Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 12:53 PM EDT

PDB ID	:	6MSB / pdb_00006msb
EMDB ID	:	EMD-9216
Title	:	Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors	:	Mao, Y.D.
Deposited on	:	2018-10-16
Resolution	:	3.00 Å(reported)

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:

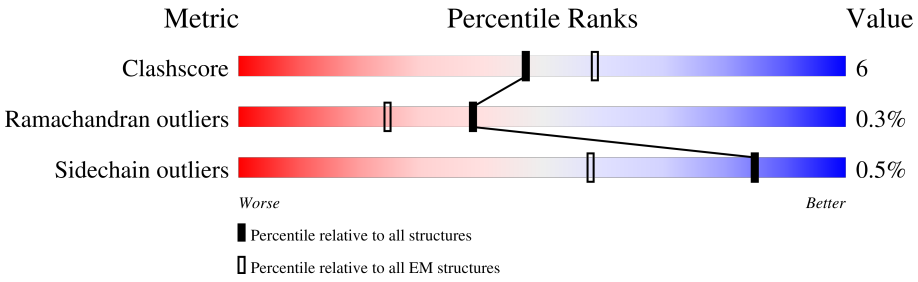
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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 <=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	U	953	68% 17% 15%
2	V	534	11% 73% 22% 5%
3	W	456	7% 80% 20%
4	X	422	80% 10% 10%
5	Y	389	79% 18%
6	Z	324	65% 23% 12%
7	a	376	78% 21%
8	b	377	40% 11% 49%

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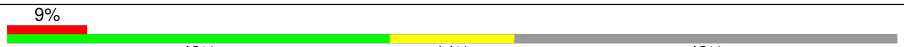
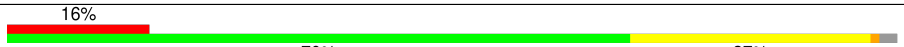
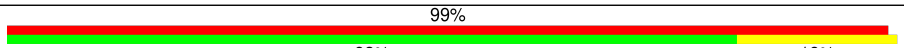
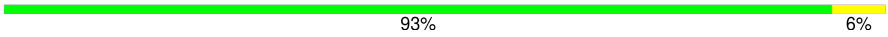
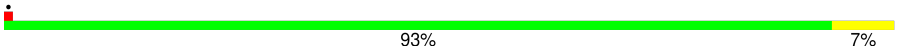
Mol	Chain	Length	Quality of chain
9	c	309	
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	u	76	
19	w	76	
20	G	245	
20	g	245	
21	H	233	
21	h	233	
22	I	260	
22	i	260	
23	J	247	
23	j	247	
24	K	240	
24	k	240	
25	L	268	
25	l	268	
26	M	254	

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Mol	Chain	Length	Quality of chain
26	m	254	
27	N	238	
27	n	238	
28	O	276	
28	o	276	
29	P	204	
29	p	204	
30	Q	201	
30	q	201	
31	R	262	
31	r	262	
32	S	240	
32	s	240	
33	T	263	
33	t	263	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 104938 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 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	812	Total	C	N	O	S	0	0
			6334	4023	1078	1189	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	508	Total	C	N	O	S	0	0
			3994	2530	712	738	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	15		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
19	w	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47
w	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
20	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
21	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
22	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		
23	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
24	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
26	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
27	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
28	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
29	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
30	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
31	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
32	s	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

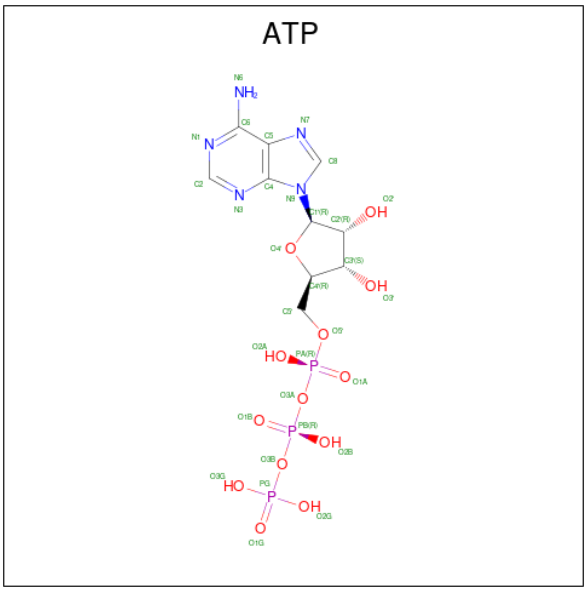
- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
33	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

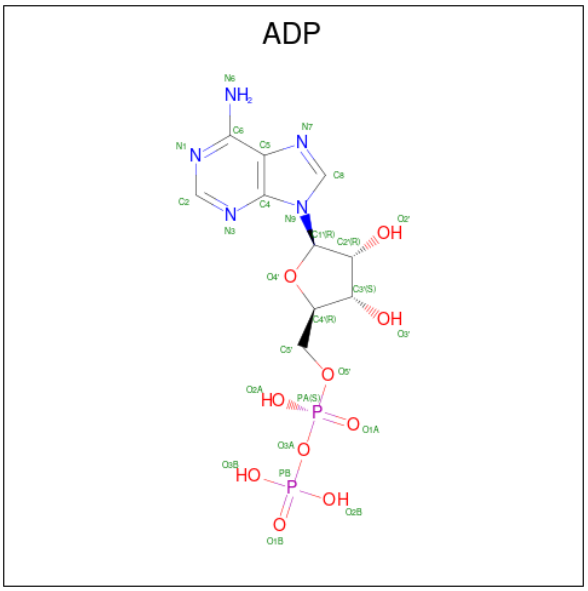


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



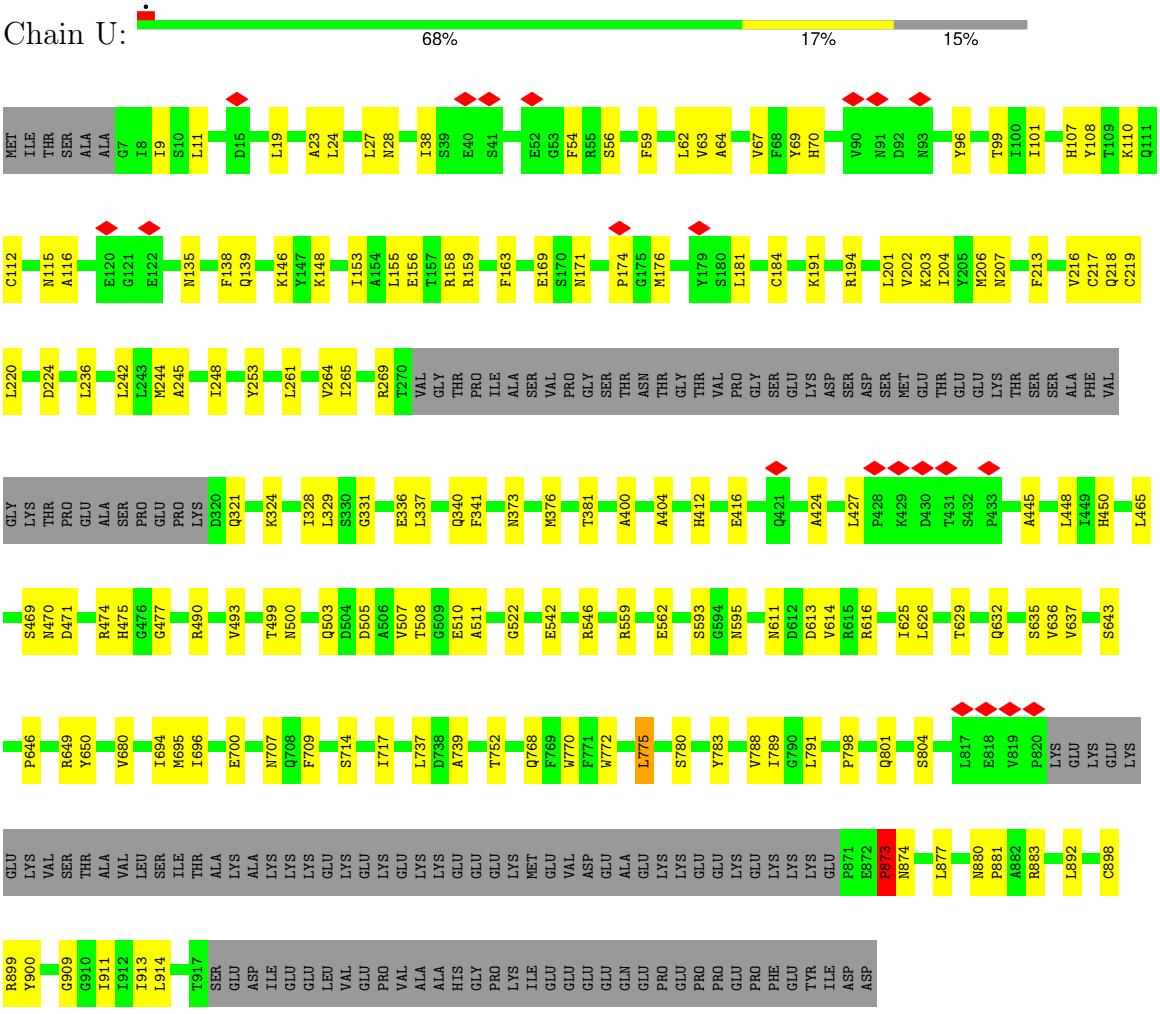
Mol	Chain	Residues	Atoms					AltConf
37	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
37	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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.

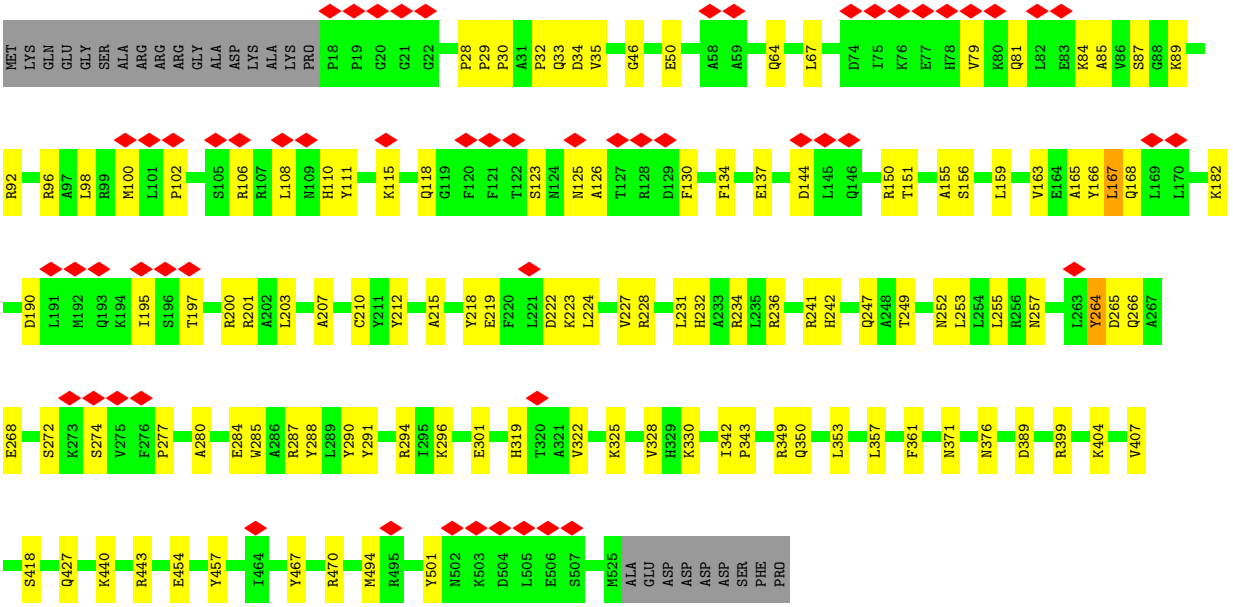
• Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

Chain U:



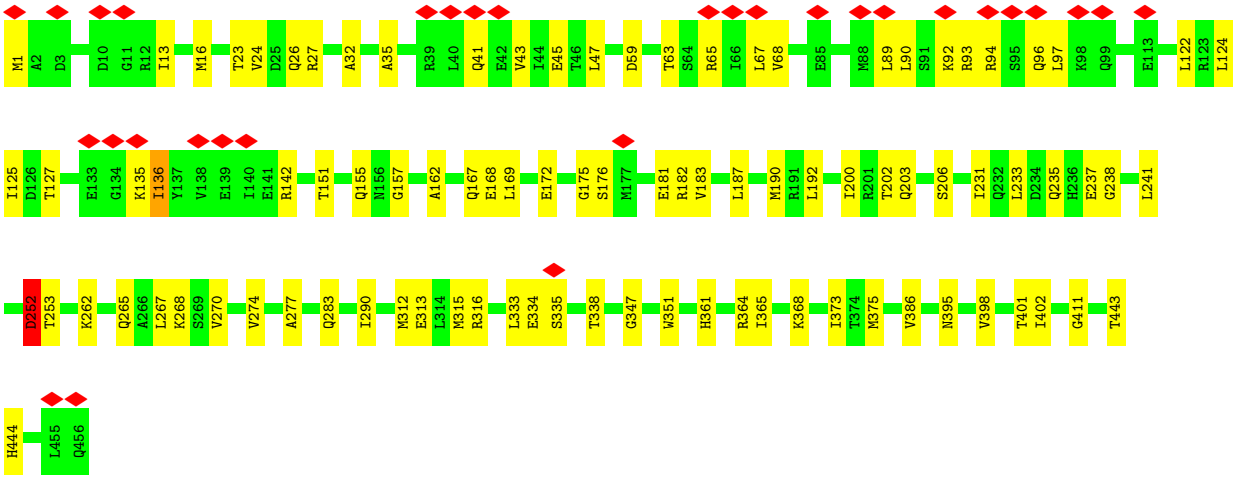
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



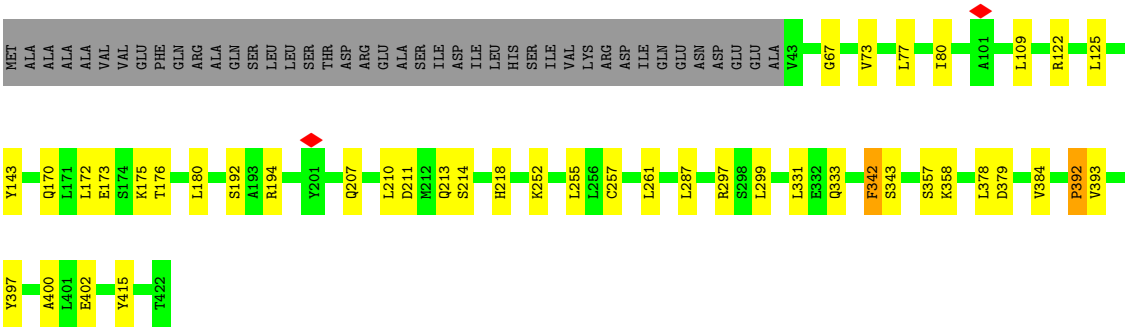
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



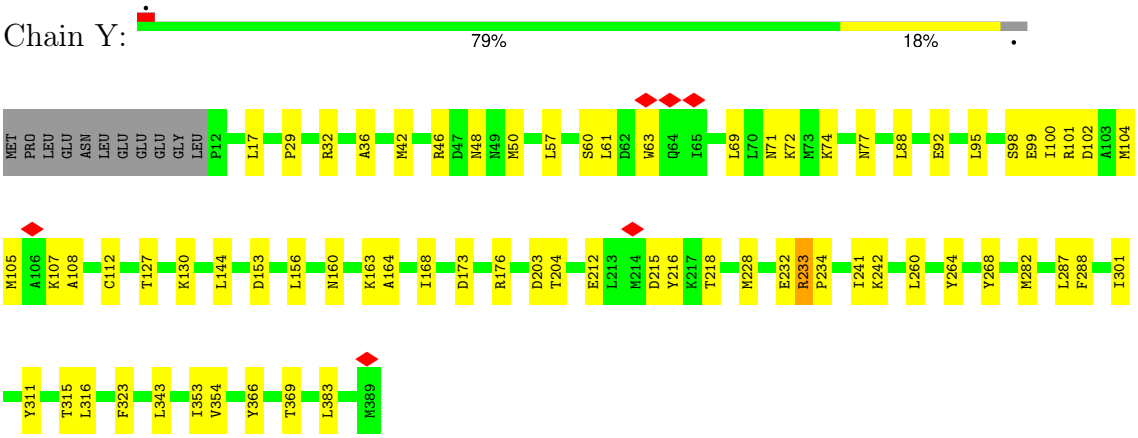
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



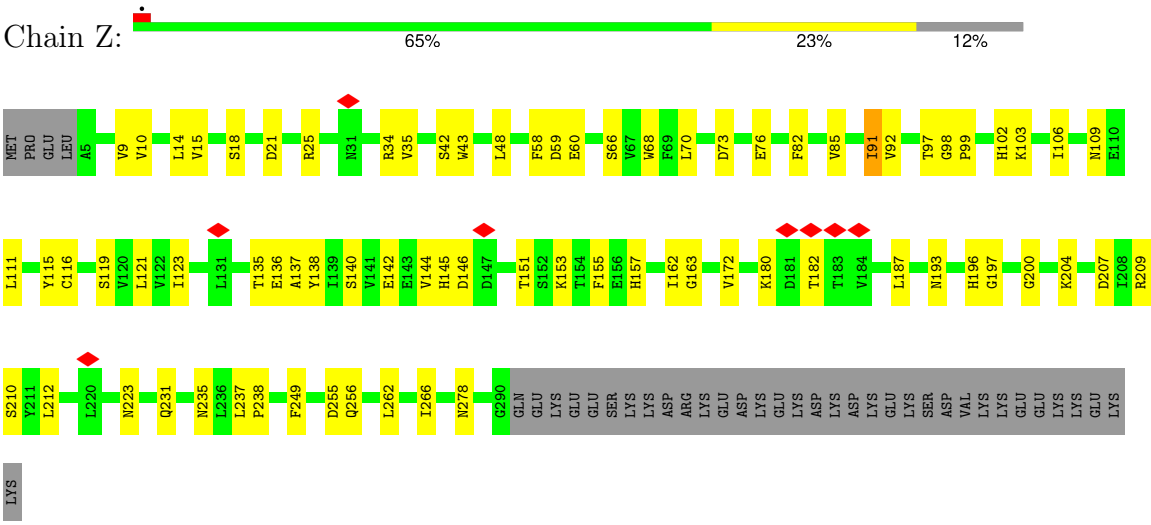
• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



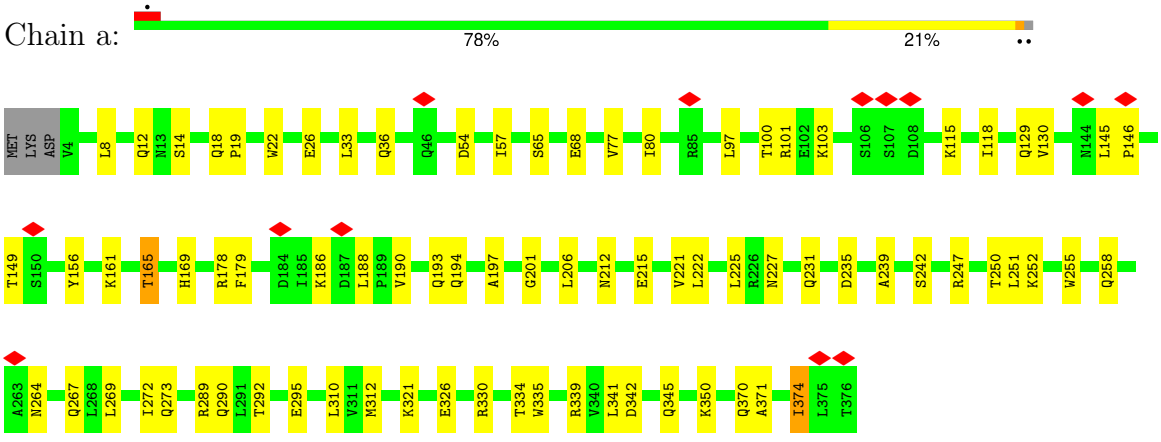
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:



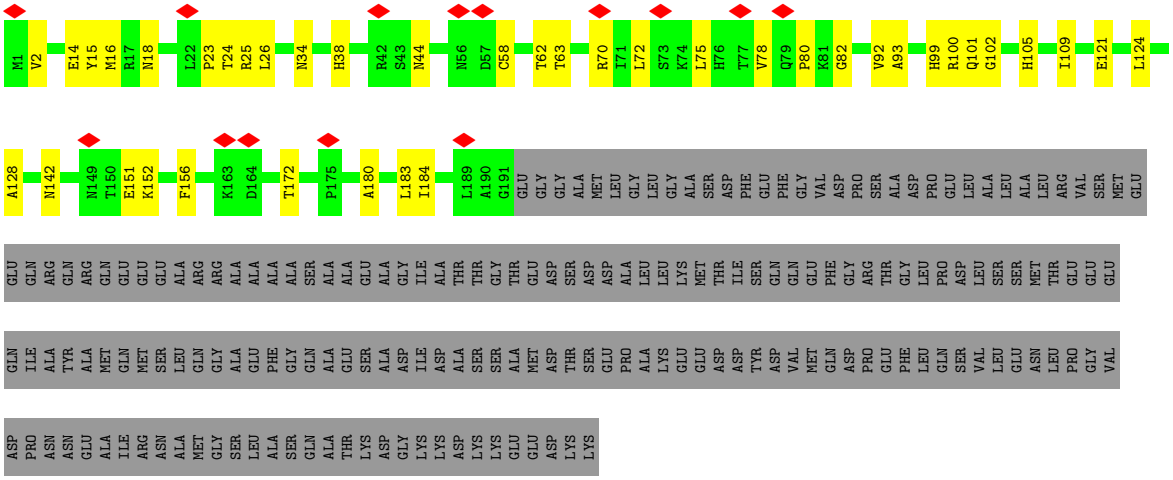
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a:



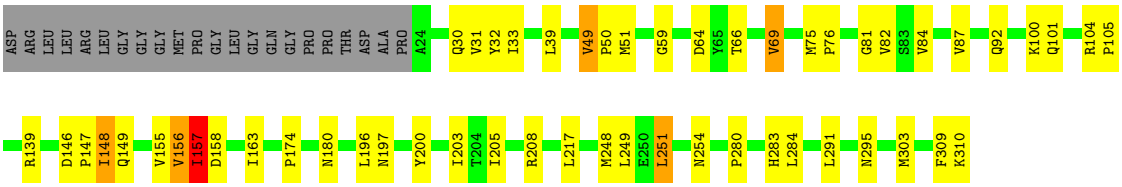
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



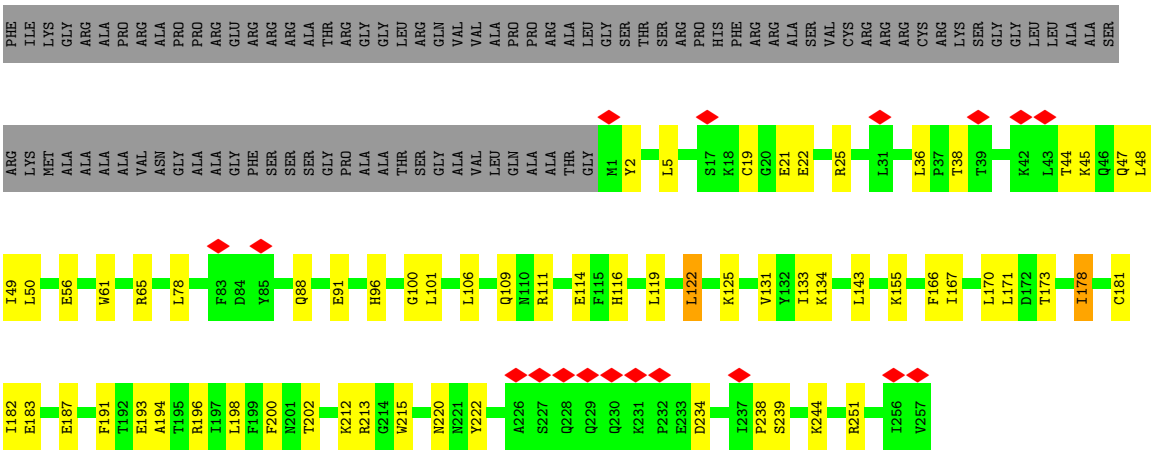
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain c:



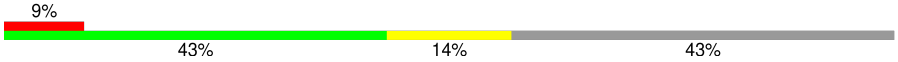
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

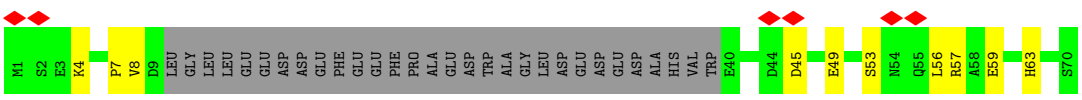
Chain d:



• Molecule 11: 26S proteasome complex subunit SEM1

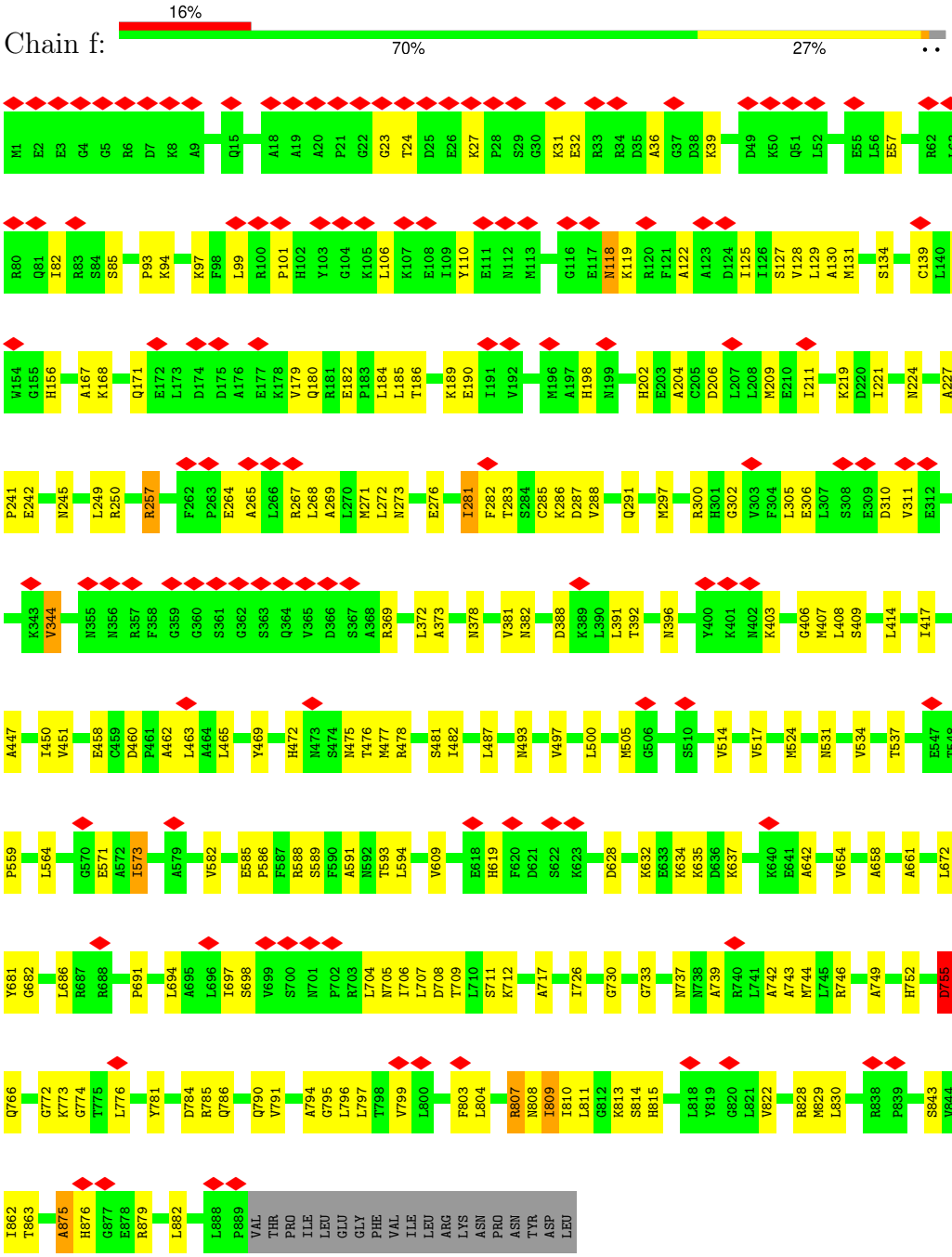
Chain e:





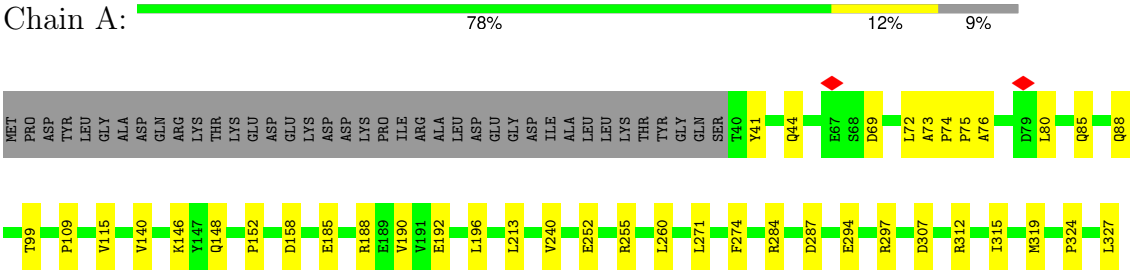
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain f:



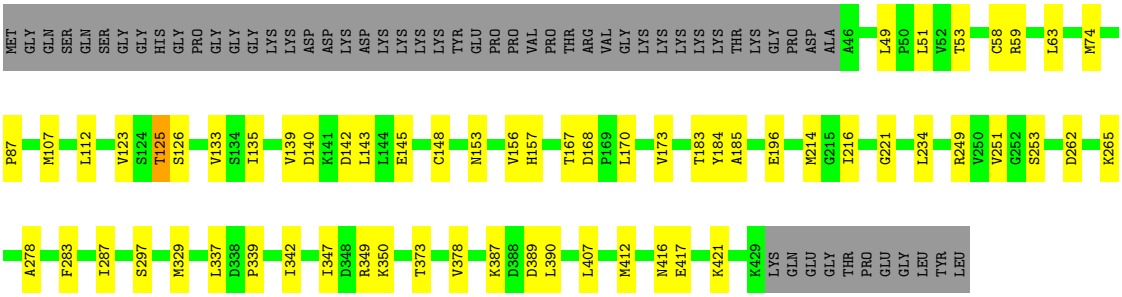
• Molecule 13: 26S proteasome regulatory subunit 7

Chain A:



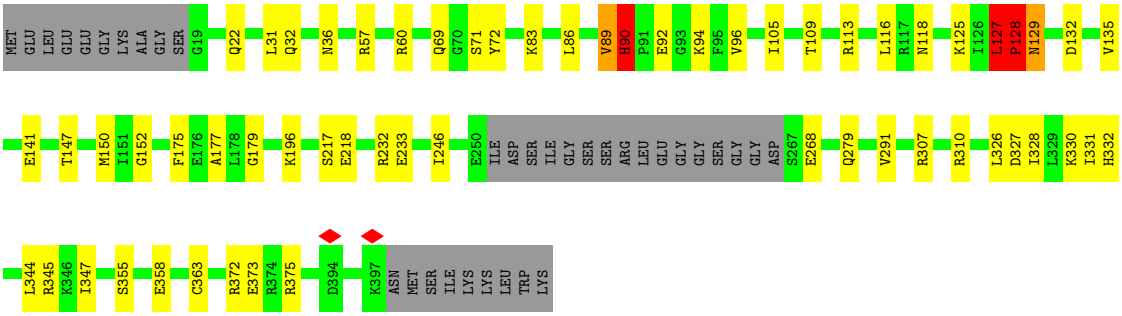
• Molecule 14: 26S proteasome regulatory subunit 4

Chain B:



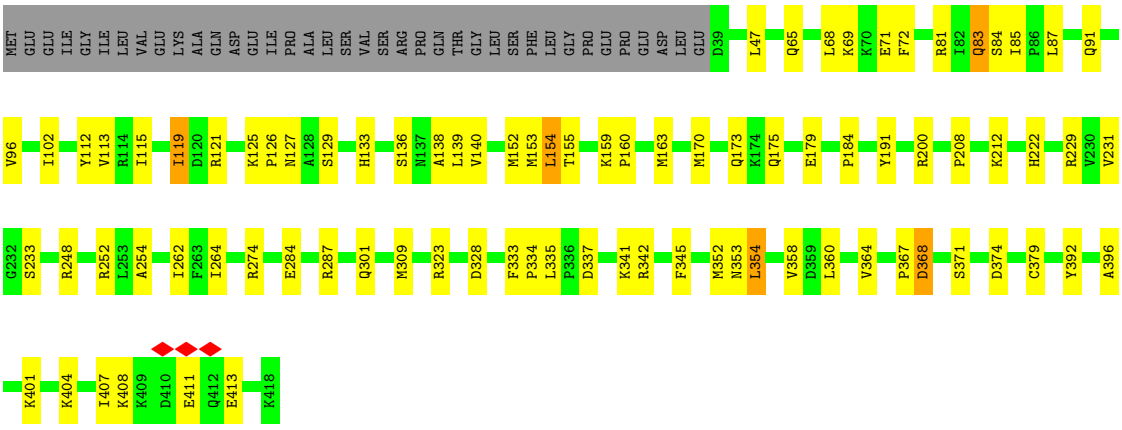
• Molecule 15: 26S proteasome regulatory subunit 8

Chain C:



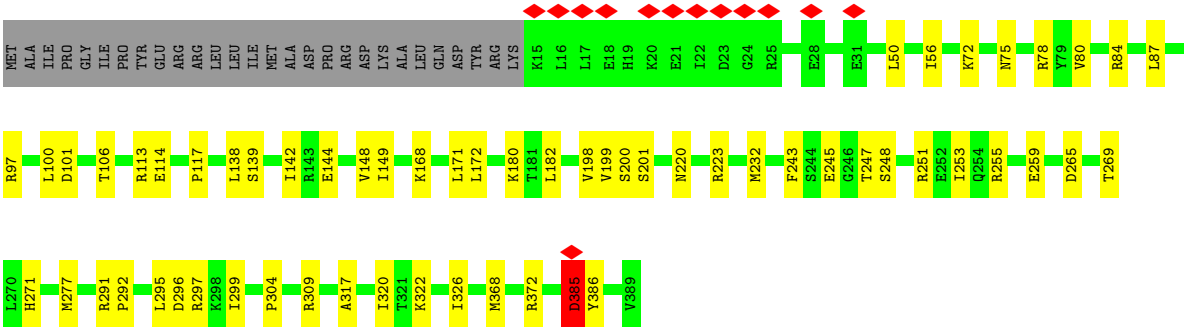
• Molecule 16: 26S proteasome regulatory subunit 6B

Chain D:



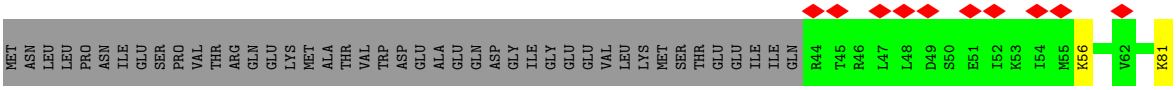
• Molecule 17: 26S proteasome regulatory subunit 10B

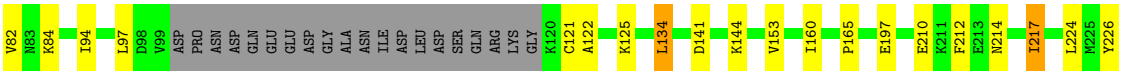
Chain E:



• Molecule 18: 26S proteasome regulatory subunit 6A

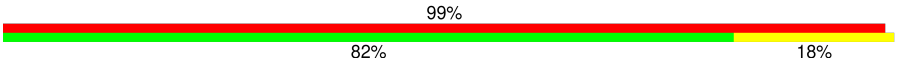
Chain F:

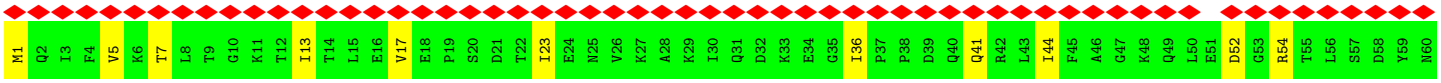


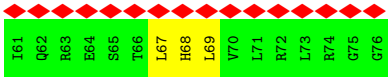


• Molecule 19: Ubiquitin

Chain u:

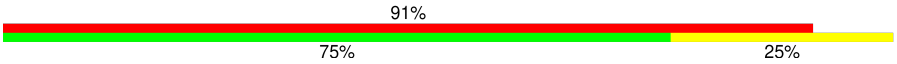


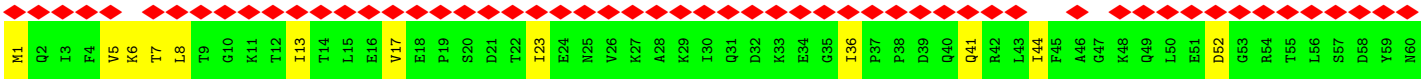


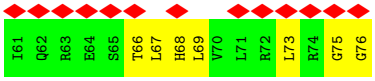


• Molecule 19: Ubiquitin

Chain w:

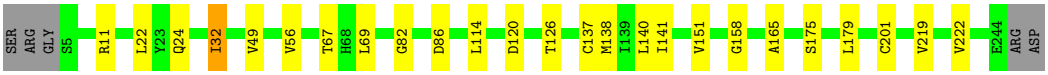






• Molecule 20: Proteasome subunit alpha type-6

Chain G:

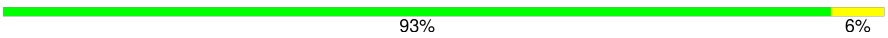


• Molecule 20: Proteasome subunit alpha type-6

Chain g:

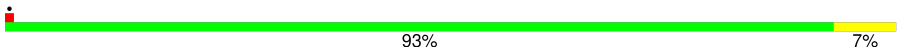
• Molecule 21: Proteasome subunit alpha type-2

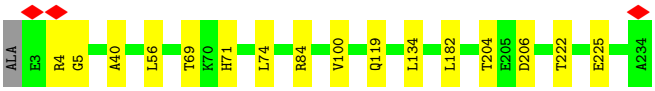
Chain H:



• Molecule 21: Proteasome subunit alpha type-2

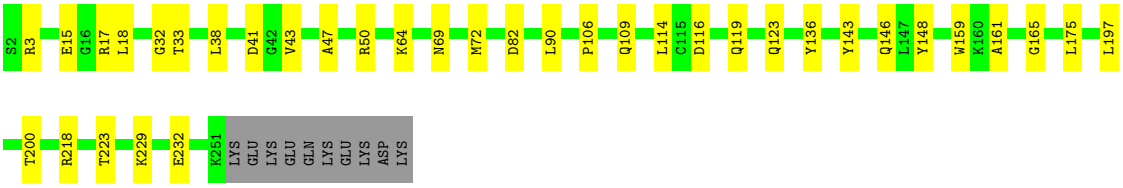
Chain h:





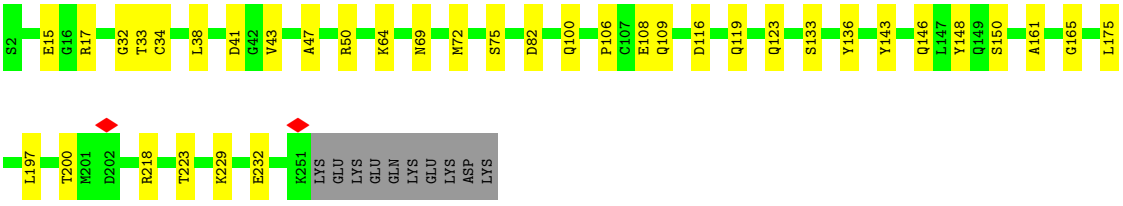
• Molecule 22: Proteasome subunit alpha type-4

Chain I:



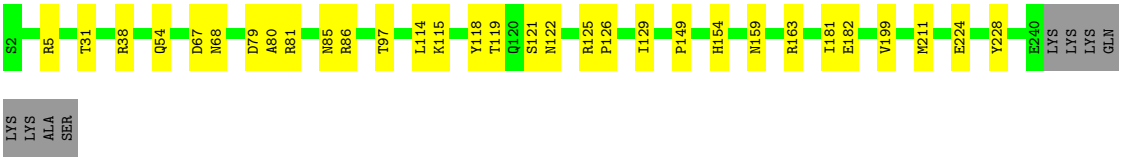
• Molecule 22: Proteasome subunit alpha type-4

Chain i:



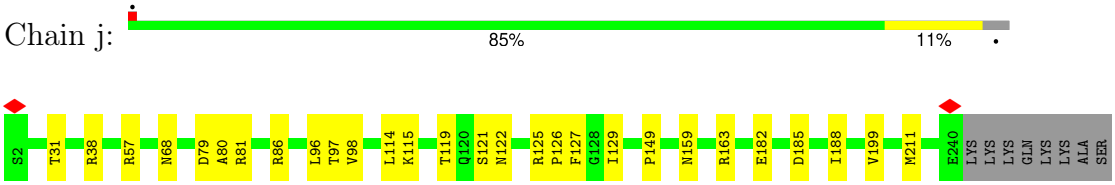
• Molecule 23: Proteasome subunit alpha type-7

Chain J:



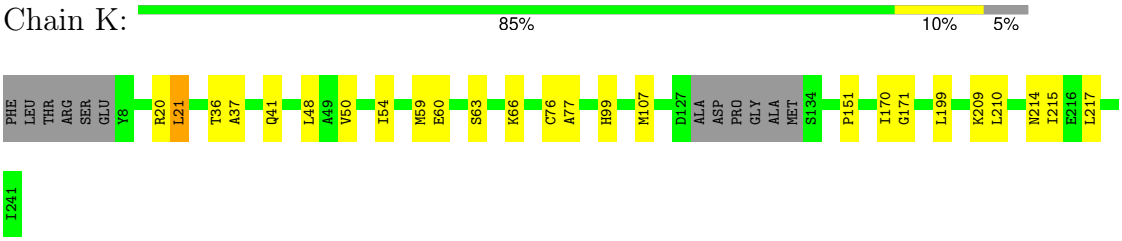
• Molecule 23: Proteasome subunit alpha type-7

Chain j:



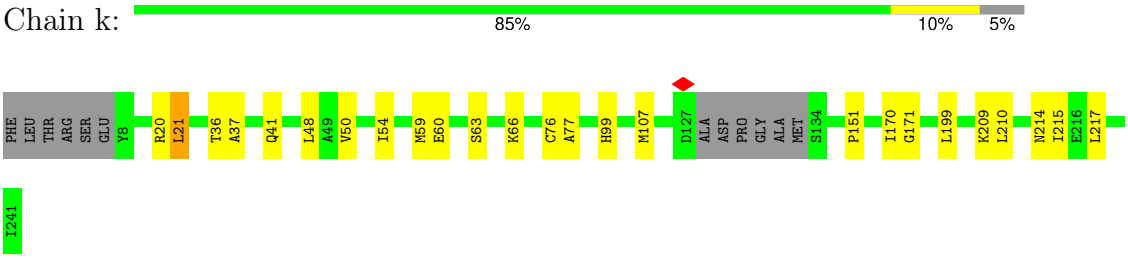
• Molecule 24: Proteasome subunit alpha type-5

Chain K:



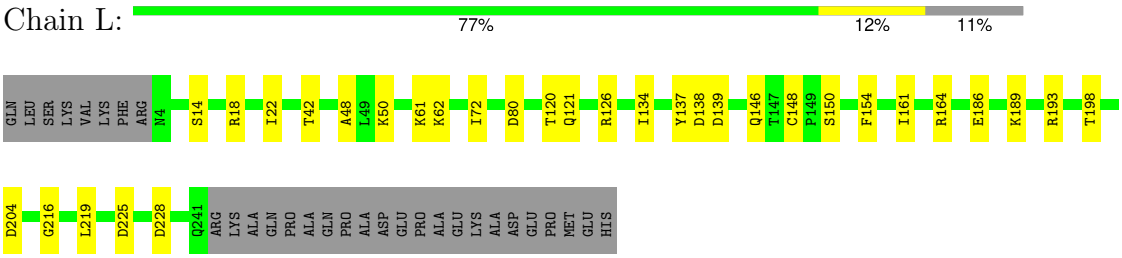
• Molecule 24: Proteasome subunit alpha type-5

Chain k:



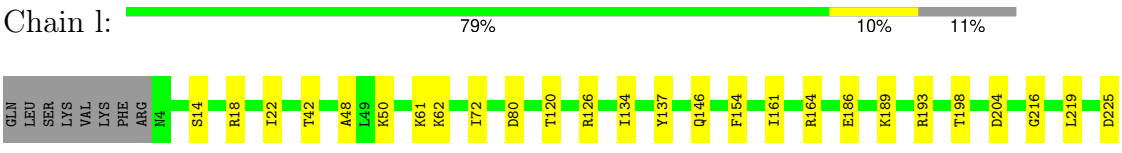
• Molecule 25: Proteasome subunit alpha type-1

Chain L:



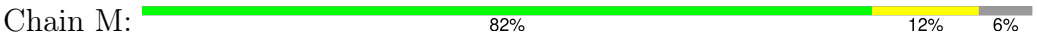
• Molecule 25: Proteasome subunit alpha type-1

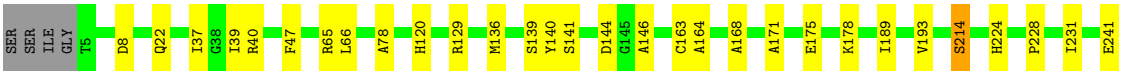
Chain l:



• Molecule 26: Proteasome subunit alpha type-3

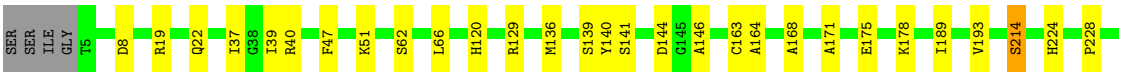
Chain M:

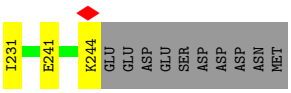




• Molecule 26: Proteasome subunit alpha type-3

Chain m:



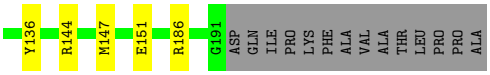


• Molecule 27: Proteasome subunit beta type-6

Chain N:

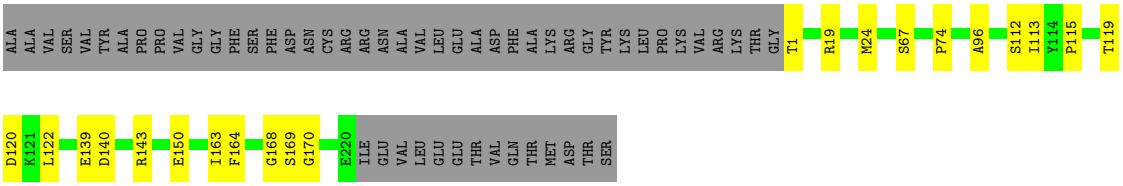
• Molecule 27: Proteasome subunit beta type-6

Chain n:

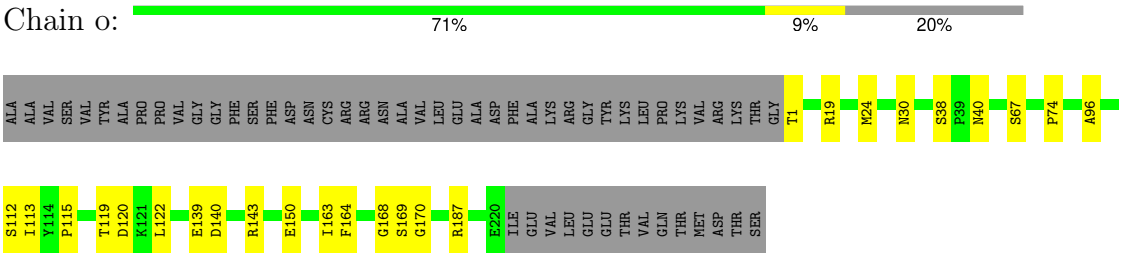


• Molecule 28: Proteasome subunit beta type-7

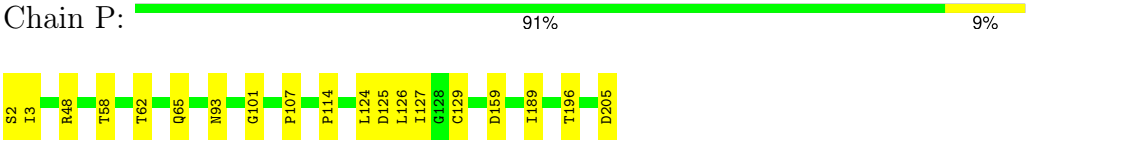
Chain O:



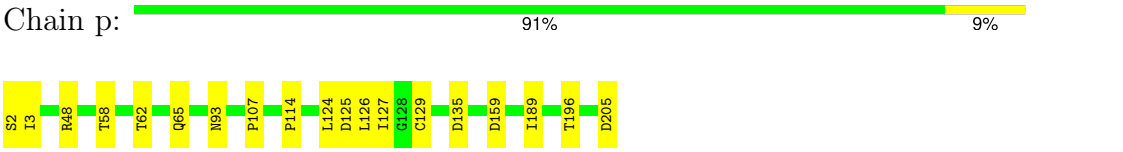
• Molecule 28: Proteasome subunit beta type-7



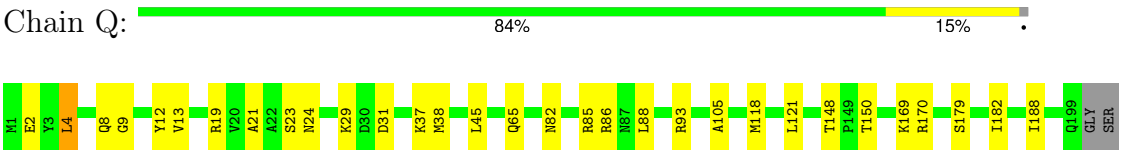
• Molecule 29: Proteasome subunit beta type-3



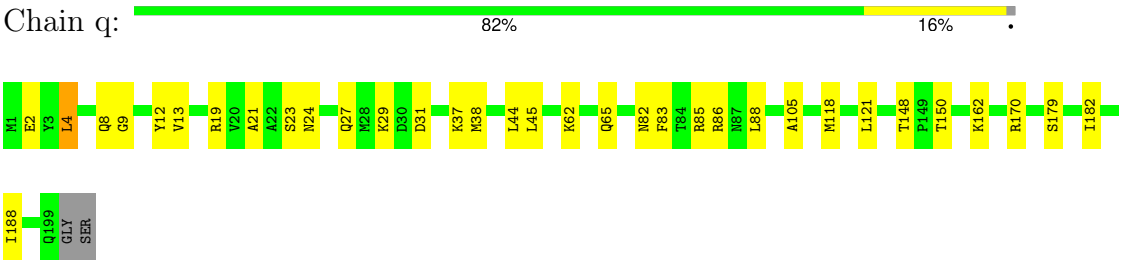
• Molecule 29: Proteasome subunit beta type-3



• Molecule 30: Proteasome subunit beta type-2

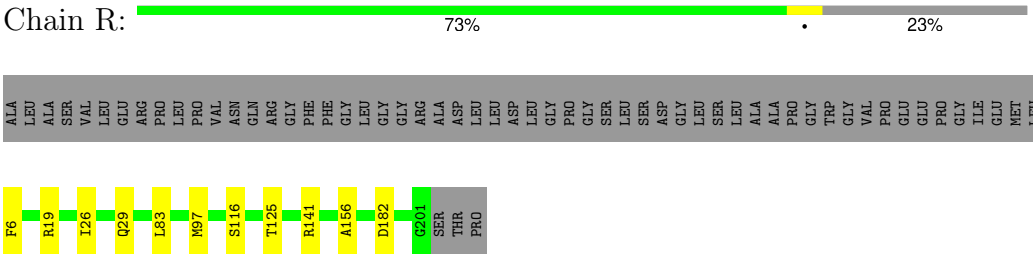


• Molecule 30: Proteasome subunit beta type-2



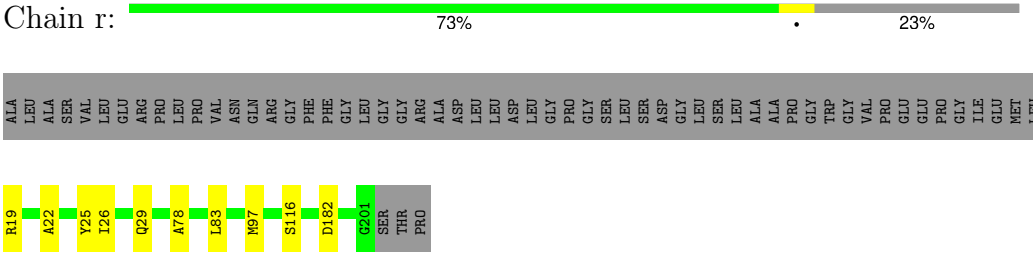
• Molecule 31: Proteasome subunit beta type-5

Chain R:



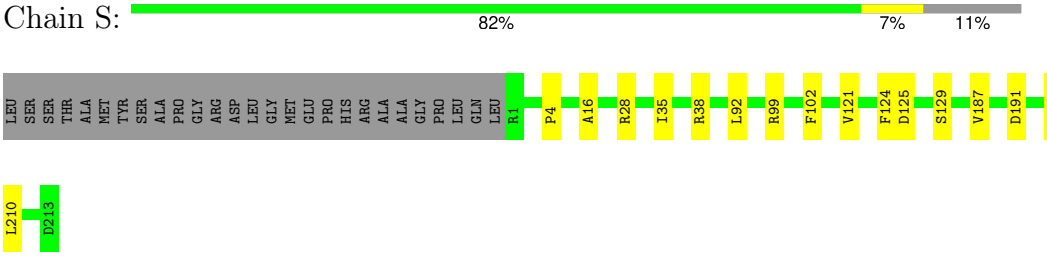
• Molecule 31: Proteasome subunit beta type-5

Chain r:



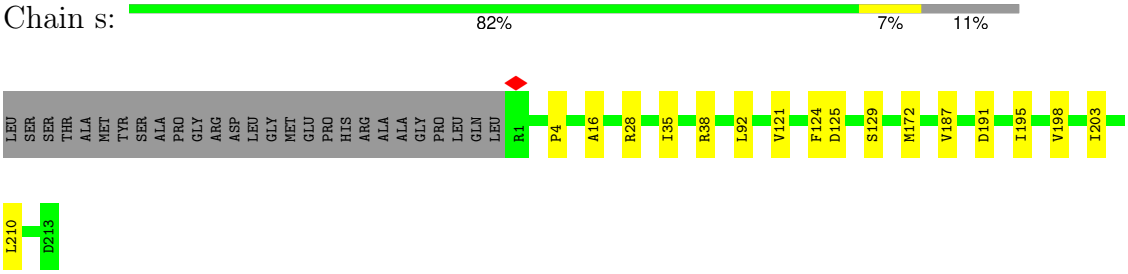
• Molecule 32: Proteasome subunit beta type-1

Chain S:



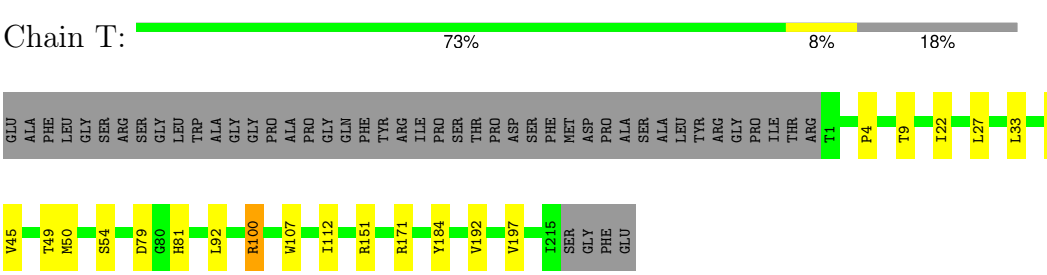
• Molecule 32: Proteasome subunit beta type-1

Chain s:



• Molecule 33: Proteasome subunit beta type-4

Chain T:



• Molecule 33: Proteasome subunit beta type-4

Chain t:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG, ZN

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	U	0.28	0/6449	0.59	2/8729 (0.0%)
2	V	0.30	0/4072	0.71	8/5510 (0.1%)
3	W	0.29	0/3751	0.67	4/5042 (0.1%)
4	X	0.26	0/3053	0.56	4/4115 (0.1%)
5	Y	0.31	0/3173	0.61	0/4273
6	Z	0.27	0/2324	0.63	2/3150 (0.1%)
7	a	0.25	0/3053	0.60	2/4133 (0.0%)
8	b	0.23	0/1478	0.58	0/2001
9	c	0.31	0/2302	0.69	2/3110 (0.1%)
10	d	0.27	0/2162	0.64	0/2919
11	e	0.26	0/338	0.67	0/450
12	f	0.28	0/6980	0.71	2/9433 (0.0%)
13	A	0.41	0/3148	0.65	0/4250
14	B	0.39	0/3061	0.61	1/4129 (0.0%)
15	C	0.37	0/2902	0.63	1/3904 (0.0%)
16	D	0.39	0/3089	0.65	2/4168 (0.0%)
17	E	0.37	0/2904	0.62	2/3924 (0.1%)
18	F	0.39	0/2896	0.57	0/3912
19	u	0.21	0/609	0.49	0/819
19	w	0.21	0/609	0.49	0/819
20	G	0.37	1/1859 (0.1%)	0.53	1/2523 (0.0%)
20	g	0.37	1/1859 (0.1%)	0.53	1/2523 (0.0%)
21	H	0.33	0/1743	0.47	0/2372
21	h	0.33	0/1743	0.47	0/2372
22	I	0.32	0/1942	0.53	0/2628
22	i	0.32	0/1942	0.53	0/2628
23	J	0.36	0/1737	0.57	0/2369
23	j	0.25	0/1728	0.51	0/2358
24	K	0.33	0/1747	0.51	0/2364
24	k	0.33	0/1747	0.51	0/2364
25	L	0.35	0/1885	0.60	2/2552 (0.1%)
25	l	0.35	0/1885	0.60	2/2552 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	M	0.33	0/1891	0.52	0/2552
26	m	0.33	0/1891	0.52	0/2552
27	N	0.31	0/1454	0.41	0/1967
27	n	0.31	0/1454	0.41	0/1967
28	O	0.32	0/1670	0.45	0/2265
28	o	0.32	0/1670	0.45	0/2265
29	P	0.32	0/1620	0.45	0/2184
29	p	0.32	0/1620	0.45	0/2184
30	Q	0.34	0/1603	0.50	0/2174
30	q	0.34	0/1603	0.50	0/2174
31	R	0.33	0/1579	0.42	0/2134
31	r	0.33	0/1579	0.42	0/2134
32	S	0.34	0/1671	0.45	0/2253
32	s	0.31	0/1674	0.44	0/2257
33	T	0.33	0/1700	0.48	0/2305
33	t	0.33	0/1700	0.48	0/2305
All	All	0.32	2/106549 (0.0%)	0.58	38/144067 (0.0%)

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	U	0	1
2	V	0	2
3	W	0	2
5	Y	0	1
6	Z	0	2
7	a	0	1
9	c	0	2
12	f	0	9
13	A	0	2
14	B	0	1
15	C	0	5
16	D	0	4
17	E	0	2
18	F	0	1
20	G	0	1
20	g	0	1
23	J	0	1
23	j	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	M	0	1
26	m	0	1
30	Q	0	1
30	q	0	1
All	All	0	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	g	56	VAL	CA-C	6.76	1.60	1.52
20	G	56	VAL	CA-C	6.67	1.59	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	106	ILE	N-CA-C	-8.15	105.96	113.71
1	U	873	PRO	CA-C-N	7.19	135.26	121.54
1	U	873	PRO	C-N-CA	7.19	135.26	121.54
16	D	160	PRO	CA-C-N	6.12	131.09	122.46
16	D	160	PRO	C-N-CA	6.12	131.09	122.46
2	V	137	GLU	N-CA-C	5.79	122.60	109.81
17	E	385	ASP	CA-C-N	5.77	132.56	121.54
17	E	385	ASP	C-N-CA	5.77	132.56	121.54
2	V	167	LEU	CA-C-N	5.64	132.32	121.54
2	V	167	LEU	C-N-CA	5.64	132.32	121.54
2	V	28	PRO	N-CA-C	5.53	117.44	110.70
25	L	225	ASP	CA-C-N	5.50	132.05	121.54
25	L	225	ASP	C-N-CA	5.50	132.05	121.54
25	l	225	ASP	CA-C-N	5.50	132.05	121.54
25	l	225	ASP	C-N-CA	5.50	132.05	121.54
9	c	157	ILE	CA-C-N	5.50	132.04	121.54
9	c	157	ILE	C-N-CA	5.50	132.04	121.54
3	W	252	ASP	CA-C-N	5.47	135.15	121.80
3	W	252	ASP	C-N-CA	5.47	135.15	121.80
20	g	56	VAL	O-C-N	5.30	127.14	121.10
2	V	165	ALA	CA-C-N	5.29	131.64	121.54
2	V	165	ALA	C-N-CA	5.29	131.64	121.54
6	Z	92	VAL	N-CA-C	-5.27	108.71	113.71
20	G	56	VAL	O-C-N	5.26	127.09	121.10
15	C	128	PRO	N-CA-C	5.25	123.28	112.47
12	f	619	HIS	CA-C-N	5.15	131.38	121.54
12	f	619	HIS	C-N-CA	5.15	131.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	342	PHE	CA-C-N	5.14	131.36	121.54
4	X	342	PHE	C-N-CA	5.14	131.36	121.54
2	V	166	TYR	CA-C-N	5.14	131.35	121.54
2	V	166	TYR	C-N-CA	5.14	131.35	121.54
4	X	392	PRO	CA-C-N	5.10	131.15	121.97
4	X	392	PRO	C-N-CA	5.10	131.15	121.97
7	a	186	LYS	CA-C-N	5.08	131.24	121.54
7	a	186	LYS	C-N-CA	5.08	131.24	121.54
14	B	53	THR	N-CA-C	5.07	121.01	109.81
3	W	92	LYS	CA-C-N	5.05	131.19	121.54
3	W	92	LYS	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	158	ASP	Peptide
13	A	400	ARG	Peptide
14	B	278	ALA	Peptide
15	C	127	LEU	Peptide
15	C	128	PRO	Peptide
15	C	129	ASN	Peptide
15	C	89	VAL	Peptide
15	C	90	HIS	Peptide
16	D	125	LYS	Peptide
16	D	354	LEU	Peptide
16	D	368	ASP	Peptide
16	D	83	GLN	Peptide
17	E	385	ASP	Peptide
17	E	75	ASN	Peptide
18	F	344	ARG	Peptide
20	G	222	VAL	Peptide
23	J	199	VAL	Peptide
26	M	214	SER	Peptide
30	Q	2	GLU	Peptide
1	U	873	PRO	Peptide
2	V	264	TYR	Peptide
2	V	501	TYR	Peptide
3	W	252	ASP	Peptide
3	W	315	MET	Peptide
5	Y	233	ARG	Peptide
6	Z	145	HIS	Peptide

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Mol	Chain	Res	Type	Group
6	Z	223	ASN	Peptide
7	a	169	HIS	Peptide
9	c	155	VAL	Peptide
9	c	84	VAL	Peptide
12	f	249	LEU	Peptide
12	f	257	ARG	Peptide
12	f	340	MET	Peptide
12	f	642	ALA	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	843	SER	Peptide
12	f	875	ALA	Peptide
20	g	222	VAL	Peptide
23	j	199	VAL	Peptide
26	m	214	SER	Peptide
30	q	2	GLU	Peptide

5.2 Too-close contacts (i)

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	U	6334	0	6366	98	0
2	V	3994	0	3960	71	0
3	W	3703	0	3822	53	0
4	X	3009	0	3113	26	0
5	Y	3115	0	3120	42	0
6	Z	2281	0	2312	58	0
7	a	2995	0	3012	53	0
8	b	1458	0	1505	26	0
9	c	2260	0	2276	39	0
10	d	2116	0	2146	38	0
11	e	334	0	294	7	0
12	f	6866	0	6866	165	0
13	A	3096	0	3138	32	0
14	B	3018	0	3081	41	0
15	C	2864	0	2971	38	0
16	D	3039	0	3075	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	E	2860	0	2827	37	0
18	F	2858	0	2853	34	0
19	u	603	0	629	11	0
19	w	603	0	629	26	0
20	G	1826	0	1796	13	0
20	g	1826	0	1796	15	0
21	H	1708	0	1594	10	0
21	h	1708	0	1594	11	0
22	I	1912	0	1851	23	0
22	i	1912	0	1851	23	0
23	J	1713	0	1537	20	0
23	j	1704	0	1517	16	0
24	K	1722	0	1673	15	0
24	k	1722	0	1673	13	0
25	L	1850	0	1822	19	0
25	l	1850	0	1822	13	0
26	M	1856	0	1814	20	0
26	m	1856	0	1814	19	0
27	N	1430	0	1398	11	0
27	n	1430	0	1398	12	0
28	O	1643	0	1644	14	0
28	o	1643	0	1644	16	0
29	P	1591	0	1609	13	0
29	p	1591	0	1609	13	0
30	Q	1570	0	1547	18	0
30	q	1570	0	1547	22	0
31	R	1548	0	1499	8	0
31	r	1548	0	1499	7	0
32	S	1641	0	1616	13	0
32	s	1644	0	1625	12	0
33	T	1667	0	1628	18	0
33	t	1667	0	1628	15	0
34	c	1	0	0	0	0
35	A	31	0	12	0	0
35	B	31	0	12	2	0
35	D	31	0	12	1	0
35	E	31	0	12	2	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	C	27	0	12	1	0
37	F	27	0	12	0	0
All	All	104938	0	104112	1208	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 6.

All (1208) 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)
12:f:310:ASP:O	19:w:75:GLY:HA3	1.40	1.18
12:f:458:GLU:HB3	19:w:8:LEU:HD21	1.39	1.02
12:f:458:GLU:HB3	19:w:8:LEU:CD2	1.95	0.95
12:f:311:VAL:HG22	19:w:75:GLY:C	1.91	0.94
18:F:56:LYS:CB	19:u:54:ARG:HE	1.84	0.90
18:F:56:LYS:CB	19:u:54:ARG:NE	2.40	0.85
12:f:458:GLU:CB	19:w:8:LEU:HD21	2.13	0.78
16:D:133:HIS:HD2	16:D:136:SER:H	1.31	0.78
12:f:311:VAL:HG22	19:w:76:GLY:N	2.02	0.73
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.70	0.73
6:Z:25:ARG:HH11	9:c:104:ARG:H	1.37	0.71
15:C:89:VAL:HB	15:C:92:GLU:HB3	1.75	0.69
23:J:86:ARG:HE	23:J:114:LEU:HD11	1.58	0.69
1:U:169:GLU:HG3	1:U:171:ASN:H	1.59	0.68
12:f:441:LYS:HB2	12:f:477:MET:HE1	1.76	0.68
3:W:142:ARG:HH12	3:W:176:SER:HB3	1.58	0.67
2:V:79:VAL:HG13	2:V:81:GLN:H	1.59	0.67
16:D:91:GLN:HE21	16:D:127:ASN:HB3	1.60	0.67
27:n:29:ARG:NH1	28:o:139:GLU:OE2	2.27	0.67
2:V:201:ARG:HE	2:V:242:HIS:HB3	1.59	0.67
3:W:169:LEU:O	3:W:182:ARG:NH1	2.27	0.67
5:Y:29:PRO:HB2	5:Y:32:ARG:HB3	1.77	0.67
7:a:212:ASN:HD21	7:a:215:GLU:HB3	1.60	0.67
26:M:47:PHE:HB2	26:M:214:SER:HB3	1.77	0.66
26:M:214:SER:HG	26:M:224:HIS:HE2	1.43	0.66
18:F:224:LEU:HB2	18:F:348:LEU:HD23	1.78	0.66
21:H:119:GLN:NE2	22:I:82:ASP:OD1	2.29	0.66
11:e:56:LEU:HB2	11:e:59:GLU:HB2	1.78	0.65
32:s:4:PRO:O	33:t:100:ARG:NH2	2.30	0.65
6:Z:73:ASP:H	8:b:63:THR:HG21	1.60	0.65
26:m:47:PHE:HB2	26:m:214:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:84:LYS:HG2	2:V:123:SER:HB2	1.78	0.65
7:a:33:LEU:HD13	7:a:36:GLN:HB2	1.79	0.65
8:b:142:ASN:HD22	8:b:172:THR:HA	1.62	0.65
23:j:86:ARG:HE	23:j:114:LEU:HD11	1.62	0.64
7:a:252:LYS:HG2	7:a:255:TRP:HE1	1.62	0.64
16:D:345:PHE:HB3	16:D:360:LEU:HD23	1.80	0.64
13:A:297:ARG:HH22	18:F:306:VAL:HG21	1.63	0.64
12:f:673:ARG:HH22	12:f:709:THR:HA	1.62	0.64
7:a:188:LEU:HD11	7:a:193:GLN:HE21	1.63	0.64
7:a:264:ASN:HB3	7:a:267:GLN:HE21	1.62	0.63
25:L:148:CYS:HG	25:L:150:SER:HG	1.45	0.63
22:i:218:ARG:NH1	22:i:223:THR:OG1	2.31	0.63
22:I:218:ARG:NH1	22:I:223:THR:OG1	2.31	0.63
1:U:337:LEU:HD21	1:U:789:ILE:HG21	1.80	0.63
25:l:186:GLU:HA	25:l:189:LYS:HG2	1.80	0.63
1:U:471:ASP:HA	1:U:474:ARG:HB2	1.79	0.63
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.81	0.63
12:f:127:SER:HA	12:f:131:MET:HB2	1.81	0.63
25:L:186:GLU:HA	25:L:189:LYS:HG2	1.80	0.63
22:I:143:TYR:HB2	22:I:146:GLN:HE21	1.64	0.63
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.81	0.62
6:Z:146:ASP:O	7:a:178:ARG:NH1	2.33	0.62
12:f:586:PRO:HA	12:f:589:SER:HB2	1.80	0.62
19:w:23:ILE:HB	19:w:52:ASP:HA	1.81	0.62
2:V:247:GLN:HE21	2:V:274:SER:HA	1.63	0.62
3:W:63:THR:HA	3:W:68:VAL:HG22	1.80	0.62
12:f:609:VAL:HG12	14:B:74:MET:HE1	1.82	0.62
22:i:143:TYR:HB2	22:i:146:GLN:HE21	1.64	0.62
2:V:223:LYS:HZ2	2:V:227:VAL:HG23	1.64	0.62
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.32	0.62
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.81	0.62
12:f:556:ARG:HD3	12:f:786:GLN:HB2	1.82	0.62
12:f:828:ARG:NH1	12:f:863:THR:OG1	2.32	0.62
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.79	0.62
17:E:148:VAL:HG13	17:E:149:ILE:HG23	1.81	0.62
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.80	0.62
12:f:571:GLU:HG3	12:f:573:ILE:H	1.63	0.62
28:O:164:PHE:O	32:s:38:ARG:NH2	2.33	0.62
1:U:219:CYS:SG	1:U:220:LEU:N	2.74	0.61
12:f:276:GLU:O	12:f:286:LYS:NZ	2.33	0.61
16:D:87:LEU:HB3	17:E:80:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:123:GLN:HG3	23:j:125:ARG:HE	1.64	0.61
5:Y:92:GLU:HB3	5:Y:100:ILE:HD11	1.81	0.61
6:Z:109:ASN:ND2	6:Z:140:SER:OG	2.34	0.61
8:b:180:ALA:HA	8:b:183:LEU:HD13	1.82	0.61
24:k:36:THR:HA	24:k:171:GLY:HA3	1.83	0.61
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.33	0.61
24:K:36:THR:HA	24:K:171:GLY:HA3	1.83	0.61
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.83	0.61
13:A:85:GLN:HA	13:A:88:GLN:HB3	1.83	0.61
12:f:813:LYS:HD3	12:f:815:HIS:HE1	1.66	0.61
16:D:411:GLU:HG2	16:D:413:GLU:H	1.66	0.61
17:E:198:VAL:HG12	17:E:200:SER:H	1.66	0.61
19:u:23:ILE:HB	19:u:52:ASP:HA	1.82	0.61
1:U:70:HIS:HB2	2:V:236:ARG:HH12	1.64	0.61
7:a:227:ASN:O	7:a:231:GLN:NE2	2.33	0.61
2:V:494:MET:SD	6:Z:278:ASN:ND2	2.74	0.60
18:F:433:ALA:HB3	24:K:20:ARG:HH22	1.65	0.60
6:Z:123:ILE:HB	6:Z:136:GLU:HB3	1.83	0.60
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.83	0.60
14:B:196:GLU:OE2	14:B:349:ARG:NH1	2.33	0.60
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.34	0.60
7:a:129:GLN:HG3	7:a:130:VAL:HG23	1.83	0.60
25:L:48:ALA:HB1	25:L:62:LYS:HE3	1.84	0.60
32:S:38:ARG:NH2	28:o:164:PHE:O	2.35	0.60
1:U:64:ALA:HA	1:U:67:VAL:HG12	1.83	0.60
26:M:37:ILE:HD11	26:M:193:VAL:HG13	1.83	0.60
26:m:37:ILE:HD11	26:m:193:VAL:HG13	1.83	0.60
32:S:38:ARG:HH12	33:T:151:ARG:HD3	1.64	0.60
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.33	0.60
12:f:209:MET:HG3	12:f:211:ILE:H	1.65	0.60
25:l:48:ALA:HB1	25:l:62:LYS:HE3	1.84	0.60
29:p:65:GLN:OE1	30:q:86:ARG:NH2	2.35	0.60
33:t:192:VAL:HG12	33:t:197:VAL:HG22	1.83	0.60
18:F:153:VAL:HG22	18:F:160:ILE:HG22	1.84	0.60
28:o:163:ILE:HG12	28:o:170:GLY:HA2	1.84	0.60
33:T:9:THR:O	33:T:41:ARG:NH2	2.35	0.60
1:U:804:SER:HA	1:U:892:LEU:HA	1.84	0.60
7:a:19:PRO:HA	7:a:22:TRP:HD1	1.67	0.60
18:F:228:PRO:O	18:F:233:LYS:NZ	2.35	0.60
33:t:9:THR:O	33:t:41:ARG:NH2	2.35	0.60
2:V:467:TYR:HH	4:X:397:TYR:HH	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:41:TYR:HB2	13:A:44:GLN:HB3	1.84	0.59
17:E:253:ILE:HG13	18:F:308:ARG:HH22	1.67	0.59
28:O:163:ILE:HG12	28:O:170:GLY:HA2	1.84	0.59
12:f:39:LYS:HD3	12:f:85:SER:HA	1.83	0.59
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.84	0.59
9:c:197:ASN:ND2	9:c:200:TYR:O	2.34	0.59
12:f:875:ALA:O	12:f:876:HIS:ND1	2.35	0.59
12:f:340:MET:SD	12:f:757:ASN:ND2	2.75	0.59
12:f:469:TYR:O	12:f:472:HIS:ND1	2.30	0.59
4:X:415:TYR:HE1	5:Y:383:LEU:HD13	1.68	0.59
27:N:29:ARG:NH1	28:O:139:GLU:OE2	2.33	0.59
2:V:224:LEU:HG	2:V:257:ASN:HD22	1.67	0.59
16:D:353:ASN:ND2	16:D:392:TYR:O	2.35	0.59
19:w:44:ILE:HB	19:w:68:HIS:HB2	1.84	0.59
14:B:412:MET:HE1	15:C:177:ALA:HB1	1.84	0.59
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.85	0.59
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.84	0.59
29:P:62:THR:OG1	30:Q:85:ARG:NH2	2.35	0.59
2:V:280:ALA:HB3	2:V:285:TRP:HB2	1.84	0.59
7:a:8:LEU:HD11	7:a:26:GLU:HB3	1.84	0.59
12:f:679:LEU:HD13	12:f:682:GLY:H	1.67	0.59
12:f:814:SER:HA	12:f:882:LEU:HD12	1.83	0.59
19:u:44:ILE:HB	19:u:68:HIS:HB2	1.84	0.59
30:q:19:ARG:HH21	30:q:31:ASP:HB2	1.68	0.59
6:Z:10:VAL:HG13	6:Z:163:GLY:HA3	1.85	0.58
16:D:352:MET:HE1	16:D:379:CYS:HB3	1.85	0.58
2:V:200:ARG:HD2	2:V:242:HIS:HB2	1.84	0.58
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.85	0.58
17:E:182:LEU:HD22	35:E:401:ATP:H2'	1.83	0.58
23:J:115:LYS:HD3	23:J:149:PRO:HA	1.84	0.58
33:T:192:VAL:HG12	33:T:197:VAL:HG22	1.83	0.58
11:e:7:PRO:HG2	11:e:8:VAL:HG23	1.86	0.58
13:A:252:GLU:OE2	13:A:255:ARG:NH1	2.36	0.58
2:V:440:LYS:NZ	10:d:143:LEU:O	2.37	0.58
12:f:168:LYS:HD3	12:f:204:ALA:HB1	1.86	0.58
22:I:197:LEU:HA	22:I:200:THR:HG22	1.85	0.58
24:K:20:ARG:HG2	24:K:21:LEU:H	1.69	0.58
8:b:2:VAL:O	8:b:44:ASN:ND2	2.37	0.58
10:d:155:LYS:HE2	10:d:167:ILE:HB	1.84	0.58
17:E:251:ARG:HB3	17:E:255:ARG:HH12	1.68	0.58
17:E:265:ASP:OD2	17:E:291:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:704:LEU:HA	12:f:707:LEU:HB2	1.84	0.58
12:f:438:ASP:HA	12:f:477:MET:HE2	1.85	0.58
13:A:284:ARG:O	18:F:334:ARG:NH2	2.32	0.58
18:F:439:ALA:HB1	25:L:62:LYS:HD3	1.86	0.58
22:I:3:ARG:HB2	23:J:5:ARG:HH12	1.68	0.58
1:U:376:MET:HA	1:U:739:ALA:HA	1.85	0.58
7:a:255:TRP:O	7:a:258:GLN:NE2	2.37	0.58
12:f:288:VAL:HA	12:f:291:GLN:HG2	1.86	0.58
22:I:106:PRO:HD2	22:I:109:GLN:HE21	1.68	0.58
6:Z:68:TRP:HE1	6:Z:111:LEU:HD22	1.67	0.57
12:f:697:ILE:HG12	12:f:737:ASN:HD21	1.68	0.57
7:a:290:GLN:O	7:a:330:ARG:NH2	2.38	0.57
22:i:119:GLN:NE2	23:j:79:ASP:OD1	2.37	0.57
22:i:197:LEU:HA	22:i:200:THR:HG22	1.84	0.57
25:l:120:THR:O	26:m:129:ARG:NH1	2.37	0.57
16:D:115:ILE:HA	16:D:139:LEU:HB2	1.85	0.57
20:G:141:ILE:HG22	20:G:151:VAL:HG22	1.87	0.57
30:Q:19:ARG:HH21	30:Q:31:ASP:HB2	1.68	0.57
24:k:20:ARG:HG2	24:k:21:LEU:H	1.69	0.57
26:m:241:GLU:O	26:m:244:LYS:NZ	2.37	0.57
1:U:217:CYS:HB2	1:U:248:ILE:HD12	1.87	0.57
23:J:38:ARG:NH1	23:J:181:ILE:O	2.38	0.57
20:g:86:ASP:OD1	26:m:120:HIS:NE2	2.31	0.57
20:g:141:ILE:HG22	20:g:151:VAL:HG22	1.87	0.57
1:U:770:TRP:HA	9:c:180:ASN:HB3	1.86	0.57
5:Y:108:ALA:O	5:Y:112:CYS:N	2.37	0.57
7:a:342:ASP:OD1	7:a:345:GLN:NE2	2.37	0.57
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.87	0.57
2:V:87:SER:HB3	2:V:126:ALA:H	1.68	0.57
12:f:680:ARG:HB3	12:f:717:ALA:H	1.70	0.57
25:L:139:ASP:H	33:T:81:HIS:HE1	1.53	0.57
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.85	0.57
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.86	0.57
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.85	0.57
1:U:522:GLY:O	1:U:559:ARG:NH2	2.38	0.56
12:f:378:ASN:OD1	12:f:382:ASN:ND2	2.38	0.56
24:K:48:LEU:HD21	24:K:77:ALA:HB2	1.87	0.56
22:i:106:PRO:HD2	22:i:109:GLN:HE21	1.68	0.56
1:U:242:LEU:HA	1:U:245:ALA:HB3	1.87	0.56
1:U:643:SER:O	15:C:57:ARG:NH1	2.38	0.56
7:a:321:LYS:HB2	7:a:335:TRP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.86	0.56
20:G:11:ARG:O	20:G:24:GLN:NE2	2.38	0.56
24:k:48:LEU:HD21	24:k:77:ALA:HB2	1.87	0.56
1:U:171:ASN:ND2	1:U:176:MET:SD	2.79	0.56
12:f:250:ARG:NH1	12:f:285:CYS:SG	2.78	0.56
26:M:241:GLU:O	26:M:244:LYS:NZ	2.37	0.56
22:i:15:GLU:OE2	22:i:17:ARG:NE	2.39	0.56
17:E:97:ARG:HH12	17:E:114:GLU:HB3	1.70	0.56
12:f:150:GLU:O	12:f:156:HIS:ND1	2.39	0.56
26:M:168:ALA:HB1	26:M:171:ALA:HB3	1.88	0.56
24:k:76:CYS:SG	24:k:77:ALA:N	2.79	0.56
2:V:255:LEU:HD22	2:V:291:TYR:HB3	1.88	0.56
3:W:63:THR:HG22	3:W:68:VAL:HG13	1.87	0.56
3:W:231:ILE:O	3:W:235:GLN:N	2.39	0.56
3:W:274:VAL:O	3:W:283:GLN:NE2	2.38	0.56
9:c:31:VAL:HB	9:c:205:ILE:HG22	1.86	0.56
14:B:49:LEU:HD13	14:B:51:LEU:H	1.71	0.56
16:D:129:SER:OG	16:D:252:ARG:NH1	2.39	0.56
18:F:282:ILE:HG22	18:F:327:LYS:HB2	1.87	0.56
24:K:76:CYS:SG	24:K:77:ALA:N	2.79	0.56
20:g:158:GLY:O	21:h:84:ARG:NH2	2.39	0.56
6:Z:172:VAL:HG13	9:c:217:LEU:HD21	1.87	0.56
10:d:2:TYR:O	10:d:25:ARG:NH2	2.38	0.56
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.87	0.56
9:c:33:ILE:HG23	9:c:69:VAL:HG13	1.87	0.56
12:f:737:ASN:O	12:f:746:ARG:NH1	2.38	0.56
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.87	0.56
7:a:374:ILE:HD11	10:d:251:ARG:HG2	1.88	0.56
11:e:53:SER:O	11:e:57:ARG:NH2	2.37	0.56
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.88	0.55
13:A:294:GLU:OE1	13:A:297:ARG:NH1	2.40	0.55
3:W:24:VAL:HG22	3:W:27:ARG:HH12	1.71	0.55
12:f:184:LEU:HD21	14:B:58:CYS:HA	1.88	0.55
7:a:221:VAL:HG23	7:a:222:LEU:HG	1.89	0.55
18:F:305:GLU:OE1	18:F:308:ARG:NH1	2.39	0.55
1:U:475:HIS:NE2	1:U:507:VAL:O	2.28	0.55
8:b:34:ASN:O	8:b:38:HIS:ND1	2.29	0.55
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.71	0.55
31:R:19:ARG:NH2	29:p:205:ASP:OD2	2.39	0.55
1:U:373:ASN:HA	1:U:376:MET:HG2	1.89	0.55
1:U:542:GLU:OE1	1:U:546:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.88	0.55
29:P:65:GLN:OE1	30:Q:86:ARG:NH2	2.40	0.55
5:Y:99:GLU:HA	5:Y:102:ASP:HB3	1.88	0.55
26:m:168:ALA:HB1	26:m:171:ALA:HB3	1.88	0.55
1:U:780:SER:HA	1:U:783:TYR:HD2	1.72	0.55
13:A:312:ARG:HB2	13:A:315:ILE:HD12	1.89	0.55
10:d:193:GLU:OE2	10:d:196:ARG:NH1	2.40	0.55
16:D:212:LYS:NZ	35:D:501:ATP:O1G	2.40	0.55
20:g:120:ASP:OD1	21:h:84:ARG:NH1	2.40	0.55
3:W:65:ARG:HG3	3:W:67:LEU:H	1.71	0.55
8:b:100:ARG:NH1	8:b:102:GLY:O	2.40	0.55
12:f:373:ALA:HB2	12:f:744:MET:HA	1.88	0.55
22:I:15:GLU:OE2	22:I:17:ARG:NE	2.39	0.55
12:f:712:LYS:HD2	12:f:781:TYR:HE2	1.72	0.55
22:i:32:GLY:H	22:i:50:ARG:HH21	1.55	0.55
12:f:24:THR:HG23	12:f:31:LYS:HG3	1.89	0.54
22:I:32:GLY:H	22:I:50:ARG:HH21	1.55	0.54
26:M:66:LEU:HD21	26:M:214:SER:HB2	1.90	0.54
20:g:11:ARG:O	20:g:24:GLN:NE2	2.38	0.54
20:g:137:CYS:SG	20:g:138:MET:N	2.79	0.54
16:D:153:MET:HE2	16:D:229:ARG:HE	1.71	0.54
20:G:158:GLY:O	21:H:84:ARG:NH2	2.39	0.54
22:I:119:GLN:NE2	23:J:79:ASP:OD1	2.40	0.54
25:L:120:THR:O	26:M:129:ARG:NH1	2.40	0.54
29:P:126:LEU:HD12	29:P:127:ILE:HG23	1.89	0.54
20:g:34:GLN:HE22	26:m:19:ARG:HB3	1.72	0.54
26:m:66:LEU:HD21	26:m:214:SER:HB2	1.90	0.54
14:B:342:ILE:HG22	14:B:350:LYS:HE3	1.89	0.54
2:V:440:LYS:HA	2:V:443:ARG:HB3	1.90	0.54
6:Z:135:THR:HG21	6:Z:162:ILE:HD11	1.88	0.54
16:D:401:LYS:HA	16:D:404:LYS:HE2	1.88	0.54
1:U:191:LYS:HD2	1:U:194:ARG:HH11	1.73	0.54
3:W:361:HIS:HA	3:W:364:ARG:HE	1.73	0.54
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.40	0.54
18:F:210:GLU:O	18:F:214:ASN:N	2.41	0.54
24:k:50:VAL:HG11	24:k:66:LYS:HB2	1.90	0.54
2:V:144:ASP:H	2:V:150:ARG:HH22	1.56	0.54
2:V:322:VAL:O	2:V:325:LYS:N	2.40	0.54
10:d:116:HIS:HA	10:d:119:LEU:HD23	1.89	0.54
12:f:198:HIS:O	12:f:202:HIS:N	2.41	0.54
22:I:116:ASP:OD1	23:J:81:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:33:GLN:HB3	2:V:115:LYS:HE2	1.90	0.54
5:Y:104:MET:HA	5:Y:107:LYS:HB2	1.88	0.54
10:d:47:GLN:HG2	10:d:48:LEU:HG	1.90	0.54
12:f:679:LEU:HD11	12:f:686:LEU:HD21	1.89	0.54
28:O:96:ALA:H	28:O:115:PRO:HB3	1.73	0.54
33:T:45:VAL:HB	33:T:49:THR:HG23	1.89	0.54
25:l:80:ASP:OD1	25:l:126:ARG:NH2	2.41	0.54
12:f:378:ASN:HD21	12:f:392:THR:HG22	1.72	0.54
22:I:159:TRP:HA	23:J:54:GLN:HA	1.90	0.54
29:p:126:LEU:HD12	29:p:127:ILE:HG23	1.89	0.54
2:V:190:ASP:OD1	2:V:234:ARG:NH1	2.41	0.54
3:W:312:MET:HE2	7:a:312:MET:HB3	1.88	0.54
3:W:334:GLU:O	3:W:338:THR:N	2.39	0.54
5:Y:69:LEU:HA	5:Y:72:LYS:HE3	1.90	0.54
10:d:212:LYS:HD2	10:d:213:ARG:HG2	1.90	0.54
12:f:425:GLY:HA3	12:f:451:VAL:HG11	1.89	0.54
2:V:325:LYS:HA	2:V:328:VAL:HG12	1.89	0.54
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.88	0.54
12:f:139:CYS:O	12:f:143:ARG:NH1	2.41	0.54
12:f:680:ARG:HB2	12:f:763:ARG:HE	1.72	0.54
15:C:69:GLN:HG3	15:C:118:ASN:HD21	1.71	0.54
20:G:137:CYS:SG	20:G:138:MET:N	2.79	0.54
26:M:228:PRO:HD2	26:M:231:ILE:HD12	1.90	0.54
12:f:106:LEU:HB2	12:f:141:LYS:HD2	1.89	0.53
12:f:594:LEU:O	12:f:635:LYS:NZ	2.41	0.53
16:D:83:GLN:HG2	16:D:140:VAL:HG13	1.91	0.53
16:D:342:ARG:HB3	16:D:364:VAL:HG11	1.90	0.53
1:U:791:LEU:HD22	1:U:911:ILE:HD11	1.90	0.53
12:f:369:ARG:NH2	12:f:791:VAL:O	2.41	0.53
15:C:147:THR:HG22	15:C:150:MET:HE3	1.91	0.53
32:S:35:ILE:HB	33:T:151:ARG:HH12	1.73	0.53
4:X:214:SER:O	4:X:218:HIS:ND1	2.39	0.53
8:b:26:LEU:HD11	8:b:80:PRO:HG3	1.91	0.53
14:B:125:THR:OG1	14:B:126:SER:N	2.40	0.53
32:s:125:ASP:OD1	32:s:129:SER:N	2.39	0.53
3:W:268:LYS:HD3	3:W:333:LEU:HD13	1.91	0.53
4:X:67:GLY:HA2	4:X:109:LEU:HD21	1.89	0.53
16:D:115:ILE:HG22	16:D:139:LEU:HD12	1.89	0.53
27:N:28:ASN:HD21	28:O:122:LEU:HD21	1.73	0.53
27:n:136:TYR:HE2	33:t:33:LEU:HD21	1.74	0.53
6:Z:34:ARG:HH12	6:Z:60:GLU:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:w:5:VAL:HB	19:w:13:ILE:HB	1.90	0.53
26:m:8:ASP:O	26:m:22:GLN:NE2	2.38	0.53
33:t:45:VAL:HB	33:t:49:THR:HG23	1.90	0.53
2:V:330:LYS:NZ	2:V:389:ASP:OD2	2.39	0.53
3:W:162:ALA:HB1	3:W:192:LEU:HB3	1.90	0.53
6:Z:151:THR:HA	7:a:146:PRO:HB2	1.90	0.53
7:a:33:LEU:HA	8:b:18:ASN:HD22	1.73	0.53
8:b:151:GLU:OE1	8:b:152:LYS:NZ	2.41	0.53
1:U:798:PRO:O	1:U:880:ASN:ND2	2.35	0.53
18:F:81:LYS:HA	18:F:84:LYS:HE3	1.90	0.53
18:F:97:LEU:HB2	18:F:121:CYS:HB2	1.91	0.53
20:g:49:VAL:HG22	20:g:219:VAL:HG23	1.91	0.53
28:o:96:ALA:H	28:o:115:PRO:HB3	1.73	0.53
6:Z:137:ALA:O	6:Z:157:HIS:ND1	2.42	0.53
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.91	0.53
14:B:262:ASP:OD1	14:B:265:LYS:NZ	2.42	0.53
20:G:49:VAL:HG22	20:G:219:VAL:HG23	1.91	0.53
3:W:444:HIS:HD2	6:Z:157:HIS:HB3	1.74	0.53
4:X:252:LYS:HA	4:X:287:LEU:HD11	1.90	0.53
8:b:93:ALA:HB1	8:b:109:ILE:HD13	1.91	0.53
10:d:234:ASP:OD1	10:d:234:ASP:N	2.39	0.53
19:u:5:VAL:HG22	19:u:67:LEU:HD12	1.91	0.53
26:m:214:SER:OG	26:m:224:HIS:NE2	2.30	0.53
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.91	0.53
3:W:347:GLY:O	3:W:351:TRP:N	2.36	0.53
6:Z:66:SER:OG	6:Z:103:LYS:NZ	2.42	0.53
9:c:59:GLY:HA3	9:c:69:VAL:HA	1.91	0.53
12:f:311:VAL:CG2	19:w:76:GLY:N	2.72	0.53
16:D:163:MET:HA	16:D:222:HIS:HE1	1.74	0.53
29:P:2:SER:OG	29:P:3:ILE:N	2.42	0.53
3:W:124:LEU:HA	3:W:127:THR:HG22	1.91	0.52
12:f:291:GLN:HE21	12:f:879:ARG:HH21	1.57	0.52
15:C:141:GLU:O	16:D:323:ARG:NH1	2.40	0.52
19:u:5:VAL:HB	19:u:13:ILE:HB	1.90	0.52
27:n:127:ILE:HG12	27:n:132:SER:HB2	1.91	0.52
12:f:717:ALA:HB1	12:f:760:PHE:HB2	1.90	0.52
19:w:5:VAL:HG22	19:w:67:LEU:HD12	1.91	0.52
29:P:48:ARG:HH12	29:P:114:PRO:HA	1.74	0.52
30:Q:38:MET:O	30:Q:65:GLN:NE2	2.42	0.52
33:T:171:ARG:NH2	28:o:140:ASP:OD2	2.42	0.52
30:q:38:MET:O	30:q:65:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:s:38:ARG:HH12	33:t:151:ARG:HD3	1.74	0.52
1:U:27:LEU:HB3	1:U:63:VAL:HG11	1.91	0.52
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.89	0.52
6:Z:193:ASN:HD22	6:Z:197:GLY:HA3	1.74	0.52
25:L:80:ASP:OD1	25:L:126:ARG:NH2	2.41	0.52
26:m:228:PRO:HD2	26:m:231:ILE:HD12	1.90	0.52
29:p:2:SER:OG	29:p:3:ILE:N	2.42	0.52
12:f:180:GLN:HB3	12:f:219:LYS:HZ2	1.75	0.52
12:f:414:LEU:HD23	12:f:417:ILE:HD12	1.90	0.52
12:f:462:ALA:H	19:w:6:LYS:NZ	2.06	0.52
27:N:127:ILE:HG12	27:N:132:SER:HB2	1.91	0.52
6:Z:180:LYS:HG2	6:Z:182:THR:HG23	1.91	0.52
18:F:94:ILE:HD11	18:F:125:LYS:HB2	1.90	0.52
23:J:119:THR:HG22	23:J:126:PRO:HB3	1.92	0.52
24:k:41:GLN:NE2	24:k:151:PRO:O	2.42	0.52
1:U:203:LYS:O	1:U:207:ASN:ND2	2.42	0.52
2:V:319:HIS:H	11:e:4:LYS:HE2	1.75	0.52
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.91	0.52
10:d:45:LYS:O	10:d:49:ILE:N	2.38	0.52
10:d:91:GLU:OE1	10:d:96:HIS:NE2	2.42	0.52
1:U:593:SER:OG	1:U:595:ASN:ND2	2.43	0.52
14:B:183:THR:OG1	14:B:184:TYR:N	2.43	0.52
4:X:299:LEU:HD21	4:X:331:LEU:HA	1.91	0.52
5:Y:228:MET:HE2	5:Y:260:LEU:HD23	1.92	0.52
17:E:199:VAL:HG23	17:E:201:SER:H	1.75	0.52
24:K:41:GLN:NE2	24:K:151:PRO:O	2.42	0.52
24:K:210:LEU:HD11	24:K:215:ILE:HG12	1.92	0.52
24:k:210:LEU:HD11	24:k:215:ILE:HG12	1.92	0.52
29:p:48:ARG:HH12	29:p:114:PRO:HA	1.74	0.52
2:V:218:TYR:HA	2:V:222:ASP:HB2	1.92	0.52
2:V:454:GLU:N	10:d:187:GLU:OE2	2.42	0.52
4:X:297:ARG:HD2	4:X:333:GLN:HE21	1.75	0.52
6:Z:144:VAL:HG22	7:a:146:PRO:HB3	1.92	0.52
25:l:42:THR:O	25:l:137:TYR:OH	2.28	0.52
1:U:153:ILE:HA	1:U:156:GLU:HB2	1.91	0.52
6:Z:151:THR:OG1	7:a:146:PRO:O	2.28	0.52
7:a:321:LYS:O	7:a:334:THR:OG1	2.28	0.52
9:c:32:TYR:HB3	9:c:208:ARG:HD2	1.92	0.52
12:f:593:THR:O	12:f:635:LYS:NZ	2.42	0.52
24:K:50:VAL:HG11	24:K:66:LYS:HB2	1.90	0.52
2:V:30:PRO:O	2:V:34:ASP:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:212:TYR:OH	2:V:287:ARG:NH2	2.43	0.51
6:Z:187:LEU:HD22	7:a:374:ILE:HG23	1.91	0.51
16:D:115:ILE:HD13	16:D:121:ARG:HH22	1.74	0.51
21:H:4:ARG:NH1	21:H:5:GLY:O	2.43	0.51
29:P:189:ILE:HG23	29:P:196:THR:HB	1.92	0.51
32:S:187:VAL:HG21	28:o:24:MET:HE3	1.92	0.51
4:X:379:ASP:HB3	4:X:384:VAL:H	1.75	0.51
5:Y:173:ASP:HB3	5:Y:176:ARG:HB2	1.92	0.51
5:Y:215:ASP:HB3	5:Y:218:THR:HG23	1.91	0.51
8:b:124:LEU:O	8:b:128:ALA:N	2.44	0.51
16:D:119:ILE:O	16:D:121:ARG:NH1	2.44	0.51
17:E:144:GLU:OE2	17:E:297:ARG:NH1	2.44	0.51
21:h:222:THR:OG1	21:h:225:GLU:OE1	2.28	0.51
1:U:898:CYS:SG	1:U:899:ARG:N	2.84	0.51
2:V:418:SER:HA	2:V:457:TYR:HA	1.93	0.51
3:W:262:LYS:HG3	3:W:265:GLN:HE21	1.75	0.51
18:F:289:ASP:OD1	18:F:289:ASP:N	2.44	0.51
25:L:189:LYS:O	25:L:193:ARG:NH1	2.44	0.51
21:h:4:ARG:NH1	21:h:5:GLY:O	2.43	0.51
12:f:130:ALA:O	12:f:134:SER:N	2.41	0.51
21:H:204:THR:OG1	21:H:206:ASP:OD1	2.28	0.51
25:l:189:LYS:O	25:l:193:ARG:NH1	2.44	0.51
1:U:328:ILE:HG13	1:U:329:LEU:HG	1.92	0.51
2:V:228:ARG:O	2:V:232:HIS:ND1	2.43	0.51
9:c:49:VAL:HG13	9:c:50:PRO:HD3	1.93	0.51
12:f:704:LEU:O	12:f:708:ASP:N	2.43	0.51
25:L:42:THR:O	25:L:137:TYR:OH	2.28	0.51
26:M:214:SER:OG	26:M:224:HIS:NE2	2.30	0.51
6:Z:249:PHE:HZ	9:c:303:MET:HG2	1.75	0.51
17:E:322:LYS:HD3	17:E:326:ILE:HG13	1.93	0.51
26:M:8:ASP:O	26:M:22:GLN:NE2	2.38	0.51
29:p:189:ILE:HG23	29:p:196:THR:HB	1.92	0.51
12:f:291:GLN:HE22	12:f:324:VAL:HG11	1.76	0.51
12:f:458:GLU:OE1	19:w:68:HIS:CG	2.63	0.51
12:f:478:ARG:HG3	12:f:514:VAL:HG11	1.92	0.51
12:f:733:GLY:O	12:f:746:ARG:NH1	2.43	0.51
13:A:390:THR:HA	14:B:216:ILE:HD11	1.93	0.51
21:H:222:THR:OG1	21:H:225:GLU:OE1	2.28	0.51
21:h:204:THR:OG1	21:h:206:ASP:OD1	2.28	0.51
1:U:768:GLN:HB2	1:U:775:LEU:HD12	1.92	0.51
5:Y:101:ARG:O	5:Y:105:MET:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:228:LYS:HB3	12:f:231:LEU:HD13	1.92	0.51
14:B:297:SER:OG	15:C:268:GLU:OE2	2.28	0.51
15:C:125:LYS:HZ2	16:D:96:VAL:HG11	1.76	0.51
16:D:152:MET:HE3	16:D:154:LEU:HD13	1.92	0.51
27:n:35:THR:OG1	27:n:45:ARG:NH2	2.44	0.51
7:a:292:THR:HG23	7:a:295:GLU:H	1.75	0.51
30:Q:4:LEU:HD22	30:Q:45:LEU:HB3	1.93	0.51
2:V:349:ARG:HA	2:V:353:LEU:HD23	1.93	0.51
9:c:51:MET:HE2	9:c:81:GLY:H	1.76	0.51
28:O:1:THR:N	28:O:168:GLY:O	2.44	0.51
32:S:4:PRO:O	33:T:100:ARG:NH2	2.41	0.51
15:C:72:TYR:N	15:C:116:LEU:O	2.43	0.50
27:N:18:SER:HB2	27:N:31:THR:H	1.75	0.50
23:j:31:THR:OG1	23:j:163:ARG:O	2.29	0.50
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.93	0.50
17:E:248:SER:HA	17:E:251:ARG:HD3	1.93	0.50
25:L:146:GLN:HE21	25:L:154:PHE:HD2	1.59	0.50
24:k:199:LEU:HD11	24:k:217:LEU:HD11	1.93	0.50
28:o:1:THR:N	28:o:168:GLY:O	2.44	0.50
3:W:142:ARG:HE	3:W:182:ARG:HB2	1.76	0.50
1:U:416:GLU:OE1	1:U:450:HIS:NE2	2.43	0.50
2:V:84:LYS:HA	2:V:87:SER:HB2	1.93	0.50
5:Y:50:MET:HE2	5:Y:74:LYS:HB3	1.94	0.50
22:I:123:GLN:HG3	23:J:125:ARG:HE	1.76	0.50
25:l:72:ILE:HG22	25:l:134:ILE:HG12	1.94	0.50
27:n:18:SER:HB2	27:n:31:THR:H	1.75	0.50
4:X:175:LYS:HG2	4:X:213:GLN:HE22	1.77	0.50
25:l:204:ASP:OD1	25:l:204:ASP:N	2.42	0.50
2:V:376:ASN:HD21	2:V:399:ARG:HH12	1.60	0.50
14:B:249:ARG:HG3	14:B:283:PHE:HD2	1.77	0.50
1:U:646:PRO:HA	1:U:649:ARG:HB2	1.94	0.50
8:b:16:MET:HA	8:b:25:ARG:HH11	1.76	0.50
13:A:80:LEU:O	13:A:85:GLN:NE2	2.44	0.50
17:E:247:THR:O	17:E:251:ARG:NH2	2.44	0.50
27:N:35:THR:OG1	27:N:45:ARG:NH2	2.44	0.50
2:V:195:ILE:HD11	2:V:241:ARG:HH21	1.77	0.50
5:Y:48:ASN:HD21	5:Y:77:ASN:HA	1.76	0.50
6:Z:98:GLY:HA3	6:Z:123:ILE:HG23	1.93	0.50
7:a:115:LYS:HD3	7:a:118:ILE:HD12	1.93	0.50
12:f:739:ALA:HB1	12:f:743:ALA:HB2	1.94	0.50
16:D:113:VAL:HB	16:D:138:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:58:THR:OG1	30:Q:121:LEU:O	2.22	0.50
30:q:4:LEU:HD22	30:q:45:LEU:HB3	1.93	0.50
1:U:146:LYS:HE2	1:U:148:LYS:HB2	1.93	0.50
12:f:369:ARG:HA	12:f:372:LEU:HD13	1.94	0.50
26:M:40:ARG:NH2	26:M:146:ALA:O	2.45	0.50
28:O:19:ARG:NH1	28:O:169:SER:O	2.45	0.50
31:R:125:THR:OG1	30:q:170:ARG:NH2	2.44	0.50
6:Z:238:PRO:HG2	9:c:309:PHE:HB3	1.94	0.49
9:c:100:LYS:HE2	9:c:105:PRO:HB3	1.93	0.49
12:f:505:MET:HE3	12:f:537:THR:HG22	1.93	0.49
15:C:175:PHE:O	15:C:179:GLY:N	2.45	0.49
26:M:141:SER:HB3	26:M:144:ASP:HB2	1.94	0.49
2:V:126:ALA:HB2	2:V:134:PHE:HE2	1.76	0.49
32:S:92:LEU:HD23	32:S:124:PHE:HE2	1.76	0.49
26:m:40:ARG:NH2	26:m:146:ALA:O	2.45	0.49
33:t:43:MET:HE3	33:t:45:VAL:HG22	1.94	0.49
1:U:490:ARG:HB2	1:U:493:VAL:HG12	1.94	0.49
12:f:267:ARG:O	12:f:271:MET:N	2.43	0.49
24:K:199:LEU:HD11	24:K:217:LEU:HD11	1.94	0.49
32:S:191:ASP:O	32:S:210:LEU:N	2.46	0.49
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.94	0.49
9:c:303:MET:HE2	10:d:239:SER:HA	1.94	0.49
12:f:257:ARG:HG2	12:f:272:LEU:HD13	1.94	0.49
12:f:463:LEU:HD23	19:w:66:THR:HG21	1.93	0.49
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.94	0.49
12:f:766:GLN:HG3	12:f:807:ARG:HH22	1.78	0.49
32:S:125:ASP:OD1	32:S:129:SER:N	2.38	0.49
25:l:146:GLN:HE21	25:l:154:PHE:HD2	1.59	0.49
28:o:19:ARG:NH1	28:o:169:SER:O	2.45	0.49
1:U:112:CYS:O	1:U:116:ALA:N	2.44	0.49
15:C:246:ILE:HB	15:C:291:VAL:HG12	1.93	0.49
26:M:175:GLU:HA	26:M:178:LYS:HD3	1.95	0.49
22:i:116:ASP:OD1	23:j:81:ARG:NH1	2.46	0.49
2:V:84:LYS:HE3	2:V:125:ASN:HB2	1.94	0.49
3:W:124:LEU:HD13	3:W:151:THR:HG22	1.95	0.49
3:W:190:MET:HB2	3:W:202:THR:HG23	1.94	0.49
6:Z:15:VAL:HA	6:Z:18:SER:HB3	1.94	0.49
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.45	0.49
13:A:192:GLU:HB2	13:A:196:LEU:HD13	1.95	0.49
17:E:117:PRO:HD3	18:F:94:ILE:HG23	1.94	0.49
1:U:59:PHE:HA	1:U:62:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:636:VAL:HG23	1:U:637:VAL:HG23	1.94	0.49
7:a:190:VAL:HB	7:a:225:LEU:HD11	1.94	0.49
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.95	0.49
16:D:91:GLN:HE22	16:D:248:ARG:HD3	1.78	0.49
2:V:470:ARG:HD2	10:d:238:PRO:HG3	1.95	0.49
12:f:300:ARG:HE	12:f:493:ASN:HB2	1.77	0.49
12:f:559:PRO:HB2	12:f:594:LEU:HG	1.94	0.49
16:D:65:GLN:O	16:D:69:LYS:NZ	2.38	0.49
23:J:80:ALA:HA	23:J:129:ILE:HD13	1.95	0.49
31:R:141:ARG:NH2	30:q:162:LYS:O	2.45	0.49
1:U:206:MET:HE3	1:U:216:VAL:HG21	1.95	0.49
3:W:142:ARG:HD3	3:W:181:GLU:HB3	1.95	0.49
3:W:373:ILE:HA	7:a:326:GLU:HB3	1.94	0.49
9:c:51:MET:HA	9:c:82:VAL:HG22	1.94	0.49
16:D:65:GLN:OE1	16:D:69:LYS:NZ	2.45	0.49
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.41	0.49
17:E:113:ARG:HH22	17:E:220:ASN:HB3	1.78	0.49
17:E:180:LYS:NZ	35:E:401:ATP:O2G	2.46	0.49
3:W:59:ASP:O	3:W:63:THR:OG1	2.26	0.49
5:Y:95:LEU:HD11	5:Y:98:SER:HA	1.95	0.49
11:e:49:GLU:O	11:e:53:SER:OG	2.23	0.49
18:F:336:ASP:OD1	18:F:336:ASP:N	2.45	0.49
33:T:43:MET:HE3	33:T:45:VAL:HG22	1.94	0.49
10:d:44:THR:O	10:d:47:GLN:NE2	2.46	0.48
13:A:240:VAL:HG21	13:A:260:LEU:HD11	1.95	0.48
14:B:183:THR:HG23	14:B:185:ALA:H	1.76	0.48
21:h:100:VAL:HG13	29:p:93:ASN:HD22	1.78	0.48
22:i:100:GLN:HE21	30:q:83:PHE:HE1	1.60	0.48
30:q:21:ALA:HB3	30:q:29:LYS:HB3	1.95	0.48
7:a:12:GLN:HE21	7:a:19:PRO:HB3	1.78	0.48
9:c:149:GLN:HB3	16:D:81:ARG:HH11	1.78	0.48
12:f:811:LEU:HD21	12:f:862:ILE:HD13	1.96	0.48
20:g:32:ILE:HA	20:g:82:GLY:HA2	1.95	0.48
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.96	0.48
6:Z:209:ARG:HD2	6:Z:212:LEU:HD22	1.95	0.48
8:b:24:THR:HG22	8:b:26:LEU:H	1.77	0.48
12:f:110:TYR:OH	12:f:118:ASN:ND2	2.46	0.48
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.94	0.48
12:f:637:LYS:HE2	12:f:673:ARG:HB2	1.95	0.48
23:J:68:ASN:HA	23:J:211:MET:HE1	1.96	0.48
25:L:72:ILE:HG22	25:L:134:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:19:ARG:HH11	30:q:179:SER:HB3	1.77	0.48
2:V:252:ASN:HD21	2:V:288:TYR:HB2	1.78	0.48
3:W:312:MET:HG3	3:W:313:GLU:H	1.78	0.48
7:a:235:ASP:HB3	7:a:251:LEU:HD11	1.94	0.48
16:D:233:SER:OG	17:E:259:GLU:OE1	2.31	0.48
17:E:269:THR:O	17:E:271:HIS:ND1	2.39	0.48
20:G:32:ILE:HA	20:G:82:GLY:HA2	1.95	0.48
3:W:183:VAL:HG12	3:W:187:LEU:HD23	1.94	0.48
3:W:443:THR:HG21	6:Z:204:LYS:HG3	1.95	0.48
6:Z:121:LEU:HD11	6:Z:138:TYR:HD2	1.78	0.48
12:f:726:ILE:O	12:f:730:GLY:N	2.38	0.48
14:B:153:ASN:HD22	14:B:156:VAL:HG22	1.78	0.48
15:C:344:LEU:HD23	15:C:347:ILE:HD12	1.96	0.48
26:m:175:GLU:HA	26:m:178:LYS:HD3	1.95	0.48
2:V:151:THR:O	2:V:155:ALA:N	2.45	0.48
10:d:178:ILE:O	10:d:182:ILE:N	2.46	0.48
16:D:335:LEU:HD11	16:D:371:SER:HA	1.95	0.48
32:s:28:ARG:NH2	32:s:191:ASP:OD1	2.45	0.48
2:V:96:ARG:HB3	2:V:98:LEU:HG	1.94	0.48
10:d:183:GLU:HA	10:d:215:TRP:HE1	1.77	0.48
12:f:711:SER:HA	12:f:749:ALA:HB2	1.95	0.48
13:A:99:THR:HG22	13:A:115:VAL:HG12	1.96	0.48
18:F:318:ASP:HB3	18:F:347:ARG:HG2	1.96	0.48
25:L:204:ASP:OD1	25:L:204:ASP:N	2.42	0.48
32:s:198:VAL:HG22	32:s:203:ILE:HG12	1.95	0.48
4:X:170:GLN:NE2	4:X:192:SER:OG	2.39	0.48
5:Y:88:LEU:HA	5:Y:100:ILE:HG12	1.96	0.48
6:Z:82:PHE:HA	6:Z:85:VAL:HG12	1.96	0.48
12:f:458:GLU:HB3	19:w:8:LEU:HD22	1.91	0.48
12:f:524:MET:HA	12:f:776:LEU:HD23	1.96	0.48
12:f:674:THR:O	12:f:678:LEU:N	2.40	0.48
13:A:73:ALA:HA	14:B:140:ASP:HB3	1.96	0.48
2:V:106:ARG:O	2:V:110:HIS:ND1	2.45	0.48
3:W:237:GLU:HG2	3:W:238:GLY:H	1.78	0.48
4:X:402:GLU:HB2	9:c:249:LEU:HD11	1.96	0.48
7:a:341:LEU:HB2	7:a:345:GLN:HE21	1.78	0.48
14:B:251:VAL:HG12	14:B:253:SER:H	1.79	0.48
1:U:9:ILE:HG12	1:U:38:ILE:HB	1.96	0.48
7:a:239:ALA:HA	7:a:242:SER:HB3	1.96	0.48
22:i:41:ASP:N	22:i:41:ASP:OD1	2.47	0.48
31:r:26:ILE:HG21	31:r:29:GLN:HE21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:469:SER:OG	1:U:470:ASN:N	2.45	0.47
8:b:124:LEU:HD21	8:b:152:LYS:HB3	1.95	0.47
12:f:310:ASP:O	19:w:75:GLY:CA	2.34	0.47
14:B:112:LEU:HD23	14:B:123:VAL:HG12	1.95	0.47
30:Q:19:ARG:HH11	30:Q:179:SER:HB3	1.77	0.47
12:f:442:SER:OG	12:f:477:MET:SD	2.71	0.47
14:B:107:MET:HB2	15:C:96:VAL:HB	1.95	0.47
22:I:41:ASP:N	22:I:41:ASP:OD1	2.46	0.47
26:m:141:SER:HB3	26:m:144:ASP:HB2	1.94	0.47
32:s:92:LEU:HD23	32:s:124:PHE:HE2	1.79	0.47
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.41	0.47
2:V:371:ASN:OD1	2:V:427:GLN:NE2	2.47	0.47
3:W:200:ILE:HD12	3:W:203:GLN:HE21	1.79	0.47
10:d:61:TRP:HZ3	10:d:65:ARG:HH21	1.61	0.47
16:D:68:LEU:O	16:D:72:PHE:N	2.42	0.47
20:g:165:ALA:HB3	21:h:56:LEU:HD22	1.94	0.47
6:Z:266:ILE:HG13	9:c:248:MET:HE1	1.96	0.47
8:b:101:GLN:OE1	9:c:101:GLN:NE2	2.47	0.47
15:C:83:LYS:HD2	15:C:105:ILE:HD11	1.95	0.47
18:F:362:ARG:NE	18:F:388:THR:O	2.47	0.47
27:N:144:ARG:H	27:N:147:MET:HE3	1.80	0.47
1:U:772:TRP:HB3	1:U:775:LEU:HB2	1.96	0.47
5:Y:233:ARG:NH1	5:Y:264:TYR:O	2.47	0.47
12:f:462:ALA:N	19:w:6:LYS:NZ	2.63	0.47
27:N:76:VAL:HG23	27:N:104:ASP:HB2	1.96	0.47
31:R:26:ILE:HG21	31:R:29:GLN:HE21	1.79	0.47
20:g:165:ALA:HB1	20:g:179:LEU:HD13	1.97	0.47
23:j:115:LYS:HD3	23:j:149:PRO:HA	1.97	0.47
1:U:611:ASN:HB3	1:U:614:VAL:HG12	1.97	0.47
2:V:108:LEU:HA	2:V:111:TYR:HD2	1.80	0.47
3:W:41:GLN:HE21	3:W:94:ARG:HD2	1.79	0.47
5:Y:160:ASN:O	5:Y:164:ALA:N	2.44	0.47
7:a:370:GLN:HB2	10:d:244:LYS:HZ3	1.80	0.47
12:f:661:ALA:HB1	13:A:76:ALA:HB1	1.96	0.47
22:I:47:ALA:HB1	22:I:64:LYS:HE3	1.97	0.47
22:i:136:TYR:HB2	22:i:148:TYR:HB2	1.97	0.47
1:U:96:TYR:O	1:U:99:THR:OG1	2.28	0.47
1:U:424:ALA:HA	1:U:427:LEU:HD13	1.97	0.47
2:V:32:PRO:HA	2:V:35:VAL:HG22	1.96	0.47
2:V:156:SER:HA	2:V:159:LEU:HB2	1.97	0.47
3:W:45:GLU:HG3	3:W:96:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:100:GLY:HA3	10:d:133:ILE:HD12	1.95	0.47
12:f:206:ASP:OD2	12:f:245:ASN:ND2	2.48	0.47
12:f:465:LEU:O	12:f:481:SER:OG	2.32	0.47
14:B:140:ASP:O	14:B:142:ASP:N	2.48	0.47
15:C:86:LEU:HD11	15:C:94:LYS:HD3	1.95	0.47
21:H:69:THR:HG23	21:H:71:HIS:H	1.80	0.47
28:O:24:MET:HE3	32:s:187:VAL:HG21	1.97	0.47
29:P:205:ASP:OD2	31:r:19:ARG:NH2	2.47	0.47
30:Q:21:ALA:HB3	30:Q:29:LYS:HB3	1.95	0.47
23:j:119:THR:HG22	23:j:126:PRO:HB3	1.97	0.47
26:m:163:CYS:SG	26:m:164:ALA:N	2.88	0.47
5:Y:168:ILE:HG23	5:Y:173:ASP:HB2	1.97	0.47
12:f:269:ALA:O	12:f:273:ASN:N	2.40	0.47
13:A:140:VAL:HG12	13:A:152:PRO:HA	1.96	0.47
27:N:32:ASP:OD1	27:N:186:ARG:NH2	2.48	0.47
23:j:115:LYS:HG3	23:j:127:PHE:HD2	1.80	0.47
33:t:27:LEU:HD22	33:t:184:TYR:HB2	1.97	0.47
3:W:13:ILE:HA	3:W:16:MET:HG2	1.97	0.47
3:W:43:VAL:O	3:W:47:LEU:N	2.43	0.47
5:Y:203:ASP:N	5:Y:203:ASP:OD1	2.45	0.47
7:a:206:LEU:HD22	7:a:264:ASN:HD22	1.79	0.47
8:b:34:ASN:HD21	8:b:72:LEU:HD21	1.78	0.47
15:C:217:SER:OG	15:C:218:GLU:N	2.48	0.47
25:L:121:GLN:HG3	26:M:129:ARG:HG2	1.96	0.47
32:S:198:VAL:HG22	32:S:203:ILE:HG12	1.97	0.47
21:h:69:THR:HG23	21:h:71:HIS:H	1.80	0.47
27:n:32:ASP:OD1	27:n:186:ARG:NH2	2.48	0.47
1:U:788:VAL:HG12	1:U:909:GLY:HA2	1.97	0.47
9:c:146:ASP:HB3	9:c:156:VAL:HB	1.97	0.47
12:f:829:MET:H	12:f:845:ARG:HB3	1.80	0.47
15:C:327:ASP:N	15:C:327:ASP:OD1	2.48	0.47
22:I:33:THR:HA	22:I:165:GLY:HA2	1.97	0.47
1:U:28:ASN:HB3	1:U:59:PHE:HZ	1.80	0.46
1:U:632:GLN:O	1:U:635:SER:OG	2.31	0.46
6:Z:70:LEU:HD12	6:Z:111:LEU:HD23	1.96	0.46
13:A:69:ASP:OD2	13:A:72:LEU:N	2.47	0.46
32:s:191:ASP:O	32:s:210:LEU:N	2.44	0.46
1:U:696:ILE:HG22	1:U:737:LEU:HA	1.96	0.46
3:W:23:THR:HA	3:W:26:GLN:HB2	1.97	0.46
8:b:100:ARG:HH12	8:b:105:HIS:HB2	1.79	0.46
26:M:163:CYS:SG	26:M:164:ALA:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:274:VAL:HG21	3:W:290:ILE:HD13	1.98	0.46
5:Y:17:LEU:HD22	5:Y:212:GLU:HB2	1.96	0.46
12:f:628:ASP:O	12:f:632:LYS:N	2.42	0.46
13:A:347:ASP:N	13:A:347:ASP:OD1	2.39	0.46
2:V:215:ALA:O	2:V:219:GLU:N	2.37	0.46
6:Z:34:ARG:HE	6:Z:102:HIS:CD2	2.34	0.46
6:Z:97:THR:HG23	6:Z:99:PRO:HD3	1.97	0.46
10:d:49:ILE:HG23	10:d:50:LEU:HD12	1.96	0.46
17:E:232:MET:HB3	17:E:277:MET:HG2	1.96	0.46
20:G:165:ALA:HB1	20:G:179:LEU:HD13	1.97	0.46
27:N:136:TYR:HE2	33:T:33:LEU:HD21	1.80	0.46
13:A:190:VAL:HG21	13:A:339:ARG:HG3	1.97	0.46
23:J:121:SER:OG	23:J:122:ASN:N	2.48	0.46
22:i:33:THR:HA	22:i:165:GLY:HA2	1.97	0.46
1:U:11:LEU:HB2	1:U:19:LEU:HD21	1.98	0.46
1:U:181:LEU:HA	1:U:184:CYS:HB2	1.98	0.46
24:K:60:GLU:OE1	24:K:63:SER:N	2.49	0.46
29:P:101:GLY:O	30:Q:93:ARG:NH1	2.48	0.46
1:U:69:TYR:CZ	1:U:99:THR:HB	2.50	0.46
2:V:264:TYR:O	2:V:266:GLN:N	2.48	0.46
3:W:241:LEU:HD12	3:W:277:ALA:HB1	1.97	0.46
12:f:171:GLN:HE21	12:f:179:VAL:HG13	1.81	0.46
12:f:305:LEU:HB2	12:f:317:LEU:HD22	1.97	0.46
19:w:7:THR:HG22	19:w:69:LEU:HD23	1.98	0.46
28:O:140:ASP:OD2	33:t:171:ARG:NH2	2.48	0.46
24:k:60:GLU:OE1	24:k:63:SER:N	2.49	0.46
25:l:50:LYS:HE2	25:l:61:LYS:HA	1.97	0.46
27:n:76:VAL:HG23	27:n:104:ASP:HB2	1.96	0.46
32:s:16:ALA:HB2	32:s:121:VAL:HG23	1.98	0.46
1:U:202:VAL:HB	1:U:216:VAL:HG23	1.98	0.46
1:U:499:THR:O	1:U:503:GLN:NE2	2.36	0.46
6:Z:91:ILE:H	6:Z:91:ILE:HG13	1.63	0.46
6:Z:196:HIS:O	6:Z:200:GLY:N	2.49	0.46
12:f:306:GLU:OE2	19:w:73:LEU:HD11	2.16	0.46
12:f:458:GLU:CG	19:w:8:LEU:HD21	2.46	0.46
13:A:74:PRO:HA	13:A:75:PRO:HD3	1.80	0.46
16:D:170:MET:HG2	16:D:173:GLN:HB2	1.98	0.46
16:D:407:ILE:HG13	16:D:408:LYS:H	1.81	0.46
27:n:144:ARG:NH2	27:n:151:GLU:OE1	2.49	0.46
1:U:505:ASP:HB3	1:U:508:THR:HG22	1.97	0.46
10:d:5:LEU:HD12	10:d:25:ARG:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:97:LEU:N	18:F:121:CYS:O	2.48	0.46
18:F:272:PHE:HD2	18:F:316:GLN:HG3	1.79	0.46
22:I:69:ASN:HD22	22:I:72:MET:HE3	1.81	0.46
22:I:229:LYS:N	22:I:232:GLU:OE2	2.49	0.46
29:P:125:ASP:OD1	29:P:129:CYS:N	2.38	0.46
10:d:191:PHE:N	10:d:220:ASN:OD1	2.38	0.46
12:f:458:GLU:HG2	19:w:8:LEU:HD21	1.98	0.46
14:B:59:ARG:O	14:B:63:LEU:N	2.46	0.46
18:F:122:ALA:HB3	18:F:134:LEU:HD11	1.97	0.46
22:I:136:TYR:HB2	22:I:148:TYR:HB2	1.97	0.46
22:i:229:LYS:N	22:i:232:GLU:OE2	2.49	0.46
27:n:144:ARG:H	27:n:147:MET:HE3	1.80	0.46
5:Y:241:ILE:HG23	5:Y:242:LYS:HG2	1.98	0.45
6:Z:231:GLN:HE22	7:a:339:ARG:H	1.64	0.45
16:D:335:LEU:HD12	16:D:335:LEU:HA	1.80	0.45
20:G:86:ASP:OD1	26:M:120:HIS:NE2	2.31	0.45
21:H:100:VAL:HG13	29:P:93:ASN:HD22	1.82	0.45
27:N:144:ARG:NH2	27:N:151:GLU:OE1	2.49	0.45
29:p:125:ASP:OD1	29:p:129:CYS:N	2.38	0.45
2:V:467:TYR:OH	6:Z:255:ASP:OD1	2.34	0.45
10:d:131:VAL:HG23	10:d:134:LYS:HE2	1.98	0.45
11:e:45:ASP:O	11:e:49:GLU:N	2.42	0.45
15:C:31:LEU:HD22	16:D:47:LEU:HB3	1.98	0.45
25:L:50:LYS:HE2	25:L:61:LYS:HA	1.97	0.45
28:o:120:ASP:OD1	28:o:120:ASP:N	2.47	0.45
29:p:62:THR:OG1	30:q:85:ARG:NH2	2.46	0.45
1:U:135:ASN:O	1:U:139:GLN:N	2.48	0.45
1:U:510:GLU:OE2	1:U:546:ARG:NH2	2.49	0.45
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.98	0.45
2:V:126:ALA:HA	2:V:130:PHE:HB2	1.99	0.45
13:A:274:PHE:HB2	13:A:319:MET:HG3	1.99	0.45
14:B:133:VAL:HG11	14:B:157:HIS:HB2	1.98	0.45
14:B:173:VAL:HG21	15:C:233:GLU:HG3	1.99	0.45
25:l:164:ARG:O	25:l:198:THR:OG1	2.30	0.45
30:q:37:LYS:HE2	30:q:188:ILE:HG13	1.98	0.45
1:U:253:TYR:CZ	1:U:331:GLY:HA3	2.51	0.45
2:V:182:LYS:NZ	2:V:210:CYS:SG	2.72	0.45
2:V:277:PRO:HD2	2:V:285:TRP:HZ3	1.82	0.45
8:b:58:CYS:HB3	8:b:92:VAL:HG21	1.97	0.45
9:c:75:MET:SD	9:c:92:GLN:NE2	2.90	0.45
15:C:32:GLN:HG3	15:C:36:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:T:27:LEU:HD22	33:T:184:TYR:HB2	1.97	0.45
22:i:47:ALA:HB1	22:i:64:LYS:HE3	1.97	0.45
12:f:316:ASP:O	12:f:320:ILE:N	2.47	0.45
15:C:132:ASP:HB2	15:C:135:VAL:HG23	1.97	0.45
28:O:113:ILE:HG12	28:O:119:THR:HG22	1.99	0.45
29:p:58:THR:OG1	30:q:121:LEU:O	2.26	0.45
1:U:135:ASN:HA	1:U:138:PHE:HB3	1.98	0.45
5:Y:32:ARG:HH12	5:Y:36:ALA:N	2.15	0.45
5:Y:60:SER:OG	5:Y:61:LEU:N	2.49	0.45
6:Z:212:LEU:HD11	7:a:350:LYS:HA	1.99	0.45
9:c:64:ASP:OD1	9:c:139:ARG:NH2	2.50	0.45
10:d:167:ILE:O	10:d:171:LEU:N	2.48	0.45
12:f:77:GLU:HB2	12:f:79:ARG:HH12	1.81	0.45
14:B:417:GLU:O	14:B:421:LYS:NZ	2.46	0.45
16:D:254:ALA:HB2	16:D:262:ILE:HD11	1.98	0.45
17:E:72:LYS:HB2	17:E:78:ARG:HG2	1.98	0.45
27:n:76:VAL:HB	27:n:110:GLN:HE21	1.81	0.45
4:X:143:TYR:HD1	4:X:180:LEU:HD13	1.81	0.45
4:X:400:ALA:HB1	6:Z:262:LEU:HD22	1.99	0.45
6:Z:14:LEU:HG	9:c:39:LEU:HB3	1.99	0.45
12:f:189:LYS:HG2	12:f:190:GLU:HG2	1.99	0.45
12:f:281:ILE:HA	12:f:282:PHE:HA	1.64	0.45
22:i:69:ASN:HD22	22:i:72:MET:HE3	1.82	0.45
26:m:39:ILE:HD11	26:m:189:ILE:HD12	1.99	0.45
28:o:112:SER:OG	28:o:120:ASP:OD1	2.35	0.45
5:Y:101:ARG:HD3	5:Y:130:LYS:HD3	1.97	0.45
6:Z:235:ASN:OD1	7:a:289:ARG:NH2	2.50	0.45
6:Z:237:LEU:HD21	9:c:310:LYS:HB2	1.97	0.45
12:f:227:ALA:HB3	12:f:232:TYR:HB2	1.99	0.45
13:A:287:ASP:OD1	13:A:287:ASP:N	2.47	0.45
27:N:76:VAL:HB	27:N:110:GLN:HE21	1.81	0.45
28:o:143:ARG:NH2	28:o:150:GLU:OE1	2.50	0.45
3:W:203:GLN:HB3	3:W:233:LEU:HD21	1.99	0.45
12:f:32:GLU:O	12:f:36:ALA:N	2.39	0.45
12:f:344:VAL:HG11	12:f:391:LEU:HG	1.99	0.45
15:C:60:ARG:NH2	16:D:71:GLU:OE2	2.49	0.45
18:F:56:LYS:CB	19:u:54:ARG:CZ	2.94	0.45
28:O:143:ARG:NH2	28:O:150:GLU:OE1	2.50	0.45
1:U:400:ALA:O	1:U:404:ALA:N	2.44	0.45
4:X:257:CYS:O	4:X:261:LEU:N	2.50	0.45
12:f:378:ASN:O	12:f:382:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:141:ASP:OD1	18:F:144:LYS:NZ	2.35	0.45
23:j:68:ASN:HA	23:j:211:MET:HE1	1.98	0.45
10:d:45:LYS:HZ1	10:d:88:GLN:HA	1.82	0.44
10:d:101:LEU:HG	10:d:166:PHE:HE2	1.81	0.44
12:f:698:SER:HB3	13:A:80:LEU:HD13	1.99	0.44
15:C:232:ARG:HD3	15:C:279:GLN:HE21	1.81	0.44
15:C:332:HIS:ND1	15:C:363:CYS:SG	2.90	0.44
16:D:96:VAL:HG23	16:D:102:ILE:HD11	1.99	0.44
19:u:1:MET:N	19:u:17:VAL:O	2.37	0.44
30:Q:37:LYS:HE2	30:Q:188:ILE:HG13	1.98	0.44
1:U:770:TRP:HD1	9:c:180:ASN:HB3	1.82	0.44
4:X:397:TYR:OH	6:Z:255:ASP:OD1	2.33	0.44
5:Y:57:LEU:HD11	5:Y:63:TRP:HB2	1.99	0.44
7:a:100:THR:HG22	7:a:103:LYS:HE2	1.98	0.44
12:f:742:ALA:O	12:f:746:ARG:NE	2.45	0.44
30:Q:23:SER:OG	30:Q:24:ASN:N	2.50	0.44
33:t:92:LEU:HD23	33:t:112:ILE:HD11	1.99	0.44
3:W:32:ALA:HA	3:W:35:ALA:HB3	1.98	0.44
9:c:291:LEU:O	9:c:295:ASN:ND2	2.50	0.44
12:f:460:ASP:OD1	12:f:460:ASP:N	2.49	0.44
19:u:7:THR:HG22	19:u:69:LEU:HD23	1.98	0.44
19:u:36:ILE:HB	19:u:41:GLN:HE21	1.82	0.44
23:j:38:ARG:HH12	23:j:182:GLU:HA	1.82	0.44
2:V:287:ARG:HH11	2:V:291:TYR:HE2	1.66	0.44
7:a:247:ARG:O	7:a:250:THR:OG1	2.31	0.44
12:f:406:GLY:HA2	12:f:409:SER:HB2	2.00	0.44
14:B:135:ILE:HG22	14:B:139:VAL:HG11	2.00	0.44
31:r:83:LEU:HD11	31:r:97:MET:HE1	2.00	0.44
33:t:79:ASP:HB3	33:t:81:HIS:HD2	1.83	0.44
8:b:14:GLU:HB3	8:b:82:GLY:H	1.82	0.44
12:f:463:LEU:HD21	19:w:66:THR:HB	1.98	0.44
16:D:173:GLN:HE22	16:D:334:PRO:HD2	1.82	0.44
17:E:101:ASP:HB3	17:E:106:THR:H	1.82	0.44
17:E:243:PHE:HB3	17:E:245:GLU:H	1.81	0.44
28:O:67:SER:HB3	28:O:74:PRO:HG3	2.00	0.44
28:O:112:SER:OG	28:O:120:ASP:OD1	2.35	0.44
2:V:228:ARG:NH1	2:V:253:LEU:O	2.49	0.44
3:W:267:LEU:HA	3:W:270:VAL:HG12	2.00	0.44
12:f:654:VAL:O	12:f:658:ALA:N	2.45	0.44
17:E:148:VAL:HB	17:E:297:ARG:HH21	1.81	0.44
18:F:212:PHE:HD1	18:F:217:ILE:HD11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:159:ASP:OD1	29:P:159:ASP:N	2.51	0.44
30:Q:170:ARG:HA	30:q:27:GLN:HG2	2.00	0.44
33:T:92:LEU:HD23	33:T:112:ILE:HD11	1.99	0.44
1:U:204:ILE:HA	1:U:207:ASN:HB2	1.99	0.44
1:U:218:GLN:HG3	1:U:752:THR:HB	2.00	0.44
2:V:296:LYS:HB3	2:V:301:GLU:HB3	2.00	0.44
4:X:207:GLN:O	4:X:211:ASP:N	2.49	0.44
7:a:100:THR:HA	7:a:103:LYS:HG2	2.00	0.44
13:A:372:LEU:HD23	13:A:375:ARG:HH21	1.82	0.44
1:U:341:PHE:HZ	1:U:883:ARG:HB3	1.81	0.44
1:U:445:ALA:HA	1:U:448:LEU:HD12	2.00	0.44
3:W:395:ASN:HA	3:W:398:VAL:HG22	1.99	0.44
18:F:311:LEU:HD23	18:F:314:LEU:HD12	1.99	0.44
19:w:36:ILE:HB	19:w:41:GLN:HE21	1.82	0.44
26:M:39:ILE:HD11	26:M:189:ILE:HD12	1.99	0.44
21:h:119:GLN:NE2	22:i:82:ASP:OD1	2.51	0.44
2:V:33:GLN:NE2	2:V:118:GLN:OE1	2.50	0.44
4:X:173:GLU:HA	4:X:176:THR:HG22	2.00	0.44
5:Y:282:MET:HG3	5:Y:288:PHE:HB3	2.00	0.44
7:a:269:LEU:HD12	7:a:272:ILE:HD11	1.99	0.44
12:f:830:LEU:HB2	12:f:859:PRO:HB2	2.00	0.44
15:C:326:LEU:HD22	15:C:345:ARG:HE	1.83	0.44
16:D:155:THR:HG23	16:D:159:LYS:HE2	2.00	0.44
25:L:164:ARG:O	25:L:198:THR:OG1	2.30	0.44
28:O:120:ASP:OD1	28:O:120:ASP:N	2.47	0.44
4:X:255:LEU:HB2	4:X:287:LEU:HD13	1.99	0.43
10:d:198:LEU:HD12	10:d:200:PHE:HE1	1.83	0.43
12:f:23:GLY:HA2	12:f:27:LYS:HD3	2.00	0.43
12:f:31:LYS:HE2	12:f:31:LYS:HB3	1.83	0.43
13:A:185:GLU:OE1	13:A:188:ARG:NH2	2.51	0.43
17:E:171:LEU:HD22	17:E:295:LEU:HD13	2.00	0.43
17:E:368:MET:HB3	17:E:372:ARG:HH12	1.83	0.43
6:Z:58:PHE:HE1	6:Z:68:TRP:HB2	1.84	0.43
6:Z:85:VAL:HA	9:c:76:PRO:HB3	2.00	0.43
12:f:297:MET:HA	12:f:772:GLY:HA2	2.01	0.43
17:E:168:LYS:N	17:E:296:ASP:OD2	2.50	0.43
33:T:79:ASP:HB3	33:T:81:HIS:HD2	1.83	0.43
30:q:148:THR:HG22	30:q:150:THR:H	1.83	0.43
1:U:341:PHE:HD1	1:U:881:PRO:HB2	1.82	0.43
1:U:500:ASN:OD1	1:U:508:THR:OG1	2.30	0.43
1:U:646:PRO:O	1:U:650:TYR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:187:LEU:HA	3:W:190:MET:HE3	2.00	0.43
4:X:122:ARG:HD2	4:X:125:LEU:HB2	1.99	0.43
5:Y:316:LEU:HB3	5:Y:354:VAL:HG23	2.01	0.43
9:c:251:LEU:HD11	9:c:283:HIS:HB3	1.99	0.43
12:f:403:LYS:HG3	12:f:406:GLY:H	1.83	0.43
17:E:172:LEU:HD23	17:E:299:ILE:HB	2.01	0.43
32:S:99:ARG:HH21	32:S:102:PHE:HD2	1.66	0.43
2:V:46:GLY:O	2:V:50:GLU:N	2.51	0.43
16:D:153:MET:SD	16:D:153:MET:N	2.90	0.43
22:i:133:SER:OG	22:i:150:SER:O	2.35	0.43
13:A:324:PRO:HA	13:A:327:LEU:HD13	2.00	0.43
14:B:387:LYS:HB3	14:B:390:LEU:HB3	2.00	0.43
16:D:264:ILE:HB	16:D:309:MET:HG2	2.01	0.43
16:D:337:ASP:O	16:D:341:LYS:NZ	2.40	0.43
23:j:96:LEU:HD12	30:q:62:LYS:HG3	2.01	0.43
23:j:98:VAL:HG22	31:r:78:ALA:HB1	2.00	0.43
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.83	0.43
3:W:1:MET:HG3	3:W:43:VAL:HG21	1.99	0.43
3:W:265:GLN:OE1	3:W:335:SER:OG	2.37	0.43
6:Z:59:ASP:HB2	8:b:99:HIS:CE1	2.53	0.43
14:B:387:LYS:HB3	14:B:390:LEU:HD23	1.99	0.43
22:I:123:GLN:NE2	23:J:118:TYR:OH	2.52	0.43
22:i:108:GLU:OE1	23:j:57:ARG:NH1	2.49	0.43
2:V:404:LYS:HA	2:V:407:VAL:HG12	2.01	0.43
5:Y:215:ASP:O	5:Y:218:THR:OG1	2.33	0.43
5:Y:232:GLU:HB3	5:Y:234:PRO:HD2	2.00	0.43
6:Z:35:VAL:HB	6:Z:97:THR:HB	1.99	0.43
9:c:31:VAL:HG23	9:c:203:ILE:HG21	2.01	0.43
16:D:374:ASP:HB3	17:E:292:PRO:HG2	2.01	0.43
26:M:136:MET:HE3	26:M:163:CYS:HB3	2.01	0.43
23:j:80:ALA:HA	23:j:129:ILE:HD13	2.00	0.43
32:s:35:ILE:HB	33:t:151:ARG:HH12	1.83	0.43
3:W:365:ILE:HG22	3:W:368:LYS:HD2	2.00	0.43
9:c:163:ILE:HG12	9:c:174:PRO:HG3	2.01	0.43
12:f:24:THR:HA	12:f:31:LYS:HB2	2.01	0.43
15:C:372:ARG:HH22	16:D:175:GLN:NE2	2.17	0.43
30:Q:148:THR:HG22	30:Q:150:THR:H	1.83	0.43
31:R:83:LEU:HD11	31:R:97:MET:HE1	2.00	0.43
26:m:136:MET:HE3	26:m:163:CYS:HB3	2.01	0.43
28:o:67:SER:HB3	28:o:74:PRO:HG3	2.00	0.43
28:o:113:ILE:HG12	28:o:119:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:101:ILE:HD11	15:C:22:GLN:HG3	2.01	0.43
4:X:378:LEU:HD23	5:Y:311:TYR:HE1	1.83	0.43
6:Z:116:CYS:O	6:Z:119:SER:OG	2.31	0.43
12:f:202:HIS:CE1	12:f:241:PRO:HB2	2.53	0.43
24:K:99:HIS:HB2	24:K:107:MET:HE3	2.01	0.43
23:j:185:ASP:HA	23:j:188:ILE:HD12	2.00	0.43
1:U:336:GLU:O	1:U:340:GLN:N	2.50	0.43
1:U:475:HIS:HD2	1:U:511:ALA:HB2	1.84	0.43
4:X:342:PHE:HB2	4:X:343:SER:H	1.61	0.43
6:Z:138:TYR:HA	6:Z:157:HIS:HA	2.01	0.43
12:f:408:LEU:HD21	12:f:797:LEU:HD13	1.99	0.43
21:h:74:LEU:HD21	21:h:134:LEU:HD22	2.01	0.43
1:U:220:LEU:O	1:U:224:ASP:N	2.51	0.42
5:Y:366:TYR:O	5:Y:369:THR:OG1	2.35	0.42
6:Z:43:TRP:HB3	6:Z:48:LEU:HD22	2.00	0.42
12:f:407:MET:HE3	12:f:439:TYR:HB2	1.99	0.42
12:f:450:ILE:HG23	12:f:804:LEU:HD13	2.01	0.42
14:B:287:ILE:HD13	14:B:329:MET:HE3	2.01	0.42
15:C:196:LYS:N	37:C:501:ADP:O3B	2.42	0.42
16:D:200:ARG:HH22	16:D:301:GLN:H	1.68	0.42
24:k:99:HIS:HB2	24:k:107:MET:HE3	2.01	0.42
3:W:375:MET:HE2	3:W:386:VAL:HB	2.01	0.42
14:B:221:GLY:HA3	14:B:347:ILE:HA	2.00	0.42
13:A:274:PHE:HD2	13:A:319:MET:HE3	1.84	0.42
14:B:145:GLU:HG2	14:B:148:CYS:HB2	2.00	0.42
2:V:100:MET:HG2	2:V:102:PRO:HD2	2.02	0.42
6:Z:212:LEU:HD21	7:a:350:LYS:HG3	2.02	0.42
12:f:180:GLN:HB3	12:f:219:LYS:NZ	2.35	0.42
12:f:755:ASP:OD1	12:f:755:ASP:N	2.48	0.42
14:B:234:LEU:HG	35:B:501:ATP:H2'	2.00	0.42
16:D:354:LEU:HD11	16:D:360:LEU:HD11	2.01	0.42
18:F:277:GLU:OE1	18:F:278:LYS:NZ	2.42	0.42
23:J:81:ARG:O	23:J:85:ASN:ND2	2.51	0.42
30:Q:13:VAL:HG11	30:Q:105:ALA:HB1	2.01	0.42
31:r:97:MET:HB3	31:r:116:SER:HB3	2.02	0.42
14:B:342:ILE:HD12	14:B:342:ILE:HG23	1.86	0.42
14:B:373:THR:OG1	14:B:412:MET:O	2.37	0.42
29:p:135:ASP:OD1	29:p:135:ASP:N	2.50	0.42
2:V:203:LEU:O	2:V:207:ALA:N	2.41	0.42
2:V:467:TYR:OH	4:X:397:TYR:OH	2.23	0.42
3:W:203:GLN:HA	3:W:206:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:21:ASP:OD1	6:Z:21:ASP:N	2.52	0.42
8:b:184:ILE:H	8:b:184:ILE:HG13	1.75	0.42
12:f:57:GLU:HG2	12:f:93:PRO:HB3	2.02	0.42
12:f:167:ALA:HB2	12:f:185:LEU:HD12	2.02	0.42
12:f:447:ALA:HA	12:f:450:ILE:HD12	2.00	0.42
18:F:226:TYR:CZ	18:F:353:GLU:HB3	2.54	0.42
25:L:216:GLY:HA3	25:L:219:LEU:HB3	2.01	0.42
31:R:97:MET:HB3	31:R:116:SER:HB3	2.02	0.42
1:U:155:LEU:O	1:U:158:ARG:NH1	2.47	0.42
3:W:155:GLN:HG2	3:W:157:GLY:H	1.85	0.42
7:a:161:LYS:O	7:a:165:THR:OG1	2.25	0.42
10:d:178:ILE:HA	10:d:181:CYS:SG	2.59	0.42
13:A:392:ALA:HA	13:A:395:PHE:HD2	1.83	0.42
15:C:71:SER:HB3	16:D:112:TYR:HB3	2.02	0.42
16:D:208:PRO:HB2	17:E:291:ARG:HD3	2.02	0.42
17:E:304:PRO:O	17:E:309:ARG:NH1	2.51	0.42
20:G:67:THR:HG22	20:G:69:LEU:H	1.85	0.42
20:G:120:ASP:OD1	21:H:84:ARG:NH1	2.53	0.42
30:Q:12:TYR:HB2	30:Q:182:ILE:HD11	2.02	0.42
25:l:14:SER:HB3	25:l:18:ARG:H	1.85	0.42
1:U:107:HIS:HA	1:U:110:LYS:HG2	2.02	0.42
1:U:714:SER:HA	1:U:717:ILE:HG22	2.02	0.42
8:b:75:LEU:HD23	8:b:78:VAL:HG21	2.02	0.42
12:f:392:THR:O	12:f:396:ASN:N	2.52	0.42
14:B:337:LEU:HD11	14:B:342:ILE:HD11	2.00	0.42
17:E:50:LEU:HD13	18:F:82:VAL:HG11	2.02	0.42
25:L:228:ASP:OD1	25:L:228:ASP:N	2.52	0.42
22:i:32:GLY:N	22:i:50:ARG:HH21	2.18	0.42
24:k:54:ILE:HG23	24:k:59:MET:HE2	2.02	0.42
25:l:216:GLY:HA3	25:l:219:LEU:HB3	2.01	0.42
6:Z:109:ASN:HD22	6:Z:155:PHE:HE1	1.67	0.42
8:b:121:GLU:HB3	8:b:152:LYS:HG2	2.01	0.42
9:c:157:ILE:HD12	9:c:157:ILE:HA	1.91	0.42
17:E:56:ILE:HB	17:E:100:LEU:HB2	2.02	0.42
17:E:84:ARG:HB2	17:E:87:LEU:HD23	2.01	0.42
17:E:139:SER:HA	17:E:142:ILE:HD12	2.02	0.42
22:I:161:ALA:HB1	22:I:175:LEU:HD13	2.02	0.42
24:K:209:LYS:O	24:K:214:ASN:ND2	2.53	0.42
33:T:9:THR:O	33:T:54:SER:OG	2.36	0.42
22:i:34:CYS:HG	22:i:75:SER:HG	1.66	0.42
24:k:209:LYS:O	24:k:214:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:227:VAL:O	2:V:231:LEU:N	2.53	0.42
10:d:194:ALA:HB3	10:d:222:TYR:HE2	1.85	0.42
12:f:556:ARG:NH1	12:f:784:ASP:O	2.53	0.42
12:f:773:LYS:HA	12:f:774:GLY:HA3	1.73	0.42
15:C:330:LYS:HE2	15:C:330:LYS:HB3	1.91	0.42
23:J:224:GLU:O	23:J:228:TYR:N	2.46	0.42
26:m:139:SER:OG	26:m:140:TYR:N	2.53	0.42
32:s:172:MET:HE1	32:s:195:ILE:HG21	2.02	0.42
1:U:213:PHE:HE2	1:U:244:MET:HB2	1.85	0.41
1:U:265:ILE:HG23	1:U:269:ARG:HH12	1.84	0.41
3:W:122:LEU:HA	3:W:125:ILE:HG22	2.02	0.41
3:W:172:GLU:C	3:W:175:GLY:H	2.28	0.41
5:Y:101:ARG:HE	5:Y:127:THR:HA	1.84	0.41
7:a:18:GLN:HG3	7:a:22:TRP:HE1	1.84	0.41
7:a:194:GLN:HB3	7:a:225:LEU:HG	2.02	0.41
7:a:371:ALA:HA	7:a:374:ILE:HD13	2.02	0.41
12:f:679:LEU:HB2	12:f:681:TYR:H	1.85	0.41
13:A:146:LYS:HD2	13:A:148:GLN:HG2	2.03	0.41
21:H:74:LEU:HD21	21:H:134:LEU:HD22	2.01	0.41
23:J:31:THR:OG1	23:J:163:ARG:O	2.38	0.41
24:K:37:ALA:N	24:K:170:ILE:O	2.53	0.41
30:Q:88:LEU:HD13	30:Q:118:MET:HE1	2.02	0.41
20:g:114:LEU:HD22	20:g:140:LEU:HD21	2.02	0.41
1:U:261:LEU:HA	1:U:264:VAL:HG12	2.03	0.41
2:V:249:THR:HG22	2:V:284:GLU:HG3	2.01	0.41
2:V:268:GLU:O	2:V:272:SER:N	2.54	0.41
5:Y:71:ASN:HA	5:Y:74:LYS:HG2	2.02	0.41
5:Y:153:ASP:HB3	5:Y:156:LEU:HB2	2.02	0.41
10:d:21:GLU:O	10:d:25:ARG:N	2.49	0.41
14:B:58:CYS:SG	14:B:59:ARG:N	2.93	0.41
19:w:1:MET:N	19:w:17:VAL:O	2.37	0.41
23:j:121:SER:OG	23:j:122:ASN:N	2.53	0.41
26:m:51:LYS:NZ	26:m:62:SER:O	2.33	0.41
30:q:13:VAL:HG11	30:q:105:ALA:HB1	2.01	0.41
1:U:381:THR:HG22	1:U:412:HIS:HA	2.01	0.41
6:Z:9:VAL:HA	6:Z:48:LEU:HB3	2.01	0.41
9:c:196:LEU:HA	9:c:197:ASN:HA	1.61	0.41
10:d:19:CYS:HA	10:d:22:GLU:HB3	2.01	0.41
12:f:149:GLU:HG3	12:f:152:ALA:HB2	2.02	0.41
12:f:265:ALA:HB3	12:f:268:LEU:HB2	2.02	0.41
12:f:531:ASN:HD22	12:f:534:VAL:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:152:GLY:HA3	15:C:328:ILE:HG12	2.02	0.41
16:D:153:MET:HE2	16:D:229:ARG:NE	2.34	0.41
16:D:284:GLU:OE1	16:D:287:ARG:NH1	2.53	0.41
16:D:328:ASP:OD1	16:D:328:ASP:N	2.50	0.41
25:L:138:ASP:HB3	33:T:81:HIS:CE1	2.56	0.41
30:q:12:TYR:HB2	30:q:182:ILE:HD11	2.02	0.41
1:U:19:LEU:O	1:U:23:ALA:N	2.54	0.41
1:U:163:PHE:HE2	1:U:201:LEU:HD11	1.84	0.41
1:U:202:VAL:HG11	1:U:219:CYS:SG	2.60	0.41
2:V:350:GLN:H	2:V:353:LEU:HB3	1.86	0.41
5:Y:268:TYR:HB3	5:Y:323:PHE:CD1	2.56	0.41
7:a:14:SER:HB2	7:a:18:GLN:HG2	2.02	0.41
9:c:254:ASN:HB3	9:c:280:PRO:HB3	2.02	0.41
12:f:221:ILE:HD12	12:f:224:ASN:HB2	2.02	0.41
13:A:393:GLY:HA2	14:B:214:MET:HE2	2.02	0.41
16:D:358:VAL:HG22	16:D:396:ALA:HB2	2.02	0.41
20:G:175:SER:OG	20:G:201:CYS:SG	2.74	0.41
23:J:154:HIS:NE2	24:K:59:MET:SD	2.91	0.41
28:o:38:SER:OG	28:o:40:ASN:OD1	2.34	0.41
1:U:24:LEU:HB2	1:U:59:PHE:CD2	2.55	0.41
1:U:112:CYS:HA	1:U:115:ASN:HB2	2.02	0.41
1:U:236:LEU:HD22	1:U:244:MET:HG3	2.01	0.41
1:U:700:GLU:OE1	1:U:707:ASN:ND2	2.53	0.41
4:X:194:ARG:HD2	4:X:210:LEU:HD21	2.03	0.41
6:Z:256:GLN:NE2	9:c:295:ASN:O	2.54	0.41
7:a:156:TYR:HB3	7:a:179:PHE:HB2	2.01	0.41
8:b:15:TYR:O	8:b:25:ARG:NH1	2.53	0.41
8:b:124:LEU:HD13	8:b:156:PHE:HB2	2.02	0.41
12:f:283:THR:O	12:f:287:ASP:N	2.45	0.41
14:B:378:VAL:HG12	14:B:416:ASN:HA	2.02	0.41
20:g:67:THR:HG22	20:g:69:LEU:H	1.84	0.41
30:q:23:SER:OG	30:q:24:ASN:N	2.50	0.41
30:q:88:LEU:HD13	30:q:118:MET:HE1	2.02	0.41
1:U:646:PRO:HB3	1:U:680:VAL:HG21	2.03	0.41
1:U:770:TRP:O	9:c:180:ASN:N	2.48	0.41
3:W:93:ARG:HG3	3:W:97:LEU:HD13	2.03	0.41
14:B:387:LYS:HG3	14:B:389:ASP:H	1.85	0.41
19:w:36:ILE:O	19:w:41:GLN:NE2	2.54	0.41
25:L:14:SER:HB3	25:L:18:ARG:H	1.85	0.41
20:g:126:THR:O	20:g:126:THR:OG1	2.36	0.41
22:i:38:LEU:HB3	22:i:43:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:p:159:ASP:OD1	29:p:159:ASP:N	2.51	0.41
2:V:89:LYS:HD3	2:V:92:ARG:NH1	2.35	0.41
5:Y:42:MET:SD	5:Y:46:ARG:NH2	2.93	0.41
5:Y:204:THR:O	5:Y:216:TYR:OH	2.38	0.41
5:Y:232:GLU:HG2	5:Y:233:ARG:H	1.86	0.41
8:b:62:THR:HG22	8:b:70:ARG:HG2	2.02	0.41
11:e:59:GLU:HG3	11:e:63:HIS:HE1	1.85	0.41
12:f:31:LYS:HE3	12:f:82:ILE:HG21	2.03	0.41
14:B:167:THR:HA	14:B:168:ASP:HA	1.88	0.41
15:C:373:GLU:HG3	15:C:375:ARG:HG3	2.02	0.41
16:D:184:PRO:HG3	16:D:191:TYR:CZ	2.56	0.41
22:I:18:LEU:HD22	23:J:125:ARG:HH12	1.86	0.41
26:M:139:SER:OG	26:M:140:TYR:N	2.53	0.41
30:Q:169:LYS:O	30:q:27:GLN:NE2	2.34	0.41
32:S:16:ALA:HB2	32:S:121:VAL:HG23	2.02	0.41
33:T:4:PRO:HG3	33:T:107:TRP:CE2	2.56	0.41
33:T:22:ILE:HD12	33:T:50:MET:HE3	2.02	0.41
33:t:22:ILE:HD12	33:t:50:MET:HE3	2.02	0.41
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.86	0.41
12:f:681:TYR:CD1	12:f:858:LYS:HG2	2.56	0.41
13:A:213:LEU:HD22	13:A:337:LEU:HD23	2.02	0.41
14:B:407:LEU:HD23	14:B:407:LEU:HA	1.88	0.41
22:I:38:LEU:HB3	22:I:43:VAL:HG23	2.02	0.41
2:V:232:HIS:O	2:V:236:ARG:N	2.52	0.41
2:V:342:ILE:HD12	2:V:343:PRO:HD2	2.02	0.41
6:Z:207:ASP:O	6:Z:210:SER:OG	2.31	0.41
7:a:197:ALA:O	7:a:201:GLY:N	2.51	0.41
9:c:147:PRO:HG2	9:c:148:ILE:HD12	2.03	0.41
10:d:106:LEU:HD21	10:d:114:GLU:HB2	2.03	0.41
12:f:311:VAL:CG2	19:w:76:GLY:CA	2.99	0.41
12:f:705:ASN:OD1	12:f:706:ILE:N	2.54	0.41
12:f:828:ARG:HG2	12:f:845:ARG:C	2.46	0.41
13:A:425:ALA:HA	14:B:339:PRO:HB2	2.03	0.41
15:C:113:ARG:HH21	15:C:129:ASN:H	1.67	0.41
15:C:307:ARG:HH21	15:C:310:ARG:CZ	2.33	0.41
18:F:81:LYS:HE2	18:F:81:LYS:HB3	1.90	0.41
21:H:40:ALA:HB1	21:H:182:LEU:HB2	2.02	0.41
23:J:67:ASP:OD1	23:J:67:ASP:N	2.53	0.41
24:K:54:ILE:HG23	24:K:59:MET:HE2	2.02	0.41
31:R:182:ASP:OD1	31:R:182:ASP:N	2.52	0.41
21:h:40:ALA:HB1	21:h:182:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:161:ALA:HB1	22:i:175:LEU:HD13	2.02	0.41
27:n:28:ASN:HD21	28:o:122:LEU:HD21	1.85	0.41
31:r:22:ALA:N	31:r:25:TYR:O	2.49	0.41
31:r:182:ASP:OD1	31:r:182:ASP:N	2.52	0.41
1:U:54:PHE:C	1:U:56:SER:H	2.29	0.41
4:X:357:SER:OG	4:X:358:LYS:N	2.54	0.41
15:C:113:ARG:HB3	15:C:127:LEU:HB3	2.03	0.41
20:G:114:LEU:HD22	20:G:140:LEU:HD21	2.02	0.41
30:Q:8:GLN:NE2	30:Q:9:GLY:O	2.54	0.41
32:S:35:ILE:O	33:T:151:ARG:NH2	2.40	0.41
5:Y:315:THR:HA	5:Y:353:ILE:HA	2.03	0.40
12:f:382:ASN:ND2	12:f:388:ASP:OD2	2.54	0.40
12:f:752:HIS:HE1	12:f:803:PHE:HZ	1.68	0.40
16:D:173:GLN:HE22	16:D:333:PHE:HA	1.86	0.40
17:E:317:ALA:HA	17:E:320:ILE:HD12	2.03	0.40
20:G:126:THR:O	20:G:126:THR:OG1	2.36	0.40
29:P:107:PRO:HG2	29:P:124:LEU:HB2	2.03	0.40
24:k:37:ALA:N	24:k:170:ILE:O	2.53	0.40
33:t:4:PRO:HG3	33:t:107:TRP:CE2	2.56	0.40
2:V:85:ALA:O	2:V:89:LYS:NZ	2.36	0.40
2:V:357:LEU:O	2:V:361:PHE:N	2.38	0.40
6:Z:42:SER:OG	6:Z:43:TRP:N	2.54	0.40
10:d:122:LEU:HB2	10:d:125:LYS:HB2	2.04	0.40
12:f:240:VAL:HG13	12:f:257:ARG:HE	1.85	0.40
12:f:785:ARG:HH22	12:f:795:GLY:HA3	1.87	0.40
18:F:197:GLU:HB2	18:F:350:ARG:HH21	1.86	0.40
32:S:28:ARG:NH2	32:S:191:ASP:OD1	2.54	0.40
30:q:8:GLN:NE2	30:q:9:GLY:O	2.54	0.40
1:U:321:GLN:HA	1:U:324:LYS:HB2	2.04	0.40
6:Z:142:GLU:HB3	6:Z:153:LYS:HE2	2.03	0.40
7:a:97:LEU:O	7:a:101:ARG:N	2.49	0.40
10:d:56:GLU:HA	10:d:78:LEU:HD11	2.03	0.40
10:d:170:LEU:HA	10:d:173:THR:HG22	2.03	0.40
12:f:182:GLU:OE2	12:f:186:THR:OG1	2.39	0.40
12:f:233:LEU:HD12	12:f:264:GLU:HG3	2.04	0.40
12:f:283:THR:HA	12:f:286:LYS:HB3	2.04	0.40
14:B:234:LEU:N	35:B:501:ATP:O1A	2.54	0.40
15:C:89:VAL:HG12	15:C:90:HIS:H	1.85	0.40
15:C:150:MET:HA	15:C:331:ILE:HG21	2.04	0.40
16:D:274:ARG:HD3	17:E:245:GLU:HB3	2.03	0.40
22:I:90:LEU:HD13	22:I:114:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:J:38:ARG:HH12	23:J:182:GLU:HA	1.86	0.40
30:q:38:MET:HE1	30:q:44:LEU:HB2	2.04	0.40
1:U:900:TYR:HB3	1:U:914:LEU:HG	2.04	0.40
2:V:64:GLN:HA	2:V:67:LEU:HD12	2.04	0.40
6:Z:76:GLU:OE2	6:Z:115:TYR:OH	2.28	0.40
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.04	0.40
9:c:75:MET:HE1	9:c:87:VAL:HA	2.03	0.40
10:d:36:LEU:HD23	10:d:38:THR:H	1.85	0.40
10:d:109:GLN:OE1	10:d:111:ARG:NH1	2.54	0.40
12:f:809:ILE:HG23	12:f:810:ILE:HG23	2.03	0.40
15:C:355:SER:OG	15:C:358:GLU:OE1	2.31	0.40
17:E:220:ASN:OD1	17:E:223:ARG:NH2	2.54	0.40
26:M:65:ARG:HH21	26:M:78:ALA:HA	1.86	0.40
20:g:112:ASP:OD1	20:g:112:ASP:N	2.54	0.40
27:n:7:GLN:HA	27:n:12:VAL:HA	2.03	0.40
33:t:126:ASP:OD1	33:t:127:MET:N	2.54	0.40
1:U:245:ALA:O	1:U:324:LYS:NZ	2.55	0.40
3:W:135:LYS:HB3	3:W:136:ILE:H	1.63	0.40
3:W:375:MET:N	3:W:411:GLY:O	2.53	0.40
4:X:73:VAL:O	4:X:77:LEU:N	2.54	0.40
7:a:65:SER:HA	7:a:68:GLU:HB2	2.02	0.40
9:c:30:GLN:HB3	9:c:66:THR:HG22	2.04	0.40
9:c:251:LEU:HD22	9:c:251:LEU:HA	1.96	0.40
12:f:437:GLU:HG3	12:f:440:ILE:HD12	2.04	0.40
18:F:252:ALA:HB3	18:F:255:GLN:HB2	2.02	0.40
19:u:36:ILE:O	19:u:41:GLN:NE2	2.54	0.40
31:R:6:PHE:HE1	31:R:156:ALA:HB2	1.87	0.40
28:o:30:ASN:OD1	28:o:187:ARG:NH2	2.55	0.40
29:p:107:PRO:HG2	29:p:124:LEU:HB2	2.03	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	U	806/953 (85%)	738 (92%)	65 (8%)	3 (0%)	30	66
2	V	506/534 (95%)	453 (90%)	49 (10%)	4 (1%)	16	51
3	W	454/456 (100%)	407 (90%)	43 (10%)	4 (1%)	14	49
4	X	378/422 (90%)	353 (93%)	24 (6%)	1 (0%)	37	70
5	Y	376/389 (97%)	342 (91%)	34 (9%)	0	100	100
6	Z	284/324 (88%)	243 (86%)	41 (14%)	0	100	100
7	a	371/376 (99%)	337 (91%)	33 (9%)	1 (0%)	37	70
8	b	189/377 (50%)	175 (93%)	13 (7%)	1 (0%)	25	61
9	c	285/309 (92%)	244 (86%)	38 (13%)	3 (1%)	12	44
10	d	255/349 (73%)	216 (85%)	39 (15%)	0	100	100
11	e	36/70 (51%)	22 (61%)	14 (39%)	0	100	100
12	f	887/908 (98%)	715 (81%)	165 (19%)	7 (1%)	16	51
13	A	392/433 (90%)	342 (87%)	48 (12%)	2 (0%)	25	61
14	B	382/440 (87%)	348 (91%)	33 (9%)	1 (0%)	37	70
15	C	359/398 (90%)	333 (93%)	24 (7%)	2 (1%)	22	57
16	D	378/418 (90%)	334 (88%)	38 (10%)	6 (2%)	8	34
17	E	373/403 (93%)	335 (90%)	36 (10%)	2 (0%)	25	61
18	F	372/439 (85%)	338 (91%)	33 (9%)	1 (0%)	37	70
19	u	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
19	w	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
20	G	238/245 (97%)	223 (94%)	15 (6%)	0	100	100
20	g	238/245 (97%)	223 (94%)	15 (6%)	0	100	100
21	H	230/233 (99%)	224 (97%)	6 (3%)	0	100	100
21	h	230/233 (99%)	224 (97%)	6 (3%)	0	100	100
22	I	248/260 (95%)	229 (92%)	19 (8%)	0	100	100
22	i	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
23	J	237/247 (96%)	218 (92%)	18 (8%)	1 (0%)	30	66
23	j	237/247 (96%)	220 (93%)	16 (7%)	1 (0%)	30	66
24	K	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
24	k	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
25	L	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
25	l	236/268 (88%)	221 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	M	238/254 (94%)	222 (93%)	16 (7%)	0	100	100
26	m	238/254 (94%)	222 (93%)	16 (7%)	0	100	100
27	N	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
27	n	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
28	O	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
28	o	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
29	P	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
29	p	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
30	Q	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
30	q	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
31	R	199/262 (76%)	188 (94%)	11 (6%)	0	100	100
31	r	199/262 (76%)	188 (94%)	11 (6%)	0	100	100
32	S	211/240 (88%)	204 (97%)	7 (3%)	0	100	100
32	s	211/240 (88%)	200 (95%)	11 (5%)	0	100	100
33	T	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
33	t	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
All	All	13391/15012 (89%)	12242 (91%)	1109 (8%)	40 (0%)	38	70

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	167	LEU
15	C	90	HIS
1	U	874	ASN
2	V	168	GLN
16	D	84	SER
17	E	386	TYR
2	V	265	ASP
3	W	252	ASP
4	X	392	PRO
7	a	149	THR
12	f	118	ASN
12	f	476	THR
12	f	808	ASN
15	C	128	PRO
16	D	126	PRO

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Mol	Chain	Res	Type
1	U	873	PRO
12	f	853	VAL
12	f	859	PRO
13	A	425	ALA
14	B	87	PRO
16	D	154	LEU
16	D	368	ASP
17	E	385	ASP
23	J	97	THR
3	W	136	ILE
9	c	158	ASP
12	f	475	ASN
13	A	109	PRO
23	j	97	THR
3	W	316	ARG
16	D	85	ILE
18	F	165	PRO
1	U	174	PRO
9	c	157	ILE
12	f	755	ASP
16	D	367	PRO
3	W	253	THR
8	b	23	PRO
2	V	29	PRO
9	c	156	VAL

5.3.2 Protein sidechains (i)

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	U	692/816 (85%)	689 (100%)	3 (0%)	89 95
2	V	415/460 (90%)	413 (100%)	2 (0%)	86 94
3	W	416/416 (100%)	414 (100%)	2 (0%)	86 94
4	X	327/362 (90%)	325 (99%)	2 (1%)	84 93
5	Y	334/344 (97%)	333 (100%)	1 (0%)	91 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	Z	257/295 (87%)	256 (100%)	1 (0%)	89 95
7	a	333/336 (99%)	330 (99%)	3 (1%)	75 89
8	b	167/312 (54%)	167 (100%)	0	100 100
9	c	252/267 (94%)	247 (98%)	5 (2%)	50 78
10	d	231/293 (79%)	228 (99%)	3 (1%)	65 85
11	e	38/63 (60%)	38 (100%)	0	100 100
12	f	745/763 (98%)	738 (99%)	7 (1%)	75 89
13	A	337/372 (91%)	334 (99%)	3 (1%)	75 89
14	B	339/385 (88%)	336 (99%)	3 (1%)	75 89
15	C	314/346 (91%)	312 (99%)	2 (1%)	84 93
16	D	333/366 (91%)	331 (99%)	2 (1%)	84 93
17	E	298/353 (84%)	297 (100%)	1 (0%)	91 96
18	F	296/379 (78%)	294 (99%)	2 (1%)	81 91
19	u	68/68 (100%)	68 (100%)	0	100 100
19	w	68/68 (100%)	68 (100%)	0	100 100
20	G	193/209 (92%)	191 (99%)	2 (1%)	73 88
20	g	193/209 (92%)	191 (99%)	2 (1%)	73 88
21	H	164/190 (86%)	164 (100%)	0	100 100
21	h	164/190 (86%)	164 (100%)	0	100 100
22	I	193/220 (88%)	193 (100%)	0	100 100
22	i	193/220 (88%)	193 (100%)	0	100 100
23	J	154/210 (73%)	153 (99%)	1 (1%)	84 93
23	j	152/210 (72%)	151 (99%)	1 (1%)	81 91
24	K	186/202 (92%)	185 (100%)	1 (0%)	86 94
24	k	186/202 (92%)	185 (100%)	1 (0%)	86 94
25	L	198/229 (86%)	196 (99%)	2 (1%)	73 88
25	l	198/229 (86%)	196 (99%)	2 (1%)	73 88
26	M	192/211 (91%)	192 (100%)	0	100 100
26	m	192/211 (91%)	192 (100%)	0	100 100
27	N	148/180 (82%)	148 (100%)	0	100 100
27	n	148/180 (82%)	148 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	177 (100%)	0	100	100
29	P	173/173 (100%)	173 (100%)	0	100	100
29	p	173/173 (100%)	173 (100%)	0	100	100
30	Q	164/171 (96%)	162 (99%)	2 (1%)	67	86
30	q	164/171 (96%)	162 (99%)	2 (1%)	67	86
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	175/198 (88%)	175 (100%)	0	100	100
33	T	175/214 (82%)	174 (99%)	1 (1%)	84	93
33	t	175/214 (82%)	174 (99%)	1 (1%)	84	93
All	All	11147/12734 (88%)	11087 (100%)	60 (0%)	85	94

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	629	THR
1	U	775	LEU
1	U	913	ILE
2	V	163	VAL
2	V	197	THR
3	W	89	LEU
3	W	90	LEU
4	X	80	ILE
4	X	393	VAL
5	Y	287	LEU
6	Z	91	ILE
7	a	145	LEU
7	a	165	THR
7	a	374	ILE
9	c	49	VAL
9	c	69	VAL
9	c	148	ILE
9	c	251	LEU
9	c	284	LEU
10	d	122	LEU
10	d	178	ILE

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Mol	Chain	Res	Type
10	d	202	THR
12	f	281	ILE
12	f	344	VAL
12	f	381	VAL
12	f	573	ILE
12	f	582	VAL
12	f	672	LEU
12	f	822	VAL
13	A	271	LEU
13	A	341	ILE
13	A	403	ILE
14	B	125	THR
14	B	143	LEU
14	B	170	LEU
15	C	109	THR
15	C	127	LEU
16	D	119	ILE
16	D	231	VAL
17	E	138	LEU
18	F	134	LEU
18	F	217	ILE
20	G	22	LEU
20	G	32	ILE
23	J	159	ASN
24	K	21	LEU
25	L	22	ILE
25	L	161	ILE
30	Q	4	LEU
30	Q	82	ASN
33	T	100	ARG
20	g	22	LEU
20	g	32	ILE
23	j	159	ASN
24	k	21	LEU
25	l	22	ILE
25	l	161	ILE
30	q	4	LEU
30	q	82	ASN
33	t	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	345	ASN
1	U	377	HIS
1	U	415	HIS
1	U	491	GLN
1	U	595	ASN
1	U	647	HIS
1	U	742	HIS
2	V	78	HIS
2	V	247	GLN
2	V	376	ASN
2	V	400	HIS
2	V	427	GLN
2	V	452	ASN
3	W	41	GLN
3	W	106	GLN
3	W	203	GLN
3	W	283	GLN
3	W	399	ASN
3	W	430	GLN
3	W	440	ASN
4	X	213	GLN
4	X	262	ASN
4	X	292	GLN
4	X	296	ASN
4	X	333	GLN
4	X	380	GLN
4	X	406	ASN
5	Y	48	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	363	ASN
6	Z	109	ASN
6	Z	194	GLN
6	Z	231	GLN
6	Z	277	ASN
7	a	12	GLN
7	a	18	GLN
7	a	23	HIS
7	a	35	HIS
7	a	144	ASN
7	a	152	HIS
7	a	164	GLN
7	a	193	GLN

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Mol	Chain	Res	Type
7	a	212	ASN
7	a	231	GLN
7	a	249	GLN
7	a	264	ASN
7	a	273	GLN
7	a	290	GLN
7	a	332	HIS
7	a	337	GLN
7	a	345	GLN
7	a	370	GLN
8	b	142	ASN
9	c	101	GLN
9	c	130	GLN
9	c	164	ASN
9	c	166	ASN
9	c	180	ASN
9	c	197	ASN
9	c	199	HIS
9	c	232	GLN
9	c	241	ASN
9	c	256	ASN
9	c	298	GLN
10	d	116	HIS
10	d	141	GLN
10	d	149	ASN
10	d	229	GLN
11	e	63	HIS
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	171	GLN
12	f	213	GLN
12	f	245	ASN
12	f	291	GLN
12	f	378	ASN
12	f	382	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	715	HIS
12	f	737	ASN

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Mol	Chain	Res	Type
12	f	747	GLN
12	f	752	HIS
12	f	766	GLN
12	f	782	HIS
12	f	786	GLN
12	f	808	ASN
12	f	848	GLN
13	A	44	GLN
13	A	85	GLN
13	A	293	ASN
13	A	304	ASN
14	B	57	GLN
14	B	154	HIS
14	B	195	GLN
14	B	242	GLN
14	B	314	ASN
14	B	315	GLN
14	B	368	HIS
15	C	36	ASN
15	C	48	GLN
15	C	53	ASN
15	C	64	GLN
15	C	90	HIS
15	C	171	HIS
15	C	279	GLN
16	D	49	GLN
16	D	67	ASN
16	D	91	GLN
16	D	133	HIS
16	D	173	GLN
16	D	187	HIS
16	D	221	HIS
16	D	222	HIS
16	D	257	ASN
16	D	412	GLN
17	E	55	GLN
17	E	359	HIS
18	F	208	HIS
19	u	25	ASN
19	u	40	GLN
19	u	41	GLN
19	w	25	ASN

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Mol	Chain	Res	Type
19	w	40	GLN
19	w	41	GLN
19	w	68	HIS
20	G	92	GLN
20	G	123	GLN
20	G	127	GLN
21	H	169	ASN
22	I	40	ASN
22	I	53	HIS
22	I	69	ASN
22	I	102	GLN
22	I	109	GLN
23	J	15	HIS
23	J	85	ASN
23	J	159	ASN
24	K	41	GLN
24	K	164	GLN
24	K	214	ASN
25	L	21	GLN
25	L	90	GLN
25	L	146	GLN
26	M	221	ASN
27	N	28	ASN
27	N	110	GLN
28	O	35	HIS
28	O	66	HIS
28	O	116	HIS
28	O	165	ASN
29	P	93	ASN
29	P	169	GLN
30	Q	71	ASN
30	Q	82	ASN
31	R	10	HIS
31	R	38	ASN
32	S	58	HIS
32	S	159	GLN
33	T	81	HIS
20	g	75	ASN
20	g	92	GLN
20	g	123	GLN
20	g	127	GLN
22	i	40	ASN

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Mol	Chain	Res	Type
22	i	69	ASN
22	i	95	GLN
22	i	100	GLN
23	j	120	GLN
23	j	159	ASN
24	k	41	GLN
24	k	155	HIS
24	k	164	GLN
24	k	214	ASN
25	l	90	GLN
25	l	146	GLN
25	l	166	GLN
26	m	221	ASN
27	n	28	ASN
27	n	110	GLN
28	o	35	HIS
28	o	66	HIS
28	o	116	HIS
28	o	165	ASN
29	p	93	ASN
30	q	82	ASN
31	r	10	HIS
31	r	38	ASN
32	s	79	ASN
32	s	151	ASN
33	t	81	HIS

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)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	ATP	A	501	36	28,33,33	0.83	0	34,52,52	1.18	2 (5%)
35	ATP	E	401	36	28,33,33	0.78	0	34,52,52	1.17	3 (8%)
35	ATP	D	501	36	28,33,33	0.78	0	34,52,52	1.29	4 (11%)
37	ADP	C	501	-	24,29,29	0.82	0	29,45,45	1.35	3 (10%)
37	ADP	F	501	36	24,29,29	0.81	0	29,45,45	1.19	2 (6%)
35	ATP	B	501	36	28,33,33	0.80	0	34,52,52	1.19	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	A	501	36	-	1/18/38/38	0/3/3/3
35	ATP	E	401	36	-	2/18/38/38	0/3/3/3
35	ATP	D	501	36	-	4/18/38/38	0/3/3/3
37	ADP	C	501	-	-	4/12/32/32	0/3/3/3
37	ADP	F	501	36	-	5/12/32/32	0/3/3/3
35	ATP	B	501	36	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	B	501	ATP	N3-C2-N1	-3.97	123.28	128.67
35	D	501	ATP	N3-C2-N1	-3.60	123.78	128.67
35	D	501	ATP	C4'-O4'-C1'	-3.59	106.64	109.92
35	E	401	ATP	N3-C2-N1	-3.59	123.80	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	501	ADP	N3-C2-N1	-3.54	123.87	128.67
35	A	501	ATP	N3-C2-N1	-3.44	124.00	128.67
37	F	501	ADP	N3-C2-N1	-3.36	124.11	128.67
37	C	501	ADP	C4'-O4'-C1'	2.46	112.18	109.92
37	C	501	ADP	C4-C5-N7	-2.37	106.83	109.34
35	E	401	ATP	O3G-PG-O2G	2.23	116.15	107.80
35	D	501	ATP	C4-C5-N7	-2.20	107.02	109.34
35	A	501	ATP	C4-C5-N7	-2.19	107.03	109.34
35	D	501	ATP	O4'-C1'-N9	2.13	111.57	108.75
35	E	401	ATP	C4-C5-N7	-2.02	107.20	109.34
37	F	501	ADP	O3B-PB-O2B	2.01	115.34	107.80

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A
37	C	501	ADP	PA-O3A-PB-O3B
37	C	501	ADP	C5'-O5'-PA-O2A
37	C	501	ADP	C5'-O5'-PA-O3A
37	F	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C3'-C4'-C5'-O5'
37	F	501	ADP	PA-O3A-PB-O1B
37	F	501	ADP	PA-O3A-PB-O2B
35	A	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	O4'-C4'-C5'-O5'
37	C	501	ADP	PA-O3A-PB-O1B
35	D	501	ATP	C3'-C4'-C5'-O5'
35	D	501	ATP	PA-O3A-PB-O2B
35	E	401	ATP	PG-O3B-PB-O2B
35	E	401	ATP	PA-O3A-PB-O2B

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	E	401	ATP	2	0

Continued on next page...

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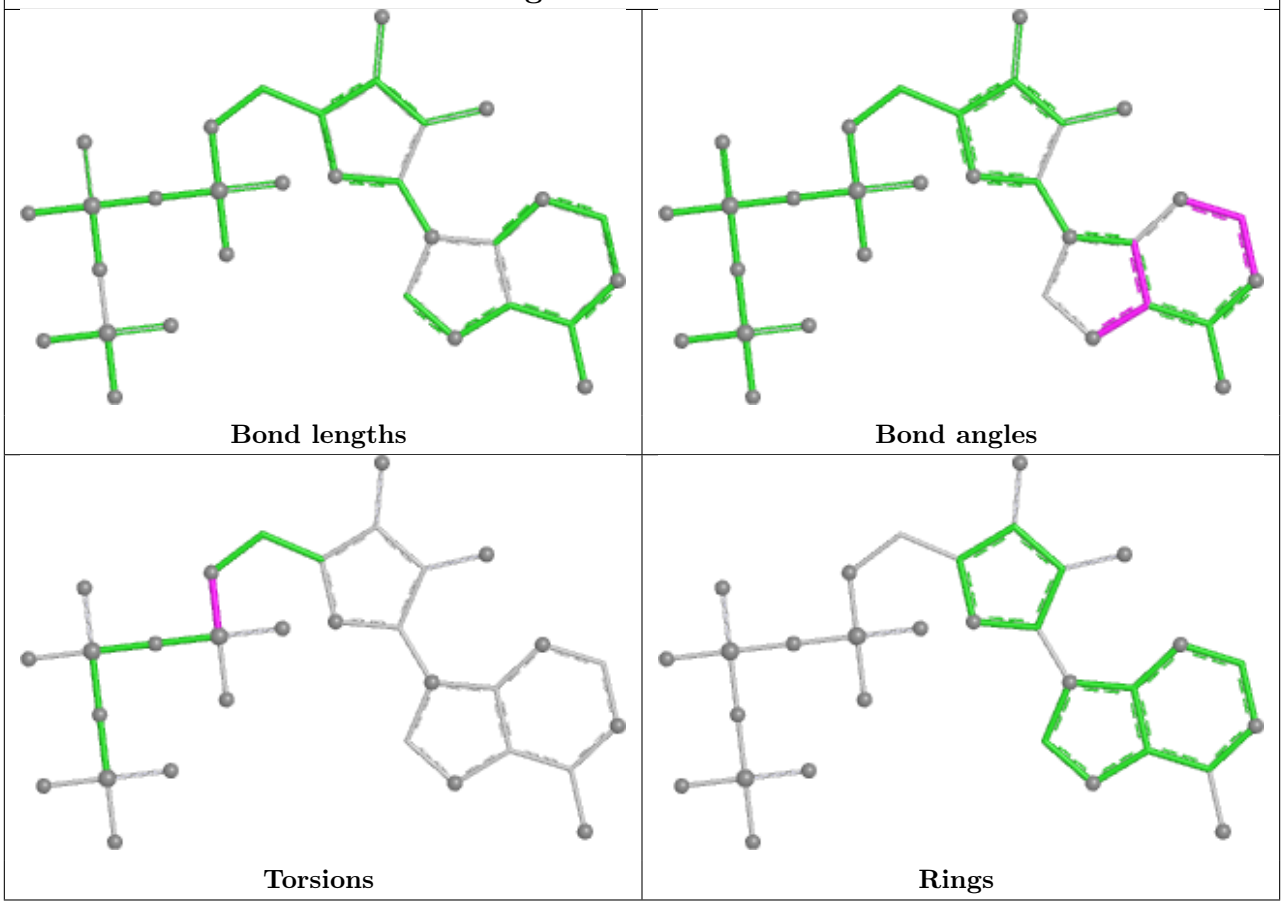
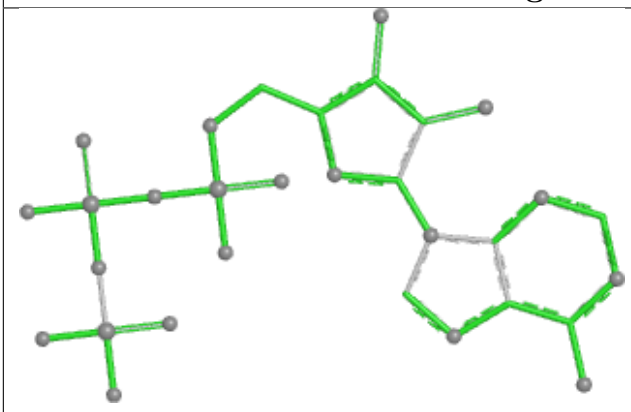
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	D	501	ATP	1	0
37	C	501	ADP	1	0
35	B	501	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

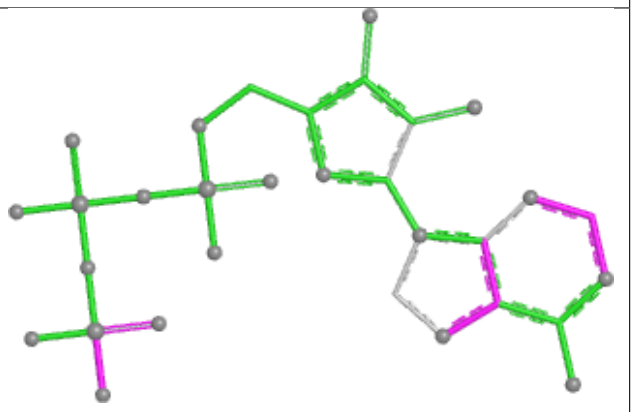
Ligand ATP A 501



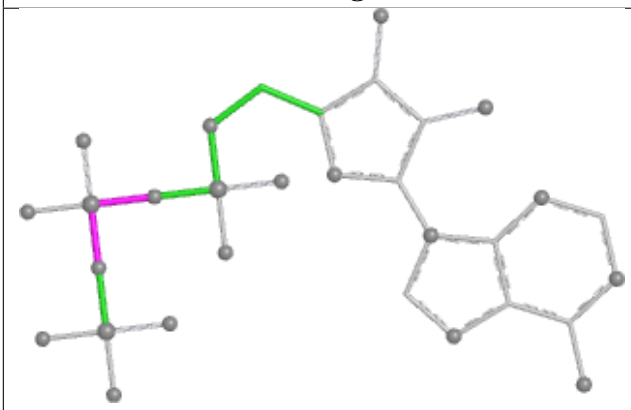
Ligand ATP E 401



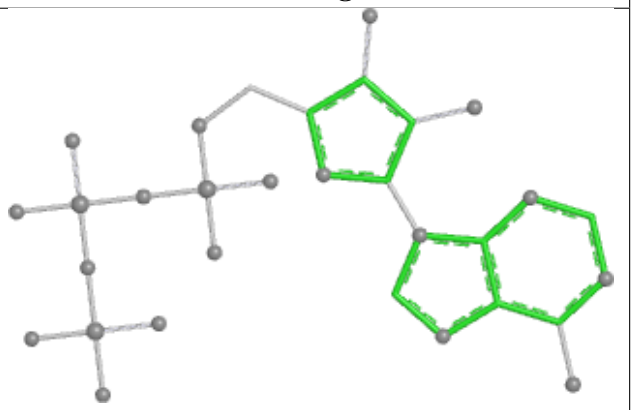
Bond lengths



Bond angles

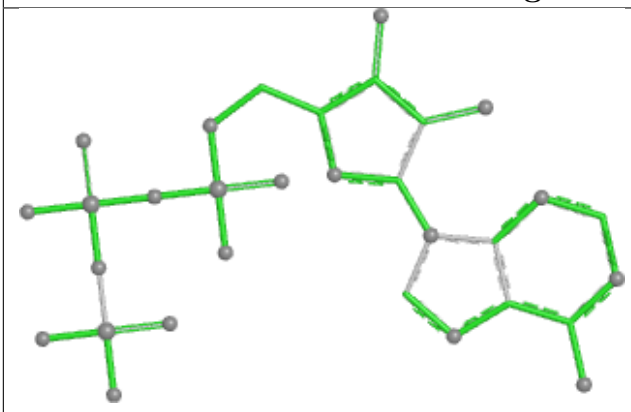


Torsions

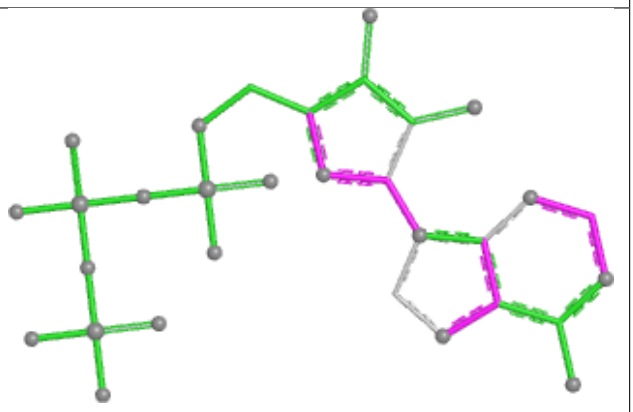


Rings

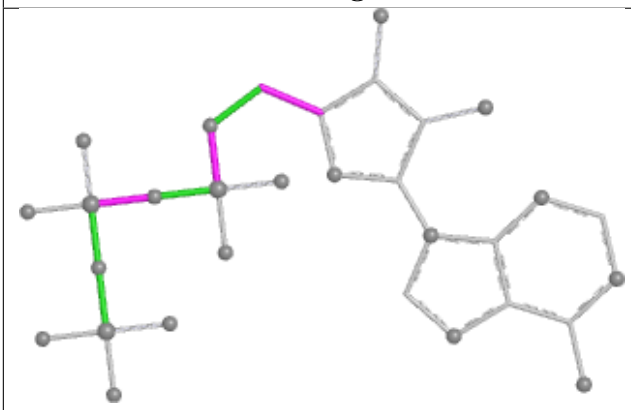
Ligand ATP D 501



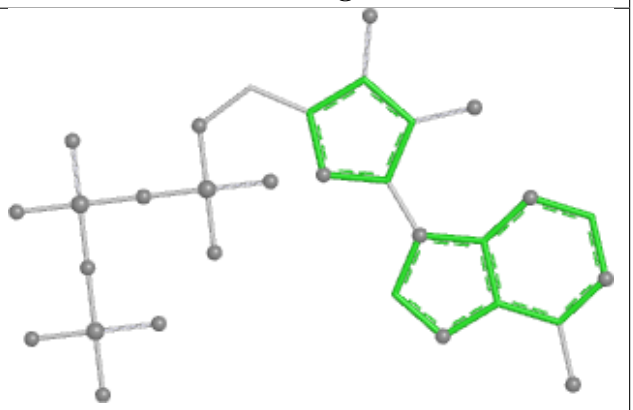
Bond lengths



Bond angles

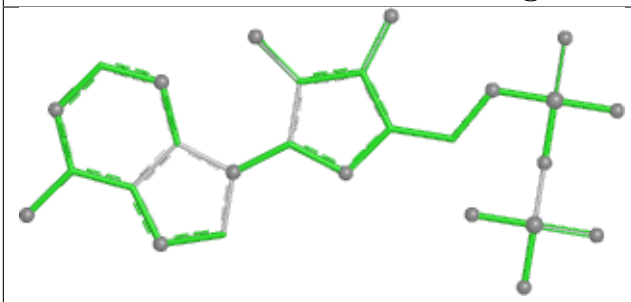


Torsions

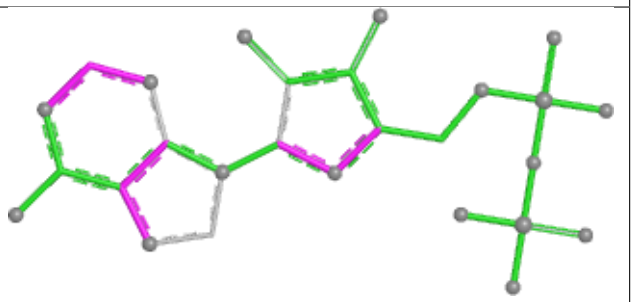


Rings

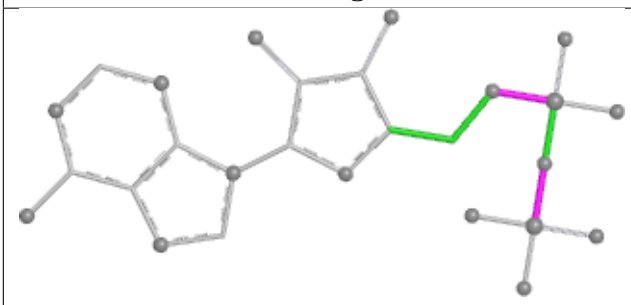
Ligand ADP C 501



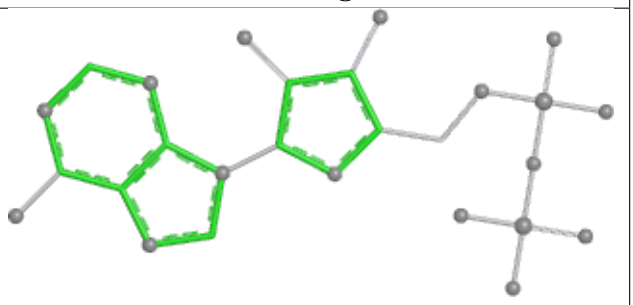
Bond lengths



Bond angles

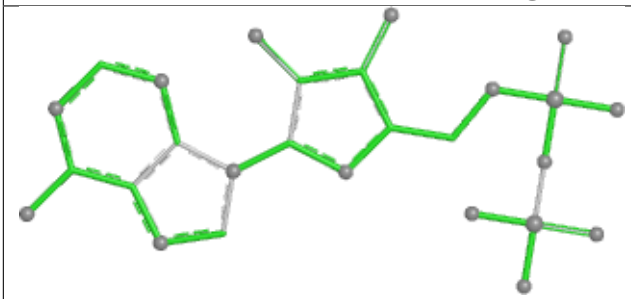


Torsions

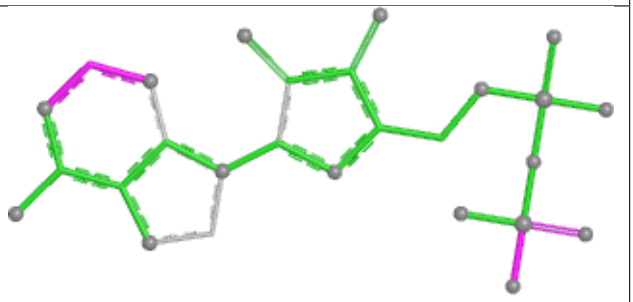


Rings

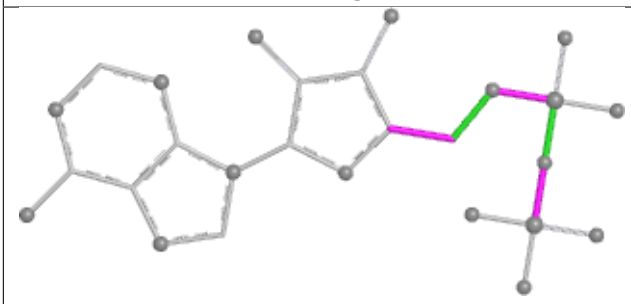
Ligand ADP F 501



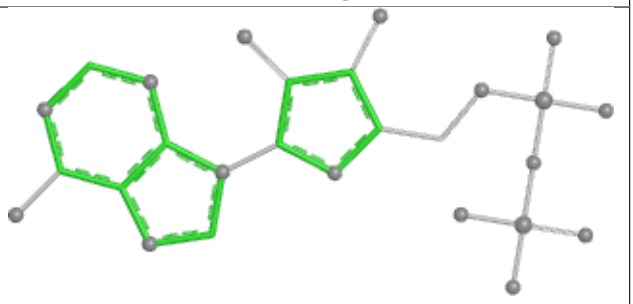
Bond lengths



Bond angles

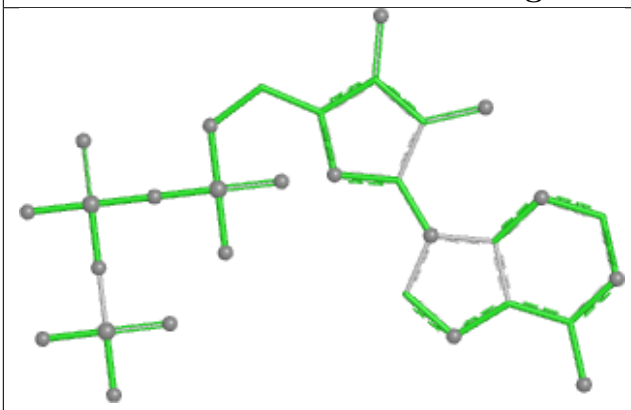


Torsions

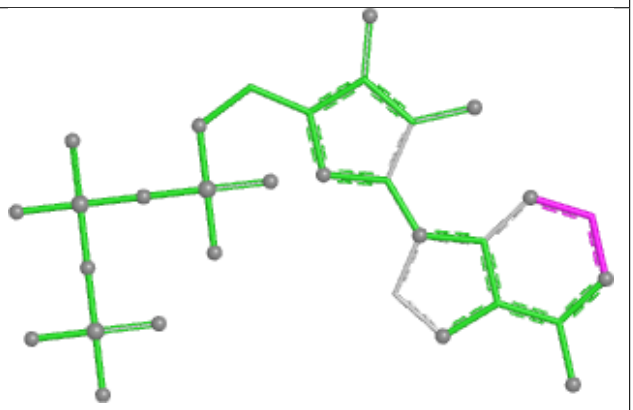


Rings

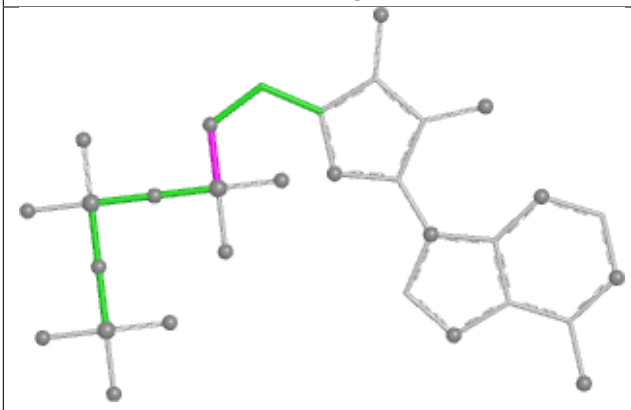
Ligand ATP B 501



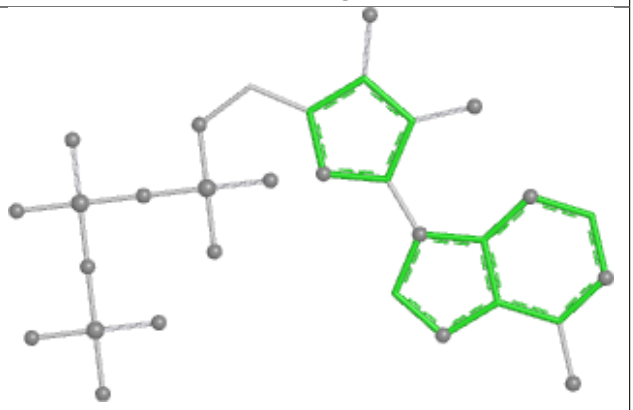
Bond lengths



Bond angles



Torsions



Rings

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.

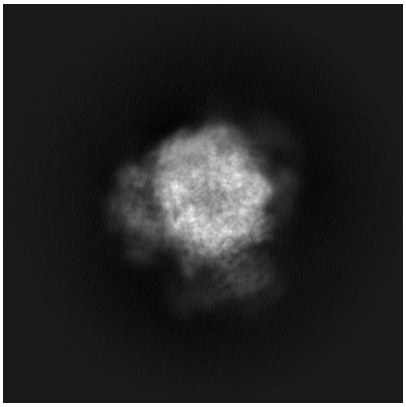
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9216. These allow visual inspection of the internal detail of the map and identification of artifacts.

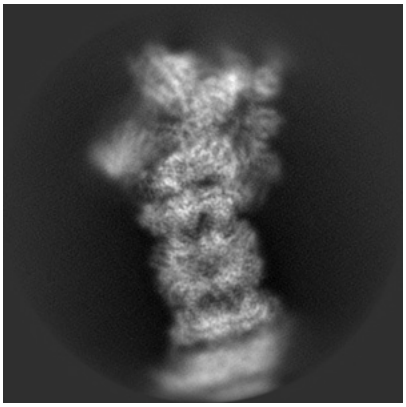
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

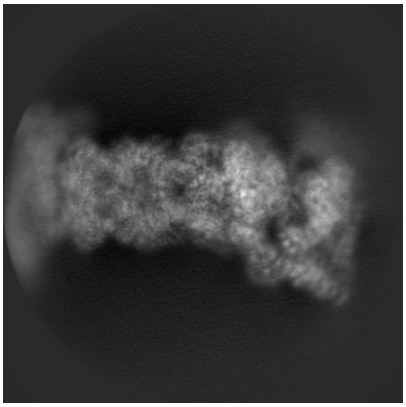
6.1.1 Primary map



X



Y

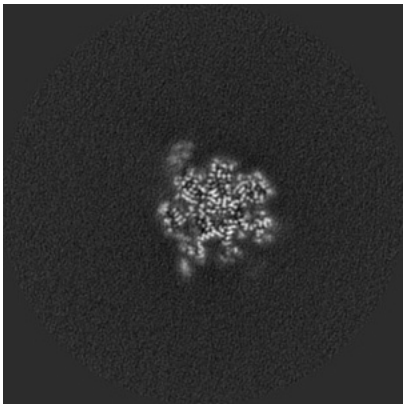


Z

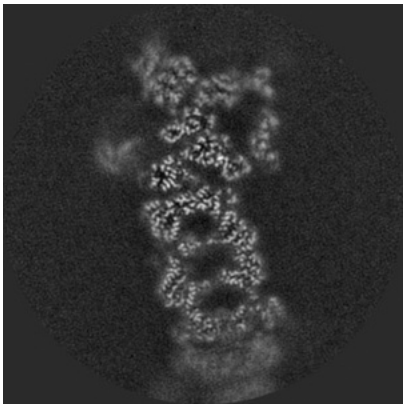
The images above show the map projected in three orthogonal directions.

6.2 Central slices

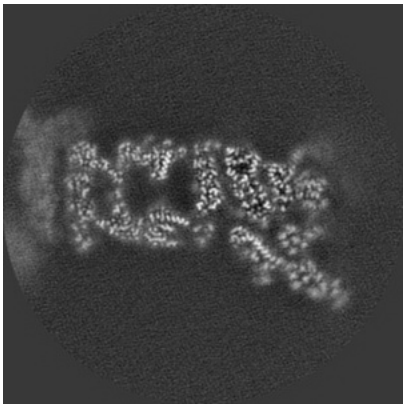
6.2.1 Primary map



X Index: 300



Y Index: 300

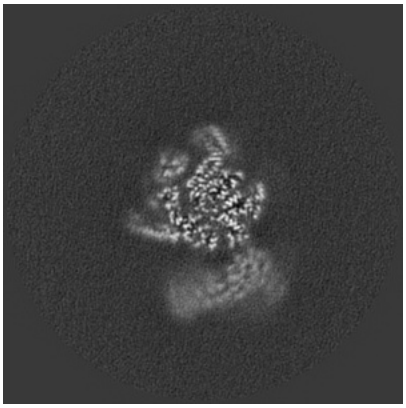


Z Index: 300

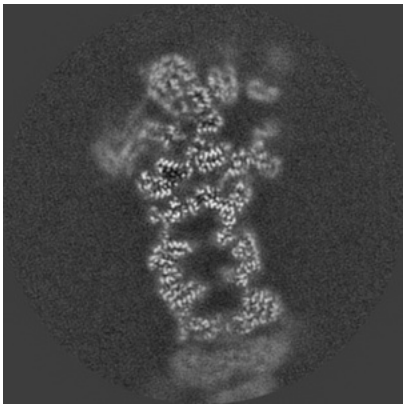
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

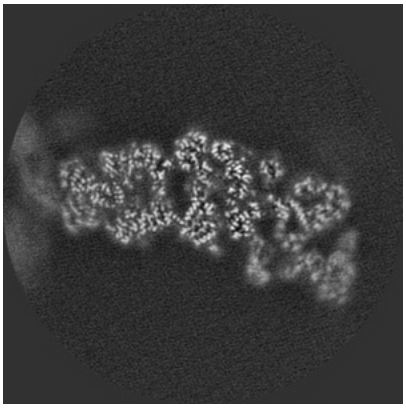
6.3.1 Primary map



X Index: 364



Y Index: 315

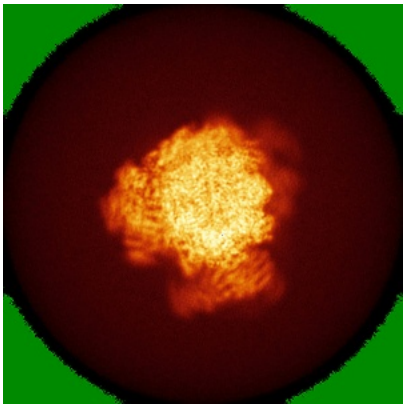


Z Index: 275

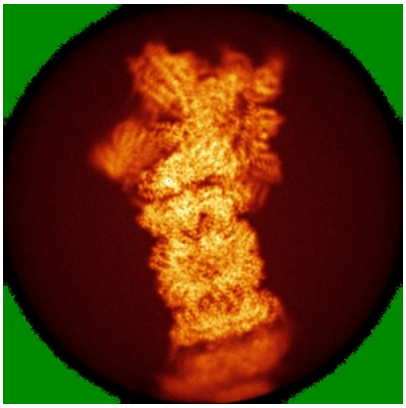
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

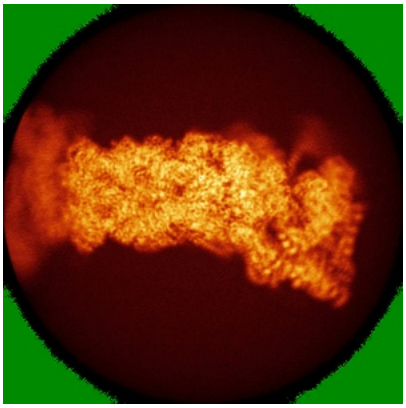
6.4.1 Primary map



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 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

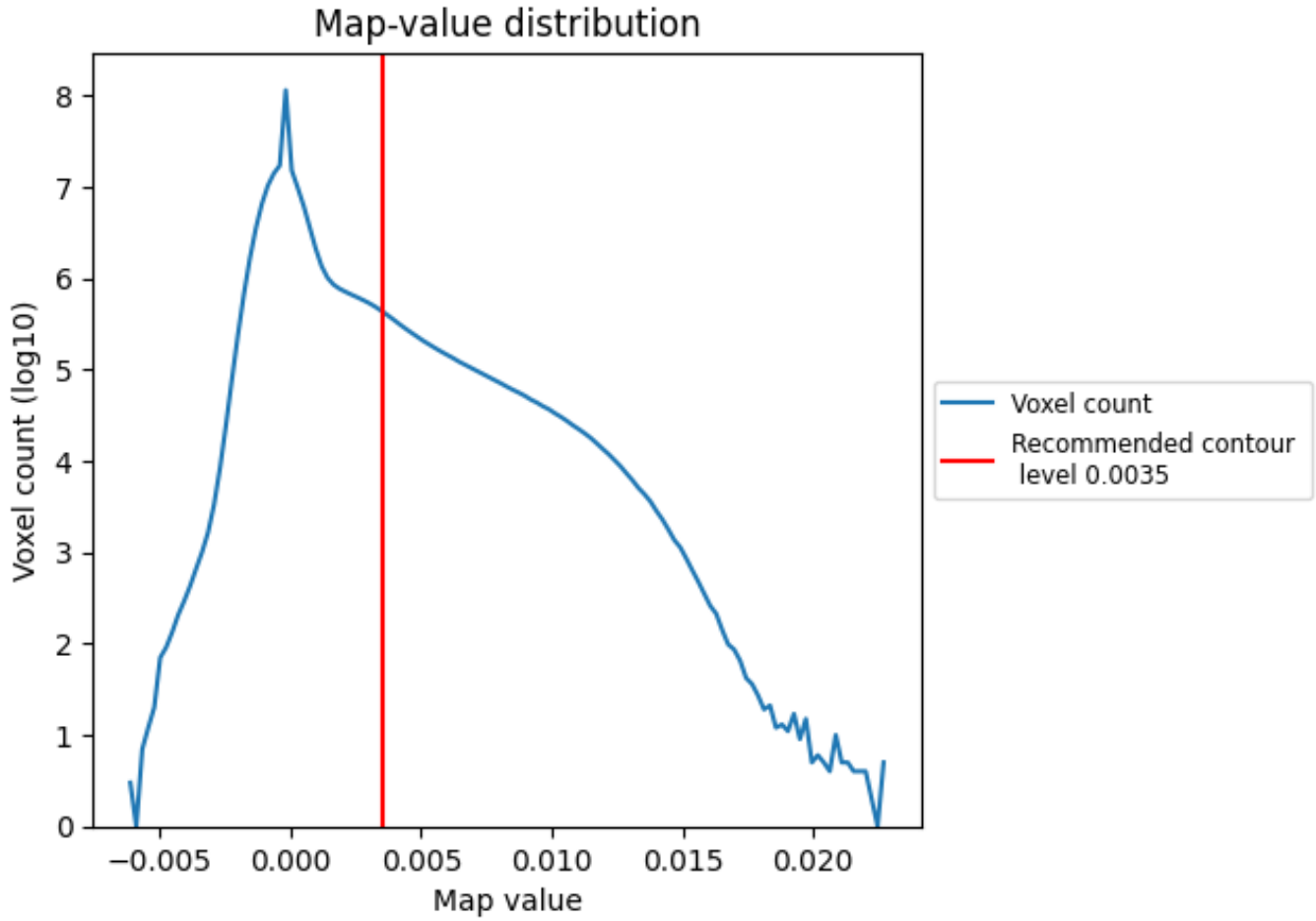
6.6 Mask visualisation (i)

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

7 Map analysis

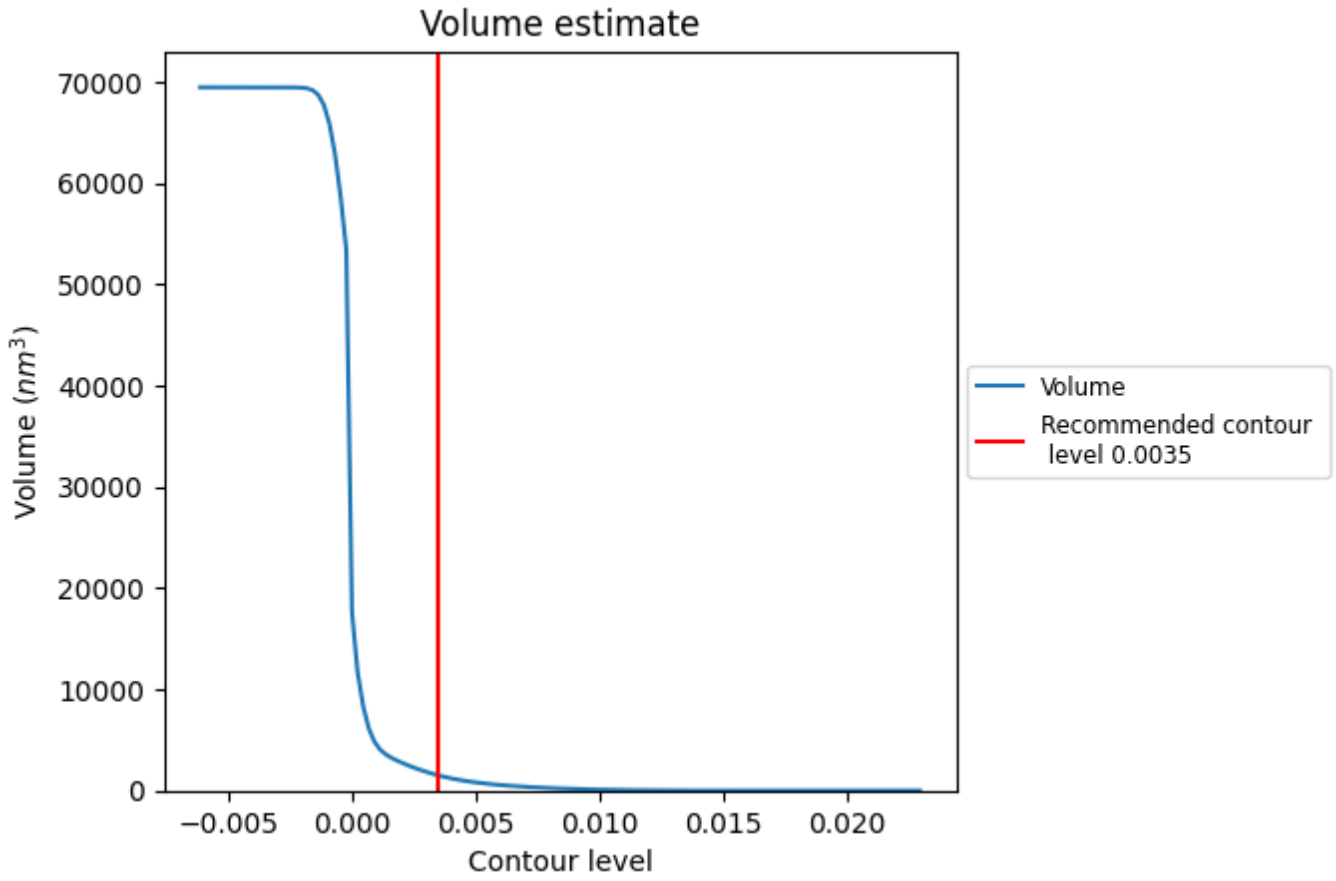
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

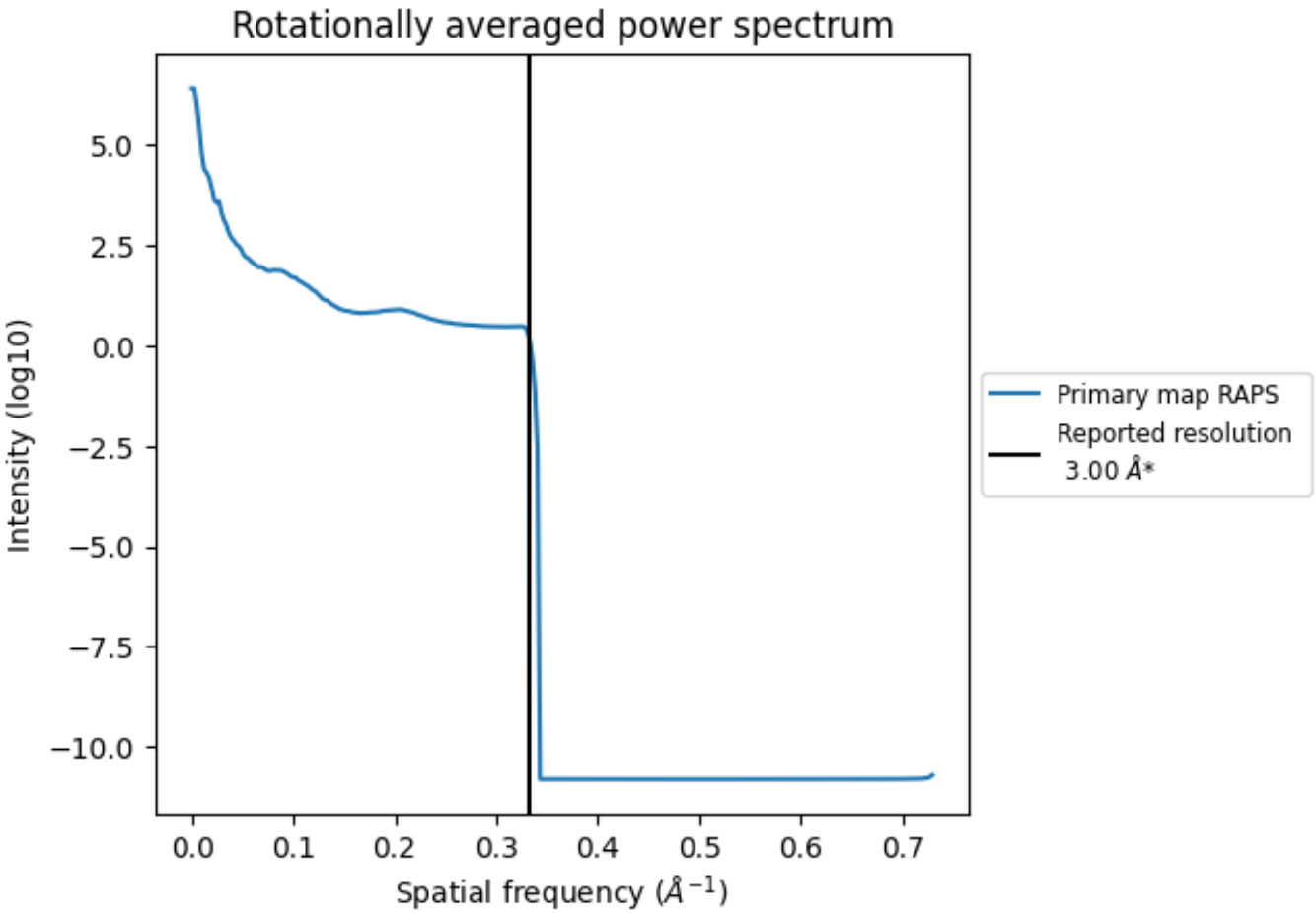
7.2 Volume estimate



The volume at the recommended contour level is 1494 nm^3; this corresponds to an approximate mass of 1350 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 (i)



*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

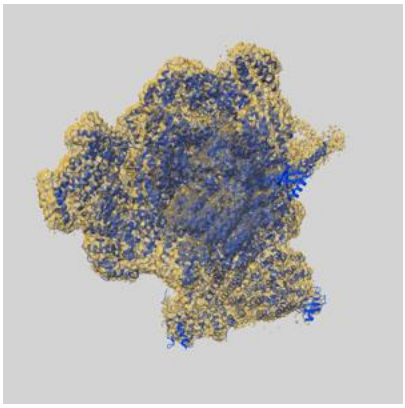
8 Fourier-Shell correlation (i)

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

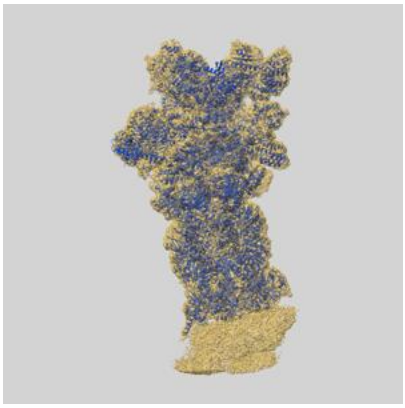
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9216 and PDB model 6MSB. Per-residue inclusion information can be found in section 3 on page 13.

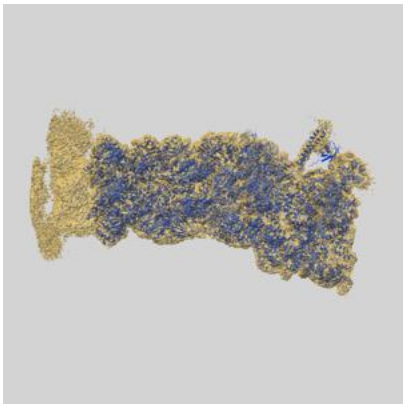
9.1 Map-model overlay



X



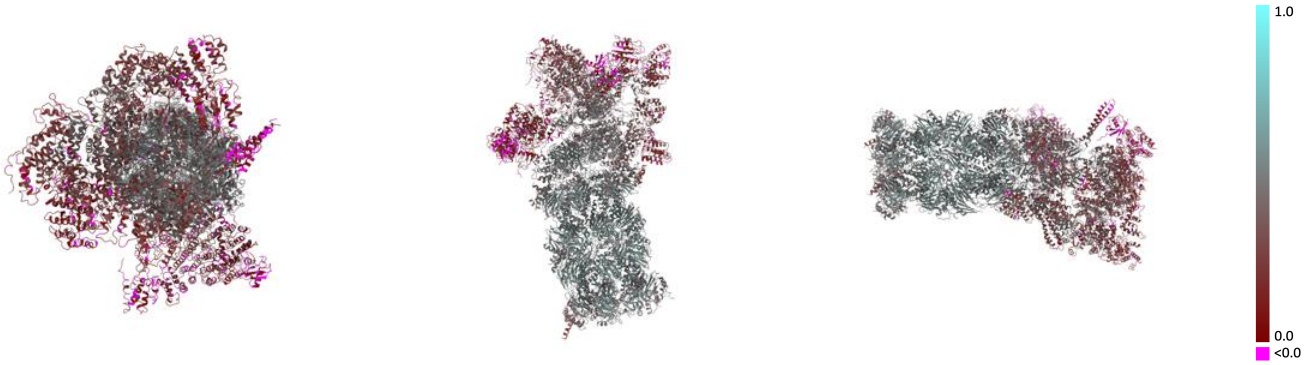
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0035 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.

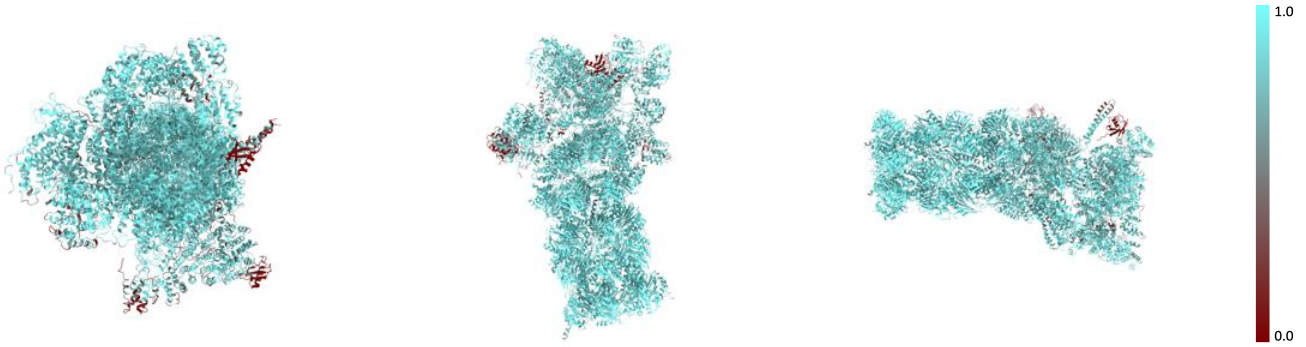
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

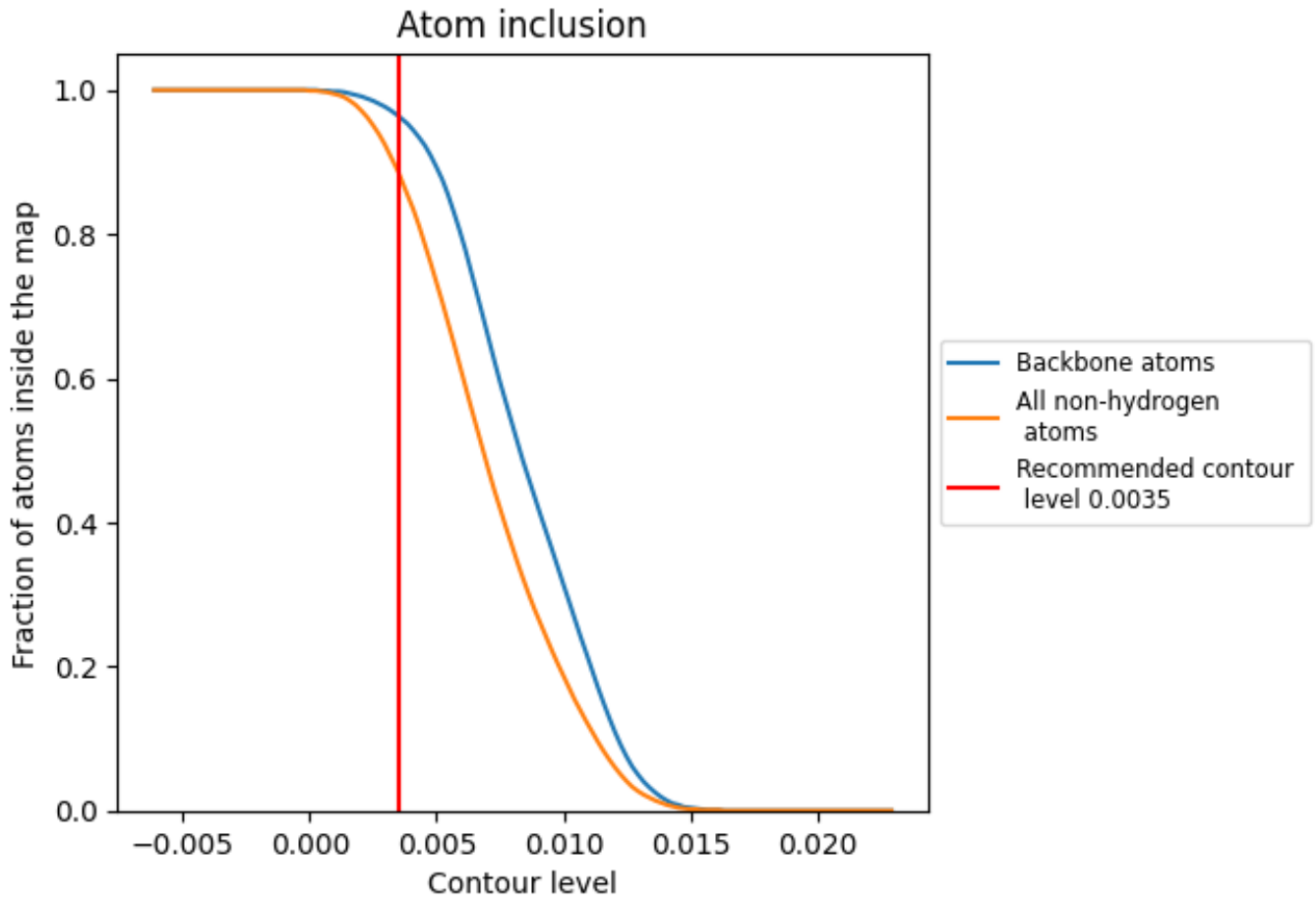
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0035).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8860	0.3890
A	0.9040	0.4330
B	0.9080	0.4270
C	0.9130	0.4390
D	0.9020	0.4280
E	0.9030	0.4250
F	0.8980	0.4340
G	0.9460	0.4920
H	0.9550	0.4990
I	0.9460	0.4700
J	0.9560	0.4710
K	0.9470	0.4850
L	0.9530	0.4930
M	0.9410	0.4780
N	0.9640	0.5170
O	0.9780	0.5130
P	0.9670	0.5180
Q	0.9670	0.5080
R	0.9710	0.5140
S	0.9600	0.5110
T	0.9620	0.5220
U	0.8620	0.2700
V	0.7860	0.2310
W	0.7960	0.2470
X	0.8470	0.3230
Y	0.8940	0.3210
Z	0.8510	0.3090
a	0.8510	0.2480
b	0.8010	0.1550
c	0.8690	0.3650
d	0.8130	0.2180
e	0.7540	0.1620
f	0.7190	0.1610
g	0.9520	0.4910
h	0.9460	0.4970

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Chain	Atom inclusion	Q-score
i	0.9080	0.4430
j	0.9310	0.4280
k	0.9420	0.4730
l	0.9560	0.4860
m	0.9340	0.4740
n	0.9700	0.5250
o	0.9730	0.5190
p	0.9710	0.5230
q	0.9720	0.5160
r	0.9810	0.5290
s	0.9680	0.5150
t	0.9690	0.5250
u	0.0200	-0.0160
w	0.1080	0.0120