Full wwPDB EM Validation Report ⓘ

Jul 24, 2024 – 04:29 PM JST

PDB ID	:	8YVG
EMDB ID	:	EMD-39600
Title	:	canine immunoproteasome 20S subunit in complex with compound 1
Authors	:	Kashima, A.; Arai, Y.
Deposited on	:	2024-03-28
Resolution	:	2.00 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:

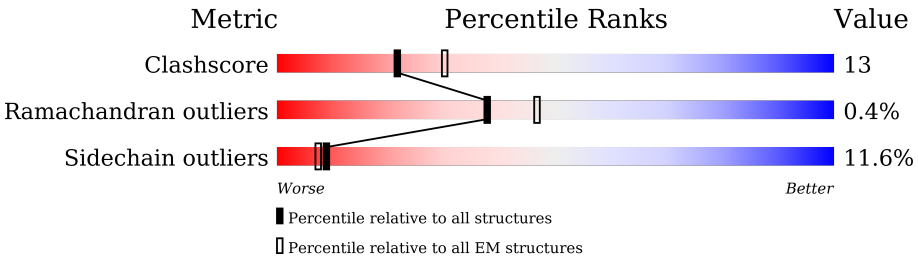
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	H	241	66% 22% 5% 7%
1	M	241	67% 22% 7%
2	I	248	24% 53% 31% 9% 7%
2	N	248	24% 54% 29% 10% 7%
3	O	261	6% 68% 20% 5% 7%
3	Z	261	6% 69% 19% 7%
4	P	234	69% 23%
4	b	234	88% 9%

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Mol	Chain	Length	Quality of chain
5	J	255	68% 24% 7%
5	Q	255	67% 24% 7%
6	T	201	74% 22%
6	V	201	74% 22%
7	U	205	75% 22%
7	Y	205	73% 24%
8	C	203	70% 28%
8	D	203	69% 28%
9	S	241	66% 22% 12%
9	X	241	66% 21% 12%
10	G	263	7% 63% 23% 11%
10	L	263	7% 63% 23% 11%
11	K	246	72% 20%
11	R	246	72% 21%
12	A	198	74% 22%
12	F	198	73% 23%
13	B	273	56% 18% 5% 20%
13	E	273	57% 18% 20%
14	W	264	62% 17% 19%
14	a	264	75% 6% 19%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47844 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 Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	225	Total	C	N	O	S	0	0
			1720	1083	286	340	11		
1	H	225	Total	C	N	O	S	0	0
			1720	1083	286	340	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	231	Total	C	N	O	S	0	0
			1815	1144	321	345	5		
2	I	231	Total	C	N	O	S	0	0
			1815	1144	321	345	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	242	Total	C	N	O	S	0	0
			1904	1204	326	364	10		
3	Z	242	Total	C	N	O	S	0	0
			1904	1204	326	364	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	226	Total	C	N	O	S	0	0
			1769	1132	298	333	6		
4	b	226	Total	C	N	O	S	0	0
			1769	1132	298	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	238	Total	C	N	O	S	0	0
			1866	1185	318	352	11		
5	J	238	Total	C	N	O	S	0	0
			1866	1185	318	352	11		

- Molecule 6 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	196	Total	C	N	O	S	0	0
			1567	1004	264	290	9		
6	V	196	Total	C	N	O	S	0	0
			1567	1004	264	290	9		

- Molecule 7 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	204	Total	C	N	O	S	0	0
			1593	1014	265	295	19		
7	Y	204	Total	C	N	O	S	0	0
			1593	1014	265	295	19		

- Molecule 8 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	200	Total	C	N	O	S	0	0
			1561	976	268	304	13		
8	D	200	Total	C	N	O	S	0	0
			1561	976	268	304	13		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	212	Total	C	N	O	S	0	0
			1644	1041	280	313	10		
9	X	212	Total	C	N	O	S	0	0
			1644	1041	280	313	10		

- Molecule 10 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	234	Total	C	N	O	S	0	0
			1832	1148	329	344	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	234	Total	C	N	O	S	0	0
			1832	1148	329	344	11		

- Molecule 11 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	236	Total	C	N	O	S	0	0
			1817	1153	302	349	13		
11	R	236	Total	C	N	O	S	0	0
			1817	1153	302	349	13		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	198	Total	C	N	O	S	0	0
			1481	930	253	288	10		
12	A	198	Total	C	N	O	S	0	0
			1481	930	253	288	10		

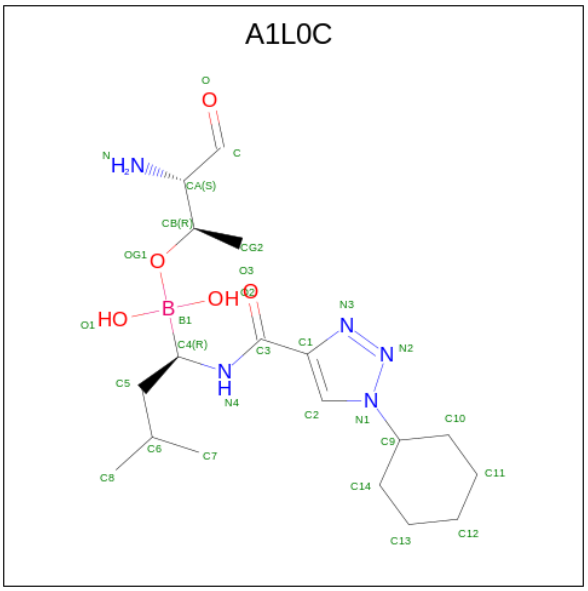
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	219	Total	C	N	O	S	0	0
			1622	1014	286	313	9		
13	B	219	Total	C	N	O	S	0	0
			1622	1014	286	313	9		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	214	Total	C	N	O	S	0	0
			1673	1056	288	317	12		
14	a	214	Total	C	N	O	S	0	0
			1673	1056	288	317	12		

- Molecule 15 is [(2 {R},3 {S})-3-azanyl-4-oxidanylidene-butan-2-yl]oxy-[(1 {R})-1-[(1-cyclohexyl-1,2,3-triazol-4-yl)carbonylamino]-3-methyl-butyl]-$l^{3}-oxidanyl-oxidanyl-boron (three-letter code: A1L0C) (formula: $C_{18}H_{33}BN_5O_5$) (labeled as "Ligand of Interest" by depositor).



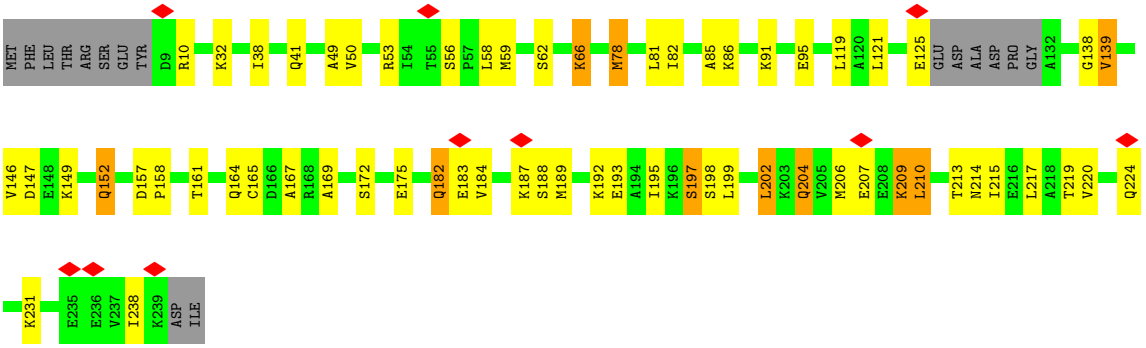
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	B	C	N	O	0
			29	1	18	5	5	
15	F	1	Total	B	C	N	O	0
			29	1	18	5	5	
15	A	1	Total	B	C	N	O	0
			29	1	18	5	5	
15	D	1	Total	B	C	N	O	0
			29	1	18	5	5	

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.

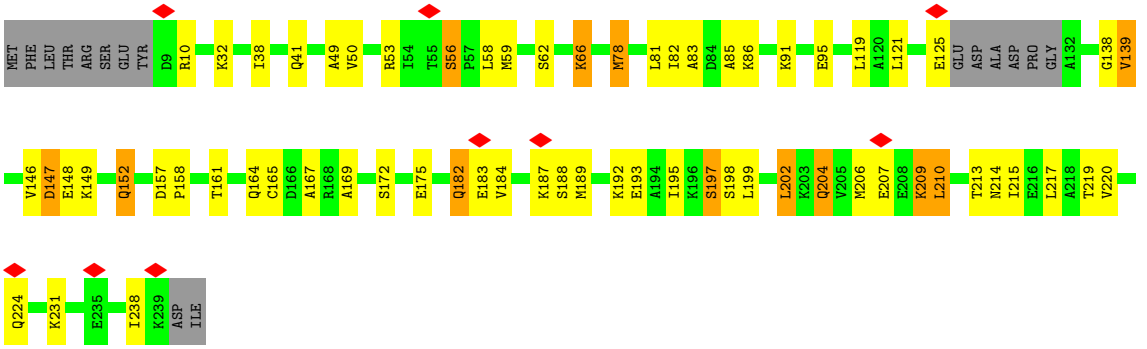
• Molecule 1: Proteasome subunit alpha type

Chain M:



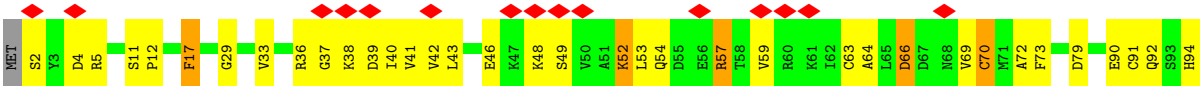
• Molecule 1: Proteasome subunit alpha type

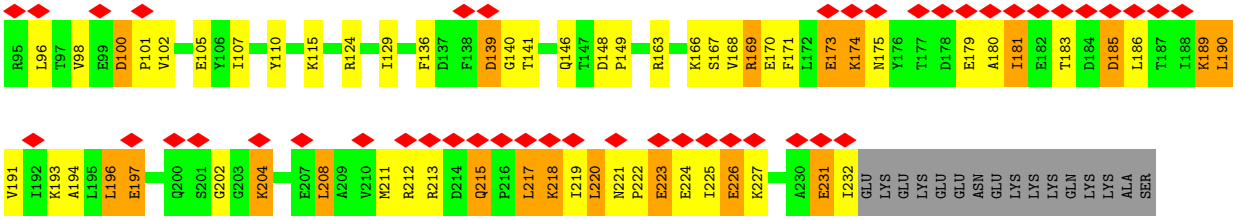
Chain H:



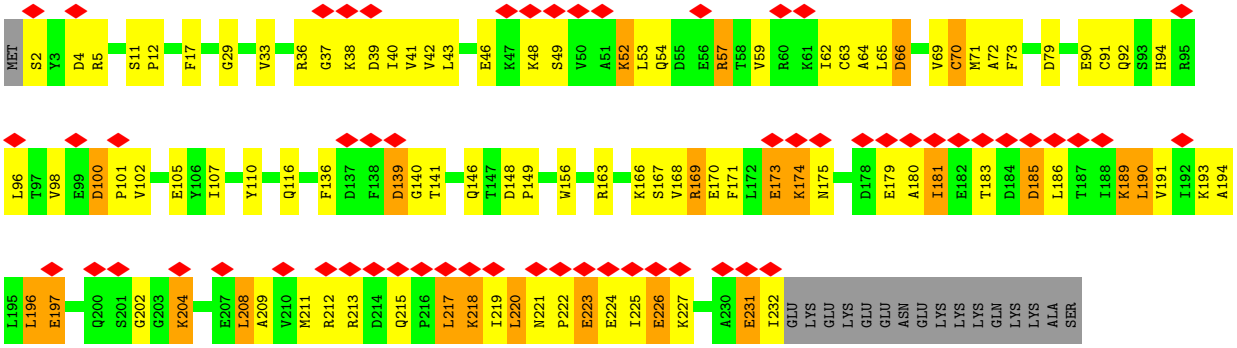
• Molecule 2: Proteasome subunit alpha type

Chain N:

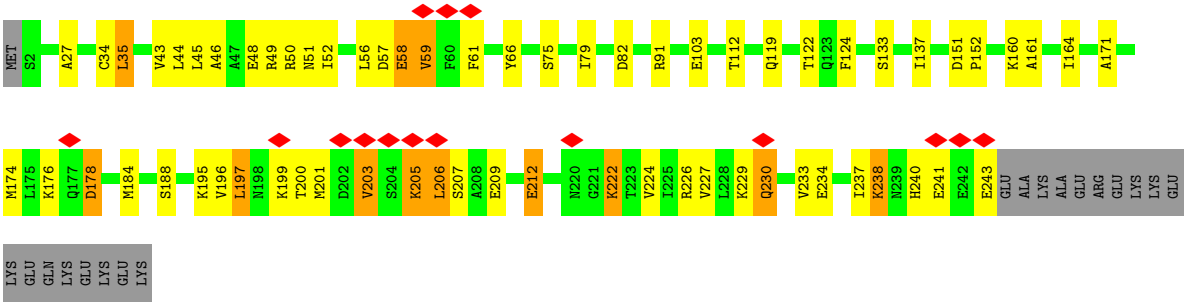




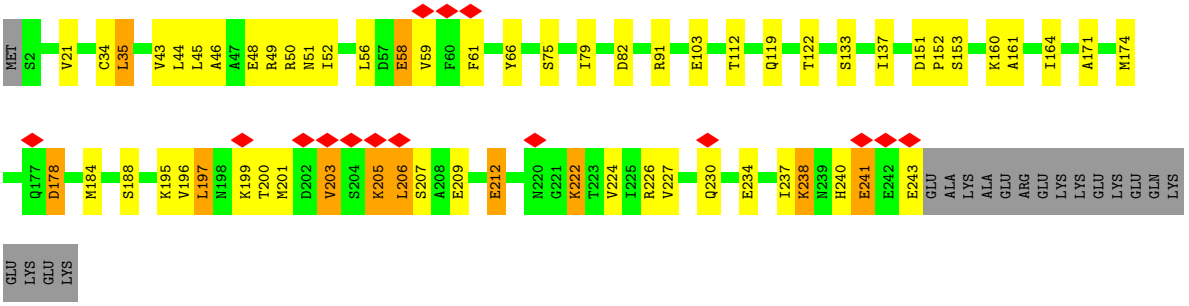
• Molecule 2: Proteasome subunit alpha type



• Molecule 3: Proteasome subunit alpha type

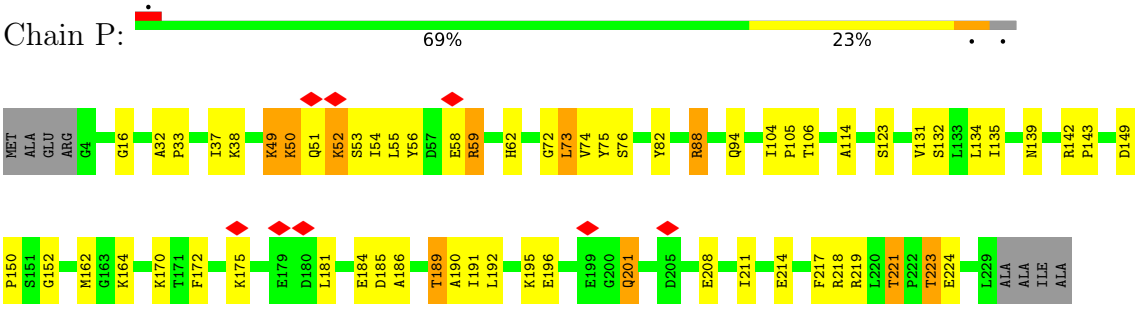


• Molecule 3: Proteasome subunit alpha type



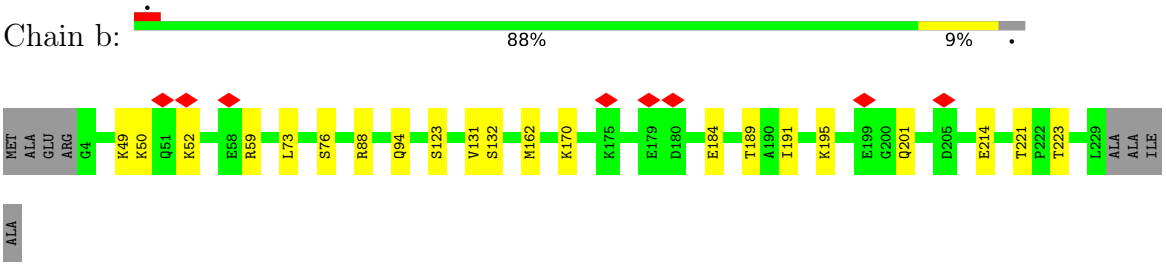
• Molecule 4: Proteasome subunit alpha type

Chain P:



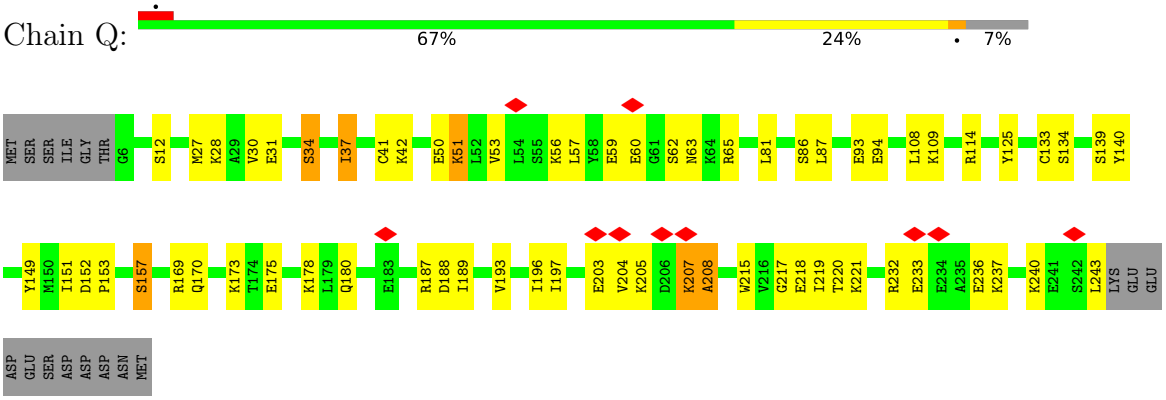
• Molecule 4: Proteasome subunit alpha type

Chain b:



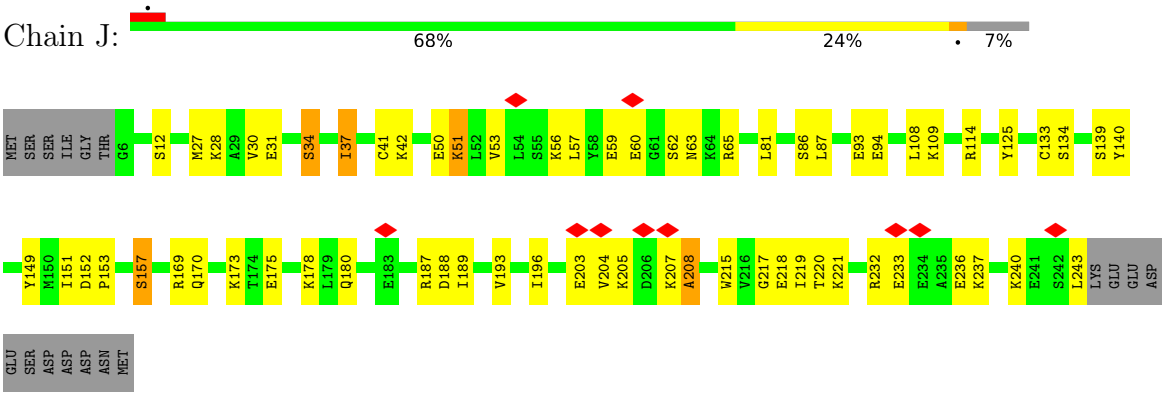
• Molecule 5: Proteasome subunit alpha type

Chain Q:



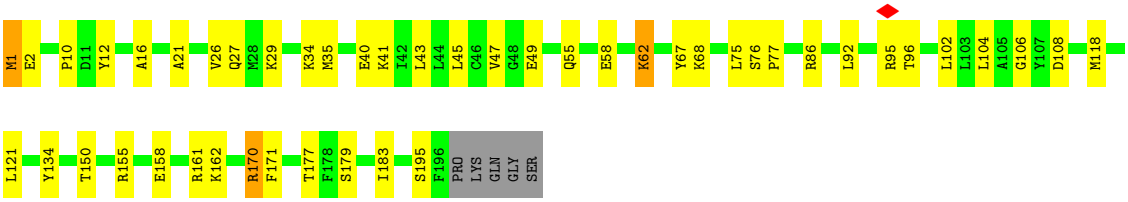
• Molecule 5: Proteasome subunit alpha type

Chain J:

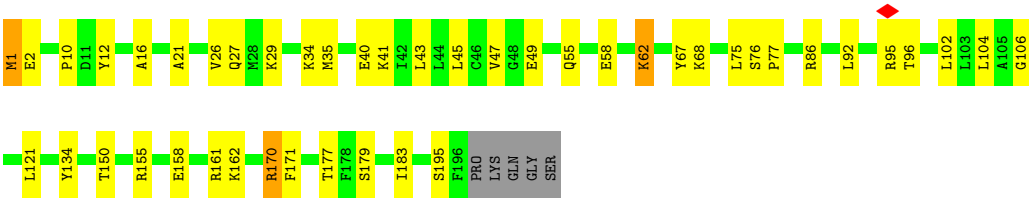


• Molecule 6: Proteasome subunit beta

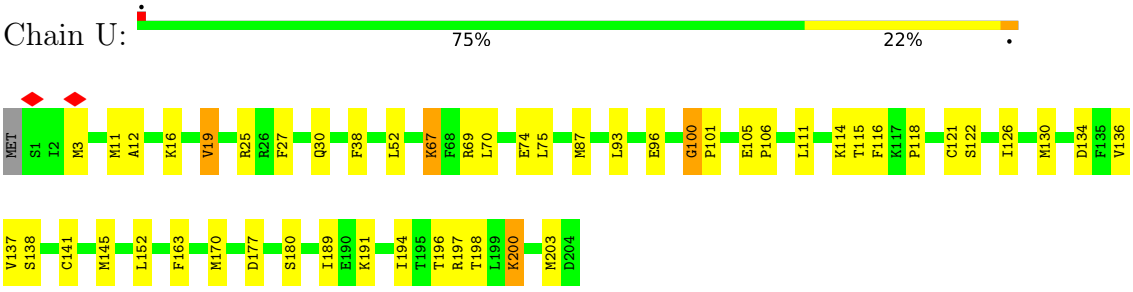
Chain T:



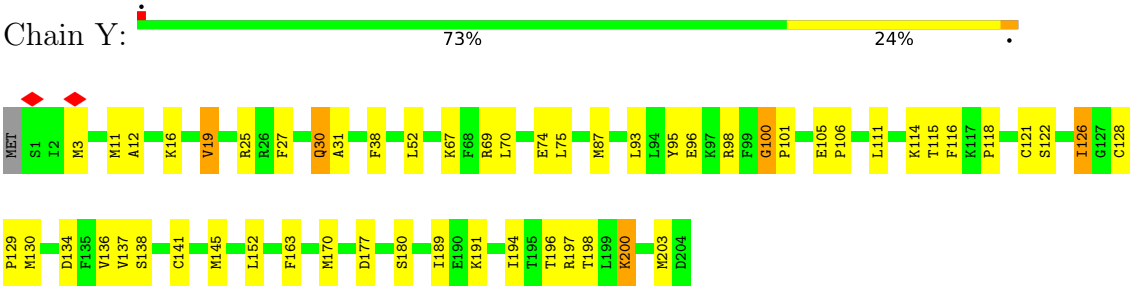
• Molecule 6: Proteasome subunit beta



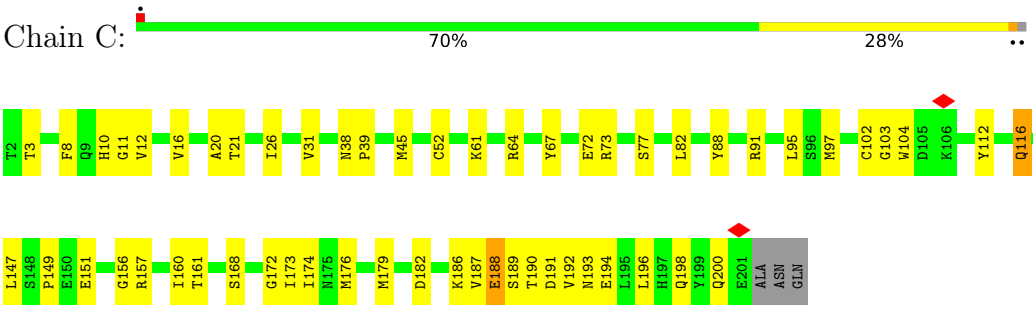
• Molecule 7: Proteasome subunit beta



• Molecule 7: Proteasome subunit beta

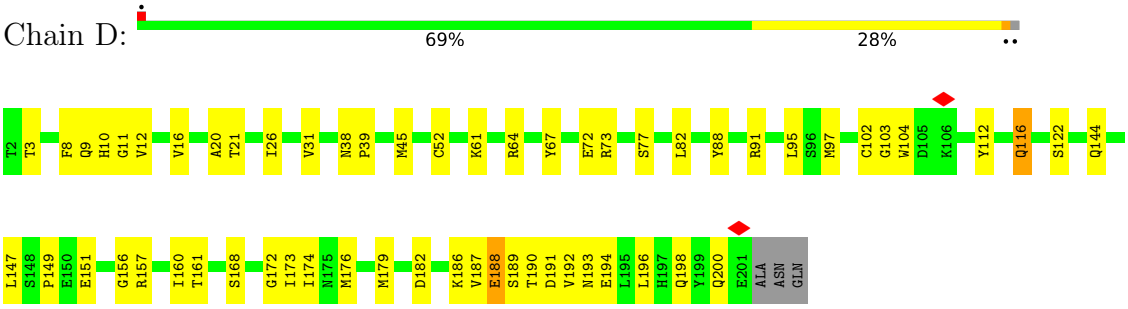


• Molecule 8: Proteasome subunit beta type-8



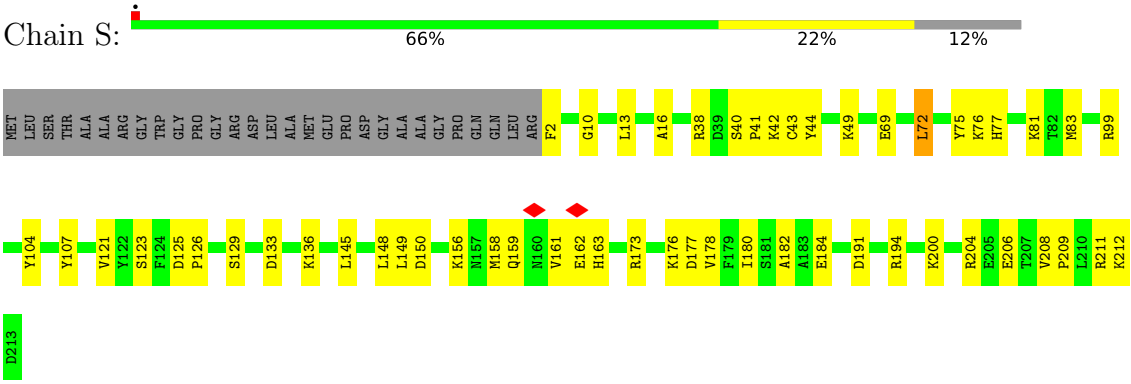
• Molecule 8: Proteasome subunit beta type-8

Chain D:



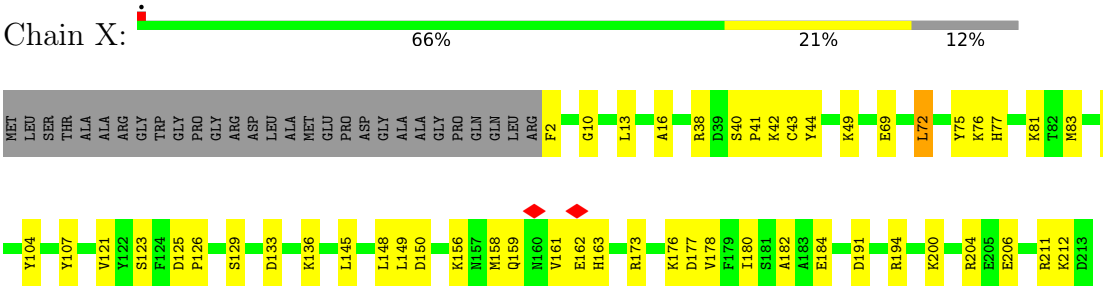
• Molecule 9: Proteasome subunit beta

Chain S:



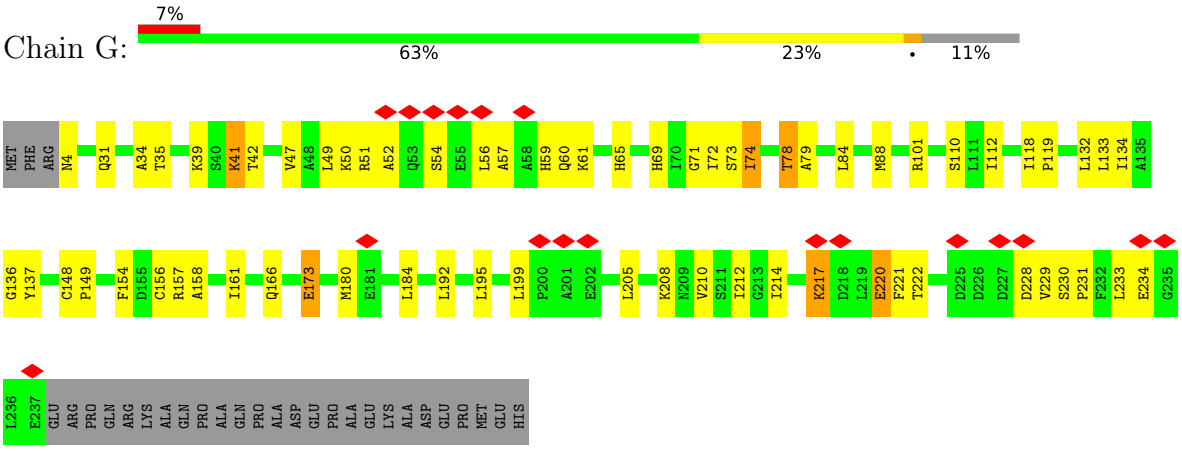
• Molecule 9: Proteasome subunit beta

Chain X:

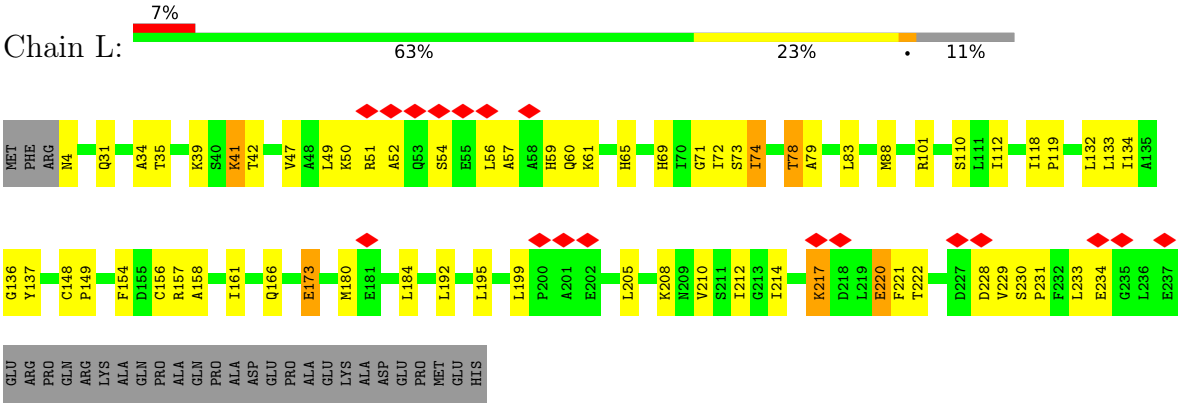


• Molecule 10: Proteasome subunit alpha type

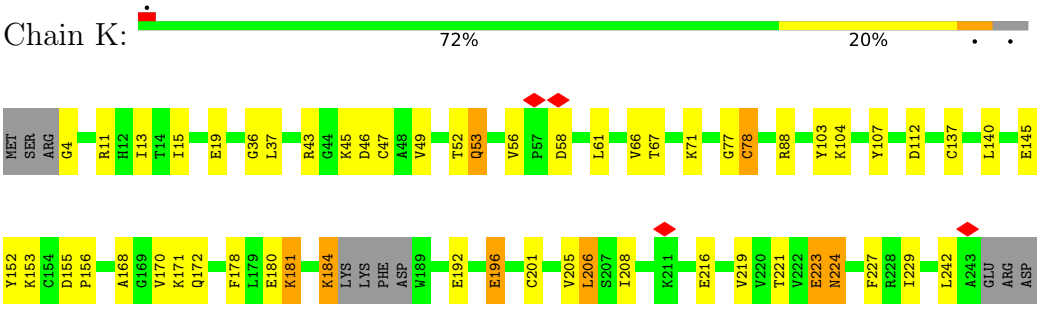
Chain G:



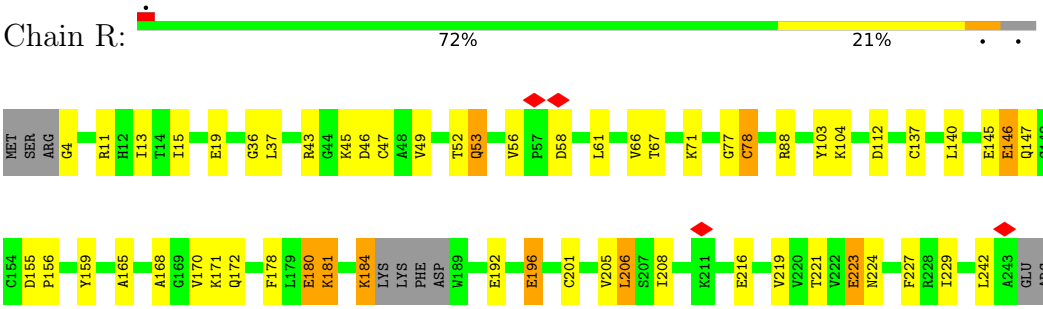
• Molecule 10: Proteasome subunit alpha type



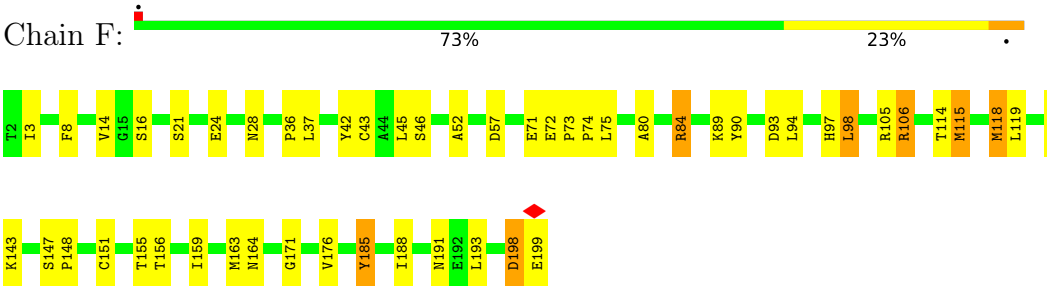
• Molecule 11: Proteasome subunit alpha type



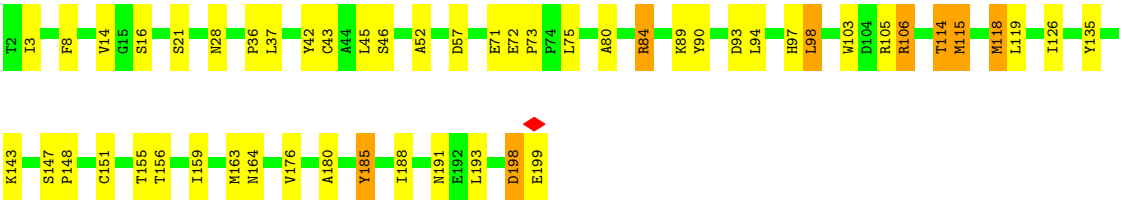
• Molecule 11: Proteasome subunit alpha type



• Molecule 12: Proteasome subunit beta

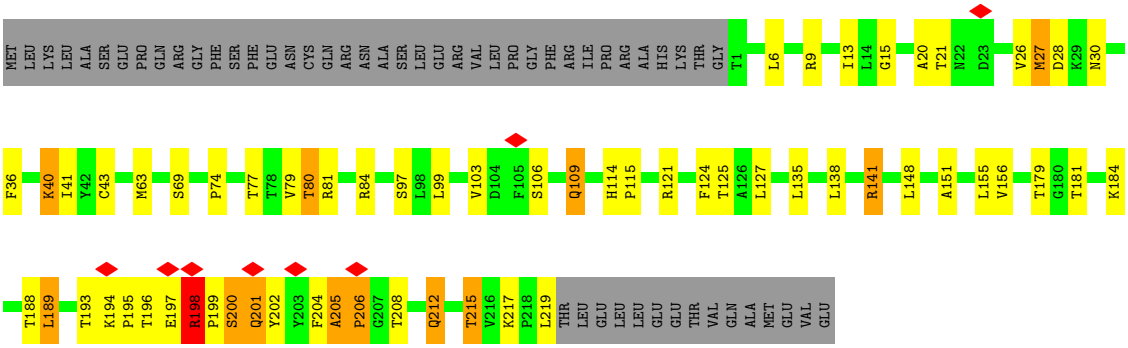


• Molecule 12: Proteasome subunit beta



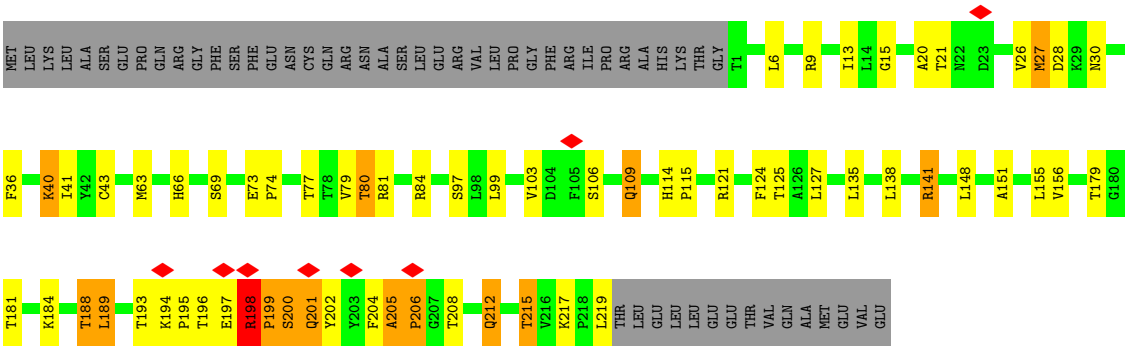
• Molecule 13: Proteasome subunit beta

Chain E:



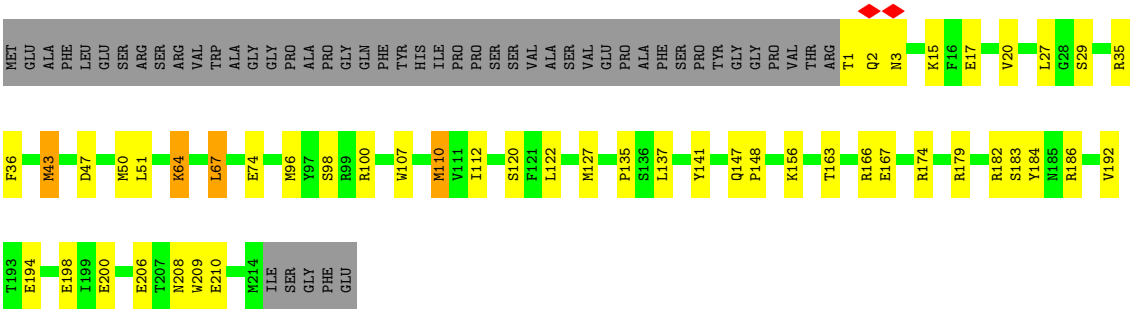
• Molecule 13: Proteasome subunit beta

Chain B:



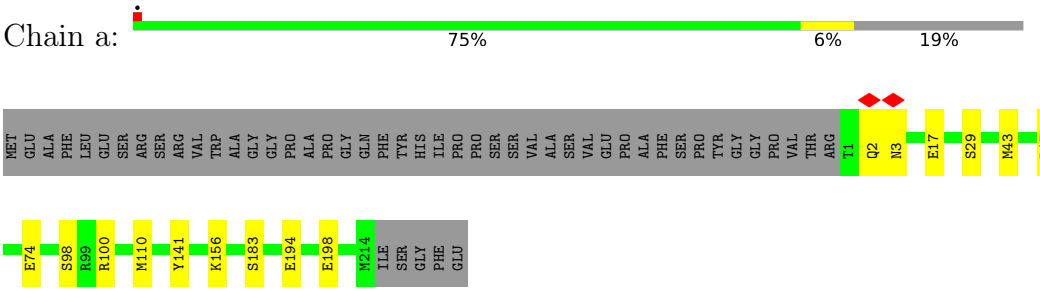
• Molecule 14: Proteasome subunit beta

Chain W:



• Molecule 14: Proteasome subunit beta

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	896501	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 ($e^-/Å^2$)	91.875	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0247	Depositor
Map size (Å)	292.16, 292.16, 292.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1L0C

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	H	0.28	0/1745	0.46	0/2354
1	M	0.28	0/1745	0.45	0/2354
2	I	0.26	0/1842	0.47	0/2489
2	N	0.26	0/1842	0.47	0/2489
3	O	0.30	0/1934	0.48	0/2608
3	Z	0.30	0/1934	0.48	0/2608
4	P	0.31	0/1808	0.49	0/2449
4	b	0.31	0/1808	0.49	0/2449
5	J	0.30	0/1901	0.50	0/2559
5	Q	0.30	0/1901	0.50	0/2559
6	T	0.32	0/1599	0.52	0/2163
6	V	0.32	0/1599	0.51	0/2163
7	U	0.31	0/1622	0.51	0/2186
7	Y	0.31	0/1622	0.51	0/2186
8	C	0.67	0/1593	0.88	0/2150
8	D	0.67	0/1593	0.88	0/2150
9	S	0.68	0/1675	0.91	0/2258
9	X	0.68	0/1675	0.91	0/2258
10	G	0.28	0/1866	0.51	0/2522
10	L	0.28	0/1866	0.51	0/2522
11	K	0.30	0/1849	0.50	0/2503
11	R	0.30	0/1849	0.50	0/2503
12	A	0.31	0/1510	0.51	0/2048
12	F	0.31	0/1510	0.51	0/2048
13	B	0.67	0/1650	0.88	0/2242
13	E	0.67	0/1650	0.88	0/2242
14	W	0.32	0/1706	0.54	0/2308
14	a	0.32	0/1706	0.54	0/2308
All	All	0.40	0/48600	0.60	0/65678

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	H	1720	0	1719	57	0
1	M	1720	0	1719	57	0
2	I	1815	0	1845	94	0
2	N	1815	0	1845	95	0
3	O	1904	0	1918	45	0
3	Z	1904	0	1918	39	0
4	P	1769	0	1761	55	0
4	b	1769	0	1761	0	0
5	J	1866	0	1855	39	0
5	Q	1866	0	1855	44	0
6	T	1567	0	1567	36	0
6	V	1567	0	1567	37	0
7	U	1593	0	1614	32	0
7	Y	1593	0	1614	34	0
8	C	1561	0	1504	42	0
8	D	1561	0	1504	45	0
9	S	1644	0	1638	43	0
9	X	1644	0	1638	40	0
10	G	1832	0	1823	59	0
10	L	1832	0	1823	61	0
11	K	1817	0	1808	43	0
11	R	1817	0	1808	47	0
12	A	1481	0	1435	41	0
12	F	1481	0	1435	41	0
13	B	1622	0	1634	73	0
13	E	1622	0	1634	73	0
14	W	1673	0	1650	29	0
14	a	1673	0	1650	0	0
15	A	29	0	0	1	0
15	C	29	0	0	1	0
15	D	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	F	29	0	0	1	0
All	All	47844	0	47542	1161	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 13.

All (1161) 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)
10:G:79:ALA:CB	1:H:121:LEU:HD12	1.38	1.53
2:I:42:VAL:CG1	2:I:191:VAL:HG21	1.37	1.52
2:N:42:VAL:CG1	2:N:191:VAL:HG21	1.37	1.51
1:M:121:LEU:HD12	10:L:79:ALA:CB	1.39	1.46
2:N:42:VAL:HG11	2:N:191:VAL:CG2	1.67	1.25
13:B:205:ALA:HB1	13:B:206:PRO:CD	1.68	1.24
2:I:42:VAL:HG11	2:I:191:VAL:CG2	1.67	1.23
5:Q:41:CYS:HB3	5:Q:189:ILE:CD1	1.68	1.22
5:J:41:CYS:HB3	5:J:189:ILE:CD1	1.68	1.22
10:G:57:ALA:HB2	1:H:165:CYS:SG	1.81	1.21
13:B:205:ALA:CB	13:B:206:PRO:HD2	1.71	1.20
13:E:205:ALA:HB1	13:E:206:PRO:CD	1.68	1.20
6:T:96:THR:HB	8:D:91:ARG:NH2	1.57	1.19
13:E:205:ALA:CB	13:E:206:PRO:HD2	1.71	1.19
10:G:79:ALA:HB3	1:H:121:LEU:CD1	1.72	1.18
8:C:91:ARG:NH2	6:V:96:THR:HB	1.58	1.17
1:M:121:LEU:CD1	10:L:79:ALA:CB	2.24	1.16
1:M:121:LEU:CD1	10:L:79:ALA:HB3	1.74	1.14
1:M:165:CYS:SG	10:L:57:ALA:HB2	1.86	1.14
10:G:79:ALA:CB	1:H:121:LEU:CD1	2.24	1.14
10:G:57:ALA:CB	1:H:165:CYS:SG	2.35	1.12
1:M:121:LEU:HD12	10:L:79:ALA:HB3	1.14	1.10
1:M:165:CYS:SG	10:L:57:ALA:CB	2.40	1.10
2:I:42:VAL:HG12	2:I:191:VAL:HG21	1.34	1.09
1:M:121:LEU:HD12	10:L:79:ALA:HB1	1.31	1.09
1:M:161:THR:OG1	10:L:78:THR:HG21	1.52	1.08
10:G:78:THR:HG21	1:H:161:THR:OG1	1.52	1.08
10:G:79:ALA:HB3	1:H:121:LEU:HD12	1.11	1.07
10:G:79:ALA:HB1	1:H:121:LEU:HD12	1.33	1.07
13:E:200:SER:OG	9:X:173:ARG:HD2	1.55	1.07
9:S:173:ARG:HD2	13:B:200:SER:OG	1.54	1.07
2:N:42:VAL:HG12	2:N:191:VAL:HG21	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:64:ARG:NH1	8:C:67:TYR:CD2	2.23	1.06
8:D:64:ARG:NH1	8:D:67:TYR:CD2	2.23	1.05
10:G:47:VAL:HG12	10:G:195:LEU:HD22	1.37	1.04
10:L:47:VAL:HG12	10:L:195:LEU:HD22	1.37	1.02
9:S:148:LEU:HD23	9:S:178:VAL:HG12	1.37	1.02
2:N:42:VAL:CG1	2:N:191:VAL:CG2	2.28	1.01
9:X:148:LEU:HD23	9:X:178:VAL:HG12	1.37	1.01
2:N:169:ARG:HB2	2:N:169:ARG:HH11	1.24	1.01
12:A:14:VAL:HG13	12:A:176:VAL:HG22	1.43	1.00
12:F:14:VAL:HG13	12:F:176:VAL:HG22	1.43	0.99
2:I:169:ARG:HH11	2:I:169:ARG:HB2	1.24	0.98
2:I:42:VAL:CG1	2:I:191:VAL:CG2	2.28	0.98
5:J:41:CYS:CB	5:J:189:ILE:CD1	2.43	0.97
9:S:173:ARG:HB3	13:B:200:SER:HB2	1.46	0.96
5:Q:41:CYS:CB	5:Q:189:ILE:CD1	2.42	0.96
4:P:59:ARG:HH11	4:P:59:ARG:HB2	1.31	0.96
6:T:96:THR:HB	8:D:91:ARG:HH21	1.27	0.96
13:E:200:SER:HB2	9:X:173:ARG:HB3	1.47	0.96
2:N:196:LEU:HD11	2:N:202:GLY:HA3	1.48	0.95
7:Y:25:ARG:HG2	7:Y:25:ARG:HH11	1.31	0.95
2:N:42:VAL:HG11	2:N:191:VAL:HG21	0.95	0.95
4:P:59:ARG:HB2	4:P:59:ARG:NH1	1.80	0.95
2:N:40:ILE:HD12	2:N:212:ARG:HG3	1.47	0.95
3:Z:174:MET:CE	3:Z:195:LYS:HG2	1.97	0.95
5:J:41:CYS:HB3	5:J:189:ILE:HD13	1.47	0.95
2:I:40:ILE:HD12	2:I:212:ARG:HG3	1.47	0.94
2:I:42:VAL:HG11	2:I:191:VAL:HG21	0.95	0.94
2:N:64:ALA:HB2	2:N:217:LEU:HD22	1.47	0.94
2:I:64:ALA:HB2	2:I:217:LEU:HD22	1.47	0.94
7:U:25:ARG:HG2	7:U:25:ARG:HH11	1.31	0.94
10:G:47:VAL:CG1	10:G:195:LEU:HD22	1.98	0.94
3:O:174:MET:CE	3:O:195:LYS:HG2	1.97	0.93
5:Q:41:CYS:HB3	5:Q:189:ILE:HD13	1.47	0.93
3:Z:151:ASP:HB2	3:Z:152:PRO:HD2	1.50	0.93
2:I:196:LEU:HD11	2:I:202:GLY:HA3	1.48	0.93
10:L:47:VAL:CG1	10:L:195:LEU:HD22	1.98	0.93
13:B:205:ALA:HB1	13:B:206:PRO:HD2	0.94	0.92
3:O:151:ASP:HB2	3:O:152:PRO:HD2	1.50	0.91
8:C:91:ARG:HH21	6:V:96:THR:HB	1.29	0.91
11:K:196:GLU:HG3	11:K:242:LEU:HD21	1.52	0.91
13:E:205:ALA:HB1	13:E:206:PRO:HD2	0.94	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:196:GLU:HG3	11:R:242:LEU:HD21	1.52	0.90
9:S:158:MET:HE2	13:B:204:PHE:HE1	1.37	0.90
4:P:88:ARG:HH21	4:P:88:ARG:HG2	1.36	0.89
2:N:100:ASP:OD1	2:N:101:PRO:HD2	1.72	0.89
10:G:56:LEU:HD13	1:H:167:ALA:HB3	1.53	0.89
11:K:155:ASP:HB2	11:K:156:PRO:CD	2.03	0.89
11:R:155:ASP:HB2	11:R:156:PRO:CD	2.03	0.89
3:O:151:ASP:HB2	3:O:152:PRO:CD	2.04	0.88
3:Z:151:ASP:HB2	3:Z:152:PRO:CD	2.03	0.88
11:R:49:VAL:HG22	11:R:219:VAL:HG12	1.56	0.88
2:I:100:ASP:OD1	2:I:101:PRO:HD2	1.73	0.87
2:I:183:THR:HG22	2:I:186:LEU:HB2	1.57	0.87
10:G:166:GLN:O	10:G:166:GLN:NE2	2.08	0.87
11:K:49:VAL:HG22	11:K:219:VAL:HG12	1.56	0.87
2:N:183:THR:HG22	2:N:186:LEU:HB2	1.57	0.87
13:B:109:GLN:HG3	13:B:121:ARG:HH11	1.40	0.87
11:R:155:ASP:HB2	11:R:156:PRO:HD2	1.56	0.87
11:K:155:ASP:HB2	11:K:156:PRO:HD2	1.56	0.86
2:N:169:ARG:HH11	2:N:169:ARG:CB	1.88	0.86
13:E:109:GLN:HG3	13:E:121:ARG:HH11	1.40	0.86
2:I:169:ARG:HH11	2:I:169:ARG:CB	1.88	0.86
10:L:166:GLN:O	10:L:166:GLN:NE2	2.08	0.85
8:C:64:ARG:NH1	8:C:67:TYR:HD2	1.71	0.85
13:E:204:PHE:HE1	9:X:158:MET:HE2	1.41	0.85
11:R:196:GLU:HG3	11:R:242:LEU:CD2	2.06	0.85
12:A:115:MET:SD	12:A:115:MET:N	2.50	0.84
11:K:196:GLU:HG3	11:K:242:LEU:CD2	2.06	0.84
2:I:29:GLY:O	2:I:163:ARG:HG2	1.78	0.84
11:K:88:ARG:HH21	11:K:88:ARG:HG2	1.42	0.84
12:F:115:MET:SD	12:F:115:MET:N	2.50	0.84
2:N:29:GLY:O	2:N:163:ARG:HG2	1.78	0.84
10:G:78:THR:CG2	1:H:161:THR:OG1	2.26	0.83
11:R:88:ARG:HG2	11:R:88:ARG:HH21	1.42	0.83
6:T:96:THR:CB	8:D:91:ARG:NH2	2.40	0.83
1:H:49:ALA:HB2	1:H:217:LEU:HD12	1.61	0.83
4:P:53:SER:HB2	11:R:180:GLU:OE2	1.78	0.83
8:D:64:ARG:NH1	8:D:67:TYR:HD2	1.71	0.83
1:M:167:ALA:HB3	10:L:56:LEU:HD13	1.58	0.82
12:A:14:VAL:HG13	12:A:176:VAL:CG2	2.09	0.82
1:M:49:ALA:HB2	1:M:217:LEU:HD12	1.61	0.82
7:U:100:GLY:H	7:U:101:PRO:HD3	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:14:VAL:CG1	12:F:176:VAL:CG2	2.58	0.82
12:F:14:VAL:HG13	12:F:176:VAL:CG2	2.09	0.82
1:M:161:THR:OG1	10:L:78:THR:CG2	2.26	0.82
12:A:14:VAL:CG1	12:A:176:VAL:CG2	2.57	0.82
7:Y:100:GLY:H	7:Y:101:PRO:HD3	1.42	0.81
7:Y:70:LEU:O	7:Y:74:GLU:HG2	1.81	0.80
6:T:1:MET:HG2	6:T:134:TYR:H	1.47	0.79
14:W:174:ARG:HD2	14:W:206:GLU:O	1.81	0.79
7:U:70:LEU:O	7:U:74:GLU:HG2	1.81	0.78
8:C:91:ARG:NH2	6:V:96:THR:CB	2.42	0.78
9:S:173:ARG:CB	13:B:200:SER:HB2	2.13	0.78
6:V:1:MET:HG2	6:V:134:TYR:H	1.47	0.78
13:E:200:SER:HB2	9:X:173:ARG:CB	2.14	0.78
5:Q:152:ASP:HB2	5:Q:153:PRO:HD2	1.66	0.77
1:H:50:VAL:HG11	1:H:66:LYS:HB2	1.67	0.77
13:E:194:LYS:HG3	13:E:195:PRO:HD2	1.66	0.77
2:N:139:ASP:OD1	2:N:139:ASP:N	2.17	0.77
14:W:174:ARG:CD	14:W:206:GLU:O	2.32	0.77
12:A:37:LEU:HD11	12:A:43:CYS:HB3	1.66	0.77
5:J:152:ASP:HB2	5:J:153:PRO:HD2	1.66	0.77
13:E:200:SER:CB	9:X:173:ARG:HD2	2.14	0.77
9:X:184:GLU:OE2	9:X:211:ARG:HD2	1.85	0.77
9:S:148:LEU:HD23	9:S:178:VAL:CG1	2.15	0.77
11:K:196:GLU:HG3	11:K:242:LEU:CG	2.15	0.77
11:R:196:GLU:HG3	11:R:242:LEU:CG	2.15	0.76
2:I:175:ASN:O	2:I:190:LEU:HD21	1.84	0.76
2:N:175:ASN:O	2:N:190:LEU:HD21	1.84	0.76
9:S:173:ARG:HD2	13:B:200:SER:CB	2.14	0.76
9:S:184:GLU:OE2	9:S:211:ARG:HD2	1.85	0.76
13:B:194:LYS:HG3	13:B:195:PRO:HD2	1.66	0.76
12:F:37:LEU:HD11	12:F:43:CYS:HB3	1.66	0.76
4:P:88:ARG:HG2	4:P:88:ARG:NH2	1.98	0.76
8:C:91:ARG:HH22	6:V:96:THR:HB	1.51	0.76
9:X:148:LEU:HD23	9:X:178:VAL:CG1	2.15	0.76
6:T:2:GLU:HG2	6:T:34:LYS:HE2	1.68	0.76
1:M:50:VAL:HG11	1:M:66:LYS:HB2	1.66	0.75
2:N:196:LEU:CD1	2:N:202:GLY:HA3	2.16	0.75
2:I:196:LEU:CD1	2:I:202:GLY:HA3	2.16	0.75
9:X:148:LEU:CD2	9:X:178:VAL:HG12	2.17	0.75
6:V:2:GLU:HG2	6:V:34:LYS:HE2	1.68	0.75
2:N:90:GLU:HG2	2:N:110:TYR:CD1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:188:ILE:HG22	12:A:193:LEU:HD23	1.69	0.74
2:I:90:GLU:HG2	2:I:110:TYR:CD1	2.23	0.74
4:P:149:ASP:HB2	4:P:150:PRO:HD2	1.68	0.74
12:F:188:ILE:HG22	12:F:193:LEU:HD23	1.69	0.74
6:T:96:THR:HB	8:D:91:ARG:HH22	1.50	0.74
9:S:148:LEU:CD2	9:S:178:VAL:HG12	2.17	0.74
11:R:196:GLU:CG	11:R:242:LEU:HD21	2.18	0.74
3:Z:35:LEU:HD23	3:Z:197:LEU:HD13	1.70	0.74
3:O:174:MET:HE2	3:O:195:LYS:HG2	1.68	0.73
11:K:196:GLU:CG	11:K:242:LEU:HD21	2.18	0.73
12:A:14:VAL:CG1	12:A:176:VAL:HG22	2.19	0.73
8:C:161:THR:HG22	8:C:196:LEU:HD13	1.70	0.73
5:J:170:GLN:HA	5:J:170:GLN:NE2	2.04	0.73
2:N:66:ASP:OD2	2:N:91:CYS:HB3	1.89	0.73
5:Q:41:CYS:HB3	5:Q:189:ILE:HD11	1.68	0.73
3:Z:174:MET:HE1	3:Z:195:LYS:HG2	1.70	0.73
8:D:161:THR:HG22	8:D:196:LEU:HD13	1.70	0.73
3:Z:174:MET:HE2	3:Z:195:LYS:HG2	1.70	0.73
3:O:35:LEU:HD23	3:O:197:LEU:HD13	1.70	0.72
5:Q:175:GLU:HB3	5:Q:196:ILE:HG12	1.71	0.72
2:I:66:ASP:OD2	2:I:91:CYS:HB3	1.89	0.72
8:C:157:ARG:NH2	8:C:188:GLU:OE2	2.21	0.72
2:I:139:ASP:OD1	2:I:139:ASP:N	2.17	0.72
5:Q:170:GLN:HA	5:Q:170:GLN:NE2	2.04	0.72
4:P:185:ASP:O	4:P:189:THR:HG22	1.89	0.72
7:Y:25:ARG:HG2	7:Y:25:ARG:NH1	2.05	0.71
13:E:40:LYS:CD	13:E:40:LYS:H	2.02	0.71
6:V:62:LYS:HD3	2:I:96:LEU:HD22	1.73	0.71
13:B:156:VAL:HG21	13:B:189:LEU:HD11	1.73	0.71
13:E:156:VAL:HG21	13:E:189:LEU:HD11	1.73	0.71
5:J:175:GLU:HB3	5:J:196:ILE:HG12	1.71	0.71
5:J:41:CYS:HB3	5:J:189:ILE:HD11	1.68	0.71
2:I:70:CYS:HB3	2:I:211:MET:SD	2.31	0.71
2:N:70:CYS:HB3	2:N:211:MET:SD	2.31	0.70
4:P:149:ASP:HB2	4:P:150:PRO:CD	2.21	0.70
2:I:180:ALA:HB1	2:I:190:LEU:CD2	2.21	0.70
8:D:156:GLY:HA3	8:D:176:MET:CE	2.22	0.70
13:B:40:LYS:H	13:B:40:LYS:CD	2.02	0.70
2:N:96:LEU:HD22	6:T:62:LYS:HD3	1.74	0.70
7:U:25:ARG:HG2	7:U:25:ARG:NH1	2.05	0.70
12:F:14:VAL:CG1	12:F:176:VAL:HG22	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:141:ARG:HG3	13:B:141:ARG:HH11	1.56	0.70
8:C:156:GLY:HA3	8:C:176:MET:CE	2.22	0.70
13:E:141:ARG:HH11	13:E:141:ARG:HG3	1.56	0.70
8:D:157:ARG:NH2	8:D:188:GLU:OE2	2.21	0.70
5:Q:152:ASP:HB2	5:Q:153:PRO:CD	2.21	0.69
12:F:90:TYR:HB2	12:F:94:LEU:HD12	1.74	0.69
13:E:198:ARG:O	13:E:198:ARG:HG2	1.90	0.69
11:K:103:TYR:O	13:B:81:ARG:HD3	1.92	0.69
12:F:75:LEU:HD21	12:F:106:ARG:HG3	1.74	0.69
13:E:135:LEU:CD1	14:W:179:ARG:HG3	2.22	0.69
12:A:75:LEU:CD2	12:A:106:ARG:HG3	2.22	0.69
12:A:75:LEU:HD21	12:A:106:ARG:HG3	1.74	0.69
12:A:90:TYR:HB2	12:A:94:LEU:HD12	1.74	0.69
10:G:56:LEU:CD1	1:H:167:ALA:HB3	2.22	0.69
8:C:157:ARG:HD3	8:C:188:GLU:OE2	1.91	0.69
7:Y:100:GLY:H	7:Y:101:PRO:CD	2.06	0.69
2:N:180:ALA:HB1	2:N:190:LEU:CD2	2.21	0.69
7:U:116:PHE:CE2	7:U:191:LYS:HE3	2.28	0.69
8:C:191:ASP:HB3	8:C:194:GLU:HG3	1.74	0.69
13:B:198:ARG:O	13:B:198:ARG:HG2	1.90	0.69
11:K:181:LYS:HA	11:K:184:LYS:HE2	1.75	0.69
8:D:157:ARG:HD3	8:D:188:GLU:OE2	1.91	0.69
1:H:213:THR:HG22	1:H:231:LYS:HE3	1.75	0.69
5:J:152:ASP:HB2	5:J:153:PRO:CD	2.21	0.69
7:Y:116:PHE:CE2	7:Y:191:LYS:HE3	2.28	0.68
3:O:174:MET:HE1	3:O:195:LYS:HG2	1.72	0.68
5:J:41:CYS:CB	5:J:189:ILE:HD12	2.23	0.68
10:L:50:LYS:HB3	10:L:59:HIS:HB3	1.75	0.68
8:D:191:ASP:HB3	8:D:194:GLU:HG3	1.74	0.68
13:E:6:LEU:HD12	13:E:6:LEU:C	2.14	0.68
11:R:181:LYS:HA	11:R:184:LYS:HE2	1.75	0.68
12:F:75:LEU:CD2	12:F:106:ARG:HG3	2.22	0.68
5:Q:41:CYS:CB	5:Q:189:ILE:HD12	2.23	0.68
1:M:213:THR:HG22	1:M:231:LYS:HE3	1.75	0.68
7:U:100:GLY:H	7:U:101:PRO:CD	2.06	0.68
1:M:165:CYS:SG	10:L:57:ALA:HB1	2.33	0.68
8:C:156:GLY:HA3	8:C:176:MET:HE1	1.76	0.68
10:G:35:THR:HG23	10:G:133:LEU:HD12	1.76	0.68
5:Q:59:GLU:OE2	10:L:157:ARG:HG2	1.94	0.67
10:G:50:LYS:HB3	10:G:59:HIS:HB3	1.75	0.67
5:J:41:CYS:CB	5:J:189:ILE:HD11	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:156:GLY:HA3	8:D:176:MET:HE1	1.76	0.67
10:G:57:ALA:HB1	1:H:165:CYS:SG	2.30	0.67
13:B:109:GLN:HG3	13:B:121:ARG:NH1	2.08	0.67
13:B:141:ARG:HG3	13:B:141:ARG:NH1	2.08	0.67
4:P:175:LYS:O	4:P:175:LYS:HG2	1.95	0.67
13:E:109:GLN:HG3	13:E:121:ARG:NH1	2.08	0.67
10:L:35:THR:HG23	10:L:133:LEU:HD12	1.76	0.67
13:E:141:ARG:HG3	13:E:141:ARG:NH1	2.08	0.67
13:B:6:LEU:C	13:B:6:LEU:HD12	2.14	0.67
13:E:81:ARG:HD3	11:R:103:TYR:O	1.95	0.66
2:I:221:ASN:HB2	2:I:222:PRO:HD2	1.78	0.66
4:P:74:VAL:CG1	4:P:134:LEU:HB2	2.26	0.66
8:D:72:GLU:HG2	8:D:72:GLU:O	1.96	0.66
10:G:157:ARG:HG2	5:J:59:GLU:OE2	1.95	0.66
12:A:42:TYR:HH	12:A:185:TYR:HE2	1.43	0.65
10:G:65:HIS:HD2	9:X:77:HIS:NE2	1.95	0.65
9:X:43:CYS:SG	9:X:194:ARG:NH2	2.69	0.65
3:O:196:VAL:O	3:O:200:THR:HG23	1.96	0.65
2:N:221:ASN:HB2	2:N:222:PRO:HD2	1.78	0.65
2:N:70:CYS:HB2	2:N:217:LEU:HD11	1.78	0.65
3:Z:196:VAL:O	3:Z:200:THR:HG23	1.96	0.65
11:K:88:ARG:HG2	11:K:88:ARG:NH2	2.12	0.65
12:A:118:MET:O	12:A:118:MET:HG3	1.97	0.65
9:S:43:CYS:SG	9:S:194:ARG:NH2	2.69	0.65
10:L:192:LEU:HD13	10:L:233:LEU:HD23	1.79	0.65
4:P:53:SER:CB	11:R:180:GLU:OE2	2.45	0.64
7:Y:19:VAL:HG23	7:Y:189:ILE:HB	1.79	0.64
2:N:96:LEU:CD1	6:T:58:GLU:HB3	2.27	0.64
4:P:88:ARG:HH21	4:P:88:ARG:CG	2.09	0.64
2:I:70:CYS:HB2	2:I:217:LEU:HD11	1.78	0.64
8:C:72:GLU:O	8:C:72:GLU:HG2	1.96	0.64
10:G:192:LEU:HD13	10:G:233:LEU:HD23	1.79	0.64
12:F:42:TYR:HH	12:F:185:TYR:HE2	1.45	0.64
9:X:176:LYS:NZ	9:X:206:GLU:OE2	2.21	0.64
2:N:170:GLU:OE1	2:N:170:GLU:HA	1.98	0.64
13:E:135:LEU:HD11	14:W:179:ARG:HG3	1.80	0.64
13:E:200:SER:OG	9:X:173:ARG:NH2	2.30	0.64
2:I:170:GLU:OE1	2:I:170:GLU:HA	1.98	0.64
3:O:57:ASP:OD2	4:P:38:LYS:HE2	1.98	0.64
4:P:172:PHE:CD2	4:P:196:GLU:OE1	2.51	0.64
12:F:118:MET:O	12:F:118:MET:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:6:LEU:HD11	13:E:151:ALA:HB1	1.80	0.64
13:B:6:LEU:HD11	13:B:151:ALA:HB1	1.80	0.64
9:S:173:ARG:NH2	13:B:200:SER:OG	2.30	0.64
7:U:19:VAL:HG23	7:U:189:ILE:HB	1.79	0.64
9:S:99:ARG:HG3	9:S:104:TYR:CE2	2.33	0.64
9:S:176:LYS:NZ	9:S:206:GLU:OE2	2.21	0.64
9:X:99:ARG:HG3	9:X:104:TYR:CE2	2.33	0.64
9:S:145:LEU:HD21	9:S:182:ALA:HB2	1.79	0.64
11:R:88:ARG:HG2	11:R:88:ARG:NH2	2.12	0.64
6:V:58:GLU:HB3	2:I:96:LEU:CD1	2.28	0.63
1:M:167:ALA:HB3	10:L:56:LEU:CD1	2.27	0.63
13:E:40:LYS:NZ	13:E:103:VAL:O	2.32	0.63
9:X:145:LEU:HD21	9:X:182:ALA:HB2	1.79	0.63
13:B:81:ARG:NH2	13:B:84:ARG:HH12	1.96	0.63
1:M:165:CYS:HG	10:L:57:ALA:HB2	1.63	0.63
11:R:196:GLU:HG3	11:R:242:LEU:HG	1.80	0.63
13:B:40:LYS:NZ	13:B:103:VAL:O	2.32	0.63
13:B:205:ALA:CB	13:B:206:PRO:CD	2.44	0.63
11:K:196:GLU:HG3	11:K:242:LEU:HG	1.80	0.63
12:F:199:GLU:HB3	14:W:186:ARG:NH1	2.14	0.63
8:D:64:ARG:HD2	8:D:64:ARG:O	2.00	0.62
13:E:81:ARG:NH2	13:E:84:ARG:HH12	1.96	0.62
5:J:151:ILE:HG12	5:J:157:SER:HB2	1.81	0.62
13:E:13:ILE:CD1	13:E:151:ALA:HB3	2.29	0.62
7:Y:200:LYS:HA	13:B:212:GLN:NE2	2.15	0.62
2:I:169:ARG:HH11	2:I:169:ARG:CG	2.13	0.62
2:I:185:ASP:N	2:I:185:ASP:OD1	2.32	0.62
13:B:13:ILE:CD1	13:B:151:ALA:HB3	2.30	0.62
6:T:171:PHE:O	6:V:27:GLN:NE2	2.32	0.62
14:W:208:ASN:HD21	14:W:210:GLU:HB2	1.64	0.62
5:Q:151:ILE:HG12	5:Q:157:SER:HB2	1.81	0.62
7:U:200:LYS:HA	13:E:212:GLN:NE2	2.14	0.62
1:H:184:VAL:O	1:H:184:VAL:HG22	2.00	0.62
12:A:156:THR:HG23	12:A:188:ILE:HD12	1.82	0.62
9:S:77:HIS:NE2	10:L:65:HIS:HD2	1.97	0.61
5:J:170:GLN:HA	5:J:170:GLN:HE21	1.65	0.61
13:E:40:LYS:H	13:E:40:LYS:HD3	1.65	0.61
4:P:54:ILE:CD1	11:R:184:LYS:HB3	2.30	0.61
1:H:91:LYS:HE2	1:H:119:LEU:HD11	1.82	0.61
2:N:185:ASP:N	2:N:185:ASP:OD1	2.32	0.61
10:L:72:ILE:HG22	10:L:134:ILE:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:72:ILE:HG22	10:G:134:ILE:HG12	1.82	0.61
9:X:43:CYS:O	9:X:194:ARG:NH2	2.33	0.61
9:S:43:CYS:O	9:S:194:ARG:NH2	2.33	0.61
2:I:40:ILE:CD1	2:I:212:ARG:HG3	2.24	0.61
1:M:184:VAL:HG22	1:M:184:VAL:O	2.00	0.61
2:N:90:GLU:OE1	2:N:90:GLU:HA	2.01	0.61
6:T:27:GLN:NE2	6:V:171:PHE:O	2.34	0.61
2:I:96:LEU:O	2:I:96:LEU:HG	2.00	0.61
11:R:58:ASP:HB3	11:R:61:LEU:HD12	1.83	0.61
8:D:38:ASN:HB2	8:D:39:PRO:CD	2.31	0.61
13:E:63:MET:CE	13:E:74:PRO:HB3	2.31	0.61
8:C:38:ASN:HB2	8:C:39:PRO:CD	2.31	0.61
8:C:64:ARG:HD2	8:C:64:ARG:O	1.99	0.61
5:J:53:VAL:HG23	5:J:53:VAL:O	2.01	0.61
1:M:91:LYS:HE2	1:M:119:LEU:HD11	1.82	0.61
2:N:57:ARG:HH11	2:N:57:ARG:CG	2.14	0.61
8:C:45:MET:HG2	8:C:52:CYS:HB3	1.82	0.61
2:N:40:ILE:CD1	2:N:212:ARG:HG3	2.24	0.60
10:G:79:ALA:HB3	1:H:121:LEU:HD11	1.79	0.60
3:Z:35:LEU:HD12	3:Z:35:LEU:C	2.21	0.60
11:K:58:ASP:HB3	11:K:61:LEU:HD12	1.83	0.60
2:I:57:ARG:HH11	2:I:57:ARG:CG	2.14	0.60
13:B:63:MET:HE3	13:B:74:PRO:HB3	1.82	0.60
8:C:116:GLN:H	8:C:116:GLN:HE21	1.47	0.60
12:A:164:ASN:ND2	12:A:198:ASP:OD1	2.34	0.60
12:F:156:THR:HG23	12:F:188:ILE:HD12	1.82	0.60
8:D:116:GLN:H	8:D:116:GLN:HE21	1.47	0.60
5:Q:63:ASN:OD1	10:L:154:PHE:CD2	2.54	0.60
13:E:109:GLN:CG	13:E:121:ARG:HH11	2.14	0.60
1:H:78:MET:HG3	1:H:82:ILE:HD12	1.83	0.60
12:F:164:ASN:ND2	12:F:198:ASP:OD1	2.34	0.60
8:D:45:MET:HG2	8:D:52:CYS:HB3	1.82	0.60
5:Q:53:VAL:HG23	5:Q:53:VAL:O	2.01	0.60
5:Q:170:GLN:HA	5:Q:170:GLN:HE21	1.65	0.60
12:A:84:ARG:HB2	12:A:119:LEU:HD13	1.84	0.60
10:L:49:LEU:HD21	10:L:199:LEU:CD2	2.32	0.60
2:N:169:ARG:HH11	2:N:169:ARG:CG	2.13	0.60
3:O:35:LEU:C	3:O:35:LEU:HD12	2.21	0.60
13:E:6:LEU:HD12	13:E:6:LEU:O	2.02	0.60
2:N:96:LEU:O	2:N:96:LEU:HG	2.00	0.60
1:M:78:MET:HG3	1:M:82:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:6:LEU:HD12	13:B:6:LEU:O	2.02	0.60
11:R:11:ARG:HG2	11:R:11:ARG:HH11	1.68	0.59
13:B:109:GLN:CG	13:B:121:ARG:HH11	2.14	0.59
5:Q:41:CYS:CB	5:Q:189:ILE:HD11	2.24	0.59
12:F:84:ARG:HB2	12:F:119:LEU:HD13	1.84	0.59
2:I:169:ARG:HB2	2:I:169:ARG:NH1	2.08	0.59
4:P:75:TYR:HB3	4:P:82:TYR:CD1	2.37	0.59
11:R:56:VAL:HG12	11:R:56:VAL:O	2.03	0.59
13:B:63:MET:CE	13:B:74:PRO:HB3	2.31	0.59
13:B:40:LYS:H	13:B:40:LYS:HD3	1.65	0.59
1:M:91:LYS:HG2	1:M:119:LEU:HD11	1.85	0.59
1:H:53:ARG:O	1:H:53:ARG:HG2	2.03	0.59
8:D:12:VAL:HG11	8:D:102:CYS:SG	2.43	0.59
5:Q:27:MET:O	5:Q:31:GLU:HG3	2.03	0.59
10:G:57:ALA:CA	1:H:165:CYS:SG	2.91	0.59
2:I:90:GLU:OE1	2:I:90:GLU:HA	2.01	0.59
13:B:13:ILE:HD12	13:B:151:ALA:HB1	1.84	0.59
5:J:27:MET:O	5:J:31:GLU:HG3	2.03	0.58
12:F:80:ALA:HB1	12:F:119:LEU:HD11	1.84	0.58
2:N:220:LEU:HD13	2:N:224:GLU:HG2	1.85	0.58
9:S:75:TYR:CD1	9:S:83:MET:HG3	2.39	0.58
13:B:13:ILE:HD12	13:B:151:ALA:CB	2.33	0.58
13:B:148:LEU:HD23	13:B:148:LEU:C	2.24	0.58
3:Z:49:ARG:NH1	3:Z:212:GLU:OE2	2.37	0.58
3:Z:161:ALA:HB3	2:I:53:LEU:HD22	1.85	0.58
13:E:13:ILE:HD12	13:E:151:ALA:HB1	1.84	0.58
13:E:148:LEU:C	13:E:148:LEU:HD23	2.24	0.58
11:R:43:ARG:HD2	11:R:149:PRO:O	2.03	0.58
1:H:157:ASP:HB2	1:H:158:PRO:CD	2.34	0.58
12:A:80:ALA:HB1	12:A:119:LEU:HD11	1.84	0.58
1:M:53:ARG:O	1:M:53:ARG:HG2	2.03	0.58
10:G:49:LEU:HD21	10:G:199:LEU:CD2	2.32	0.58
10:G:49:LEU:HD21	10:G:199:LEU:HD21	1.85	0.58
13:B:81:ARG:HH21	13:B:84:ARG:HH12	1.50	0.58
1:H:91:LYS:HG2	1:H:119:LEU:HD11	1.84	0.58
12:F:171:GLY:HA2	14:W:209:TRP:CH2	2.39	0.58
13:E:13:ILE:HD12	13:E:151:ALA:CB	2.33	0.58
10:G:154:PHE:CD2	5:J:63:ASN:OD1	2.57	0.58
11:K:11:ARG:HH11	11:K:11:ARG:HG2	1.68	0.58
13:E:63:MET:HE3	13:E:74:PRO:HB3	1.83	0.58
3:O:171:ALA:HB2	3:O:200:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:12:VAL:HG11	8:C:102:CYS:SG	2.43	0.57
9:S:159:GLN:HG2	13:B:208:THR:O	2.04	0.57
9:X:123:SER:HB3	9:X:136:LYS:HG2	1.85	0.57
9:X:75:TYR:CD1	9:X:83:MET:HG3	2.39	0.57
9:S:123:SER:HB3	9:S:136:LYS:HG2	1.85	0.57
13:E:81:ARG:HH21	13:E:84:ARG:HH12	1.50	0.57
11:K:56:VAL:HG12	11:K:56:VAL:O	2.03	0.57
13:E:208:THR:O	9:X:159:GLN:HG2	2.04	0.57
2:N:11:SER:OG	2:N:12:PRO:HD2	2.05	0.57
11:K:43:ARG:HD2	11:K:149:PRO:O	2.03	0.57
2:I:42:VAL:HG12	2:I:191:VAL:CG2	2.14	0.57
1:M:157:ASP:HB2	1:M:158:PRO:CD	2.34	0.57
3:O:49:ARG:NH1	3:O:212:GLU:OE2	2.37	0.57
7:Y:93:LEU:C	7:Y:93:LEU:HD23	2.25	0.57
10:L:49:LEU:HD21	10:L:199:LEU:HD21	1.85	0.57
1:M:121:LEU:HD11	10:L:79:ALA:HB3	1.79	0.57
3:Z:171:ALA:HB2	3:Z:200:THR:HG21	1.86	0.57
2:I:220:LEU:HD13	2:I:224:GLU:HG2	1.85	0.57
9:X:41:PRO:HB3	9:X:194:ARG:HD2	1.86	0.57
2:I:11:SER:OG	2:I:12:PRO:HD2	2.05	0.57
2:I:42:VAL:HG11	2:I:191:VAL:HG23	1.78	0.57
11:K:37:LEU:HD22	11:K:53:GLN:HB3	1.87	0.56
6:V:67:TYR:CD1	6:V:75:LEU:HG	2.40	0.56
10:L:59:HIS:CD2	10:L:208:LYS:O	2.58	0.56
1:M:91:LYS:HG2	1:M:119:LEU:CD1	2.35	0.56
5:Q:53:VAL:HG22	5:Q:208:ALA:O	2.06	0.56
10:G:59:HIS:CD2	10:G:208:LYS:O	2.58	0.56
1:H:91:LYS:HG2	1:H:119:LEU:CD1	2.35	0.56
11:K:56:VAL:HG22	11:K:66:VAL:HG11	1.87	0.56
12:F:147:SER:HB2	12:F:148:PRO:HD2	1.87	0.56
12:A:188:ILE:CG2	12:A:193:LEU:HD23	2.35	0.56
10:L:230:SER:HB2	10:L:231:PRO:HD3	1.88	0.56
10:G:230:SER:HB2	10:G:231:PRO:HD3	1.88	0.56
12:A:147:SER:HB2	12:A:148:PRO:HD2	1.87	0.56
2:N:148:ASP:HB2	2:N:149:PRO:HD2	1.87	0.56
6:T:67:TYR:CD1	6:T:75:LEU:HG	2.40	0.56
13:E:20:ALA:HB3	13:E:28:ASP:HB3	1.88	0.56
11:R:78:CYS:HB2	11:R:140:LEU:HD23	1.86	0.56
13:B:40:LYS:CD	13:B:40:LYS:N	2.69	0.56
8:C:160:ILE:HB	8:C:174:ILE:HD12	1.87	0.56
9:S:41:PRO:HB3	9:S:194:ARG:HD2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:37:LEU:HD22	11:R:53:GLN:HB3	1.87	0.56
8:D:112:TYR:CE2	8:D:122:SER:HB2	2.41	0.56
8:D:160:ILE:HB	8:D:174:ILE:HD12	1.87	0.56
14:W:174:ARG:HD3	14:W:206:GLU:O	2.05	0.56
11:K:78:CYS:HB2	11:K:140:LEU:HD23	1.86	0.56
9:X:43:CYS:SG	9:X:194:ARG:HD3	2.46	0.56
9:S:10:GLY:HA3	9:S:42:LYS:HE2	1.87	0.55
13:B:20:ALA:HB3	13:B:28:ASP:HB3	1.88	0.55
9:S:43:CYS:SG	9:S:194:ARG:HD3	2.46	0.55
7:U:93:LEU:C	7:U:93:LEU:HD23	2.25	0.55
11:R:223:GLU:OE2	11:R:223:GLU:HA	2.06	0.55
5:J:53:VAL:HG22	5:J:208:ALA:O	2.06	0.55
11:R:56:VAL:HG22	11:R:66:VAL:HG11	1.87	0.55
11:R:201:CYS:O	11:R:205:VAL:HG13	2.07	0.55
9:X:10:GLY:HA3	9:X:42:LYS:HE2	1.87	0.55
8:C:112:TYR:CE2	8:C:122:SER:HB2	2.41	0.55
9:S:158:MET:HE2	13:B:204:PHE:CE1	2.30	0.55
12:F:188:ILE:CG2	12:F:193:LEU:HD23	2.35	0.55
13:E:201:GLN:H	13:E:201:GLN:NE2	2.05	0.55
2:I:148:ASP:HB2	2:I:149:PRO:HD2	1.88	0.55
2:N:148:ASP:HB2	2:N:149:PRO:CD	2.37	0.55
6:V:2:GLU:HG2	6:V:34:LYS:CE	2.37	0.55
12:A:57:ASP:OD2	13:B:84:ARG:NH1	2.33	0.55
11:K:223:GLU:HA	11:K:223:GLU:OE2	2.06	0.55
13:E:13:ILE:CD1	13:E:151:ALA:CB	2.85	0.55
4:P:106:THR:OG1	4:P:139:ASN:ND2	2.30	0.55
6:T:43:LEU:HB2	6:T:183:ILE:HD11	1.89	0.55
8:C:64:ARG:NH1	8:C:67:TYR:CE2	2.66	0.55
3:Z:34:CYS:HB2	3:Z:164:ILE:HG13	1.89	0.55
2:I:183:THR:CG2	2:I:186:LEU:HB2	2.34	0.55
2:N:40:ILE:CA	2:N:136:PHE:HZ	2.20	0.55
2:N:42:VAL:HG12	2:N:191:VAL:CG2	2.14	0.55
2:N:227:LYS:O	2:N:231:GLU:HG2	2.07	0.55
6:V:43:LEU:HB2	6:V:183:ILE:HD11	1.89	0.55
11:R:137:CYS:SG	11:R:153:LYS:HD2	2.47	0.55
13:B:201:GLN:H	13:B:201:GLN:NE2	2.05	0.55
6:V:102:LEU:HD11	6:V:118:MET:CE	2.37	0.54
11:K:201:CYS:O	11:K:205:VAL:HG13	2.07	0.54
1:M:165:CYS:SG	10:L:57:ALA:CA	2.95	0.54
2:I:227:LYS:O	2:I:231:GLU:HG2	2.07	0.54
11:K:77:GLY:HA3	11:K:227:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:137:CYS:SG	11:K:153:LYS:HD2	2.47	0.54
12:F:57:ASP:OD2	13:E:84:ARG:NH1	2.33	0.54
4:P:74:VAL:HG12	4:P:134:LEU:HB2	1.90	0.54
10:G:220:GLU:O	10:G:222:THR:HG23	2.08	0.54
6:T:102:LEU:HD11	6:T:118:MET:CE	2.37	0.54
12:F:14:VAL:HG12	12:F:176:VAL:HG23	1.90	0.54
2:I:148:ASP:HB2	2:I:149:PRO:CD	2.37	0.54
13:B:13:ILE:CD1	13:B:151:ALA:CB	2.85	0.54
13:B:15:GLY:HA3	13:B:155:LEU:HD11	1.90	0.54
4:P:181:LEU:HD21	4:P:186:ALA:HA	1.89	0.54
5:Q:34:SER:CB	5:Q:65:ARG:HH12	2.21	0.54
12:F:126:ILE:HD11	12:F:135:TYR:CE1	2.43	0.54
2:I:40:ILE:CA	2:I:136:PHE:HZ	2.20	0.54
4:P:51:GLN:HA	4:P:51:GLN:NE2	2.23	0.54
10:G:199:LEU:HD11	10:G:205:LEU:HD23	1.90	0.54
11:R:77:GLY:HA3	11:R:227:PHE:CD1	2.43	0.54
5:J:41:CYS:SG	5:J:189:ILE:HD12	2.48	0.54
7:U:137:VAL:HG11	7:U:145:MET:HB3	1.90	0.53
1:H:32:LYS:O	1:H:172:SER:HA	2.09	0.53
5:J:34:SER:CB	5:J:65:ARG:HH12	2.21	0.53
10:L:220:GLU:O	10:L:222:THR:HG23	2.08	0.53
8:D:161:THR:HG22	8:D:196:LEU:CD1	2.38	0.53
5:Q:41:CYS:SG	5:Q:189:ILE:HD12	2.48	0.53
7:Y:137:VAL:HG11	7:Y:145:MET:HB3	1.90	0.53
13:E:15:GLY:HA3	13:E:155:LEU:HD11	1.90	0.53
3:O:34:CYS:HB2	3:O:164:ILE:HG13	1.89	0.53
11:K:78:CYS:CB	11:K:140:LEU:HD23	2.38	0.53
12:A:72:GLU:HB2	12:A:73:PRO:HD2	1.91	0.53
8:C:161:THR:HG22	8:C:196:LEU:CD1	2.38	0.53
12:A:14:VAL:HG12	12:A:176:VAL:HG23	1.90	0.53
12:A:126:ILE:HD11	12:A:135:TYR:CE1	2.43	0.53
8:D:20:ALA:HB2	8:D:31:VAL:HG21	1.91	0.53
2:N:208:LEU:HB2	2:N:225:ILE:HD11	1.90	0.53
12:F:45:LEU:CD2	12:F:98:LEU:HD11	2.39	0.53
12:A:37:LEU:HD21	12:A:43:CYS:SG	2.49	0.53
11:R:4:GLY:N	11:R:19:GLU:OE2	2.41	0.53
11:K:4:GLY:N	11:K:19:GLU:OE2	2.41	0.53
1:M:32:LYS:O	1:M:172:SER:HA	2.09	0.53
4:P:54:ILE:HD13	11:R:184:LYS:HB3	1.90	0.53
10:G:41:LYS:HD3	10:G:180:MET:HB3	1.90	0.53
1:H:91:LYS:CE	1:H:119:LEU:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:58:GLU:CD	3:Z:58:GLU:H	2.13	0.53
10:L:199:LEU:HD11	10:L:205:LEU:HD23	1.90	0.53
11:R:78:CYS:CB	11:R:140:LEU:HD23	2.38	0.53
10:G:78:THR:HG21	1:H:161:THR:HG1	1.70	0.53
8:D:64:ARG:HH11	8:D:67:TYR:HD2	1.43	0.53
1:M:91:LYS:CE	1:M:119:LEU:HD11	2.38	0.52
2:N:183:THR:CG2	2:N:186:LEU:HB2	2.34	0.52
4:P:149:ASP:CB	4:P:150:PRO:CD	2.86	0.52
8:C:20:ALA:HB2	8:C:31:VAL:HG21	1.91	0.52
12:A:45:LEU:CD2	12:A:98:LEU:HD11	2.39	0.52
2:I:136:PHE:HE1	2:I:211:MET:O	1.92	0.52
3:Z:51:ASN:HB3	3:Z:56:LEU:HD13	1.91	0.52
7:Y:69:ARG:NH2	7:Y:96:GLU:OE2	2.40	0.52
13:B:99:LEU:HD22	13:B:125:THR:OG1	2.10	0.52
1:M:91:LYS:CD	1:M:119:LEU:HD11	2.40	0.52
2:N:40:ILE:N	2:N:136:PHE:HZ	2.08	0.52
3:O:51:ASN:HB3	3:O:56:LEU:HD13	1.91	0.52
6:T:102:LEU:HD11	6:T:118:MET:HE1	1.91	0.52
1:H:91:LYS:CD	1:H:119:LEU:HD11	2.40	0.52
6:V:58:GLU:HB3	2:I:96:LEU:HD13	1.92	0.52
12:F:37:LEU:HD21	12:F:43:CYS:SG	2.49	0.52
11:R:88:ARG:NH2	11:R:88:ARG:CG	2.73	0.52
6:T:35:MET:HG2	6:T:45:LEU:HG	1.91	0.52
8:C:64:ARG:HH11	8:C:67:TYR:HD2	1.43	0.52
2:I:208:LEU:HB2	2:I:225:ILE:HD11	1.90	0.52
1:H:204:GLN:O	1:H:204:GLN:HG2	2.10	0.52
5:J:175:GLU:OE2	5:J:175:GLU:HA	2.10	0.52
5:Q:51:LYS:HE2	5:Q:62:SER:O	2.10	0.52
2:N:57:ARG:CG	2:N:57:ARG:NH1	2.73	0.52
8:C:173:ILE:HG22	8:C:191:ASP:HA	1.92	0.52
10:G:74:ILE:HG22	10:G:132:LEU:CD2	2.40	0.52
13:E:99:LEU:HD22	13:E:125:THR:OG1	2.10	0.52
10:L:41:LYS:HD3	10:L:180:MET:HB3	1.91	0.52
2:N:136:PHE:HE1	2:N:211:MET:O	1.92	0.52
12:F:156:THR:CG2	12:F:188:ILE:HD12	2.40	0.52
13:B:99:LEU:HG	13:B:127:LEU:HD12	1.92	0.52
6:T:96:THR:CG2	8:D:91:ARG:NH2	2.73	0.51
12:F:155:THR:O	12:F:159:ILE:HG13	2.10	0.51
3:Z:61:PHE:CZ	3:Z:227:VAL:CG2	2.93	0.51
12:F:72:GLU:HB2	12:F:73:PRO:HD2	1.91	0.51
13:E:179:THR:HG23	13:E:181:THR:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:40:ILE:N	2:I:136:PHE:HZ	2.08	0.51
2:I:57:ARG:CG	2:I:57:ARG:NH1	2.73	0.51
2:N:79:ASP:OD1	3:O:119:GLN:NE2	2.43	0.51
2:I:180:ALA:HB1	2:I:190:LEU:HD23	1.92	0.51
8:D:173:ILE:HG22	8:D:191:ASP:HA	1.92	0.51
3:O:61:PHE:CZ	3:O:227:VAL:CG2	2.93	0.51
6:V:35:MET:HG2	6:V:45:LEU:HG	1.91	0.51
14:W:1:THR:O	14:W:107:TRP:HE3	1.93	0.51
2:N:42:VAL:HG11	2:N:191:VAL:HG23	1.78	0.51
2:N:169:ARG:HB2	2:N:169:ARG:NH1	2.08	0.51
6:T:86:ARG:O	6:T:86:ARG:HD3	2.11	0.51
10:G:210:VAL:HG12	10:G:210:VAL:O	2.10	0.51
12:A:155:THR:O	12:A:159:ILE:HG13	2.10	0.51
12:A:156:THR:CG2	12:A:188:ILE:HD12	2.40	0.51
8:D:95:LEU:O	8:D:116:GLN:HG3	2.11	0.51
7:U:69:ARG:NH2	7:U:96:GLU:OE2	2.40	0.51
10:L:74:ILE:HG22	10:L:132:LEU:CD2	2.40	0.51
11:R:88:ARG:HH21	11:R:88:ARG:CG	2.16	0.51
2:N:180:ALA:HB1	2:N:190:LEU:HD23	1.92	0.51
10:G:71:GLY:HA3	10:G:221:PHE:CZ	2.46	0.51
5:J:51:LYS:HE2	5:J:62:SER:O	2.10	0.51
6:V:155:ARG:NE	6:V:158:GLU:OE2	2.36	0.51
13:E:21:THR:HG22	13:E:26:VAL:HA	1.93	0.51
8:C:3:THR:HG22	8:C:16:VAL:HG12	1.93	0.51
13:E:99:LEU:HG	13:E:127:LEU:HD12	1.92	0.51
3:O:58:GLU:H	3:O:58:GLU:CD	2.13	0.51
6:T:16:ALA:HA	6:T:179:SER:O	2.11	0.51
9:X:16:ALA:HB2	9:X:121:VAL:HG23	1.93	0.51
1:M:204:GLN:O	1:M:204:GLN:HG2	2.09	0.51
6:V:86:ARG:O	6:V:86:ARG:HD3	2.11	0.51
13:E:205:ALA:CB	13:E:206:PRO:CD	2.44	0.51
10:L:210:VAL:HG12	10:L:210:VAL:O	2.10	0.51
4:P:221:THR:HG23	4:P:223:THR:H	1.77	0.50
5:J:34:SER:HB2	5:J:65:ARG:HH12	1.76	0.50
5:Q:175:GLU:OE2	5:Q:175:GLU:HA	2.10	0.50
2:N:92:GLN:OE1	2:N:92:GLN:HA	2.10	0.50
4:P:208:GLU:OE2	4:P:219:ARG:HD2	2.12	0.50
8:C:95:LEU:O	8:C:116:GLN:HG3	2.11	0.50
9:S:16:ALA:HB2	9:S:121:VAL:HG23	1.93	0.50
10:G:57:ALA:HA	1:H:165:CYS:SG	2.51	0.50
1:H:157:ASP:HB2	1:H:158:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:92:GLN:OE1	2:I:92:GLN:HA	2.10	0.50
6:T:2:GLU:HG2	6:T:34:LYS:CE	2.37	0.50
13:E:156:VAL:HG21	13:E:189:LEU:CD1	2.41	0.50
11:R:13:ILE:HG13	11:R:15:ILE:HG12	1.92	0.50
7:U:27:PHE:HB2	7:U:38:PHE:HB2	1.94	0.50
3:Z:49:ARG:HD3	3:Z:209:GLU:O	2.12	0.50
7:Y:116:PHE:CD2	7:Y:191:LYS:HE3	2.47	0.50
13:B:179:THR:HG23	13:B:181:THR:H	1.75	0.50
1:H:206:MET:HE3	1:H:214:ASN:ND2	2.27	0.50
7:Y:27:PHE:HB2	7:Y:38:PHE:HB2	1.94	0.50
13:B:21:THR:HG22	13:B:26:VAL:HA	1.93	0.50
2:N:218:LYS:C	2:N:218:LYS:HD3	2.32	0.50
6:T:155:ARG:NE	6:T:158:GLU:OE2	2.36	0.50
6:V:34:LYS:HD3	6:V:47:VAL:HG12	1.94	0.50
5:Q:34:SER:HB2	5:Q:65:ARG:HH12	1.76	0.50
5:Q:56:LYS:HD2	10:L:173:GLU:HG2	1.93	0.50
11:K:196:GLU:CG	11:K:242:LEU:CD2	2.82	0.50
14:W:147:GLN:HB3	14:W:148:PRO:HD3	1.94	0.50
2:N:171:PHE:CD1	2:N:171:PHE:C	2.85	0.50
8:C:91:ARG:NH2	6:V:96:THR:CG2	2.75	0.50
9:S:38:ARG:NH1	9:S:191:ASP:OD1	2.38	0.50
9:S:177:ASP:OD1	13:B:198:ARG:HB2	2.12	0.50
1:H:183:GLU:O	1:H:183:GLU:HG3	2.12	0.50
13:E:201:GLN:NE2	13:E:201:GLN:N	2.60	0.50
10:L:71:GLY:HA3	10:L:221:PHE:CZ	2.46	0.50
1:M:183:GLU:O	1:M:183:GLU:HG3	2.12	0.49
5:Q:37:ILE:HD11	5:Q:193:VAL:HG13	1.94	0.49
11:K:36:GLY:HA2	11:K:170:VAL:HG21	1.94	0.49
13:E:204:PHE:CE1	9:X:158:MET:HE2	2.33	0.49
2:I:69:VAL:HG11	2:I:107:ILE:HG21	1.94	0.49
2:N:180:ALA:HB1	2:N:190:LEU:HD22	1.93	0.49
3:Z:119:GLN:NE2	2:I:79:ASP:OD1	2.44	0.49
7:U:116:PHE:CD2	7:U:191:LYS:HE3	2.47	0.49
6:V:16:ALA:HA	6:V:179:SER:O	2.11	0.49
7:Y:152:LEU:HD13	13:B:204:PHE:HE2	1.78	0.49
11:R:196:GLU:CG	11:R:242:LEU:CD2	2.82	0.49
8:D:3:THR:HG22	8:D:16:VAL:HG12	1.93	0.49
3:Z:44:LEU:C	3:Z:44:LEU:HD12	2.32	0.49
10:L:69:HIS:O	10:L:136:GLY:HA2	2.13	0.49
3:O:49:ARG:HD3	3:O:209:GLU:O	2.12	0.49
1:H:58:LEU:HD21	2:I:173:GLU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:206:LEU:HB3	3:Z:237:ILE:HD13	1.94	0.49
13:E:198:ARG:HB2	9:X:177:ASP:OD1	2.12	0.49
12:A:90:TYR:HB2	12:A:94:LEU:CD1	2.42	0.49
13:B:201:GLN:NE2	13:B:201:GLN:N	2.60	0.49
11:K:13:ILE:HG13	11:K:15:ILE:HG12	1.92	0.49
12:F:24:GLU:HG2	14:W:182:ARG:HG2	1.94	0.49
13:B:141:ARG:HH11	13:B:141:ARG:CG	2.25	0.49
2:I:171:PHE:CD1	2:I:171:PHE:C	2.85	0.49
3:O:44:LEU:HD12	3:O:44:LEU:C	2.32	0.49
4:P:74:VAL:HG13	4:P:134:LEU:HB2	1.94	0.49
10:G:69:HIS:O	10:G:136:GLY:HA2	2.13	0.49
5:J:37:ILE:HD11	5:J:193:VAL:HG13	1.94	0.49
11:K:88:ARG:NH2	11:K:88:ARG:CG	2.73	0.49
1:M:206:MET:CE	1:M:214:ASN:ND2	2.76	0.49
6:T:34:LYS:HD3	6:T:47:VAL:HG12	1.94	0.49
1:M:157:ASP:HB2	1:M:158:PRO:HD2	1.94	0.49
2:N:69:VAL:HG11	2:N:107:ILE:HG21	1.94	0.49
7:U:100:GLY:N	7:U:101:PRO:CD	2.69	0.49
6:V:77:PRO:HD2	6:V:108:ASP:HB2	1.95	0.49
1:M:195:ILE:HD11	1:M:219:THR:HG21	1.95	0.48
3:O:206:LEU:HB3	3:O:237:ILE:HD13	1.95	0.48
7:U:152:LEU:HD13	13:E:204:PHE:HE2	1.77	0.48
2:N:179:GLU:O	2:N:186:LEU:HD13	2.14	0.48
1:H:209:LYS:O	1:H:214:ASN:ND2	2.47	0.48
5:J:219:ILE:HG23	5:J:220:THR:HG23	1.95	0.48
4:P:50:LYS:NZ	4:P:50:LYS:HB3	2.28	0.48
9:S:44:TYR:N	9:S:44:TYR:CD1	2.81	0.48
13:B:156:VAL:HG21	13:B:189:LEU:CD1	2.41	0.48
1:M:165:CYS:SG	10:L:57:ALA:HA	2.54	0.48
1:H:85:ALA:HB2	1:H:139:VAL:HG21	1.96	0.48
2:I:221:ASN:ND2	2:I:224:GLU:HB2	2.28	0.48
2:N:96:LEU:HD13	6:T:58:GLU:HB3	1.93	0.48
6:T:41:LYS:O	6:T:106:GLY:HA2	2.13	0.48
12:A:45:LEU:HD22	12:A:52:ALA:HB1	1.96	0.48
9:X:125:ASP:HB2	9:X:126:PRO:CD	2.44	0.48
2:N:221:ASN:ND2	2:N:224:GLU:HB2	2.28	0.48
13:E:135:LEU:HD11	14:W:179:ARG:CG	2.44	0.48
2:I:218:LYS:HD3	2:I:218:LYS:C	2.32	0.48
11:R:36:GLY:HA2	11:R:170:VAL:HG21	1.94	0.48
4:P:37:ILE:HD12	4:P:190:ALA:HB2	1.96	0.48
9:S:125:ASP:HB2	9:S:126:PRO:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:LEU:HA	1:H:202:LEU:HD23	1.74	0.48
1:H:206:MET:CE	1:H:214:ASN:ND2	2.76	0.48
2:I:169:ARG:CG	2:I:169:ARG:NH1	2.73	0.48
9:X:13:LEU:HD11	9:X:149:LEU:HD11	1.95	0.48
13:B:81:ARG:NH2	13:B:84:ARG:NH1	2.62	0.48
13:B:189:LEU:HD13	13:B:189:LEU:C	2.33	0.48
5:Q:219:ILE:HG23	5:Q:220:THR:HG23	1.96	0.48
12:F:45:LEU:HD22	12:F:52:ALA:HB1	1.96	0.48
2:I:220:LEU:N	2:I:220:LEU:HD23	2.29	0.48
9:X:75:TYR:CG	9:X:83:MET:HG3	2.48	0.48
9:X:125:ASP:OD2	9:X:129:SER:HB3	2.14	0.48
9:S:180:ILE:CD1	13:B:196:THR:HB	2.44	0.48
2:N:220:LEU:N	2:N:220:LEU:HD23	2.29	0.48
12:A:14:VAL:CG1	12:A:176:VAL:HG23	2.42	0.48
1:M:157:ASP:CB	1:M:158:PRO:CD	2.91	0.47
2:N:189:LYS:HG3	2:N:193:LYS:HE3	1.96	0.47
7:U:105:GLU:HB2	7:U:138:SER:OG	2.14	0.47
8:C:21:THR:HG22	8:C:26:ILE:HA	1.96	0.47
9:S:13:LEU:HD11	9:S:149:LEU:HD11	1.95	0.47
9:S:75:TYR:CG	9:S:83:MET:HG3	2.48	0.47
1:H:195:ILE:HD11	1:H:219:THR:HG21	1.95	0.47
6:V:41:LYS:O	6:V:106:GLY:HA2	2.14	0.47
13:E:189:LEU:C	13:E:189:LEU:HD13	2.33	0.47
2:I:189:LYS:HG3	2:I:193:LYS:HE3	1.96	0.47
2:N:179:GLU:OE1	2:N:179:GLU:N	2.38	0.47
7:Y:105:GLU:HB2	7:Y:138:SER:OG	2.14	0.47
13:E:196:THR:HB	9:X:180:ILE:CD1	2.44	0.47
14:W:15:LYS:HD2	14:W:135:PRO:HA	1.96	0.47
2:I:197:GLU:OE1	2:I:197:GLU:HA	2.14	0.47
8:D:21:THR:HG22	8:D:26:ILE:HA	1.96	0.47
1:M:209:LYS:O	1:M:214:ASN:ND2	2.47	0.47
9:S:13:LEU:CD1	9:S:149:LEU:HD11	2.44	0.47
14:W:122:LEU:HG	14:W:137:LEU:HD12	1.96	0.47
12:A:14:VAL:HG12	12:A:176:VAL:CG2	2.41	0.47
10:L:184:LEU:HD11	10:L:214:ILE:HG21	1.96	0.47
2:I:179:GLU:O	2:I:186:LEU:HD13	2.14	0.47
9:X:184:GLU:OE2	9:X:211:ARG:CD	2.61	0.47
1:M:85:ALA:HB2	1:M:139:VAL:HG21	1.96	0.47
1:M:182:GLN:HA	10:L:56:LEU:HD11	1.97	0.47
4:P:59:ARG:HH11	4:P:59:ARG:CB	2.14	0.47
4:P:221:THR:HG22	4:P:224:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:184:LEU:HD11	10:G:214:ILE:HG21	1.96	0.47
1:H:213:THR:HG22	1:H:231:LYS:CE	2.44	0.47
13:E:135:LEU:HD12	14:W:179:ARG:HG3	1.96	0.47
9:S:125:ASP:OD2	9:S:129:SER:HB3	2.14	0.47
10:G:49:LEU:CD2	10:G:199:LEU:HD21	2.45	0.47
2:I:180:ALA:HB1	2:I:190:LEU:HD22	1.93	0.47
8:D:10:HIS:CD2	8:D:149:PRO:HD3	2.50	0.47
6:T:77:PRO:HD2	6:T:108:ASP:HB2	1.95	0.47
8:C:91:ARG:HH22	6:V:96:THR:CB	2.20	0.47
13:E:81:ARG:NH2	13:E:84:ARG:NH1	2.62	0.47
5:Q:151:ILE:HG12	5:Q:157:SER:CB	2.45	0.47
7:U:25:ARG:NH1	7:U:25:ARG:CG	2.73	0.47
8:C:12:VAL:HB	8:C:179:MET:HB3	1.97	0.47
1:H:157:ASP:CB	1:H:158:PRO:CD	2.91	0.47
3:Z:240:HIS:HA	3:Z:243:GLU:HB2	1.97	0.47
5:J:108:LEU:HD22	5:J:139:SER:HB3	1.97	0.47
6:V:76:SER:HB2	6:V:108:ASP:OD2	2.15	0.47
9:X:13:LEU:CD1	9:X:149:LEU:HD11	2.44	0.47
9:X:44:TYR:N	9:X:44:TYR:CD1	2.81	0.47
2:N:169:ARG:CG	2:N:169:ARG:NH1	2.73	0.47
4:P:49:LYS:HB2	4:P:49:LYS:HE2	1.51	0.47
6:T:10:PRO:HG3	6:T:150:THR:HA	1.97	0.47
7:Y:100:GLY:N	7:Y:101:PRO:CD	2.69	0.47
13:E:204:PHE:HE1	9:X:158:MET:CE	2.21	0.47
10:L:49:LEU:CD2	10:L:199:LEU:HD21	2.45	0.47
2:I:64:ALA:HB2	2:I:217:LEU:CD2	2.33	0.47
13:B:40:LYS:HD3	13:B:40:LYS:N	2.27	0.47
1:M:213:THR:HG22	1:M:231:LYS:CE	2.44	0.47
14:W:35:ARG:HG2	14:W:36:PHE:CE2	2.50	0.47
2:I:98:VAL:HG12	2:I:98:VAL:O	2.15	0.47
8:D:12:VAL:HB	8:D:179:MET:HB3	1.97	0.47
2:N:98:VAL:HG12	2:N:98:VAL:O	2.15	0.47
14:W:43:MET:HG3	14:W:64:LYS:HD2	1.97	0.47
2:N:197:GLU:OE1	2:N:197:GLU:HA	2.14	0.46
5:Q:108:LEU:HD22	5:Q:139:SER:HB3	1.97	0.46
11:K:155:ASP:CB	11:K:156:PRO:CD	2.78	0.46
13:E:197:GLU:OE1	13:E:197:GLU:HA	2.16	0.46
10:L:74:ILE:HG22	10:L:132:LEU:HD22	1.96	0.46
11:R:53:GLN:CD	11:R:206:LEU:HD21	2.35	0.46
2:N:52:LYS:HB2	2:N:52:LYS:HE2	1.35	0.46
2:N:94:HIS:CG	2:N:102:VAL:HG12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:10:HIS:CD2	8:C:149:PRO:HD3	2.50	0.46
6:V:10:PRO:HG3	6:V:150:THR:HA	1.97	0.46
12:F:90:TYR:HB2	12:F:94:LEU:CD1	2.42	0.46
2:I:90:GLU:HG2	2:I:110:TYR:CE1	2.51	0.46
11:K:53:GLN:CD	11:K:206:LEU:HD21	2.35	0.46
14:W:112:ILE:HD12	14:W:112:ILE:N	2.30	0.46
10:L:35:THR:HG23	10:L:133:LEU:CD1	2.46	0.46
2:I:174:LYS:H	2:I:174:LYS:HG2	1.45	0.46
9:X:38:ARG:NH1	9:X:191:ASP:OD1	2.38	0.46
3:O:240:HIS:HA	3:O:243:GLU:HB2	1.97	0.46
10:G:137:TYR:CZ	10:G:217:LYS:HA	2.51	0.46
5:J:50:GLU:HG2	5:J:50:GLU:O	2.14	0.46
7:Y:52:LEU:HD23	7:Y:106:PRO:HB3	1.97	0.46
7:Y:203:MET:H	8:D:193:ASN:ND2	2.14	0.46
10:L:71:GLY:HA3	10:L:221:PHE:CE1	2.51	0.46
2:N:90:GLU:HG2	2:N:110:TYR:CE1	2.51	0.46
3:Z:178:ASP:OD2	3:Z:195:LYS:HE2	2.15	0.46
6:V:109:GLU:H	6:V:109:GLU:HG2	1.56	0.46
14:W:27:LEU:HD22	14:W:184:TYR:HB2	1.98	0.46
3:O:174:MET:HE3	3:O:195:LYS:NZ	2.31	0.46
5:Q:50:GLU:O	5:Q:50:GLU:HG2	2.14	0.46
13:B:124:PHE:HB2	13:B:138:LEU:HD13	1.97	0.46
2:N:124:ARG:HB3	3:O:124:PHE:HB3	1.98	0.46
8:D:64:ARG:NH1	8:D:67:TYR:CE2	2.66	0.46
1:M:58:LEU:HD21	2:N:173:GLU:HA	1.98	0.46
3:O:178:ASP:OD2	3:O:195:LYS:HE2	2.15	0.46
10:L:118:ILE:N	10:L:119:PRO:HD2	2.31	0.46
2:I:94:HIS:CG	2:I:102:VAL:HG12	2.50	0.46
2:N:64:ALA:HB2	2:N:217:LEU:CD2	2.33	0.46
6:T:76:SER:HB2	6:T:108:ASP:OD2	2.15	0.46
7:U:12:ALA:HB3	7:U:136:VAL:CG2	2.46	0.46
7:U:196:THR:HB	13:E:215:THR:HG23	1.98	0.46
10:L:137:TYR:CZ	10:L:217:LYS:HA	2.51	0.46
3:O:59:VAL:HG13	4:P:142:ARG:NH2	2.30	0.45
4:P:164:LYS:HB3	4:P:164:LYS:HE2	1.55	0.45
8:C:103:GLY:HA2	8:C:179:MET:HE3	1.98	0.45
10:G:74:ILE:HG22	10:G:132:LEU:HD22	1.96	0.45
2:I:52:LYS:HE2	2:I:52:LYS:HB2	1.35	0.45
2:I:196:LEU:HD13	2:I:196:LEU:HA	1.72	0.45
8:C:172:GLY:O	8:C:192:VAL:HG22	2.17	0.45
10:G:35:THR:HG22	10:G:161:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:230:SER:CB	10:G:231:PRO:HD3	2.46	0.45
1:H:83:ALA:HB1	2:I:116:GLN:HG3	1.98	0.45
11:K:67:THR:OG1	11:K:216:GLU:OE2	2.22	0.45
15:A:201:A1L0C:CB	15:A:201:A1L0C:O2	2.64	0.45
13:B:197:GLU:OE1	13:B:197:GLU:HA	2.16	0.45
3:O:59:VAL:CG1	4:P:142:ARG:NH2	2.79	0.45
3:O:205:LYS:HB2	3:O:205:LYS:HE2	1.38	0.45
7:U:3:MET:CE	7:U:105:GLU:HG3	2.47	0.45
10:G:35:THR:HG23	10:G:133:LEU:CD1	2.46	0.45
5:J:12:SER:HB3	5:J:125:TYR:HA	1.99	0.45
13:E:124:PHE:HB2	13:E:138:LEU:HD13	1.97	0.45
2:I:37:GLY:HA2	2:I:181:ILE:HD12	1.99	0.45
2:N:37:GLY:HA2	2:N:181:ILE:HD12	1.98	0.45
2:N:174:LYS:H	2:N:174:LYS:HG2	1.45	0.45
5:Q:57:LEU:HB3	10:L:158:ALA:O	2.17	0.45
10:G:57:ALA:HA	1:H:165:CYS:HA	1.98	0.45
1:H:56:SER:HG	2:I:156:TRP:HZ3	1.63	0.45
5:J:151:ILE:HG12	5:J:157:SER:CB	2.45	0.45
7:Y:12:ALA:HB3	7:Y:136:VAL:CG2	2.46	0.45
9:X:107:TYR:CE1	9:X:126:PRO:HD3	2.51	0.45
3:O:50:ARG:HD3	3:O:50:ARG:HA	1.80	0.45
3:O:197:LEU:HD12	3:O:197:LEU:HA	1.65	0.45
10:G:118:ILE:N	10:G:119:PRO:HD2	2.31	0.45
1:H:193:GLU:O	1:H:197:SER:HB2	2.17	0.45
6:V:102:LEU:HD11	6:V:118:MET:HE3	1.97	0.45
12:A:3:ILE:HG22	12:A:16:SER:HB3	1.99	0.45
10:G:71:GLY:HA3	10:G:221:PHE:CE1	2.51	0.45
3:Z:151:ASP:CB	3:Z:152:PRO:CD	2.77	0.45
7:Y:30:GLN:HB3	7:Y:31:ALA:H	1.65	0.45
11:R:52:THR:CG2	11:R:216:GLU:HB2	2.47	0.45
2:N:73:PHE:CD1	2:N:73:PHE:C	2.90	0.45
7:U:52:LEU:HD23	7:U:106:PRO:HB3	1.97	0.45
9:S:208:VAL:HA	9:S:209:PRO:HD3	1.84	0.45
10:L:148:CYS:HB3	10:L:149:PRO:HD2	1.99	0.45
10:L:230:SER:CB	10:L:231:PRO:HD3	2.46	0.45
11:R:168:ALA:HA	11:R:172:GLN:HG3	1.99	0.45
8:D:172:GLY:O	8:D:192:VAL:HG22	2.17	0.45
3:O:174:MET:CE	3:O:195:LYS:NZ	2.80	0.45
5:Q:30:VAL:HG22	5:Q:133:CYS:HA	1.99	0.45
5:Q:109:LYS:HG3	5:Q:149:TYR:OH	2.17	0.45
9:S:107:TYR:CE1	9:S:126:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:184:GLU:OE2	9:S:211:ARG:CD	2.61	0.45
10:G:173:GLU:HG2	5:J:56:LYS:HD2	1.99	0.45
11:K:112:ASP:HB3	11:K:152:TYR:CZ	2.52	0.45
2:I:218:LYS:C	2:I:218:LYS:CD	2.85	0.45
4:P:49:LYS:O	4:P:49:LYS:HG3	2.17	0.45
7:U:203:MET:H	8:C:193:ASN:ND2	2.14	0.45
8:C:88:TYR:CZ	6:V:55:GLN:HG3	2.51	0.45
10:G:154:PHE:HD2	5:J:63:ASN:OD1	1.99	0.45
3:Z:50:ARG:HD3	3:Z:50:ARG:HA	1.80	0.45
5:J:30:VAL:HG22	5:J:133:CYS:HA	1.99	0.45
2:N:204:LYS:HB2	2:N:204:LYS:HE3	1.60	0.45
6:T:21:ALA:HB3	6:T:29:LYS:HB3	1.99	0.45
5:J:109:LYS:HG3	5:J:149:TYR:OH	2.17	0.45
7:Y:3:MET:CE	7:Y:105:GLU:HG3	2.47	0.45
12:A:3:ILE:HG22	12:A:16:SER:CB	2.47	0.45
11:R:112:ASP:HB3	11:R:152:TYR:CZ	2.52	0.45
2:N:59:VAL:O	2:N:59:VAL:HG23	2.17	0.44
2:N:218:LYS:C	2:N:218:LYS:CD	2.85	0.44
2:N:220:LEU:N	2:N:220:LEU:CD2	2.80	0.44
8:C:45:MET:CG	8:C:52:CYS:HB3	2.47	0.44
11:K:52:THR:CG2	11:K:216:GLU:HB2	2.47	0.44
15:F:201:A1L0C:CB	15:F:201:A1L0C:O2	2.64	0.44
14:W:50:MET:HE2	14:W:192:VAL:HG12	1.98	0.44
12:A:8:PHE:HB3	12:A:151:CYS:SG	2.58	0.44
2:I:73:PHE:CD1	2:I:73:PHE:C	2.90	0.44
4:P:72:GLY:HA3	4:P:217:PHE:CE1	2.52	0.44
3:Z:238:LYS:HB2	3:Z:238:LYS:HE2	1.26	0.44
13:B:6:LEU:C	13:B:6:LEU:CD1	2.83	0.44
1:M:206:MET:HE3	1:M:214:ASN:ND2	2.31	0.44
4:P:51:GLN:HA	4:P:51:GLN:HE21	1.82	0.44
5:Q:12:SER:HB3	5:Q:125:TYR:HA	1.99	0.44
12:F:45:LEU:HD22	12:F:98:LEU:HD11	1.99	0.44
2:I:40:ILE:HA	2:I:136:PHE:HZ	1.82	0.44
13:B:36:PHE:CD1	13:B:36:PHE:C	2.91	0.44
1:M:49:ALA:CB	1:M:217:LEU:HD12	2.40	0.44
4:P:54:ILE:HD11	11:R:184:LYS:HB3	1.98	0.44
4:P:62:HIS:HB3	4:P:208:GLU:OE2	2.17	0.44
6:T:86:ARG:HD3	6:T:86:ARG:C	2.38	0.44
10:G:148:CYS:HB3	10:G:149:PRO:HD2	1.99	0.44
3:Z:174:MET:CE	3:Z:195:LYS:NZ	2.80	0.44
5:J:63:ASN:HD22	5:J:81:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:21:ALA:HB3	6:V:29:LYS:HB3	1.99	0.44
10:L:35:THR:HG22	10:L:161:ILE:HG13	1.99	0.44
1:M:193:GLU:O	1:M:197:SER:HB2	2.17	0.44
4:P:59:ARG:H	4:P:59:ARG:HG3	1.56	0.44
4:P:114:ALA:HB1	4:P:152:GLY:O	2.18	0.44
7:Y:196:THR:HB	13:B:215:THR:HG23	1.98	0.44
2:N:148:ASP:CB	2:N:149:PRO:CD	2.96	0.44
4:P:142:ARG:HG2	4:P:143:PRO:HD2	1.99	0.44
5:Q:41:CYS:HB2	5:Q:189:ILE:HD11	2.00	0.44
5:Q:63:ASN:OD1	10:L:154:PHE:HD2	1.96	0.44
5:Q:63:ASN:HD22	5:Q:81:LEU:HD23	1.83	0.44
6:T:55:GLN:HG3	8:D:88:TYR:CZ	2.52	0.44
6:T:67:TYR:CG	6:T:75:LEU:HG	2.53	0.44
12:F:8:PHE:HB3	12:F:151:CYS:SG	2.58	0.44
13:E:41:ILE:HD13	13:E:79:VAL:HG21	2.00	0.44
2:I:59:VAL:O	2:I:59:VAL:HG23	2.17	0.44
2:N:40:ILE:HA	2:N:136:PHE:HZ	1.83	0.44
2:N:53:LEU:HD22	3:O:161:ALA:HB3	2.00	0.44
12:F:3:ILE:HG22	12:F:16:SER:CB	2.47	0.44
12:F:3:ILE:HG22	12:F:16:SER:HB3	1.99	0.44
13:E:36:PHE:CD1	13:E:36:PHE:C	2.91	0.44
12:A:45:LEU:HD22	12:A:98:LEU:HD11	1.99	0.44
7:U:130:MET:HG3	13:E:27:MET:SD	2.58	0.44
6:V:67:TYR:CG	6:V:75:LEU:HG	2.53	0.44
13:E:196:THR:HB	9:X:180:ILE:HD13	1.99	0.44
12:A:97:HIS:CG	12:A:115:MET:HB3	2.53	0.44
13:B:41:ILE:HD13	13:B:79:VAL:HG21	2.00	0.44
1:M:91:LYS:CG	1:M:119:LEU:HD11	2.47	0.44
1:H:146:VAL:HG23	1:H:220:VAL:HG22	1.99	0.44
13:E:77:THR:O	13:E:80:THR:HG22	2.18	0.44
13:B:77:THR:O	13:B:80:THR:HG22	2.18	0.44
3:O:238:LYS:HE2	3:O:238:LYS:HB2	1.26	0.43
1:H:38:ILE:HD13	1:H:169:ALA:HB2	2.00	0.43
7:Y:130:MET:HG3	13:B:27:MET:SD	2.57	0.43
13:B:198:ARG:HA	13:B:199:PRO:HD3	1.83	0.43
7:U:11:MET:HG2	7:U:170:MET:SD	2.58	0.43
9:S:173:ARG:HD2	13:B:200:SER:HB2	1.98	0.43
11:K:168:ALA:HA	11:K:172:GLN:HG3	1.99	0.43
3:O:151:ASP:CB	3:O:152:PRO:CD	2.77	0.43
4:P:221:THR:HG23	4:P:223:THR:N	2.33	0.43
5:Q:87:LEU:HD23	5:Q:87:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:19:VAL:HG13	7:U:118:PRO:HB3	2.00	0.43
9:S:180:ILE:HD13	13:B:196:THR:HB	1.99	0.43
3:Z:35:LEU:HG	3:Z:46:ALA:HB3	2.00	0.43
3:Z:197:LEU:HD12	3:Z:197:LEU:HA	1.65	0.43
12:F:97:HIS:CG	12:F:115:MET:HB3	2.53	0.43
14:W:51:LEU:HD21	14:W:110:MET:HG2	2.01	0.43
14:W:96:MET:HE3	14:W:127:MET:HA	1.99	0.43
2:I:148:ASP:CB	2:I:149:PRO:CD	2.96	0.43
2:I:179:GLU:OE1	2:I:179:GLU:N	2.38	0.43
3:O:91:ARG:HG2	7:U:75:LEU:HD13	2.01	0.43
8:C:88:TYR:CE2	6:V:55:GLN:HG3	2.53	0.43
7:Y:11:MET:HG2	7:Y:170:MET:SD	2.58	0.43
2:I:65:LEU:HD23	2:I:65:LEU:HA	1.83	0.43
1:M:38:ILE:HD13	1:M:169:ALA:HB2	2.00	0.43
5:J:140:TYR:CG	5:J:217:GLY:HA2	2.54	0.43
6:V:86:ARG:HD3	6:V:86:ARG:C	2.38	0.43
2:I:181:ILE:O	2:I:181:ILE:HG13	2.19	0.43
2:I:220:LEU:N	2:I:220:LEU:CD2	2.80	0.43
2:N:215:GLN:HE21	2:N:215:GLN:HB2	1.61	0.43
5:J:87:LEU:HD23	5:J:87:LEU:HA	1.86	0.43
2:I:70:CYS:CB	2:I:217:LEU:HD11	2.48	0.43
10:G:84:LEU:HD23	10:G:84:LEU:HA	1.86	0.43
1:H:49:ALA:CB	1:H:217:LEU:HD12	2.40	0.43
1:H:91:LYS:CG	1:H:119:LEU:HD11	2.47	0.43
10:L:49:LEU:HD21	10:L:199:LEU:HD23	2.01	0.43
10:L:166:GLN:HE21	10:L:166:GLN:C	2.15	0.43
2:I:204:LYS:HB2	2:I:204:LYS:HE3	1.60	0.43
8:D:38:ASN:HB2	8:D:39:PRO:HD3	2.01	0.43
1:M:202:LEU:HA	1:M:202:LEU:HD23	1.74	0.43
2:N:43:LEU:HD13	2:N:72:ALA:HB2	2.01	0.43
4:P:104:ILE:HA	4:P:105:PRO:HD3	1.94	0.43
1:M:149:LYS:HB2	1:M:152:GLN:HE22	1.84	0.43
5:Q:41:CYS:HB3	5:Q:189:ILE:HD12	1.77	0.43
7:U:194:ILE:HG12	13:E:219:LEU:HD21	2.01	0.43
1:H:49:ALA:HB2	1:H:217:LEU:CD1	2.42	0.43
11:K:206:LEU:HB3	11:K:208:ILE:HD12	2.00	0.43
7:Y:141:CYS:HB3	7:Y:177:ASP:HB2	2.00	0.43
12:F:126:ILE:HD11	12:F:135:TYR:CD1	2.54	0.43
8:D:45:MET:CG	8:D:52:CYS:HB3	2.47	0.43
1:M:146:VAL:HG23	1:M:220:VAL:HG22	1.99	0.42
3:O:174:MET:SD	3:O:199:LYS:HD2	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:LYS:HB2	1:H:152:GLN:HE22	1.84	0.42
11:K:181:LYS:H	11:K:181:LYS:HG3	1.65	0.42
2:I:223:GLU:HA	2:I:226:GLU:HB2	2.01	0.42
10:G:52:ALA:HB2	10:G:59:HIS:CE1	2.54	0.42
7:Y:111:LEU:HD23	7:Y:118:PRO:HA	2.00	0.42
7:Y:128:CYS:HA	7:Y:129:PRO:HD3	1.83	0.42
14:W:163:THR:O	14:W:167:GLU:HG3	2.19	0.42
11:R:178:PHE:CD1	11:R:178:PHE:C	2.93	0.42
8:D:187:VAL:HG12	8:D:188:GLU:CG	2.49	0.42
1:M:81:LEU:HD12	1:M:138:GLY:HA3	2.02	0.42
2:N:181:ILE:O	2:N:181:ILE:HG13	2.19	0.42
2:N:40:ILE:HA	2:N:136:PHE:CZ	2.55	0.42
3:O:222:LYS:NZ	3:O:224:VAL:HG22	2.35	0.42
4:P:134:LEU:HD23	4:P:134:LEU:HA	1.85	0.42
8:C:147:LEU:HD22	8:C:151:GLU:HB3	2.02	0.42
8:C:187:VAL:HG12	8:C:188:GLU:CG	2.49	0.42
3:Z:174:MET:SD	3:Z:199:LYS:HD2	2.58	0.42
6:V:92:LEU:HD11	6:V:121:LEU:HD23	2.01	0.42
7:Y:19:VAL:HG13	7:Y:118:PRO:HB3	2.00	0.42
12:A:159:ILE:HG22	12:A:163:MET:SD	2.59	0.42
3:O:35:LEU:HG	3:O:46:ALA:HB3	2.01	0.42
5:Q:203:GLU:CD	5:Q:203:GLU:N	2.72	0.42
9:S:150:ASP:HB3	9:S:156:LYS:HD2	2.01	0.42
11:K:107:TYR:OH	13:B:66:HIS:HE1	2.02	0.42
10:L:52:ALA:HB2	10:L:59:HIS:CE1	2.54	0.42
1:M:49:ALA:HB2	1:M:217:LEU:CD1	2.42	0.42
1:M:210:LEU:HD12	1:M:215:ILE:HG21	2.02	0.42
3:O:35:LEU:HD12	3:O:35:LEU:O	2.19	0.42
5:Q:175:GLU:CB	5:Q:196:ILE:HG12	2.46	0.42
11:K:178:PHE:CD1	11:K:178:PHE:C	2.93	0.42
12:F:159:ILE:HG22	12:F:163:MET:SD	2.59	0.42
2:I:40:ILE:HG13	2:I:211:MET:O	2.20	0.42
2:I:43:LEU:HD23	2:I:43:LEU:HA	1.87	0.42
7:U:141:CYS:HB3	7:U:177:ASP:HB2	2.00	0.42
15:C:301:A1L0C:CB	15:C:301:A1L0C:O2	2.68	0.42
3:Z:137:ILE:O	3:Z:137:ILE:HG13	2.20	0.42
5:J:203:GLU:CD	5:J:203:GLU:N	2.73	0.42
11:K:146:GLU:H	11:K:146:GLU:HG3	1.66	0.42
7:Y:194:ILE:HG12	13:B:219:LEU:HD21	2.02	0.42
2:I:43:LEU:HD13	2:I:72:ALA:HB2	2.01	0.42
5:Q:94:GLU:OE2	5:Q:114:ARG:CZ	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:207:LYS:HB2	5:Q:207:LYS:HE3	1.49	0.42
9:S:123:SER:CB	9:S:136:LYS:HG2	2.50	0.42
10:G:56:LEU:HD11	1:H:182:GLN:HA	2.02	0.42
10:G:88:MET:HG2	10:G:112:ILE:HD11	2.02	0.42
3:Z:222:LYS:NZ	3:Z:224:VAL:HG22	2.35	0.42
11:K:178:PHE:HA	11:K:181:LYS:NZ	2.35	0.42
12:A:36:PRO:HB3	12:A:42:TYR:CE1	2.55	0.42
11:R:206:LEU:HB3	11:R:208:ILE:HD12	2.00	0.42
8:D:11:GLY:HA2	8:D:104:TRP:HZ3	1.84	0.42
2:N:231:GLU:HG2	2:N:231:GLU:H	1.62	0.42
7:U:67:LYS:HD3	7:U:67:LYS:HA	1.81	0.42
7:U:111:LEU:HD23	7:U:118:PRO:HA	2.00	0.42
3:Z:79:ILE:HB	3:Z:82:ASP:HB2	2.02	0.42
7:Y:87:MET:HG3	7:Y:121:CYS:SG	2.60	0.42
2:N:43:LEU:HD23	2:N:43:LEU:HA	1.87	0.42
2:N:57:ARG:HH11	2:N:57:ARG:HG3	1.84	0.42
3:O:79:ILE:HB	3:O:82:ASP:HB2	2.02	0.42
4:P:56:TYR:HE2	11:R:159:TYR:OH	2.02	0.42
5:Q:240:LYS:HE3	5:Q:240:LYS:HB2	1.91	0.42
7:U:163:PHE:CE1	7:U:197:ARG:HD2	2.55	0.42
10:G:158:ALA:O	5:J:57:LEU:HB3	2.20	0.42
3:Z:174:MET:HE3	3:Z:195:LYS:NZ	2.35	0.42
5:J:94:GLU:OE2	5:J:114:ARG:CZ	2.68	0.42
12:A:126:ILE:HD11	12:A:135:TYR:CD1	2.54	0.42
10:L:83:LEU:HD23	10:L:83:LEU:HA	1.88	0.42
2:N:40:ILE:HG13	2:N:211:MET:O	2.20	0.41
2:N:223:GLU:HA	2:N:226:GLU:HB2	2.01	0.41
5:Q:140:TYR:CG	5:Q:217:GLY:HA2	2.54	0.41
6:T:92:LEU:HD11	6:T:121:LEU:HD23	2.02	0.41
8:C:38:ASN:CB	8:C:39:PRO:CD	2.96	0.41
9:S:72:LEU:HD22	9:S:83:MET:SD	2.60	0.41
13:E:6:LEU:C	13:E:6:LEU:CD1	2.83	0.41
14:W:166:ARG:NH2	14:W:200:GLU:OE2	2.45	0.41
2:I:40:ILE:HA	2:I:136:PHE:CZ	2.55	0.41
4:P:32:ALA:HA	4:P:33:PRO:HD3	1.87	0.41
4:P:52:LYS:H	4:P:52:LYS:HG2	1.49	0.41
4:P:73:LEU:HD11	4:P:135:ILE:HG13	2.02	0.41
6:T:12:TYR:CD1	6:T:12:TYR:C	2.93	0.41
7:U:87:MET:HG3	7:U:121:CYS:SG	2.60	0.41
10:G:49:LEU:HD21	10:G:199:LEU:HD23	2.01	0.41
3:Z:35:LEU:HD12	3:Z:35:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:205:LYS:HB2	3:Z:205:LYS:HE2	1.38	0.41
7:Y:163:PHE:CE1	7:Y:197:ARG:HD2	2.55	0.41
13:E:40:LYS:HD3	13:E:40:LYS:N	2.27	0.41
13:E:114:HIS:HB3	13:E:115:PRO:HD2	2.02	0.41
10:L:88:MET:HG2	10:L:112:ILE:HD11	2.02	0.41
11:R:47:CYS:HB2	11:R:221:THR:HG22	2.02	0.41
11:R:178:PHE:HA	11:R:181:LYS:NZ	2.35	0.41
9:X:150:ASP:HB3	9:X:156:LYS:HD2	2.02	0.41
1:M:50:VAL:CG1	1:M:66:LYS:HB2	2.45	0.41
2:N:227:LYS:HB3	2:N:227:LYS:HE3	1.51	0.41
6:T:96:THR:CB	8:D:91:ARG:HH22	2.18	0.41
10:L:50:LYS:HB2	10:L:50:LYS:HE2	1.98	0.41
2:I:168:VAL:HG13	2:I:194:ALA:HB1	2.02	0.41
2:I:173:GLU:H	2:I:173:GLU:HG2	1.54	0.41
11:R:67:THR:OG1	11:R:216:GLU:OE2	2.22	0.41
9:X:123:SER:CB	9:X:136:LYS:HG2	2.50	0.41
9:S:158:MET:CE	13:B:204:PHE:HE1	2.20	0.41
1:H:204:GLN:HE21	1:H:204:GLN:HB3	1.60	0.41
3:Z:45:LEU:HD13	3:Z:75:SER:HB2	2.03	0.41
8:D:147:LEU:HD22	8:D:151:GLU:HB3	2.02	0.41
6:T:55:GLN:HG3	8:D:88:TYR:CE2	2.55	0.41
12:F:73:PRO:HA	12:F:74:PRO:HD3	1.86	0.41
14:W:67:LEU:HD12	14:W:67:LEU:HA	1.92	0.41
14:W:110:MET:HB2	14:W:110:MET:HE2	1.76	0.41
1:M:204:GLN:HE21	1:M:204:GLN:HB3	1.60	0.41
3:O:27:ALA:HB2	4:P:16:GLY:O	2.20	0.41
6:T:104:LEU:C	6:T:104:LEU:HD23	2.41	0.41
6:T:170:ARG:HA	6:T:170:ARG:HD3	1.51	0.41
6:V:12:TYR:CD1	6:V:12:TYR:C	2.93	0.41
14:W:51:LEU:C	14:W:51:LEU:HD23	2.41	0.41
10:L:230:SER:N	10:L:231:PRO:CD	2.83	0.41
2:I:57:ARG:HH11	2:I:57:ARG:HG3	1.84	0.41
2:N:53:LEU:HD11	3:O:176:LYS:HG2	2.03	0.41
3:O:66:TYR:CD1	3:O:66:TYR:N	2.89	0.41
3:O:137:ILE:O	3:O:137:ILE:HG13	2.20	0.41
4:P:189:THR:HA	4:P:192:LEU:HD12	2.02	0.41
1:H:210:LEU:HD12	1:H:215:ILE:HG21	2.02	0.41
12:F:36:PRO:HB3	12:F:42:TYR:CE1	2.55	0.41
10:L:69:HIS:HB2	10:L:137:TYR:O	2.21	0.41
11:R:146:GLU:H	11:R:146:GLU:HG3	1.65	0.41
8:D:38:ASN:CB	8:D:39:PRO:CD	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:206:MET:HE1	1:M:214:ASN:HD21	1.86	0.41
1:H:81:LEU:HD12	1:H:138:GLY:HA3	2.02	0.41
6:V:104:LEU:C	6:V:104:LEU:HD23	2.41	0.41
7:Y:126:ILE:H	7:Y:126:ILE:HG13	1.60	0.41
12:A:97:HIS:CD2	12:A:97:HIS:C	2.94	0.41
2:I:33:VAL:CG2	2:I:168:VAL:HG11	2.51	0.41
13:B:73:GLU:HA	13:B:74:PRO:HD3	1.88	0.41
8:C:11:GLY:HA2	8:C:104:TRP:HZ3	1.84	0.41
9:S:125:ASP:HB2	9:S:126:PRO:HD2	2.02	0.41
3:Z:91:ARG:HG2	7:Y:75:LEU:HD13	2.02	0.41
11:K:47:CYS:HB2	11:K:221:THR:HG22	2.02	0.41
11:K:224:ASN:C	11:K:224:ASN:HD22	2.24	0.41
6:V:170:ARG:HD3	6:V:170:ARG:HA	1.51	0.41
13:E:135:LEU:HD11	14:W:179:ARG:CD	2.51	0.41
12:A:103:TRP:CZ2	12:A:180:ALA:HB2	2.56	0.41
10:L:34:ALA:HA	10:L:161:ILE:O	2.21	0.41
15:D:301:A1L0C:CB	15:D:301:A1L0C:O2	2.68	0.41
13:B:114:HIS:HB3	13:B:115:PRO:HD2	2.02	0.41
2:N:168:VAL:HG13	2:N:194:ALA:HB1	2.02	0.41
2:N:179:GLU:H	2:N:179:GLU:CD	2.21	0.41
4:P:201:GLN:NE2	4:P:201:GLN:HA	2.36	0.41
4:P:211:ILE:HD11	4:P:218:ARG:HG2	2.03	0.41
3:Z:66:TYR:CD1	3:Z:66:TYR:N	2.89	0.41
13:E:63:MET:HE2	13:E:74:PRO:HB3	2.03	0.41
14:W:20:VAL:HG23	14:W:120:SER:HB2	2.03	0.41
12:A:114:THR:O	12:A:114:THR:OG1	2.38	0.41
2:I:90:GLU:HG2	2:I:110:TYR:CG	2.55	0.41
8:D:103:GLY:HA2	8:D:179:MET:CE	2.51	0.41
8:D:103:GLY:HA2	8:D:179:MET:HE3	2.03	0.41
9:X:72:LEU:HD22	9:X:83:MET:SD	2.60	0.41
1:M:91:LYS:O	1:M:95:GLU:HG2	2.21	0.40
2:N:33:VAL:CG2	2:N:168:VAL:HG11	2.51	0.40
10:G:34:ALA:HA	10:G:161:ILE:O	2.21	0.40
1:H:91:LYS:O	1:H:95:GLU:HG2	2.22	0.40
3:Z:241:GLU:N	3:Z:241:GLU:OE1	2.55	0.40
13:E:135:LEU:C	13:E:135:LEU:HD13	2.41	0.40
8:D:9:GLN:HG3	8:D:10:HIS:CD2	2.56	0.40
13:B:188:THR:CG2	13:B:188:THR:O	2.70	0.40
1:M:152:GLN:HE21	1:M:152:GLN:HB2	1.73	0.40
1:M:182:GLN:HE21	1:M:182:GLN:HB3	1.70	0.40
2:N:70:CYS:CB	2:N:217:LEU:HD11	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:90:GLU:HG2	2:N:110:TYR:CG	2.55	0.40
3:O:230:GLN:HE21	3:O:230:GLN:HB2	1.65	0.40
10:G:230:SER:N	10:G:231:PRO:CD	2.83	0.40
5:J:240:LYS:HE3	5:J:240:LYS:HB2	1.91	0.40
13:E:109:GLN:HE21	13:E:109:GLN:HB2	1.78	0.40
10:L:74:ILE:O	10:L:74:ILE:HG12	2.22	0.40
2:I:62:ILE:HD13	2:I:209:ALA:HB3	2.04	0.40
2:I:65:LEU:HD11	2:I:71:MET:SD	2.62	0.40
13:B:135:LEU:C	13:B:135:LEU:HD13	2.41	0.40
3:O:45:LEU:HD13	3:O:75:SER:HB2	2.03	0.40
3:O:229:LYS:O	3:O:233:VAL:HG23	2.21	0.40
10:G:69:HIS:HB2	10:G:137:TYR:O	2.21	0.40
1:H:147:ASP:HB2	1:H:148:GLU:H	1.72	0.40
12:F:97:HIS:CD2	12:F:97:HIS:C	2.94	0.40
4:P:55:LEU:HD22	11:R:165:ALA:HB3	2.03	0.40
4:P:58:GLU:CD	4:P:58:GLU:H	2.24	0.40
3:Z:21:VAL:HG11	3:Z:153:SER:HB3	2.03	0.40
2:N:17:PHE:HD1	2:N:17:PHE:HA	1.80	0.40
2:N:115:LYS:HE2	2:N:129:ILE:HD12	2.04	0.40
4:P:221:THR:CG2	4:P:224:GLU:H	2.35	0.40
5:Q:50:GLU:HB2	5:Q:197:ILE:HG23	2.03	0.40
7:Y:95:TYR:CE1	7:Y:98:ARG:HD3	2.57	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	H	221/241 (92%)	215 (97%)	6 (3%)	0	100 100
1	M	221/241 (92%)	215 (97%)	6 (3%)	0	100 100
2	I	229/248 (92%)	213 (93%)	12 (5%)	4 (2%)	9 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	N	229/248 (92%)	213 (93%)	12 (5%)	4 (2%)	9 4
3	O	240/261 (92%)	229 (95%)	9 (4%)	2 (1%)	19 13
3	Z	240/261 (92%)	229 (95%)	9 (4%)	2 (1%)	19 13
4	P	224/234 (96%)	213 (95%)	10 (4%)	1 (0%)	34 30
4	b	224/234 (96%)	213 (95%)	10 (4%)	1 (0%)	34 30
5	J	236/255 (92%)	231 (98%)	4 (2%)	1 (0%)	34 30
5	Q	236/255 (92%)	231 (98%)	4 (2%)	1 (0%)	34 30
6	T	194/201 (96%)	191 (98%)	3 (2%)	0	100 100
6	V	194/201 (96%)	191 (98%)	3 (2%)	0	100 100
7	U	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	29 23
7	Y	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	29 23
8	C	198/203 (98%)	192 (97%)	6 (3%)	0	100 100
8	D	198/203 (98%)	192 (97%)	6 (3%)	0	100 100
9	S	210/241 (87%)	206 (98%)	4 (2%)	0	100 100
9	X	210/241 (87%)	206 (98%)	4 (2%)	0	100 100
10	G	232/263 (88%)	225 (97%)	7 (3%)	0	100 100
10	L	232/263 (88%)	225 (97%)	7 (3%)	0	100 100
11	K	232/246 (94%)	228 (98%)	4 (2%)	0	100 100
11	R	232/246 (94%)	228 (98%)	4 (2%)	0	100 100
12	A	196/198 (99%)	193 (98%)	3 (2%)	0	100 100
12	F	196/198 (99%)	193 (98%)	3 (2%)	0	100 100
13	B	217/273 (80%)	206 (95%)	7 (3%)	4 (2%)	8 3
13	E	217/273 (80%)	206 (95%)	7 (3%)	4 (2%)	8 3
14	W	212/264 (80%)	202 (95%)	10 (5%)	0	100 100
14	a	212/264 (80%)	202 (95%)	10 (5%)	0	100 100
All	All	6086/6666 (91%)	5876 (96%)	184 (3%)	26 (0%)	38 30

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	E	205	ALA
13	B	205	ALA
2	N	49	SER

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Mol	Chain	Res	Type
13	E	199	PRO
13	E	206	PRO
2	I	49	SER
13	B	199	PRO
13	B	206	PRO
2	N	140	GLY
2	N	217	LEU
2	I	140	GLY
2	I	217	LEU
3	O	207	SER
3	Z	207	SER
13	E	198	ARG
13	B	198	ARG
2	N	48	LYS
4	P	201	GLN
5	Q	208	ALA
4	b	201	GLN
5	J	208	ALA
2	I	48	LYS
3	O	203	VAL
7	U	100	GLY
7	Y	100	GLY
3	Z	203	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	H	189/203 (93%)	160 (85%)	29 (15%)	2 1
1	M	189/203 (93%)	160 (85%)	29 (15%)	2 1
2	I	195/211 (92%)	153 (78%)	42 (22%)	1 0
2	N	195/211 (92%)	153 (78%)	42 (22%)	1 0
3	O	204/221 (92%)	178 (87%)	26 (13%)	4 2
3	Z	204/221 (92%)	178 (87%)	26 (13%)	4 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	P	187/191 (98%)	167 (89%)	20 (11%)	6 3
4	b	187/191 (98%)	167 (89%)	20 (11%)	6 3
5	J	196/212 (92%)	169 (86%)	27 (14%)	3 2
5	Q	196/212 (92%)	169 (86%)	27 (14%)	3 2
6	T	167/171 (98%)	155 (93%)	12 (7%)	14 9
6	V	167/171 (98%)	155 (93%)	12 (7%)	14 9
7	U	174/175 (99%)	162 (93%)	12 (7%)	15 11
7	Y	174/175 (99%)	162 (93%)	12 (7%)	15 11
8	C	167/169 (99%)	151 (90%)	16 (10%)	8 5
8	D	167/169 (99%)	151 (90%)	16 (10%)	8 5
9	S	178/197 (90%)	164 (92%)	14 (8%)	12 8
9	X	178/197 (90%)	164 (92%)	14 (8%)	12 8
10	G	199/223 (89%)	177 (89%)	22 (11%)	6 3
10	L	199/223 (89%)	177 (89%)	22 (11%)	6 3
11	K	197/210 (94%)	178 (90%)	19 (10%)	8 5
11	R	197/210 (94%)	178 (90%)	19 (10%)	8 5
12	A	151/151 (100%)	133 (88%)	18 (12%)	5 3
12	F	151/151 (100%)	134 (89%)	17 (11%)	6 3
13	B	174/221 (79%)	152 (87%)	22 (13%)	4 2
13	E	174/221 (79%)	152 (87%)	22 (13%)	4 2
14	W	176/215 (82%)	159 (90%)	17 (10%)	8 4
14	a	176/215 (82%)	159 (90%)	17 (10%)	8 4
All	All	5108/5540 (92%)	4517 (88%)	591 (12%)	9 3

All (591) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	10	ARG
1	M	41	GLN
1	M	56	SER
1	M	59	MET
1	M	62	SER
1	M	66	LYS
1	M	78	MET

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Mol	Chain	Res	Type
1	M	86	LYS
1	M	125	GLU
1	M	139	VAL
1	M	147	ASP
1	M	152	GLN
1	M	164	GLN
1	M	175	GLU
1	M	182	GLN
1	M	187	LYS
1	M	188	SER
1	M	189	MET
1	M	192	LYS
1	M	197	SER
1	M	198	SER
1	M	199	LEU
1	M	202	LEU
1	M	204	GLN
1	M	207	GLU
1	M	209	LYS
1	M	210	LEU
1	M	224	GLN
1	M	238	ILE
2	N	2	SER
2	N	4	ASP
2	N	5	ARG
2	N	17	PHE
2	N	36	ARG
2	N	38	LYS
2	N	39	ASP
2	N	41	VAL
2	N	46	GLU
2	N	52	LYS
2	N	54	GLN
2	N	57	ARG
2	N	63	CYS
2	N	66	ASP
2	N	70	CYS
2	N	100	ASP
2	N	105	GLU
2	N	139	ASP
2	N	141	THR
2	N	146	GLN

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Mol	Chain	Res	Type
2	N	166	LYS
2	N	167	SER
2	N	169	ARG
2	N	173	GLU
2	N	174	LYS
2	N	181	ILE
2	N	185	ASP
2	N	189	LYS
2	N	190	LEU
2	N	196	LEU
2	N	197	GLU
2	N	204	LYS
2	N	208	LEU
2	N	213	ARG
2	N	215	GLN
2	N	218	LYS
2	N	219	ILE
2	N	220	LEU
2	N	223	GLU
2	N	226	GLU
2	N	231	GLU
2	N	232	ILE
3	O	35	LEU
3	O	43	VAL
3	O	48	GLU
3	O	52	ILE
3	O	58	GLU
3	O	59	VAL
3	O	103	GLU
3	O	112	THR
3	O	122	THR
3	O	133	SER
3	O	160	LYS
3	O	178	ASP
3	O	184	MET
3	O	188	SER
3	O	197	LEU
3	O	201	MET
3	O	203	VAL
3	O	205	LYS
3	O	206	LEU
3	O	212	GLU

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Mol	Chain	Res	Type
3	O	222	LYS
3	O	226	ARG
3	O	230	GLN
3	O	234	GLU
3	O	238	LYS
3	O	241	GLU
4	P	49	LYS
4	P	50	LYS
4	P	52	LYS
4	P	59	ARG
4	P	73	LEU
4	P	76	SER
4	P	88	ARG
4	P	94	GLN
4	P	123	SER
4	P	131	VAL
4	P	132	SER
4	P	162	MET
4	P	170	LYS
4	P	184	GLU
4	P	189	THR
4	P	191	ILE
4	P	195	LYS
4	P	214	GLU
4	P	221	THR
4	P	223	THR
5	Q	28	LYS
5	Q	34	SER
5	Q	37	ILE
5	Q	42	LYS
5	Q	51	LYS
5	Q	60	GLU
5	Q	86	SER
5	Q	93	GLU
5	Q	134	SER
5	Q	157	SER
5	Q	169	ARG
5	Q	173	LYS
5	Q	178	LYS
5	Q	180	GLN
5	Q	187	ARG
5	Q	188	ASP

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Mol	Chain	Res	Type
5	Q	204	VAL
5	Q	205	LYS
5	Q	207	LYS
5	Q	215	TRP
5	Q	218	GLU
5	Q	221	LYS
5	Q	232	ARG
5	Q	233	GLU
5	Q	236	GLU
5	Q	237	LYS
5	Q	243	LEU
6	T	1	MET
6	T	26	VAL
6	T	40	GLU
6	T	49	GLU
6	T	62	LYS
6	T	68	LYS
6	T	95	ARG
6	T	161	ARG
6	T	162	LYS
6	T	170	ARG
6	T	177	THR
6	T	195	SER
7	U	16	LYS
7	U	19	VAL
7	U	30	GLN
7	U	67	LYS
7	U	114	LYS
7	U	115	THR
7	U	122	SER
7	U	126	ILE
7	U	134	ASP
7	U	180	SER
7	U	198	THR
7	U	200	LYS
8	C	8	PHE
8	C	61	LYS
8	C	73	ARG
8	C	77	SER
8	C	82	LEU
8	C	97	MET
8	C	116	GLN

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Mol	Chain	Res	Type
8	C	144	GLN
8	C	168	SER
8	C	182	ASP
8	C	186	LYS
8	C	188	GLU
8	C	189	SER
8	C	190	THR
8	C	198	GLN
8	C	200	GLN
9	S	2	PHE
9	S	40	SER
9	S	49	LYS
9	S	69	GLU
9	S	72	LEU
9	S	76	LYS
9	S	81	LYS
9	S	133	ASP
9	S	161	VAL
9	S	162	GLU
9	S	163	HIS
9	S	200	LYS
9	S	204	ARG
9	S	212	LYS
10	G	4	ASN
10	G	31	GLN
10	G	39	LYS
10	G	41	LYS
10	G	42	THR
10	G	51	ARG
10	G	54	SER
10	G	60	GLN
10	G	61	LYS
10	G	73	SER
10	G	74	ILE
10	G	78	THR
10	G	101	ARG
10	G	110	SER
10	G	156	CYS
10	G	173	GLU
10	G	212	ILE
10	G	217	LYS
10	G	220	GLU

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Mol	Chain	Res	Type
10	G	228	ASP
10	G	229	VAL
10	G	234	GLU
1	H	10	ARG
1	H	41	GLN
1	H	56	SER
1	H	59	MET
1	H	62	SER
1	H	66	LYS
1	H	78	MET
1	H	86	LYS
1	H	125	GLU
1	H	139	VAL
1	H	147	ASP
1	H	152	GLN
1	H	164	GLN
1	H	175	GLU
1	H	182	GLN
1	H	187	LYS
1	H	188	SER
1	H	189	MET
1	H	192	LYS
1	H	197	SER
1	H	198	SER
1	H	199	LEU
1	H	202	LEU
1	H	204	GLN
1	H	207	GLU
1	H	209	LYS
1	H	210	LEU
1	H	224	GLN
1	H	238	ILE
3	Z	35	LEU
3	Z	43	VAL
3	Z	48	GLU
3	Z	52	ILE
3	Z	58	GLU
3	Z	59	VAL
3	Z	103	GLU
3	Z	112	THR
3	Z	122	THR
3	Z	133	SER

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Mol	Chain	Res	Type
3	Z	160	LYS
3	Z	178	ASP
3	Z	184	MET
3	Z	188	SER
3	Z	197	LEU
3	Z	201	MET
3	Z	203	VAL
3	Z	205	LYS
3	Z	206	LEU
3	Z	212	GLU
3	Z	222	LYS
3	Z	226	ARG
3	Z	230	GLN
3	Z	234	GLU
3	Z	238	LYS
3	Z	241	GLU
4	b	49	LYS
4	b	50	LYS
4	b	52	LYS
4	b	59	ARG
4	b	73	LEU
4	b	76	SER
4	b	88	ARG
4	b	94	GLN
4	b	123	SER
4	b	131	VAL
4	b	132	SER
4	b	162	MET
4	b	170	LYS
4	b	184	GLU
4	b	189	THR
4	b	191	ILE
4	b	195	LYS
4	b	214	GLU
4	b	221	THR
4	b	223	THR
5	J	28	LYS
5	J	34	SER
5	J	37	ILE
5	J	42	LYS
5	J	51	LYS
5	J	60	GLU

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Mol	Chain	Res	Type
5	J	86	SER
5	J	93	GLU
5	J	134	SER
5	J	157	SER
5	J	169	ARG
5	J	173	LYS
5	J	178	LYS
5	J	180	GLN
5	J	187	ARG
5	J	188	ASP
5	J	204	VAL
5	J	205	LYS
5	J	207	LYS
5	J	215	TRP
5	J	218	GLU
5	J	221	LYS
5	J	232	ARG
5	J	233	GLU
5	J	236	GLU
5	J	237	LYS
5	J	243	LEU
11	K	45	LYS
11	K	46	ASP
11	K	53	GLN
11	K	71	LYS
11	K	78	CYS
11	K	104	LYS
11	K	145	GLU
11	K	146	GLU
11	K	147	GLN
11	K	171	LYS
11	K	180	GLU
11	K	181	LYS
11	K	184	LYS
11	K	192	GLU
11	K	196	GLU
11	K	206	LEU
11	K	223	GLU
11	K	224	ASN
11	K	229	ILE
6	V	1	MET
6	V	26	VAL

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Mol	Chain	Res	Type
6	V	40	GLU
6	V	49	GLU
6	V	62	LYS
6	V	68	LYS
6	V	95	ARG
6	V	161	ARG
6	V	162	LYS
6	V	170	ARG
6	V	177	THR
6	V	195	SER
7	Y	16	LYS
7	Y	19	VAL
7	Y	30	GLN
7	Y	67	LYS
7	Y	114	LYS
7	Y	115	THR
7	Y	122	SER
7	Y	126	ILE
7	Y	134	ASP
7	Y	180	SER
7	Y	198	THR
7	Y	200	LYS
12	F	21	SER
12	F	28	ASN
12	F	46	SER
12	F	71	GLU
12	F	84	ARG
12	F	89	LYS
12	F	93	ASP
12	F	98	LEU
12	F	105	ARG
12	F	106	ARG
12	F	114	THR
12	F	115	MET
12	F	118	MET
12	F	143	LYS
12	F	185	TYR
12	F	191	ASN
12	F	198	ASP
13	E	9	ARG
13	E	27	MET
13	E	30	ASN

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Mol	Chain	Res	Type
13	E	40	LYS
13	E	43	CYS
13	E	69	SER
13	E	80	THR
13	E	97	SER
13	E	106	SER
13	E	109	GLN
13	E	141	ARG
13	E	184	LYS
13	E	188	THR
13	E	189	LEU
13	E	193	THR
13	E	198	ARG
13	E	200	SER
13	E	201	GLN
13	E	202	TYR
13	E	212	GLN
13	E	215	THR
13	E	217	LYS
14	W	2	GLN
14	W	3	ASN
14	W	17	GLU
14	W	29	SER
14	W	43	MET
14	W	47	ASP
14	W	64	LYS
14	W	67	LEU
14	W	74	GLU
14	W	98	SER
14	W	100	ARG
14	W	110	MET
14	W	141	TYR
14	W	156	LYS
14	W	183	SER
14	W	194	GLU
14	W	198	GLU
12	A	21	SER
12	A	28	ASN
12	A	46	SER
12	A	71	GLU
12	A	84	ARG
12	A	89	LYS

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Mol	Chain	Res	Type
12	A	93	ASP
12	A	98	LEU
12	A	105	ARG
12	A	106	ARG
12	A	114	THR
12	A	115	MET
12	A	118	MET
12	A	143	LYS
12	A	185	TYR
12	A	191	ASN
12	A	198	ASP
12	A	199	GLU
14	a	2	GLN
14	a	3	ASN
14	a	17	GLU
14	a	29	SER
14	a	43	MET
14	a	47	ASP
14	a	64	LYS
14	a	67	LEU
14	a	74	GLU
14	a	98	SER
14	a	100	ARG
14	a	110	MET
14	a	141	TYR
14	a	156	LYS
14	a	183	SER
14	a	194	GLU
14	a	198	GLU
10	L	4	ASN
10	L	31	GLN
10	L	39	LYS
10	L	41	LYS
10	L	42	THR
10	L	51	ARG
10	L	54	SER
10	L	60	GLN
10	L	61	LYS
10	L	73	SER
10	L	74	ILE
10	L	78	THR
10	L	101	ARG

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Mol	Chain	Res	Type
10	L	110	SER
10	L	156	CYS
10	L	173	GLU
10	L	212	ILE
10	L	217	LYS
10	L	220	GLU
10	L	228	ASP
10	L	229	VAL
10	L	234	GLU
2	I	2	SER
2	I	4	ASP
2	I	5	ARG
2	I	17	PHE
2	I	36	ARG
2	I	38	LYS
2	I	39	ASP
2	I	41	VAL
2	I	46	GLU
2	I	52	LYS
2	I	54	GLN
2	I	57	ARG
2	I	63	CYS
2	I	66	ASP
2	I	70	CYS
2	I	100	ASP
2	I	105	GLU
2	I	139	ASP
2	I	141	THR
2	I	146	GLN
2	I	166	LYS
2	I	167	SER
2	I	169	ARG
2	I	173	GLU
2	I	174	LYS
2	I	181	ILE
2	I	185	ASP
2	I	189	LYS
2	I	190	LEU
2	I	196	LEU
2	I	197	GLU
2	I	204	LYS
2	I	208	LEU

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Mol	Chain	Res	Type
2	I	213	ARG
2	I	215	GLN
2	I	218	LYS
2	I	219	ILE
2	I	220	LEU
2	I	223	GLU
2	I	226	GLU
2	I	231	GLU
2	I	232	ILE
11	R	45	LYS
11	R	46	ASP
11	R	53	GLN
11	R	71	LYS
11	R	78	CYS
11	R	104	LYS
11	R	145	GLU
11	R	146	GLU
11	R	147	GLN
11	R	171	LYS
11	R	180	GLU
11	R	181	LYS
11	R	184	LYS
11	R	192	GLU
11	R	196	GLU
11	R	206	LEU
11	R	223	GLU
11	R	224	ASN
11	R	229	ILE
8	D	8	PHE
8	D	61	LYS
8	D	73	ARG
8	D	77	SER
8	D	82	LEU
8	D	97	MET
8	D	116	GLN
8	D	144	GLN
8	D	168	SER
8	D	182	ASP
8	D	186	LYS
8	D	188	GLU
8	D	189	SER
8	D	190	THR

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Mol	Chain	Res	Type
8	D	198	GLN
8	D	200	GLN
9	X	2	PHE
9	X	40	SER
9	X	49	LYS
9	X	69	GLU
9	X	72	LEU
9	X	76	LYS
9	X	81	LYS
9	X	133	ASP
9	X	161	VAL
9	X	162	GLU
9	X	163	HIS
9	X	200	LYS
9	X	204	ARG
9	X	212	LYS
13	B	9	ARG
13	B	27	MET
13	B	30	ASN
13	B	40	LYS
13	B	43	CYS
13	B	69	SER
13	B	80	THR
13	B	97	SER
13	B	106	SER
13	B	109	GLN
13	B	141	ARG
13	B	184	LYS
13	B	188	THR
13	B	189	LEU
13	B	193	THR
13	B	198	ARG
13	B	200	SER
13	B	201	GLN
13	B	202	TYR
13	B	212	GLN
13	B	215	THR
13	B	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	41	GLN
1	M	118	ASN
1	M	152	GLN
1	M	164	GLN
1	M	182	GLN
1	M	204	GLN
2	N	215	GLN
3	O	230	GLN
4	P	51	GLN
4	P	139	ASN
4	P	188	HIS
4	P	201	GLN
5	Q	63	ASN
5	Q	170	GLN
6	T	63	ASN
6	T	174	ASN
7	U	172	ASN
8	C	9	GLN
8	C	10	HIS
8	C	116	GLN
8	C	117	ASN
8	C	124	ASN
8	C	193	ASN
9	S	157	ASN
9	S	159	GLN
10	G	4	ASN
10	G	31	GLN
10	G	59	HIS
10	G	60	GLN
10	G	65	HIS
10	G	203	GLN
1	H	41	GLN
1	H	118	ASN
1	H	152	GLN
1	H	164	GLN
1	H	182	GLN
1	H	204	GLN
3	Z	230	GLN
4	b	51	GLN
4	b	139	ASN
4	b	188	HIS
4	b	201	GLN
5	J	63	ASN

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Mol	Chain	Res	Type
5	J	170	GLN
11	K	53	GLN
11	K	90	GLN
11	K	147	GLN
11	K	224	ASN
6	V	63	ASN
6	V	174	ASN
7	Y	172	ASN
12	F	28	ASN
12	F	39	GLN
12	F	62	GLN
13	E	30	ASN
13	E	66	HIS
13	E	201	GLN
13	E	212	GLN
14	W	208	ASN
14	W	213	HIS
12	A	28	ASN
12	A	39	GLN
12	A	62	GLN
14	a	208	ASN
14	a	213	HIS
10	L	4	ASN
10	L	31	GLN
10	L	59	HIS
10	L	60	GLN
10	L	65	HIS
10	L	203	GLN
2	I	215	GLN
11	R	53	GLN
11	R	90	GLN
11	R	147	GLN
11	R	224	ASN
8	D	9	GLN
8	D	116	GLN
8	D	117	ASN
8	D	124	ASN
8	D	193	ASN
9	X	157	ASN
9	X	159	GLN
13	B	30	ASN
13	B	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	B	201	GLN
13	B	212	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)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
15	A1L0C	F	201	12	21,30,30	0.63	1 (4%)	21,42,42	1.38	2 (9%)
15	A1L0C	A	201	12	21,30,30	0.62	1 (4%)	21,42,42	1.39	2 (9%)
15	A1L0C	D	301	8	21,30,30	0.77	1 (4%)	21,42,42	1.33	2 (9%)
15	A1L0C	C	301	8	21,30,30	0.77	1 (4%)	21,42,42	1.33	2 (9%)

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
15	A1L0C	F	201	12	-	3/10/41/41	0/2/2/2
15	A1L0C	A	201	12	-	3/10/41/41	0/2/2/2
15	A1L0C	D	301	8	-	1/10/41/41	0/2/2/2
15	A1L0C	C	301	8	-	1/10/41/41	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	301	A1L0C	N3-N2	-2.05	1.30	1.34
15	D	301	A1L0C	N3-N2	-2.05	1.30	1.34
15	F	201	A1L0C	N3-N2	-2.03	1.30	1.34
15	A	201	A1L0C	N3-N2	-2.01	1.30	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	201	A1L0C	C2-N1-C9	5.23	130.11	125.48
15	F	201	A1L0C	C2-N1-C9	5.21	130.10	125.48
15	C	301	A1L0C	C2-N1-C9	4.74	129.68	125.48
15	D	301	A1L0C	C2-N1-C9	4.74	129.68	125.48
15	F	201	A1L0C	O-C-CA	-2.50	118.22	124.78
15	A	201	A1L0C	O-C-CA	-2.50	118.22	124.78
15	C	301	A1L0C	O-C-CA	-2.12	119.23	124.78
15	D	301	A1L0C	O-C-CA	-2.12	119.23	124.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	301	A1L0C	CG2-CB-OG1-B1
15	F	201	A1L0C	O3-C3-N4-C4
15	A	201	A1L0C	O3-C3-N4-C4
15	D	301	A1L0C	CG2-CB-OG1-B1
15	F	201	A1L0C	N4-C4-C5-C6
15	A	201	A1L0C	N4-C4-C5-C6
15	F	201	A1L0C	O-C-CA-CB
15	A	201	A1L0C	O-C-CA-CB

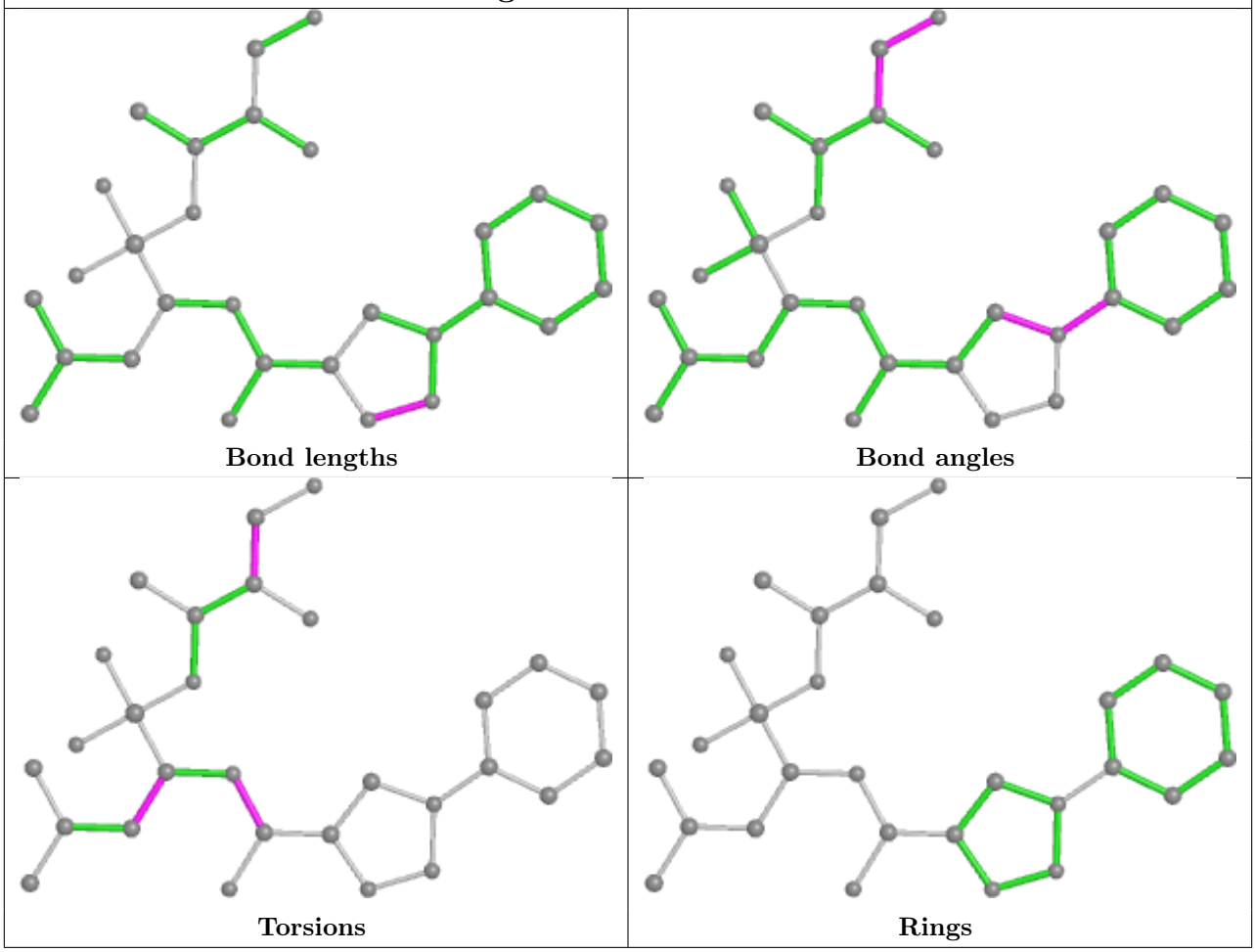
There are no ring outliers.

4 monomers are involved in 4 short contacts:

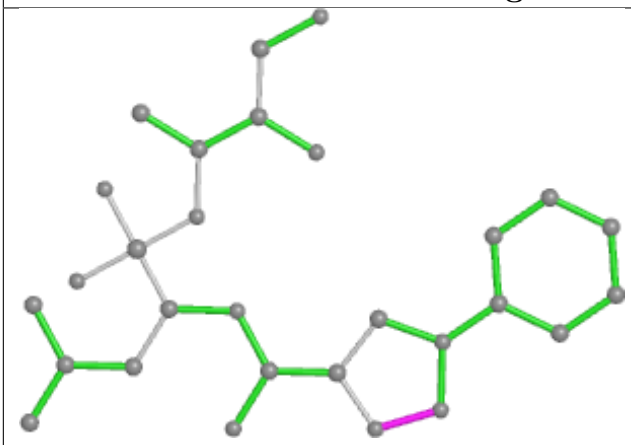
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	201	A1L0C	1	0
15	A	201	A1L0C	1	0
15	D	301	A1L0C	1	0
15	C	301	A1L0C	1	0

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.

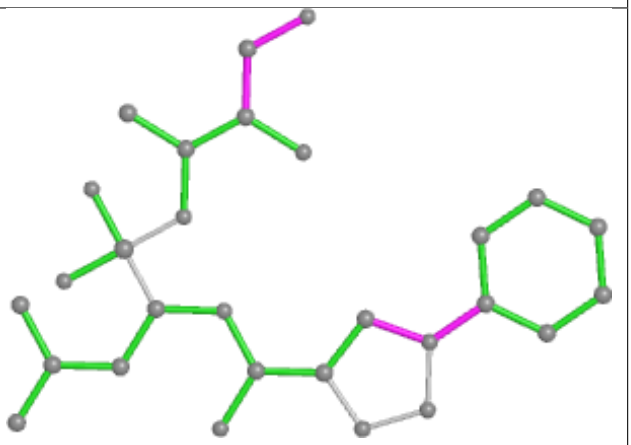
Ligand A1L0C F 201



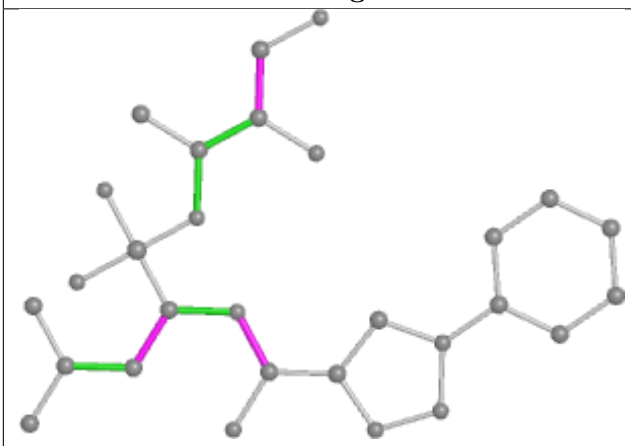
Ligand A1L0C A 201



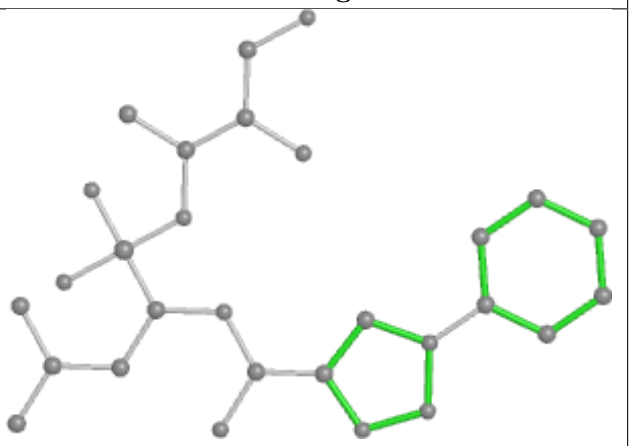
Bond lengths



Bond angles

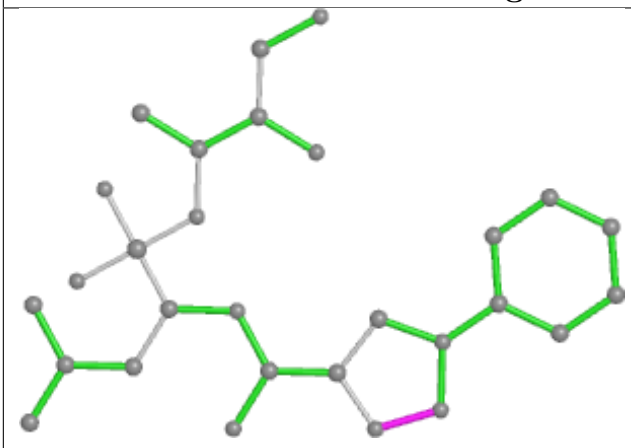


Torsions

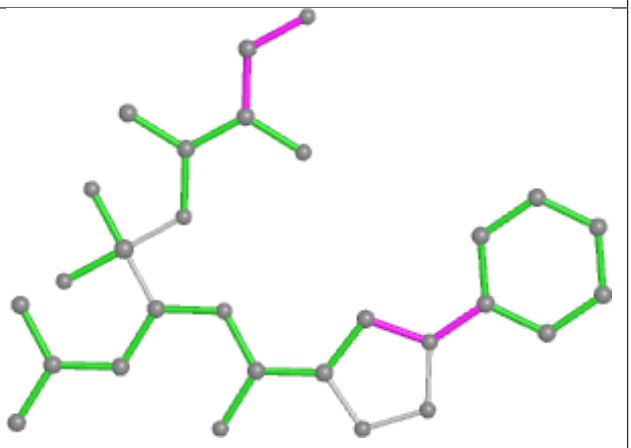


Rings

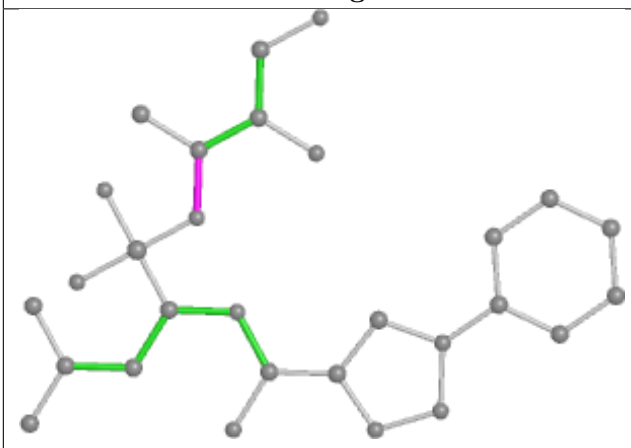
Ligand A1L0C D 301



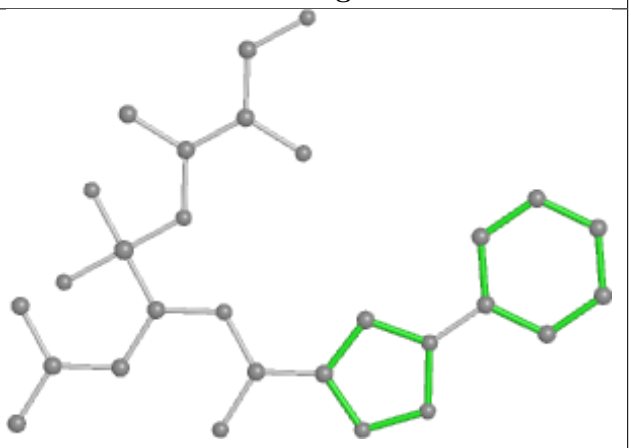
Bond lengths



Bond angles

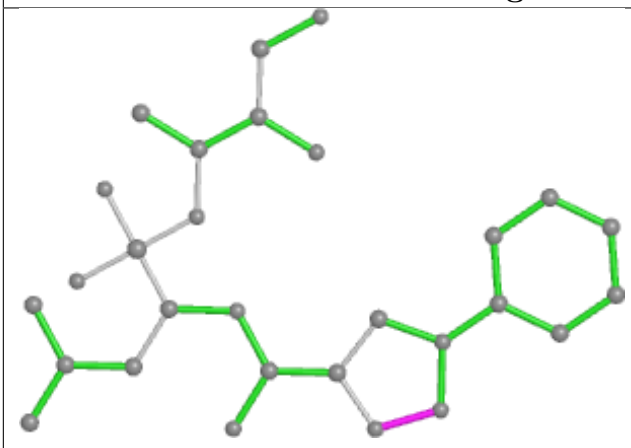


Torsions

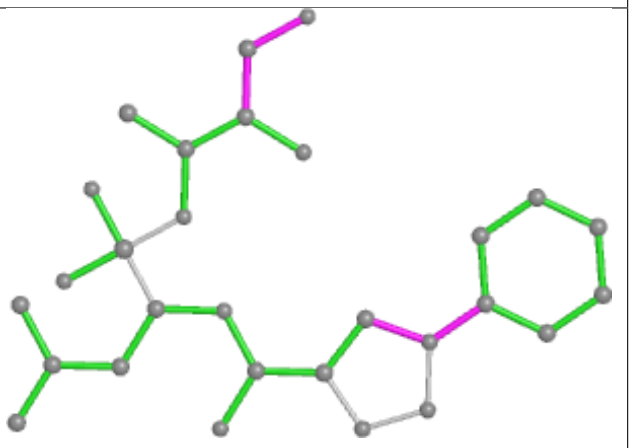


Rings

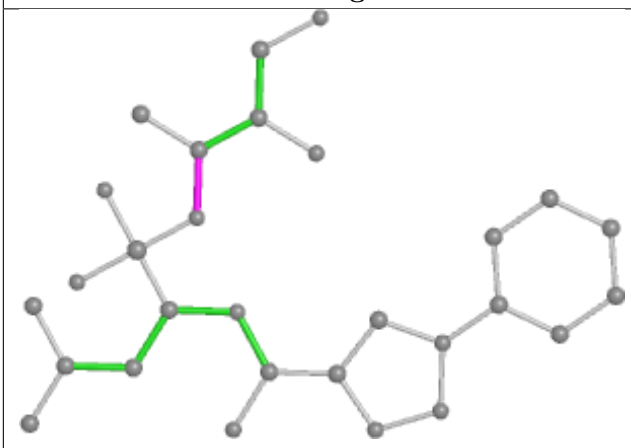
Ligand A1L0C C 301



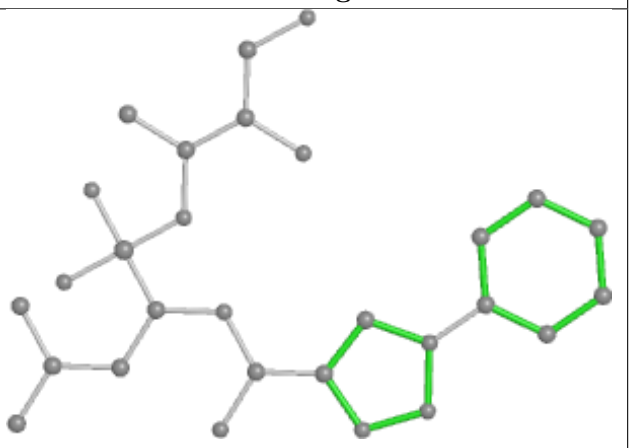
Bond lengths



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.

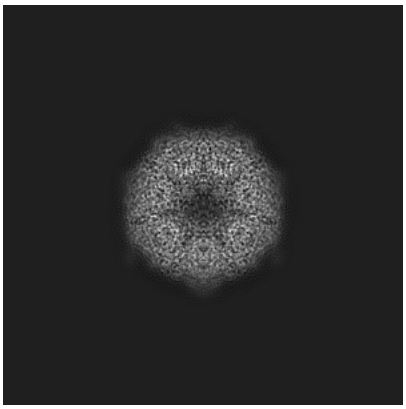
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39600. These allow visual inspection of the internal detail of the map and identification of artifacts.

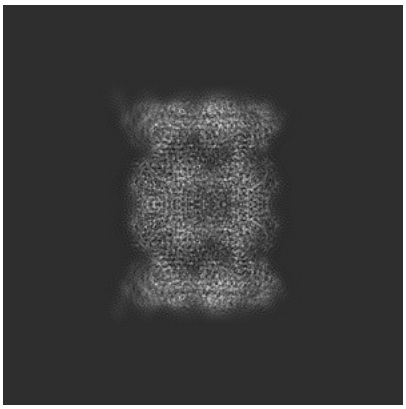
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

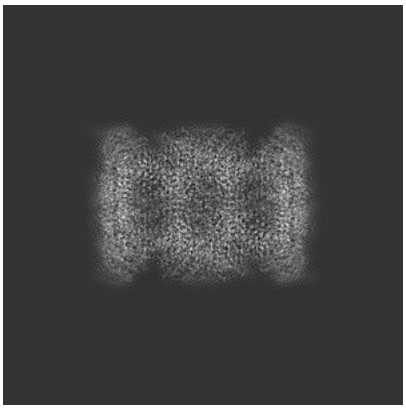
6.1.1 Primary map



X

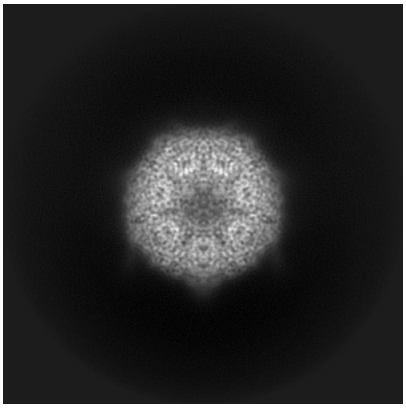


Y

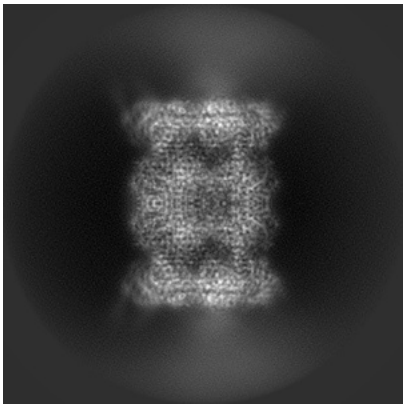


Z

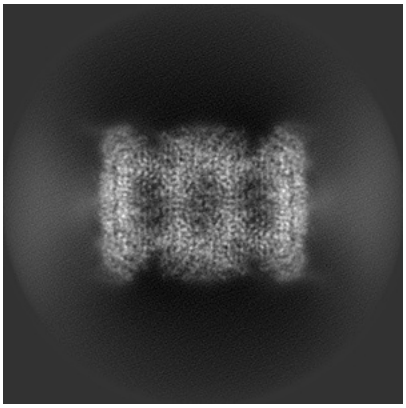
6.1.2 Raw map



X



Y

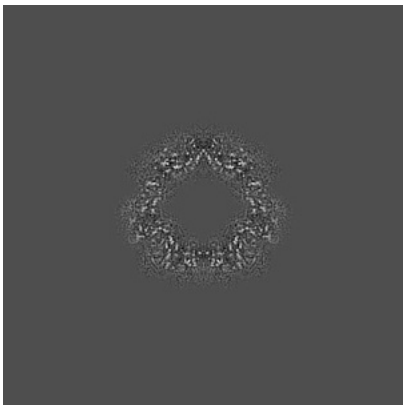


Z

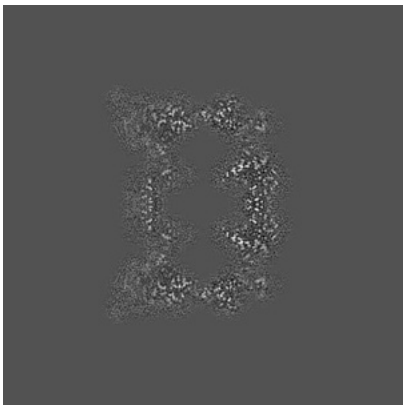
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

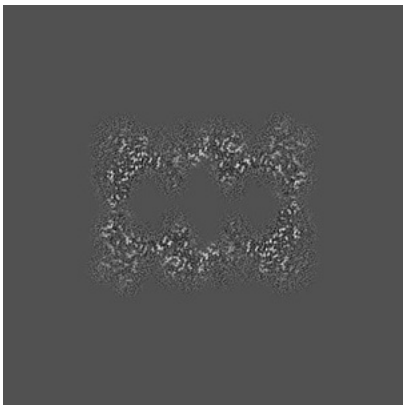
6.2.1 Primary map



X Index: 176

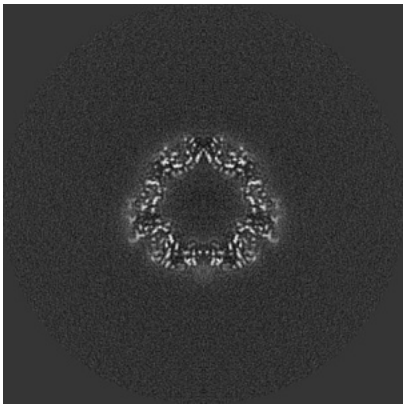


Y Index: 176

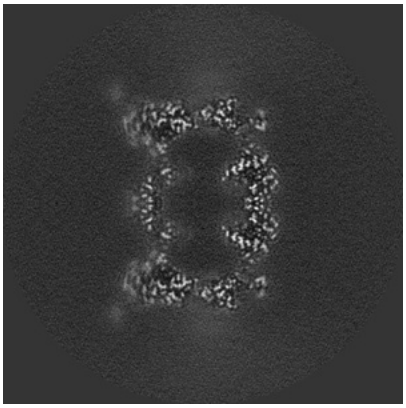


Z Index: 176

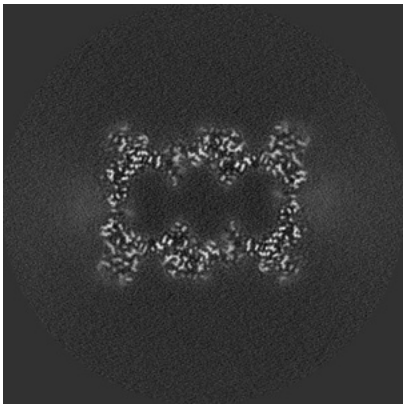
6.2.2 Raw map



X Index: 176



Y Index: 176

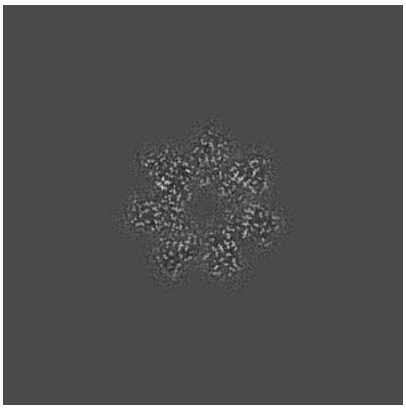


Z Index: 176

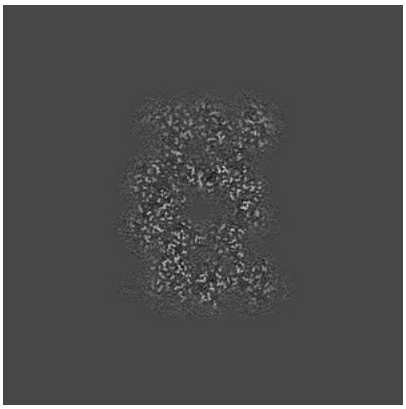
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

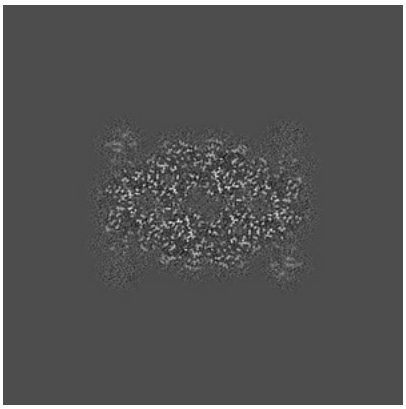
6.3.1 Primary map



X Index: 154

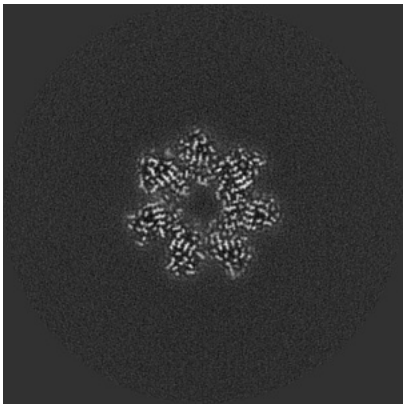


Y Index: 204

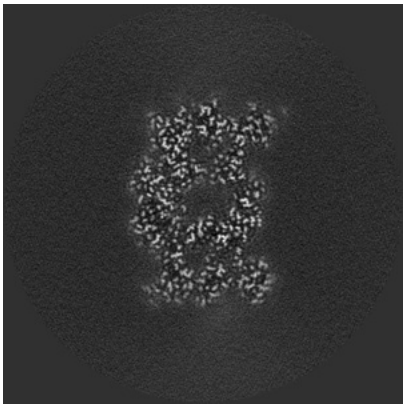


Z Index: 206

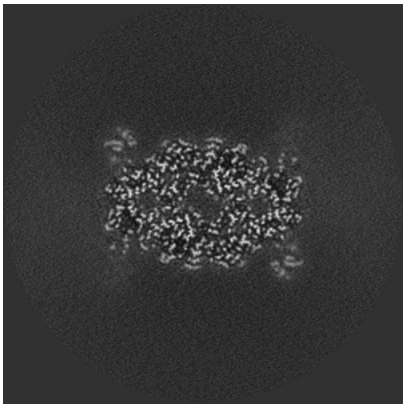
6.3.2 Raw map



X Index: 198



Y Index: 148

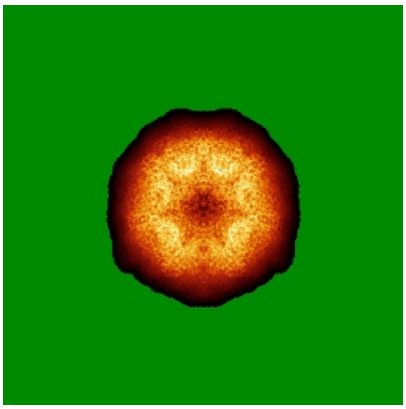


Z Index: 206

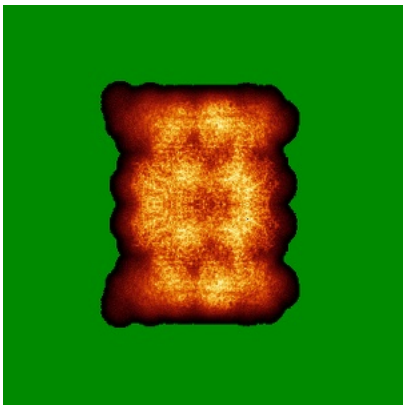
The images above show the largest variance slices of the map in three orthogonal directions.

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

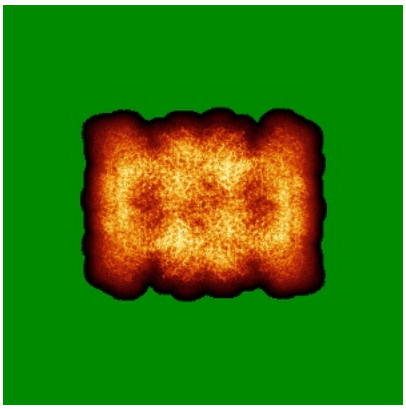
6.4.1 Primary map



X

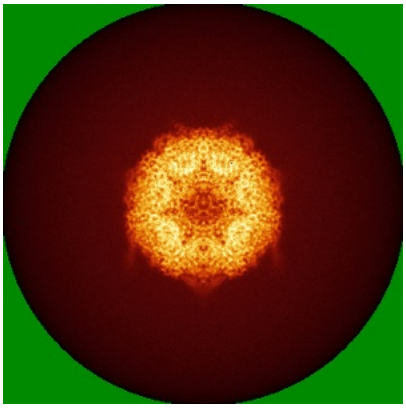


Y

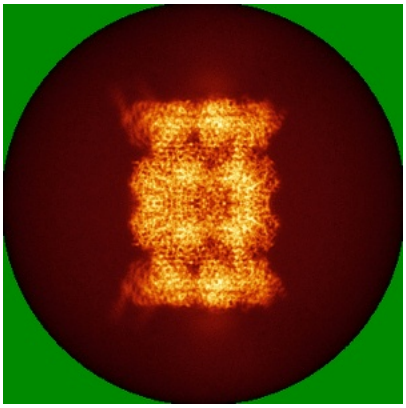


Z

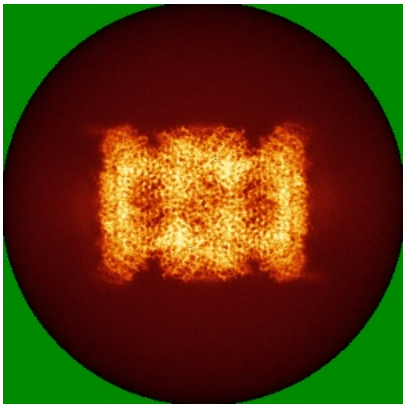
6.4.2 Raw map



X



Y

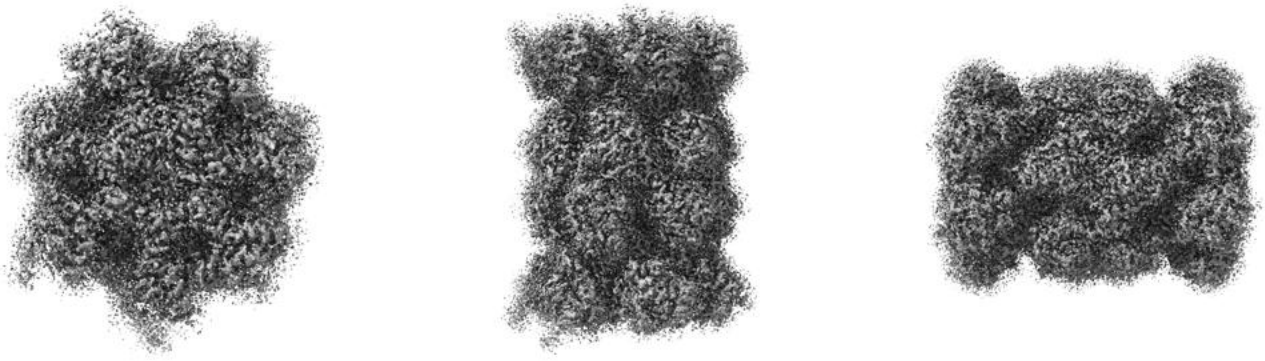


Z

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)

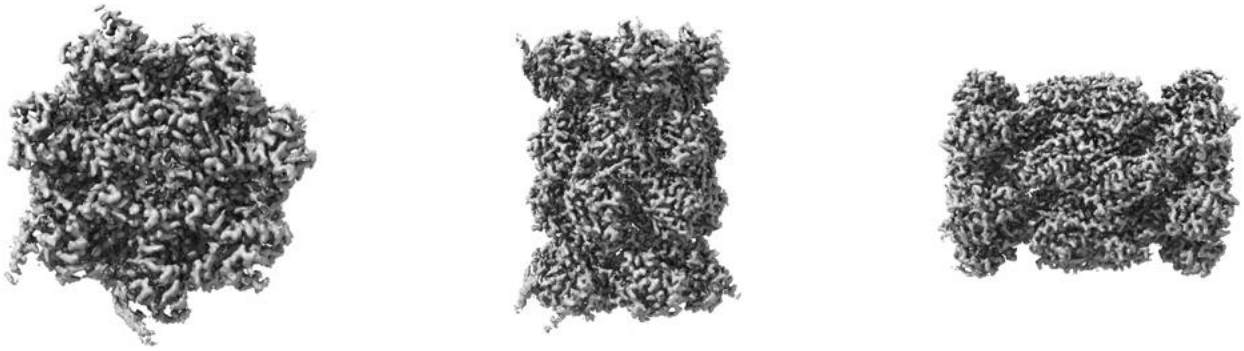
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0247. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

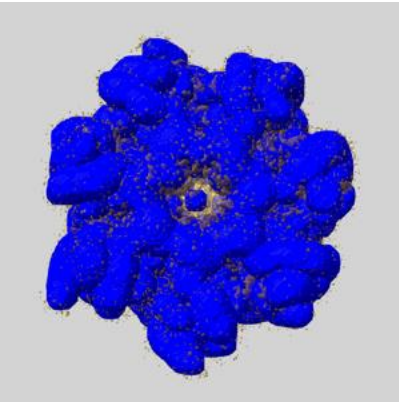
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

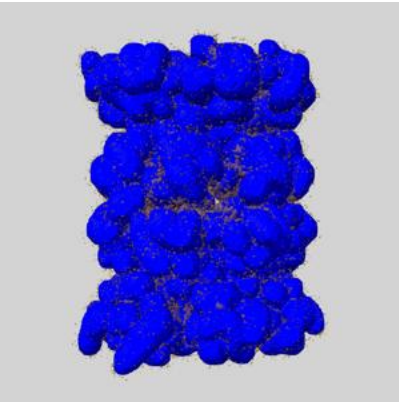
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

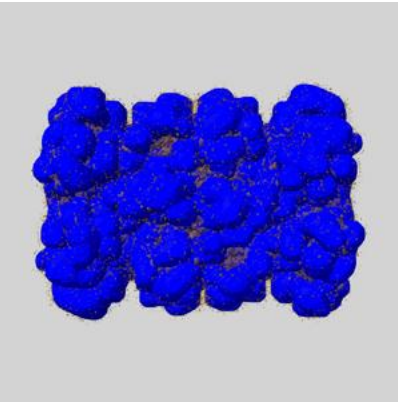
6.6.1 emd_39600_msk_1.map (i)



X



Y

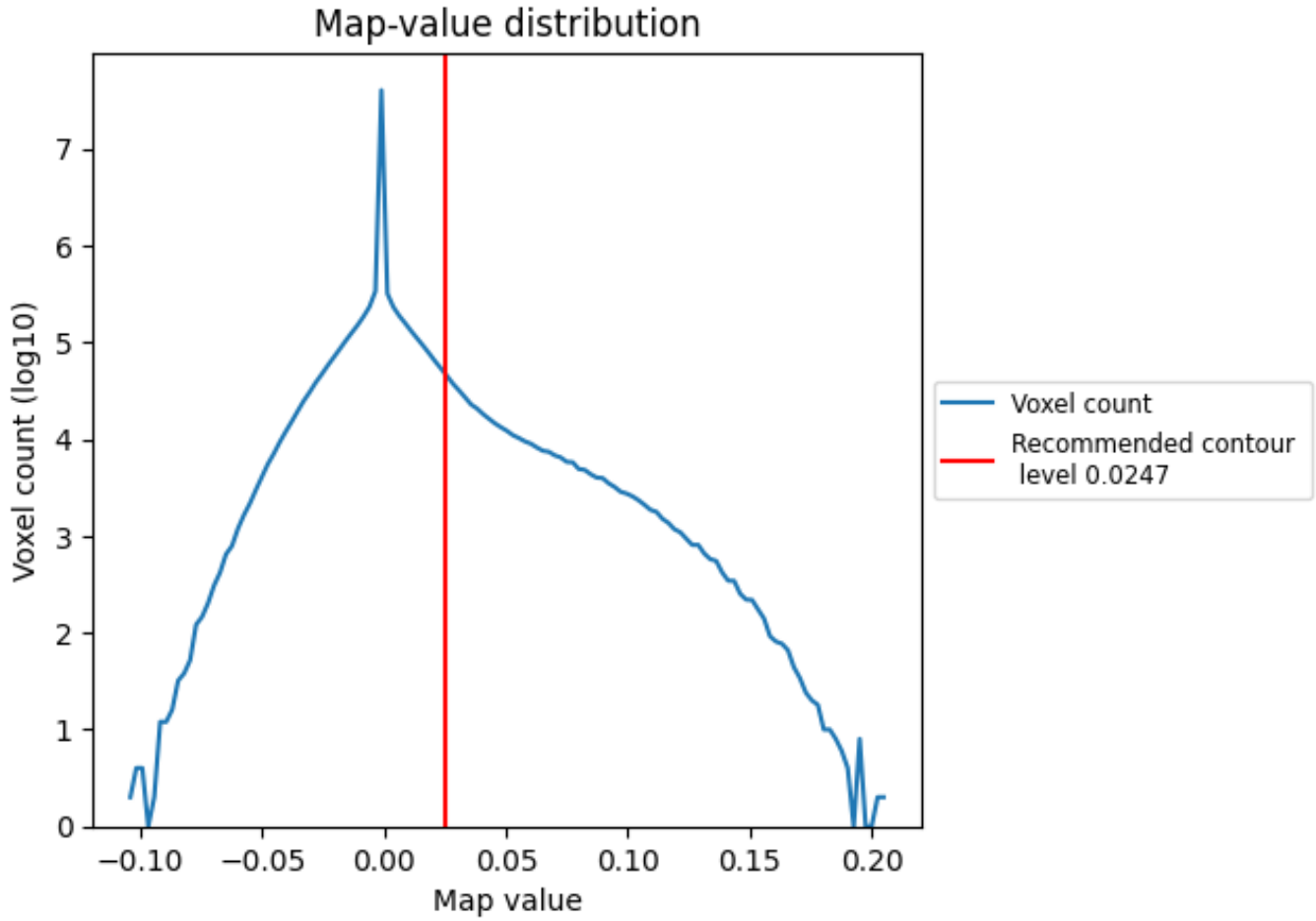


Z

7 Map analysis

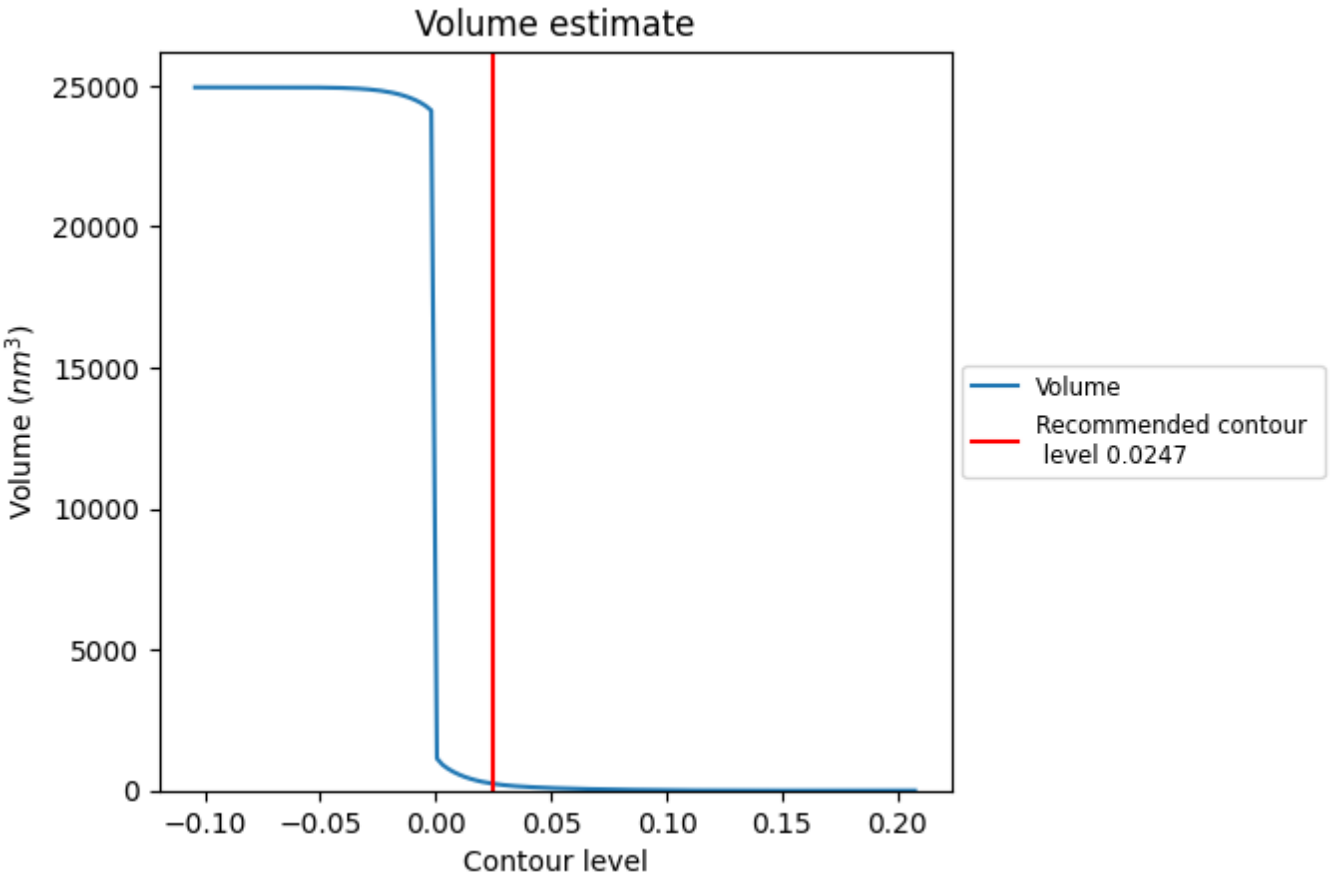
This section contains the results of statistical analysis of the map.

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.

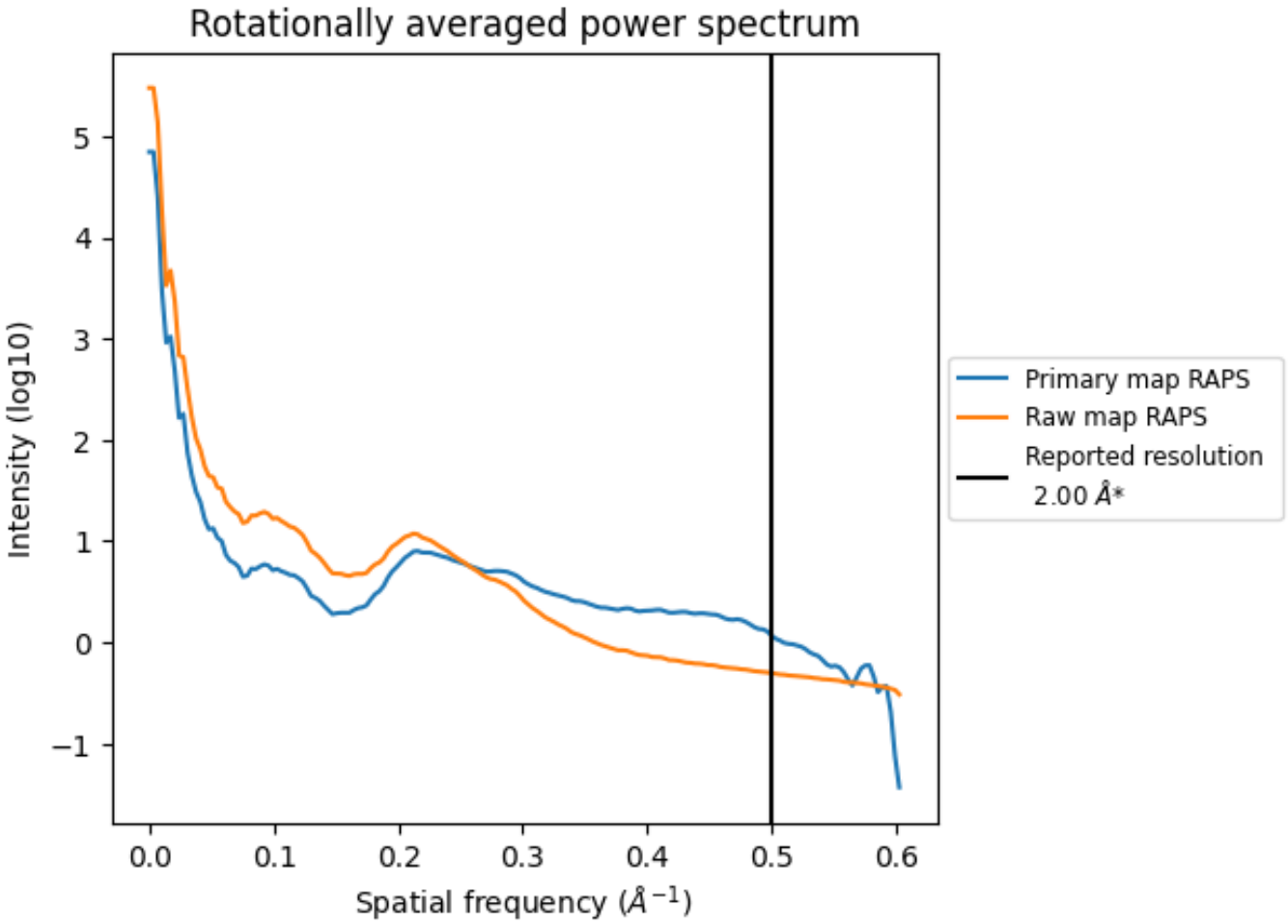
7.2 Volume estimate



The volume at the recommended contour level is 245 nm^3; this corresponds to an approximate mass of 221 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)

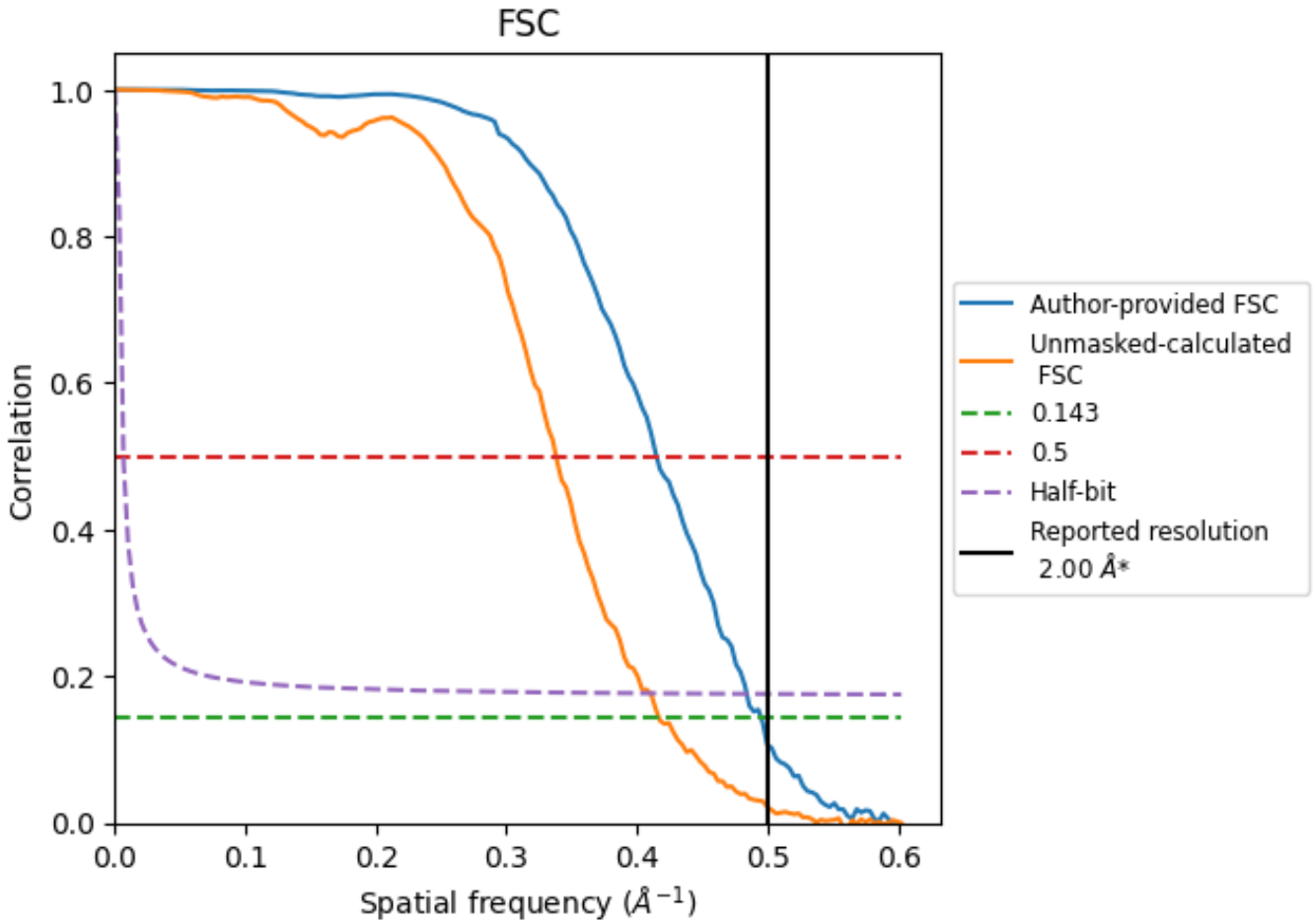


*Reported resolution corresponds to spatial frequency of 0.500 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.500 Å^{-1}

8.2 Resolution estimates (i)

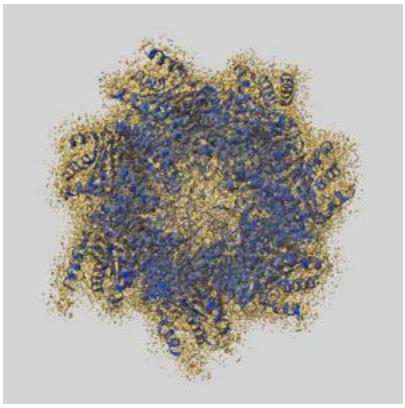
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.02	2.41	2.07
Unmasked-calculated*	2.40	2.96	2.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.40 differs from the reported value 2.0 by more than 10 %

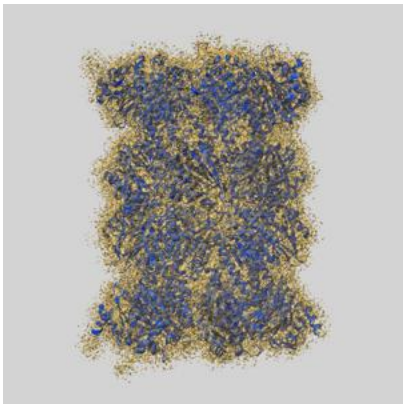
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39600 and PDB model 8YVG. Per-residue inclusion information can be found in section 3 on page 8.

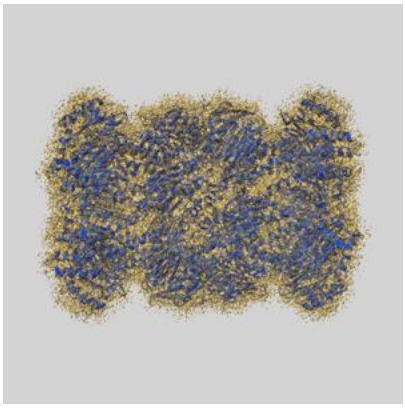
9.1 Map-model overlay



X



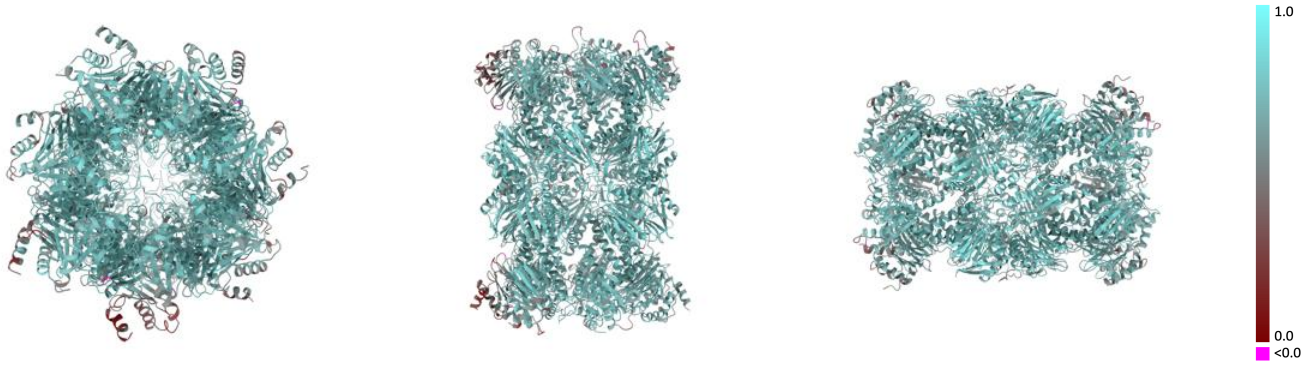
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0247 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.

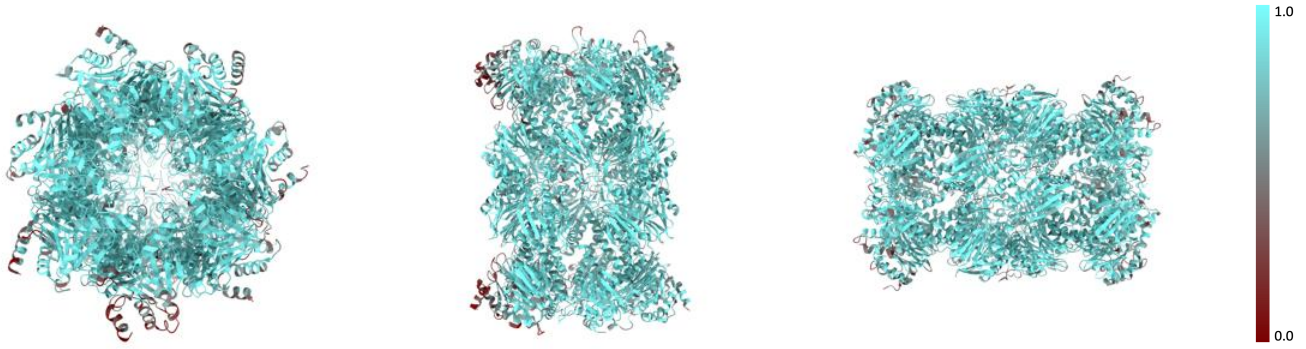
9.2 Q-score mapped to coordinate model (i)



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.

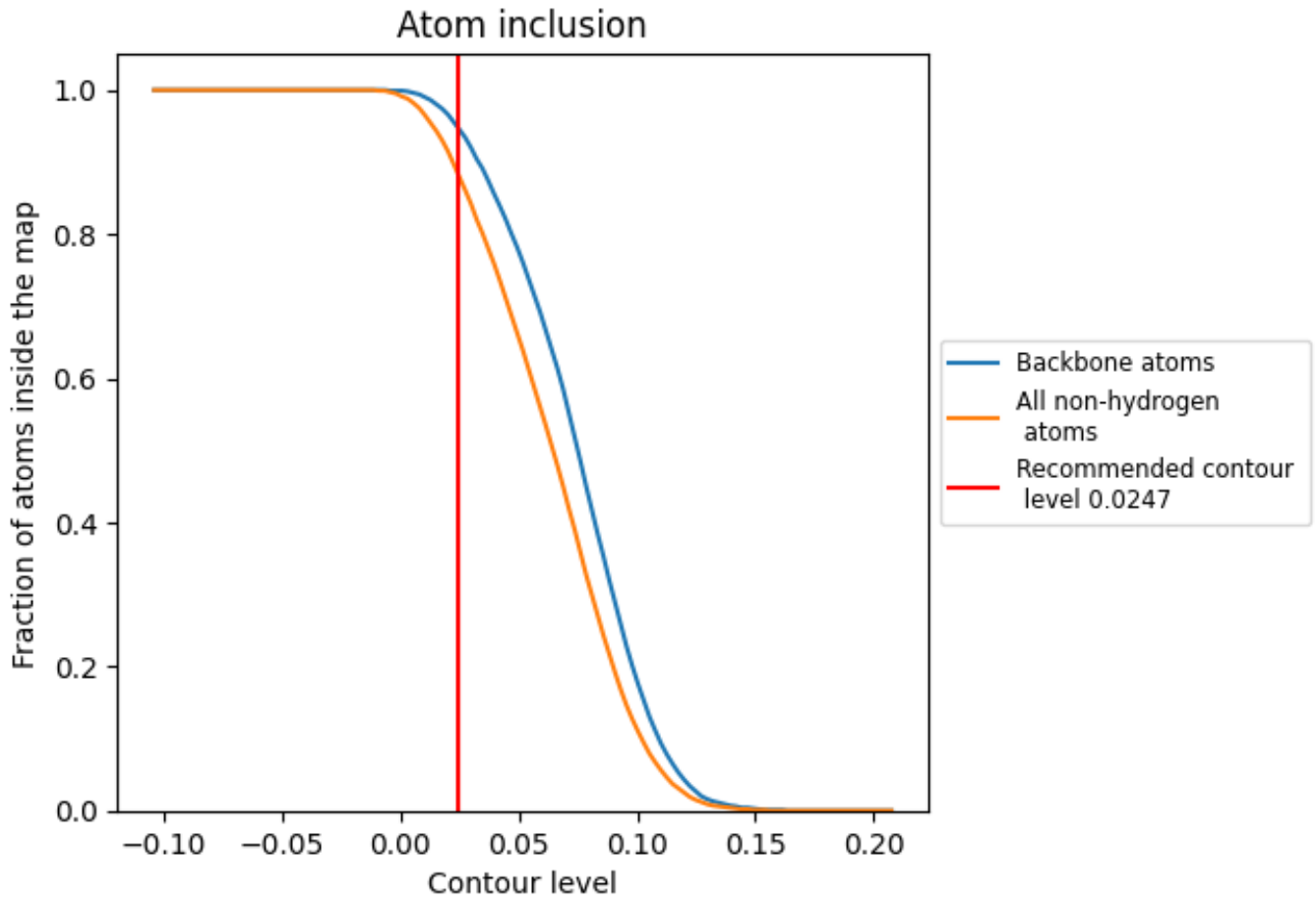
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0247).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.0247) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.7070
A	0.9300	0.7450
B	0.8910	0.7200
C	0.9320	0.7430
D	0.9320	0.7420
E	0.8920	0.7200
F	0.9300	0.7440
G	0.8470	0.6690
H	0.8530	0.6760
I	0.6600	0.5580
J	0.8660	0.6920
K	0.8980	0.7110
L	0.8450	0.6730
M	0.8490	0.6770
N	0.6640	0.5600
O	0.8530	0.6870
P	0.8900	0.6990
Q	0.8650	0.6880
R	0.8990	0.7110
S	0.9290	0.7610
T	0.9430	0.7510
U	0.9400	0.7590
V	0.9420	0.7530
W	0.9400	0.7670
X	0.9290	0.7590
Y	0.9390	0.7590
Z	0.8540	0.6880
a	0.9400	0.7650
b	0.8890	0.7000