54:ALA:CB	2:5E:281:TYR:O	2.61	0.48
2:5H:289:LEU:HD12	2:5H:365:VAL:HG12	1.96	0.48
1:2I:5:ILE:HG12	1:2I:132:LEU:HD11	1.96	0.48
2:3A:267:LEU:CD2	2:3A:374:ILE:HD11	2.34	0.48
2:3C:122:LYS:CE	2:3D:281:TYR:OH	2.62	0.48
2:3C:311:LEU:HD12	2:3C:342:VAL:HG11	1.95	0.48
2:3F:25:SER:HG	2:3F:81:PHE:HE2	1.60	0.48
1:4E:151:CYS:SG	1:4E:193:SER:OG	2.40	0.48
1:4G:136:LEU:HD22	1:4G:167:LEU:HD23	1.96	0.48
1:4H:178:SER:HB2	2:5H:347:ASN:ND2	2.29	0.48
1:4I:53:PHE:HB3	1:4I:61:HIS:HB3	1.95	0.48
2:5D:178:THR:OG1	2:5D:181:GLU:OE2	2.31	0.48
2:5D:284:LEU:HD23	2:5D:362:LYS:HG2	1.95	0.48
2:5E:213:ARG:HH12	2:5E:297:LYS:HB2	1.79	0.48
2:5I:193:VAL:HG21	2:5I:418:LEU:HD12	1.94	0.48
1:2D:75:VAL:O	1:2D:78:VAL:HG12	2.14	0.48
1:2E:174:SER:HB3	1:2E:207:GLU:HG2	1.96	0.48
1:2H:4:VAL:HG21	1:2H:136:LEU:HD13	1.95	0.48
1:2H:210:TYR:CG	2:3H:324:LYS:HE3	2.42	0.48
2:3A:258:ILE:HG13	2:3A:258:ILE:O	2.13	0.48
1:4D:99:ALA:O	1:4D:105:ARG:HD3	2.13	0.48
1:4E:11:GLN:HG3	1:4E:74:VAL:HG21	1.95	0.48
2:5A:109:GLY:O	2:5A:113:ILE:HG12	2.14	0.48
2:5G:55:THR:HG23	2:5H:283:ALA:CB	2.44	0.48
1:2H:71:GLU:HB3	1:2H:98:ASP:HB3	1.96	0.48
2:3C:181:GLU:CG	2:3C:182:PRO:HD3	2.44	0.48
2:3E:274:THR:HG21	2:3E:282:ARG:HD2	1.95	0.48
2:3F:202:ILE:HD11	2:3F:268:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3G:107:THR:OG1	2:3G:401:GLU:OE2	2.31	0.48
2:3G:196:ALA:O	2:3G:264:HIS:NE2	2.47	0.48
1:4E:178:SER:OG	2:5E:347:ASN:ND2	2.47	0.48
1:4F:306:ASP:HB3	1:4F:309:HIS:HE1	1.79	0.48
2:5A:133:PHE:HZ	2:5A:159:TYR:HD2	1.62	0.48
2:5B:311:LEU:HD12	2:5B:342:VAL:HG11	1.96	0.48
2:5F:173:PRO:HD2	2:5F:205:GLU:OE2	2.14	0.48
1:2E:76:ASP:OD2	2:3E:46:ARG:NH1	2.40	0.48
1:2G:212:ILE:HG23	1:2G:275:ILE:CD1	2.41	0.48
1:2G:269:LEU:HD11	1:2G:384:ILE:HD11	1.95	0.48
1:2H:406:HIS:HA	1:2H:409:VAL:HG22	1.96	0.48
2:3E:55:THR:HG22	2:3F:283:ALA:HA	1.90	0.48
2:3H:64:ILE:HD12	2:3H:119:VAL:HG12	1.96	0.48
1:4A:301:MET:HE2	1:4A:301:MET:HB3	1.76	0.48
2:5F:98:GLY:H	2:5F:103:LYS:HD3	1.78	0.48
1:2A:397:LEU:HD23	2:3A:346:PRO:HD3	1.96	0.47
1:2D:269:LEU:CD2	1:2D:301:MET:HG2	2.43	0.47
1:2H:223:THR:OG1	2:3H:245:GLN:OE1	2.32	0.47
2:3F:323:THR:HA	2:3F:326:VAL:HG12	1.95	0.47
1:4C:105:ARG:HH12	2:5C:251:ARG:HD3	1.79	0.47
1:4F:335:ILE:HG23	1:4F:341:ILE:HD13	1.96	0.47
2:5D:375:GLN:HG3	2:5D:419:VAL:HG13	1.96	0.47
1:2H:51:THR:HG23	1:2H:52:PHE:HD1	1.79	0.47
1:2I:52:PHE:HD2	1:2I:243:ARG:HD3	1.78	0.47
2:3C:86:ARG:HG3	2:3D:280:GLN:OE1	2.13	0.47
1:4E:5:ILE:HD13	1:4E:64:ARG:HB3	1.95	0.47
1:4E:217:LEU:HD11	1:4E:275:ILE:CG2	2.43	0.47
1:4H:399:TYR:OH	1:4H:415:GLU:OE2	2.32	0.47
2:5A:272:PRO:HD2	2:5A:361:LEU:HD21	1.95	0.47
2:5C:88:ASP:OD2	2:5D:281:TYR:CE2	2.67	0.47
1:2G:100:ALA:O	2:3G:255:VAL:HG11	2.14	0.47
2:3A:220:PRO:HD2	1:4A:326:LYS:HE3	1.78	0.47
2:3E:258:ILE:HG13	2:3E:258:ILE:O	2.14	0.47
2:3F:334:GLN:HE22	2:3F:348:ASN:H	1.61	0.47
2:3G:220:PRO:CD	1:4G:326:LYS:HD3	2.45	0.47
1:4B:72:PRO:HD2	2:5B:2:ARG:HH22	1.79	0.47
1:4D:178:SER:CB	2:5D:347:ASN:HD22	2.19	0.47
1:4I:70:LEU:HD12	1:4I:99:ALA:HB2	1.96	0.47
2:5C:86:ARG:C	2:5D:281:TYR:OH	2.53	0.47
2:5E:114:ASP:N	2:5E:114:ASP:OD1	2.47	0.47
2:5G:311:LEU:HD12	2:5G:342:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5H:10:GLY:O	2:5H:14:ASN:ND2	2.48	0.47
2:5H:249:ASP:H	2:5H:252:LYS:HB2	1.79	0.47
1:2E:403:ALA:HB2	2:3E:344:TRP:CZ3	2.48	0.47
1:2F:168:ASN:ND2	1:2F:170:CYS:SG	2.88	0.47
1:2G:189:LEU:HD11	1:2G:418:PHE:CD1	2.49	0.47
1:2H:178:SER:HB3	2:3H:347:ASN:ND2	2.29	0.47
2:3A:179:VAL:HG11	1:4A:258:ASN:O	2.15	0.47
2:3B:309:ARG:NH1	2:3B:341:PHE:O	2.48	0.47
2:3C:163:ILE:HD12	2:3C:250:LEU:HB2	1.95	0.47
2:3D:73:MET:HE3	2:3D:92:PHE:CD1	2.50	0.47
2:3E:98:GLY:O	1:4E:257:THR:HG21	2.14	0.47
2:3F:58:ARG:HD3	2:3G:281:TYR:CD1	2.49	0.47
1:4A:50:ASN:O	1:4A:64:ARG:NH2	2.46	0.47
1:4A:70:LEU:HD12	1:4A:99:ALA:HB2	1.96	0.47
1:4F:60:LYS:HZ3	1:4F:62:VAL:HB	1.79	0.47
2:5E:215:LEU:HB3	2:5E:217:LEU:HD13	1.96	0.47
2:5G:169:VAL:HG12	2:5G:202:ILE:HB	1.96	0.47
1:2B:221:ARG:HD2	1:2B:221:ARG:HA	1.43	0.47
1:2C:223:THR:OG1	2:3C:245:GLN:NE2	2.47	0.47
1:4D:16:ILE:HD11	1:4D:138:PHE:HB3	1.96	0.47
2:5A:200:GLN:HG3	2:5A:268:ILE:HD11	1.96	0.47
2:5D:135:ILE:HG22	2:5D:137:HIS:CD2	2.49	0.47
1:2H:11:GLN:NE2	1:2H:15:GLN:OE1	2.48	0.47
1:2H:168:ASN:HD22	1:2H:198:THR:HG21	1.80	0.47
1:2I:71:GLU:OE2	1:2I:73:THR:HG23	2.14	0.47
1:2I:123:ARG:HH12	1:2I:160:ASP:CG	2.18	0.47
2:3A:121:ARG:NH2	2:3A:158:GLU:OE2	2.47	0.47
2:3C:99:ASN:HD21	1:4C:258:ASN:HD21	1.61	0.47
2:3D:309:ARG:NH1	2:3D:341:PHE:O	2.48	0.47
2:3G:52:ASN:ND2	2:3G:123:GLU:OE2	2.34	0.47
2:3G:69:GLU:HG2	1:4G:2:ARG:NH2	2.29	0.47
1:4A:269:LEU:HD11	1:4A:384:ILE:HD11	1.97	0.47
1:4C:8:HIS:CD2	1:4C:65:CYS:SG	3.07	0.47
1:4G:154:LEU:HD21	1:4G:198:THR:OG1	2.14	0.47
1:2A:406:HIS:HA	1:2A:409:VAL:HG22	1.96	0.47
1:2B:221:ARG:NH2	2:3B:325:GLU:N	2.61	0.47
1:2C:50:ASN:O	1:2C:64:ARG:NH2	2.48	0.47
1:2E:269:LEU:HD11	1:2E:384:ILE:HD11	1.97	0.47
1:2G:60:LYS:CE	1:2H:283:HIS:CD2	2.98	0.47
1:2G:137:MET:HB3	1:2G:168:ASN:HA	1.95	0.47
1:2H:100:ALA:O	2:3H:255:VAL:HG11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3A:169:VAL:HG12	2:3A:202:ILE:HB	1.96	0.47
2:3D:64:ILE:HD12	2:3D:119:VAL:HG12	1.96	0.47
2:3E:55:THR:HG21	2:3F:284:LEU:H	1.80	0.47
2:3H:391:ARG:HD2	1:4H:346:TRP:CD1	2.49	0.47
1:4A:407:TRP:CZ2	2:5A:258:ILE:HD11	2.50	0.47
1:4D:57:GLY:N	1:4E:285:GLN:CB	2.67	0.47
1:4E:181:VAL:HG22	2:5E:256:ASN:ND2	2.30	0.47
1:4E:260:VAL:HG23	1:4E:260:VAL:O	2.15	0.47
2:5A:207:LEU:HD21	2:5A:225:LEU:CB	2.38	0.47
2:5A:313:ALA:HB1	2:5A:367:PHE:HE1	1.79	0.47
2:5D:239:CYS:SG	2:5D:248:SER:N	2.83	0.47
1:2A:90:GLU:O	1:2A:93:ILE:HD11	2.15	0.47
1:2H:411:GLU:N	1:2H:411:GLU:OE1	2.48	0.47
1:2I:396:ASP:OD2	1:2I:422:ARG:NH2	2.47	0.47
2:3B:213:ARG:HH12	2:3B:297:LYS:HB3	1.80	0.47
2:3C:181:GLU:HG2	2:3C:182:PRO:HD3	1.97	0.47
2:3D:290:THR:HG21	2:3D:329:GLN:HB3	1.97	0.47
2:3F:347:ASN:OD1	2:3F:349:MET:HB3	2.15	0.47
1:4C:212:ILE:HD11	1:4C:300:SER:HA	1.97	0.47
1:4G:340:THR:HG23	1:4G:341:ILE:HG13	1.97	0.47
2:5D:309:ARG:H	2:5D:372:THR:HG22	1.80	0.47
2:5I:211:CYS:SG	2:5I:220:PRO:HB3	2.55	0.47
1:2B:12:ALA:HB3	1:2B:140:ALA:HB2	1.96	0.47
1:2D:203:MET:HE1	1:2D:387:VAL:HG11	1.96	0.47
1:2E:60:LYS:NZ	1:2F:283:HIS:CD2	2.83	0.47
1:2F:30:ILE:HG22	1:2F:36:MET:HG2	1.97	0.47
1:2F:105:ARG:HH12	2:3F:251:ARG:HG2	1.80	0.47
2:3G:175:VAL:HG21	1:4G:332:VAL:HG23	1.96	0.47
2:3H:12:CYS:HB3	2:3H:138:SER:OG	2.14	0.47
1:4A:57:GLY:CA	1:4B:285:GLN:HG2	2.45	0.47
1:4A:68:LEU:HD23	1:4A:149:LEU:HD21	1.97	0.47
1:4H:142:GLY:CA	1:4H:183:GLU:HG2	2.45	0.47
1:4H:404:PHE:HE2	2:5H:345:ILE:HD12	1.80	0.47
2:5D:58:ARG:CD	2:5E:280:GLN:C	2.83	0.47
2:5E:155:VAL:HG13	2:5E:164:MET:CE	2.45	0.47
2:5E:192:LEU:HD21	2:5E:199:VAL:HG11	1.97	0.47
2:5H:20:PHE:HD2	2:5H:233:MET:HE2	1.79	0.47
1:2D:57:GLY:N	1:2E:285:GLN:CB	2.76	0.47
1:2G:108:TYR:O	1:2G:112:LYS:NZ	2.47	0.47
2:3F:417:ASP:O	2:3F:421:GLU:OE1	2.33	0.47
2:3I:137:HIS:HE1	2:3I:166:THR:CG2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4F:60:LYS:NZ	1:4G:283:HIS:ND1	2.57	0.47
1:4G:135:PHE:HB2	1:4G:166:LYS:HG2	1.97	0.47
1:4G:181:VAL:HB	2:5G:256:ASN:OD1	2.14	0.47
2:5D:58:ARG:NH2	2:5E:281:TYR:CD1	2.78	0.47
2:5G:135:ILE:HD13	2:5G:152:ILE:HG12	1.96	0.47
1:2A:60:LYS:NZ	1:2B:283:HIS:HD2	2.13	0.46
1:2A:181:VAL:HG13	1:2A:398:MET:HE1	1.97	0.46
1:2A:306:ASP:N	1:2A:386:GLU:OE2	2.45	0.46
1:2B:215:ARG:HH21	1:2B:299:ALA:C	2.18	0.46
1:2H:35:GLN:OE1	1:2H:35:GLN:N	2.47	0.46
2:3D:309:ARG:H	2:3D:372:THR:HG22	1.80	0.46
2:3G:135:ILE:CG1	2:3G:166:THR:HG22	2.45	0.46
2:3I:178:THR:HA	1:4I:258:ASN:HD21	1.79	0.46
1:4D:11:GLN:NE2	2:5D:247:ASN:OD1	2.48	0.46
1:4D:60:LYS:CE	1:4E:283:HIS:HA	2.40	0.46
1:4G:398:MET:SD	2:5G:346:PRO:HD2	2.55	0.46
1:4I:246:GLY:HA2	1:4I:357:TYR:HD1	1.79	0.46
2:5B:284:LEU:HB3	2:5B:362:LYS:HE3	1.96	0.46
1:2A:402:ARG:NH1	1:2A:405:VAL:HG11	2.30	0.46
1:2G:401:LYS:NZ	2:3G:425:TYR:CD1	2.83	0.46
1:2I:241:SER:HB2	1:2I:249:ASN:HB2	1.97	0.46
2:3D:10:GLY:HA2	2:3D:143:THR:HG23	1.96	0.46
2:3E:205:GLU:CD	1:4E:329:ASN:HD21	2.17	0.46
2:3F:309:ARG:H	2:3F:372:THR:HG22	1.80	0.46
2:3G:97:ALA:HB3	2:3G:143:THR:HB	1.98	0.46
2:3H:169:VAL:HG12	2:3H:202:ILE:HB	1.96	0.46
1:4B:306:ASP:HB3	1:4B:309:HIS:CE1	2.49	0.46
1:4C:70:LEU:HD12	1:4C:99:ALA:HB2	1.97	0.46
1:4D:238:LEU:HD11	1:4D:255:PHE:CE2	2.50	0.46
1:4I:213:CYS:SG	1:4I:222:PRO:HG3	2.56	0.46
2:5H:181:GLU:CG	2:5H:182:PRO:HD3	2.45	0.46
2:5I:272:PRO:HG3	2:5I:284:LEU:HD11	1.96	0.46
1:2B:98:ASP:O	1:2B:105:ARG:NH1	2.48	0.46
1:2G:287:SER:N	1:2G:290:GLU:OE2	2.45	0.46
2:3A:311:LEU:HD12	2:3A:342:VAL:HG11	1.96	0.46
2:3F:238:CYS:SG	2:3F:318:ARG:NE	2.88	0.46
2:3H:397:TRP:CH2	1:4H:260:VAL:HG23	2.50	0.46
2:3I:192:LEU:HD21	2:3I:199:VAL:HG21	1.97	0.46
1:4A:340:THR:HG23	1:4A:341:ILE:HG13	1.96	0.46
1:4D:33:ASP:O	1:4D:60:LYS:NZ	2.48	0.46
1:4E:241:SER:OG	1:4E:250:VAL:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4G:358:GLN:OE1	1:4G:359:PRO:HD2	2.15	0.46
2:5B:105:HIS:CD2	2:5B:150:LEU:HB2	2.51	0.46
2:5I:252:LYS:HG3	2:5I:350:LYS:HE3	1.98	0.46
1:2E:398:MET:HE1	2:3E:346:PRO:HD2	1.94	0.46
1:2H:183:GLU:HG3	1:2H:184:PRO:HD3	1.97	0.46
2:3A:55:THR:HG21	2:3B:283:ALA:HB1	1.90	0.46
2:3C:249:ASP:OD1	2:3C:252:LYS:HG2	2.15	0.46
2:3G:55:THR:HG23	2:3H:283:ALA:CB	2.46	0.46
2:3H:179:VAL:HG11	1:4H:258:ASN:O	2.15	0.46
2:3I:267:LEU:HB3	2:3I:299:MET:HE2	1.98	0.46
1:4B:419:SER:O	1:4B:423:GLU:OE1	2.33	0.46
1:4H:406:HIS:HA	1:4H:409:VAL:HG22	1.98	0.46
2:5B:19:LYS:HE3	2:5B:227:HIS:HB2	1.97	0.46
2:5B:156:ARG:NH1	2:5B:162:ARG:O	2.49	0.46
2:5B:284:LEU:HD23	2:5B:362:LYS:HG3	1.97	0.46
1:2C:124:LYS:CD	1:2D:283:HIS:NE2	2.69	0.46
1:2G:403:ALA:HB2	2:3G:344:TRP:CH2	2.51	0.46
2:3B:16:ILE:HD11	2:3B:136:THR:HB	1.97	0.46
2:3G:189:VAL:HG11	2:3G:415:MET:SD	2.55	0.46
2:3G:407:GLU:OE1	2:3G:407:GLU:N	2.47	0.46
1:4B:316:CYS:SG	1:4B:378:ILE:HB	2.55	0.46
1:4D:1:MET:N	1:4D:3:GLU:OE2	2.35	0.46
1:4G:244:PHE:HB2	1:4G:356:ASN:HD21	1.81	0.46
2:5E:404:ASP:OD1	2:5E:405:GLU:N	2.47	0.46
1:2A:10:GLY:HA2	1:2A:145:THR:HG23	1.96	0.46
1:2A:137:MET:HE3	1:2A:154:LEU:HD12	1.98	0.46
1:2C:192:HIS:NE2	1:2C:420:GLU:OE2	2.49	0.46
1:2D:306:ASP:HB3	1:2D:309:HIS:CE1	2.50	0.46
2:3D:324:LYS:O	2:3D:328:GLU:HG2	2.15	0.46
2:3E:169:VAL:HG12	2:3E:202:ILE:HB	1.96	0.46
2:3G:265:PHE:CE2	2:3G:418:LEU:HD21	2.51	0.46
2:3H:372:THR:HA	2:3H:422:TYR:HD2	1.79	0.46
1:4A:80:THR:HA	1:4A:84:ARG:HE	1.80	0.46
1:4C:298:PRO:HB3	1:4C:307:PRO:HD2	1.98	0.46
1:4D:50:ASN:O	1:4D:64:ARG:NH2	2.49	0.46
1:4E:179:THR:HG21	2:5E:327:ASP:OD1	2.16	0.46
1:4G:121:ARG:NH1	1:4G:124:LYS:HE3	2.28	0.46
2:5A:7:VAL:HG22	2:5A:64:ILE:HG21	1.98	0.46
2:5D:16:ILE:HG22	2:5D:136:THR:HG21	1.98	0.46
1:2A:323:VAL:HG13	1:2A:355:ILE:HG23	1.97	0.46
1:2A:397:LEU:HG	2:3A:344:TRP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2B:256:GLN:HE21	1:2B:256:GLN:H	1.63	0.46
1:2I:223:THR:HG22	2:3I:322:SER:HA	1.96	0.46
2:3A:171:PRO:HG3	2:3A:181:GLU:OE1	2.16	0.46
2:3B:94:GLN:O	1:4B:2:ARG:CZ	2.63	0.46
2:3D:282:ARG:NH1	2:3D:288:GLU:OE2	2.49	0.46
1:4C:238:LEU:HD13	1:4C:255:PHE:HE2	1.79	0.46
1:4F:377:MET:HE2	1:4F:379:SER:HB3	1.98	0.46
1:4G:135:PHE:HD2	1:4G:166:LYS:HG2	1.81	0.46
1:4G:259:LEU:HD11	1:4G:316:CYS:HB2	1.98	0.46
2:5C:178:THR:HG23	2:5C:181:GLU:HG3	1.98	0.46
1:2C:234:VAL:HG21	1:2C:302:MET:HE1	1.97	0.46
1:2F:215:ARG:NH2	1:2F:300:SER:HB2	2.31	0.46
1:2H:133:GLN:NE2	1:2H:253:THR:HG23	2.31	0.46
2:3C:397:TRP:HZ2	1:4C:260:VAL:HB	1.81	0.46
2:3D:94:GLN:O	1:4D:2:ARG:NH2	2.49	0.46
2:3E:397:TRP:NE1	1:4E:256:GLN:OE1	2.49	0.46
2:3F:10:GLY:HA2	2:3F:143:THR:HG23	1.98	0.46
2:3F:54:ALA:HB1	2:3G:281:TYR:O	2.16	0.46
2:3G:397:TRP:CZ3	1:4G:256:GLN:O	2.69	0.46
1:4G:167:LEU:HA	1:4G:200:VAL:HG13	1.98	0.46
2:5E:169:VAL:HG12	2:5E:202:ILE:HB	1.98	0.46
2:5F:135:ILE:HB	2:5F:166:THR:HG22	1.97	0.46
2:5G:7:VAL:HG11	2:5G:151:LEU:HD22	1.98	0.46
1:2A:60:LYS:HE2	1:2B:283:HIS:CD2	2.50	0.46
1:2G:213:CYS:SG	1:2G:222:PRO:HG3	2.56	0.46
2:3A:7:VAL:HB	2:3A:135:ILE:CD1	2.46	0.46
2:3D:326:VAL:HG22	2:3D:351:SER:HB2	1.98	0.46
2:3E:10:GLY:HA2	2:3E:143:THR:HG23	1.98	0.46
2:3F:2:ARG:HB3	2:3F:131:GLN:HB2	1.98	0.46
2:3G:99:ASN:OD1	2:3G:99:ASN:N	2.49	0.46
2:3H:113:ILE:HA	2:3H:116:VAL:HG12	1.98	0.46
1:4H:200:VAL:HG13	1:4H:268:MET:HE3	1.98	0.46
1:4I:274:PRO:HB2	1:4I:276:ILE:HG12	1.98	0.46
2:5B:407:GLU:OE2	2:5B:407:GLU:N	2.47	0.46
2:5D:54:ALA:HA	2:5E:283:ALA:CA	2.45	0.46
2:5D:139:LEU:HD11	2:5D:192:LEU:HD13	1.97	0.46
2:5E:54:ALA:CB	2:5F:281:TYR:O	2.45	0.46
1:2A:65:CYS:O	1:2A:91:GLN:HG3	2.16	0.46
1:2A:301:MET:HE2	1:2A:301:MET:HB3	1.80	0.46
1:2D:398:MET:HE2	2:3D:345:ILE:HG23	1.97	0.46
1:2F:27:GLU:OE1	1:2F:320:ARG:NH2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3A:5:VAL:HB	2:3A:133:PHE:HD1	1.81	0.46
2:3B:68:LEU:HD11	2:3B:147:MET:CE	2.46	0.46
2:3G:174:LYS:HE2	1:4G:333:ALA:HB1	1.97	0.46
2:3H:149:THR:HG22	2:3H:191:GLN:NE2	2.31	0.46
1:4A:97:GLU:HG3	1:4A:105:ARG:HH21	1.81	0.46
1:4E:172:TRP:HZ2	1:4E:391:MET:HE1	1.80	0.46
1:4E:261:PRO:HG3	1:4E:313:MET:HE2	1.97	0.46
1:4H:269:LEU:CD2	1:4H:384:ILE:HD11	2.46	0.46
2:5A:172:SER:HB2	2:5A:205:GLU:OE1	2.16	0.46
2:5C:103:LYS:HA	2:5C:107:THR:HB	1.98	0.46
1:2C:76:ASP:HA	1:2C:79:ARG:HD2	1.98	0.45
2:3G:175:VAL:HG11	1:4G:332:VAL:CG2	2.47	0.45
1:4C:238:LEU:HD21	1:4C:378:ILE:HD11	1.98	0.45
2:5C:274:THR:HG21	2:5C:282:ARG:HD3	1.98	0.45
2:5E:68:LEU:HB3	2:5E:96:GLY:HA2	1.98	0.45
2:5G:403:MET:HB3	2:5G:408:PHE:HE1	1.81	0.45
1:2D:138:PHE:CZ	1:2D:235:ILE:HD12	2.47	0.45
1:2H:312:TYR:HD2	1:2H:379:SER:HG	1.63	0.45
2:3B:94:GLN:C	1:4B:2:ARG:NH2	2.70	0.45
2:3B:173:PRO:HB3	2:3B:380:ARG:CZ	2.46	0.45
2:3G:309:ARG:H	2:3G:372:THR:HG22	1.82	0.45
1:4A:256:GLN:O	1:4A:260:VAL:HG22	2.16	0.45
1:4F:99:ALA:HA	1:4F:105:ARG:HG2	1.97	0.45
1:4F:309:HIS:HE2	1:4F:386:GLU:CD	2.17	0.45
1:4G:88:HIS:HB3	1:4G:91:GLN:HE22	1.82	0.45
1:4H:72:PRO:HD2	2:5H:2:ARG:NH2	2.31	0.45
1:4H:251:ASP:OD1	1:4H:254:GLU:N	2.49	0.45
1:4I:167:LEU:HD22	1:4I:200:VAL:HB	1.98	0.45
1:4I:397:LEU:CD2	2:5I:344:TRP:HA	2.43	0.45
2:5G:86:ARG:NE	2:5G:86:ARG:HA	2.31	0.45
2:5H:169:VAL:HG12	2:5H:202:ILE:HB	1.97	0.45
1:2C:306:ASP:OD1	1:2C:308:ARG:NH1	2.50	0.45
1:2I:181:VAL:HG22	2:3I:347:ASN:O	2.16	0.45
2:3E:113:ILE:HD12	2:3E:113:ILE:HA	1.86	0.45
2:3F:14:ASN:ND2	2:3F:67:ASP:OD2	2.50	0.45
2:3G:7:VAL:HG11	2:3G:151:LEU:HD23	1.98	0.45
1:4A:51:THR:HG23	1:4A:52:PHE:CD2	2.51	0.45
1:4H:269:LEU:HD21	1:4H:384:ILE:HD11	1.99	0.45
1:4I:269:LEU:HD12	1:4I:303:ALA:HB3	1.99	0.45
2:5E:58:ARG:NH1	2:5F:281:TYR:CE1	2.84	0.45
1:2D:57:GLY:N	1:2E:285:GLN:CA	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3F:208:TYR:HA	1:4F:326:LYS:HE2	1.98	0.45
1:4C:75:VAL:HG21	1:4C:94:SER:HB2	1.98	0.45
1:4F:230:LEU:HD21	1:4F:368:LEU:HD21	1.98	0.45
1:4G:241:SER:HB2	1:4G:249:ASN:HB2	1.97	0.45
2:5G:5:VAL:HB	2:5G:133:PHE:CD1	2.51	0.45
1:2A:17:GLY:HA2	1:2A:20:CYS:SG	2.56	0.45
1:2B:221:ARG:HH12	2:3B:324:LYS:CB	2.29	0.45
1:2D:5:ILE:HG12	1:2D:132:LEU:HD11	1.99	0.45
1:2F:217:LEU:CD2	1:2F:275:ILE:HG22	2.46	0.45
1:2F:377:MET:SD	1:2F:379:SER:HB3	2.56	0.45
1:2G:48:ALA:O	1:2G:51:THR:HG22	2.16	0.45
2:3C:60:VAL:CG1	2:3D:280:GLN:NE2	2.69	0.45
2:3C:284:LEU:HD23	2:3C:362:LYS:HG2	1.97	0.45
2:3E:177:ASP:OD1	1:4E:353:CYS:SG	2.74	0.45
2:3H:94:GLN:O	1:4H:2:ARG:NH2	2.50	0.45
2:3I:274:THR:HG21	2:3I:282:ARG:HD2	1.98	0.45
1:4A:238:LEU:HD13	1:4A:378:ILE:HD13	1.99	0.45
1:4C:101:ASN:ND2	2:5C:256:ASN:OD1	2.50	0.45
1:4F:50:ASN:O	1:4F:64:ARG:NH2	2.48	0.45
1:4G:173:PRO:HG2	1:4G:391:MET:HE3	1.98	0.45
1:4G:287:SER:OG	1:4G:290:GLU:OE2	2.35	0.45
2:5E:201:VAL:HG11	2:5E:377:MET:HE1	1.99	0.45
2:5H:7:VAL:HB	2:5H:135:ILE:HD13	1.98	0.45
2:5I:313:ALA:HB3	2:5I:349:MET:CE	2.47	0.45
1:2B:210:TYR:CE1	2:3B:324:LYS:HB2	2.51	0.45
1:2C:89:PRO:HD3	1:2D:282:TYR:CD2	2.52	0.45
1:2F:11:GLN:OE1	2:3F:247:ASN:ND2	2.49	0.45
1:2I:70:LEU:HD12	1:2I:99:ALA:HB2	1.98	0.45
2:3C:10:GLY:HA2	2:3C:143:THR:HG23	1.96	0.45
2:3F:98:GLY:CA	1:4F:254:GLU:HB3	2.47	0.45
2:3F:220:PRO:CG	1:4F:326:LYS:HE3	2.39	0.45
2:3G:5:VAL:HB	2:3G:133:PHE:CD1	2.52	0.45
2:3G:329:GLN:OE1	2:3G:332:ASN:ND2	2.42	0.45
2:3H:35:THR:OG1	2:3H:36:TYR:N	2.50	0.45
1:4A:100:ALA:O	2:5A:255:VAL:HG11	2.17	0.45
1:4F:401:LYS:HE2	2:5F:344:TRP:CD2	2.52	0.45
2:5B:172:SER:HB3	2:5B:205:GLU:CD	2.37	0.45
2:5D:150:LEU:CD2	2:5D:154:LYS:HD2	2.46	0.45
2:5F:202:ILE:HD11	2:5F:268:ILE:HG21	1.99	0.45
2:5I:354:CYS:SG	2:5I:355:ASP:N	2.90	0.45
1:2B:301:MET:SD	1:2B:307:PRO:HG3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2C:244:PHE:HB2	1:2C:356:ASN:HD21	1.82	0.45
2:3B:211:CYS:SG	2:3B:220:PRO:HB3	2.57	0.45
2:3E:294:PHE:HE1	2:3E:367:PHE:CE1	2.35	0.45
1:4A:105:ARG:NH2	2:5A:251:ARG:HH12	2.13	0.45
1:4C:107:HIS:NE2	1:4C:151:CYS:SG	2.89	0.45
1:4D:132:LEU:HG	1:4D:164:LYS:HD3	1.99	0.45
2:5C:284:LEU:CD2	2:5C:363:MET:HB2	2.46	0.45
2:5H:35:THR:OG1	2:5H:36:TYR:N	2.50	0.45
1:2G:186:ASN:OD1	1:2G:408:TYR:OH	2.34	0.45
2:3C:332:ASN:HD21	2:3C:336:LYS:NZ	2.15	0.45
2:3G:100:ASN:HB3	2:3G:103:LYS:HG2	1.98	0.45
2:3G:239:CYS:SG	2:3G:248:SER:N	2.89	0.45
1:4C:216:ASN:O	1:4C:280:LYS:HE2	2.17	0.45
1:4E:306:ASP:HB3	1:4E:309:HIS:CE1	2.51	0.45
1:4F:306:ASP:HB3	1:4F:309:HIS:CE1	2.51	0.45
2:5A:156:ARG:NH2	2:5A:197:ASP:OD1	2.50	0.45
2:5B:176:SER:OG	2:5B:181:GLU:OE1	2.34	0.45
2:5D:54:ALA:HA	2:5E:283:ALA:N	2.31	0.45
2:5F:173:PRO:HD3	2:5F:380:ARG:CZ	2.46	0.45
2:5G:309:ARG:H	2:5G:372:THR:HG22	1.81	0.45
1:2D:154:LEU:HB3	1:2D:197:HIS:HB3	1.98	0.45
1:2D:301:MET:HG3	1:2D:302:MET:H	1.81	0.45
1:2G:121:ARG:NH1	1:2G:121:ARG:HA	2.32	0.45
2:3A:133:PHE:HB2	2:3A:164:MET:HB3	1.99	0.45
2:3B:248:SER:HA	2:3B:252:LYS:HG2	1.98	0.45
2:3D:113:ILE:HA	2:3D:116:VAL:HG12	1.99	0.45
2:5A:358:PRO:HG2	2:5A:361:LEU:HB3	1.98	0.45
2:5E:239:CYS:SG	2:5E:248:SER:N	2.85	0.45
2:5G:267:LEU:HD21	2:5G:374:ILE:CG2	2.47	0.45
1:2A:265:ILE:HG23	1:2A:432:TYR:HE1	1.82	0.45
1:2D:102:ASN:ND2	1:2D:411:GLU:OE1	2.50	0.45
1:2E:195:LEU:HD22	1:2E:264:ARG:HG3	1.99	0.45
1:2I:88:HIS:HB3	1:2I:91:GLN:HG3	1.99	0.45
2:3B:20:PHE:HA	2:3B:230:SER:OG	2.17	0.45
2:3D:323:THR:O	2:3D:326:VAL:HG12	2.16	0.45
2:3E:67:ASP:OD1	2:3E:68:LEU:N	2.50	0.45
2:3I:10:GLY:HA2	2:3I:143:THR:HG23	1.98	0.45
1:4A:306:ASP:HB3	1:4A:309:HIS:CE1	2.51	0.45
1:4D:35:GLN:OE1	1:4E:282:TYR:CZ	2.70	0.45
1:4G:172:TRP:HB3	1:4G:205:ASP:OD1	2.17	0.45
1:4H:142:GLY:HA2	1:4H:183:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5B:7:VAL:HG11	2:5B:151:LEU:HD22	1.99	0.45
2:5B:211:CYS:SG	2:5B:220:PRO:HG3	2.56	0.45
2:5C:368:VAL:HG23	2:5C:368:VAL:O	2.17	0.45
2:5E:238:CYS:SG	2:5E:318:ARG:NE	2.90	0.45
2:5I:318:ARG:HD3	2:5I:356:ILE:O	2.16	0.45
1:2F:298:PRO:HB3	1:2F:307:PRO:HD2	1.98	0.44
1:2H:269:LEU:HD21	1:2H:384:ILE:HD11	1.97	0.44
1:2I:195:LEU:HD21	1:2I:264:ARG:HE	1.81	0.44
2:3C:391:ARG:HD2	1:4C:346:TRP:CD1	2.53	0.44
2:3E:397:TRP:CZ2	1:4E:260:VAL:CG2	2.99	0.44
2:3H:117:LEU:HD13	2:3H:154:LYS:HG2	1.99	0.44
1:4B:183:GLU:HG3	1:4B:184:PRO:HD3	1.99	0.44
1:4C:215:ARG:NH2	1:4C:300:SER:HB2	2.32	0.44
1:4F:269:LEU:HD12	1:4F:384:ILE:HD11	1.98	0.44
1:4I:88:HIS:HB3	1:4I:91:GLN:HG3	1.99	0.44
2:5D:54:ALA:HB1	2:5E:281:TYR:O	2.16	0.44
1:2A:225:THR:O	1:2A:229:ARG:HG2	2.17	0.44
1:2E:33:ASP:OD1	1:2E:34:GLY:N	2.51	0.44
1:2H:122:ILE:HG21	1:2H:157:LEU:HD11	2.00	0.44
2:3B:68:LEU:HD13	2:3B:143:THR:OG1	2.16	0.44
2:3D:27:GLU:OE1	2:3D:318:ARG:NH2	2.46	0.44
2:3F:113:ILE:HA	2:3F:116:VAL:HG12	2.00	0.44
2:3F:317:PHE:HB3	2:3F:321:MET:HE1	1.99	0.44
2:3H:318:ARG:HD3	2:3H:358:PRO:HD3	1.99	0.44
1:4B:210:TYR:CE1	2:5B:324:LYS:HB2	2.53	0.44
1:4D:204:LEU:HD13	1:4D:231:ILE:HD12	1.98	0.44
1:4I:246:GLY:HA2	1:4I:357:TYR:CD1	2.52	0.44
1:4I:250:VAL:HG23	1:4I:254:GLU:HG2	1.99	0.44
2:5D:58:ARG:HH11	2:5E:280:GLN:HB2	1.82	0.44
1:2A:271:SER:HB3	1:2A:377:MET:HB3	2.00	0.44
1:2F:259:LEU:HD21	1:2F:316:CYS:HB2	1.99	0.44
1:2I:220:GLU:O	2:3I:324:LYS:HD3	2.17	0.44
2:3B:169:VAL:HG12	2:3B:202:ILE:HB	1.99	0.44
2:3G:334:GLN:HG3	2:3G:341:PHE:CD2	2.53	0.44
2:3H:211:CYS:HA	2:3H:215:LEU:HB2	2.00	0.44
2:3I:165:GLU:HG2	2:3I:198:GLU:HG3	2.00	0.44
1:4B:250:VAL:HA	1:4B:254:GLU:HG2	2.00	0.44
1:4D:262:TYR:HB2	1:4D:265:ILE:HD12	2.00	0.44
1:4F:107:HIS:NE2	1:4F:151:CYS:SG	2.90	0.44
2:5A:30:ILE:HD12	2:5A:51:TYR:HE2	1.82	0.44
2:5A:77:ARG:HH22	2:5A:92:PHE:HZ	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5C:87:PRO:CA	2:5D:281:TYR:OH	2.65	0.44
2:5C:169:VAL:HG12	2:5C:202:ILE:HB	1.98	0.44
1:2A:306:ASP:HB3	1:2A:309:HIS:CE1	2.52	0.44
1:2B:338:LYS:HE3	1:2B:338:LYS:HB3	1.91	0.44
1:2C:271:SER:OG	1:2C:377:MET:HB3	2.18	0.44
2:3H:257:LEU:HD21	2:3H:314:SER:HB2	2.00	0.44
2:3I:137:HIS:HE1	2:3I:166:THR:HG23	1.82	0.44
1:4A:265:ILE:HG23	1:4A:432:TYR:HE1	1.81	0.44
1:4C:392:ASP:OD1	1:4C:422:ARG:NH1	2.50	0.44
2:5A:268:ILE:HB	2:5A:300:MET:HE2	1.99	0.44
2:5B:139:LEU:HA	2:5B:145:SER:HB2	2.00	0.44
2:5D:267:LEU:HD11	2:5D:374:ILE:CG2	2.47	0.44
2:5F:55:THR:CG2	2:5G:283:ALA:CA	2.90	0.44
2:5H:187:LEU:HD13	2:5H:190:HIS:HE1	1.82	0.44
2:5I:67:ASP:OD1	2:5I:68:LEU:N	2.50	0.44
1:2B:164:LYS:HB3	1:2B:164:LYS:HE3	1.74	0.44
1:2C:221:ARG:HG3	2:3C:325:GLU:OE1	2.18	0.44
1:2F:217:LEU:HD21	1:2F:275:ILE:HG22	1.99	0.44
1:2F:401:LYS:NZ	2:3F:344:TRP:CG	2.83	0.44
1:2I:10:GLY:HA2	1:2I:145:THR:HG23	1.99	0.44
1:2I:339:ARG:NH1	1:2I:342:GLN:OE1	2.51	0.44
2:3A:398:TYR:HB3	2:3A:403:MET:HG3	1.99	0.44
2:3D:257:LEU:HD23	2:3D:312:THR:HG22	1.99	0.44
2:3D:383:ASP:HA	2:3D:386:THR:HG22	2.00	0.44
2:3G:178:THR:HA	1:4G:352:LYS:HD3	2.00	0.44
1:4C:50:ASN:O	1:4C:64:ARG:NH2	2.50	0.44
1:4I:188:VAL:HG23	1:4I:189:LEU:HD12	1.99	0.44
2:5C:16:ILE:HD11	2:5C:229:VAL:HG11	1.99	0.44
2:5G:53:GLU:OE2	2:5G:54:ALA:N	2.48	0.44
2:5G:325:GLU:HA	2:5G:328:GLU:HG2	1.99	0.44
2:5H:200:GLN:HG3	2:5H:268:ILE:HD11	1.98	0.44
2:5H:267:LEU:HD11	2:5H:374:ILE:HD13	1.98	0.44
2:5I:241:ARG:HH11	2:5I:241:ARG:HD2	1.67	0.44
1:2D:390:ARG:NH2	1:2D:390:ARG:HB3	2.32	0.44
1:2F:28:HIS:CE1	1:2F:243:ARG:HH11	2.36	0.44
1:2G:154:LEU:HD21	1:2G:198:THR:HB	1.99	0.44
1:2I:241:SER:OG	1:2I:250:VAL:O	2.23	0.44
2:3A:109:GLY:O	2:3A:113:ILE:HG12	2.17	0.44
2:3A:391:ARG:NH2	1:4A:346:TRP:NE1	2.66	0.44
2:3F:7:VAL:HB	2:3F:135:ILE:HG12	1.99	0.44
2:3F:137:HIS:HE1	2:3F:166:THR:HB	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:175:PRO:HA	1:4A:390:ARG:NE	2.33	0.44
1:4E:269:LEU:HD23	1:4E:303:ALA:HB3	1.98	0.44
1:4G:427:ALA:O	1:4G:430:LYS:HG3	2.17	0.44
1:4H:155:GLU:HG2	1:4H:197:HIS:CD2	2.53	0.44
2:5D:55:THR:OG1	2:5E:283:ALA:CA	2.66	0.44
1:2D:57:GLY:N	1:2E:285:GLN:HB3	2.31	0.44
1:2D:223:THR:OG1	2:3D:245:GLN:OE1	2.34	0.44
1:2E:225:THR:O	1:2E:229:ARG:HG2	2.18	0.44
1:2H:12:ALA:HB3	1:2H:140:ALA:HB2	1.99	0.44
1:2I:100:ALA:O	2:3I:255:VAL:HG11	2.17	0.44
2:3A:208:TYR:CD1	1:4A:326:LYS:HB3	2.52	0.44
1:4B:88:HIS:ND1	1:4C:283:HIS:CB	2.80	0.44
1:4D:56:THR:HA	1:4E:285:GLN:CB	2.47	0.44
2:5D:113:ILE:HA	2:5D:116:VAL:HG12	1.99	0.44
2:5H:211:CYS:HA	2:5H:215:LEU:HB2	2.00	0.44
1:2A:212:ILE:HD11	1:2A:300:SER:HA	1.99	0.44
1:2B:269:LEU:HD23	1:2B:303:ALA:HB3	1.99	0.44
1:2H:222:PRO:HD2	2:3H:324:LYS:HG2	2.00	0.44
2:3A:186:THR:HG23	2:3A:415:MET:HE2	2.00	0.44
2:3H:309:ARG:H	2:3H:372:THR:HG22	1.83	0.44
1:4G:121:ARG:NH1	1:4G:121:ARG:HA	2.33	0.44
2:5E:201:VAL:HG11	2:5E:377:MET:CE	2.47	0.44
2:5E:383:ASP:HA	2:5E:386:THR:HG22	1.98	0.44
2:5G:1:MET:N	2:5G:128:ASP:OD2	2.41	0.44
2:5I:6:HIS:CD2	2:5I:8:GLN:HG3	2.53	0.44
1:2D:204:LEU:HD13	1:2D:231:ILE:HD12	1.99	0.44
1:2F:323:VAL:HG13	1:2F:323:VAL:O	2.18	0.44
1:2I:252:VAL:HG22	1:2I:252:VAL:O	2.18	0.44
2:3B:105:HIS:HD2	2:3B:150:LEU:HD22	1.83	0.44
2:3B:139:LEU:HA	2:3B:145:SER:HB2	1.99	0.44
2:3B:156:ARG:HD2	2:3B:156:ARG:HA	1.86	0.44
2:3C:16:ILE:HG22	2:3C:136:THR:HG21	2.00	0.44
2:3E:317:PHE:CD2	2:3E:365:VAL:HG22	2.53	0.44
2:3H:200:GLN:HG3	2:3H:268:ILE:HD11	2.00	0.44
1:4A:9:VAL:HG13	1:4A:149:LEU:HD23	2.00	0.44
1:4E:225:THR:O	1:4E:229:ARG:HG2	2.18	0.44
2:5D:12:CYS:SG	2:5D:138:SER:N	2.91	0.44
2:5G:83:GLN:N	2:5G:83:GLN:OE1	2.51	0.44
1:2F:7:ILE:HG21	1:2F:153:LEU:HD21	2.00	0.43
1:2G:195:LEU:HD21	1:2G:264:ARG:HE	1.83	0.43
1:2G:217:LEU:HD23	1:2G:217:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:309:ARG:H	2:3B:372:THR:HG22	1.83	0.43
2:3B:326:VAL:O	2:3B:330:MET:HG2	2.18	0.43
2:3D:178:THR:HA	1:4D:352:LYS:HD3	2.00	0.43
2:3E:325:GLU:HA	2:3E:328:GLU:HG2	1.99	0.43
2:3F:101:TRP:HB3	2:3F:398:TYR:HE1	1.82	0.43
1:4A:60:LYS:HE3	1:4A:60:LYS:HB3	1.90	0.43
1:4G:198:THR:O	1:4G:266:HIS:NE2	2.51	0.43
1:4G:276:ILE:HD12	1:4G:281:ALA:HA	1.99	0.43
1:4H:259:LEU:HD21	1:4H:316:CYS:HB2	2.00	0.43
1:4H:425:LEU:HD23	1:4H:425:LEU:HA	1.87	0.43
1:4I:108:TYR:O	1:4I:112:LYS:NZ	2.50	0.43
1:4I:223:THR:HG22	2:5I:322:SER:HA	2.00	0.43
2:5D:200:GLN:HG2	2:5D:268:ILE:HD11	2.00	0.43
2:5G:5:VAL:HB	2:5G:133:PHE:HD1	1.83	0.43
2:3A:105:HIS:CD2	2:3A:150:LEU:HD12	2.51	0.43
2:3D:267:LEU:HD21	2:3D:374:ILE:CG2	2.48	0.43
2:3E:309:ARG:H	2:3E:372:THR:HG22	1.82	0.43
2:3F:220:PRO:CG	1:4F:326:LYS:HG3	2.44	0.43
2:3F:244:GLY:HA2	2:3F:355:ASP:HB2	2.00	0.43
2:3G:203:ASP:O	2:3G:207:LEU:HD13	2.18	0.43
1:4B:70:LEU:HD23	1:4B:145:THR:OG1	2.18	0.43
1:4B:107:HIS:NE2	1:4B:151:CYS:SG	2.84	0.43
1:2A:292:THR:HG21	1:2A:331:ALA:HB1	2.00	0.43
1:2B:272:TYR:HB3	1:2B:275:ILE:HD11	2.00	0.43
1:2B:309:HIS:NE2	1:2B:386:GLU:OE1	2.40	0.43
1:2C:88:HIS:HD1	1:2C:90:GLU:H	1.65	0.43
1:2E:265:ILE:HD11	1:2E:435:VAL:HG21	1.99	0.43
1:2G:398:MET:HE1	2:3G:346:PRO:HD2	2.00	0.43
2:3A:28:HIS:HB2	2:3A:30:ILE:HD12	2.00	0.43
2:3C:394:PHE:HD1	2:3C:397:TRP:HZ3	1.66	0.43
2:3F:170:PHE:HD1	2:3F:171:PRO:HD2	1.83	0.43
1:4A:338:LYS:HG2	1:4A:340:THR:HG22	2.00	0.43
1:4F:175:PRO:HB3	1:4F:390:ARG:HD3	2.00	0.43
2:5G:68:LEU:HD13	2:5G:93:GLY:HA3	1.99	0.43
1:2A:214:ARG:HH22	1:2A:220:GLU:HG2	1.83	0.43
1:2B:352:LYS:HD3	1:2B:352:LYS:HA	1.87	0.43
1:2D:402:ARG:HG3	1:2D:405:VAL:CG2	2.48	0.43
1:2F:15:GLN:HE21	1:2F:74:VAL:CG2	2.32	0.43
1:2G:205:ASP:HB2	1:2G:303:ALA:HA	2.01	0.43
2:3F:203:ASP:O	2:3F:207:LEU:HD23	2.18	0.43
2:3F:353:VAL:HG13	2:3F:353:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3G:164:MET:SD	2:3G:196:ALA:HA	2.58	0.43
2:3H:392:LYS:HA	2:3H:395:LEU:HD23	1.99	0.43
1:4D:225:THR:O	1:4D:229:ARG:HG2	2.19	0.43
1:4D:276:ILE:HD12	1:4D:281:ALA:HA	2.01	0.43
1:4G:309:HIS:HE2	1:4G:386:GLU:CD	2.22	0.43
1:4H:205:ASP:HB2	1:4H:303:ALA:HA	2.00	0.43
2:5B:420:SER:O	2:5B:424:GLN:HG3	2.19	0.43
2:5D:54:ALA:HB1	2:5E:282:ARG:C	2.39	0.43
2:5D:124:ALA:HB1	2:5D:130:LEU:HD22	2.01	0.43
2:5G:107:THR:OG1	2:5G:401:GLU:OE2	2.29	0.43
1:2C:166:LYS:N	1:2C:199:ASP:OD2	2.48	0.43
1:2C:282:TYR:HB2	1:2C:283:HIS:CD2	2.53	0.43
1:2D:85:HIS:HB3	1:2E:283:HIS:NE2	2.33	0.43
1:2D:133:GLN:NE2	1:2D:251:ASP:OD1	2.52	0.43
2:3B:394:PHE:CE1	1:4B:261:PRO:HB3	2.53	0.43
2:3C:156:ARG:NH1	2:3C:162:ARG:O	2.51	0.43
2:3E:94:GLN:OE1	1:4E:2:ARG:HG3	2.18	0.43
1:4B:223:THR:CG2	1:4B:225:THR:HG22	2.47	0.43
1:4E:391:MET:HE3	1:4E:391:MET:HB2	1.85	0.43
1:4I:183:GLU:HG3	1:4I:184:PRO:HD3	1.99	0.43
2:5D:54:ALA:CA	2:5E:283:ALA:N	2.81	0.43
1:2A:210:TYR:HE2	2:3A:327:ASP:OD2	2.01	0.43
1:2B:306:ASP:HB3	1:2B:309:HIS:HE1	1.83	0.43
1:2C:311:LYS:NZ	1:2C:342:GLN:OE1	2.47	0.43
1:2G:153:LEU:O	1:2G:157:LEU:HD23	2.18	0.43
1:2H:210:TYR:HE1	1:2H:227:LEU:HD11	1.84	0.43
1:2I:269:LEU:CD2	1:2I:384:ILE:HD11	2.47	0.43
2:3D:16:ILE:HG22	2:3D:136:THR:HG21	2.01	0.43
2:3D:176:SER:HB2	1:4D:349:THR:OG1	2.18	0.43
2:3E:68:LEU:HB3	2:3E:96:GLY:HA2	2.01	0.43
2:3G:169:VAL:HG12	2:3G:202:ILE:HB	1.99	0.43
2:3G:207:LEU:HB3	2:3G:225:LEU:CD1	2.48	0.43
2:3G:209:ASP:HA	2:3G:212:PHE:CD2	2.54	0.43
1:4F:7:ILE:HG21	1:4F:153:LEU:HD21	2.00	0.43
1:4G:28:HIS:HE1	1:4G:243:ARG:HD2	1.84	0.43
1:4H:358:GLN:OE1	1:4H:359:PRO:HD2	2.18	0.43
2:5A:117:LEU:HB3	2:5A:121:ARG:HH22	1.83	0.43
2:5C:293:MET:HG3	2:5C:367:PHE:HB2	2.01	0.43
2:5D:58:ARG:HD3	2:5E:280:GLN:O	2.01	0.43
2:5G:165:GLU:HG3	2:5G:198:GLU:HG3	1.99	0.43
1:2D:181:VAL:H	2:3D:256:ASN:HD22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2F:98:ASP:OD1	1:2F:99:ALA:N	2.52	0.43
1:2F:164:LYS:O	1:2F:166:LYS:NZ	2.51	0.43
2:3B:303:SER:HB3	2:3B:377:MET:HE3	2.00	0.43
2:3E:165:GLU:HG3	2:3E:198:GLU:HG3	2.00	0.43
2:3E:238:CYS:SG	2:3E:318:ARG:NE	2.92	0.43
1:4C:224:TYR:HD1	1:4C:227:LEU:HD12	1.84	0.43
1:4E:181:VAL:HG21	2:5E:256:ASN:O	2.18	0.43
2:5A:237:THR:O	2:5A:241:ARG:NH1	2.51	0.43
2:5C:141:GLY:O	2:5C:145:SER:OG	2.32	0.43
2:5C:257:LEU:HD11	2:5C:368:VAL:CG2	2.48	0.43
2:5G:100:ASN:HB3	2:5G:103:LYS:HG2	1.99	0.43
2:5H:69:GLU:HG2	2:5H:71:GLY:H	1.83	0.43
2:5H:141:GLY:O	2:5H:145:SER:OG	2.27	0.43
2:5H:274:THR:OG1	2:5H:279:GLN:OE1	2.32	0.43
1:2I:77:GLU:OE1	2:3I:243:PRO:HB3	2.18	0.43
1:4A:223:THR:O	1:4A:227:LEU:HD23	2.18	0.43
1:4F:210:TYR:CG	2:5F:324:LYS:HD2	2.54	0.43
1:4G:168:ASN:ND2	1:4G:194:LEU:HD11	2.20	0.43
1:4H:105:ARG:HH21	1:4H:110:ILE:HG21	1.84	0.43
1:4H:141:VAL:HG21	1:4H:172:TRP:CZ3	2.53	0.43
2:5F:10:GLY:O	2:5F:14:ASN:ND2	2.51	0.43
2:5G:295:ASP:HB3	2:5G:298:ASN:HB2	2.01	0.43
2:5H:318:ARG:HD3	2:5H:358:PRO:HD3	1.99	0.43
1:2A:88:HIS:HB3	1:2A:91:GLN:NE2	2.33	0.43
1:2C:183:GLU:HG3	1:2C:184:PRO:HD3	2.01	0.43
1:2F:241:SER:OG	1:2F:250:VAL:O	2.22	0.43
1:2H:225:THR:O	1:2H:229:ARG:HG2	2.18	0.43
1:2H:259:LEU:HD21	1:2H:316:CYS:HB2	2.01	0.43
2:3F:330:MET:CB	2:3F:349:MET:SD	3.04	0.43
2:3I:169:VAL:HG12	2:3I:202:ILE:HB	2.01	0.43
1:4F:370:LYS:O	1:4F:370:LYS:HG3	2.18	0.43
2:5A:67:ASP:OD1	2:5A:68:LEU:N	2.48	0.43
2:5D:176:SER:OG	2:5D:181:GLU:HG3	2.19	0.43
1:2C:98:ASP:OD1	1:2C:99:ALA:N	2.52	0.43
1:2D:119:LEU:HA	1:2D:122:ILE:HG22	2.01	0.43
1:2I:269:LEU:HD21	1:2I:384:ILE:CD1	2.49	0.43
2:3A:139:LEU:HD23	2:3A:139:LEU:HA	1.87	0.43
2:3C:20:PHE:HA	2:3C:230:SER:OG	2.19	0.43
2:3E:155:VAL:HG13	2:3E:164:MET:HE1	2.00	0.43
2:3G:151:LEU:HD12	2:3G:151:LEU:HA	1.90	0.43
1:4B:181:VAL:N	2:5B:350:LYS:HZ2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4G:177:VAL:HB	1:4G:207:GLU:HB3	2.01	0.43
1:4G:251:ASP:N	1:4G:254:GLU:OE2	2.40	0.43
1:4G:298:PRO:O	1:4G:301:MET:SD	2.77	0.43
2:5E:139:LEU:HD12	2:5E:170:PHE:HE1	1.83	0.43
2:5F:268:ILE:HG23	2:5F:300:MET:HB2	2.01	0.43
1:2D:11:GLN:NE2	1:2D:15:GLN:OE1	2.44	0.42
1:2D:60:LYS:HZ1	1:2E:283:HIS:CD2	2.33	0.42
1:2G:222:PRO:HD2	2:3G:324:LYS:HB3	2.01	0.42
1:2I:239:THR:OG1	1:2I:243:ARG:NH1	2.52	0.42
2:3C:103:LYS:HG2	2:3C:108:GLU:HG2	2.01	0.42
2:3E:58:ARG:HD2	2:3F:281:TYR:CD1	2.52	0.42
2:3G:68:LEU:HD12	2:3G:97:ALA:HB2	2.01	0.42
2:3G:320:ARG:NH1	2:3G:320:ARG:HB2	2.34	0.42
2:5C:295:ASP:OD2	2:5C:297:LYS:HG2	2.19	0.42
2:5D:150:LEU:HD23	2:5D:154:LYS:HD2	2.01	0.42
2:5E:318:ARG:HB3	2:5E:357:PRO:HA	2.00	0.42
2:5F:192:LEU:HD21	2:5F:199:VAL:HG11	2.01	0.42
2:5G:10:GLY:HA2	2:5G:143:THR:OG1	2.19	0.42
1:2A:76:ASP:OD2	2:3A:46:ARG:NH1	2.52	0.42
1:2D:222:PRO:HD2	2:3D:324:LYS:HE3	2.01	0.42
1:2F:306:ASP:HB3	1:2F:309:HIS:CE1	2.54	0.42
1:2H:109:THR:OG1	1:2H:110:ILE:N	2.52	0.42
2:3B:94:GLN:C	1:4B:2:ARG:HH22	2.22	0.42
2:3C:141:GLY:O	2:3C:145:SER:OG	2.33	0.42
2:3D:117:LEU:HA	2:3D:120:VAL:HG12	1.99	0.42
2:3F:19:LYS:HA	2:3F:22:GLU:OE1	2.19	0.42
2:3H:149:THR:O	2:3H:191:GLN:NE2	2.52	0.42
1:4G:26:LEU:HD21	1:4G:363:VAL:HG12	2.00	0.42
2:5B:68:LEU:HD23	2:5B:112:LEU:HD13	2.01	0.42
2:5F:55:THR:HG23	2:5G:283:ALA:CA	2.48	0.42
1:2A:96:LYS:CG	2:3A:129:CYS:SG	3.07	0.42
1:2B:224:TYR:HA	1:2B:227:LEU:HD23	2.02	0.42
1:2D:298:PRO:HG2	1:2D:308:ARG:HH11	1.84	0.42
1:2E:97:GLU:OE2	2:3E:162:ARG:NH1	2.51	0.42
1:2H:31:GLN:HG2	1:2H:35:GLN:O	2.19	0.42
2:3B:105:HIS:CD2	2:3B:150:LEU:HB2	2.53	0.42
2:3D:69:GLU:OE2	2:3D:96:GLY:HA3	2.19	0.42
2:3F:320:ARG:HD2	2:3F:320:ARG:HA	1.79	0.42
1:4A:26:LEU:HD21	1:4A:363:VAL:HG12	2.00	0.42
1:4B:181:VAL:N	2:5B:350:LYS:HE3	2.29	0.42
1:4F:98:ASP:OD1	1:4F:99:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4G:121:ARG:HH11	1:4G:121:ARG:HD2	1.69	0.42
2:5B:87:PRO:CD	2:5C:281:TYR:HE2	2.25	0.42
2:5F:140:GLY:O	2:5F:184:ASN:ND2	2.49	0.42
2:5F:309:ARG:H	2:5F:372:THR:HG22	1.84	0.42
2:5H:113:ILE:HA	2:5H:116:VAL:HG12	2.01	0.42
2:5I:13:GLY:HA2	2:5I:136:THR:HG22	2.01	0.42
2:5I:246:LEU:HA	2:5I:246:LEU:HD12	1.81	0.42
1:2A:296:PHE:CZ	1:2A:317:LEU:HD21	2.55	0.42
1:2B:10:GLY:HA2	1:2B:145:THR:HG23	2.01	0.42
1:2B:221:ARG:CZ	2:3B:322:SER:OG	2.67	0.42
1:2B:404:PHE:HZ	2:3B:312:THR:HG21	1.85	0.42
1:2C:65:CYS:SG	1:2C:66:VAL:N	2.93	0.42
1:2D:60:LYS:HE2	1:2E:283:HIS:CD2	2.45	0.42
1:2D:178:SER:CB	2:3D:347:ASN:ND2	2.82	0.42
1:2D:259:LEU:HD21	1:2D:316:CYS:HB2	2.01	0.42
1:2E:60:LYS:HZ3	1:2F:283:HIS:CD2	2.37	0.42
1:2F:154:LEU:HB3	1:2F:197:HIS:HB3	2.01	0.42
1:2G:401:LYS:HE3	2:3G:344:TRP:CE2	2.54	0.42
1:2I:52:PHE:CD2	1:2I:243:ARG:HD3	2.54	0.42
2:3B:206:ALA:HB2	2:3B:302:ALA:HB2	2.00	0.42
2:3C:131:GLN:OE1	2:3C:163:ILE:HD11	2.20	0.42
2:3D:8:GLN:NE2	2:3D:65:LEU:HD22	2.34	0.42
2:3E:155:VAL:HG13	2:3E:164:MET:CE	2.50	0.42
2:3H:372:THR:HA	2:3H:422:TYR:CD2	2.54	0.42
1:4D:2:ARG:HG3	1:4D:51:THR:HG22	2.00	0.42
1:4E:294:SER:O	1:4E:297:GLU:HG2	2.19	0.42
1:4F:145:THR:O	1:4F:149:LEU:HB2	2.20	0.42
1:4G:14:ILE:HD12	1:4G:67:PHE:CD1	2.55	0.42
1:4H:100:ALA:O	2:5H:255:VAL:HG11	2.20	0.42
2:5A:404:ASP:HB3	2:5A:406:MET:HG3	2.01	0.42
2:5F:7:VAL:HB	2:5F:135:ILE:HG12	2.02	0.42
2:5I:8:GLN:O	2:5I:66:MET:HB2	2.19	0.42
1:2B:71:GLU:HB3	1:2B:98:ASP:HB2	2.02	0.42
1:2B:256:GLN:HE21	1:2B:256:GLN:N	2.17	0.42
1:2E:261:PRO:HG3	1:2E:313:MET:HE2	2.02	0.42
1:2G:60:LYS:HD2	1:2H:283:HIS:CD2	2.52	0.42
1:2H:398:MET:HE1	2:3H:345:ILE:HA	2.01	0.42
2:3I:179:VAL:HG22	1:4I:258:ASN:OD1	2.19	0.42
1:4G:79:ARG:NH1	1:4G:92:LEU:O	2.53	0.42
1:4G:100:ALA:HA	2:5G:252:LYS:HB3	2.00	0.42
1:4H:35:GLN:OE1	1:4H:35:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5E:321:MET:HE1	2:5E:353:VAL:HG13	2.01	0.42
2:5G:200:GLN:HB3	2:5G:266:PHE:HB2	2.02	0.42
1:2B:109:THR:HG23	1:2B:411:GLU:OE1	2.20	0.42
1:2D:81:GLY:O	1:2D:84:ARG:HG3	2.19	0.42
1:2F:170:CYS:HB2	1:2F:203:MET:HE1	2.01	0.42
1:2H:269:LEU:HD21	1:2H:384:ILE:CD1	2.49	0.42
2:3G:135:ILE:CD1	2:3G:152:ILE:HD11	2.45	0.42
2:3H:25:SER:HB2	2:3H:30:ILE:HG22	2.01	0.42
2:3H:391:ARG:NH2	1:4H:437:ILE:O	2.52	0.42
1:4B:213:CYS:SG	1:4B:222:PRO:HG3	2.60	0.42
1:4C:406:HIS:HA	1:4C:409:VAL:HG12	2.01	0.42
1:4D:393:HIS:O	1:4D:397:LEU:HD13	2.19	0.42
1:4E:60:LYS:HD3	1:4F:283:HIS:HA	2.01	0.42
1:4I:107:HIS:CE1	1:4I:151:CYS:HB3	2.55	0.42
2:5D:267:LEU:HB3	2:5D:299:MET:CE	2.46	0.42
2:5E:64:ILE:HD11	2:5E:123:GLU:HG3	2.01	0.42
2:5G:19:LYS:HD2	2:5G:227:HIS:ND1	2.35	0.42
2:5G:135:ILE:CD1	2:5G:152:ILE:HG12	2.49	0.42
2:5I:16:ILE:CG2	2:5I:136:THR:HG21	2.49	0.42
1:2C:386:GLU:OE1	1:2C:390:ARG:NH1	2.53	0.42
1:2E:338:LYS:HG2	1:2E:340:THR:HG22	2.02	0.42
1:2I:152:LEU:O	1:2I:155:GLU:HG3	2.18	0.42
2:3E:180:VAL:O	2:3E:184:ASN:ND2	2.52	0.42
2:3E:383:ASP:HA	2:3E:386:THR:HG22	2.00	0.42
1:4C:209:ILE:CD1	1:4C:302:MET:HG3	2.47	0.42
1:4E:326:LYS:NZ	1:4E:327:ASP:OD1	2.40	0.42
1:4G:114:ILE:HD12	1:4G:114:ILE:HA	1.92	0.42
2:5D:58:ARG:HD2	2:5E:280:GLN:C	2.36	0.42
2:5H:309:ARG:H	2:5H:372:THR:HG22	1.85	0.42
1:2A:100:ALA:O	2:3A:255:VAL:HG11	2.20	0.42
1:2E:172:TRP:NE1	1:2E:391:MET:SD	2.90	0.42
1:2F:153:LEU:O	1:2F:157:LEU:HD23	2.20	0.42
2:3D:326:VAL:O	2:3D:330:MET:HG2	2.20	0.42
2:3E:282:ARG:NH2	2:3E:292:GLN:OE1	2.48	0.42
2:3F:311:LEU:HD12	2:3F:342:VAL:HG11	2.01	0.42
1:4F:298:PRO:HB3	1:4F:307:PRO:HD2	2.02	0.42
1:4G:177:VAL:HG13	2:5G:327:ASP:CB	2.49	0.42
1:4H:313:MET:HE1	1:4H:344:VAL:HG21	2.01	0.42
1:4H:414:GLU:HG2	1:4H:417:GLU:OE2	2.20	0.42
2:5A:7:VAL:HG11	2:5A:151:LEU:HD23	2.01	0.42
2:5A:249:ASP:H	2:5A:252:LYS:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5B:309:ARG:NH2	2:5B:343:GLU:OE2	2.53	0.42
2:5D:107:THR:HG1	2:5D:108:GLU:CD	2.22	0.42
2:5E:385:PHE:HE2	2:5E:412:GLU:HB2	1.84	0.42
2:5F:407:GLU:HA	2:5F:410:GLU:HG3	2.02	0.42
2:5G:6:HIS:CD2	2:5G:134:GLN:HG3	2.55	0.42
1:2D:98:ASP:OD1	1:2D:99:ALA:N	2.52	0.42
1:2H:121:ARG:HD2	1:2H:121:ARG:HA	1.75	0.42
1:2H:176:GLN:O	2:3H:347:ASN:ND2	2.53	0.42
1:2I:151:CYS:HG	1:2I:193:SER:HG	1.29	0.42
2:3A:135:ILE:HB	2:3A:166:THR:HG22	2.02	0.42
2:3C:211:CYS:HB3	2:3C:220:PRO:HG3	2.02	0.42
2:3D:267:LEU:HD21	2:3D:374:ILE:HG22	2.02	0.42
2:3F:54:ALA:O	2:3G:280:GLN:O	2.38	0.42
2:3F:236:VAL:HG13	2:3F:237:THR:HG23	2.02	0.42
2:3H:16:ILE:HG22	2:3H:136:THR:HG21	2.01	0.42
2:3H:130:LEU:HD11	2:3H:133:PHE:HE1	1.85	0.42
2:3H:295:ASP:HB3	2:3H:297:LYS:HG2	2.01	0.42
2:3H:330:MET:HB3	2:3H:349:MET:HG2	2.02	0.42
1:4B:64:ARG:HB3	1:4B:125:LEU:HD21	2.02	0.42
1:4I:81:GLY:O	1:4I:84:ARG:HG3	2.19	0.42
2:5B:67:ASP:OD1	2:5B:68:LEU:N	2.50	0.42
2:5C:10:GLY:HA2	2:5C:143:THR:HG23	2.02	0.42
2:5D:2:ARG:HD3	2:5D:240:LEU:HD22	2.02	0.42
2:5E:237:THR:HG22	2:5E:250:LEU:HD21	2.02	0.42
2:5F:27:GLU:OE1	2:5F:318:ARG:NH2	2.47	0.42
2:5G:167:PHE:HZ	2:5G:236:VAL:HG11	1.85	0.42
2:5I:5:VAL:HB	2:5I:133:PHE:HD1	1.85	0.42
1:2A:269:LEU:CD2	1:2A:384:ILE:HD11	2.50	0.42
1:2A:323:VAL:CG1	1:2A:355:ILE:HG23	2.50	0.42
1:2F:189:LEU:HD11	1:2F:418:PHE:CD1	2.55	0.42
2:3C:77:ARG:HH22	2:3C:92:PHE:HZ	1.67	0.42
2:3D:112:LEU:HD12	2:3D:112:LEU:HA	1.92	0.42
2:3E:73:MET:HG2	2:3E:90:PHE:HD2	1.85	0.42
2:3G:186:THR:O	2:3G:189:VAL:HG12	2.20	0.42
1:4E:276:ILE:HD12	1:4E:281:ALA:HA	2.02	0.42
2:5D:139:LEU:HD12	2:5D:170:PHE:CE1	2.55	0.42
2:5E:68:LEU:HD12	2:5E:143:THR:HG22	2.02	0.42
2:5E:172:SER:HB3	2:5E:205:GLU:HG2	2.02	0.42
2:5G:55:THR:CG2	2:5H:283:ALA:CB	2.98	0.42
2:5G:138:SER:HA	2:5G:169:VAL:HG22	2.01	0.42
1:2A:398:MET:HE2	2:3A:345:ILE:HG23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2E:6:SER:OG	1:2E:8:HIS:NE2	2.52	0.41
1:2E:81:GLY:O	1:2E:84:ARG:HG3	2.20	0.41
1:2E:145:THR:O	1:2E:149:LEU:HB2	2.20	0.41
1:2F:403:ALA:HB2	2:3F:344:TRP:HZ3	1.84	0.41
2:3C:388:MET:HG2	1:4C:346:TRP:O	2.19	0.41
2:3C:397:TRP:CZ2	1:4C:260:VAL:HB	2.54	0.41
2:3F:189:VAL:HG11	2:3F:415:MET:SD	2.60	0.41
2:3G:113:ILE:HA	2:3G:116:VAL:HG12	2.02	0.41
2:3H:25:SER:HA	2:3H:30:ILE:HG22	2.00	0.41
1:4A:231:ILE:O	1:4A:235:ILE:HG12	2.20	0.41
1:4C:124:LYS:HD2	1:4D:283:HIS:NE2	2.35	0.41
1:4E:75:VAL:HG11	1:4E:94:SER:HB3	2.01	0.41
1:4F:181:VAL:HG22	2:5F:347:ASN:O	2.20	0.41
1:4G:231:ILE:O	1:4G:235:ILE:HG12	2.20	0.41
1:4G:287:SER:HG	1:4G:290:GLU:CD	2.22	0.41
1:4H:210:TYR:CZ	2:5H:324:LYS:HG2	2.55	0.41
1:4H:260:VAL:O	1:4H:260:VAL:HG23	2.19	0.41
2:5A:215:LEU:HB3	2:5A:217:LEU:HD23	2.02	0.41
2:5A:292:GLN:O	2:5A:298:ASN:ND2	2.41	0.41
2:5B:315:ALA:HB3	2:5B:330:MET:HE1	2.02	0.41
2:5I:113:ILE:HD12	2:5I:113:ILE:HA	1.91	0.41
2:5I:192:LEU:HD21	2:5I:199:VAL:HG21	2.02	0.41
1:2A:274:PRO:HG3	1:2A:286:LEU:HD13	2.01	0.41
1:2E:250:VAL:CG1	1:2E:318:MET:HE1	2.50	0.41
1:2G:399:TYR:OH	1:2G:415:GLU:OE2	2.37	0.41
2:3A:208:TYR:HE2	1:4A:329:ASN:ND2	2.17	0.41
2:3C:259:PRO:HD2	2:3C:263:LEU:HD11	2.03	0.41
2:3H:268:ILE:CD1	2:3H:368:VAL:HG12	2.50	0.41
2:3I:139:LEU:HD23	2:3I:139:LEU:HA	1.86	0.41
1:4A:224:TYR:CD2	2:5A:323:THR:HG21	2.55	0.41
1:4A:427:ALA:O	1:4A:430:LYS:HG3	2.19	0.41
1:4B:328:VAL:HG12	1:4B:353:CYS:SG	2.60	0.41
1:4G:103:PHE:HB3	1:4G:189:LEU:HD23	2.02	0.41
1:4G:212:ILE:HD13	1:4G:215:ARG:HH22	1.85	0.41
2:5B:130:LEU:HD23	2:5B:130:LEU:H	1.85	0.41
2:5D:272:PRO:HB2	2:5D:282:ARG:HH22	1.85	0.41
2:5F:375:GLN:HG3	2:5F:419:VAL:HG13	2.02	0.41
2:5I:19:LYS:HA	2:5I:22:GLU:HG2	2.02	0.41
1:2B:221:ARG:NH2	2:3B:322:SER:C	2.74	0.41
2:3D:238:CYS:SG	2:3D:318:ARG:NE	2.94	0.41
2:3E:239:CYS:SG	2:3E:248:SER:N	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3I:156:ARG:HG3	2:3I:195:ASN:O	2.20	0.41
1:4A:10:GLY:O	1:4A:14:ILE:HG12	2.20	0.41
1:4C:183:GLU:HG3	1:4C:184:PRO:HD3	2.02	0.41
1:4E:269:LEU:HD11	1:4E:384:ILE:HD11	2.02	0.41
1:4H:70:LEU:HD12	1:4H:99:ALA:HB2	2.03	0.41
1:4I:98:ASP:OD1	1:4I:99:ALA:N	2.52	0.41
1:4I:265:ILE:HG21	1:4I:313:MET:CE	2.50	0.41
1:4I:265:ILE:HG22	1:4I:380:ASN:HD21	1.85	0.41
2:5D:238:CYS:SG	2:5D:318:ARG:NE	2.94	0.41
1:2A:65:CYS:SG	1:2A:66:VAL:N	2.93	0.41
1:2A:91:GLN:OE1	1:2A:91:GLN:N	2.53	0.41
1:2D:56:THR:CA	1:2E:285:GLN:H	2.28	0.41
1:2D:183:GLU:HG3	1:2D:184:PRO:HD3	2.03	0.41
1:2H:54:SER:OG	1:2H:55:GLU:N	2.53	0.41
2:3C:113:ILE:HA	2:3C:116:VAL:HG12	2.03	0.41
2:3E:16:ILE:HD11	2:3E:229:VAL:HG11	2.02	0.41
2:3I:8:GLN:HG2	2:3I:14:ASN:HA	2.03	0.41
1:4A:230:LEU:HD21	1:4A:368:LEU:HD21	2.02	0.41
1:4A:259:LEU:HD21	1:4A:316:CYS:HB2	2.02	0.41
1:4D:56:THR:HA	1:4E:285:GLN:HB3	2.02	0.41
1:4H:173:PRO:O	1:4H:390:ARG:NH1	2.50	0.41
1:4I:133:GLN:HG3	1:4I:252:VAL:HB	2.01	0.41
2:5B:323:THR:HA	2:5B:326:VAL:HG12	2.02	0.41
2:5E:4:ILE:HD11	2:5E:240:LEU:HD13	2.03	0.41
1:2E:11:GLN:HE21	1:2E:15:GLN:NE2	2.19	0.41
1:2E:259:LEU:HD21	1:2E:316:CYS:HB2	2.02	0.41
1:2G:60:LYS:NZ	1:2H:283:HIS:HD2	2.05	0.41
1:2G:132:LEU:HB3	1:2G:164:LYS:NZ	2.35	0.41
1:2I:34:GLY:HA3	1:2I:60:LYS:NZ	2.35	0.41
2:3A:66:MET:HE3	2:3A:66:MET:HB3	2.02	0.41
2:3B:117:LEU:HA	2:3B:120:VAL:HG12	2.02	0.41
2:3B:163:ILE:HD13	2:3B:250:LEU:HB3	2.03	0.41
2:3F:53:GLU:OE2	2:3F:54:ALA:N	2.46	0.41
2:3F:245:GLN:HB2	2:3F:353:VAL:CG1	2.51	0.41
2:3I:141:GLY:O	2:3I:145:SER:OG	2.32	0.41
1:4A:218:ASP:OD2	1:4A:280:LYS:NZ	2.42	0.41
1:4I:306:ASP:OD2	1:4I:308:ARG:NH2	2.52	0.41
2:5B:107:THR:HG21	2:5B:401:GLU:OE2	2.20	0.41
2:5C:7:VAL:HG11	2:5C:151:LEU:HD23	2.02	0.41
2:5F:68:LEU:HD13	2:5F:108:GLU:OE2	2.21	0.41
2:5H:73:MET:HB3	2:5H:77:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5H:119:VAL:O	2:5H:122:LYS:HG3	2.19	0.41
2:5I:200:GLN:HB2	2:5I:268:ILE:HD11	2.02	0.41
1:2D:96:LYS:CE	2:3D:129:CYS:HB2	2.49	0.41
2:3H:391:ARG:HD2	1:4H:346:TRP:CG	2.56	0.41
1:4G:154:LEU:HG	1:4G:197:HIS:HB3	2.01	0.41
1:4H:432:TYR:O	1:4H:436:GLY:N	2.52	0.41
1:4I:224:TYR:HB2	2:5I:245:GLN:NE2	2.36	0.41
2:5I:5:VAL:HB	2:5I:133:PHE:CD1	2.55	0.41
1:2B:401:LYS:HE2	2:3B:344:TRP:CE2	2.55	0.41
1:2D:276:ILE:HD12	1:2D:281:ALA:HA	2.03	0.41
1:2F:15:GLN:HE21	1:2F:74:VAL:HG23	1.86	0.41
1:2G:135:PHE:HB2	1:2G:166:LYS:HA	2.02	0.41
2:3B:67:ASP:OD1	2:3B:68:LEU:N	2.54	0.41
2:3C:13:GLY:HA2	2:3C:136:THR:HG22	2.03	0.41
2:3I:16:ILE:CG2	2:3I:136:THR:HG21	2.50	0.41
2:3I:137:HIS:CE1	2:3I:166:THR:HG23	2.55	0.41
1:4E:66:VAL:HG21	1:4E:122:ILE:HD11	2.03	0.41
1:4G:71:GLU:HB3	1:4G:98:ASP:HB3	2.03	0.41
1:4G:168:ASN:HB2	1:4G:201:ALA:HA	2.03	0.41
2:5A:386:THR:HG23	2:5A:412:GLU:OE2	2.21	0.41
2:5G:65:LEU:CD1	2:5G:76:VAL:HG11	2.51	0.41
2:5G:133:PHE:HB2	2:5G:164:MET:HB3	2.02	0.41
2:5G:324:LYS:HG3	2:5G:325:GLU:N	2.36	0.41
1:2G:114:ILE:HD12	1:2G:114:ILE:HA	1.88	0.41
1:2G:191:THR:HB	1:2G:425:LEU:HD21	2.03	0.41
1:2H:60:LYS:HE2	1:2H:60:LYS:HB2	1.90	0.41
2:3D:139:LEU:HA	2:3D:145:SER:HB2	2.02	0.41
2:3E:99:ASN:CG	1:4E:254:GLU:OE1	2.59	0.41
2:3E:191:GLN:HA	2:3E:194:GLU:HG2	2.02	0.41
2:3E:385:PHE:HE2	2:3E:412:GLU:HB2	1.85	0.41
2:3F:388:MET:HG2	1:4F:346:TRP:O	2.20	0.41
2:3G:391:ARG:NE	2:3G:391:ARG:HA	2.35	0.41
2:3H:113:ILE:HA	2:3H:113:ILE:HD13	1.96	0.41
1:4A:152:LEU:HD11	1:4A:156:ARG:HH11	1.84	0.41
1:4D:269:LEU:HD21	1:4D:384:ILE:CD1	2.50	0.41
1:4F:36:MET:SD	1:4F:61:HIS:NE2	2.78	0.41
1:4G:230:LEU:HD11	1:4G:275:ILE:HD13	2.02	0.41
2:5A:209:ASP:OD1	2:5A:213:ARG:NH1	2.54	0.41
2:5D:272:PRO:HB2	2:5D:282:ARG:NH2	2.35	0.41
2:5E:92:PHE:O	2:5E:112:LEU:HD11	2.21	0.41
2:5I:156:ARG:HG3	2:5I:195:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:193:SER:O	1:2A:197:HIS:ND1	2.52	0.41
1:2B:221:ARG:HH12	2:3B:324:LYS:N	2.19	0.41
1:2B:241:SER:OG	1:2B:250:VAL:O	2.23	0.41
1:2D:12:ALA:HB3	1:2D:140:ALA:HB2	2.01	0.41
1:2D:76:ASP:HA	1:2D:79:ARG:HG2	2.03	0.41
1:2F:7:ILE:HD13	1:2F:153:LEU:HD21	2.02	0.41
1:2F:50:ASN:O	1:2F:64:ARG:NH2	2.46	0.41
1:2G:231:ILE:O	1:2G:235:ILE:HG12	2.21	0.41
1:2G:306:ASP:HB3	1:2G:309:HIS:CE1	2.56	0.41
1:2H:176:GLN:O	2:3H:331:LEU:HD21	2.21	0.41
1:2I:77:GLU:OE1	2:3I:243:PRO:CB	2.69	0.41
2:3A:309:ARG:H	2:3A:372:THR:HG22	1.85	0.41
2:3E:7:VAL:HG11	2:3E:151:LEU:HD23	2.03	0.41
2:3F:18:ALA:O	2:3F:22:GLU:OE1	2.39	0.41
2:3G:265:PHE:HE2	2:3G:418:LEU:HD21	1.86	0.41
2:3G:293:MET:HE1	2:3G:365:VAL:HG21	2.02	0.41
2:3H:121:ARG:NH2	2:3H:158:GLU:OE1	2.54	0.41
1:4B:259:LEU:HD11	1:4B:316:CYS:SG	2.61	0.41
1:4E:28:HIS:CE1	1:4E:243:ARG:HD2	2.56	0.41
1:4H:107:HIS:NE2	1:4H:151:CYS:SG	2.83	0.41
1:4I:215:ARG:HH22	1:4I:299:ALA:C	2.25	0.41
2:5A:47:ILE:HD12	2:5A:47:ILE:HA	1.97	0.41
2:5A:263:LEU:H	2:5A:263:LEU:HD23	1.86	0.41
2:5A:374:ILE:O	2:5A:374:ILE:CG2	2.67	0.41
2:5A:403:MET:HB3	2:5A:403:MET:HE2	2.01	0.41
1:2A:296:PHE:CE2	1:2A:335:ILE:HG21	2.56	0.41
1:2B:60:LYS:CE	1:2C:282:TYR:HD2	2.30	0.41
1:2G:211:ASP:HA	1:2G:214:ARG:HG2	2.03	0.41
1:2H:231:ILE:HD13	1:2H:231:ILE:HA	1.89	0.41
2:3D:19:LYS:HD2	2:3D:19:LYS:HA	1.89	0.41
2:3F:397:TRP:HZ2	1:4F:260:VAL:HB	1.86	0.41
2:3G:334:GLN:HG3	2:3G:341:PHE:HD2	1.86	0.41
1:4A:90:GLU:O	1:4A:93:ILE:HD11	2.20	0.41
1:4A:274:PRO:HG3	1:4A:286:LEU:HD13	2.02	0.41
1:4B:102:ASN:HB3	1:4B:105:ARG:HB2	2.02	0.41
1:4D:251:ASP:H	1:4D:254:GLU:HG3	1.85	0.41
1:4F:76:ASP:O	1:4F:79:ARG:HG2	2.20	0.41
1:4H:180:ALA:HB3	1:4H:183:GLU:HB2	2.02	0.41
2:5B:66:MET:CG	2:5B:116:VAL:HG21	2.51	0.41
2:5B:289:LEU:HD12	2:5B:365:VAL:HG12	2.02	0.41
2:5F:169:VAL:HG12	2:5F:202:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5F:270:PHE:O	2:5F:298:ASN:ND2	2.54	0.41
1:2B:98:ASP:OD1	1:2B:99:ALA:N	2.54	0.40
1:2C:422:ARG:HH12	1:2C:426:ALA:HB2	1.86	0.40
1:2G:96:LYS:HA	1:2G:96:LYS:HE2	2.03	0.40
1:2I:339:ARG:O	1:2I:339:ARG:HG3	2.21	0.40
2:3A:5:VAL:HG22	2:3A:123:GLU:OE1	2.21	0.40
2:3A:7:VAL:HB	2:3A:135:ILE:HD13	2.02	0.40
2:3A:133:PHE:HB2	2:3A:164:MET:CB	2.51	0.40
2:3F:54:ALA:HB1	2:3G:281:TYR:C	2.42	0.40
2:3F:64:ILE:HD11	2:3F:123:GLU:HG3	2.04	0.40
2:3F:173:PRO:HB3	2:3F:380:ARG:HD3	2.02	0.40
2:3G:173:PRO:HD2	2:3G:205:GLU:HG2	2.03	0.40
2:3I:107:THR:HG21	2:3I:401:GLU:OE2	2.20	0.40
1:4C:151:CYS:SG	1:4C:193:SER:OG	2.40	0.40
1:4I:338:LYS:NZ	1:4I:340:THR:OG1	2.44	0.40
2:5B:113:ILE:HA	2:5B:116:VAL:HG12	2.03	0.40
2:5C:113:ILE:HA	2:5C:116:VAL:HG12	2.03	0.40
2:5D:54:ALA:CA	2:5E:283:ALA:CA	2.98	0.40
2:5D:103:LYS:HB2	2:5D:108:GLU:OE1	2.21	0.40
2:5F:42:LEU:HD12	2:5F:42:LEU:HA	1.94	0.40
2:5G:20:PHE:O	2:5G:24:ILE:HG12	2.22	0.40
2:5G:86:ARG:HB2	2:5G:89:ASN:OD1	2.21	0.40
2:5G:97:ALA:HB3	2:5G:143:THR:HG22	2.02	0.40
1:2D:10:GLY:HA2	1:2D:145:THR:HG23	2.04	0.40
1:2E:332:VAL:O	1:2E:336:LYS:HG3	2.21	0.40
1:2G:296:PHE:CE2	1:2G:335:ILE:HG21	2.57	0.40
1:2H:275:ILE:HD12	1:2H:368:LEU:HD11	2.03	0.40
2:3A:177:ASP:OD1	1:4A:353:CYS:SG	2.77	0.40
2:3D:99:ASN:ND2	1:4D:254:GLU:OE1	2.54	0.40
2:3D:284:LEU:HD23	2:3D:362:LYS:HG2	2.01	0.40
1:4A:103:PHE:CD2	1:4A:189:LEU:HB3	2.56	0.40
1:4E:185:TYR:HE1	1:4E:398:MET:HB3	1.85	0.40
1:4G:15:GLN:HA	1:4G:18:ASN:ND2	2.36	0.40
2:5D:83:GLN:HB3	2:5E:281:TYR:OH	2.21	0.40
1:2A:219:ILE:HD13	1:2A:219:ILE:HA	1.83	0.40
1:2A:231:ILE:O	1:2A:235:ILE:HG12	2.21	0.40
1:2D:292:THR:CG2	1:2D:331:ALA:HB1	2.50	0.40
1:2H:269:LEU:CD2	1:2H:384:ILE:HD11	2.51	0.40
2:3C:207:LEU:HB3	2:3C:225:LEU:HD22	2.02	0.40
2:3E:391:ARG:CD	1:4E:346:TRP:CD1	3.04	0.40
1:4A:301:MET:CE	1:4A:307:PRO:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4B:65:CYS:SG	1:4B:66:VAL:N	2.93	0.40
1:4F:231:ILE:O	1:4F:235:ILE:HG12	2.21	0.40
1:4G:15:GLN:HA	1:4G:18:ASN:HD21	1.86	0.40
1:4G:176:GLN:HB3	2:5G:331:LEU:HD22	2.03	0.40
1:4H:225:THR:O	1:4H:229:ARG:HG2	2.22	0.40
1:4H:346:TRP:HZ2	1:4H:435:VAL:HG13	1.86	0.40
2:5G:171:PRO:HG3	2:5G:181:GLU:OE1	2.21	0.40
2:5H:211:CYS:SG	2:5H:217:LEU:HB2	2.61	0.40
2:5I:290:THR:HA	2:5I:293:MET:HE3	2.04	0.40
1:2A:2:ARG:NE	1:2A:133:GLN:HE21	2.16	0.40
1:2E:98:ASP:OD1	1:2E:99:ALA:N	2.54	0.40
1:2F:101:ASN:ND2	2:3F:256:ASN:HD21	2.19	0.40
1:2H:155:GLU:HG2	1:2H:197:HIS:CE1	2.57	0.40
2:3B:95:THR:C	1:4B:2:ARG:HH12	2.24	0.40
2:3B:246:LEU:HD12	2:3B:246:LEU:HA	1.84	0.40
2:3C:284:LEU:HD12	2:3C:284:LEU:HA	1.95	0.40
2:3E:117:LEU:HA	2:3E:120:VAL:HG12	2.03	0.40
2:3F:25:SER:OG	2:3F:81:PHE:HE2	2.04	0.40
2:3F:66:MET:HE2	2:3F:116:VAL:HG21	2.04	0.40
2:3I:290:THR:HA	2:3I:293:MET:HG2	2.03	0.40
1:4A:88:HIS:HB3	1:4A:91:GLN:HE22	1.85	0.40
1:4C:274:PRO:HB2	1:4C:276:ILE:HG12	2.04	0.40
2:5B:117:LEU:HA	2:5B:120:VAL:HG12	2.04	0.40
2:5F:355:ASP:O	2:5F:355:ASP:OD1	2.40	0.40
1:2D:50:ASN:O	1:2D:64:ARG:NH2	2.52	0.40
1:2E:243:ARG:HH11	1:2E:243:ARG:HD2	1.72	0.40
1:2G:189:LEU:HD11	1:2G:418:PHE:HD1	1.87	0.40
1:2G:310:GLY:HA3	1:2G:383:ALA:HB2	2.03	0.40
1:2H:108:TYR:CE2	1:2H:413:MET:HB3	2.56	0.40
2:3B:258:ILE:HD11	2:3B:266:PHE:CZ	2.56	0.40
2:3B:280:GLN:HG2	2:3B:281:TYR:CD1	2.56	0.40
2:3E:100:ASN:ND2	2:3E:397:TRP:O	2.54	0.40
2:3E:396:HIS:HE1	1:4E:262:TYR:HA	1.86	0.40
2:3G:294:PHE:O	2:3G:306:ARG:NH2	2.41	0.40
2:3I:11:GLN:HE22	1:4I:248:LEU:HD12	1.86	0.40
2:3I:16:ILE:HG22	2:3I:136:THR:HG21	2.02	0.40
2:3I:354:CYS:SG	2:3I:355:ASP:N	2.95	0.40
1:4C:88:HIS:HD1	1:4C:90:GLU:H	1.68	0.40
1:4C:185:TYR:HE2	1:4C:404:PHE:HB2	1.86	0.40
1:4H:306:ASP:N	1:4H:386:GLU:OE2	2.54	0.40
1:4H:395:PHE:O	1:4H:398:MET:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4I:65:CYS:SG	1:4I:66:VAL:N	2.94	0.40
1:4I:230:LEU:HD21	1:4I:368:LEU:HD11	2.03	0.40
2:5A:256:ASN:ND2	2:5A:350:LYS:HG3	2.37	0.40
2:5F:151:LEU:HD12	2:5F:151:LEU:HA	1.90	0.40
2:5H:192:LEU:HD21	2:5H:199:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2A	424/437 (97%)	416 (98%)	7 (2%)	1 (0%)	44	78
1	2B	424/437 (97%)	416 (98%)	8 (2%)	0	100	100
1	2C	424/437 (97%)	419 (99%)	5 (1%)	0	100	100
1	2D	424/437 (97%)	418 (99%)	6 (1%)	0	100	100
1	2E	424/437 (97%)	417 (98%)	7 (2%)	0	100	100
1	2F	424/437 (97%)	415 (98%)	9 (2%)	0	100	100
1	2G	424/437 (97%)	411 (97%)	13 (3%)	0	100	100
1	2H	424/437 (97%)	414 (98%)	10 (2%)	0	100	100
1	2I	424/437 (97%)	418 (99%)	6 (1%)	0	100	100
1	4A	424/437 (97%)	414 (98%)	10 (2%)	0	100	100
1	4B	424/437 (97%)	413 (97%)	11 (3%)	0	100	100
1	4C	424/437 (97%)	416 (98%)	8 (2%)	0	100	100
1	4D	424/437 (97%)	417 (98%)	7 (2%)	0	100	100
1	4E	424/437 (97%)	414 (98%)	10 (2%)	0	100	100
1	4F	424/437 (97%)	417 (98%)	7 (2%)	0	100	100
1	4G	424/437 (97%)	415 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4H	424/437 (97%)	411 (97%)	13 (3%)	0	100	100
1	4I	424/437 (97%)	419 (99%)	5 (1%)	0	100	100
2	3A	424/426 (100%)	411 (97%)	13 (3%)	0	100	100
2	3B	424/426 (100%)	408 (96%)	16 (4%)	0	100	100
2	3C	424/426 (100%)	409 (96%)	15 (4%)	0	100	100
2	3D	424/426 (100%)	410 (97%)	14 (3%)	0	100	100
2	3E	424/426 (100%)	406 (96%)	18 (4%)	0	100	100
2	3F	424/426 (100%)	406 (96%)	18 (4%)	0	100	100
2	3G	424/426 (100%)	413 (97%)	11 (3%)	0	100	100
2	3H	424/426 (100%)	411 (97%)	13 (3%)	0	100	100
2	3I	424/426 (100%)	411 (97%)	13 (3%)	0	100	100
2	5A	424/426 (100%)	410 (97%)	14 (3%)	0	100	100
2	5B	424/426 (100%)	406 (96%)	18 (4%)	0	100	100
2	5C	424/426 (100%)	410 (97%)	14 (3%)	0	100	100
2	5D	424/426 (100%)	409 (96%)	15 (4%)	0	100	100
2	5E	424/426 (100%)	405 (96%)	19 (4%)	0	100	100
2	5F	424/426 (100%)	407 (96%)	17 (4%)	0	100	100
2	5G	424/426 (100%)	410 (97%)	14 (3%)	0	100	100
2	5H	424/426 (100%)	411 (97%)	12 (3%)	1 (0%)	44	78
2	5I	424/426 (100%)	412 (97%)	12 (3%)	0	100	100
All	All	15264/15534 (98%)	14845 (97%)	417 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2A	304	LYS
2	5H	180	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2A	359/368 (98%)	353 (98%)	6 (2%)	56	72
1	2B	359/368 (98%)	354 (99%)	5 (1%)	62	75
1	2C	359/368 (98%)	356 (99%)	3 (1%)	79	85
1	2D	359/368 (98%)	356 (99%)	3 (1%)	79	85
1	2E	359/368 (98%)	358 (100%)	1 (0%)	91	92
1	2F	359/368 (98%)	356 (99%)	3 (1%)	79	85
1	2G	359/368 (98%)	355 (99%)	4 (1%)	70	80
1	2H	359/368 (98%)	354 (99%)	5 (1%)	62	75
1	2I	359/368 (98%)	354 (99%)	5 (1%)	62	75
1	4A	359/368 (98%)	350 (98%)	9 (2%)	42	61
1	4B	359/368 (98%)	356 (99%)	3 (1%)	79	85
1	4C	359/368 (98%)	355 (99%)	4 (1%)	70	80
1	4D	359/368 (98%)	355 (99%)	4 (1%)	70	80
1	4E	359/368 (98%)	356 (99%)	3 (1%)	79	85
1	4F	359/368 (98%)	357 (99%)	2 (1%)	84	88
1	4G	359/368 (98%)	352 (98%)	7 (2%)	52	69
1	4H	359/368 (98%)	355 (99%)	4 (1%)	70	80
1	4I	359/368 (98%)	356 (99%)	3 (1%)	79	85
2	3A	364/366 (100%)	360 (99%)	4 (1%)	70	80
2	3B	364/366 (100%)	362 (100%)	2 (0%)	86	89
2	3C	364/366 (100%)	363 (100%)	1 (0%)	91	92
2	3D	364/366 (100%)	360 (99%)	4 (1%)	70	80
2	3E	364/366 (100%)	359 (99%)	5 (1%)	62	75
2	3F	364/366 (100%)	361 (99%)	3 (1%)	79	85
2	3G	364/366 (100%)	361 (99%)	3 (1%)	79	85
2	3H	364/366 (100%)	362 (100%)	2 (0%)	86	89
2	3I	364/366 (100%)	361 (99%)	3 (1%)	79	85
2	5A	364/366 (100%)	362 (100%)	2 (0%)	86	89
2	5B	364/366 (100%)	358 (98%)	6 (2%)	58	73
2	5C	364/366 (100%)	360 (99%)	4 (1%)	70	80
2	5D	364/366 (100%)	362 (100%)	2 (0%)	86	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5E	364/366 (100%)	360 (99%)	4 (1%)	70	80
2	5F	364/366 (100%)	359 (99%)	5 (1%)	62	75
2	5G	364/366 (100%)	359 (99%)	5 (1%)	62	75
2	5H	364/366 (100%)	361 (99%)	3 (1%)	79	85
2	5I	364/366 (100%)	361 (99%)	3 (1%)	79	85
All	All	13014/13212 (98%)	12879 (99%)	135 (1%)	71	82

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2A	36	MET
1	2A	112	LYS
1	2A	123	ARG
1	2A	154	LEU
1	2A	227	LEU
1	2A	430	LYS
1	2B	86	LEU
1	2B	121	ARG
1	2B	153	LEU
1	2B	238	LEU
1	2B	256	GLN
1	2C	221	ARG
1	2C	302	MET
1	2C	386	GLU
1	2D	163	LYS
1	2D	229	ARG
1	2D	339	ARG
1	2E	370	LYS
1	2F	32	PRO
1	2F	166	LYS
1	2F	390	ARG
1	2G	124	LYS
1	2G	390	ARG
1	2G	401	LYS
1	2G	422	ARG
1	2H	107	HIS
1	2H	154	LEU
1	2H	196	GLU
1	2H	258	ASN
1	2H	372	MET

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Mol	Chain	Res	Type
1	2I	123	ARG
1	2I	125	LEU
1	2I	308	ARG
1	2I	334	THR
1	2I	342	GLN
2	3A	69	GLU
2	3A	122	LYS
2	3A	375	GLN
2	3A	391	ARG
2	3B	179	VAL
2	3B	306	ARG
2	3C	328	GLU
2	3D	52	ASN
2	3D	53	GLU
2	3D	117	LEU
2	3D	306	ARG
2	3E	44	LEU
2	3E	48	ASN
2	3E	77	ARG
2	3E	84	LEU
2	3E	191	GLN
2	3F	86	ARG
2	3F	147	MET
2	3F	426	GLN
2	3G	155	VAL
2	3G	213	ARG
2	3G	359	LYS
2	3H	45	GLU
2	3H	117	LEU
2	3I	162	ARG
2	3I	256	ASN
2	3I	375	GLN
1	4A	112	LYS
1	4A	128	ASN
1	4A	167	LEU
1	4A	174	SER
1	4A	280	LYS
1	4A	320	ARG
1	4A	336	LYS
1	4A	401	LYS
1	4A	430	LYS
1	4B	217	LEU

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Mol	Chain	Res	Type
1	4B	221	ARG
1	4B	238	LEU
1	4C	96	LYS
1	4C	107	HIS
1	4C	221	ARG
1	4C	308	ARG
1	4D	96	LYS
1	4D	125	LEU
1	4D	153	LEU
1	4D	326	LYS
1	4E	124	LYS
1	4E	315	CYS
1	4E	407	TRP
1	4F	112	LYS
1	4F	402	ARG
1	4G	31	GLN
1	4G	124	LYS
1	4G	183	GLU
1	4G	238	LEU
1	4G	280	LYS
1	4G	422	ARG
1	4G	430	LYS
1	4H	196	GLU
1	4H	256	GLN
1	4H	325	PRO
1	4H	326	LYS
1	4I	125	LEU
1	4I	308	ARG
1	4I	425	LEU
2	5A	2	ARG
2	5A	123	GLU
2	5B	213	ARG
2	5B	262	ARG
2	5B	297	LYS
2	5B	323	THR
2	5B	347	ASN
2	5B	362	LYS
2	5C	39	ASP
2	5C	147	MET
2	5C	247	ASN
2	5C	320	ARG
2	5D	52	ASN

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Mol	Chain	Res	Type
2	5D	336	LYS
2	5E	48	ASN
2	5E	190	HIS
2	5E	297	LYS
2	5E	298	ASN
2	5F	46	ARG
2	5F	66	MET
2	5F	99	ASN
2	5F	117	LEU
2	5F	192	LEU
2	5G	2	ARG
2	5G	306	ARG
2	5G	362	LYS
2	5G	364	SER
2	5G	365	VAL
2	5H	117	LEU
2	5H	122	LYS
2	5H	297	LYS
2	5I	162	ARG
2	5I	164	MET
2	5I	280	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	2A	133	GLN
1	2B	18	ASN
1	2B	31	GLN
1	2B	256	GLN
1	2B	283	HIS
1	2C	31	GLN
1	2D	356	ASN
1	2D	393	HIS
1	2E	11	GLN
1	2E	101	ASN
1	2F	11	GLN
1	2F	15	GLN
1	2F	28	HIS
1	2F	168	ASN
1	2F	206	ASN
1	2F	283	HIS
1	2G	133	GLN

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Mol	Chain	Res	Type
1	2G	258	ASN
1	2H	139	ASN
1	2H	283	HIS
1	2H	309	HIS
2	3A	99	ASN
2	3B	247	ASN
2	3B	256	ASN
2	3B	347	ASN
2	3B	423	GLN
2	3C	11	GLN
2	3C	14	ASN
2	3C	347	ASN
2	3D	11	GLN
2	3D	14	ASN
2	3D	99	ASN
2	3D	190	HIS
2	3D	191	GLN
2	3D	204	ASN
2	3D	334	GLN
2	3D	347	ASN
2	3E	99	ASN
2	3E	134	GLN
2	3E	247	ASN
2	3E	256	ASN
2	3E	396	HIS
2	3F	11	GLN
2	3F	14	ASN
2	3F	99	ASN
2	3F	247	ASN
2	3F	334	GLN
2	3H	99	ASN
2	3I	137	HIS
1	4B	31	GLN
1	4B	283	HIS
1	4B	329	ASN
1	4C	101	ASN
1	4C	258	ASN
1	4D	283	HIS
1	4E	11	GLN
1	4E	35	GLN
1	4E	285	GLN
1	4F	139	ASN

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Mol	Chain	Res	Type
1	4F	258	ASN
1	4F	283	HIS
1	4G	168	ASN
1	4G	342	GLN
1	4H	139	ASN
1	4H	226	ASN
1	4H	233	GLN
1	4H	329	ASN
1	4I	8	HIS
1	4I	15	GLN
2	5A	14	ASN
2	5A	105	HIS
2	5A	134	GLN
2	5A	247	ASN
2	5A	279	GLN
2	5A	348	ASN
2	5B	11	GLN
2	5B	414	ASN
2	5C	256	ASN
2	5C	347	ASN
2	5D	6	HIS
2	5D	8	GLN
2	5D	134	GLN
2	5D	204	ASN
2	5D	280	GLN
2	5D	334	GLN
2	5D	347	ASN
2	5E	134	GLN
2	5E	137	HIS
2	5E	347	ASN
2	5F	11	GLN
2	5F	99	ASN
2	5G	8	GLN
2	5G	134	GLN
2	5G	347	ASN
2	5H	14	ASN
2	5H	105	HIS
2	5H	190	HIS
2	5H	347	ASN
2	5I	245	GLN
2	5I	347	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

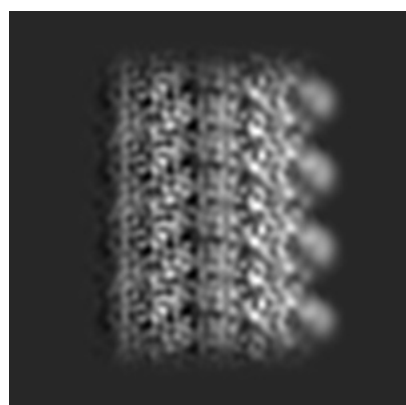
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26020. These allow visual inspection of the internal detail of the map and identification of artifacts.

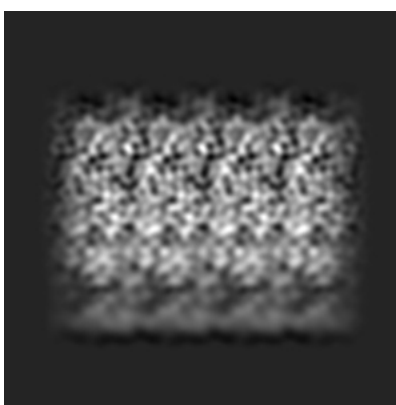
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

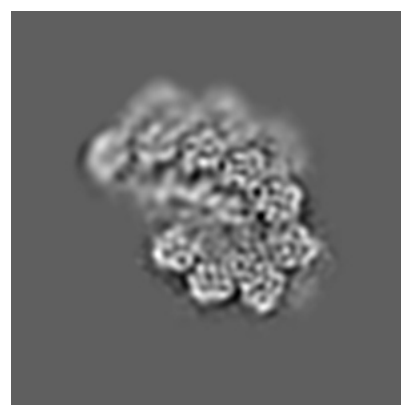
6.1.1 Primary map



X



Y

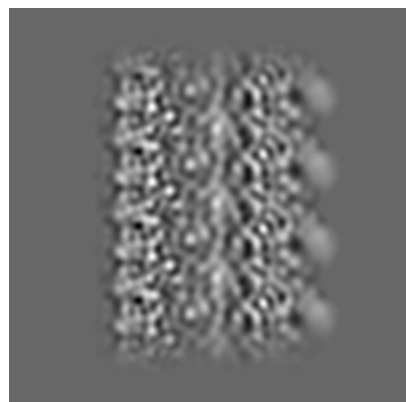


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

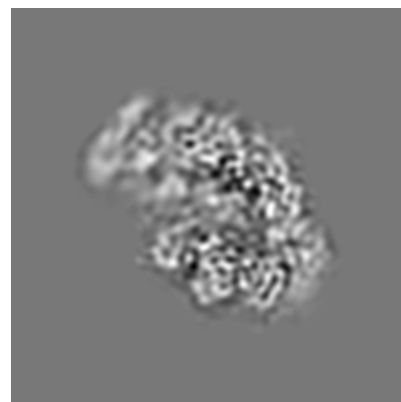
6.2.1 Primary map



X Index: 64



Y Index: 64

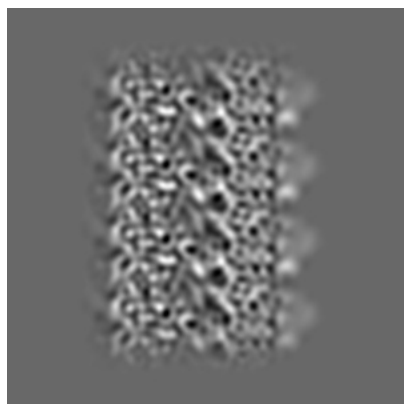


Z Index: 64

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

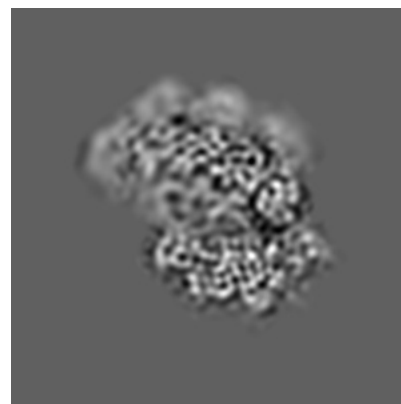
6.3.1 Primary map



X Index: 76



Y Index: 79

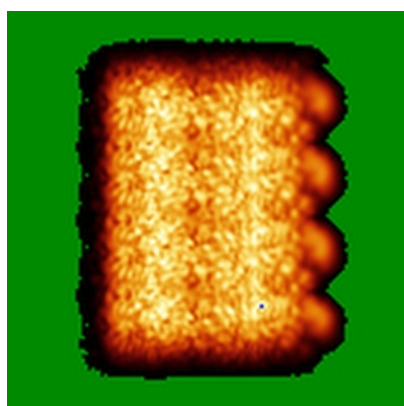


Z Index: 32

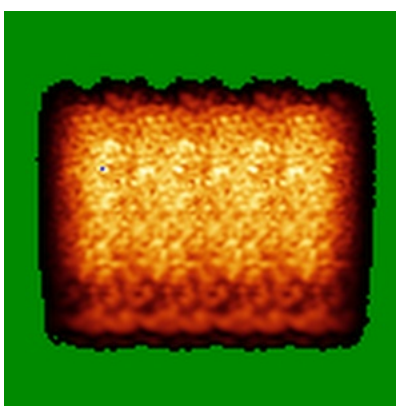
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

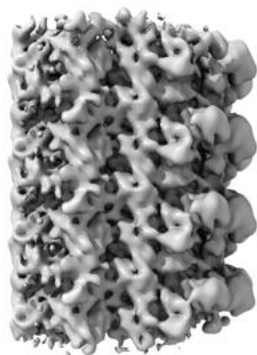


Z

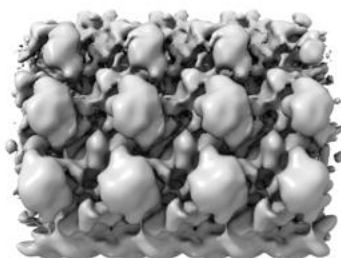
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

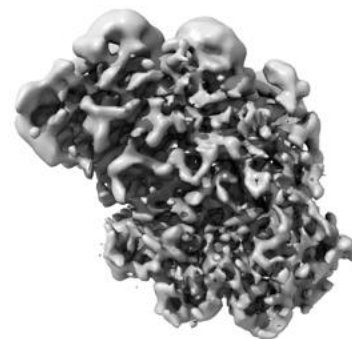
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

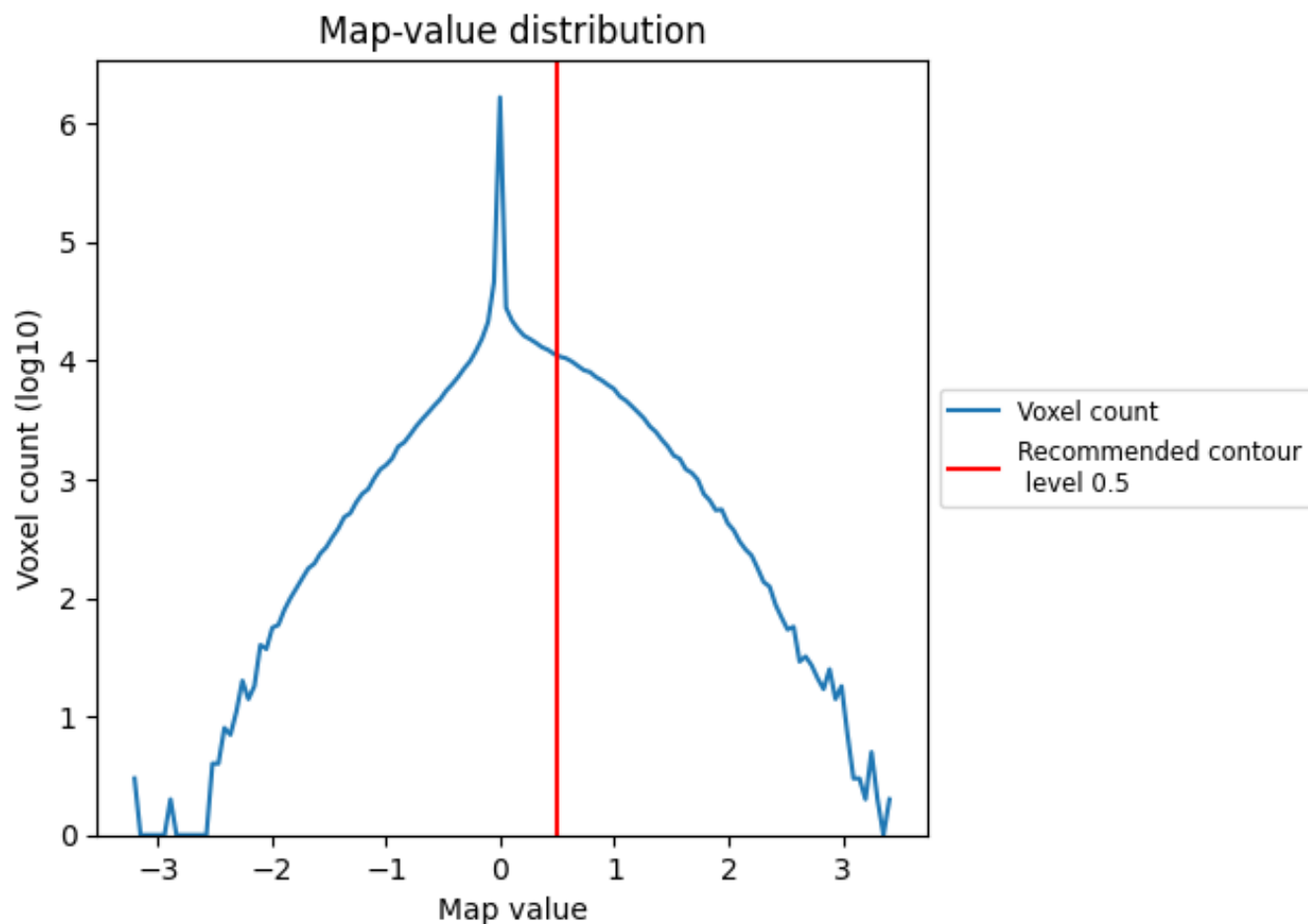
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

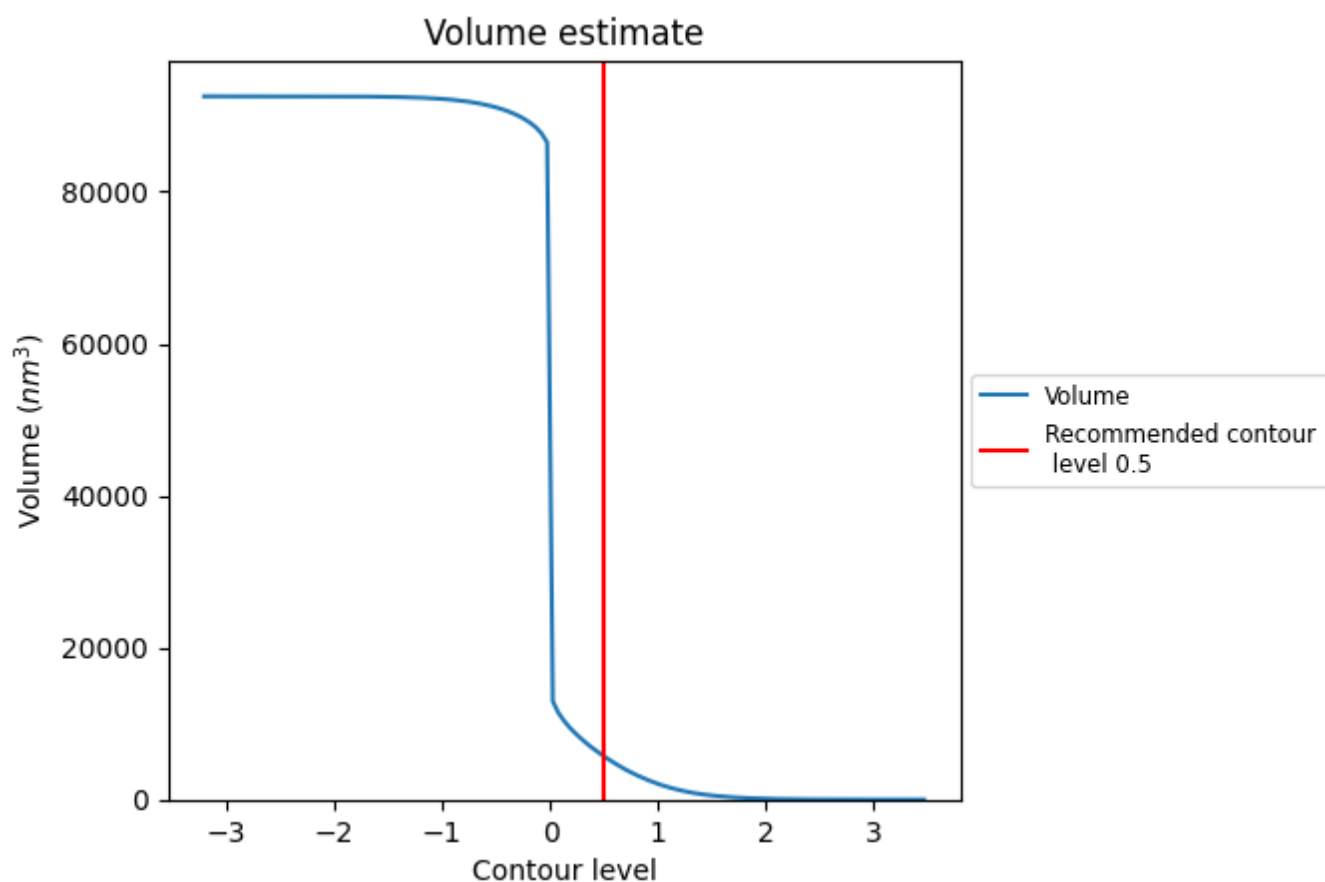
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

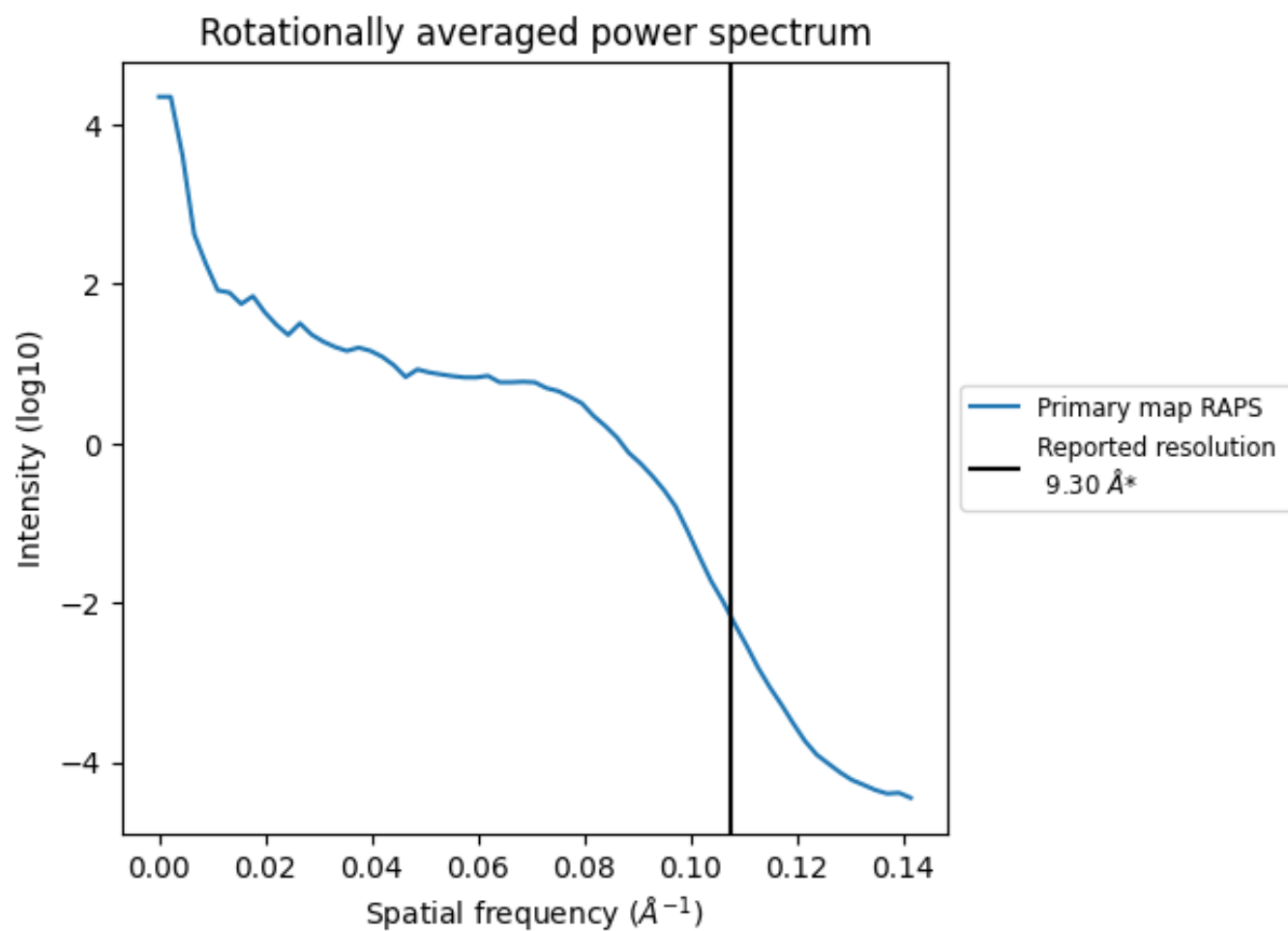
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5688 nm³; this corresponds to an approximate mass of 5138 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.108 Å⁻¹

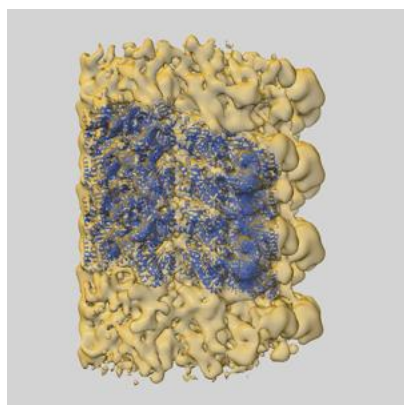
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

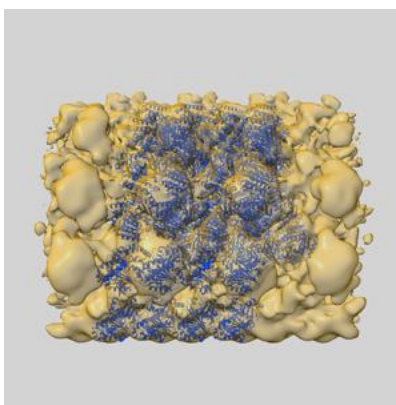
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26020 and PDB model 7TNT. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

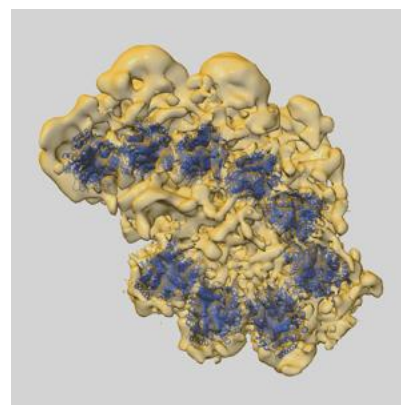
9.1 Map-model overlay [i](#)



X



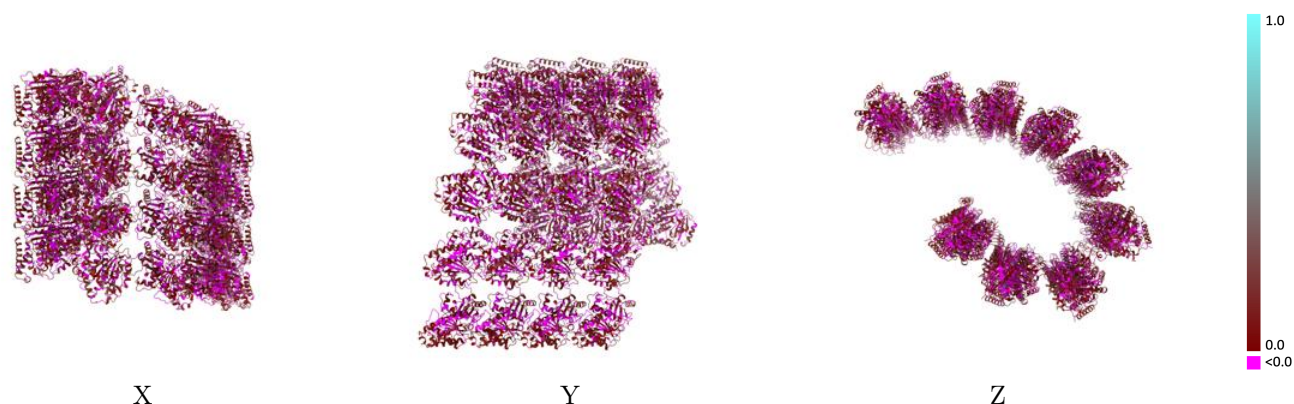
Y



Z

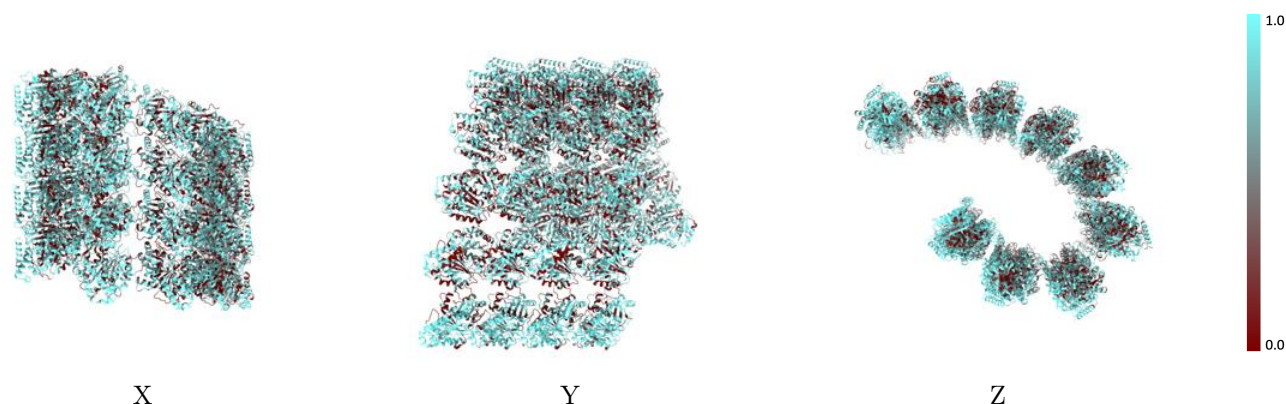
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



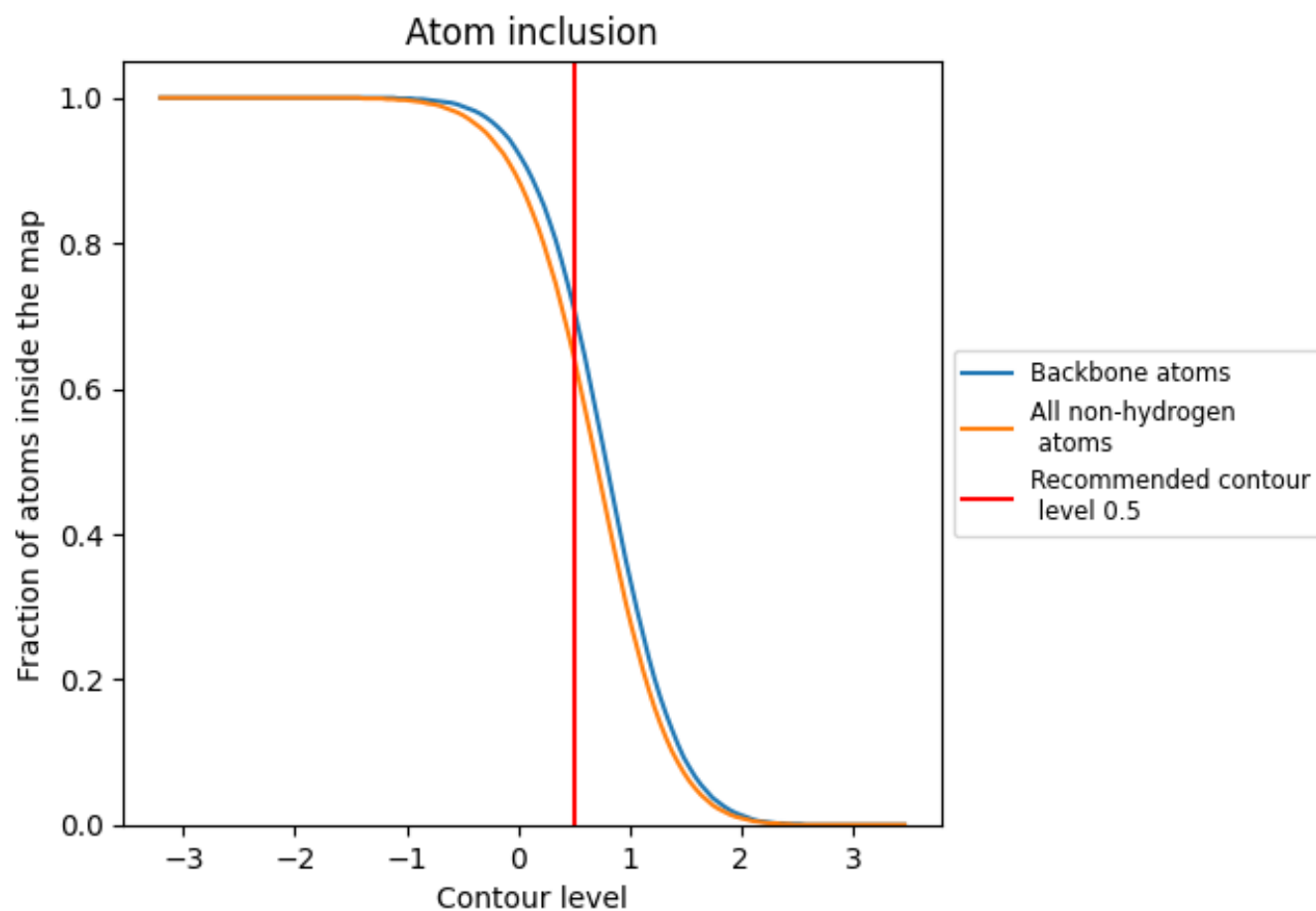
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.0530
2A	 0.7180	 0.0590
2B	 0.6580	 0.0530
2C	 0.6420	 0.0620
2D	 0.5940	 0.0530
2E	 0.5920	 0.0500
2F	 0.5900	 0.0480
2G	 0.6300	 0.0580
2H	 0.6000	 0.0350
2I	 0.7640	 0.0390
3A	 0.7140	 0.0620
3B	 0.6630	 0.0700
3C	 0.6540	 0.0620
3D	 0.6530	 0.0650
3E	 0.6030	 0.0510
3F	 0.5930	 0.0610
3G	 0.5680	 0.0410
3H	 0.5900	 0.0380
3I	 0.7520	 0.0330
4A	 0.7220	 0.0590
4B	 0.6720	 0.0680
4C	 0.6470	 0.0650
4D	 0.6030	 0.0540
4E	 0.6060	 0.0530
4F	 0.6110	 0.0610
4G	 0.6360	 0.0590
4H	 0.6160	 0.0390
4I	 0.7810	 0.0400
5A	 0.7070	 0.0650
5B	 0.6580	 0.0640
5C	 0.6430	 0.0630
5D	 0.6500	 0.0700
5E	 0.5900	 0.0470
5F	 0.5820	 0.0490
5G	 0.5630	 0.0350



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Chain	Atom inclusion	Q-score
5H	 0.5740	 0.0330
5I	 0.7390	 0.0260