



Full wwPDB X-ray Structure Validation Report i

Jul 4, 2024 – 12:28 PM JST

PDB ID : 8XK5
Title : SNB1G11 Fab bound to SFTSV glycoprotein Gn
Authors : Deng, Z.
Deposited on : 2023-12-22
Resolution : 3.05 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>
with specific help available everywhere you see the i 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

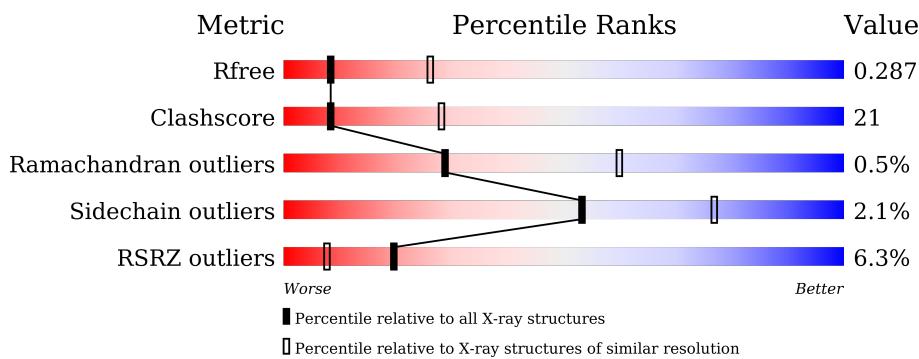
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



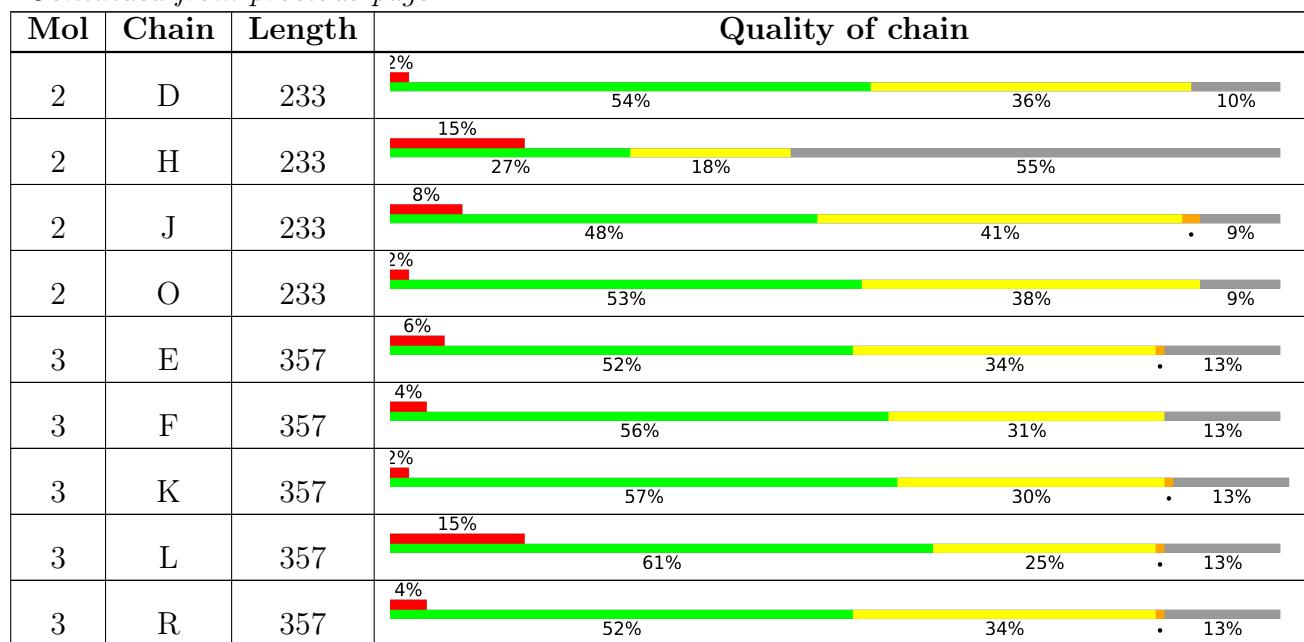
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27019 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 mAb SNB1G11 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1686	1070	276	332	8			
1	C	220	Total	C	N	O	S	0	0	0
			1695	1076	278	333	8			
1	I	220	Total	C	N	O	S	0	0	0
			1695	1076	278	333	8			
1	N	219	Total	C	N	O	S	0	0	0
			1689	1073	277	331	8			
1	G	124	Total	C	N	O	S	0	0	0
			997	632	164	195	6			

- Molecule 2 is a protein called mAb SNB1G11 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1620	1016	269	330	5			
2	D	210	Total	C	N	O	S	0	0	0
			1620	1016	269	330	5			
2	J	213	Total	C	N	O	S	0	0	0
			1639	1026	272	335	6			
2	O	212	Total	C	N	O	S	0	0	0
			1633	1023	271	334	5			
2	H	105	Total	C	N	O	S	0	0	0
			804	507	130	164	3			

- Molecule 3 is a protein called Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	309	Total	C	N	O	S	0	0	0
			2384	1495	412	451	26			
3	F	309	Total	C	N	O	S	0	0	0
			2384	1495	412	451	26			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	311	Total	C	N	O	S	0	0	0
			2402	1506	415	455	26			
3	R	309	Total	C	N	O	S	0	0	0
			2387	1498	413	450	26			
3	L	309	Total	C	N	O	S	0	0	0
			2384	1495	412	451	26			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	13	LEU	PHE	conflict	UNP R4V2Q5
E	18	GLY	SER	conflict	UNP R4V2Q5
E	21	THR	SER	conflict	UNP R4V2Q5
E	161	ARG	GLY	conflict	UNP R4V2Q5
E	340	SER	ASN	conflict	UNP R4V2Q5
E	341	GLY	-	expression tag	UNP R4V2Q5
E	342	SER	-	expression tag	UNP R4V2Q5
E	343	THR	-	expression tag	UNP R4V2Q5
E	344	LEU	-	expression tag	UNP R4V2Q5
E	345	GLU	-	expression tag	UNP R4V2Q5
E	346	VAL	-	expression tag	UNP R4V2Q5
E	347	LEU	-	expression tag	UNP R4V2Q5
E	348	PHE	-	expression tag	UNP R4V2Q5
E	349	GLN	-	expression tag	UNP R4V2Q5
E	350	GLY	-	expression tag	UNP R4V2Q5
E	351	PRO	-	expression tag	UNP R4V2Q5
E	352	HIS	-	expression tag	UNP R4V2Q5
E	353	HIS	-	expression tag	UNP R4V2Q5
E	354	HIS	-	expression tag	UNP R4V2Q5
E	355	HIS	-	expression tag	UNP R4V2Q5
E	356	HIS	-	expression tag	UNP R4V2Q5
E	357	HIS	-	expression tag	UNP R4V2Q5
F	13	LEU	PHE	conflict	UNP R4V2Q5
F	18	GLY	SER	conflict	UNP R4V2Q5
F	21	THR	SER	conflict	UNP R4V2Q5
F	161	ARG	GLY	conflict	UNP R4V2Q5
F	340	SER	ASN	conflict	UNP R4V2Q5
F	341	GLY	-	expression tag	UNP R4V2Q5
F	342	SER	-	expression tag	UNP R4V2Q5
F	343	THR	-	expression tag	UNP R4V2Q5
F	344	LEU	-	expression tag	UNP R4V2Q5
F	345	GLU	-	expression tag	UNP R4V2Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	346	VAL	-	expression tag	UNP R4V2Q5
F	347	LEU	-	expression tag	UNP R4V2Q5
F	348	PHE	-	expression tag	UNP R4V2Q5
F	349	GLN	-	expression tag	UNP R4V2Q5
F	350	GLY	-	expression tag	UNP R4V2Q5
F	351	PRO	-	expression tag	UNP R4V2Q5
F	352	HIS	-	expression tag	UNP R4V2Q5
F	353	HIS	-	expression tag	UNP R4V2Q5
F	354	HIS	-	expression tag	UNP R4V2Q5
F	355	HIS	-	expression tag	UNP R4V2Q5
F	356	HIS	-	expression tag	UNP R4V2Q5
F	357	HIS	-	expression tag	UNP R4V2Q5
K	13	LEU	PHE	conflict	UNP R4V2Q5
K	18	GLY	SER	conflict	UNP R4V2Q5
K	21	THR	SER	conflict	UNP R4V2Q5
K	161	ARG	GLY	conflict	UNP R4V2Q5
K	340	SER	ASN	conflict	UNP R4V2Q5
K	341	GLY	-	expression tag	UNP R4V2Q5
K	342	SER	-	expression tag	UNP R4V2Q5
K	343	THR	-	expression tag	UNP R4V2Q5
K	344	LEU	-	expression tag	UNP R4V2Q5
K	345	GLU	-	expression tag	UNP R4V2Q5
K	346	VAL	-	expression tag	UNP R4V2Q5
K	347	LEU	-	expression tag	UNP R4V2Q5
K	348	PHE	-	expression tag	UNP R4V2Q5
K	349	GLN	-	expression tag	UNP R4V2Q5
K	350	GLY	-	expression tag	UNP R4V2Q5
K	351	PRO	-	expression tag	UNP R4V2Q5
K	352	HIS	-	expression tag	UNP R4V2Q5
K	353	HIS	-	expression tag	UNP R4V2Q5
K	354	HIS	-	expression tag	UNP R4V2Q5
K	355	HIS	-	expression tag	UNP R4V2Q5
K	356	HIS	-	expression tag	UNP R4V2Q5
K	357	HIS	-	expression tag	UNP R4V2Q5
R	13	LEU	PHE	conflict	UNP R4V2Q5
R	18	GLY	SER	conflict	UNP R4V2Q5
R	21	THR	SER	conflict	UNP R4V2Q5
R	161	ARG	GLY	conflict	UNP R4V2Q5
R	340	SER	ASN	conflict	UNP R4V2Q5
R	341	GLY	-	expression tag	UNP R4V2Q5
R	342	SER	-	expression tag	UNP R4V2Q5
R	343	THR	-	expression tag	UNP R4V2Q5

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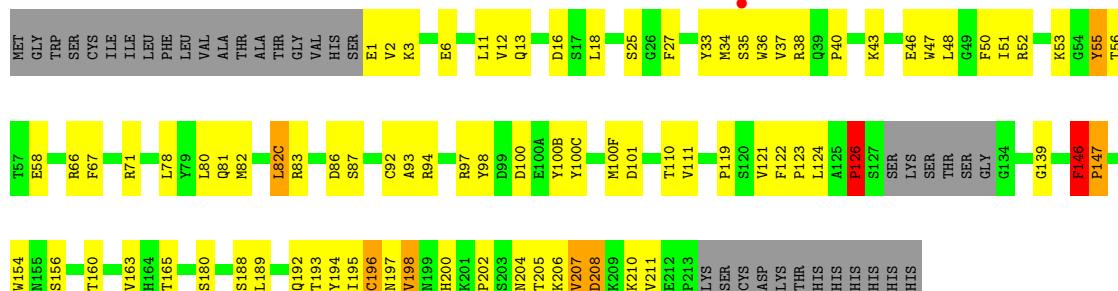
Chain	Residue	Modelled	Actual	Comment	Reference
R	344	LEU	-	expression tag	UNP R4V2Q5
R	345	GLU	-	expression tag	UNP R4V2Q5
R	346	VAL	-	expression tag	UNP R4V2Q5
R	347	LEU	-	expression tag	UNP R4V2Q5
R	348	PHE	-	expression tag	UNP R4V2Q5
R	349	GLN	-	expression tag	UNP R4V2Q5
R	350	GLY	-	expression tag	UNP R4V2Q5
R	351	PRO	-	expression tag	UNP R4V2Q5
R	352	HIS	-	expression tag	UNP R4V2Q5
R	353	HIS	-	expression tag	UNP R4V2Q5
R	354	HIS	-	expression tag	UNP R4V2Q5
R	355	HIS	-	expression tag	UNP R4V2Q5
R	356	HIS	-	expression tag	UNP R4V2Q5
R	357	HIS	-	expression tag	UNP R4V2Q5
L	13	LEU	PHE	conflict	UNP R4V2Q5
L	18	GLY	SER	conflict	UNP R4V2Q5
L	21	THR	SER	conflict	UNP R4V2Q5
L	161	ARG	GLY	conflict	UNP R4V2Q5
L	340	SER	ASN	conflict	UNP R4V2Q5
L	341	GLY	-	expression tag	UNP R4V2Q5
L	342	SER	-	expression tag	UNP R4V2Q5
L	343	THR	-	expression tag	UNP R4V2Q5
L	344	LEU	-	expression tag	UNP R4V2Q5
L	345	GLU	-	expression tag	UNP R4V2Q5
L	346	VAL	-	expression tag	UNP R4V2Q5
L	347	LEU	-	expression tag	UNP R4V2Q5
L	348	PHE	-	expression tag	UNP R4V2Q5
L	349	GLN	-	expression tag	UNP R4V2Q5
L	350	GLY	-	expression tag	UNP R4V2Q5
L	351	PRO	-	expression tag	UNP R4V2Q5
L	352	HIS	-	expression tag	UNP R4V2Q5
L	353	HIS	-	expression tag	UNP R4V2Q5
L	354	HIS	-	expression tag	UNP R4V2Q5
L	355	HIS	-	expression tag	UNP R4V2Q5
L	356	HIS	-	expression tag	UNP R4V2Q5
L	357	HIS	-	expression tag	UNP R4V2Q5

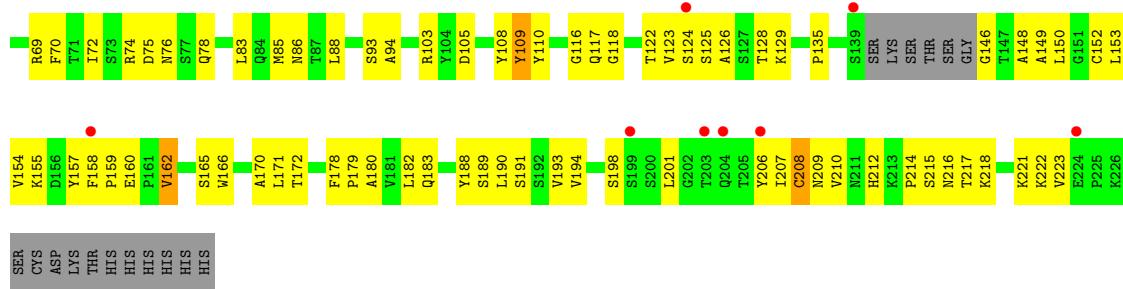
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

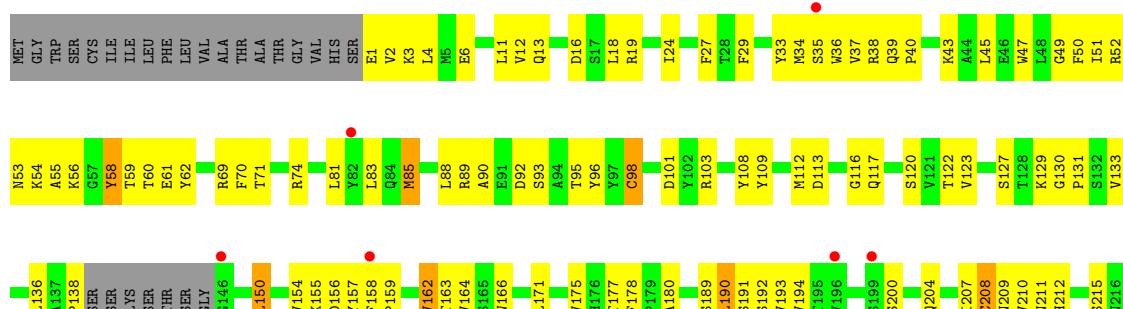
- Molecule 1: mAb SNB1G11 Fab heavy chain

Chain A:  52% 30% 14%

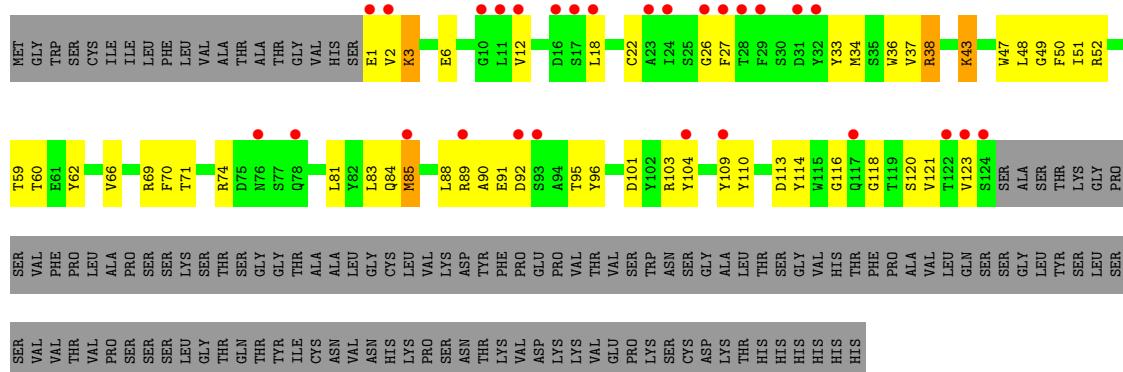
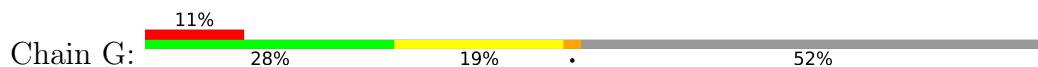




- Molecule 1: mAb SNB1G11 Fab heavy chain

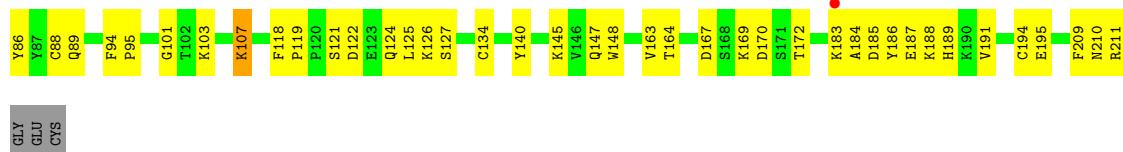


- Molecule 1: mAb SNB1G11 Fab heavy chain



- Molecule 2: mAb SNB1G11 Fab light chain





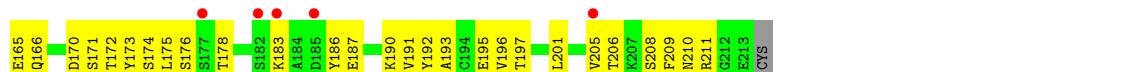
- Molecule 2: mAb SNB1G11 Fab light chain



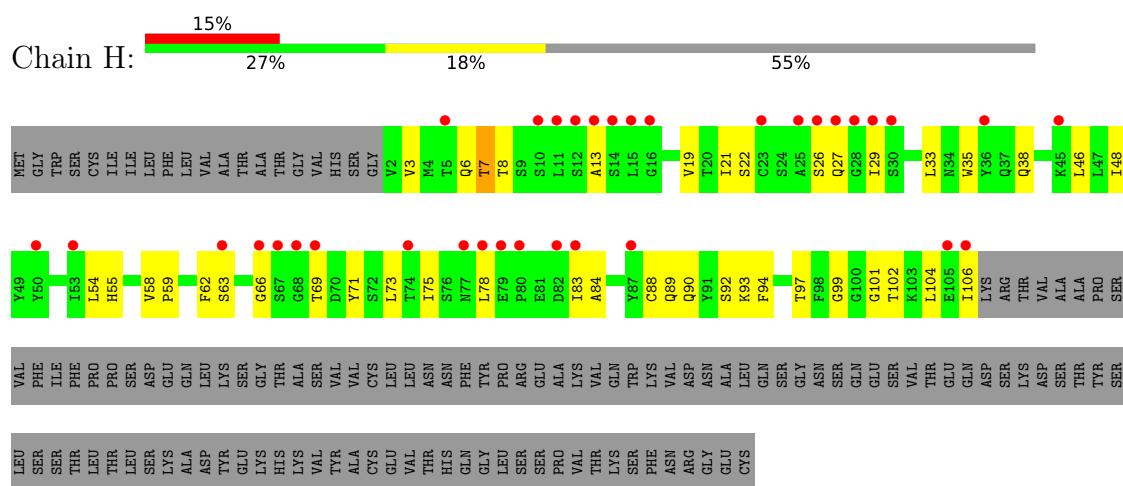
- Molecule 2: mAb SNB1G11 Fab light chain



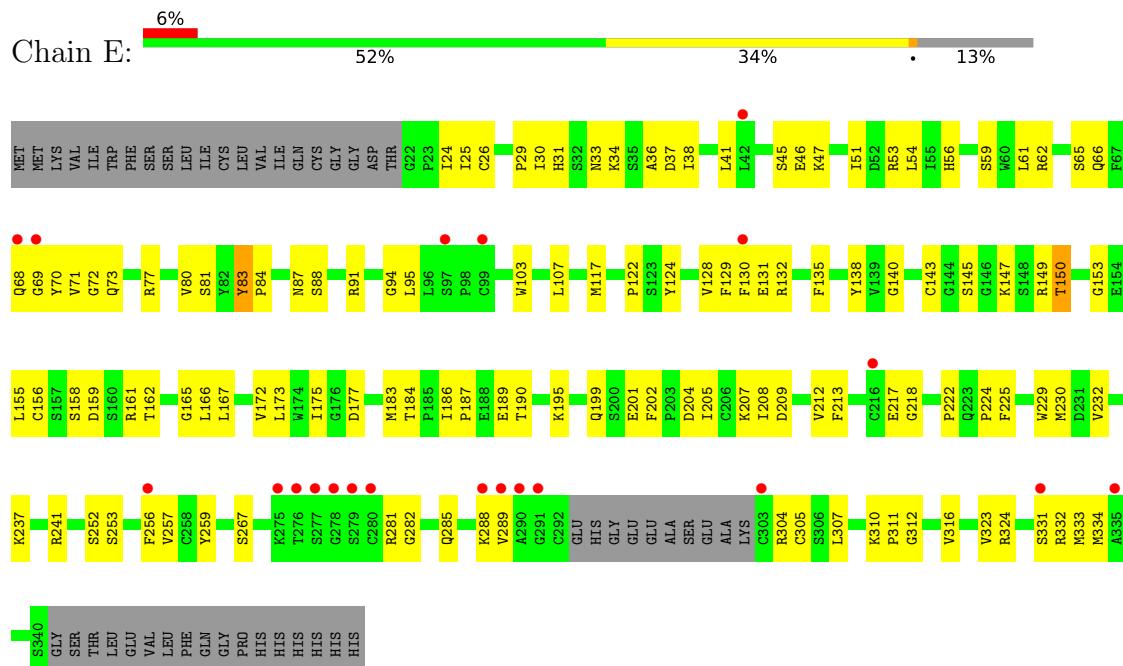
- Molecule 2: mAb SNB1G11 Fab light chain



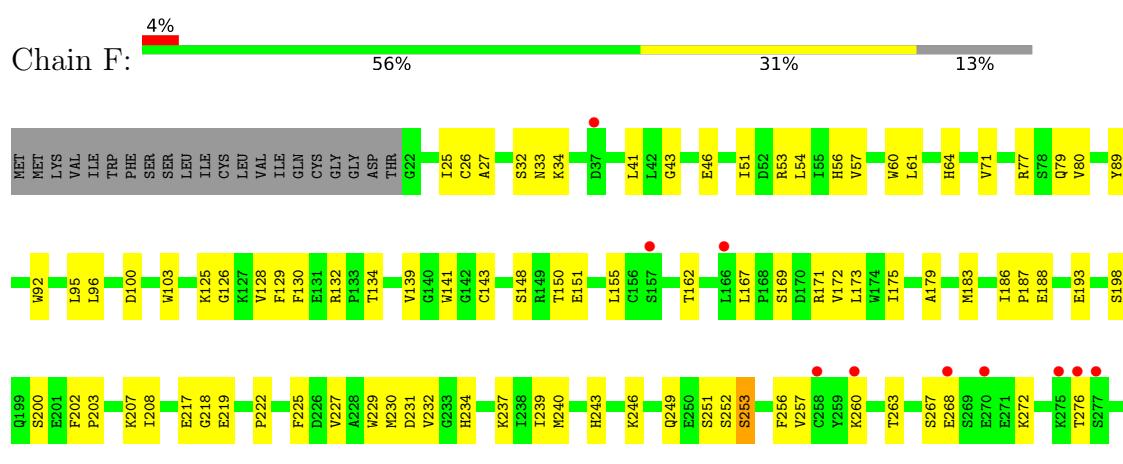
- Molecule 2: mAb SNB1G11 Fab light chain

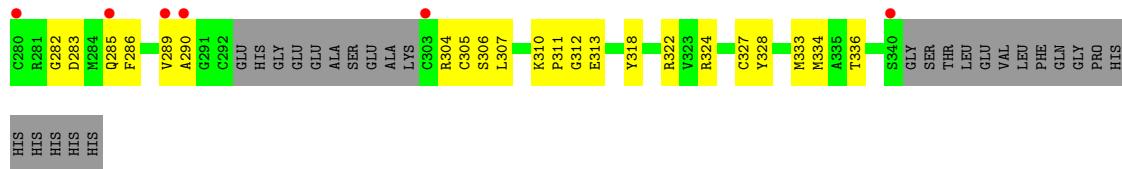


- Molecule 3: Envelopment polyprotein

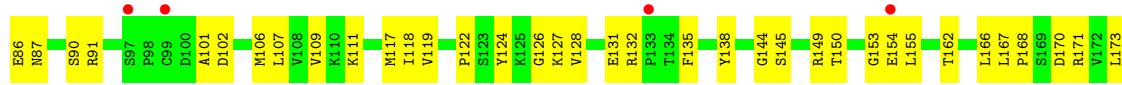


- Molecule 3: Envelopment polyprotein

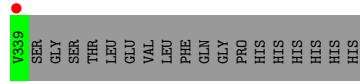




- Molecule 3: Envelopment polyprotein

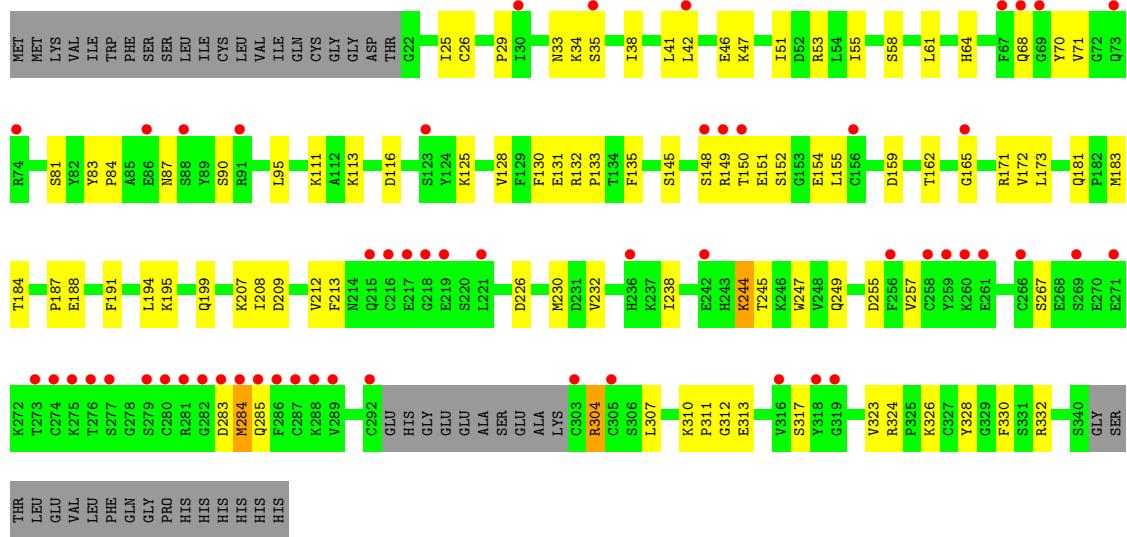


- Molecule 3: Envelopment polyprotein



- Molecule 3: Envelopment polyprotein





4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.67 Å 180.96 Å 263.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.05 29.97 – 3.05	Depositor EDS
% Data completeness (in resolution range)	76.4 (29.97-3.05) 99.9 (29.97-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.67 (at 3.06 Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R , R_{free}	0.215 , 0.281 0.236 , 0.287	Depositor DCC
R_{free} test set	5281 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	91.7	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.8	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27019	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	A	0.78	3/1729 (0.2%)	0.93	3/2352 (0.1%)
1	C	0.82	0/1738	0.95	2/2363 (0.1%)
1	G	0.39	0/1022	0.63	0/1382
1	I	0.68	0/1738	0.89	3/2363 (0.1%)
1	N	0.63	0/1732	0.89	5/2355 (0.2%)
2	B	0.72	0/1654	0.89	1/2246 (0.0%)
2	D	0.72	1/1654 (0.1%)	0.88	1/2246 (0.0%)
2	H	0.35	0/821	0.62	0/1115
2	J	0.56	0/1673	0.79	1/2271 (0.0%)
2	O	0.61	0/1667	0.80	0/2263
3	E	0.56	0/2444	0.76	0/3295
3	F	0.57	0/2444	0.75	0/3295
3	K	0.59	0/2462	0.77	0/3318
3	L	0.44	0/2444	0.71	1/3295 (0.0%)
3	R	0.56	0/2447	0.78	0/3298
All	All	0.62	4/27669 (0.0%)	0.81	17/37457 (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	A	0	2
1	C	0	1
2	J	0	1
3	R	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	VAL	CB-CG1	-5.78	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	TYR	CA-CB	-5.52	1.41	1.53
1	A	198	VAL	CB-CG1	-5.47	1.41	1.52
2	D	111	ALA	C-N	-5.02	1.22	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	PRO	CA-N-CD	-7.38	101.17	111.50
1	A	146	PHE	C-N-CD	-7.13	104.91	120.60
2	D	111	ALA	C-N-CA	-6.47	105.52	121.70
1	N	150	LEU	CA-CB-CG	6.43	130.09	115.30
1	I	109	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	I	109	TYR	CA-CB-CG	5.96	124.72	113.40
1	A	198	VAL	CG1-CB-CG2	-5.95	101.39	110.90
1	N	162	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	I	208	CYS	CA-CB-SG	5.42	123.75	114.00
1	N	56	LYS	C-N-CA	-5.41	110.94	122.30
2	B	54	LEU	CB-CG-CD2	-5.39	101.84	111.00
2	J	41	ASP	N-CA-CB	-5.36	100.96	110.60
1	C	190	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	N	208	CYS	CA-CB-SG	5.19	123.34	114.00
3	L	244	LYS	CA-CB-CG	5.18	124.80	113.40
1	A	82(C)	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	N	190	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	PRO	Peptide
1	A	146	PHE	Peptide
1	C	158	PHE	Peptide
2	J	192	TYR	Peptide
3	R	151	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	A	1686	0	1628	69	0
1	C	1695	0	1641	74	0
1	G	997	0	941	45	0
1	I	1695	0	1641	108	0
1	N	1689	0	1636	101	0
2	B	1620	0	1577	49	0
2	D	1620	0	1577	65	0
2	H	804	0	779	28	0
2	J	1639	0	1593	100	0
2	O	1633	0	1586	82	0
3	E	2384	0	2295	113	0
3	F	2384	0	2295	83	0
3	K	2402	0	2314	80	0
3	L	2384	0	2295	55	0
3	R	2387	0	2303	103	0
All	All	27019	0	26101	1112	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 21.

All (1112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:LYS:HG2	1:N:13:GLN:NE2	1.45	1.28
3:E:217:GLU:HG2	3:E:218:GLY:H	1.20	1.06
3:E:201:GLU:O	3:E:241:ARG:NH2	1.92	1.00
1:A:52:ARG:NH2	1:A:58:GLU:OE2	1.95	0.98
1:I:14:PRO:HD2	1:I:125:SER:HB2	1.47	0.95
3:E:31:HIS:H	3:E:73:GLN:HE22	1.15	0.94
1:I:180:ALA:HB2	1:I:190:LEU:HB3	1.49	0.94
2:B:185:ASP:HA	2:B:188:LYS:HD2	1.51	0.93
2:O:41:ASP:HB2	2:O:43:THR:HG22	1.51	0.93
1:N:164:VAL:HG22	1:N:210:VAL:HG22	1.51	0.92
1:I:218:LYS:CG	1:N:13:GLN:NE2	2.33	0.92
2:O:108:ARG:HH12	2:O:111:ALA:HB2	1.33	0.91
1:N:52:ARG:HG3	1:N:59:THR:HB	1.52	0.91
1:A:87:SER:HB3	1:A:111:VAL:H	1.34	0.91
1:I:135:PRO:HB3	1:I:223:VAL:HG22	1.51	0.91
1:A:121:VAL:HG11	1:A:198:VAL:HG11	1.52	0.90
2:J:187:GLU:HA	2:J:211:ARG:NH1	1.86	0.89
1:G:89:ARG:HE	1:G:90:ALA:H	1.21	0.89
1:I:218:LYS:HG2	1:N:13:GLN:HE22	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:ILE:HD13	1:I:74:ARG:HG2	1.57	0.87
2:J:195:GLU:HB3	2:J:206:THR:HB	1.54	0.86
1:A:47:TRP:HZ2	1:A:50:PHE:HD2	1.21	0.86
2:J:197:THR:HG22	2:J:198:HIS:H	1.38	0.86
2:B:36:TYR:HE2	2:B:89:GLN:HG2	1.40	0.84
1:I:93:SER:HB2	1:I:122:THR:HA	1.59	0.84
1:G:48:LEU:HD22	1:G:66:VAL:HG11	1.58	0.84
2:O:115:VAL:HG21	2:O:196:VAL:HG11	1.59	0.84
1:C:35:SER:HB3	1:C:50:PHE:HB3	1.60	0.83
3:F:80:VAL:HG13	3:F:172:VAL:HG23	1.60	0.83
1:I:218:LYS:HG2	1:N:13:GLN:HE21	1.42	0.82
3:E:199:GLN:NE2	3:E:213:PHE:O	2.13	0.82
1:I:51:ILE:HG13	1:I:60:THR:HG22	1.62	0.82
3:R:202:PHE:HB3	3:R:205:ILE:HD12	1.59	0.82
3:L:29:PRO:HG3	3:L:53:ARG:HB3	1.61	0.82
3:R:73:GLN:HG3	3:R:166:LEU:HB3	1.61	0.81
2:J:115:VAL:HG22	2:J:136:LEU:HG	1.62	0.81
2:J:123:GLU:HA	2:J:126:LYS:HG3	1.60	0.81
2:J:148:TRP:HB3	2:J:194:CYS:HB2	1.63	0.81
3:K:25:ILE:HD11	3:K:257:VAL:HB	1.61	0.81
1:A:3:LYS:HB2	1:A:25:SER:HB2	1.64	0.80
3:F:310:LYS:HG3	3:F:312:GLY:H	1.47	0.80
1:C:40:PRO:HG2	1:C:43:LYS:HB2	1.64	0.79
2:J:139:PHE:HD2	2:J:199:GLN:HE22	1.26	0.79
3:F:286:PHE:CE2	3:F:305:CYS:HB2	2.17	0.79
2:D:186:TYR:O	2:D:211:ARG:NH2	2.17	0.78
3:E:38:ILE:HD11	3:E:59:SER:HB3	1.65	0.78
1:I:124:SER:HB2	1:I:158:PHE:HZ	1.49	0.78
3:K:222:PRO:HA	3:K:336:THR:HG22	1.65	0.77
3:E:132:ARG:HH12	3:E:333:MET:HA	1.50	0.77
3:R:162:THR:HA	3:R:167:LEU:HD21	1.66	0.77
1:N:29:PHE:O	1:N:74:ARG:NH2	2.18	0.77
3:E:217:GLU:HG2	3:E:218:GLY:N	1.98	0.77
3:E:37:ASP:HA	3:E:62:ARG:HH12	1.48	0.76
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.66	0.76
3:K:87:ASN:HD22	3:K:90:SER:HB3	1.49	0.76
1:I:215:SER:O	1:I:217:THR:N	2.18	0.76
3:E:70:TYR:HD2	3:E:166:LEU:HD21	1.51	0.76
2:D:94:PHE:HB3	2:D:95:PRO:HD3	1.66	0.75
3:K:118:ILE:HD12	3:K:154:GLU:HB2	1.67	0.75
3:F:79:GLN:HB3	3:F:169:SER:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:THR:HG23	2:B:8:THR:HG23	1.67	0.74
2:J:141:PRO:O	2:J:199:GLN:NE2	2.20	0.74
1:I:36:TRP:HD1	1:I:72:ILE:HG12	1.51	0.74
2:J:61:ARG:NH2	2:J:82:ASP:OD1	2.21	0.74
1:A:38:ARG:HD3	1:A:48:LEU:HD11	1.68	0.74
1:A:52:ARG:HE	1:A:56:THR:HB	1.52	0.74
3:L:83:TYR:OH	3:L:332:ARG:NH1	2.21	0.74
1:N:90:ALA:HA	1:N:123:VAL:HG23	1.69	0.74
1:A:165:THR:HG23	1:A:180:SER:HB2	1.69	0.73
3:E:162:THR:HA	3:E:167:LEU:HD11	1.71	0.73
3:L:95:LEU:HD21	3:L:311:PRO:HD2	1.71	0.73
1:C:12:VAL:HG11	1:C:18:LEU:HD13	1.71	0.73
1:I:36:TRP:CD1	1:I:72:ILE:HG12	2.24	0.73
1:A:146:PHE:CD2	1:A:147:PRO:HD3	2.25	0.72
1:I:14:PRO:HD2	1:I:125:SER:CB	2.18	0.72
3:R:51:ILE:HG23	3:R:56:HIS:CE1	2.24	0.72
2:O:10:SER:OG	2:O:11:LEU:N	2.22	0.72
3:F:183:MET:HG3	3:F:324:ARG:O	1.90	0.71
2:O:195:GLU:HG2	2:O:206:THR:HB	1.71	0.71
2:J:187:GLU:HA	2:J:211:ARG:HH12	1.55	0.71
2:D:30:SER:OG	2:D:31:ASN:N	2.21	0.71
1:G:51:ILE:HD12	1:G:60:THR:HG22	1.72	0.71
3:F:283:ASP:OD1	3:F:306:SER:HA	1.89	0.71
3:E:132:ARG:NH1	3:E:333:MET:HA	2.06	0.71
2:D:187:GLU:HA	2:D:211:ARG:HH12	1.55	0.71
3:K:54:LEU:HD13	3:K:77:ARG:HA	1.72	0.71
2:J:19:VAL:HG21	2:J:78:LEU:HD13	1.72	0.71
3:E:51:ILE:HG22	3:E:77:ARG:HD2	1.72	0.70
3:E:24:ILE:HD11	3:E:94:GLY:HA2	1.72	0.70
1:N:4:LEU:HD23	1:N:98:CYS:SG	2.31	0.70
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.26	0.70
2:J:149:LYS:HZ2	2:J:155:GLN:H	1.40	0.70
2:O:28:GLY:HA2	2:O:69:THR:HG22	1.74	0.70
2:D:151:ASP:N	2:D:191:VAL:O	2.22	0.70
2:D:150:VAL:HG13	2:D:155:GLN:HG3	1.73	0.69
2:J:141:PRO:HD2	2:J:199:GLN:OE1	1.92	0.69
1:N:209:ASN:HA	1:N:220:ASP:HB3	1.74	0.69
3:F:95:LEU:HD11	3:F:311:PRO:HD2	1.74	0.69
2:O:35:TRP:CZ3	2:O:88:CYS:HB3	2.26	0.69
3:E:31:HIS:H	3:E:73:GLN:NE2	1.89	0.68
1:A:47:TRP:CZ2	1:A:50:PHE:HD2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:64:HIS:ND1	3:K:111:LYS:HB2	2.07	0.68
1:I:52:ARG:HD3	1:I:59:THR:OG1	1.93	0.68
3:K:253:SER:O	3:K:275:LYS:NZ	2.27	0.68
1:G:37:VAL:HG22	1:G:47:TRP:HA	1.74	0.68
1:N:200:SER:HB2	1:N:204:GLN:HB3	1.76	0.68
3:L:199:GLN:NE2	3:L:213:PHE:O	2.26	0.68
2:D:167:ASP:OD2	2:D:169:LYS:HG2	1.94	0.68
2:O:13:ALA:O	2:O:107:LYS:N	2.25	0.68
3:F:230:MET:HG3	3:F:232:VAL:HG13	1.76	0.68
3:K:250:GLU:OE2	3:K:324:ARG:NH2	2.27	0.68
3:E:150:THR:HG23	3:E:153:GLY:H	1.58	0.67
2:J:139:PHE:HD2	2:J:199:GLN:NE2	1.91	0.67
1:N:39:GLN:HB2	1:N:45:LEU:HD23	1.76	0.67
1:A:122:PHE:HB3	2:B:121:SER:OG	1.95	0.67
2:B:34:ASN:HD22	2:B:89:GLN:HE21	1.39	0.67
1:I:218:LYS:CD	1:N:13:GLN:HE21	2.06	0.67
1:N:70:PHE:CZ	1:N:85:MET:HG2	2.28	0.67
3:L:47:LYS:O	3:L:51:ILE:HG13	1.95	0.67
1:I:148:ALA:HB3	1:I:201:LEU:HD21	1.77	0.67
2:H:35:TRP:HB2	2:H:48:ILE:HB	1.75	0.67
3:E:259:TYR:OH	3:E:304:ARG:NH1	2.25	0.67
2:D:30:SER:O	2:D:71:TYR:OH	2.12	0.67
1:G:89:ARG:HE	1:G:90:ALA:N	1.91	0.67
1:I:198:SER:HA	1:I:201:LEU:HG	1.77	0.67
3:K:150:THR:HG23	3:K:155:LEU:O	1.95	0.67
1:C:9:GLY:H	1:C:119:THR:HG21	1.60	0.66
2:J:145:LYS:C	2:J:196:VAL:HG23	2.15	0.66
3:L:310:LYS:HG3	3:L:312:GLY:H	1.60	0.66
1:A:13:GLN:O	1:A:16:ASP:HB2	1.94	0.66
3:K:128:VAL:HG23	3:K:171:ARG:HB3	1.78	0.66
2:B:147:GLN:HB2	2:B:195:GLU:HB2	1.76	0.66
2:J:108:ARG:HG3	2:J:109:THR:N	2.10	0.66
3:L:87:ASN:HB3	3:L:90:SER:OG	1.96	0.66
3:K:87:ASN:ND2	3:K:90:SER:HB3	2.10	0.66
3:L:34:LYS:HD3	3:L:165:GLY:HA3	1.76	0.66
1:I:193:VAL:HG21	2:J:135:LEU:HD22	1.78	0.66
1:A:97:ARG:NH2	3:E:189:GLU:OE1	2.28	0.66
1:N:35:SER:HB3	1:N:50:PHE:HB3	1.78	0.65
3:R:119:VAL:HA	3:R:334:MET:HE3	1.78	0.65
1:N:162:VAL:HG23	1:N:212:HIS:HD2	1.61	0.65
3:K:162:THR:HA	3:K:167:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:GLU:O	2:B:211:ARG:NH2	2.28	0.65
3:R:254:LYS:NZ	3:R:255:ASP:OD1	2.29	0.65
3:E:229:TRP:HE1	3:E:331:SER:HB3	1.62	0.65
3:L:25:ILE:HD11	3:L:257:VAL:HB	1.79	0.65
3:K:218:GLY:HA3	3:K:339:VAL:HG22	1.77	0.65
3:E:61:LEU:HD21	3:E:129:PHE:HB2	1.78	0.65
1:I:36:TRP:CE2	1:I:83:LEU:HB2	2.32	0.65
1:I:88:LEU:HD12	1:I:123:VAL:HG21	1.78	0.65
1:N:51:ILE:HD13	1:N:60:THR:HG22	1.78	0.65
3:R:310:LYS:HG3	3:R:312:GLY:H	1.62	0.65
1:I:155:LYS:HG2	1:I:189:SER:OG	1.97	0.65
1:I:218:LYS:CG	1:N:13:GLN:HE21	2.02	0.65
1:I:159:PRO:HD2	1:I:212:HIS:CE1	2.32	0.64
2:O:111:ALA:HB3	2:O:140:TYR:H	1.62	0.64
2:J:30:SER:O	2:J:71:TYR:OH	2.14	0.64
3:R:46:GLU:O	3:R:50:GLN:HG3	1.97	0.64
2:H:19:VAL:HG21	2:H:78:LEU:HD22	1.79	0.64
1:N:193:VAL:HG21	2:O:135:LEU:HD13	1.78	0.64
3:R:246:LYS:NZ	3:R:322:ARG:HH22	1.95	0.64
3:K:154:GLU:O	3:K:155:LEU:HG	1.97	0.64
2:B:167:ASP:OD2	2:B:169:LYS:HB3	1.97	0.64
3:F:251:SER:OG	3:F:285:GLN:NE2	2.30	0.64
3:K:202:PHE:HB3	3:K:205:ILE:HD12	1.78	0.64
2:O:32:TYR:CZ	3:R:187:PRO:HD3	2.33	0.64
2:B:94:PHE:HB3	2:B:95:PRO:HD3	1.80	0.64
1:C:32:TYR:O	1:C:74:ARG:NH2	2.26	0.64
3:R:120:PRO:HD2	3:R:334:MET:CE	2.28	0.64
1:I:150:LEU:HD12	1:I:223:VAL:HG12	1.80	0.64
3:R:240:MET:HE3	3:R:316:VAL:HG11	1.80	0.63
3:R:125:LYS:HB2	3:R:151:GLU:HB3	1.78	0.63
2:H:7:THR:HG23	2:H:8:THR:H	1.64	0.63
1:N:129:LYS:HE2	1:N:156:ASP:O	1.99	0.63
2:D:78:LEU:HD21	2:D:83:ILE:HD11	1.80	0.63
1:I:52:ARG:HB3	1:I:56:LYS:HB3	1.80	0.63
2:O:66:GLY:HA3	2:O:71:TYR:CD1	2.34	0.63
2:J:197:THR:OG1	2:J:204:PRO:HB3	1.98	0.63
1:N:47:TRP:CH2	1:N:49:GLY:HA2	2.34	0.63
1:C:131:PRO:HD2	1:C:217:THR:HG21	1.81	0.63
2:J:145:LYS:O	2:J:196:VAL:HG23	1.99	0.62
1:A:2:VAL:HG13	1:A:27:PHE:CD1	2.34	0.62
2:O:46:LEU:HD23	2:O:55:HIS:CG	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:71:VAL:HG11	3:F:172:VAL:HG13	1.79	0.62
2:O:120:PRO:HG3	2:O:130:ALA:HB1	1.81	0.62
3:L:226:ASP:OD1	3:L:332:ARG:HG3	1.99	0.62
1:C:6:GLU:HG3	1:C:22:CYS:HB2	1.82	0.62
3:F:286:PHE:CD2	3:F:305:CYS:HB2	2.34	0.62
3:K:286:PHE:CE2	3:K:305:CYS:HB2	2.34	0.62
1:C:207:ILE:HD12	1:C:222:LYS:HB3	1.81	0.62
1:I:12:VAL:HG23	1:I:123:VAL:HG22	1.80	0.62
1:C:6:GLU:OE2	1:C:98:CYS:N	2.25	0.62
2:D:166:GLN:HE21	2:D:171:SER:HB3	1.63	0.62
1:N:51:ILE:HG21	1:N:74:ARG:HD2	1.82	0.62
2:D:190:LYS:HG2	2:D:191:VAL:HG23	1.80	0.61
3:F:43:GLY:HA2	3:F:268:GLU:HB2	1.81	0.61
1:I:124:SER:HB2	1:I:158:PHE:CZ	2.35	0.61
1:N:175:VAL:HG22	1:N:194:VAL:HB	1.81	0.61
2:O:120:PRO:HB2	2:O:125:LEU:HD21	1.81	0.61
1:I:182:LEU:HB3	1:I:188:TYR:CE1	2.35	0.61
3:K:219:GLU:OE2	3:K:336:THR:OG1	2.18	0.61
3:R:43:GLY:HA3	3:R:46:GLU:HG3	1.82	0.61
3:F:25:ILE:HG22	3:F:26:CYS:SG	2.41	0.61
3:R:25:ILE:HD11	3:R:257:VAL:HB	1.82	0.61
3:R:110:LYS:HZ3	3:R:138:TYR:H	1.48	0.61
1:C:210:VAL:HG13	1:C:219:VAL:HG13	1.82	0.61
2:O:66:GLY:HA3	2:O:71:TYR:HD1	1.66	0.61
3:R:38:ILE:HD12	3:R:59:SER:OG	2.00	0.61
3:E:130:PHE:HE1	3:E:149:ARG:HD2	1.64	0.61
2:B:34:ASN:HD22	2:B:89:GLN:NE2	1.99	0.61
3:E:33:ASN:OD1	3:E:36:ALA:N	2.33	0.61
2:D:187:GLU:HA	2:D:211:ARG:NH1	2.16	0.61
1:N:155:LYS:HA	1:N:189:SER:HB2	1.83	0.61
1:N:162:VAL:CG2	1:N:212:HIS:CD2	2.84	0.60
2:B:186:TYR:CZ	2:B:211:ARG:HD3	2.36	0.60
3:E:37:ASP:HA	3:E:62:ARG:NH1	2.16	0.60
3:F:260:LYS:HB2	3:F:263:THR:OG1	2.00	0.60
3:R:31:HIS:HB2	3:R:73:GLN:HE21	1.66	0.60
3:R:120:PRO:HD2	3:R:334:MET:HE1	1.83	0.60
2:B:189:HIS:O	2:B:211:ARG:NH2	2.32	0.60
1:I:13:GLN:HG2	1:I:125:SER:HA	1.82	0.60
1:G:71:THR:HB	1:G:84:GLN:HB3	1.83	0.60
1:A:35:SER:HB2	1:A:100(F):MET:HE1	1.81	0.60
3:F:150:THR:HG22	3:F:155:LEU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:240:MET:HG2	3:R:318:TYR:CG	2.36	0.60
1:I:38:ARG:HB2	1:I:48:LEU:HD11	1.82	0.60
3:F:313:GLU:OE1	3:F:324:ARG:NH1	2.35	0.60
1:I:183:GLN:HE22	1:I:189:SER:HB2	1.67	0.60
3:E:34:LYS:HD3	3:E:165:GLY:HA3	1.84	0.60
1:I:24:ILE:HG13	1:I:29:PHE:CE1	2.36	0.60
2:B:19:VAL:HG21	2:B:78:LEU:HD22	1.84	0.60
1:C:4:LEU:HD22	1:C:24:ILE:CD1	2.32	0.59
1:C:33:TYR:OH	3:F:193:GLU:OE2	2.19	0.59
2:J:150:VAL:HG12	2:J:192:TYR:CE1	2.37	0.59
1:N:6:GLU:OE2	1:N:116:GLY:HA3	2.02	0.59
2:H:88:CYS:O	2:H:99:GLY:N	2.33	0.59
1:C:151:GLY:HA3	1:C:193:VAL:HG12	1.83	0.59
2:O:190:LYS:HA	2:O:211:ARG:HD2	1.85	0.59
2:J:192:TYR:HB2	2:J:209:PHE:CE1	2.37	0.59
3:R:54:LEU:HD21	3:R:77:ARG:HA	1.83	0.59
1:G:22:CYS:HB3	1:G:81:LEU:HB3	1.84	0.59
1:N:69:ARG:NH2	1:N:92:ASP:OD2	2.35	0.59
2:D:6:GLN:NE2	2:D:86:TYR:O	2.35	0.59
2:D:89:GLN:HB2	2:D:98:PHE:CD1	2.38	0.59
3:F:231:ASP:HB3	3:F:327:CYS:H	1.67	0.59
1:I:6:GLU:OE2	1:I:118:GLY:N	2.28	0.59
1:C:158:PHE:CG	1:C:159:PRO:HD2	2.37	0.59
3:K:68:GLN:H	3:K:145:SER:HB3	1.68	0.59
1:N:38:ARG:HD3	1:N:96:TYR:CZ	2.38	0.59
1:N:93:SER:HB2	1:N:123:VAL:H	1.67	0.59
1:N:162:VAL:CG2	1:N:212:HIS:HD2	2.16	0.59
1:G:47:TRP:HZ2	1:G:50:PHE:HD2	1.51	0.59
3:L:71:VAL:HG11	3:L:172:VAL:HG23	1.84	0.59
2:J:30:SER:OG	2:J:31:ASN:N	2.27	0.58
3:R:31:HIS:HB2	3:R:73:GLN:NE2	2.17	0.58
1:G:52:ARG:HG3	1:G:59:THR:O	2.03	0.58
2:B:36:TYR:CE2	2:B:89:GLN:HG2	2.30	0.58
1:C:57:GLY:O	1:C:59:THR:N	2.33	0.58
2:D:90:GLN:OE1	2:D:92:SER:N	2.36	0.58
1:N:129:LYS:HZ3	1:N:156:ASP:HB3	1.68	0.58
2:D:124:GLN:HG2	2:D:129:THR:O	2.03	0.58
3:K:206:CYS:HB2	3:K:219:GLU:CD	2.24	0.58
2:H:33:LEU:HD13	2:H:71:TYR:CD2	2.38	0.58
3:E:38:ILE:HG23	3:E:70:TYR:HE1	1.68	0.58
3:E:45:SER:OG	3:E:257:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:145:LYS:HB3	2:O:197:THR:HG22	1.85	0.58
3:K:47:LYS:O	3:K:51:ILE:HG13	2.03	0.58
1:A:51:ILE:HG12	1:A:71:ARG:HD2	1.86	0.58
1:C:62:TYR:OH	1:C:71:THR:HA	2.03	0.58
1:C:175:VAL:HG22	1:C:194:VAL:HB	1.85	0.58
1:A:204:ASN:OD1	1:C:13:GLN:HG3	2.04	0.58
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.85	0.58
3:E:122:PRO:HB2	3:E:124:TYR:CZ	2.39	0.58
2:O:193:ALA:HB2	2:O:208:SER:HB3	1.84	0.58
3:F:217:GLU:OE1	3:F:217:GLU:N	2.37	0.58
1:A:93:ALA:HB3	1:A:100(F):MET:HE2	1.86	0.57
3:E:83:TYR:HB3	3:E:84:PRO:HD3	1.86	0.57
3:E:122:PRO:HB2	3:E:124:TYR:CE1	2.38	0.57
3:R:31:HIS:H	3:R:73:GLN:NE2	2.02	0.57
1:I:2:VAL:HG13	1:I:27:PHE:CD2	2.39	0.57
3:E:73:GLN:OE1	3:E:166:LEU:HD22	2.04	0.57
3:E:117:MET:HE1	3:E:222:PRO:HB3	1.87	0.57
3:L:207:LYS:HG2	3:L:212:VAL:HA	1.86	0.57
3:L:283:ASP:HB3	3:L:304:ARG:HH21	1.70	0.57
3:R:46:GLU:OE2	3:R:267:SER:HA	2.04	0.57
1:G:34:MET:HB3	1:G:81:LEU:HD22	1.85	0.57
2:O:8:THR:OG1	2:O:10:SER:O	2.21	0.57
2:O:14:SER:HB3	2:O:17:ASP:OD2	2.03	0.57
3:R:77:ARG:NH2	3:R:95:LEU:O	2.38	0.57
2:B:148:TRP:CZ3	2:B:194:CYS:HB2	2.40	0.57
1:A:156:SER:H	1:A:197:ASN:HD21	1.52	0.57
3:F:225:PHE:CZ	3:F:227:VAL:HB	2.40	0.57
3:K:240:MET:HB3	3:K:318:TYR:CE1	2.40	0.57
1:N:38:ARG:HD3	1:N:96:TYR:CE2	2.39	0.57
3:R:199:GLN:HG2	3:R:214:ASN:ND2	2.19	0.57
2:B:51:THR:HG23	2:B:71:TYR:HD2	1.70	0.57
3:E:68:GLN:HG3	3:E:145:SER:OG	2.05	0.57
2:J:148:TRP:NE1	2:J:179:LEU:HB2	2.20	0.57
3:E:202:PHE:HB3	3:E:205:ILE:HD12	1.86	0.56
3:R:110:LYS:NZ	3:R:138:TYR:H	2.03	0.56
3:F:77:ARG:NH2	3:F:95:LEU:O	2.38	0.56
3:R:39:PRO:HB2	3:R:41:LEU:HD21	1.88	0.56
1:G:36:TRP:CE2	1:G:83:LEU:HB2	2.40	0.56
1:A:11:LEU:HD22	1:A:147:PRO:HG3	1.87	0.56
2:D:15:LEU:HD21	2:D:80:PRO:HG3	1.88	0.56
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:217:GLU:HG2	3:F:218:GLY:H	1.69	0.56
1:A:160:THR:O	1:A:163:VAL:HG12	2.05	0.56
1:C:158:PHE:CD2	1:C:159:PRO:HD2	2.39	0.56
2:B:187:GLU:HA	2:B:211:ARG:CZ	2.35	0.56
2:D:189:HIS:O	2:D:211:ARG:NH2	2.35	0.56
1:I:108:TYR:OH	3:K:323:VAL:HG22	2.05	0.56
2:O:175:LEU:HD23	2:O:176:SER:N	2.19	0.56
2:J:39:LYS:HE2	2:J:81:GLU:O	2.06	0.56
2:O:118:PHE:HB2	2:O:133:VAL:HG23	1.88	0.56
1:A:33:TYR:CE2	1:A:52:ARG:HG2	2.40	0.56
2:D:150:VAL:CG2	2:D:155:GLN:HE21	2.19	0.56
1:I:207:ILE:HG12	1:I:222:LYS:HG2	1.86	0.56
2:J:139:PHE:CD2	2:J:199:GLN:NE2	2.73	0.56
3:K:51:ILE:HG23	3:K:56:HIS:CE1	2.39	0.56
1:N:220:ASP:OD1	1:N:220:ASP:N	2.38	0.56
1:A:146:PHE:HD2	1:A:147:PRO:HD3	1.71	0.56
3:K:127:LYS:HE3	3:K:170:ASP:O	2.05	0.56
1:N:88:LEU:HD13	1:N:123:VAL:HG11	1.88	0.56
1:G:51:ILE:CD1	1:G:60:THR:HG22	2.36	0.56
3:E:41:LEU:HD13	3:E:46:GLU:HB3	1.87	0.56
1:I:162:VAL:HG13	1:I:162:VAL:O	2.05	0.56
2:O:48:ILE:HD13	2:O:54:LEU:HA	1.88	0.56
2:O:150:VAL:HG13	2:O:155:GLN:HG3	1.87	0.56
3:R:281:ARG:NH2	3:R:302:LYS:O	2.32	0.56
1:A:67:PHE:HA	1:A:81:GLN:O	2.06	0.56
1:N:162:VAL:HG23	1:N:212:HIS:CD2	2.41	0.55
3:E:41:LEU:O	3:E:47:LYS:HE2	2.07	0.55
3:E:187:PRO:HG2	3:E:190:THR:OG1	2.07	0.55
2:J:78:LEU:HD21	2:J:83:ILE:HD11	1.87	0.55
1:N:166:TRP:CZ3	1:N:208:CYS:HB3	2.42	0.55
1:G:70:PHE:CE1	1:G:85:MET:HB3	2.40	0.55
3:E:30:ILE:HA	3:E:73:GLN:HE21	1.71	0.55
1:G:88:LEU:HD22	1:G:123:VAL:HG21	1.88	0.55
1:A:197:ASN:HB3	1:A:208:ASP:OD2	2.05	0.55
1:A:200:HIS:NE2	1:A:202:PRO:HG2	2.20	0.55
3:E:257:VAL:O	3:E:305:CYS:HA	2.06	0.55
3:F:92:TRP:CZ2	3:F:311:PRO:HG3	2.41	0.55
2:O:211:ARG:HG3	2:O:211:ARG:HH11	1.71	0.55
1:I:126:ALA:HB3	1:I:158:PHE:CE2	2.42	0.55
1:I:150:LEU:HD11	1:I:206:TYR:HD2	1.71	0.55
2:O:183:LYS:O	2:O:187:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:51:ILE:HD11	3:F:103:TRP:HB3	1.89	0.55
3:F:57:VAL:HG11	3:F:172:VAL:HG11	1.87	0.55
3:L:130:PHE:HE1	3:L:149:ARG:HD2	1.72	0.55
1:C:37:VAL:HG21	1:C:112:MET:HE1	1.89	0.55
2:D:151:ASP:HA	2:D:191:VAL:HB	1.88	0.55
1:I:166:TRP:CZ3	1:I:208:CYS:HB3	2.41	0.55
1:N:166:TRP:CH2	1:N:208:CYS:HB3	2.42	0.55
3:E:310:LYS:HG3	3:E:312:GLY:H	1.72	0.55
1:I:35:SER:HB3	1:I:50:PHE:HB3	1.89	0.55
1:A:101:ASP:HA	2:B:46:LEU:HD22	1.89	0.54
3:E:207:LYS:HE3	3:E:212:VAL:HG22	1.88	0.54
2:D:105:GLU:HB2	2:D:166:GLN:OE1	2.07	0.54
1:I:24:ILE:HG13	1:I:29:PHE:CD1	2.42	0.54
2:J:61:ARG:HH21	2:J:82:ASP:CG	2.10	0.54
2:O:14:SER:HB2	2:O:107:LYS:HE3	1.90	0.54
3:K:51:ILE:HG22	3:K:77:ARG:HD2	1.89	0.54
3:E:70:TYR:CD2	3:E:166:LEU:HD21	2.38	0.54
1:I:157:TYR:CZ	1:I:162:VAL:HG11	2.43	0.54
3:E:230:MET:HG3	3:E:232:VAL:HG13	1.87	0.54
2:O:108:ARG:NH1	2:O:111:ALA:HB2	2.13	0.54
3:L:58:SER:HB3	3:L:70:TYR:HA	1.90	0.54
1:A:66:ARG:NH1	1:A:83:ARG:NE	2.56	0.54
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.43	0.54
2:D:48:ILE:HD13	2:D:54:LEU:HA	1.90	0.54
1:I:93:SER:CB	1:I:123:VAL:H	2.21	0.54
1:N:138:PRO:HG3	1:N:150:LEU:HD12	1.90	0.54
1:A:37:VAL:HG13	1:A:46:GLU:O	2.07	0.54
1:C:78:GLN:HB3	1:C:80:ILE:HD12	1.88	0.54
3:R:220:SER:N	3:R:337:LEU:O	2.38	0.54
3:F:150:THR:OG1	3:F:151:GLU:N	2.39	0.54
1:I:150:LEU:HD11	1:I:206:TYR:CD2	2.41	0.54
2:J:148:TRP:HB3	2:J:194:CYS:CB	2.36	0.54
2:J:193:ALA:HB3	2:J:208:SER:HB2	1.89	0.54
2:D:120:PRO:HG3	2:D:130:ALA:HB1	1.90	0.54
2:J:89:GLN:HG2	2:J:90:GLN:N	2.22	0.54
3:K:249:GLN:N	3:K:249:GLN:OE1	2.40	0.54
3:E:95:LEU:CD1	3:E:310:LYS:HB2	2.38	0.53
1:C:104:TYR:O	1:C:106:ASP:N	2.41	0.53
2:H:55:HIS:HB3	2:H:58:VAL:HG21	1.89	0.53
1:I:128:THR:CG2	1:N:215:SER:HA	2.38	0.53
1:N:177:THR:HG23	1:N:192:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:THR:HA	1:G:120:SER:HA	1.90	0.53
3:F:95:LEU:CD1	3:F:310:LYS:HB2	2.38	0.53
1:N:129:LYS:NZ	1:N:156:ASP:HB3	2.23	0.53
2:J:108:ARG:HB3	2:J:140:TYR:CD1	2.43	0.53
2:O:47:LEU:HA	2:O:58:VAL:HG21	1.90	0.53
2:O:94:PHE:HB3	2:O:95:PRO:HD3	1.91	0.53
3:E:130:PHE:HA	3:E:173:LEU:O	2.08	0.53
2:J:6:GLN:HG2	2:J:100:GLY:H	1.74	0.53
2:J:120:PRO:HG3	2:J:130:ALA:HB1	1.91	0.53
1:A:34:MET:HE1	1:A:94:ARG:HB2	1.90	0.53
3:E:26:CYS:HB3	3:E:53:ARG:HD3	1.90	0.53
3:R:125:LYS:N	3:R:151:GLU:HB3	2.24	0.53
2:D:12:SER:HA	2:D:105:GLU:HG3	1.90	0.53
1:A:100(B):TYR:CE2	3:E:186:ILE:HG22	2.44	0.53
2:B:107:LYS:HA	2:B:140:TYR:OH	2.09	0.53
3:F:310:LYS:HG3	3:F:312:GLY:N	2.21	0.53
3:K:224:PRO:HA	3:K:334:MET:HE1	1.91	0.53
2:O:190:LYS:HD2	2:O:211:ARG:HG2	1.90	0.53
1:C:24:ILE:HD12	1:C:27:PHE:CZ	2.43	0.53
2:D:21:ILE:HG23	2:D:102:THR:HG21	1.91	0.53
1:I:182:LEU:HB3	1:I:188:TYR:CD1	2.44	0.53
2:H:59:PRO:HD2	2:H:62:PHE:HD2	1.73	0.53
1:I:93:SER:HB3	1:I:123:VAL:H	1.74	0.53
3:R:130:PHE:HB3	3:R:173:LEU:HB3	1.92	0.53
3:R:245:THR:HG21	3:R:328:TYR:OH	2.09	0.53
3:R:240:MET:HG2	3:R:318:TYR:CD1	2.44	0.52
1:G:110:TYR:HE2	3:L:187:PRO:HG2	1.73	0.52
3:K:207:LYS:HG2	3:K:212:VAL:HA	1.91	0.52
1:G:2:VAL:HG13	1:G:27:PHE:CD1	2.44	0.52
3:F:128:VAL:HG23	3:F:171:ARG:HB3	1.91	0.52
3:F:128:VAL:HG23	3:F:171:ARG:HD2	1.91	0.52
3:F:283:ASP:OD1	3:F:283:ASP:N	2.32	0.52
2:J:149:LYS:HD3	2:J:154:LEU:HA	1.91	0.52
1:N:130:GLY:HA3	1:N:217:THR:HG21	1.92	0.52
2:B:31:ASN:HB3	2:B:50:TYR:CE1	2.44	0.52
1:C:24:ILE:HG23	1:C:27:PHE:CE1	2.44	0.52
1:C:158:PHE:O	1:C:212:HIS:CE1	2.63	0.52
2:J:125:LEU:C	2:J:127:SER:H	2.12	0.52
3:K:202:PHE:HB3	3:K:205:ILE:CD1	2.39	0.52
1:N:34:MET:CG	1:N:81:LEU:HD22	2.39	0.52
1:A:198:VAL:CG1	1:A:207:VAL:HG13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:TRP:CH2	1:C:49:GLY:HA2	2.44	0.52
3:F:92:TRP:CE2	3:F:311:PRO:HG3	2.44	0.52
1:I:154:VAL:HG11	1:I:210:VAL:HG21	1.92	0.52
2:H:29:ILE:HD11	2:H:71:TYR:HE2	1.73	0.52
3:L:131:GLU:OE2	3:L:133:PRO:HD3	2.09	0.52
1:A:12:VAL:HG11	1:A:18:LEU:HD22	1.92	0.52
1:C:1:GLU:HB2	1:I:31:ASP:OD2	2.09	0.52
1:I:159:PRO:HB2	1:I:214:PRO:HG2	1.91	0.52
2:O:55:HIS:CG	2:O:56:SER:N	2.78	0.52
2:O:125:LEU:C	2:O:127:SER:H	2.13	0.52
2:D:192:TYR:O	2:D:208:SER:HB2	2.10	0.52
3:K:286:PHE:CD2	3:K:305:CYS:HB2	2.44	0.52
2:D:27:GLN:O	2:D:29:ILE:HG23	2.10	0.52
1:I:51:ILE:HG23	1:I:74:ARG:HH11	1.75	0.52
1:I:75:ASP:OD2	1:I:78:GLN:HB2	2.08	0.52
3:F:96:LEU:HB3	3:F:100:ASP:HB2	1.92	0.51
3:R:219:GLU:HA	3:R:337:LEU:O	2.10	0.51
3:F:41:LEU:HB3	3:F:46:GLU:OE1	2.10	0.51
1:I:17:SER:OG	1:I:86:ASN:HA	2.10	0.51
2:J:94:PHE:HB2	3:K:188:GLU:HG2	1.92	0.51
1:N:40:PRO:HG2	1:N:43:LYS:HB2	1.92	0.51
1:N:52:ARG:HG3	1:N:59:THR:CB	2.35	0.51
1:G:33:TYR:CD2	1:G:52:ARG:HA	2.45	0.51
3:L:226:ASP:HB3	3:L:330:PHE:CE1	2.45	0.51
1:G:89:ARG:HG3	1:G:91:GLU:HG2	1.91	0.51
1:A:121:VAL:HG11	1:A:198:VAL:CG1	2.32	0.51
3:K:183:MET:HG3	3:K:324:ARG:O	2.10	0.51
2:H:29:ILE:HD11	2:H:71:TYR:CE2	2.44	0.51
2:H:90:GLN:HE21	2:H:97:THR:HG23	1.74	0.51
1:C:136:LEU:HD21	1:C:153:LEU:HB2	1.93	0.51
1:N:158:PHE:HB3	1:N:159:PRO:HD3	1.93	0.51
2:O:125:LEU:HD11	2:O:130:ALA:HB2	1.92	0.51
1:C:9:GLY:N	1:C:119:THR:HG21	2.24	0.51
2:D:32:TYR:CZ	3:F:187:PRO:HD3	2.45	0.51
3:F:249:GLN:OE1	3:F:249:GLN:N	2.43	0.51
2:O:115:VAL:HG22	2:O:136:LEU:HG	1.92	0.51
3:E:24:ILE:HD11	3:E:94:GLY:CA	2.38	0.51
3:R:101:ALA:HB1	3:R:106:MET:HB2	1.93	0.51
1:I:150:LEU:HD12	1:I:223:VAL:CG1	2.40	0.51
1:I:157:TYR:OH	1:I:190:LEU:HD23	2.10	0.51
1:I:159:PRO:HD2	1:I:212:HIS:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2:VAL:O	2:J:97:THR:HG21	2.11	0.51
1:N:37:VAL:HG21	1:N:112:MET:CE	2.41	0.51
1:I:125:SER:O	1:I:125:SER:OG	2.22	0.51
2:B:36:TYR:CE1	2:B:46:LEU:HD13	2.46	0.51
2:D:21:ILE:HD12	2:D:73:LEU:HD23	1.92	0.51
3:F:132:ARG:NH1	3:F:333:MET:HA	2.26	0.51
1:I:38:ARG:CB	1:I:48:LEU:HD11	2.40	0.51
2:O:190:LYS:HE2	2:O:210:ASN:HB3	1.93	0.51
3:R:283:ASP:OD2	3:R:306:SER:HA	2.11	0.51
3:E:29:PRO:HB2	3:E:31:HIS:CD2	2.45	0.50
3:E:147:LYS:HE2	3:E:158:SER:HB3	1.93	0.50
2:O:18:ARG:HG2	2:O:76:SER:O	2.11	0.50
3:R:186:ILE:HD11	3:R:232:VAL:HB	1.92	0.50
1:A:100(C):TYR:HE1	2:B:50:TYR:CD2	2.28	0.50
2:D:166:GLN:NE2	2:D:171:SER:HB3	2.24	0.50
3:F:229:TRP:CZ3	3:F:237:LYS:HE3	2.47	0.50
2:J:14:SER:OG	2:J:107:LYS:HE2	2.11	0.50
3:K:54:LEU:HD23	3:K:72:GLY:HA3	1.93	0.50
1:N:52:ARG:NH2	1:N:61:GLU:OE2	2.43	0.50
3:R:34:LYS:HE3	3:R:68:GLN:HG2	1.93	0.50
3:R:73:GLN:NE2	3:R:166:LEU:HD13	2.26	0.50
1:G:69:ARG:NH2	1:G:92:ASP:OD2	2.40	0.50
1:I:149:ALA:HB3	2:J:116:PHE:CD2	2.46	0.50
2:J:123:GLU:HA	2:J:126:LYS:CG	2.38	0.50
2:J:134:CYS:HB2	2:J:148:TRP:CZ3	2.46	0.50
1:C:106:ASP:OD2	3:F:322:ARG:NH1	2.45	0.50
2:D:36:TYR:CE1	2:D:46:LEU:HD13	2.47	0.50
3:F:260:LYS:HB2	3:F:263:THR:HG1	1.77	0.50
1:I:69:ARG:O	1:I:86:ASN:HB2	2.12	0.50
1:I:221:LYS:HE2	1:I:221:LYS:HA	1.93	0.50
3:L:128:VAL:HG22	3:L:171:ARG:HB3	1.94	0.50
2:D:166:GLN:HE21	2:D:171:SER:CB	2.25	0.50
1:I:171:LEU:HD21	1:I:194:VAL:HG21	1.93	0.50
2:J:94:PHE:HB3	2:J:95:PRO:HD3	1.92	0.50
2:J:108:ARG:HG3	2:J:109:THR:H	1.77	0.50
1:N:101:ASP:OD1	1:N:112:MET:HG3	2.12	0.50
1:C:3:LYS:C	1:C:4:LEU:HD23	2.31	0.50
2:J:158:ASN:N	2:J:158:ASN:OD1	2.45	0.50
3:R:165:GLY:O	3:R:166:LEU:HD23	2.12	0.50
1:A:198:VAL:HG13	1:A:207:VAL:HG13	1.94	0.49
1:I:105:ASP:OD1	1:I:110:TYR:OH	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:PHE:CD1	1:I:191:SER:HB2	2.48	0.49
3:K:91:ARG:HG3	3:K:91:ARG:HH11	1.77	0.49
1:N:178:PHE:HD2	1:N:191:SER:HB2	1.77	0.49
1:G:6:GLU:OE1	1:G:118:GLY:N	2.33	0.49
2:D:131:SER:OG	2:D:180:THR:HG22	2.12	0.49
2:J:90:GLN:OE1	2:J:92:SER:N	2.45	0.49
2:O:33:LEU:HD22	2:O:71:TYR:CG	2.47	0.49
3:R:80:VAL:HG13	3:R:172:VAL:O	2.13	0.49
3:R:225:PHE:CZ	3:R:227:VAL:HB	2.47	0.49
2:H:7:THR:HB	2:H:22:SER:OG	2.12	0.49
3:E:51:ILE:HG23	3:E:56:HIS:CE1	2.47	0.49
3:E:71:VAL:HG11	3:E:172:VAL:HG23	1.93	0.49
3:E:147:LYS:HD2	3:E:156:CYS:O	2.12	0.49
2:J:12:SER:HB2	2:J:107:LYS:HG3	1.93	0.49
3:K:102:ASP:HB2	3:K:109:VAL:HG23	1.94	0.49
1:C:13:GLN:HA	1:C:124:SER:O	2.12	0.49
1:I:30:SER:HB3	1:I:76:ASN:HD22	1.77	0.49
1:N:51:ILE:CD1	1:N:60:THR:HG22	2.40	0.49
3:L:283:ASP:HB3	3:L:304:ARG:NH2	2.27	0.49
2:B:36:TYR:HE2	2:B:89:GLN:CG	2.18	0.49
3:E:132:ARG:HB3	3:E:175:ILE:HD12	1.95	0.49
1:C:11:LEU:HD12	1:C:122:THR:O	2.11	0.49
1:C:37:VAL:HG22	1:C:47:TRP:HA	1.94	0.49
3:F:60:TRP:O	3:F:64:HIS:HB2	2.12	0.49
2:O:166:GLN:HB2	2:O:173:TYR:CZ	2.47	0.49
3:R:53:ARG:HB2	3:R:55:ILE:HG13	1.93	0.49
3:E:51:ILE:HD11	3:E:103:TRP:HB3	1.95	0.49
1:I:217:THR:HG22	1:N:127:SER:OG	2.12	0.49
2:O:83:ILE:HG23	2:O:104:LEU:O	2.13	0.49
3:R:148:SER:O	3:R:156:CYS:HA	2.12	0.49
1:I:6:GLU:OE1	1:I:116:GLY:HA3	2.12	0.49
1:I:146:GLY:N	1:I:198:SER:HG	2.10	0.49
2:O:118:PHE:HB2	2:O:133:VAL:CG2	2.43	0.49
2:O:147:GLN:HG2	2:O:195:GLU:HB2	1.94	0.49
1:A:51:ILE:CG1	1:A:71:ARG:HD2	2.43	0.49
2:B:184:ALA:C	2:B:188:LYS:HE3	2.33	0.49
3:E:95:LEU:HD12	3:E:310:LYS:HB2	1.94	0.49
3:L:68:GLN:HG2	3:L:145:SER:OG	2.13	0.49
1:I:37:VAL:HG22	1:I:47:TRP:HA	1.94	0.49
3:K:282:GLY:HA2	3:K:304:ARG:HG3	1.94	0.49
1:N:51:ILE:HG22	1:N:52:ARG:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:PHE:HB3	2:D:95:PRO:CD	2.42	0.49
3:F:251:SER:HB3	3:F:289:VAL:HG21	1.95	0.49
1:A:206:LYS:NZ	1:C:16:ASP:OD1	2.42	0.48
2:D:166:GLN:HE21	2:D:171:SER:CA	2.26	0.48
3:K:29:PRO:HB3	3:K:53:ARG:HD2	1.94	0.48
3:R:102:ASP:OD2	3:R:109:VAL:HG22	2.13	0.48
1:G:18:LEU:HD23	1:G:121:VAL:HG13	1.95	0.48
3:F:126:GLY:O	3:F:148:SER:HB2	2.13	0.48
2:J:90:GLN:CG	2:J:97:THR:HG22	2.43	0.48
3:E:83:TYR:CD1	3:E:122:PRO:HG3	2.49	0.48
1:N:24:ILE:HG23	1:N:27:PHE:CE1	2.48	0.48
3:E:34:LYS:O	3:E:69:GLY:HA2	2.12	0.48
3:E:256:PHE:HD1	3:E:307:LEU:HA	1.77	0.48
3:F:257:VAL:O	3:F:305:CYS:HA	2.13	0.48
2:O:187:GLU:HG2	2:O:211:ARG:NH2	2.28	0.48
3:R:240:MET:HB3	3:R:318:TYR:CE1	2.48	0.48
2:H:21:ILE:HG12	2:H:102:THR:HG21	1.95	0.48
3:E:256:PHE:HE1	3:E:307:LEU:HB2	1.79	0.48
3:L:249:GLN:HG3	3:L:249:GLN:O	2.12	0.48
3:E:159:ASP:OD1	3:E:161:ARG:HB2	2.13	0.48
1:C:13:GLN:HG2	1:C:124:SER:O	2.13	0.48
3:F:128:VAL:HG21	3:F:167:LEU:HD13	1.95	0.48
2:J:14:SER:HB2	2:J:17:ASP:OD1	2.13	0.48
3:K:107:LEU:HD13	3:K:138:TYR:CD2	2.49	0.48
3:K:222:PRO:CA	3:K:336:THR:HG22	2.38	0.48
1:N:70:PHE:CE2	1:N:85:MET:HG2	2.49	0.48
1:N:95:THR:HA	1:N:120:SER:HA	1.96	0.48
3:E:225:PHE:O	3:E:332:ARG:HA	2.12	0.48
3:E:230:MET:SD	3:E:316:VAL:HG21	2.53	0.48
1:C:11:LEU:HD22	1:C:159:PRO:HG3	1.96	0.48
1:C:33:TYR:CE2	1:C:52:ARG:HD2	2.49	0.48
1:C:158:PHE:CG	1:C:159:PRO:CD	2.97	0.48
1:I:103:ARG:NH2	3:K:189:GLU:OE1	2.46	0.48
2:O:28:GLY:CA	2:O:69:THR:HG22	2.44	0.48
2:H:63:SER:O	2:H:73:LEU:HD12	2.14	0.48
1:C:38:ARG:HD2	1:C:96:TYR:OH	2.13	0.48
2:J:159:SER:HB2	2:J:179:LEU:HD12	1.96	0.48
2:O:145:LYS:O	2:O:196:VAL:HA	2.14	0.48
3:R:31:HIS:H	3:R:73:GLN:HE22	1.61	0.48
3:R:32:SER:OG	3:R:33:ASN:N	2.47	0.48
3:R:71:VAL:HG11	3:R:172:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:130:PHE:HA	3:L:173:LEU:O	2.14	0.48
2:J:90:GLN:HG3	2:J:97:THR:HG22	1.96	0.48
3:K:65:SER:O	3:K:144:GLY:HA2	2.14	0.48
3:K:168:PRO:HG2	3:K:170:ASP:OD1	2.14	0.48
3:R:246:LYS:HZ3	3:R:322:ARG:HH22	1.61	0.48
2:H:3:VAL:O	2:H:26:SER:HB3	2.13	0.48
1:C:37:VAL:HG21	1:C:112:MET:CE	2.44	0.48
2:J:136:LEU:HD11	2:J:146:VAL:HG21	1.95	0.48
3:K:206:CYS:HB2	3:K:219:GLU:OE2	2.13	0.48
2:H:13:ALA:O	2:H:106:ILE:HA	2.14	0.48
3:E:25:ILE:HD11	3:E:257:VAL:CG1	2.44	0.47
1:I:128:THR:HG21	1:N:215:SER:HA	1.95	0.47
2:J:158:ASN:HD22	2:J:181:LEU:HD21	1.79	0.47
2:J:211:ARG:O	2:J:211:ARG:HG3	2.13	0.47
1:N:36:TRP:NE1	1:N:83:LEU:HB2	2.29	0.47
1:N:178:PHE:CD2	2:O:176:SER:HB3	2.48	0.47
3:R:79:GLN:O	3:R:169:SER:HB2	2.14	0.47
3:E:95:LEU:HD11	3:E:311:PRO:HD2	1.95	0.47
3:E:135:PHE:HB2	3:E:208:ILE:HG22	1.95	0.47
1:C:34:MET:HB3	1:C:81:LEU:HD22	1.96	0.47
3:F:217:GLU:CD	3:F:217:GLU:H	2.16	0.47
3:R:126:GLY:HA2	3:R:148:SER:OG	2.14	0.47
1:A:82(C):LEU:HA	1:A:82(C):LEU:HD23	1.47	0.47
3:L:113:LYS:HG2	3:L:116:ASP:OD2	2.14	0.47
1:N:16:ASP:O	1:N:88:LEU:HB2	2.14	0.47
3:R:120:PRO:HD2	3:R:334:MET:HE3	1.96	0.47
3:E:130:PHE:HB3	3:E:173:LEU:HB3	1.97	0.47
3:F:128:VAL:HG21	3:F:167:LEU:CD1	2.44	0.47
3:F:267:SER:OG	3:F:268:GLU:N	2.47	0.47
2:O:150:VAL:HG12	2:O:192:TYR:CD1	2.49	0.47
3:L:38:ILE:HD13	3:L:55:ILE:HG23	1.96	0.47
2:J:6:GLN:HG3	2:J:101:GLY:N	2.30	0.47
3:K:149:ARG:HD2	3:K:153:GLY:O	2.14	0.47
1:N:3:LYS:C	1:N:4:LEU:HD12	2.34	0.47
2:H:6:GLN:OE1	2:H:102:THR:N	2.48	0.47
1:A:193:THR:HG23	1:A:210:LYS:HE3	1.97	0.47
2:D:118:PHE:O	2:D:132:VAL:HG13	2.15	0.47
3:F:41:LEU:HD13	3:F:46:GLU:HB3	1.97	0.47
1:I:85:MET:HB2	1:I:88:LEU:HD21	1.96	0.47
2:J:47:LEU:HD23	2:J:47:LEU:HA	1.47	0.47
2:J:148:TRP:HE1	2:J:179:LEU:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:193:ALA:HB3	2:J:208:SER:CB	2.45	0.47
3:K:206:CYS:HB3	3:K:216:CYS:HB2	1.62	0.47
3:R:83:TYR:CD1	3:R:83:TYR:C	2.88	0.47
3:L:154:GLU:O	3:L:155:LEU:HG	2.13	0.47
2:D:150:VAL:HG21	2:D:155:GLN:HE21	1.80	0.47
2:J:147:GLN:N	2:J:194:CYS:SG	2.88	0.47
1:N:207:ILE:HD11	1:N:222:LYS:HG3	1.97	0.47
3:R:31:HIS:N	3:R:73:GLN:HE22	2.12	0.47
1:G:52:ARG:HE	1:G:59:THR:HB	1.79	0.47
3:E:130:PHE:CB	3:E:173:LEU:HB3	2.45	0.47
1:C:160:GLU:N	1:C:161:PRO:HD2	2.30	0.47
2:O:35:TRP:CH2	2:O:88:CYS:HB3	2.50	0.47
3:R:60:TRP:O	3:R:64:HIS:HB2	2.15	0.47
3:E:25:ILE:CG1	3:E:257:VAL:HG11	2.45	0.47
3:E:73:GLN:OE1	3:E:166:LEU:HB3	2.14	0.47
1:C:159:PRO:C	1:C:161:PRO:HD2	2.35	0.47
1:C:193:VAL:HG21	2:D:135:LEU:HD22	1.97	0.47
1:N:108:TYR:CZ	3:R:186:ILE:HG22	2.50	0.47
3:R:154:GLU:O	3:R:155:LEU:HG	2.14	0.47
1:C:24:ILE:HD13	1:C:24:ILE:HA	1.61	0.46
2:O:133:VAL:CG1	2:O:178:THR:HG23	2.45	0.46
1:G:2:VAL:HG13	1:G:27:PHE:CE1	2.50	0.46
1:A:82:MET:HB3	1:A:82(C):LEU:HD21	1.98	0.46
3:E:51:ILE:HA	3:E:56:HIS:CE1	2.50	0.46
3:F:129:PHE:HA	3:F:141:TRP:O	2.15	0.46
1:I:129:LYS:O	1:I:157:TYR:HA	2.16	0.46
3:K:280:CYS:O	3:K:292:CYS:HB2	2.15	0.46
2:O:29:ILE:HD11	2:O:71:TYR:CE2	2.51	0.46
1:N:171:LEU:HD11	1:N:194:VAL:HG21	1.97	0.46
2:H:6:GLN:OE1	2:H:101:GLY:N	2.49	0.46
3:L:208:ILE:HD12	3:L:213:PHE:HB2	1.97	0.46
3:E:54:LEU:HD11	3:E:80:VAL:CG2	2.45	0.46
2:D:187:GLU:HA	2:D:211:ARG:HH22	1.79	0.46
3:F:272:LYS:O	3:F:276:THR:HG23	2.16	0.46
1:N:54:LYS:HB2	1:N:58:TYR:OH	2.15	0.46
3:R:56:HIS:HB3	3:R:103:TRP:CD2	2.50	0.46
3:R:227:VAL:HG21	3:R:239:ILE:HB	1.96	0.46
1:C:42:GLY:O	1:C:43:LYS:HD3	2.15	0.46
3:F:130:PHE:HA	3:F:173:LEU:O	2.16	0.46
1:I:58:TYR:HE1	1:I:74:ARG:CZ	2.28	0.46
2:J:89:GLN:HB2	2:J:98:PHE:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:LEU:HD22	2:O:133:VAL:HG21	1.96	0.46
3:R:132:ARG:NH1	3:R:333:MET:HA	2.30	0.46
1:G:2:VAL:HB	1:G:114:TYR:CD2	2.51	0.46
1:A:1:GLU:HG2	1:A:3:LYS:HE3	1.96	0.46
1:A:154:TRP:CH2	1:A:196:CYS:HB3	2.51	0.46
3:E:36:ALA:O	3:E:62:ARG:NH2	2.40	0.46
3:F:27:ALA:O	3:F:53:ARG:NE	2.47	0.46
3:L:83:TYR:HB3	3:L:84:PRO:HD3	1.98	0.46
3:L:184:THR:HG22	3:L:324:ARG:HB3	1.97	0.46
1:A:122:PHE:CE2	2:B:124:GLN:HG3	2.51	0.46
3:F:285:GLN:HG2	3:F:307:LEU:HD22	1.97	0.46
2:J:148:TRP:CB	2:J:194:CYS:HB2	2.40	0.46
2:O:170:ASP:OD2	2:O:172:THR:OG1	2.28	0.46
2:B:32:TYR:CZ	3:E:187:PRO:HD3	2.51	0.46
3:E:29:PRO:HB2	3:E:31:HIS:NE2	2.31	0.46
3:E:38:ILE:CD1	3:E:59:SER:HB3	2.42	0.46
1:I:166:TRP:CH2	1:I:208:CYS:HB3	2.50	0.46
3:K:122:PRO:HB2	3:K:124:TYR:CE1	2.51	0.46
3:K:207:LYS:HB2	3:K:219:GLU:OE2	2.16	0.46
1:N:34:MET:HG2	1:N:81:LEU:HD22	1.97	0.46
2:O:140:TYR:CD2	2:O:141:PRO:HA	2.51	0.46
3:R:130:PHE:CB	3:R:173:LEU:HB3	2.45	0.46
2:B:23:CYS:HB2	2:B:35:TRP:CH2	2.51	0.46
3:E:230:MET:SD	3:E:316:VAL:HG11	2.56	0.46
3:E:282:GLY:HA2	3:E:304:ARG:HG3	1.97	0.46
3:F:188:GLU:HB2	3:F:234:HIS:CE1	2.51	0.46
1:I:70:PHE:CE1	1:I:85:MET:HB3	2.50	0.46
2:O:103:LYS:HB2	2:O:103:LYS:HE2	1.69	0.46
2:O:111:ALA:HB3	2:O:140:TYR:N	2.30	0.46
3:R:82:TYR:O	3:R:85:ALA:HA	2.15	0.46
2:B:47:LEU:HD23	2:B:47:LEU:HA	1.70	0.46
3:E:131:GLU:HA	3:E:140:GLY:HA2	1.97	0.46
1:C:135:PRO:HB2	1:C:223:VAL:HG13	1.98	0.46
2:D:191:VAL:HG22	2:D:210:ASN:OD1	2.16	0.46
2:J:36:TYR:CE1	2:J:46:LEU:HD13	2.51	0.46
3:L:25:ILE:HG22	3:L:26:CYS:SG	2.56	0.46
3:E:288:LYS:O	3:E:288:LYS:HD3	2.16	0.45
1:C:6:GLU:OE2	1:C:116:GLY:HA3	2.16	0.45
3:F:89:TYR:CD2	3:F:179:ALA:HB2	2.50	0.45
2:J:3:VAL:HB	2:J:26:SER:HB3	1.98	0.45
3:K:281:ARG:HB2	3:K:304:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:6:GLU:CD	1:N:116:GLY:HA3	2.37	0.45
2:O:164:THR:HG23	2:O:165:GLU:O	2.15	0.45
3:E:132:ARG:NH2	3:E:209:ASP:OD1	2.42	0.45
3:F:162:THR:HG22	3:F:171:ARG:HE	1.80	0.45
2:J:150:VAL:HG12	2:J:192:TYR:CD1	2.51	0.45
1:N:6:GLU:OE1	1:N:116:GLY:HA3	2.16	0.45
1:I:38:ARG:NH1	1:I:46:GLU:OE1	2.50	0.45
3:K:218:GLY:CA	3:K:339:VAL:HG22	2.45	0.45
2:O:147:GLN:CG	2:O:195:GLU:HB2	2.46	0.45
3:R:208:ILE:HA	3:R:334:MET:O	2.17	0.45
2:H:66:GLY:HA3	2:H:71:TYR:HA	1.98	0.45
1:A:67:PHE:CZ	1:A:82:MET:HE3	2.51	0.45
3:E:25:ILE:HD13	3:E:25:ILE:HG21	1.67	0.45
3:E:232:VAL:HG12	3:E:323:VAL:HG11	1.98	0.45
1:C:124:SER:OG	1:C:125:SER:N	2.48	0.45
3:F:43:GLY:CA	3:F:268:GLU:HB2	2.45	0.45
2:J:9:SER:O	2:J:102:THR:HA	2.17	0.45
3:K:135:PHE:HB2	3:K:208:ILE:HG22	1.99	0.45
3:L:255:ASP:O	3:L:307:LEU:HA	2.16	0.45
3:L:284:MET:HE3	3:L:284:MET:H	1.80	0.45
1:A:36:TRP:CE2	1:A:80:LEU:HB2	2.52	0.45
3:F:207:LYS:NZ	3:F:219:GLU:OE2	2.49	0.45
3:F:285:GLN:O	3:F:289:VAL:HG22	2.16	0.45
2:J:161:GLU:OE2	2:J:175:LEU:HD11	2.17	0.45
2:O:21:ILE:HG23	2:O:102:THR:HG21	1.99	0.45
3:R:24:ILE:HD11	3:R:77:ARG:HH12	1.81	0.45
3:R:41:LEU:HG	3:R:50:GLN:OE1	2.17	0.45
3:R:152:SER:HB2	3:R:154:GLU:HG2	1.98	0.45
2:B:34:ASN:OD1	2:B:49:TYR:HA	2.16	0.45
3:F:71:VAL:HG11	3:F:172:VAL:CG1	2.45	0.45
3:R:119:VAL:HB	3:R:332:ARG:HG2	1.98	0.45
1:G:60:THR:HG1	1:G:62:TYR:HE1	1.61	0.45
2:J:208:SER:OG	2:J:209:PHE:N	2.49	0.45
1:N:36:TRP:CE2	1:N:83:LEU:HB2	2.51	0.45
1:C:36:TRP:O	1:C:48:LEU:HB2	2.17	0.45
1:N:88:LEU:HA	1:N:88:LEU:HD23	1.51	0.45
2:O:108:ARG:HD2	2:O:171:SER:HB2	1.99	0.45
2:O:164:THR:HG22	2:O:174:SER:H	1.82	0.45
1:G:47:TRP:CH2	1:G:49:GLY:HA2	2.52	0.45
3:L:135:PHE:HB2	3:L:208:ILE:HG22	1.98	0.45
1:C:108:TYR:CZ	3:F:186:ILE:HG22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:50:PHE:HE1	1:I:52:ARG:HE	1.65	0.45
3:K:126:GLY:O	3:K:171:ARG:NH1	2.36	0.45
1:N:2:VAL:HG13	1:N:27:PHE:CD1	2.51	0.45
3:R:247:TRP:CE3	3:R:311:PRO:HB2	2.52	0.45
3:E:281:ARG:HB2	3:E:304:ARG:HB2	1.99	0.45
3:F:198:SER:OG	3:F:239:ILE:O	2.32	0.45
3:K:280:CYS:HB3	3:K:303:CYS:O	2.17	0.45
3:R:183:MET:HE2	3:R:183:MET:HB3	1.93	0.45
1:A:124:LEU:N	1:A:139:GLY:O	2.47	0.44
3:E:80:VAL:HG13	3:E:172:VAL:O	2.17	0.44
3:E:107:LEU:HD13	3:E:138:TYR:CD2	2.52	0.44
1:C:3:LYS:O	1:C:4:LEU:HD23	2.17	0.44
1:C:21:SER:HB3	1:C:82:TYR:CD1	2.53	0.44
1:C:126:ALA:HB3	1:C:158:PHE:CE2	2.52	0.44
1:I:33:TYR:CE2	1:I:52:ARG:HG3	2.52	0.44
1:I:158:PHE:O	1:I:158:PHE:CD1	2.69	0.44
3:K:135:PHE:CE2	3:K:236:HIS:ND1	2.86	0.44
1:N:89:ARG:O	1:N:123:VAL:HG21	2.17	0.44
3:R:215:GLN:OE1	3:R:215:GLN:HA	2.17	0.44
3:L:195:LYS:O	3:L:199:GLN:HG3	2.17	0.44
1:A:87:SER:HB2	1:A:110:THR:HA	1.98	0.44
2:B:59:PRO:HD2	2:B:62:PHE:CD2	2.53	0.44
1:C:133:VAL:HG21	1:C:210:VAL:HG11	1.98	0.44
3:F:32:SER:OG	3:F:33:ASN:N	2.50	0.44
2:J:90:GLN:HE21	2:J:97:THR:HG22	1.81	0.44
2:J:120:PRO:CG	2:J:130:ALA:HB1	2.47	0.44
1:N:1:GLU:HG2	1:N:3:LYS:HE3	1.99	0.44
2:H:54:LEU:HD21	2:H:62:PHE:O	2.17	0.44
3:L:244:LYS:HB2	3:L:317:SER:O	2.16	0.44
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.52	0.44
2:B:145:LYS:HD2	2:B:145:LYS:HA	1.70	0.44
3:E:25:ILE:HD11	3:E:257:VAL:HG11	1.99	0.44
3:E:46:GLU:OE2	3:E:267:SER:HA	2.17	0.44
3:E:225:PHE:HB3	3:E:333:MET:O	2.16	0.44
1:C:185:SER:HB2	1:C:187:LEU:H	1.82	0.44
1:I:5:MET:HA	1:I:117:GLN:OE1	2.17	0.44
1:I:58:TYR:CD1	1:I:74:ARG:HG3	2.52	0.44
2:J:167:ASP:OD1	2:J:168:SER:N	2.50	0.44
2:J:194:CYS:SG	2:J:195:GLU:N	2.90	0.44
1:N:93:SER:CB	1:N:122:THR:HA	2.48	0.44
3:R:266:CYS:HB3	3:R:270:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:38:ILE:HG13	3:R:38:ILE:O	2.18	0.44
1:A:194:TYR:O	1:A:211:VAL:HG12	2.18	0.44
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.17	0.44
2:D:143:GLU:O	2:D:198:HIS:HD2	1.99	0.44
3:F:54:LEU:HD21	3:F:172:VAL:HG21	2.00	0.44
2:J:148:TRP:HE1	2:J:179:LEU:HD13	1.83	0.44
2:J:193:ALA:CB	2:J:208:SER:HA	2.48	0.44
3:K:224:PRO:HA	3:K:334:MET:CE	2.46	0.44
3:R:131:GLU:HA	3:R:140:GLY:HA2	2.00	0.44
1:G:36:TRP:HE1	1:G:81:LEU:HG	1.81	0.44
3:E:128:VAL:HG13	3:E:143:CYS:HB2	2.00	0.44
1:I:2:VAL:HG13	1:I:27:PHE:HD2	1.81	0.44
1:I:38:ARG:HG3	1:I:94:ALA:HB3	1.99	0.44
1:N:159:PRO:HD2	1:N:212:HIS:CE1	2.53	0.44
3:R:50:GLN:HE22	3:R:103:TRP:HZ2	1.65	0.44
1:A:33:TYR:O	1:A:34:MET:HG2	2.16	0.44
1:A:195:ILE:HG22	1:A:210:LYS:HA	2.00	0.44
1:C:41:PRO:O	1:C:43:LYS:HG2	2.18	0.44
2:D:25:ALA:O	2:D:69:THR:HB	2.17	0.44
1:I:158:PHE:HB3	1:I:159:PRO:HD3	1.99	0.44
2:J:183:LYS:O	2:J:187:GLU:HG3	2.18	0.44
3:L:183:MET:HB2	3:L:326:LYS:HA	2.00	0.44
1:A:123:PRO:HB2	1:A:211:VAL:HG23	1.99	0.44
1:I:159:PRO:HD2	1:I:212:HIS:HE2	1.83	0.44
3:R:261:GLU:H	3:R:261:GLU:HG3	1.46	0.44
3:E:25:ILE:HG22	3:E:26:CYS:SG	2.58	0.44
1:C:211:ASN:HB3	1:C:218:LYS:HG3	2.00	0.44
1:I:182:LEU:HD23	1:I:188:TYR:HE1	1.83	0.44
3:K:332:ARG:HE	3:K:332:ARG:HB2	1.55	0.44
2:O:125:LEU:HD12	2:O:183:LYS:HG3	2.00	0.44
1:G:70:PHE:HD1	1:G:85:MET:HA	1.83	0.44
1:A:51:ILE:HG21	1:A:78:LEU:HD11	2.00	0.43
2:D:125:LEU:HD13	2:D:125:LEU:HA	1.86	0.43
1:I:14:PRO:CD	1:I:125:SER:HB2	2.35	0.43
2:J:148:TRP:CE2	2:J:179:LEU:HB2	2.53	0.43
1:N:34:MET:HG3	1:N:81:LEU:HD22	2.00	0.43
1:N:180:ALA:HA	1:N:190:LEU:HB3	1.99	0.43
2:O:6:GLN:HE21	2:O:35:TRP:HZ3	1.64	0.43
2:O:46:LEU:HD23	2:O:55:HIS:ND1	2.32	0.43
3:L:81:SER:O	3:L:173:LEU:HA	2.18	0.43
1:A:188:SER:HB2	1:A:192:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:ILE:HA	3:E:56:HIS:ND1	2.33	0.43
1:C:24:ILE:HD12	1:C:27:PHE:HZ	1.83	0.43
1:C:38:ARG:HB2	1:C:48:LEU:HD11	2.01	0.43
1:C:69:ARG:O	1:C:86:ASN:HB2	2.17	0.43
3:F:79:GLN:O	3:F:169:SER:HB2	2.18	0.43
1:I:179:PRO:O	1:I:180:ALA:HB3	2.18	0.43
3:K:83:TYR:CG	3:K:122:PRO:HG3	2.53	0.43
3:E:150:THR:HG22	3:E:155:LEU:H	1.84	0.43
1:C:79:SER:O	1:C:80:ILE:HG13	2.18	0.43
1:C:135:PRO:O	1:C:136:LEU:HD23	2.18	0.43
3:K:227:VAL:HG22	3:K:228:ALA:O	2.18	0.43
2:O:201:LEU:HD23	2:O:201:LEU:HA	1.74	0.43
3:R:272:LYS:HB3	3:R:272:LYS:HE2	1.71	0.43
1:A:12:VAL:HG21	1:A:82(C):LEU:HD12	1.99	0.43
1:A:67:PHE:HD1	1:A:67:PHE:N	2.17	0.43
1:A:208:ASP:OD1	1:A:208:ASP:N	2.51	0.43
3:E:31:HIS:ND1	3:E:70:TYR:CD2	2.87	0.43
2:O:193:ALA:CB	2:O:208:SER:HB3	2.49	0.43
3:R:61:LEU:HD23	3:R:61:LEU:HA	1.91	0.43
2:D:19:VAL:O	2:D:74:THR:HA	2.18	0.43
3:F:200:SER:O	3:F:203:PRO:HD3	2.17	0.43
1:I:154:VAL:HG23	1:I:157:TYR:HE2	1.83	0.43
3:K:302:LYS:HA	3:K:302:LYS:HD3	1.67	0.43
3:L:247:TRP:CE3	3:L:311:PRO:HB2	2.54	0.43
1:A:66:ARG:NH2	1:A:86:ASP:OD1	2.52	0.43
2:D:120:PRO:HB2	2:D:125:LEU:CD2	2.48	0.43
3:K:31:HIS:HB2	3:K:166:LEU:HD22	2.00	0.43
2:O:85:THR:HA	2:O:103:LYS:HA	2.00	0.43
2:H:62:PHE:CE1	2:H:75:ILE:HG12	2.54	0.43
3:L:33:ASN:ND2	3:L:35:SER:HB3	2.34	0.43
3:L:125:LYS:HD3	3:L:151:GLU:HB2	2.01	0.43
3:L:150:THR:HG22	3:L:152:SER:H	1.83	0.43
2:D:46:LEU:HG	2:D:55:HIS:HB2	2.00	0.43
2:D:195:GLU:HG3	2:D:206:THR:OG1	2.19	0.43
3:F:217:GLU:HG2	3:F:218:GLY:N	2.34	0.43
1:I:159:PRO:HG2	1:I:214:PRO:HB2	2.01	0.43
2:J:150:VAL:HG12	2:J:192:TYR:HE1	1.79	0.43
3:R:150:THR:HG23	3:R:153:GLY:H	1.83	0.43
1:G:1:GLU:HG2	1:G:3:LYS:HE3	1.99	0.43
1:G:38:ARG:HB3	1:G:96:TYR:CE2	2.54	0.43
3:L:181:GLN:HB2	3:L:313:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:207:LYS:HA	3:K:211:ILE:O	2.19	0.43
3:E:81:SER:O	3:E:173:LEU:HD12	2.18	0.43
2:D:107:LYS:HA	2:D:140:TYR:OH	2.18	0.43
2:D:187:GLU:HA	2:D:211:ARG:NH2	2.34	0.43
2:J:113:PRO:HB3	2:J:139:PHE:HB3	2.01	0.43
3:R:67:PHE:HE1	3:R:69:GLY:C	2.22	0.43
3:R:302:LYS:HA	3:R:302:LYS:HD3	1.90	0.43
1:G:1:GLU:HB3	1:G:3:LYS:HE3	1.99	0.43
1:G:6:GLU:OE2	1:G:116:GLY:HA3	2.19	0.43
1:A:156:SER:N	1:A:197:ASN:HD21	2.15	0.43
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.24	0.43
3:F:208:ILE:HA	3:F:334:MET:O	2.19	0.43
1:I:153:LEU:HD12	1:I:190:LEU:O	2.19	0.43
2:J:161:GLU:OE2	2:J:175:LEU:HD21	2.19	0.43
2:H:94:PHE:HB2	3:L:188:GLU:OE2	2.19	0.43
3:L:230:MET:HG3	3:L:232:VAL:HG13	2.00	0.43
3:L:245:THR:HG21	3:L:328:TYR:CZ	2.54	0.43
2:B:147:GLN:N	2:B:195:GLU:O	2.40	0.42
2:J:141:PRO:HD2	2:J:199:GLN:CD	2.39	0.42
1:A:67:PHE:N	1:A:67:PHE:CD1	2.86	0.42
2:B:184:ALA:HB1	2:B:188:LYS:HE3	2.00	0.42
2:D:175:LEU:HD23	2:D:176:SER:N	2.34	0.42
3:F:202:PHE:CE2	3:F:239:ILE:HG13	2.54	0.42
3:R:54:LEU:CD2	3:R:77:ARG:HA	2.50	0.42
2:H:92:SER:O	2:H:93:LYS:HD2	2.19	0.42
1:A:55:TYR:CD1	1:A:71:ARG:HD3	2.54	0.42
2:B:19:VAL:O	2:B:74:THR:HA	2.19	0.42
3:E:130:PHE:CE1	3:E:149:ARG:HD2	2.51	0.42
1:I:170:ALA:O	1:I:172:THR:HG23	2.19	0.42
3:K:192:LEU:HD23	3:K:192:LEU:HA	1.73	0.42
1:N:89:ARG:HG3	1:N:89:ARG:HH11	1.84	0.42
2:O:125:LEU:C	2:O:127:SER:N	2.72	0.42
3:R:67:PHE:CD1	3:R:67:PHE:C	2.92	0.42
3:E:88:SER:O	3:E:91:ARG:HB2	2.19	0.42
3:E:184:THR:HG23	3:E:324:ARG:HD2	2.01	0.42
3:F:252:SER:OG	3:F:253:SER:N	2.51	0.42
2:J:187:GLU:HA	2:J:211:ARG:HH11	1.77	0.42
3:R:47:LYS:O	3:R:51:ILE:HG13	2.20	0.42
3:R:71:VAL:HG12	3:R:72:GLY:N	2.34	0.42
2:H:38:GLN:O	2:H:84:ALA:HB1	2.19	0.42
1:A:119:PRO:HD2	1:A:205:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:HIS:CD2	1:C:214:PRO:HD2	2.54	0.42
2:J:183:LYS:HD2	2:J:183:LYS:HA	1.74	0.42
3:K:39:PRO:HB2	3:K:41:LEU:HD21	2.02	0.42
1:N:11:LEU:HA	1:N:11:LEU:HD23	1.62	0.42
1:N:131:PRO:HB2	1:N:154:VAL:HG22	2.00	0.42
1:N:163:THR:HG23	1:N:211:ASN:OD1	2.18	0.42
2:O:151:ASP:HA	2:O:191:VAL:HG13	2.01	0.42
3:L:194:LEU:HD11	3:L:323:VAL:HG21	2.01	0.42
2:B:103:LYS:HB3	2:B:103:LYS:HE2	1.77	0.42
2:D:11:LEU:C	2:D:11:LEU:HD23	2.39	0.42
3:F:268:GLU:O	3:F:272:LYS:HB2	2.19	0.42
1:I:182:LEU:HD23	1:I:188:TYR:CE1	2.54	0.42
2:J:54:LEU:HA	2:J:54:LEU:HD23	1.79	0.42
1:N:51:ILE:CG2	1:N:74:ARG:HD2	2.47	0.42
1:A:126:PRO:CB	1:A:189:LEU:HD21	2.50	0.42
3:E:167:LEU:HA	3:E:167:LEU:HD13	1.79	0.42
3:F:222:PRO:HA	3:F:336:THR:HG22	2.01	0.42
3:F:286:PHE:CD1	3:F:286:PHE:C	2.93	0.42
2:J:108:ARG:CG	2:J:109:THR:N	2.81	0.42
3:K:119:VAL:HG12	3:K:334:MET:HE3	2.01	0.42
3:K:197:PHE:CE2	3:K:319:GLY:HA2	2.54	0.42
2:O:201:LEU:HD11	2:O:205:VAL:HG12	2.01	0.42
3:R:94:GLY:HA3	3:R:308:VAL:HG12	2.02	0.42
1:G:51:ILE:HG12	1:G:74:ARG:CD	2.49	0.42
3:E:195:LYS:O	3:E:199:GLN:HG3	2.19	0.42
2:D:55:HIS:CG	2:D:56:SER:N	2.87	0.42
3:K:211:ILE:HD13	3:K:211:ILE:HA	1.85	0.42
1:N:33:TYR:HB2	1:N:101:ASP:HB2	2.02	0.42
1:N:131:PRO:HB3	1:N:157:TYR:HB3	2.01	0.42
3:R:87:ASN:OD1	3:R:90:SER:HB3	2.19	0.42
2:H:19:VAL:HG11	2:H:104:LEU:HD21	2.02	0.42
3:E:229:TRP:CD2	3:E:237:LYS:HD3	2.55	0.42
1:C:146:GLY:N	1:C:198:SER:HG	2.18	0.42
1:I:179:PRO:HG2	2:J:162:SER:OG	2.19	0.42
1:G:104:TYR:HD2	1:G:109:TYR:CD2	2.37	0.42
1:A:47:TRP:HZ2	1:A:50:PHE:CD2	2.13	0.42
1:C:39:GLN:HB2	1:C:45:LEU:HD23	2.02	0.42
1:C:66:VAL:HB	1:C:70:PHE:HB2	2.02	0.42
1:I:128:THR:HG22	1:N:215:SER:HA	2.02	0.42
1:I:157:TYR:OH	1:I:162:VAL:HG11	2.20	0.42
3:K:119:VAL:O	3:K:124:TYR:OH	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:6:GLU:OE2	1:N:98:CYS:N	2.33	0.42
1:N:113:ASP:HA	2:O:46:LEU:HD22	2.02	0.42
1:G:12:VAL:HG21	1:G:88:LEU:HD13	2.01	0.42
3:L:159:ASP:O	3:L:162:THR:OG1	2.34	0.42
2:B:86:TYR:O	2:B:101:GLY:HA2	2.20	0.41
3:E:71:VAL:HG12	3:E:72:GLY:H	1.84	0.41
2:J:166:GLN:HB2	2:J:173:TYR:CZ	2.55	0.41
1:N:12:VAL:HG23	1:N:123:VAL:HG12	2.02	0.41
1:N:18:LEU:HD12	1:N:19:ARG:N	2.35	0.41
1:N:53:ASN:HD21	1:N:55:ALA:HB3	1.85	0.41
2:O:125:LEU:O	2:O:127:SER:N	2.52	0.41
3:R:198:SER:OG	3:R:239:ILE:O	2.26	0.41
3:R:199:GLN:HG2	3:R:214:ASN:HD21	1.84	0.41
3:L:64:HIS:CE1	3:L:111:LYS:HB2	2.55	0.41
3:L:132:ARG:NH2	3:L:209:ASP:OD1	2.33	0.41
2:B:163:VAL:HG12	2:B:164:THR:O	2.20	0.41
1:C:113:ASP:OD1	1:C:114:TYR:HD1	2.04	0.41
2:D:41:ASP:CG	2:D:43:THR:HG23	2.40	0.41
2:J:78:LEU:HD11	2:J:104:LEU:HD23	2.02	0.41
3:K:310:LYS:HG3	3:K:312:GLY:H	1.85	0.41
1:G:113:ASP:HA	2:H:46:LEU:HD22	2.01	0.41
3:L:191:PHE:CE1	3:L:238:ILE:HD11	2.55	0.41
3:L:284:MET:HG2	3:L:285:GLN:HG2	2.00	0.41
3:E:256:PHE:CD1	3:E:307:LEU:HA	2.53	0.41
3:E:285:GLN:O	3:E:289:VAL:HG22	2.20	0.41
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.55	0.41
2:J:115:VAL:HA	2:J:135:LEU:O	2.19	0.41
3:K:186:ILE:HD11	3:K:232:VAL:HB	2.01	0.41
2:O:119:PRO:HB3	2:O:209:PHE:CZ	2.56	0.41
2:O:120:PRO:HB3	2:O:131:SER:H	1.85	0.41
3:R:255:ASP:OD1	3:R:310:LYS:NZ	2.25	0.41
1:G:51:ILE:HG12	1:G:74:ARG:HG3	2.02	0.41
1:A:66:ARG:HH12	1:A:83:ARG:NE	2.17	0.41
2:B:122:ASP:O	2:B:126:LYS:HG3	2.21	0.41
2:D:151:ASP:HB3	2:D:191:VAL:H	1.84	0.41
1:I:76:ASN:OD1	1:I:76:ASN:C	2.58	0.41
2:J:46:LEU:HD12	2:J:47:LEU:H	1.86	0.41
3:K:117:MET:CB	3:K:334:MET:HG3	2.51	0.41
3:K:117:MET:HB3	3:K:334:MET:HG3	2.02	0.41
1:N:12:VAL:CG2	1:N:123:VAL:HG12	2.50	0.41
3:R:122:PRO:HG2	3:R:175:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:227:VAL:HG22	3:R:228:ALA:O	2.21	0.41
1:G:70:PHE:CD1	1:G:85:MET:HA	2.55	0.41
1:G:88:LEU:HD23	1:G:88:LEU:HA	1.93	0.41
2:H:62:PHE:CD1	2:H:75:ILE:HG12	2.55	0.41
2:B:78:LEU:HD12	2:B:82:ASP:HB2	2.03	0.41
3:E:87:ASN:HD21	3:E:177:ASP:HA	1.86	0.41
3:E:166:LEU:HD23	3:E:166:LEU:HA	1.79	0.41
2:O:118:PHE:HA	2:O:119:PRO:HD3	1.89	0.41
2:O:125:LEU:HB3	2:O:183:LYS:HE2	2.02	0.41
3:R:213:PHE:CZ	3:R:239:ILE:HD11	2.56	0.41
1:A:53:LYS:HA	1:A:53:LYS:HD2	1.89	0.41
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.90	0.41
3:E:65:SER:O	3:E:66:GLN:HB2	2.19	0.41
1:C:9:GLY:HA3	1:C:119:THR:HG22	2.03	0.41
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.56	0.41
3:F:134:THR:HG21	3:F:139:VAL:CG2	2.51	0.41
2:J:193:ALA:HB3	2:J:208:SER:HA	2.02	0.41
2:O:186:TYR:CE1	2:O:192:TYR:CE2	3.08	0.41
3:R:232:VAL:HG12	3:R:323:VAL:HG11	2.03	0.41
3:E:252:SER:OG	3:E:253:SER:N	2.54	0.41
3:F:256:PHE:HA	3:F:306:SER:O	2.21	0.41
1:I:165:SER:O	1:I:209:ASN:N	2.45	0.41
1:I:218:LYS:HD2	1:N:13:GLN:HE21	1.83	0.41
2:J:27:GLN:C	2:J:69:THR:HG22	2.41	0.41
3:K:259:TYR:HA	3:K:265:PRO:HA	2.02	0.41
2:H:83:ILE:HG23	2:H:104:LEU:O	2.20	0.41
3:E:207:LYS:HG2	3:E:212:VAL:HA	2.02	0.41
3:F:61:LEU:HD21	3:F:129:PHE:HB2	2.03	0.41
1:N:207:ILE:HD11	1:N:222:LYS:CG	2.50	0.41
1:N:212:HIS:HB3	1:N:217:THR:HG22	2.03	0.41
3:R:281:ARG:CZ	3:R:304:ARG:HB2	2.51	0.41
2:H:27:GLN:C	2:H:69:THR:HG22	2.40	0.41
1:A:33:TYR:C	1:A:34:MET:HG2	2.41	0.41
2:B:30:SER:O	2:B:30:SER:OG	2.39	0.41
3:E:71:VAL:HG12	3:E:72:GLY:N	2.35	0.41
1:C:90:ALA:O	1:C:93:SER:HB3	2.20	0.41
2:D:41:ASP:N	2:D:41:ASP:OD1	2.54	0.41
2:D:94:PHE:O	2:D:96:ARG:N	2.53	0.41
2:D:143:GLU:H	2:D:143:GLU:CD	2.24	0.41
3:F:79:GLN:HB3	3:F:169:SER:CB	2.43	0.41
2:J:4:MET:HB2	2:J:99:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:197:THR:HG22	2:J:198:HIS:N	2.20	0.41
3:K:43:GLY:HA3	3:K:46:GLU:HG3	2.03	0.41
3:K:101:ALA:HB1	3:K:106:MET:HB2	2.02	0.41
3:K:205:ILE:HG23	3:K:335:ALA:HB1	2.02	0.41
1:N:37:VAL:HG22	1:N:47:TRP:HA	2.01	0.41
1:N:62:TYR:OH	1:N:71:THR:HA	2.20	0.41
1:N:103:ARG:HA	1:N:109:TYR:O	2.20	0.41
2:O:186:TYR:HE1	2:O:192:TYR:CE2	2.39	0.41
3:R:51:ILE:HA	3:R:56:HIS:CE1	2.56	0.41
3:R:280:CYS:O	3:R:292:CYS:HB2	2.21	0.41
1:G:113:ASP:CG	1:G:114:TYR:HD1	2.24	0.41
2:B:125:LEU:C	2:B:127:SER:H	2.24	0.41
3:E:29:PRO:HG3	3:E:53:ARG:HB3	2.03	0.41
3:F:240:MET:HB3	3:F:318:TYR:CE1	2.56	0.41
3:F:282:GLY:HA2	3:F:304:ARG:HG3	2.03	0.41
1:I:1:GLU:O	1:I:26:GLY:HA3	2.20	0.41
1:I:50:PHE:C	1:I:50:PHE:CD1	2.95	0.41
1:I:153:LEU:HD23	2:J:124:GLN:HE22	1.86	0.41
2:J:35:TRP:CG	2:J:73:LEU:HD13	2.56	0.41
2:O:21:ILE:O	2:O:72:SER:HA	2.20	0.41
3:R:130:PHE:HA	3:R:173:LEU:O	2.20	0.41
1:G:43:LYS:N	1:G:43:LYS:HD2	2.36	0.41
1:A:6:GLU:OE2	1:A:92:CYS:N	2.39	0.40
2:B:134:CYS:HB2	2:B:148:TRP:CZ2	2.55	0.40
3:E:147:LYS:HD3	3:E:158:SER:HA	2.04	0.40
1:C:158:PHE:HD1	1:C:158:PHE:HA	1.72	0.40
3:F:132:ARG:HB3	3:F:175:ILE:HD12	2.03	0.40
1:N:133:VAL:HG11	1:N:219:VAL:HG23	2.02	0.40
1:N:175:VAL:HA	1:N:194:VAL:HA	2.02	0.40
1:N:177:THR:HA	1:N:192:SER:HA	2.04	0.40
2:O:154:LEU:CD1	3:L:154:GLU:HG2	2.51	0.40
3:L:61:LEU:CD1	3:L:71:VAL:HG21	2.51	0.40
3:E:147:LYS:HZ3	3:E:158:SER:N	2.19	0.40
2:D:30:SER:HB3	2:D:32:TYR:CD2	2.56	0.40
2:D:31:ASN:HB3	2:D:51:THR:OG1	2.21	0.40
2:D:132:VAL:HG12	2:D:148:TRP:HH2	1.86	0.40
1:I:157:TYR:CE1	1:I:188:TYR:HB2	2.55	0.40
1:I:207:ILE:HA	1:I:222:LYS:HA	2.03	0.40
2:J:149:LYS:HZ2	2:J:154:LEU:HA	1.86	0.40
2:J:149:LYS:HB3	2:J:153:ALA:O	2.21	0.40
2:J:175:LEU:HD23	2:J:176:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:119:VAL:HG13	3:K:132:ARG:NE	2.37	0.40
2:O:161:GLU:CG	2:O:175:LEU:HD21	2.52	0.40
3:R:240:MET:HB2	3:R:243:HIS:ND1	2.37	0.40
3:E:30:ILE:HA	3:E:73:GLN:NE2	2.34	0.40
1:C:21:SER:HB3	1:C:82:TYR:HD1	1.87	0.40
3:F:243:HIS:NE2	3:F:328:TYR:OH	2.39	0.40
2:J:121:SER:O	2:J:124:GLN:HB3	2.21	0.40
3:K:205:ILE:CG2	3:K:335:ALA:HB1	2.51	0.40
3:R:48:ILE:HG21	3:R:257:VAL:HG11	2.04	0.40
1:G:33:TYR:HB2	1:G:101:ASP:HB2	2.03	0.40
3:L:41:LEU:HD13	3:L:46:GLU:HG2	2.02	0.40
2:B:39:LYS:HZ3	2:B:39:LYS:HG2	1.73	0.40
2:J:83:ILE:HG23	2:J:104:LEU:O	2.22	0.40
3:K:25:ILE:HG22	3:K:26:CYS:SG	2.61	0.40
3:K:131:GLU:HG2	3:K:132:ARG:N	2.36	0.40
2:O:120:PRO:HG2	2:O:186:TYR:CE2	2.56	0.40
3:R:92:TRP:CE2	3:R:311:PRO:HG3	2.57	0.40
1:G:1:GLU:O	1:G:26:GLY:HA3	2.21	0.40
1:G:103:ARG:HA	1:G:109:TYR:O	2.21	0.40
1:A:40:PRO:HB2	1:A:43:LYS:CD	2.52	0.40
3:E:224:PRO:HA	3:E:334:MET:CE	2.51	0.40
1:C:131:PRO:HB2	1:C:154:VAL:CG1	2.51	0.40
3:F:162:THR:CG2	3:F:171:ARG:HE	2.35	0.40
2:J:118:PHE:HA	2:J:119:PRO:HD3	1.85	0.40
3:K:81:SER:O	3:K:173:LEU:HA	2.22	0.40
3:R:24:ILE:HD13	3:R:24:ILE:HG21	1.84	0.40
3:L:29:PRO:HG3	3:L:53:ARG:CB	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	215/256 (84%)	198 (92%)	14 (6%)	3 (1%)	11 36
1	C	216/256 (84%)	202 (94%)	11 (5%)	3 (1%)	11 36
1	G	122/256 (48%)	116 (95%)	6 (5%)	0	100 100
1	I	216/256 (84%)	200 (93%)	13 (6%)	3 (1%)	11 36
1	N	215/256 (84%)	200 (93%)	14 (6%)	1 (0%)	29 60
2	B	208/233 (89%)	201 (97%)	7 (3%)	0	100 100
2	D	208/233 (89%)	195 (94%)	13 (6%)	0	100 100
2	H	103/233 (44%)	93 (90%)	9 (9%)	1 (1%)	15 45
2	J	211/233 (91%)	193 (92%)	16 (8%)	2 (1%)	17 47
2	O	210/233 (90%)	198 (94%)	11 (5%)	1 (0%)	29 60
3	E	305/357 (85%)	292 (96%)	11 (4%)	2 (1%)	22 52
3	F	305/357 (85%)	288 (94%)	16 (5%)	1 (0%)	41 70
3	K	307/357 (86%)	293 (95%)	14 (5%)	0	100 100
3	L	305/357 (85%)	293 (96%)	12 (4%)	0	100 100
3	R	305/357 (85%)	291 (95%)	14 (5%)	0	100 100
All	All	3451/4230 (82%)	3253 (94%)	181 (5%)	17 (0%)	29 60

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	147	PRO
1	C	105	ASP
1	C	159	PRO
1	I	160	GLU
2	J	193	ALA
1	I	216	ASN
3	E	150	THR
2	H	7	THR
3	F	290	ALA
1	I	162	VAL
2	O	126	LYS
1	A	126	PRO
1	C	58	TYR
2	J	126	LYS
1	N	58	TYR
3	E	83	TYR

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	187/219 (85%)	184 (98%)	3 (2%)	62 83
1	C	188/219 (86%)	182 (97%)	6 (3%)	39 68
1	G	105/219 (48%)	101 (96%)	4 (4%)	33 63
1	I	188/219 (86%)	185 (98%)	3 (2%)	62 83
1	N	187/219 (85%)	183 (98%)	4 (2%)	53 77
2	B	187/204 (92%)	184 (98%)	3 (2%)	62 83
2	D	187/204 (92%)	182 (97%)	5 (3%)	44 71
2	H	92/204 (45%)	91 (99%)	1 (1%)	73 88
2	J	189/204 (93%)	181 (96%)	8 (4%)	30 60
2	O	188/204 (92%)	186 (99%)	2 (1%)	73 88
3	E	268/309 (87%)	266 (99%)	2 (1%)	84 92
3	F	268/309 (87%)	262 (98%)	6 (2%)	52 76
3	K	270/309 (87%)	263 (97%)	7 (3%)	46 72
3	L	268/309 (87%)	263 (98%)	5 (2%)	57 79
3	R	268/309 (87%)	263 (98%)	5 (2%)	57 79
All	All	3040/3660 (83%)	2976 (98%)	64 (2%)	53 77

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	196	CYS
1	A	208	ASP
2	B	30	SER
2	B	107	LYS
2	B	183	LYS
3	E	183	MET
3	E	204	ASP
1	C	22	CYS
1	C	89	ARG

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Mol	Chain	Res	Type
1	C	117	GLN
1	C	150	LEU
1	C	158	PHE
1	C	208	CYS
2	D	108	ARG
2	D	145	LYS
2	D	152	ASN
2	D	169	LYS
2	D	207	LYS
3	F	34	LYS
3	F	56	HIS
3	F	125	LYS
3	F	143	CYS
3	F	246	LYS
3	F	253	SER
1	I	50	PHE
1	I	109	TYR
1	I	152	CYS
2	J	18	ARG
2	J	22	SER
2	J	27	GLN
2	J	33	LEU
2	J	108	ARG
2	J	126	LYS
2	J	148	TRP
2	J	182	SER
3	K	40	HIS
3	K	86	GLU
3	K	183	MET
3	K	197	PHE
3	K	216	CYS
3	K	241	ARG
3	K	274	CYS
1	N	85	MET
1	N	98	CYS
1	N	117	GLN
1	N	220	ASP
2	O	17	ASP
2	O	134	CYS
3	R	91	ARG
3	R	158	SER
3	R	183	MET

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Mol	Chain	Res	Type
3	R	283	ASP
3	R	322	ARG
1	G	3	LYS
1	G	38	ARG
1	G	43	LYS
1	G	85	MET
2	H	89	GLN
3	L	42	LEU
3	L	148	SER
3	L	267	SER
3	L	284	MET
3	L	304	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	89	GLN
3	E	73	GLN
2	D	155	GLN
2	D	198	HIS
3	F	285	GLN
3	K	87	ASN
1	N	13	GLN
1	N	53	ASN
2	O	189	HIS
3	R	50	GLN
3	R	73	GLN
3	R	214	ASN
1	G	39	GLN
2	H	38	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/256 (85%)	-0.08	1 (0%) 91 79	5, 16, 39, 47	0
1	C	220/256 (85%)	0.02	5 (2%) 60 36	5, 16, 53, 70	0
1	G	124/256 (48%)	1.19	28 (22%) 0 0	75, 93, 114, 127	0
1	I	220/256 (85%)	0.14	8 (3%) 42 21	11, 33, 97, 106	0
1	N	219/256 (85%)	0.04	6 (2%) 54 28	9, 38, 74, 86	0
2	B	210/233 (90%)	-0.15	1 (0%) 91 79	6, 21, 58, 76	0
2	D	210/233 (90%)	0.05	5 (2%) 59 34	5, 18, 58, 64	0
2	H	105/233 (45%)	1.53	34 (32%) 0 0	85, 110, 129, 137	0
2	J	213/233 (91%)	0.33	18 (8%) 10 4	8, 49, 105, 116	0
2	O	212/233 (90%)	0.11	5 (2%) 59 34	10, 42, 78, 105	0
3	E	309/357 (86%)	0.26	21 (6%) 17 6	10, 56, 83, 101	0
3	F	309/357 (86%)	0.21	16 (5%) 27 11	11, 39, 80, 93	0
3	K	311/357 (87%)	0.07	6 (1%) 66 43	14, 33, 67, 85	0
3	L	309/357 (86%)	0.85	55 (17%) 1 0	56, 81, 117, 143	0
3	R	309/357 (86%)	0.17	13 (4%) 36 17	16, 44, 73, 99	0
All	All	3499/4230 (82%)	0.25	222 (6%) 20 8	5, 40, 103, 143	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	18	LEU	14.1
2	H	13	ALA	8.2
2	H	12	SER	7.6
2	H	106	ILE	7.3
1	G	16	ASP	6.5
3	L	303	CYS	6.3
3	L	242	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
3	L	258	CYS	6.0
3	L	277	SER	6.0
3	L	276	THR	5.9
3	L	217	GLU	5.8
3	F	289	VAL	5.6
2	J	197	THR	5.5
2	O	183	LYS	5.4
1	G	28	THR	5.4
2	H	83	ILE	5.3
3	L	273	THR	5.0
2	H	63	SER	5.0
3	L	305	CYS	5.0
1	G	1	GLU	5.0
2	J	187	GLU	4.9
1	G	17	SER	4.8
2	H	74	THR	4.7
3	L	288	LYS	4.7
2	H	105	GLU	4.6
1	G	85	MET	4.5
2	H	5	THR	4.5
2	H	15	LEU	4.5
2	H	14	SER	4.5
3	R	288	LYS	4.4
2	H	80	PRO	4.4
3	E	277	SER	4.4
3	L	215	GLN	4.4
1	G	93	SER	4.3
1	I	203	THR	4.3
1	G	109	TYR	4.2
1	G	24	ILE	4.2
3	L	275	LYS	4.1
2	H	78	LEU	4.0
2	H	26	SER	3.9
1	G	10	GLY	3.9
3	L	289	VAL	3.9
3	E	275	LYS	3.8
2	H	67	SER	3.8
2	J	204	PRO	3.8
1	G	11	LEU	3.8
2	H	36	TYR	3.7
3	F	303	CYS	3.7
3	L	282	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	92	ASP	3.6
2	H	27	GLN	3.6
1	G	123	VAL	3.6
3	L	274	CYS	3.6
1	G	122	THR	3.6
3	E	280	CYS	3.6
2	J	134	CYS	3.6
3	L	216	CYS	3.5
3	L	286	PHE	3.4
1	G	23	ALA	3.4
3	R	285	GLN	3.4
2	H	79	GLU	3.4
1	N	158	PHE	3.4
3	L	67	PHE	3.3
3	L	68	GLN	3.3
2	H	16	GLY	3.3
3	F	37	ASP	3.2
3	E	291	GLY	3.2
2	O	182	SER	3.2
2	D	134	CYS	3.2
1	G	2	VAL	3.2
3	E	216	CYS	3.2
3	F	276	THR	3.2
1	I	124	SER	3.2
1	G	12	VAL	3.2
3	E	289	VAL	3.1
1	G	124	SER	3.1
2	D	177	SER	3.1
2	H	11	LEU	3.1
3	R	275	LYS	3.1
1	G	27	PHE	3.1
2	J	151	ASP	3.1
3	L	292	CYS	3.1
2	H	25	ALA	3.1
3	L	88	SER	3.0
2	J	205	VAL	3.0
3	K	97	SER	3.0
3	L	150	THR	3.0
2	J	144	ALA	3.0
2	J	143	GLU	3.0
2	J	198	HIS	3.0
1	I	204	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	199	SER	2.9
3	L	280	CYS	2.9
3	L	42	LEU	2.9
3	L	281	ARG	2.9
2	H	69	THR	2.9
3	L	156	CYS	2.9
3	L	266	CYS	2.9
3	L	236	HIS	2.9
3	R	217	GLU	2.9
3	L	318	TYR	2.9
3	E	69	GLY	2.9
3	F	275	LYS	2.9
2	D	210	ASN	2.8
2	J	153	ALA	2.8
3	R	155	LEU	2.8
2	B	183	LYS	2.8
2	H	66	GLY	2.8
2	H	77	ASN	2.8
3	L	316	VAL	2.8
1	G	104	TYR	2.8
3	L	69	GLY	2.8
3	E	288	LYS	2.8
2	J	213	GLU	2.8
3	L	256	PHE	2.8
1	C	225	PRO	2.7
3	E	256	PHE	2.7
2	H	29	ILE	2.7
3	E	279	SER	2.7
3	E	68	GLN	2.7
3	K	38	ILE	2.7
3	L	149	ARG	2.7
1	N	82	TYR	2.7
1	G	29	PHE	2.7
3	R	289	VAL	2.6
1	G	31	ASP	2.6
1	G	117	GLN	2.6
2	O	185	ASP	2.6
3	L	73	GLN	2.6
1	N	146	GLY	2.6
3	L	261	GLU	2.6
2	J	154	LEU	2.6
3	F	277	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	178	THR	2.6
1	C	151	GLY	2.6
1	C	35	SER	2.6
3	L	285	GLN	2.6
2	J	177	SER	2.6
2	O	205	VAL	2.5
3	L	271	GLU	2.5
3	L	165	GLY	2.5
1	N	35	SER	2.5
2	H	53	ILE	2.5
3	L	287	CYS	2.5
2	H	68	GLY	2.5
3	L	35	SER	2.5
3	L	123	SER	2.5
2	H	28	GLY	2.4
3	F	280	CYS	2.4
1	A	35	SER	2.4
3	L	221	LEU	2.4
1	I	224	GLU	2.4
3	L	284	MET	2.4
3	L	279	SER	2.4
3	L	219	GLU	2.4
3	F	166	LEU	2.4
3	R	216	CYS	2.4
3	E	290	ALA	2.4
2	J	150	VAL	2.4
3	L	269	SER	2.4
3	F	157	SER	2.3
2	H	30	SER	2.3
3	K	99	CYS	2.3
1	G	78	GLN	2.3
2	H	82	ASP	2.3
2	J	188	LYS	2.3
3	R	339	VAL	2.3
3	E	276	THR	2.3
1	C	152	CYS	2.3
1	N	196	VAL	2.3
3	L	218	GLY	2.3
3	L	260	LYS	2.3
3	K	289	VAL	2.3
3	E	42	LEU	2.3
3	F	258	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	158	PHE	2.3
2	H	87	TYR	2.3
2	H	50	TYR	2.3
3	L	91	ARG	2.2
2	D	176	SER	2.2
3	L	283	ASP	2.2
3	E	303	CYS	2.2
3	R	99	CYS	2.2
3	E	278	GLY	2.2
2	O	177	SER	2.2
3	F	268	GLU	2.2
1	I	206	TYR	2.2
3	F	270	GLU	2.2
3	E	130	PHE	2.2
3	E	331	SER	2.2
3	L	319	GLY	2.2
3	L	30	ILE	2.2
1	G	89	ARG	2.2
3	L	86	GLU	2.1
3	E	99	CYS	2.1
3	E	335	ALA	2.1
2	H	45	LYS	2.1
3	F	260	LYS	2.1
3	F	285	GLN	2.1
3	R	281	ARG	2.1
1	N	199	SER	2.1
2	J	140	TYR	2.1
1	C	226	LYS	2.1
3	F	340	SER	2.1
3	R	97	SER	2.1
2	J	145	LYS	2.1
3	K	154	GLU	2.1
3	L	148	SER	2.1
3	R	304	ARG	2.1
2	J	184	ALA	2.1
3	R	290	ALA	2.1
3	L	259	TYR	2.1
3	L	74	ARG	2.1
1	G	32	TYR	2.1
3	K	133	PRO	2.1
1	G	26	GLY	2.1
2	H	10	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	23	CYS	2.1
3	E	97	SER	2.0
1	I	139	SER	2.0
3	F	290	ALA	2.0
1	G	76	ASN	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.