



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:41 PM UTC

PDB ID : 6TCZ / pdb_00006tcz
EMDB ID : EMD-10462
Title : Leishmania tarentolae proteasome 20S subunit complexed with LXE408
Authors : Srinivas, H.
Deposited on : 2019-11-07
Resolution : 3.40 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:

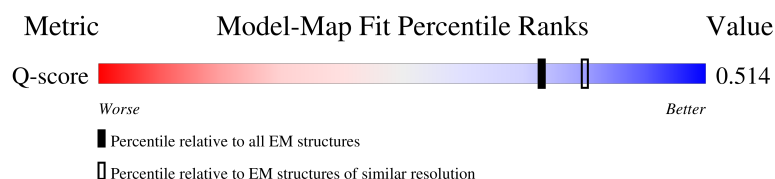
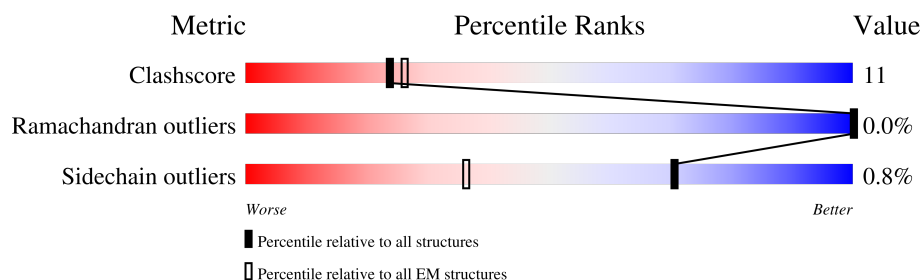
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	
1	a	250	
2	B	231	
2	b	231	

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Mol	Chain	Length	Quality of chain
3	C	285	
3	c	285	
4	D	248	
4	d	248	
5	E	344	
5	e	344	
6	F	428	
6	f	428	
7	G	238	
7	g	238	
8	H	283	
8	h	283	
9	I	254	
9	i	254	
10	J	205	
10	j	205	
11	K	206	
11	k	206	
12	L	302	
12	l	302	
13	M	339	
13	m	339	
14	N	220	
14	n	220	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 49248 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	A	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		
1	a	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		
2	b	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		
3	c	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		

- Molecule 4 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		
4	d	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	235	Total	C	N	O	S	0	0
			1802	1119	315	356	12		
5	e	235	Total	C	N	O	S	0	0
			1802	1119	315	356	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		
6	f	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		

- Molecule 7 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1741	1085	308	338	10		
7	g	230	Total	C	N	O	S	0	0
			1741	1085	308	338	10		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total	C	N	O	S	0	0
			1709	1062	295	340	12		
8	h	229	Total	C	N	O	S	0	0
			1709	1062	295	340	12		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		
9	i	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

- Molecule 11 is a protein called Proteasome subunit family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		
11	k	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	202	Total	C	N	O	S	0	0
			1577	997	277	296	7		
12	l	202	Total	C	N	O	S	0	0
			1577	997	277	296	7		

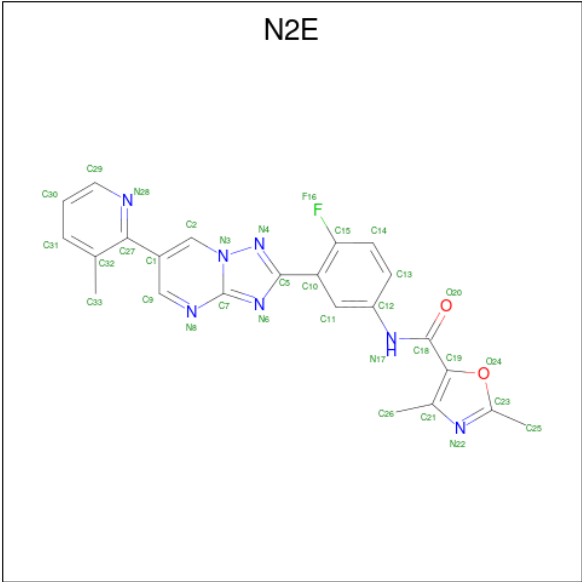
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		
13	m	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		
14	n	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		

- Molecule 15 is {N}-[4-fluoranyl-3-[6-(3-methylpyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-2-yl]phenyl]-2,4-dimethyl-1,3-oxazole-5-carboxamide (CCD ID: N2E) (formula: C₂₃H₁₈FN₇O₂) (labeled as "Ligand of Interest" by depositor).

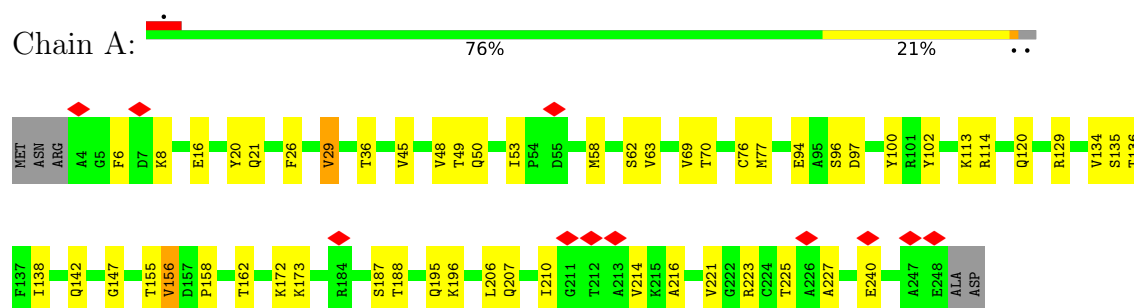


Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	F	N	O	0
			33	23	1	7	2	
15	1	1	Total	C	F	N	O	0
			33	23	1	7	2	

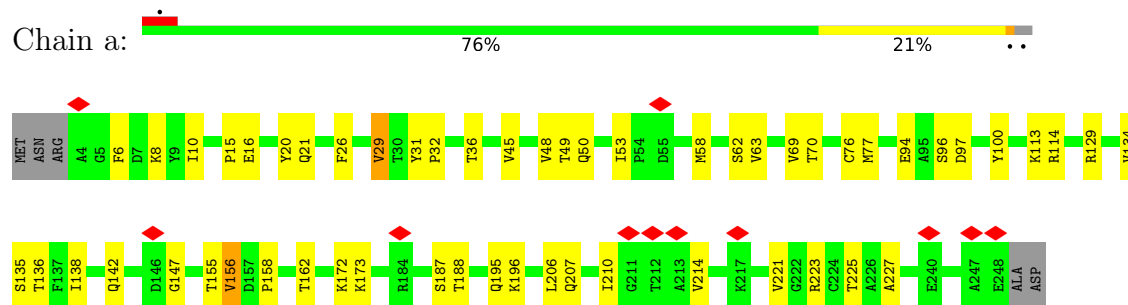
3 Residue-property plots

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

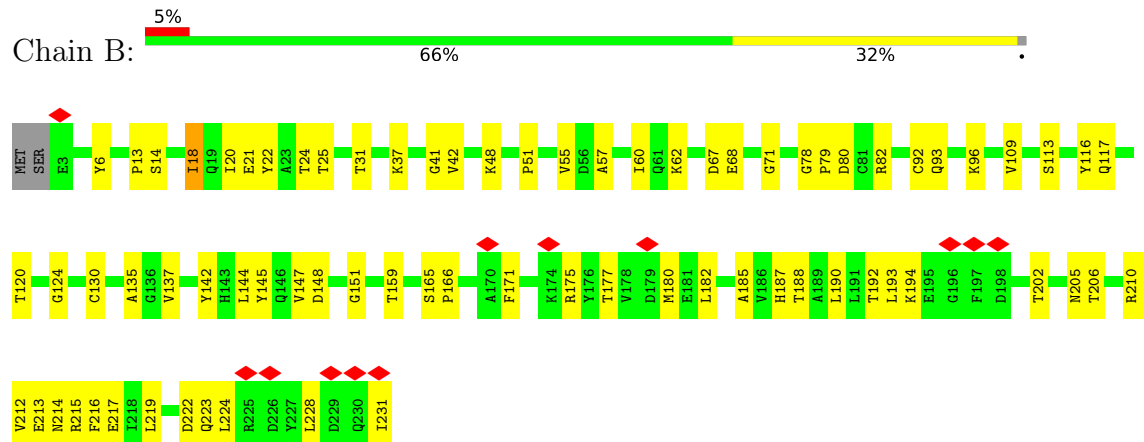
- Molecule 1: Proteasome subunit alpha type



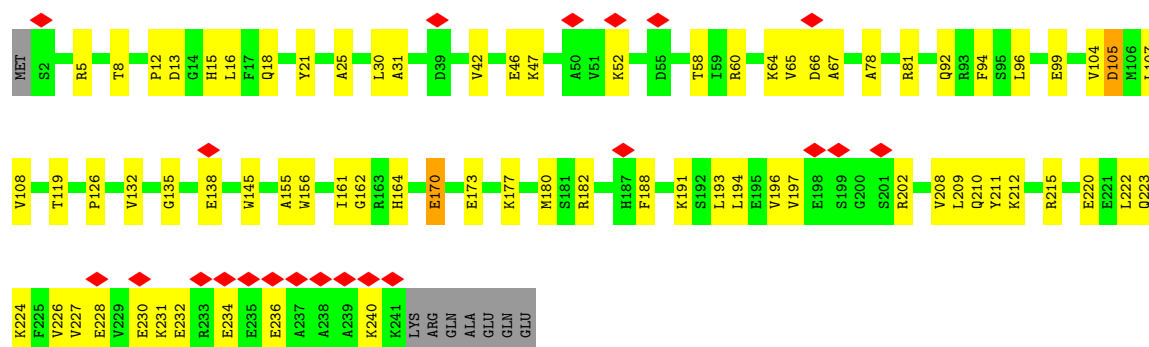
- Molecule 1: Proteasome subunit alpha type



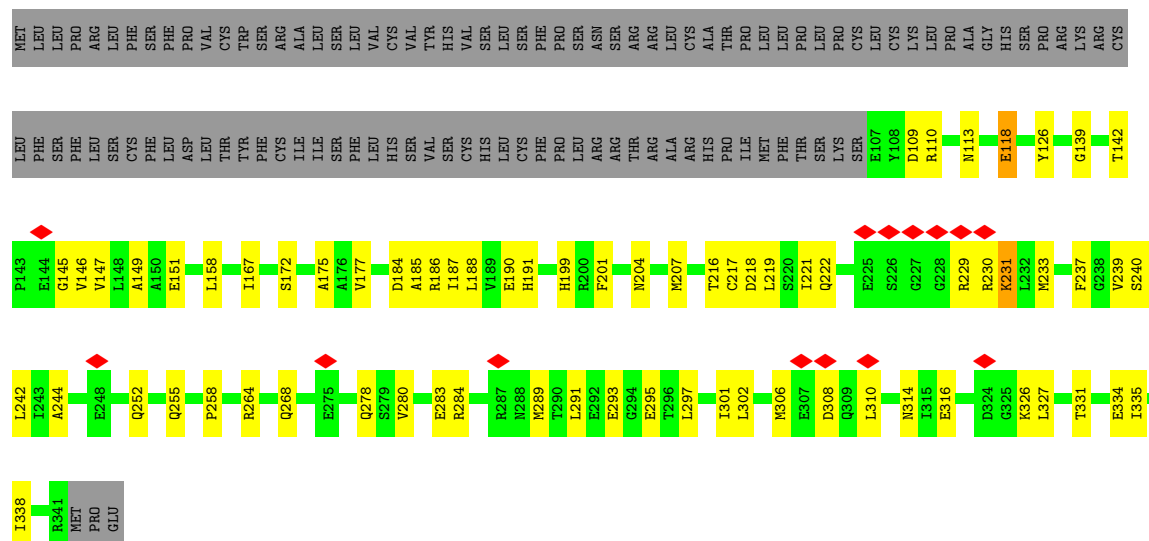
- Molecule 2: Proteasome subunit alpha type



- Molecule 4: Proteasome endopeptidase complex

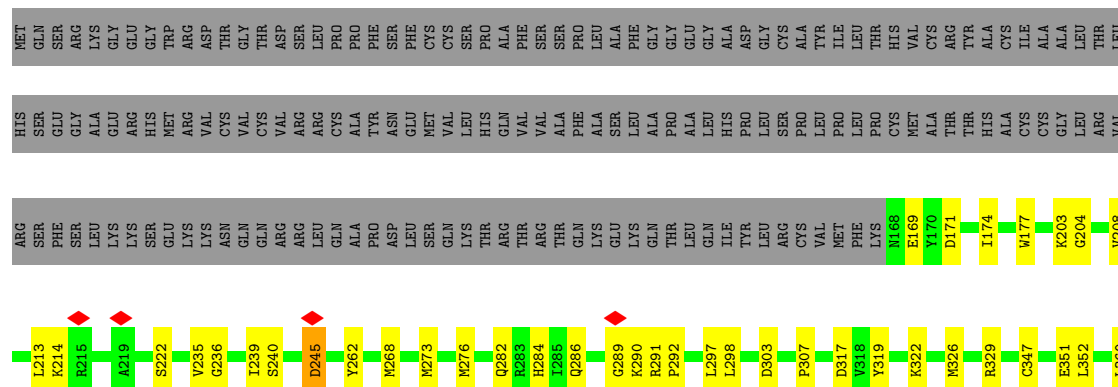


- Molecule 5: Proteasome subunit alpha type



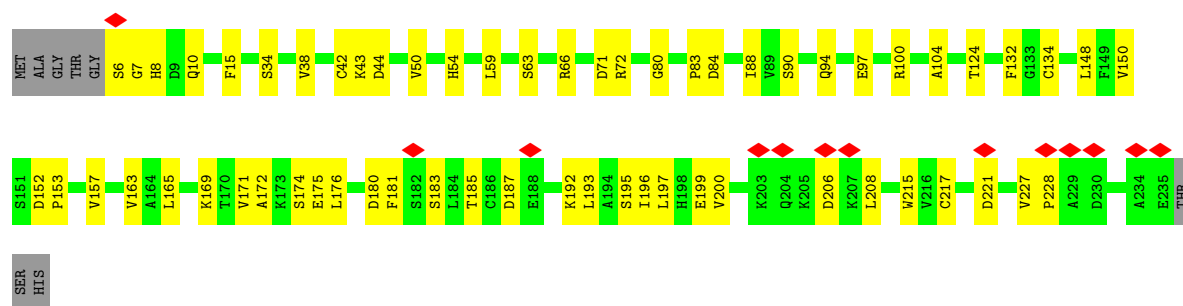
- Molecule 5: Proteasome subunit alpha type



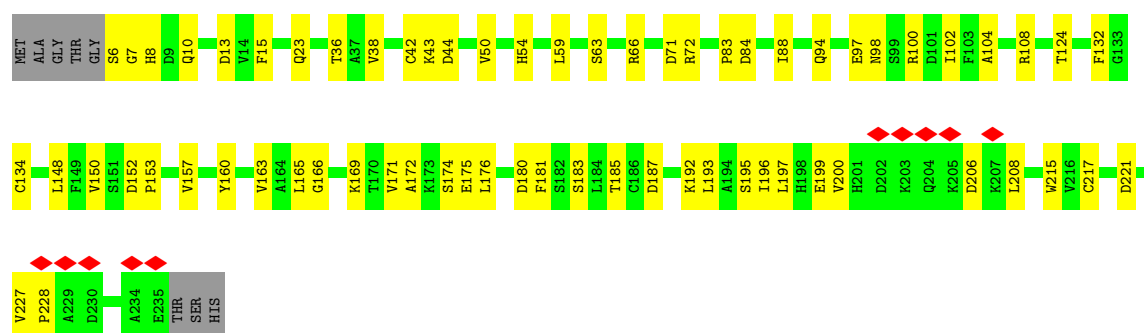


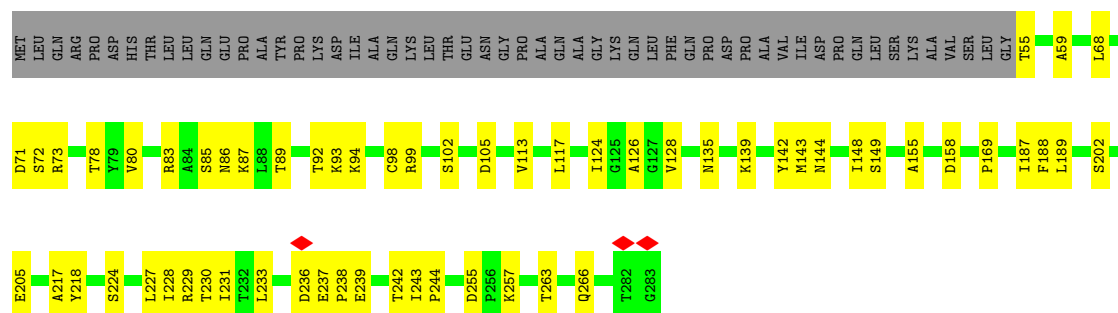


- Molecule 7: Proteasome endopeptidase complex

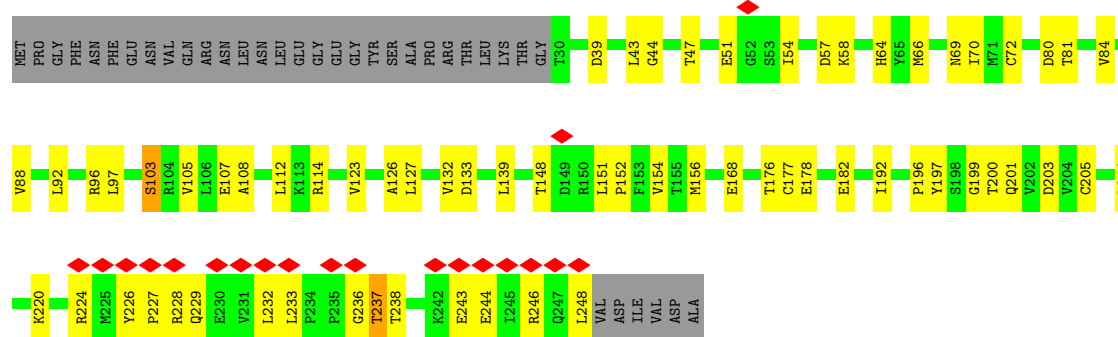


- Molecule 7: Proteasome endopeptidase complex

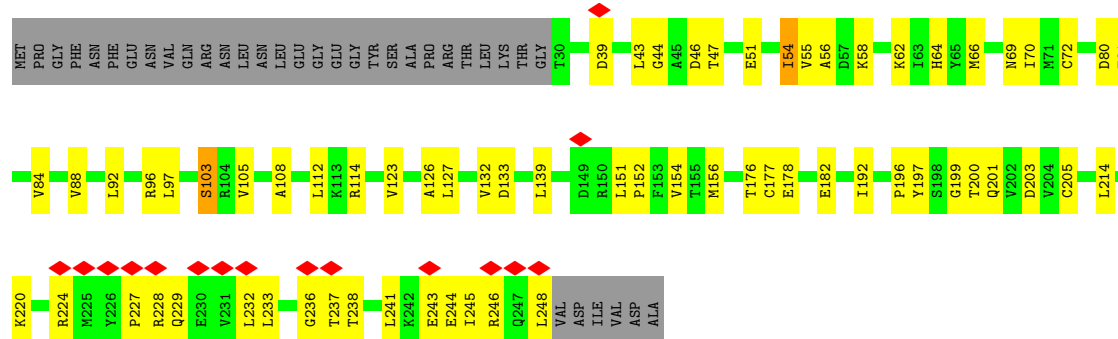




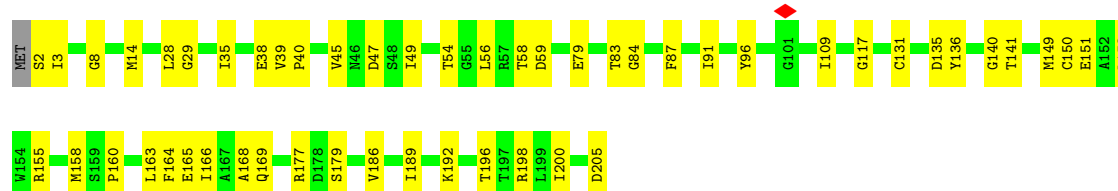
• Molecule 9: Proteasome subunit beta



• Molecule 9: Proteasome subunit beta



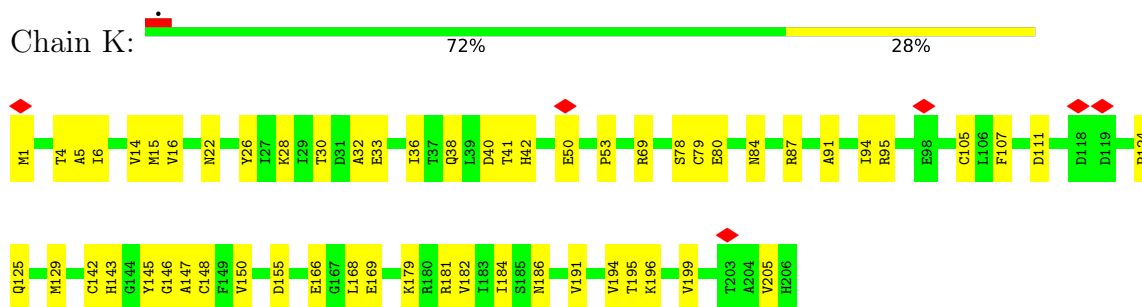
• Molecule 10: Proteasome subunit beta



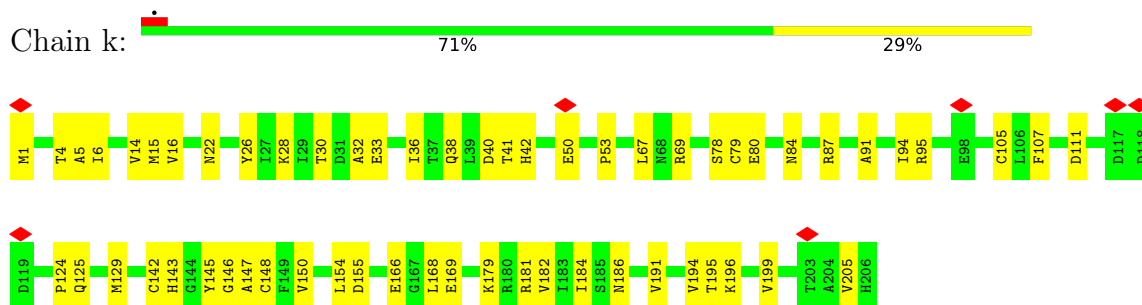
- Molecule 10: Proteasome subunit beta



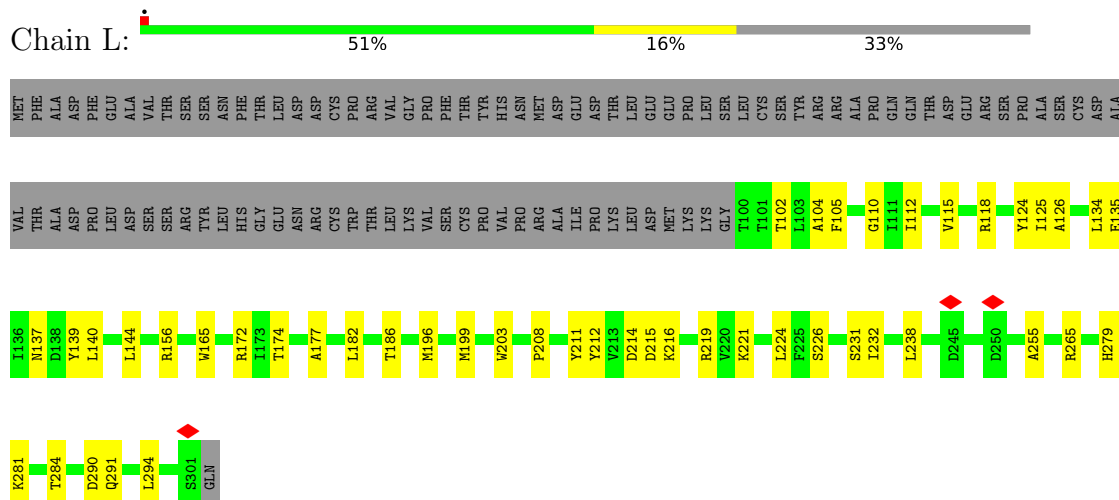
- Molecule 11: Proteasome subunit family protein



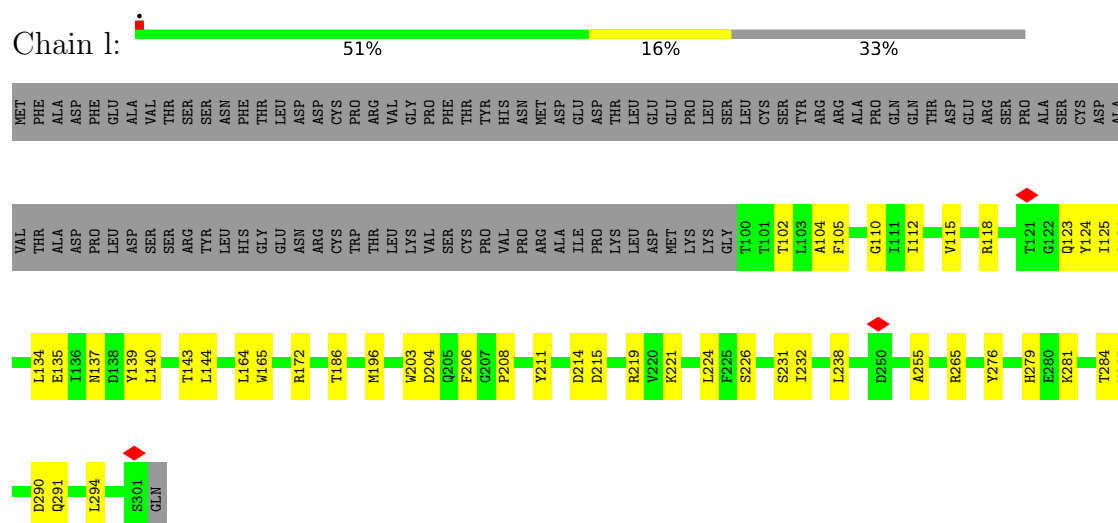
- Molecule 11: Proteasome subunit family protein



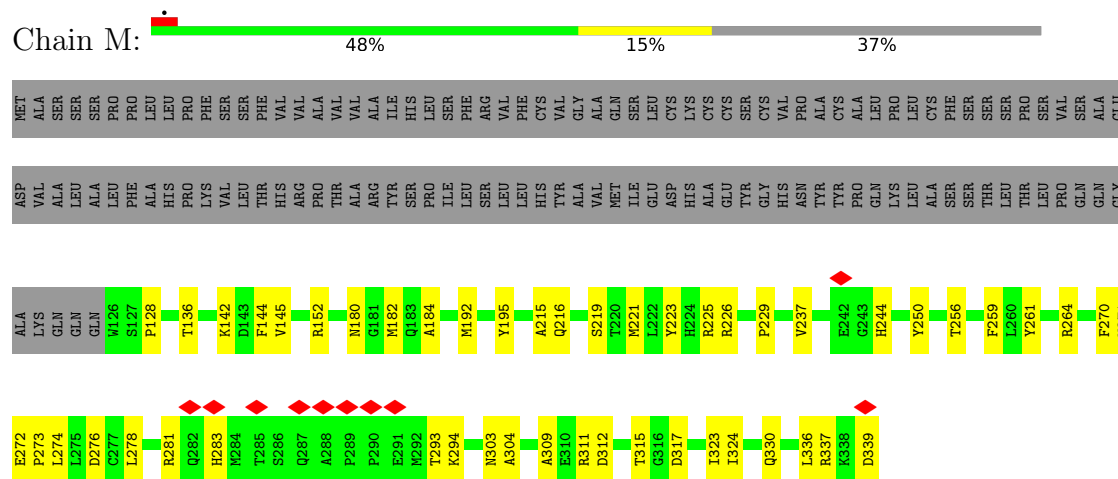
- Molecule 12: Proteasome subunit beta



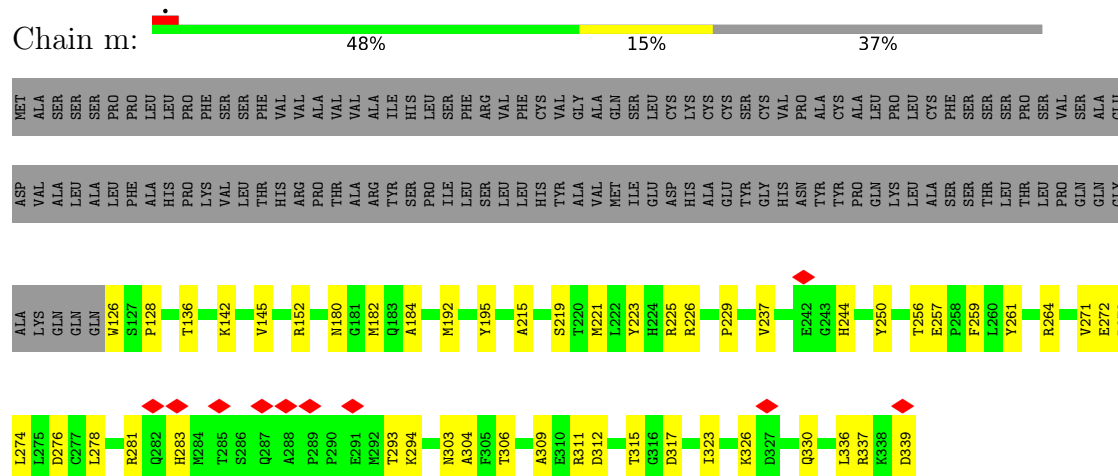
- Molecule 12: Proteasome subunit beta



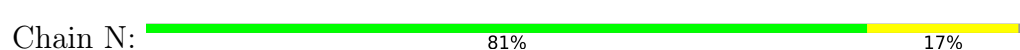
- Molecule 13: Proteasome subunit beta

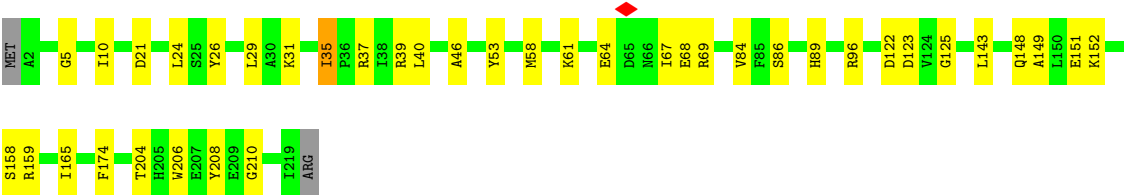


- Molecule 13: Proteasome subunit beta



- Molecule 14: Proteasome subunit beta



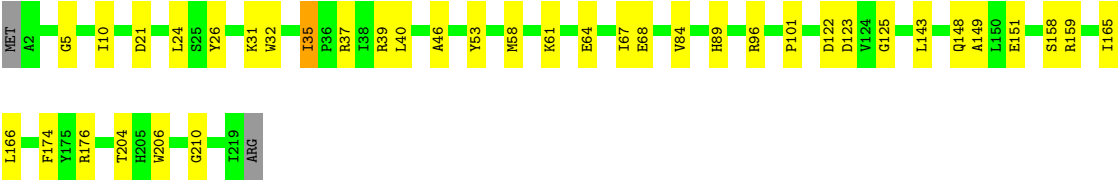


● Molecule 14: Proteasome subunit beta

Chain n:

82%

17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	38000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0154	Depositor
Map size ($\text{\AA}$)	255.6, 255.6, 255.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.852, 0.852, 0.852	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N2E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/1893	0.47	0/2567
1	a	0.30	0/1893	0.47	0/2567
2	B	0.34	0/1786	0.49	0/2421
2	b	0.34	0/1786	0.49	0/2421
3	C	0.28	0/2202	0.46	0/2982
3	c	0.28	0/2202	0.46	0/2982
4	D	0.28	0/1911	0.50	0/2573
4	d	0.28	0/1911	0.50	0/2573
5	E	0.29	0/1831	0.51	0/2476
5	e	0.28	0/1831	0.51	0/2476
6	F	0.29	0/1907	0.46	0/2575
6	f	0.29	0/1907	0.46	0/2575
7	G	0.30	0/1773	0.49	0/2398
7	g	0.30	0/1773	0.49	0/2398
8	H	0.37	0/1741	0.51	0/2359
8	h	0.37	0/1741	0.51	0/2359
9	I	0.33	0/1685	0.49	0/2284
9	i	0.33	0/1685	0.49	0/2284
10	J	0.37	0/1583	0.48	0/2135
10	j	0.37	0/1583	0.48	0/2135
11	K	0.34	0/1643	0.51	0/2222
11	k	0.34	0/1643	0.51	0/2222
12	L	0.37	0/1611	0.46	0/2180
12	l	0.37	0/1611	0.47	0/2180
13	M	0.35	0/1743	0.46	0/2354
13	m	0.35	0/1743	0.46	0/2354
14	N	0.37	0/1748	0.49	0/2363
14	n	0.37	0/1748	0.49	0/2363
All	All	0.33	0/50114	0.48	0/67778

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1861	0	1874	36	0
1	a	1861	0	1874	40	0
2	B	1753	0	1741	53	0
2	b	1753	0	1741	57	0
3	C	2155	0	2102	48	0
3	c	2155	0	2102	47	0
4	D	1882	0	1881	50	0
4	d	1882	0	1881	51	0
5	E	1802	0	1784	53	0
5	e	1802	0	1784	49	0
6	F	1869	0	1823	35	0
6	f	1869	0	1823	38	0
7	G	1741	0	1702	45	0
7	g	1741	0	1702	48	0
8	H	1709	0	1665	46	0
8	h	1709	0	1665	43	0
9	I	1659	0	1684	56	0
9	i	1659	0	1684	53	0
10	J	1557	0	1552	43	0
10	j	1557	0	1552	44	0
11	K	1612	0	1571	35	0
11	k	1612	0	1571	39	0
12	L	1577	0	1534	35	0
12	l	1577	0	1534	33	0
13	M	1702	0	1638	37	0
13	m	1702	0	1638	40	0
14	N	1712	0	1668	28	0
14	n	1712	0	1668	28	0
15	L	33	0	0	0	0
15	l	33	0	0	0	0
All	All	49248	0	48438	1062	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 11.

All (1062) 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)
3:C:229:ILE:HG13	9:I:246:ARG:HH12	1.25	0.97
11:K:30:THR:HG22	11:K:32:ALA:H	1.39	0.87
9:i:238:THR:HG22	10:j:169:GLN:HE21	1.41	0.85
11:k:30:THR:HG22	11:k:32:ALA:H	1.39	0.85
1:A:100:TYR:O	9:I:114:ARG:NH1	2.10	0.83
3:c:12:PHE:H	4:d:18:GLN:HE22	1.26	0.82
13:M:136:THR:HG22	13:M:180:ASN:HD21	1.48	0.79
13:M:283:HIS:O	10:j:169:GLN:NE2	2.15	0.79
13:m:136:THR:HG22	13:m:180:ASN:HD21	1.48	0.78
5:E:230:ARG:NH1	5:E:231:LYS:O	2.17	0.78
5:e:230:ARG:NH1	5:e:231:LYS:O	2.17	0.77
3:c:160:GLY:O	4:d:81:ARG:NH2	2.18	0.77
10:J:169:GLN:NE2	13:m:283:HIS:O	2.18	0.77
4:D:13:ASP:OD2	4:D:15:HIS:ND1	2.18	0.76
4:d:13:ASP:OD2	4:d:15:HIS:ND1	2.18	0.76
9:i:243:GLU:OE2	10:j:198:ARG:NE	2.17	0.76
2:B:210:ARG:HE	2:B:219:LEU:HD21	1.51	0.75
2:b:210:ARG:HE	2:b:219:LEU:HD21	1.51	0.75
3:C:12:PHE:H	4:D:18:GLN:HE22	1.32	0.75
9:i:58:LYS:NZ	10:j:151:GLU:OE2	2.20	0.74
11:k:111:ASP:OD2	11:k:125:GLN:NE2	2.21	0.73
11:K:111:ASP:OD2	11:K:125:GLN:NE2	2.21	0.72
1:a:69:VAL:HG12	1:a:70:THR:HG23	1.71	0.72
2:b:214:ASN:OD1	2:b:215:ARG:NH1	2.23	0.72
10:J:136:TYR:OH	10:J:151:GLU:OE1	2.07	0.72
13:M:337:ARG:HH22	9:i:200:THR:HG22	1.54	0.72
1:a:100:TYR:O	9:i:114:ARG:NH1	2.22	0.72
12:l:134:LEU:HD11	12:l:144:LEU:HD12	1.72	0.72
9:i:192:ILE:HG12	9:i:199:GLY:HA2	1.71	0.72
10:j:136:TYR:OH	10:j:151:GLU:OE1	2.07	0.72
2:B:214:ASN:OD1	2:B:215:ARG:NH1	2.23	0.71
12:l:102:THR:HG23	12:l:115:VAL:HG12	1.72	0.71
1:A:69:VAL:HG12	1:A:70:THR:HG23	1.71	0.71
3:C:122:ASP:OD1	4:D:81:ARG:NH1	2.23	0.71
9:I:192:ILE:HG12	9:I:199:GLY:HA2	1.72	0.71
8:H:111:GLU:CD	9:I:114:ARG:HH21	2.00	0.70
8:h:263:THR:OG1	8:h:266:GLN:NE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:21:ASP:OD1	14:N:37:ARG:NH1	2.23	0.70
14:n:21:ASP:OD1	14:n:37:ARG:NH1	2.24	0.70
8:h:89:THR:OG1	8:h:99:ARG:NH1	2.24	0.70
8:H:263:THR:OG1	8:H:266:GLN:NE2	2.24	0.70
8:H:89:THR:OG1	8:H:99:ARG:NH1	2.24	0.70
12:L:124:TYR:OH	13:M:272:GLU:OE1	2.07	0.70
8:H:191:SER:OG	8:h:188:PHE:O	2.05	0.69
12:L:134:LEU:HD11	12:L:144:LEU:HD12	1.73	0.69
3:C:160:GLY:O	4:D:81:ARG:NH2	2.25	0.69
4:D:223:GLN:HA	4:D:226:VAL:HG12	1.75	0.69
4:d:194:LEU:HA	4:d:197:VAL:HG12	1.75	0.69
5:e:185:ALA:HB2	5:e:239:VAL:HG21	1.75	0.68
3:C:109:GLU:OE1	11:K:78:SER:OG	2.12	0.68
8:H:55:THR:N	8:H:224:SER:HG	1.92	0.68
4:D:194:LEU:HA	4:D:197:VAL:HG12	1.76	0.68
1:a:21:GLN:HE22	7:g:15:PHE:H	1.41	0.68
7:g:150:VAL:HG21	7:g:163:VAL:HG21	1.75	0.68
10:J:40:PRO:HB3	10:J:186:VAL:HG11	1.75	0.68
10:J:91:ILE:HD11	10:J:109:ILE:HD11	1.75	0.68
10:j:91:ILE:HD11	10:j:109:ILE:HD11	1.75	0.67
9:I:248:LEU:HD13	10:J:47:ASP:HB2	1.76	0.67
4:D:47:LYS:NZ	4:D:202:ARG:O	2.28	0.67
4:d:223:GLN:HA	4:d:226:VAL:HG12	1.75	0.67
10:j:40:PRO:HB3	10:j:186:VAL:HG11	1.75	0.67
13:m:152:ARG:NH1	13:m:317:ASP:OD2	2.27	0.67
13:M:152:ARG:NH1	13:M:317:ASP:OD2	2.27	0.67
1:a:142:GLN:NE2	1:a:147:GLY:O	2.28	0.67
12:l:124:TYR:OH	13:m:272:GLU:OE1	2.08	0.67
7:G:150:VAL:HG21	7:G:163:VAL:HG21	1.75	0.66
7:G:165:LEU:HA	7:G:169:LYS:HE2	1.78	0.66
6:f:282:GLN:NE2	6:f:286:GLN:OE1	2.29	0.66
1:A:142:GLN:NE2	1:A:147:GLY:O	2.28	0.66
5:E:185:ALA:HB2	5:E:239:VAL:HG21	1.75	0.66
8:h:55:THR:N	8:h:224:SER:HG	1.94	0.66
6:F:282:GLN:NE2	6:F:286:GLN:OE1	2.29	0.66
10:j:153:LEU:HB3	10:j:166:ILE:HD12	1.77	0.66
10:j:28:LEU:HB2	10:j:39:VAL:HG11	1.77	0.66
2:B:113:SER:OG	2:B:151:GLY:O	2.13	0.65
10:J:28:LEU:HB2	10:J:39:VAL:HG11	1.77	0.65
10:J:153:LEU:HB3	10:J:166:ILE:HD12	1.77	0.65
4:D:132:VAL:HG23	4:D:161:ILE:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:66:MET:HE1	9:I:88:VAL:HG23	1.79	0.65
14:N:24:LEU:HD13	14:N:35:ILE:HD11	1.79	0.65
1:a:155:THR:O	1:a:162:THR:HA	1.97	0.65
1:a:195:GLN:HE22	1:a:223:ARG:HH11	1.45	0.65
2:b:113:SER:OG	2:b:151:GLY:O	2.13	0.65
4:d:47:LYS:NZ	4:d:202:ARG:O	2.28	0.65
8:H:227:LEU:HD23	8:H:244:PRO:HA	1.78	0.65
5:e:231:LYS:NZ	5:e:231:LYS:HB3	2.12	0.65
8:h:227:LEU:HD23	8:h:244:PRO:HA	1.79	0.65
7:g:215:TRP:CD1	7:g:227:VAL:HG22	2.32	0.65
13:m:128:PRO:O	14:n:96:ARG:NH2	2.30	0.65
5:E:231:LYS:HB3	5:E:231:LYS:NZ	2.12	0.64
9:i:66:MET:HE1	9:i:88:VAL:HG23	1.79	0.64
1:A:50:GLN:HE21	1:A:210:ILE:HD13	1.61	0.64
2:B:206:THR:HG23	2:B:224:LEU:HD21	1.79	0.64
8:H:107:GLN:HE22	9:I:148:THR:H	1.43	0.64
14:N:26:TYR:HB2	14:N:31:LYS:HD2	1.78	0.64
3:c:167:ALA:HB1	3:c:181:LEU:HD22	1.80	0.64
14:n:26:TYR:HB2	14:n:31:LYS:HD2	1.78	0.64
8:H:73:ARG:NH1	8:H:224:SER:O	2.31	0.64
14:n:24:LEU:HD13	14:n:35:ILE:HD11	1.79	0.64
3:c:229:ILE:HG13	9:i:246:ARG:HH12	1.63	0.64
7:g:42:CYS:O	7:g:43:LYS:HG3	1.98	0.64
7:g:165:LEU:HA	7:g:169:LYS:HE2	1.78	0.64
1:A:155:THR:O	1:A:162:THR:HA	1.97	0.64
6:F:319:TYR:HB3	7:G:59:LEU:HD21	1.80	0.64
1:a:129:ARG:NH1	7:g:124:THR:O	2.30	0.64
9:i:92:LEU:HD11	9:i:108:ALA:HB2	1.80	0.64
9:I:205:CYS:HB3	9:I:214:LEU:HD13	1.80	0.64
1:a:50:GLN:HE21	1:a:210:ILE:HD13	1.61	0.64
6:f:174:ILE:HD12	6:f:292:PRO:HD3	1.80	0.64
5:E:331:THR:HG22	5:E:334:GLU:HG2	1.80	0.63
4:d:132:VAL:HG23	4:d:161:ILE:HD13	1.79	0.63
9:i:205:CYS:HB3	9:i:214:LEU:HD13	1.80	0.63
5:e:331:THR:HG22	5:e:334:GLU:HG2	1.80	0.63
2:b:206:THR:HG23	2:b:224:LEU:HD21	1.79	0.63
7:g:172:ALA:HB2	7:g:200:VAL:HG21	1.80	0.63
8:h:73:ARG:NH1	8:h:224:SER:O	2.31	0.63
13:M:303:ASN:HD21	9:i:229:GLN:HG3	1.62	0.63
5:e:240:SER:OG	5:e:255:GLN:NE2	2.31	0.63
7:G:42:CYS:O	7:G:43:LYS:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:126:ALA:O	10:j:177:ARG:NH1	2.31	0.63
5:E:186:ARG:O	5:E:190:GLU:HG2	1.99	0.63
11:K:4:THR:HA	11:K:143:HIS:O	1.99	0.63
11:K:181:ARG:NH1	11:k:28:LYS:O	2.32	0.63
7:G:215:TRP:CD1	7:G:227:VAL:HG22	2.32	0.63
12:L:280:GLU:HG3	12:L:281:LYS:HE2	1.80	0.63
7:g:50:VAL:HG21	7:g:66:ARG:HD3	1.81	0.63
1:A:195:GLN:HE22	1:A:223:ARG:HH11	1.45	0.63
3:C:167:ALA:HB1	3:C:181:LEU:HD22	1.80	0.63
5:E:240:SER:OG	5:E:255:GLN:NE2	2.31	0.63
1:A:120:GLN:NE2	2:B:80:ASP:OD1	2.32	0.62
9:I:92:LEU:HD11	9:I:108:ALA:HB2	1.80	0.62
11:k:4:THR:HA	11:k:143:HIS:O	1.99	0.62
11:k:182:VAL:HG12	11:k:184:ILE:H	1.63	0.62
6:F:174:ILE:HD12	6:F:292:PRO:HD3	1.80	0.62
9:I:236:GLY:N	10:J:165:GLU:OE2	2.31	0.62
11:K:182:VAL:HG12	11:K:184:ILE:H	1.63	0.62
7:G:6:SER:OG	7:G:8:HIS:ND1	2.23	0.62
9:i:244:GLU:OE2	9:i:246:ARG:NH1	2.29	0.62
5:e:186:ARG:O	5:e:190:GLU:HG2	1.99	0.62
13:m:192:MET:HB3	13:m:221:MET:HE1	1.82	0.62
7:G:172:ALA:HB2	7:G:200:VAL:HG21	1.80	0.61
13:M:192:MET:HB3	13:M:221:MET:HE1	1.82	0.61
7:g:6:SER:OG	7:g:8:HIS:ND1	2.23	0.61
7:g:104:ALA:HB2	8:h:135:ASN:HD22	1.65	0.61
6:F:263:MET:O	14:N:86:SER:OG	2.18	0.61
1:A:8:LYS:HB3	1:A:20:TYR:HD2	1.64	0.61
3:C:177:ALA:HB2	3:C:205:THR:HG21	1.82	0.61
4:D:157:ARG:NH2	5:E:158:LEU:O	2.32	0.61
7:G:50:VAL:HG21	7:G:66:ARG:HD3	1.81	0.61
1:a:8:LYS:HB3	1:a:20:TYR:HD2	1.64	0.61
12:L:196:MET:H	12:L:215:ASP:HB3	1.65	0.61
9:I:244:GLU:OE2	9:I:246:ARG:NH1	2.29	0.61
10:J:177:ARG:NH1	12:l:126:ALA:O	2.32	0.61
8:h:68:LEU:HD21	8:h:155:ALA:HB3	1.83	0.61
11:k:15:MET:HE1	11:k:168:LEU:HD22	1.83	0.60
9:I:44:GLY:HA2	9:I:203:ASP:O	2.02	0.60
11:K:15:MET:HE1	11:K:168:LEU:HD22	1.83	0.60
3:C:57:ASP:OD1	3:C:58:SER:N	2.34	0.60
3:c:85:VAL:HG23	3:c:88:ASP:HB3	1.84	0.60
3:c:177:ALA:HB2	3:c:205:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:92:THR:HG22	8:H:93:LYS:H	1.67	0.60
9:i:44:GLY:HA2	9:i:203:ASP:O	2.02	0.60
14:N:39:ARG:NH2	14:N:64:GLU:OE1	2.35	0.59
3:c:57:ASP:OD1	3:c:58:SER:N	2.34	0.59
8:h:92:THR:HG22	8:h:93:LYS:H	1.67	0.59
4:D:135:GLY:HA2	4:D:209:LEU:HD21	1.84	0.59
4:d:135:GLY:HA2	4:d:209:LEU:HD21	1.83	0.59
6:f:372:VAL:HG11	6:f:395:ARG:HG3	1.83	0.59
6:F:372:VAL:HG11	6:F:395:ARG:HG3	1.83	0.59
11:K:80:GLU:O	11:K:84:ASN:ND2	2.27	0.59
1:A:225:THR:HG22	1:A:227:ALA:H	1.67	0.59
8:H:68:LEU:HD21	8:H:155:ALA:HB3	1.83	0.59
14:n:39:ARG:NH2	14:n:64:GLU:OE1	2.35	0.59
11:K:22:ASN:ND2	11:K:33:GLU:OE1	2.36	0.59
3:c:257:HIS:HD2	3:c:260:ARG:HH22	1.51	0.59
1:A:29:VAL:HG11	1:A:134:VAL:HG23	1.84	0.59
3:C:257:HIS:HD2	3:C:260:ARG:HH22	1.51	0.59
10:J:179:SER:HB3	12:l:125:ILE:HD11	1.83	0.59
1:a:225:THR:HG22	1:a:227:ALA:H	1.67	0.59
11:k:194:VAL:HG22	11:k:199:VAL:HG12	1.84	0.59
14:N:61:LYS:HA	14:N:64:GLU:HG2	1.85	0.58
1:a:29:VAL:HG11	1:a:134:VAL:HG23	1.83	0.58
3:c:163:SER:OG	3:c:165:TRP:NE1	2.36	0.58
12:l:196:MET:H	12:l:215:ASP:HB3	1.69	0.58
3:C:85:VAL:HG23	3:C:88:ASP:HB3	1.85	0.58
5:E:204:ASN:HB2	13:M:216:GLN:HG2	1.85	0.58
11:K:28:LYS:O	11:k:181:ARG:NH1	2.35	0.58
11:K:194:VAL:HG22	11:K:199:VAL:HG12	1.84	0.58
4:d:188:PHE:HA	4:d:191:LYS:HG2	1.86	0.58
3:C:43:VAL:HG13	3:C:221:MET:HB3	1.86	0.58
9:I:224:ARG:NH2	9:I:227:PRO:HA	2.19	0.58
14:N:210:GLY:HA3	9:i:152:PRO:HG3	1.86	0.58
9:i:224:ARG:NH2	9:i:227:PRO:HA	2.19	0.58
1:A:26:PHE:HE1	1:A:158:PRO:HD2	1.69	0.58
11:k:22:ASN:ND2	11:k:33:GLU:OE1	2.36	0.58
14:n:61:LYS:HA	14:n:64:GLU:HG2	1.85	0.58
5:E:218:ASP:O	5:E:222:GLN:NE2	2.37	0.57
14:n:10:ILE:HD13	14:n:165:ILE:HD11	1.86	0.57
3:C:163:SER:OG	3:C:165:TRP:NE1	2.36	0.57
3:C:187:GLU:OE1	3:C:187:GLU:N	2.36	0.57
3:C:220:VAL:HG13	3:C:249:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:43:VAL:HG13	3:c:221:MET:HB3	1.86	0.57
3:C:95:TYR:CE2	3:C:123:GLU:HG3	2.40	0.57
7:g:72:ARG:NH1	7:g:221:ASP:OD2	2.38	0.57
11:k:80:GLU:O	11:k:84:ASN:ND2	2.27	0.57
4:D:188:PHE:HA	4:D:191:LYS:HG2	1.86	0.57
3:c:220:VAL:HG13	3:c:249:LEU:HD11	1.86	0.57
7:g:180:ASP:OD1	7:g:183:SER:N	2.35	0.57
3:C:190:THR:HG23	3:C:193:ASP:H	1.70	0.57
8:h:233:LEU:HD23	8:h:238:PRO:HB3	1.87	0.57
12:L:110:GLY:HA2	12:L:203:TRP:HZ3	1.67	0.57
1:a:26:PHE:HE1	1:a:158:PRO:HD2	1.69	0.57
5:e:218:ASP:O	5:e:222:GLN:NE2	2.37	0.57
1:a:172:LYS:HG3	1:a:173:LYS:HG3	1.86	0.57
1:A:207:GLN:HE21	1:A:214:VAL:HG22	1.70	0.56
1:a:207:GLN:HE21	1:a:214:VAL:HG22	1.70	0.56
9:I:243:GLU:OE2	10:J:198:ARG:NE	2.38	0.56
12:L:104:ALA:HA	12:L:112:ILE:O	2.06	0.56
13:M:145:VAL:HG11	13:M:237:VAL:HG13	1.87	0.56
9:I:238:THR:HG21	10:J:168:ALA:HB3	1.87	0.56
12:L:125:ILE:HD11	10:j:179:SER:HB3	1.87	0.56
12:L:279:HIS:HE1	12:L:284:THR:HG23	1.70	0.56
1:a:135:SER:HB2	1:a:156:VAL:HG13	1.86	0.56
4:d:105:ASP:N	4:d:105:ASP:OD2	2.38	0.56
5:e:110:ARG:H	5:e:110:ARG:HD3	1.70	0.56
12:l:110:GLY:HA2	12:l:203:TRP:HZ3	1.69	0.56
13:m:145:VAL:HG11	13:m:237:VAL:HG13	1.87	0.56
13:m:271:VAL:HG13	13:m:304:ALA:HB1	1.87	0.56
5:E:110:ARG:HD3	5:E:110:ARG:H	1.70	0.56
8:H:233:LEU:HD23	8:H:238:PRO:HB3	1.87	0.56
1:a:58:MET:HE2	7:g:160:TYR:CZ	2.41	0.56
2:B:13:PRO:HA	3:C:23:TYR:CD1	2.40	0.56
14:N:122:ASP:OD2	14:N:123:ASP:N	2.33	0.56
2:b:51:PRO:HD2	2:b:55:VAL:HG21	1.87	0.56
3:c:4:ARG:HH12	7:g:10:GLN:HG3	1.71	0.56
6:F:235:VAL:HG21	6:F:273:MET:HE1	1.88	0.56
3:c:190:THR:HG23	3:c:193:ASP:H	1.70	0.56
14:N:10:ILE:HD13	14:N:165:ILE:HD11	1.86	0.56
1:A:135:SER:HB2	1:A:156:VAL:HG13	1.86	0.56
1:A:172:LYS:HG3	1:A:173:LYS:HG3	1.86	0.55
4:D:138:GLU:OE2	4:D:212:LYS:NZ	2.39	0.55
13:m:182:MET:HE2	13:m:184:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:PRO:HD2	2:B:55:VAL:HG21	1.87	0.55
4:D:177:LYS:H	4:D:180:MET:HE3	1.72	0.55
13:M:271:VAL:HG13	13:M:304:ALA:HB1	1.87	0.55
3:c:187:GLU:OE1	3:c:187:GLU:N	2.36	0.55
4:d:65:VAL:HG11	4:d:107:LEU:HD21	1.88	0.55
9:I:80:ASP:OD1	10:J:96:TYR:OH	2.21	0.55
3:c:95:TYR:CE2	3:c:123:GLU:HG3	2.40	0.55
4:d:177:LYS:H	4:d:180:MET:HE3	1.72	0.55
5:E:167:ILE:HD12	5:E:316:GLU:HG3	1.89	0.55
2:b:48:LYS:NZ	2:b:57:ALA:O	2.34	0.55
4:d:138:GLU:OE2	4:d:212:LYS:NZ	2.39	0.55
5:e:289:MET:HE2	5:e:293:GLU:HB3	1.88	0.55
7:G:72:ARG:NH1	7:G:221:ASP:OD2	2.38	0.55
3:c:122:ASP:OD1	4:d:81:ARG:NH1	2.39	0.55
6:f:235:VAL:HG21	6:f:273:MET:HE1	1.88	0.55
8:h:255:ASP:OD2	8:h:257:LYS:NZ	2.32	0.55
12:l:279:HIS:HE1	12:l:284:THR:HG23	1.72	0.55
5:E:289:MET:HE2	5:E:293:GLU:HB3	1.88	0.55
7:g:215:TRP:HE1	7:g:227:VAL:HA	1.72	0.55
4:D:65:VAL:HG11	4:D:107:LEU:HD21	1.88	0.55
10:j:29:GLY:HA2	10:j:35:ILE:H	1.72	0.54
2:B:109:VAL:HG21	2:B:145:TYR:HD2	1.71	0.54
6:F:203:LYS:HE2	6:F:322:LYS:HA	1.90	0.54
7:G:215:TRP:HE1	7:G:227:VAL:HA	1.71	0.54
11:K:148:CYS:SG	12:l:232:ILE:HD12	2.48	0.54
1:a:10:ILE:HD12	2:b:8:LEU:HD11	1.90	0.54
2:B:182:LEU:HD11	2:B:212:VAL:HG12	1.90	0.54
3:c:52:PRO:HG3	3:c:214:ASP:HB2	1.89	0.54
4:d:182:ARG:HH22	4:d:215:ARG:HH22	1.54	0.54
6:f:303:ASP:N	6:f:303:ASP:OD1	2.40	0.54
13:m:261:TYR:OH	13:m:276:ASP:OD1	2.19	0.54
6:F:329:ARG:NH1	6:F:363:ALA:O	2.41	0.54
10:J:59:ASP:OD2	11:K:95:ARG:NH2	2.40	0.54
8:h:202:SER:OG	8:h:205:GLU:OE2	2.26	0.54
2:B:48:LYS:NZ	2:B:57:ALA:O	2.34	0.54
13:M:182:MET:HE2	13:M:184:ALA:HB3	1.88	0.54
5:e:149:ALA:HB1	5:e:302:LEU:HD11	1.90	0.54
4:D:105:ASP:N	4:D:105:ASP:OD2	2.38	0.54
9:I:238:THR:HG22	10:J:169:GLN:HE21	1.72	0.54
12:l:224:LEU:HD11	12:l:238:LEU:HG	1.90	0.54
13:M:261:TYR:OH	13:M:276:ASP:OD1	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:ARG:HH22	4:D:215:ARG:HH22	1.55	0.54
1:a:15:PRO:HA	2:b:22:TYR:CE1	2.43	0.54
2:b:182:LEU:HD11	2:b:212:VAL:HG12	1.90	0.54
6:F:303:ASP:N	6:F:303:ASP:OD1	2.40	0.53
2:b:109:VAL:HG21	2:b:145:TYR:HD2	1.71	0.53
6:f:203:LYS:HE2	6:f:322:LYS:HA	1.89	0.53
13:m:126:TRP:CZ2	14:n:101:PRO:HB3	2.43	0.53
5:e:167:ILE:HD12	5:e:316:GLU:HG3	1.89	0.53
3:C:21:VAL:O	3:C:25:VAL:HG23	2.08	0.53
6:f:329:ARG:NH1	6:f:363:ALA:O	2.41	0.53
10:j:135:ASP:OD1	10:j:135:ASP:N	2.42	0.53
5:E:149:ALA:HB1	5:E:302:LEU:HD11	1.90	0.53
9:I:229:GLN:HG3	13:m:303:ASN:HD21	1.74	0.53
6:F:169:GLU:OE1	6:F:169:GLU:N	2.42	0.53
3:c:21:VAL:O	3:c:25:VAL:HG23	2.08	0.53
1:A:21:GLN:HE22	7:G:15:PHE:H	1.56	0.53
8:H:187:ILE:HD12	8:h:187:ILE:HD12	1.91	0.53
8:H:202:SER:OG	8:H:205:GLU:OE2	2.26	0.53
3:C:52:PRO:HG3	3:C:214:ASP:HB2	1.89	0.53
8:H:190:TYR:CE2	14:N:29:LEU:HD21	2.44	0.53
9:I:58:LYS:NZ	10:J:151:GLU:OE2	2.36	0.53
1:a:45:VAL:HG11	1:a:138:ILE:HB	1.91	0.53
8:H:255:ASP:OD2	8:H:257:LYS:NZ	2.32	0.53
7:g:206:ASP:OD1	7:g:206:ASP:N	2.42	0.53
10:J:29:GLY:HA2	10:J:35:ILE:H	1.72	0.53
14:N:206:TRP:HB2	8:h:244:PRO:HB3	1.91	0.53
13:m:337:ARG:NH2	13:m:339:ASP:OD2	2.42	0.53
1:A:129:ARG:NH1	7:G:124:THR:O	2.42	0.53
12:L:203:TRP:CZ3	12:L:208:PRO:HG3	2.44	0.53
12:L:224:LEU:HD11	12:L:238:LEU:HG	1.91	0.53
13:m:223:TYR:O	13:m:226:ARG:HB2	2.09	0.53
9:I:237:THR:HG23	10:J:165:GLU:OE1	2.09	0.52
12:L:232:ILE:HD12	11:k:148:CYS:SG	2.49	0.52
2:b:117:GLN:HA	2:b:120:THR:HG22	1.92	0.52
1:A:6:PHE:O	1:A:8:LYS:HG2	2.09	0.52
5:e:229:ARG:HE	5:e:230:ARG:HB2	1.74	0.52
1:A:45:VAL:HG11	1:A:138:ILE:HB	1.91	0.52
13:M:223:TYR:O	13:M:226:ARG:HB2	2.09	0.52
13:M:337:ARG:NH2	13:M:339:ASP:OD2	2.42	0.52
4:d:92:GLN:HG3	11:k:67:LEU:HB2	1.90	0.52
6:f:319:TYR:HB3	7:g:59:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HG3	2:B:82:ARG:HH21	1.74	0.52
2:B:117:GLN:HA	2:B:120:THR:HG22	1.92	0.52
5:E:229:ARG:HE	5:E:230:ARG:HB2	1.74	0.52
5:E:291:LEU:O	5:E:295:GLU:HG2	2.10	0.52
8:H:68:LEU:HD22	8:H:98:CYS:SG	2.50	0.52
13:M:250:TYR:CE2	13:M:256:THR:HB	2.45	0.52
1:a:6:PHE:O	1:a:8:LYS:HG2	2.09	0.52
4:D:220:GLU:O	4:D:224:LYS:HG2	2.09	0.52
7:G:180:ASP:OD1	7:G:183:SER:N	2.35	0.52
6:f:169:GLU:OE1	6:f:169:GLU:N	2.42	0.52
12:l:203:TRP:CZ3	12:l:208:PRO:HG3	2.44	0.52
5:E:109:ASP:OD1	5:E:109:ASP:N	2.43	0.52
6:F:171:ASP:OD1	6:F:171:ASP:N	2.42	0.52
10:J:14:MET:HE3	10:J:150:CYS:SG	2.50	0.52
3:c:146:ASP:OD2	3:c:152:GLN:NE2	2.43	0.52
4:d:220:GLU:O	4:d:224:LYS:HG2	2.09	0.52
2:B:177:THR:HB	2:B:180:MET:HG3	1.92	0.52
4:D:231:LYS:O	4:D:234:GLU:HG2	2.10	0.52
8:H:111:GLU:OE2	9:I:114:ARG:NH2	2.42	0.52
6:f:236:GLY:HA3	6:f:386:PHE:CE1	2.45	0.52
7:g:215:TRP:HZ3	7:g:217:CYS:HG	1.53	0.52
8:h:68:LEU:HD22	8:h:98:CYS:SG	2.50	0.52
2:B:187:HIS:CE1	2:B:231:ILE:HG22	2.45	0.52
3:C:146:ASP:OD2	3:C:152:GLN:NE2	2.43	0.52
2:b:67:ASP:OD1	2:b:92:CYS:HB3	2.10	0.52
9:i:80:ASP:HB3	9:i:123:VAL:HG13	1.91	0.52
8:H:72:SER:O	8:H:72:SER:OG	2.26	0.51
9:I:152:PRO:HG3	14:n:210:GLY:HA3	1.91	0.51
12:L:105:PHE:HE2	12:L:255:ALA:HB2	1.74	0.51
1:a:206:LEU:O	1:a:210:ILE:HG12	2.10	0.51
2:b:187:HIS:CE1	2:b:231:ILE:HG22	2.45	0.51
5:e:191:HIS:CG	5:e:219:LEU:HD12	2.45	0.51
6:f:171:ASP:OD1	6:f:171:ASP:N	2.42	0.51
7:g:108:ARG:HH21	8:h:124:ILE:HD12	1.75	0.51
2:B:67:ASP:OD1	2:B:92:CYS:HB3	2.10	0.51
8:h:71:ASP:OD1	8:h:87:LYS:NZ	2.43	0.51
13:m:293:THR:OG1	13:m:294:LYS:N	2.43	0.51
6:F:204:GLY:HA3	6:F:352:LEU:HD11	1.91	0.51
3:c:139:SER:OG	3:c:156:THR:O	2.26	0.51
13:m:250:TYR:CE2	13:m:256:THR:HB	2.45	0.51
5:E:191:HIS:CG	5:E:219:LEU:HD12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:135:ASP:OD1	10:J:135:ASP:N	2.42	0.51
12:L:102:THR:HG23	12:L:115:VAL:HG12	1.92	0.51
5:e:237:PHE:HB3	5:e:239:VAL:HG12	1.93	0.51
5:e:291:LEU:O	5:e:295:GLU:HG2	2.10	0.51
12:l:105:PHE:HE2	12:l:255:ALA:HB2	1.75	0.51
3:C:28:ILE:HD13	3:C:139:SER:HB2	1.93	0.51
2:b:177:THR:HB	2:b:180:MET:HG3	1.92	0.51
5:e:109:ASP:N	5:e:109:ASP:OD1	2.43	0.51
6:f:204:GLY:HA3	6:f:352:LEU:HD11	1.91	0.51
13:m:250:TYR:O	13:m:264:ARG:NH2	2.44	0.51
2:B:68:GLU:O	2:B:215:ARG:HA	2.11	0.51
5:E:229:ARG:NE	5:E:230:ARG:HB2	2.26	0.51
6:F:236:GLY:HA3	6:F:386:PHE:CE1	2.45	0.51
10:j:14:MET:HE3	10:j:150:CYS:SG	2.50	0.51
13:m:309:ALA:HB2	13:m:336:LEU:HD13	1.92	0.51
12:l:186:THR:HG21	12:l:214:ASP:O	2.10	0.51
9:I:80:ASP:HB3	9:I:123:VAL:HG13	1.92	0.51
3:c:262:ASP:OD1	3:c:265:ARG:NH1	2.43	0.51
8:h:72:SER:O	8:h:72:SER:OG	2.26	0.51
14:N:40:LEU:HA	14:N:46:ALA:HA	1.93	0.51
5:e:229:ARG:NE	5:e:230:ARG:HB2	2.26	0.51
14:n:122:ASP:OD2	14:n:123:ASP:N	2.33	0.51
9:i:241:LEU:HD22	10:j:201:LYS:HE2	1.93	0.51
2:B:109:VAL:HG21	2:B:145:TYR:CD2	2.46	0.50
2:B:215:ARG:NE	2:B:217:GLU:OE2	2.44	0.50
5:E:237:PHE:HB3	5:E:239:VAL:HG12	1.93	0.50
13:M:128:PRO:O	14:N:96:ARG:NH2	2.43	0.50
4:d:231:LYS:O	4:d:234:GLU:HG2	2.10	0.50
3:C:262:ASP:OD1	3:C:265:ARG:NH1	2.43	0.50
7:g:176:LEU:HD22	7:g:181:PHE:HZ	1.75	0.50
11:k:16:VAL:HG23	11:k:36:ILE:HD13	1.93	0.50
13:M:293:THR:OG1	13:M:294:LYS:N	2.43	0.50
12:l:104:ALA:HA	12:l:112:ILE:O	2.11	0.50
1:A:206:LEU:O	1:A:210:ILE:HG12	2.10	0.50
7:G:44:ASP:O	7:G:217:CYS:HB2	2.12	0.50
7:G:176:LEU:HD22	7:G:181:PHE:HZ	1.75	0.50
10:j:56:LEU:HG	10:j:58:THR:HG22	1.94	0.50
2:B:37:LYS:HG2	2:B:42:VAL:HG22	1.93	0.50
13:M:309:ALA:HB2	13:M:336:LEU:HD13	1.92	0.50
5:e:268:GLN:OE1	5:e:278:GLN:NE2	2.45	0.50
1:A:53:ILE:HG21	1:A:58:MET:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:HG3	2:B:79:PRO:HB2	1.93	0.50
7:G:227:VAL:HG12	7:G:228:PRO:O	2.12	0.50
7:g:94:GLN:HA	7:g:97:GLU:OE1	2.11	0.50
7:g:104:ALA:HB2	8:h:135:ASN:ND2	2.26	0.50
9:i:80:ASP:CG	10:j:99:ARG:HH21	2.19	0.50
3:C:139:SER:OG	3:C:156:THR:O	2.26	0.50
7:G:206:ASP:OD1	7:G:206:ASP:N	2.42	0.50
11:K:16:VAL:HG23	11:K:36:ILE:HD13	1.93	0.50
12:L:265:ARG:HD3	11:k:155:ASP:OD1	2.11	0.50
2:b:31:THR:OG1	2:b:62:LYS:HE2	2.12	0.50
2:b:109:VAL:HG21	2:b:145:TYR:CD2	2.46	0.50
3:c:109:GLU:OE1	11:k:78:SER:OG	2.28	0.50
6:f:262:TYR:HB2	13:m:195:TYR:HE2	1.75	0.50
10:j:45:VAL:HG22	10:j:49:ILE:HB	1.93	0.50
2:B:31:THR:OG1	2:B:62:LYS:HE2	2.12	0.50
6:F:392:GLU:N	6:F:392:GLU:OE1	2.44	0.50
7:G:71:ASP:OD1	7:G:100:ARG:NH2	2.44	0.50
13:M:250:TYR:O	13:M:264:ARG:NH2	2.44	0.50
1:a:36:THR:HG22	1:a:49:THR:HB	1.94	0.50
3:c:229:ILE:O	9:i:246:ARG:NH1	2.45	0.50
7:g:44:ASP:O	7:g:217:CYS:HB2	2.12	0.50
7:G:94:GLN:HA	7:G:97:GLU:OE1	2.11	0.50
10:J:45:VAL:HG22	10:J:49:ILE:HB	1.93	0.50
2:b:68:GLU:O	2:b:215:ARG:HA	2.11	0.50
3:c:82:VAL:HG12	3:c:140:PHE:CE1	2.47	0.50
5:E:268:GLN:OE1	5:E:278:GLN:NE2	2.45	0.49
1:a:53:ILE:HG21	1:a:58:MET:HB3	1.94	0.49
4:d:227:VAL:O	4:d:230:GLU:HG3	2.12	0.49
2:b:101:GLU:OE2	10:j:80:ARG:NH2	2.41	0.49
2:B:13:PRO:HA	3:C:23:TYR:CE1	2.47	0.49
2:B:18:ILE:HD11	2:B:22:TYR:OH	2.12	0.49
2:B:188:THR:O	2:B:192:THR:HG22	2.13	0.49
3:C:82:VAL:HG12	3:C:140:PHE:CE1	2.47	0.49
8:H:138:GLN:NE2	14:N:58:MET:HE3	2.27	0.49
3:c:71:MET:HG3	3:c:81:SER:HB2	1.95	0.49
5:e:113:ASN:HB3	6:f:291:ARG:HB3	1.93	0.49
6:f:235:VAL:HG12	6:f:236:GLY:H	1.77	0.49
7:g:227:VAL:HG12	7:g:228:PRO:O	2.12	0.49
12:l:290:ASP:OD1	12:l:291:GLN:N	2.45	0.49
14:n:40:LEU:HA	14:n:46:ALA:HA	1.93	0.49
4:D:227:VAL:O	4:D:230:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:28:ILE:HD13	3:c:139:SER:HB2	1.93	0.49
14:n:24:LEU:HD21	14:n:53:TYR:CG	2.47	0.49
6:F:214:LYS:HG3	6:F:374:ASN:HA	1.93	0.49
6:F:361:ALA:HB2	6:F:370:LEU:HG	1.95	0.49
2:b:18:ILE:HD11	2:b:22:TYR:OH	2.12	0.49
2:b:37:LYS:HG2	2:b:42:VAL:HG22	1.93	0.49
6:f:214:LYS:HG3	6:f:374:ASN:HA	1.93	0.49
3:C:53:HIS:CG	3:C:54:PRO:HD2	2.48	0.49
2:b:188:THR:O	2:b:192:THR:HG22	2.13	0.49
2:b:215:ARG:NE	2:b:217:GLU:OE2	2.44	0.49
3:c:4:ARG:HH22	7:g:10:GLN:HB2	1.78	0.49
9:i:248:LEU:HD13	10:j:47:ASP:HB2	1.95	0.49
13:m:272:GLU:HB2	13:m:273:PRO:HD3	1.95	0.49
8:H:71:ASP:OD1	8:H:87:LYS:NZ	2.43	0.49
2:b:121:GLN:O	3:c:133:VAL:HG21	2.13	0.49
6:f:361:ALA:HB2	6:f:370:LEU:HG	1.95	0.49
3:C:64:LYS:HA	10:J:79:GLU:OE2	2.13	0.49
5:E:310:LEU:HA	5:E:314:ASN:HD22	1.78	0.49
10:J:58:THR:O	11:K:87:ARG:NH2	2.46	0.49
3:c:53:HIS:CG	3:c:54:PRO:HD2	2.48	0.49
6:f:392:GLU:OE1	6:f:392:GLU:N	2.44	0.49
1:A:36:THR:HG22	1:A:49:THR:HB	1.94	0.48
3:C:146:ASP:OD1	3:C:146:ASP:N	2.46	0.48
9:I:58:LYS:HZ3	13:m:311:ARG:NH2	2.11	0.48
10:J:56:LEU:HG	10:J:58:THR:HG22	1.94	0.48
7:G:104:ALA:HB2	8:H:135:ASN:HD22	1.78	0.48
7:G:215:TRP:HZ3	7:G:217:CYS:SG	2.36	0.48
13:M:259:PHE:HE2	13:M:261:TYR:CE2	2.31	0.48
2:B:41:GLY:HA2	2:B:142:TYR:CD1	2.49	0.48
3:C:71:MET:HG3	3:C:81:SER:HB2	1.95	0.48
2:b:116:TYR:OH	2:b:130:CYS:O	2.18	0.48
14:N:24:LEU:HD21	14:N:53:TYR:CG	2.47	0.48
6:f:222:SER:O	6:f:222:SER:OG	2.32	0.48
9:i:47:THR:OG1	9:i:201:GLN:HB2	2.14	0.48
9:i:64:HIS:HE1	9:i:81:THR:HG22	1.79	0.48
9:I:47:THR:OG1	9:I:201:GLN:HB2	2.14	0.48
9:I:57:ASP:HB2	10:J:131:CYS:SG	2.53	0.48
13:M:272:GLU:HB2	13:M:273:PRO:HD3	1.95	0.48
2:b:6:TYR:O	2:b:124:GLY:N	2.46	0.48
5:e:188:LEU:HD22	5:e:216:THR:HG23	1.95	0.48
6:f:262:TYR:HB2	13:m:195:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:102:SER:OG	8:h:105:ASP:OD1	2.28	0.48
14:N:148:GLN:HG3	14:N:149:ALA:N	2.28	0.48
5:e:151:GLU:HG2	5:e:306:MET:SD	2.54	0.48
1:A:102:TYR:O	9:I:107:GLU:HA	2.13	0.48
6:F:222:SER:O	6:F:222:SER:OG	2.32	0.48
7:G:150:VAL:O	7:G:157:VAL:HA	2.14	0.48
9:I:64:HIS:HE1	9:I:81:THR:HG22	1.79	0.48
9:I:196:PRO:HG2	9:I:197:TYR:CD2	2.48	0.48
5:e:310:LEU:HA	5:e:314:ASN:HD22	1.78	0.48
13:m:259:PHE:HE2	13:m:261:TYR:CE2	2.31	0.48
4:D:66:ASP:OD2	4:D:67:ALA:N	2.40	0.48
5:E:188:LEU:HD22	5:E:216:THR:HG23	1.95	0.48
8:H:229:ARG:HG2	8:H:242:THR:HG22	1.96	0.48
2:b:41:GLY:HA2	2:b:142:TYR:CD1	2.49	0.48
5:E:151:GLU:HG2	5:E:306:MET:SD	2.54	0.48
9:I:168:GLU:OE2	14:n:176:ARG:NE	2.47	0.48
11:K:40:ASP:OD1	11:K:69:ARG:NE	2.47	0.48
13:M:312:ASP:OD2	13:M:315:THR:OG1	2.31	0.48
1:a:48:VAL:HG12	1:a:221:VAL:HG13	1.96	0.48
4:d:119:THR:HG22	4:d:126:PRO:HB3	1.96	0.48
6:F:393:SER:O	6:F:396:LYS:HE3	2.14	0.48
13:M:303:ASN:ND2	9:i:229:GLN:HG3	2.29	0.48
4:d:66:ASP:OD2	4:d:67:ALA:N	2.40	0.48
7:g:54:HIS:HB2	7:g:208:LEU:HB3	1.96	0.48
7:g:150:VAL:O	7:g:157:VAL:HA	2.14	0.48
8:h:229:ARG:HG2	8:h:242:THR:HG22	1.96	0.48
2:B:6:TYR:O	2:B:124:GLY:N	2.46	0.47
6:f:208:VAL:HG23	6:f:307:PRO:HB2	1.96	0.47
1:A:8:LYS:HE2	1:A:20:TYR:CD2	2.49	0.47
5:E:231:LYS:HB3	5:E:231:LYS:HZ3	1.77	0.47
11:K:195:THR:HG22	11:K:196:LYS:H	1.79	0.47
12:L:186:THR:HG21	12:L:214:ASP:O	2.14	0.47
3:c:9:THR:HB	3:c:20:GLN:HG3	1.96	0.47
7:g:38:VAL:HG13	7:g:193:LEU:HD13	1.96	0.47
7:g:215:TRP:HZ3	7:g:217:CYS:SG	2.36	0.47
8:h:169:PRO:HG3	14:n:32:TRP:HH2	1.79	0.47
11:k:40:ASP:OD1	11:k:69:ARG:NE	2.47	0.47
2:B:78:GLY:N	2:B:79:PRO:HD2	2.30	0.47
3:C:229:ILE:O	9:I:246:ARG:NH1	2.48	0.47
4:D:119:THR:HG22	4:D:126:PRO:HB3	1.96	0.47
5:E:177:VAL:HG13	5:E:242:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:235:VAL:HG12	6:F:236:GLY:H	1.77	0.47
7:G:54:HIS:HB2	7:G:208:LEU:HB3	1.95	0.47
11:K:195:THR:HG22	11:K:196:LYS:N	2.30	0.47
4:d:8:THR:HG22	4:d:16:LEU:HD22	1.97	0.47
4:d:8:THR:HG23	4:d:18:GLN:HB2	1.96	0.47
9:i:196:PRO:HG2	9:i:197:TYR:CD2	2.48	0.47
10:j:117:GLY:HA2	10:j:192:LYS:HD3	1.96	0.47
14:n:148:GLN:HG3	14:n:149:ALA:N	2.28	0.47
6:F:208:VAL:HG23	6:F:307:PRO:HB2	1.96	0.47
9:I:236:GLY:H	10:J:165:GLU:CD	2.21	0.47
1:a:8:LYS:HE2	1:a:20:TYR:CD2	2.49	0.47
4:D:8:THR:HG22	4:D:16:LEU:HD22	1.97	0.47
5:E:172:SER:HB2	5:E:326:LYS:HE3	1.96	0.47
2:b:78:GLY:N	2:b:79:PRO:HD2	2.30	0.47
9:i:178:GLU:O	9:i:182:GLU:HG3	2.15	0.47
4:D:30:LEU:HB3	4:D:46:GLU:HB2	1.96	0.47
13:M:270:PHE:HZ	9:i:54:ILE:HG22	1.79	0.47
4:d:94:PHE:C	4:d:96:LEU:H	2.23	0.47
6:f:245:ASP:OD1	6:f:245:ASP:N	2.48	0.47
8:h:189:LEU:HD21	8:h:217:ALA:HB2	1.97	0.47
9:i:245:ILE:HG23	10:j:196:THR:OG1	2.14	0.47
12:l:135:GLU:O	12:l:135:GLU:HG2	2.14	0.47
3:C:9:THR:HB	3:C:20:GLN:HG3	1.96	0.47
5:E:199:HIS:CG	5:E:207:MET:HG3	2.50	0.47
6:F:279:GLU:OE2	7:G:90:SER:OG	2.26	0.47
12:L:212:TYR:OH	12:L:214:ASP:OD2	2.20	0.47
2:b:18:ILE:HD11	2:b:22:TYR:CZ	2.50	0.47
11:k:50:GLU:HB3	11:k:53:PRO:HD2	1.97	0.47
7:G:38:VAL:HG13	7:G:193:LEU:HD13	1.96	0.47
10:J:117:GLY:HA2	10:J:192:LYS:HD3	1.96	0.47
12:L:290:ASP:OD2	12:L:291:GLN:N	2.48	0.47
3:c:146:ASP:N	3:c:146:ASP:OD1	2.46	0.47
5:e:177:VAL:HG13	5:e:242:LEU:HB3	1.96	0.47
5:e:199:HIS:CG	5:e:207:MET:HG3	2.50	0.47
6:f:393:SER:O	6:f:396:LYS:HE3	2.14	0.47
2:B:96:LYS:HB3	2:B:96:LYS:HE3	1.71	0.47
4:D:8:THR:HG23	4:D:18:GLN:HB2	1.96	0.47
8:H:189:LEU:HD21	8:H:217:ALA:HB2	1.97	0.47
11:K:155:ASP:OD1	12:l:265:ARG:HD3	2.14	0.47
11:k:195:THR:HG22	11:k:196:LYS:H	1.80	0.47
12:l:226:SER:O	12:l:231:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:ARG:HD2	4:D:60:ARG:N	2.30	0.47
9:I:66:MET:HB2	9:I:70:ILE:O	2.15	0.47
9:I:178:GLU:O	9:I:182:GLU:HG3	2.15	0.47
11:K:1:MET:HE3	11:K:145:TYR:HE1	1.80	0.47
12:L:174:THR:HG23	12:L:177:ALA:H	1.80	0.47
5:e:252:GLN:HE21	5:e:264:ARG:NH1	2.13	0.47
7:g:71:ASP:OD1	7:g:100:ARG:NH2	2.44	0.47
12:l:102:THR:HG21	12:l:143:THR:HB	1.97	0.47
1:A:48:VAL:HG12	1:A:221:VAL:HG13	1.96	0.46
5:E:229:ARG:HG3	5:E:230:ARG:H	1.79	0.46
11:k:1:MET:HE3	11:k:145:TYR:HE1	1.80	0.46
4:D:173:GLU:HA	5:E:158:LEU:HD11	1.96	0.46
5:e:172:SER:HB2	5:e:326:LYS:HE3	1.96	0.46
5:e:229:ARG:HG3	5:e:230:ARG:H	1.79	0.46
9:i:66:MET:HB2	9:i:70:ILE:O	2.15	0.46
2:B:67:ASP:OD2	2:B:93:GLN:NE2	2.49	0.46
7:G:6:SER:OG	7:G:7:GLY:N	2.48	0.46
8:H:158:ASP:OD1	8:H:158:ASP:N	2.49	0.46
2:b:190:LEU:HD13	2:b:228:LEU:HD23	1.97	0.46
4:d:30:LEU:HB3	4:d:46:GLU:HB2	1.97	0.46
4:d:60:ARG:HD2	4:d:60:ARG:N	2.30	0.46
7:g:6:SER:OG	7:g:7:GLY:N	2.48	0.46
11:k:1:MET:HE3	11:k:145:TYR:CE1	2.50	0.46
14:n:67:ILE:HD11	14:n:84:VAL:HG21	1.98	0.46
2:B:18:ILE:HD11	2:B:22:TYR:CZ	2.50	0.46
4:D:94:PHE:C	4:D:96:LEU:H	2.23	0.46
4:D:193:LEU:O	4:D:196:VAL:HG12	2.15	0.46
4:d:193:LEU:O	4:d:196:VAL:HG12	2.15	0.46
2:B:190:LEU:HD13	2:B:228:LEU:HD23	1.97	0.46
11:K:50:GLU:HB3	11:K:53:PRO:HD2	1.97	0.46
12:L:135:GLU:O	12:L:135:GLU:HG2	2.14	0.46
13:M:281:ARG:HA	13:M:281:ARG:HD3	1.74	0.46
4:d:104:VAL:O	4:d:108:VAL:HG23	2.15	0.46
11:k:195:THR:HG22	11:k:196:LYS:N	2.30	0.46
12:L:215:ASP:OD1	12:L:216:LYS:HG3	2.15	0.46
1:A:76:CYS:SG	1:A:136:THR:HB	2.56	0.46
5:E:252:GLN:HE21	5:E:264:ARG:NH1	2.13	0.46
3:c:64:LYS:HA	10:j:79:GLU:OE2	2.16	0.46
9:i:43:LEU:HB2	9:i:205:CYS:SG	2.56	0.46
9:i:224:ARG:HH22	9:i:228:ARG:H	1.63	0.46
13:m:136:THR:HG22	13:m:180:ASN:ND2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:326:LYS:HE3	13:m:326:LYS:HB3	1.81	0.46
8:H:228:ILE:HD12	8:H:243:ILE:HD11	1.98	0.46
1:a:76:CYS:SG	1:a:136:THR:HB	2.56	0.46
6:f:379:ILE:HD12	6:f:389:PHE:HE2	1.80	0.46
8:h:158:ASP:OD1	8:h:158:ASP:N	2.49	0.46
4:D:104:VAL:O	4:D:108:VAL:HG23	2.15	0.46
11:K:1:MET:HE3	11:K:145:TYR:CE1	2.50	0.46
12:L:211:TYR:CE2	12:L:221:LYS:HB2	2.51	0.46
8:h:218:TYR:HE1	8:h:228:ILE:HG12	1.80	0.46
12:l:139:TYR:CD1	12:l:172:ARG:HD3	2.51	0.46
12:l:165:TRP:CD1	12:l:165:TRP:C	2.93	0.46
1:A:77:MET:SD	1:A:135:SER:OG	2.59	0.46
2:B:42:VAL:HG11	2:B:135:ALA:HB1	1.98	0.46
5:E:142:THR:OG1	5:E:145:GLY:O	2.30	0.46
6:F:317:ASP:OD1	7:G:83:PRO:HD3	2.15	0.46
12:L:102:THR:O	12:L:226:SER:HA	2.16	0.46
1:a:96:SER:O	1:a:100:TYR:N	2.44	0.46
1:a:129:ARG:HB2	7:g:13:ASP:HA	1.98	0.46
2:b:42:VAL:HG11	2:b:135:ALA:HB1	1.98	0.46
9:I:43:LEU:HB2	9:I:205:CYS:SG	2.56	0.45
9:I:226:TYR:HB3	13:m:306:THR:HG21	1.98	0.45
2:b:62:LYS:HB3	2:b:62:LYS:HE3	1.70	0.45
2:b:67:ASP:OD2	2:b:93:GLN:NE2	2.49	0.45
3:c:8:ARG:HD3	4:d:5:ARG:NH1	2.31	0.45
10:j:59:ASP:OD2	11:k:95:ARG:NH2	2.49	0.45
8:H:218:TYR:HE1	8:H:228:ILE:HG12	1.80	0.45
5:e:139:GLY:HA2	5:e:147:VAL:O	2.17	0.45
8:h:142:TYR:CE2	14:n:58:MET:HG3	2.51	0.45
2:B:194:LYS:NZ	2:B:231:ILE:HG13	2.32	0.45
3:C:14:PRO:HA	4:D:21:TYR:CE1	2.52	0.45
8:H:78:THR:HG22	8:H:78:THR:O	2.17	0.45
8:H:149:SER:O	8:H:149:SER:OG	2.34	0.45
9:I:224:ARG:HH22	9:I:228:ARG:H	1.63	0.45
2:b:101:GLU:CD	10:j:80:ARG:HH22	2.23	0.45
10:j:58:THR:O	11:k:87:ARG:NH2	2.49	0.45
4:D:31:ALA:HA	4:D:162:GLY:HA3	1.98	0.45
2:b:144:LEU:HD21	2:b:159:THR:HG22	1.99	0.45
14:n:148:GLN:HA	14:n:151:GLU:HG2	1.99	0.45
2:B:48:LYS:HD2	2:B:60:ILE:HG13	1.99	0.45
3:C:235:PRO:HG2	10:J:38:GLU:HG2	1.98	0.45
6:F:379:ILE:HD12	6:F:389:PHE:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:59:LEU:HD22	7:G:63:SER:OG	2.17	0.45
9:I:126:ALA:HB1	9:I:156:MET:HE3	1.99	0.45
11:K:91:ALA:O	11:K:94:ILE:HG12	2.16	0.45
13:M:311:ARG:NH1	9:i:56:ALA:O	2.50	0.45
4:d:99:GLU:O	4:d:99:GLU:HG2	2.17	0.45
5:e:142:THR:OG1	5:e:145:GLY:O	2.30	0.45
9:i:112:LEU:HD22	9:i:127:LEU:HD13	1.99	0.45
13:m:312:ASP:OD2	13:m:315:THR:OG1	2.31	0.45
12:L:226:SER:O	12:L:231:SER:HB2	2.16	0.45
14:N:148:GLN:HA	14:N:151:GLU:HG2	1.99	0.45
5:e:297:LEU:O	5:e:301:ILE:HG13	2.17	0.45
9:i:151:LEU:HD12	9:i:154:VAL:HG12	1.98	0.45
14:n:5:GLY:H	14:n:37:ARG:NH1	2.14	0.45
5:E:175:ALA:HB2	5:E:327:LEU:HD13	1.99	0.45
5:E:297:LEU:O	5:E:301:ILE:HG13	2.17	0.45
6:F:329:ARG:NH1	6:F:364:THR:O	2.44	0.45
9:I:39:ASP:N	9:I:39:ASP:OD1	2.50	0.45
9:I:176:THR:HG22	9:I:177:CYS:H	1.82	0.45
13:M:136:THR:HG22	13:M:180:ASN:ND2	2.26	0.45
2:b:96:LYS:HB3	2:b:96:LYS:HE3	1.71	0.45
4:d:31:ALA:HA	4:d:162:GLY:HA3	1.97	0.45
9:i:39:ASP:N	9:i:39:ASP:OD1	2.49	0.45
2:B:116:TYR:OH	2:B:130:CYS:O	2.18	0.45
8:H:144:ASN:O	8:H:148:ILE:HG12	2.17	0.45
14:N:5:GLY:H	14:N:37:ARG:NH1	2.14	0.45
14:N:67:ILE:HD11	14:N:84:VAL:HG21	1.97	0.45
2:b:48:LYS:HD2	2:b:60:ILE:HG13	1.99	0.45
4:D:99:GLU:O	4:D:99:GLU:HG2	2.17	0.45
9:I:112:LEU:HD22	9:I:127:LEU:HD13	1.99	0.45
12:L:165:TRP:CD1	12:L:165:TRP:C	2.94	0.45
2:b:137:VAL:HG22	2:b:142:TYR:CD1	2.52	0.45
2:b:194:LYS:NZ	2:b:231:ILE:HG13	2.32	0.45
2:b:222:ASP:OD1	2:b:223:GLN:N	2.50	0.45
4:d:236:GLU:O	4:d:240:LYS:HG3	2.17	0.45
7:g:59:LEU:HD22	7:g:63:SER:OG	2.17	0.45
13:m:182:MET:HE1	14:n:96:ARG:CZ	2.47	0.45
14:N:158:SER:OG	14:N:159:ARG:N	2.50	0.45
3:c:185:TRP:HA	3:c:189:MET:HE1	1.99	0.45
8:h:144:ASN:O	8:h:148:ILE:HG12	2.17	0.45
11:k:91:ALA:O	11:k:94:ILE:HG12	2.16	0.45
7:G:152:ASP:OD1	7:G:153:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:231:LYS:HB3	5:e:231:LYS:HZ2	1.82	0.44
8:h:78:THR:HG22	8:h:78:THR:O	2.17	0.44
10:j:2:SER:OG	10:j:3:ILE:N	2.50	0.44
2:B:222:ASP:OD1	2:B:223:GLN:N	2.50	0.44
3:C:214:ASP:OD1	3:C:214:ASP:N	2.46	0.44
8:H:68:LEU:O	8:H:230:THR:HA	2.17	0.44
10:J:2:SER:OG	10:J:3:ILE:N	2.50	0.44
10:J:205:ASP:OD2	12:l:118:ARG:NH2	2.51	0.44
14:N:64:GLU:O	14:N:68:GLU:HG2	2.18	0.44
2:b:18:ILE:O	2:b:18:ILE:HG13	2.16	0.44
3:c:121:CYS:HB3	3:c:160:GLY:O	2.17	0.44
6:f:375:THR:HB	6:f:398:LEU:HD11	1.99	0.44
9:i:126:ALA:HB1	9:i:156:MET:HE3	1.98	0.44
9:i:176:THR:HG22	9:i:177:CYS:H	1.82	0.44
12:l:211:TYR:CE2	12:l:221:LYS:HB2	2.52	0.44
14:n:166:LEU:HD23	14:n:166:LEU:HA	1.76	0.44
2:B:18:ILE:O	2:B:18:ILE:HG13	2.16	0.44
11:K:191:VAL:HG21	11:K:205:VAL:HG23	2.00	0.44
8:h:228:ILE:HD12	8:h:243:ILE:HD11	1.98	0.44
10:j:189:ILE:HG23	10:j:196:THR:HB	1.99	0.44
12:l:137:ASN:ND2	12:l:139:TYR:OH	2.50	0.44
2:B:137:VAL:HG22	2:B:142:TYR:CD1	2.52	0.44
2:B:182:LEU:CD1	2:B:212:VAL:HG12	2.47	0.44
4:D:236:GLU:O	4:D:240:LYS:HG3	2.17	0.44
5:E:139:GLY:HA2	5:E:147:VAL:O	2.17	0.44
9:I:229:GLN:HG3	13:m:303:ASN:ND2	2.33	0.44
6:f:317:ASP:OD1	7:g:83:PRO:HD3	2.18	0.44
7:g:152:ASP:OD1	7:g:153:PRO:HD2	2.17	0.44
13:m:215:ALA:O	13:m:250:TYR:OH	2.31	0.44
3:C:185:TRP:HA	3:C:189:MET:HE1	1.99	0.44
4:D:12:PRO:HA	5:E:126:TYR:CE1	2.52	0.44
4:D:170:GLU:OE1	4:D:170:GLU:HA	2.18	0.44
7:G:148:LEU:HD21	7:G:163:VAL:HG12	2.00	0.44
3:c:188:SER:O	3:c:188:SER:OG	2.31	0.44
8:H:244:PRO:HB3	14:n:206:TRP:HB2	2.00	0.44
9:I:151:LEU:HD12	9:I:154:VAL:HG12	1.98	0.44
14:N:89:HIS:NE2	14:N:125:GLY:O	2.51	0.44
5:e:335:ILE:HA	5:e:338:ILE:HD12	2.00	0.44
8:h:68:LEU:O	8:h:230:THR:HA	2.17	0.44
10:j:28:LEU:HB2	10:j:39:VAL:CG1	2.45	0.44
10:j:83:THR:OG1	10:j:84:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:HD21	2:B:159:THR:HG22	1.99	0.44
4:d:231:LYS:HA	4:d:234:GLU:CD	2.43	0.44
11:k:14:VAL:HG23	11:k:124:PRO:HB3	2.00	0.44
11:k:181:ARG:HA	11:k:181:ARG:HD3	1.72	0.44
5:E:146:VAL:HG11	5:E:244:ALA:HB1	2.00	0.44
7:G:171:VAL:HG23	7:G:200:VAL:HG23	2.00	0.44
11:K:14:VAL:HG23	11:K:124:PRO:HB3	2.00	0.44
5:e:175:ALA:HB2	5:e:327:LEU:HD13	1.99	0.44
6:f:298:LEU:HD23	6:f:298:LEU:HA	1.81	0.44
9:i:80:ASP:OD2	10:j:99:ARG:NH2	2.41	0.44
14:n:64:GLU:O	14:n:68:GLU:HG2	2.17	0.44
3:C:176:VAL:O	3:C:180:LEU:HG	2.18	0.44
5:E:280:VAL:HG11	5:E:301:ILE:HG12	1.99	0.44
6:F:245:ASP:OD1	6:F:245:ASP:N	2.48	0.44
7:G:124:THR:O	7:G:124:THR:OG1	2.36	0.44
10:J:28:LEU:HB2	10:J:39:VAL:CG1	2.44	0.44
11:K:6:ILE:HG23	11:K:142:CYS:SG	2.58	0.44
3:c:230:ASP:OD2	3:c:230:ASP:N	2.49	0.44
4:d:12:PRO:HA	5:e:126:TYR:CE1	2.53	0.44
5:e:280:VAL:HG11	5:e:301:ILE:HG12	1.99	0.44
3:C:4:ARG:HH12	7:G:10:GLN:HG3	1.83	0.43
7:G:215:TRP:HZ3	7:G:217:CYS:HG	1.58	0.43
10:J:155:ARG:O	10:J:158:MET:HG3	2.18	0.43
11:K:142:CYS:HB3	11:K:147:ALA:HA	1.99	0.43
12:L:139:TYR:CD1	12:L:172:ARG:HD3	2.53	0.43
10:j:164:PHE:CE1	10:j:200:ILE:HD11	2.53	0.43
11:k:6:ILE:HG23	11:k:142:CYS:SG	2.58	0.43
11:k:191:VAL:HG21	11:k:205:VAL:HG23	2.00	0.43
2:B:21:GLU:O	2:B:24:THR:HG22	2.18	0.43
2:B:147:VAL:HG12	2:B:148:ASP:H	1.83	0.43
6:F:375:THR:HB	6:F:398:LEU:HD11	1.99	0.43
12:L:137:ASN:ND2	12:L:139:TYR:OH	2.47	0.43
1:a:58:MET:HE3	1:a:58:MET:HB2	1.84	0.43
2:b:21:GLU:O	2:b:24:THR:HG22	2.18	0.43
2:b:182:LEU:CD1	2:b:212:VAL:HG12	2.48	0.43
5:e:237:PHE:O	5:e:258:PRO:HB3	2.19	0.43
14:n:143:LEU:HA	14:n:143:LEU:HD12	1.75	0.43
2:B:202:THR:HG22	2:B:205:ASN:HB2	2.00	0.43
1:a:196:LYS:HB2	1:a:196:LYS:HE2	1.81	0.43
4:d:64:LYS:HE2	4:d:67:ALA:HA	2.01	0.43
4:d:170:GLU:OE1	4:d:170:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:32:LEU:HD23	10:j:32:LEU:HA	1.86	0.43
10:j:155:ARG:O	10:j:158:MET:HG3	2.18	0.43
11:k:105:CYS:SG	11:k:129:MET:HB3	2.59	0.43
14:n:89:HIS:NE2	14:n:125:GLY:O	2.51	0.43
2:B:212:VAL:O	2:B:213:GLU:HG2	2.18	0.43
3:C:121:CYS:HB3	3:C:160:GLY:O	2.17	0.43
5:E:335:ILE:HA	5:E:338:ILE:HD12	2.00	0.43
13:M:215:ALA:O	13:M:250:TYR:OH	2.31	0.43
3:c:176:VAL:O	3:c:180:LEU:HG	2.18	0.43
14:n:158:SER:OG	14:n:159:ARG:N	2.50	0.43
10:J:83:THR:OG1	10:J:84:GLY:N	2.51	0.43
2:b:202:THR:HG22	2:b:205:ASN:HB2	2.00	0.43
3:c:14:PRO:HA	4:d:21:TYR:CE1	2.53	0.43
4:d:145:TRP:CE2	4:d:155:ALA:HB2	2.54	0.43
10:j:14:MET:HB3	10:j:163:LEU:HD11	2.01	0.43
4:D:64:LYS:HE2	4:D:67:ALA:HA	2.00	0.43
8:H:139:LYS:HE3	8:H:143:MET:HE3	2.01	0.43
10:J:14:MET:HB3	10:J:163:LEU:HD11	2.01	0.43
12:L:182:LEU:HD12	12:L:182:LEU:HA	1.87	0.43
1:a:195:GLN:HE22	1:a:223:ARG:NH1	2.14	0.43
8:h:59:ALA:HB2	8:h:68:LEU:HD23	2.01	0.43
8:h:117:LEU:CD1	8:h:128:VAL:HG11	2.48	0.43
1:A:195:GLN:HE22	1:A:223:ARG:NH1	2.14	0.43
4:D:182:ARG:HG3	4:D:210:GLN:NE2	2.34	0.43
6:F:268:MET:HE1	6:F:276:MET:SD	2.58	0.43
9:I:201:GLN:HG2	9:I:220:LYS:HG2	2.00	0.43
11:K:105:CYS:SG	11:K:129:MET:HB3	2.59	0.43
13:M:311:ARG:HA	9:i:55:VAL:HB	2.00	0.43
3:c:141:LEU:HD23	3:c:141:LEU:HA	1.89	0.43
5:e:146:VAL:HG11	5:e:244:ALA:HB1	2.00	0.43
7:g:171:VAL:HG23	7:g:200:VAL:HG23	2.00	0.43
9:i:96:ARG:HH21	9:i:103:SER:HB3	1.84	0.43
4:D:228:GLU:O	4:D:232:GLU:HG2	2.19	0.43
5:E:216:THR:HG21	5:E:241:LEU:HD12	2.01	0.43
5:E:237:PHE:O	5:E:258:PRO:HB3	2.18	0.43
11:K:166:GLU:HA	11:K:169:GLU:HG2	2.01	0.43
3:c:16:GLY:HA3	4:d:25:ALA:HB2	2.00	0.43
6:f:268:MET:HE1	6:f:276:MET:SD	2.58	0.43
7:g:148:LEU:HD21	7:g:163:VAL:HG12	2.00	0.43
9:i:97:LEU:HD23	9:i:97:LEU:HA	1.92	0.43
2:B:71:GLY:HA3	2:B:216:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:221:MET:HB3	13:M:221:MET:HE2	1.81	0.43
5:e:229:ARG:NH2	5:e:230:ARG:HB2	2.34	0.43
6:f:213:LEU:HB2	6:f:360:LEU:HD11	2.01	0.43
11:k:129:MET:HE3	11:k:129:MET:HB2	1.71	0.43
11:k:142:CYS:HB3	11:k:147:ALA:HA	1.99	0.43
4:D:231:LYS:HA	4:D:234:GLU:CD	2.43	0.43
5:E:199:HIS:HB2	5:E:207:MET:HE3	2.01	0.43
5:E:217:CYS:O	5:E:221:ILE:HG23	2.19	0.43
2:b:71:GLY:HA3	2:b:216:PHE:CZ	2.54	0.43
2:b:147:VAL:HG12	2:b:148:ASP:H	1.83	0.43
3:c:125:GLN:HG3	4:d:78:ALA:HB1	2.01	0.43
12:l:164:LEU:HD23	12:l:164:LEU:HA	1.81	0.43
1:A:187:SER:OG	1:A:188:THR:HG23	2.19	0.42
7:G:104:ALA:HB2	8:H:135:ASN:ND2	2.33	0.42
10:J:164:PHE:CE1	10:J:200:ILE:HD11	2.53	0.42
5:e:191:HIS:ND1	5:e:219:LEU:HD12	2.34	0.42
9:i:72:CYS:SG	9:i:127:LEU:HD22	2.60	0.42
1:A:62:SER:OG	1:A:63:VAL:N	2.51	0.42
5:E:229:ARG:NH2	5:E:230:ARG:HB2	2.34	0.42
1:a:15:PRO:HA	2:b:22:TYR:CD1	2.54	0.42
12:l:281:LYS:HE2	12:l:281:LYS:HB3	1.91	0.42
4:D:99:GLU:OE2	12:L:219:ARG:NH2	2.52	0.42
8:H:124:ILE:HG13	8:H:126:ALA:H	1.85	0.42
9:I:72:CYS:SG	9:I:127:LEU:HD22	2.59	0.42
9:I:105:VAL:HG23	9:I:133:ASP:OD2	2.19	0.42
10:J:189:ILE:HG23	10:J:196:THR:HB	2.00	0.42
11:K:146:GLY:O	11:K:150:VAL:HG22	2.19	0.42
12:L:118:ARG:NH2	10:j:205:ASP:OD2	2.52	0.42
4:d:156:TRP:HA	5:e:159:VAL:HA	2.01	0.42
8:h:85:SER:OG	8:h:86:ASN:N	2.52	0.42
9:i:46:ASP:OD2	9:i:62:LYS:NZ	2.51	0.42
12:l:139:TYR:HD2	12:l:140:LEU:HG	1.85	0.42
2:B:20:ILE:HD11	2:B:120:THR:OG1	2.20	0.42
6:F:320:ASP:HB3	7:G:63:SER:HB3	2.02	0.42
9:I:232:LEU:O	9:I:233:LEU:HD23	2.20	0.42
13:M:219:SER:HB2	13:M:250:TYR:HE2	1.85	0.42
1:a:62:SER:OG	1:a:63:VAL:N	2.51	0.42
2:b:212:VAL:O	2:b:213:GLU:HG2	2.18	0.42
9:i:232:LEU:O	9:i:233:LEU:HD23	2.20	0.42
11:k:38:GLN:NE2	11:k:199:VAL:HG21	2.35	0.42
11:k:146:GLY:O	11:k:150:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:204:ASP:OD1	12:l:206:PHE:N	2.49	0.42
5:E:283:GLU:CD	5:E:284:ARG:HB2	2.45	0.42
8:H:85:SER:OG	8:H:86:ASN:N	2.52	0.42
8:H:102:SER:OG	8:H:105:ASP:OD1	2.29	0.42
8:H:117:LEU:CD1	8:H:128:VAL:HG11	2.48	0.42
1:a:187:SER:OG	1:a:188:THR:HG23	2.20	0.42
4:d:42:VAL:HG12	4:d:208:VAL:HA	2.01	0.42
4:d:228:GLU:O	4:d:232:GLU:HG2	2.19	0.42
5:e:216:THR:HG21	5:e:241:LEU:HD12	2.01	0.42
6:f:177:TRP:H	7:g:23:GLN:HE22	1.67	0.42
7:g:197:LEU:HA	7:g:200:VAL:HG12	2.01	0.42
9:i:139:LEU:HD21	9:i:154:VAL:HG22	2.02	0.42
11:k:166:GLU:HA	11:k:169:GLU:HG2	2.01	0.42
13:m:323:ILE:HD12	13:m:330:GLN:HE21	1.84	0.42
4:D:145:TRP:CE2	4:D:155:ALA:HB2	2.54	0.42
5:E:191:HIS:ND1	5:E:219:LEU:HD12	2.34	0.42
6:F:347:CYS:HB3	6:F:351:GLU:HB2	2.02	0.42
8:H:59:ALA:HB2	8:H:68:LEU:HD23	2.01	0.42
9:I:200:THR:HG22	13:m:337:ARG:HH22	1.85	0.42
10:J:54:THR:HG21	10:J:140:GLY:HA2	2.02	0.42
12:L:139:TYR:HD2	12:L:140:LEU:HG	1.85	0.42
4:d:164:HIS:ND1	4:d:196:VAL:HG23	2.35	0.42
5:e:306:MET:HE2	5:e:306:MET:HB3	1.89	0.42
6:f:240:SER:HB2	6:f:326:MET:HE3	2.02	0.42
8:h:231:ILE:HG13	8:h:239:GLU:O	2.20	0.42
9:i:248:LEU:HG	10:j:194:LYS:HA	2.02	0.42
9:I:80:ASP:O	9:I:84:VAL:HG12	2.19	0.42
9:I:232:LEU:HD23	9:I:232:LEU:H	1.85	0.42
14:N:143:LEU:HD12	14:N:143:LEU:HA	1.74	0.42
5:e:225:GLU:OE2	6:f:289:GLY:HA2	2.19	0.42
8:h:139:LYS:HE3	8:h:143:MET:HE3	2.01	0.42
6:F:213:LEU:HB2	6:F:360:LEU:HD11	2.00	0.42
7:G:34:SER:OG	7:G:80:GLY:HA2	2.20	0.42
13:M:142:LYS:HD3	13:M:244:HIS:CD2	2.55	0.42
13:M:225:ARG:O	13:M:229:PRO:HA	2.20	0.42
2:b:82:ARG:HD2	2:b:82:ARG:HA	1.81	0.42
4:d:182:ARG:HG3	4:d:210:GLN:NE2	2.34	0.42
5:e:199:HIS:HB2	5:e:207:MET:HE3	2.01	0.42
9:i:66:MET:HE3	9:i:66:MET:HB3	1.92	0.42
9:i:201:GLN:HG2	9:i:220:LYS:HG2	2.00	0.42
5:E:201:PHE:HD1	12:L:156:ARG:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:240:SER:HB2	6:F:326:MET:HE3	2.02	0.42
9:I:96:ARG:HH21	9:I:103:SER:HB3	1.84	0.42
2:b:171:PHE:CZ	2:b:175:ARG:HG3	2.55	0.42
5:e:217:CYS:O	5:e:221:ILE:HG23	2.19	0.42
7:g:175:GLU:HG3	7:g:196:ILE:HG23	2.02	0.42
9:i:80:ASP:O	9:i:84:VAL:HG12	2.19	0.42
9:i:232:LEU:HD23	9:i:232:LEU:H	1.85	0.42
1:A:94:GLU:OE2	1:A:114:ARG:HD3	2.20	0.42
2:B:37:LYS:HE2	2:B:37:LYS:HB3	1.81	0.42
3:C:177:ALA:O	3:C:181:LEU:HD12	2.20	0.42
7:G:175:GLU:HG3	7:G:196:ILE:HG23	2.02	0.42
7:G:197:LEU:HA	7:G:200:VAL:HG12	2.01	0.42
8:H:105:ASP:OD2	8:H:148:ILE:HG22	2.19	0.42
11:K:38:GLN:NE2	11:K:199:VAL:HG21	2.35	0.42
14:N:208:TYR:HE2	8:h:83:ARG:HH22	1.66	0.42
1:a:94:GLU:OE2	1:a:114:ARG:HD3	2.20	0.42
2:b:165:SER:OG	2:b:166:PRO:HD3	2.20	0.42
3:c:116:LEU:HD12	3:c:119:ILE:HG22	2.02	0.42
7:g:84:ASP:HB3	7:g:132:PHE:HD1	1.85	0.42
9:i:105:VAL:HG23	9:i:133:ASP:OD2	2.19	0.42
12:l:102:THR:O	12:l:226:SER:HA	2.20	0.42
13:m:142:LYS:HD3	13:m:244:HIS:CD2	2.55	0.42
2:B:171:PHE:CZ	2:B:175:ARG:HG3	2.55	0.41
2:B:193:LEU:HD23	2:B:193:LEU:HA	1.83	0.41
5:E:184:ASP:O	5:E:187:ILE:HG22	2.20	0.41
8:H:92:THR:HG22	8:H:93:LYS:N	2.34	0.41
8:H:236:ASP:CG	8:H:237:GLU:H	2.28	0.41
11:K:5:ALA:O	11:K:142:CYS:HA	2.20	0.41
5:e:184:ASP:O	5:e:187:ILE:HG22	2.20	0.41
10:j:8:GLY:HA2	10:j:141:THR:HG21	2.02	0.41
11:k:154:LEU:HD23	11:k:154:LEU:HA	1.93	0.41
13:m:221:MET:HE2	13:m:221:MET:HB3	1.81	0.41
13:m:281:ARG:HD3	13:m:281:ARG:HA	1.75	0.41
1:A:196:LYS:HB2	1:A:196:LYS:HE2	1.81	0.41
2:B:165:SER:OG	2:B:166:PRO:HD3	2.20	0.41
3:C:33:THR:HA	3:C:170:ILE:O	2.20	0.41
7:G:192:LYS:O	7:G:196:ILE:HG12	2.20	0.41
10:J:87:PHE:O	10:J:91:ILE:HG23	2.20	0.41
10:J:149:MET:HE3	10:J:149:MET:HB3	1.89	0.41
2:b:49:LYS:HD3	2:b:49:LYS:HA	1.96	0.41
7:g:185:THR:HG22	7:g:187:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:160:PRO:HB3	10:j:189:ILE:HD11	2.02	0.41
3:C:64:LYS:H	3:C:64:LYS:HG2	1.56	0.41
3:C:116:LEU:HD12	3:C:119:ILE:HG22	2.02	0.41
7:G:97:GLU:HB2	14:N:69:ARG:NH2	2.35	0.41
9:I:139:LEU:HD21	9:I:154:VAL:HG22	2.02	0.41
1:a:50:GLN:NE2	1:a:210:ILE:HD13	2.33	0.41
1:a:113:LYS:HG3	2:b:82:ARG:HH21	1.85	0.41
2:b:20:ILE:HD11	2:b:120:THR:OG1	2.20	0.41
6:f:347:CYS:HB3	6:f:351:GLU:HB2	2.02	0.41
7:g:195:SER:O	7:g:199:GLU:HG3	2.20	0.41
8:h:94:LYS:HE3	8:h:238:PRO:HD3	2.03	0.41
11:k:5:ALA:O	11:k:142:CYS:HA	2.20	0.41
11:k:41:THR:HG23	11:k:42:HIS:ND1	2.35	0.41
11:k:179:LYS:HG2	11:k:186:ASN:O	2.21	0.41
7:G:195:SER:O	7:G:199:GLU:HG3	2.20	0.41
8:H:73:ARG:HD2	8:H:80:VAL:HG22	2.02	0.41
9:I:66:MET:HE3	9:I:66:MET:HB3	1.92	0.41
10:J:141:THR:HB	12:l:123:GLN:NE2	2.35	0.41
6:f:284:HIS:HA	6:f:290:LYS:HD3	2.02	0.41
9:i:236:GLY:H	10:j:165:GLU:CD	2.29	0.41
10:j:87:PHE:O	10:j:91:ILE:HG23	2.20	0.41
2:B:62:LYS:HB3	2:B:62:LYS:HE3	1.70	0.41
7:G:88:ILE:HD12	7:G:134:CYS:SG	2.61	0.41
7:G:185:THR:HG22	7:G:187:ASP:H	1.85	0.41
13:M:323:ILE:HD12	13:M:330:GLN:HE21	1.84	0.41
2:b:185:ALA:HA	2:b:188:THR:HG22	2.03	0.41
2:b:219:LEU:HD23	2:b:219:LEU:HA	1.81	0.41
7:g:98:ASN:O	7:g:102:ILE:N	2.48	0.41
7:g:192:LYS:O	7:g:196:ILE:HG12	2.20	0.41
8:h:105:ASP:OD2	8:h:148:ILE:HG22	2.19	0.41
13:m:225:ARG:O	13:m:229:PRO:HA	2.20	0.41
8:H:94:LYS:HE3	8:H:238:PRO:HD3	2.03	0.41
8:H:231:ILE:HG13	8:H:239:GLU:O	2.20	0.41
9:I:97:LEU:HD23	9:I:97:LEU:HA	1.92	0.41
9:I:200:THR:O	9:I:201:GLN:HG3	2.20	0.41
11:K:79:CYS:HB3	11:K:107:PHE:HE2	1.86	0.41
14:N:174:PHE:HE2	14:N:204:THR:HG21	1.86	0.41
3:c:177:ALA:O	3:c:181:LEU:HD12	2.20	0.41
8:h:73:ARG:HD2	8:h:80:VAL:HG22	2.02	0.41
8:h:113:VAL:O	8:h:117:LEU:HD23	2.21	0.41
8:h:124:ILE:HG13	8:h:126:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:142:TYR:CZ	14:n:58:MET:HG3	2.55	0.41
4:D:108:VAL:HG11	4:D:145:TRP:HB3	2.03	0.41
5:E:113:ASN:HB3	6:F:291:ARG:HB3	2.03	0.41
5:E:229:ARG:HH21	5:E:230:ARG:HB2	1.86	0.41
10:J:160:PRO:HB3	10:J:189:ILE:HD11	2.03	0.41
11:K:179:LYS:HG2	11:K:186:ASN:O	2.21	0.41
12:L:102:THR:HG22	12:L:199:MET:HE2	2.02	0.41
12:L:203:TRP:CE2	12:L:280:GLU:HB3	2.55	0.41
12:L:294:LEU:HD23	12:L:294:LEU:HA	1.81	0.41
1:a:77:MET:SD	1:a:135:SER:OG	2.59	0.41
5:e:283:GLU:CD	5:e:284:ARG:HB2	2.45	0.41
6:f:329:ARG:NH1	6:f:364:THR:O	2.44	0.41
9:i:69:ASN:ND2	9:i:132:VAL:O	2.50	0.41
9:i:200:THR:O	9:i:201:GLN:HG3	2.20	0.41
14:n:174:PHE:HE2	14:n:204:THR:HG21	1.86	0.41
1:A:96:SER:O	1:A:100:TYR:N	2.44	0.41
3:C:213:LEU:HD11	3:C:254:LEU:HB3	2.03	0.41
4:D:164:HIS:ND1	4:D:196:VAL:HG23	2.35	0.41
7:G:84:ASP:HB3	7:G:132:PHE:HD1	1.85	0.41
3:c:33:THR:HA	3:c:170:ILE:O	2.20	0.41
10:j:15:ALA:HB1	10:j:119:VAL:HG11	2.03	0.41
12:l:294:LEU:HD23	12:l:294:LEU:HA	1.83	0.41
13:m:257:GLU:HG2	13:m:257:GLU:O	2.21	0.41
2:B:211:VAL:HG23	2:B:215:ARG:O	2.21	0.41
4:D:170:GLU:OE1	4:D:173:GLU:HG2	2.21	0.41
4:D:222:LEU:HA	4:D:222:LEU:HD12	1.88	0.41
4:D:230:GLU:HA	4:D:233:ARG:NH1	2.36	0.41
6:F:262:TYR:HB2	13:M:195:TYR:CE2	2.55	0.41
6:F:298:LEU:HD23	6:F:298:LEU:HA	1.81	0.41
10:J:151:GLU:CD	13:m:311:ARG:HE	2.29	0.41
13:M:274:LEU:O	13:M:278:LEU:HG	2.21	0.41
2:b:4:ALA:O	2:b:124:GLY:HA3	2.21	0.41
6:f:239:ILE:HG22	6:f:297:LEU:HD22	2.03	0.41
10:j:54:THR:HG21	10:j:140:GLY:HA2	2.02	0.41
11:k:79:CYS:HB3	11:k:107:PHE:HE2	1.86	0.41
13:m:274:LEU:O	13:m:278:LEU:HG	2.21	0.41
2:B:185:ALA:HA	2:B:188:THR:HG22	2.03	0.41
3:C:223:LYS:HA	3:C:244:PRO:HA	2.02	0.41
5:E:151:GLU:N	5:E:151:GLU:OE1	2.54	0.41
4:d:170:GLU:OE1	4:d:173:GLU:HG2	2.21	0.41
4:d:222:LEU:HD12	4:d:222:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:377:ILE:O	6:f:389:PHE:HB2	2.21	0.41
10:j:124:THR:HG22	10:j:130:PRO:HA	2.03	0.41
6:F:284:HIS:HA	6:F:290:LYS:HD3	2.01	0.40
8:H:91:LEU:HD11	8:H:137:PHE:HE2	1.86	0.40
10:J:8:GLY:HA2	10:J:141:THR:HG21	2.02	0.40
14:N:148:GLN:O	14:N:152:LYS:HG3	2.22	0.40
2:b:37:LYS:HB3	2:b:37:LYS:HE2	1.81	0.40
3:c:213:LEU:HD11	3:c:254:LEU:HB3	2.03	0.40
3:c:223:LYS:HA	3:c:244:PRO:HA	2.02	0.40
4:d:52:LYS:HA	4:d:52:LYS:HD3	1.91	0.40
6:f:398:LEU:HD23	6:f:398:LEU:HA	1.94	0.40
4:D:79:ASP:O	4:D:82:VAL:HG12	2.22	0.40
4:D:140:GLY:H	4:D:211:TYR:HE1	1.69	0.40
11:K:41:THR:HG23	11:K:42:HIS:ND1	2.35	0.40
13:M:144:PHE:HA	13:M:324:ILE:O	2.21	0.40
4:d:108:VAL:HG11	4:d:145:TRP:HB3	2.03	0.40
4:d:211:TYR:CE2	4:d:212:LYS:HD3	2.56	0.40
5:e:187:ILE:HA	5:e:187:ILE:HD12	1.84	0.40
7:g:36:THR:HA	7:g:166:GLY:HA3	2.04	0.40
1:A:50:GLN:NE2	1:A:210:ILE:HG21	2.36	0.40
4:D:42:VAL:HG12	4:D:208:VAL:HA	2.01	0.40
5:E:118:GLU:OE2	5:E:118:GLU:HA	2.22	0.40
9:I:69:ASN:ND2	9:I:132:VAL:O	2.50	0.40
14:N:174:PHE:CE2	14:N:204:THR:HG21	2.57	0.40
5:e:110:ARG:HH21	5:e:126:TYR:HE2	1.70	0.40
8:h:236:ASP:CG	8:h:237:GLU:H	2.28	0.40
13:m:219:SER:HB2	13:m:250:TYR:HE2	1.85	0.40
3:C:157:GLU:C	3:C:159:SER:H	2.30	0.40
3:C:221:MET:HE3	3:C:244:PRO:HB2	2.04	0.40
5:E:306:MET:HG2	5:E:308:ASP:H	1.87	0.40
8:H:113:VAL:O	8:H:117:LEU:HD23	2.21	0.40
1:a:50:GLN:NE2	1:a:210:ILE:HG21	2.37	0.40
4:d:99:GLU:OE2	12:l:219:ARG:NH2	2.55	0.40
7:g:71:ASP:CG	7:g:72:ARG:H	2.29	0.40
1:A:216:ALA:HB2	1:A:240:GLU:HG2	2.03	0.40
3:C:89:ALA:HB2	3:C:138:VAL:HG21	2.04	0.40
3:C:125:GLN:HG3	4:D:78:ALA:HB1	2.03	0.40
5:E:110:ARG:HH21	5:E:126:TYR:HE2	1.70	0.40
1:a:31:TYR:HB3	1:a:32:PRO:HD3	2.03	0.40
7:g:88:ILE:HD12	7:g:134:CYS:SG	2.61	0.40
12:l:276:TYR:CE2	12:l:285:LYS:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	243/250 (97%)	228 (94%)	15 (6%)	0	100	100
1	a	243/250 (97%)	228 (94%)	15 (6%)	0	100	100
2	B	227/231 (98%)	212 (93%)	15 (7%)	0	100	100
2	b	227/231 (98%)	212 (93%)	15 (7%)	0	100	100
3	C	270/285 (95%)	251 (93%)	19 (7%)	0	100	100
3	c	270/285 (95%)	251 (93%)	19 (7%)	0	100	100
4	D	238/248 (96%)	221 (93%)	17 (7%)	0	100	100
4	d	238/248 (96%)	221 (93%)	17 (7%)	0	100	100
5	E	233/344 (68%)	220 (94%)	13 (6%)	0	100	100
5	e	233/344 (68%)	220 (94%)	13 (6%)	0	100	100
6	F	236/428 (55%)	220 (93%)	16 (7%)	0	100	100
6	f	236/428 (55%)	220 (93%)	16 (7%)	0	100	100
7	G	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
7	g	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
8	H	227/283 (80%)	215 (95%)	12 (5%)	0	100	100
8	h	227/283 (80%)	215 (95%)	12 (5%)	0	100	100
9	I	217/254 (85%)	203 (94%)	14 (6%)	0	100	100
9	i	217/254 (85%)	203 (94%)	14 (6%)	0	100	100
10	J	202/205 (98%)	184 (91%)	18 (9%)	0	100	100
10	j	202/205 (98%)	184 (91%)	18 (9%)	0	100	100
11	K	204/206 (99%)	195 (96%)	8 (4%)	1 (0%)	24	54
11	k	204/206 (99%)	196 (96%)	7 (3%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	200/302 (66%)	194 (97%)	6 (3%)	0	100	100
12	l	200/302 (66%)	196 (98%)	4 (2%)	0	100	100
13	M	212/339 (62%)	203 (96%)	9 (4%)	0	100	100
13	m	212/339 (62%)	203 (96%)	9 (4%)	0	100	100
14	N	216/220 (98%)	200 (93%)	16 (7%)	0	100	100
14	n	216/220 (98%)	200 (93%)	16 (7%)	0	100	100
All	All	6306/7666 (82%)	5935 (94%)	369 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	26	TYR
11	k	26	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/197 (98%)	189 (98%)	4 (2%)	47	64
1	a	193/197 (98%)	189 (98%)	4 (2%)	47	64
2	B	188/190 (99%)	185 (98%)	3 (2%)	55	68
2	b	188/190 (99%)	185 (98%)	3 (2%)	55	68
3	C	229/241 (95%)	228 (100%)	1 (0%)	84	83
3	c	229/241 (95%)	228 (100%)	1 (0%)	84	83
4	D	201/208 (97%)	198 (98%)	3 (2%)	57	69
4	d	201/208 (97%)	198 (98%)	3 (2%)	57	69
5	E	197/301 (65%)	194 (98%)	3 (2%)	57	69
5	e	197/301 (65%)	194 (98%)	3 (2%)	57	69
6	F	200/363 (55%)	199 (100%)	1 (0%)	81	81
6	f	200/363 (55%)	199 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	185/190 (97%)	184 (100%)	1 (0%)	81	81
7	g	185/190 (97%)	184 (100%)	1 (0%)	81	81
8	H	184/229 (80%)	183 (100%)	1 (0%)	81	81
8	h	184/229 (80%)	183 (100%)	1 (0%)	81	81
9	I	180/209 (86%)	176 (98%)	4 (2%)	45	63
9	i	180/209 (86%)	176 (98%)	4 (2%)	45	63
10	J	167/168 (99%)	167 (100%)	0	100	100
10	j	167/168 (99%)	167 (100%)	0	100	100
11	K	172/172 (100%)	172 (100%)	0	100	100
11	k	172/172 (100%)	172 (100%)	0	100	100
12	L	162/253 (64%)	162 (100%)	0	100	100
12	l	162/253 (64%)	162 (100%)	0	100	100
13	M	181/288 (63%)	181 (100%)	0	100	100
13	m	181/288 (63%)	181 (100%)	0	100	100
14	N	181/183 (99%)	180 (99%)	1 (1%)	78	80
14	n	181/183 (99%)	180 (99%)	1 (1%)	78	80
All	All	5240/6384 (82%)	5196 (99%)	44 (1%)	70	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	29	VAL
1	A	97	ASP
1	A	156	VAL
2	B	14	SER
2	B	18	ILE
2	B	25	THR
3	C	181	LEU
4	D	58	THR
4	D	105	ASP
4	D	170	GLU
5	E	118	GLU
5	E	231	LYS
5	E	233	MET
6	F	245	ASP

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Mol	Chain	Res	Type
7	G	174	SER
8	H	149	SER
9	I	51	GLU
9	I	54	ILE
9	I	103	SER
9	I	237	THR
14	N	35	ILE
1	a	16	GLU
1	a	29	VAL
1	a	97	ASP
1	a	156	VAL
2	b	14	SER
2	b	18	ILE
2	b	25	THR
3	c	181	LEU
4	d	58	THR
4	d	105	ASP
4	d	170	GLU
5	e	118	GLU
5	e	231	LYS
5	e	233	MET
6	f	245	ASP
7	g	174	SER
8	h	149	SER
9	i	51	GLU
9	i	54	ILE
9	i	103	SER
9	i	237	THR
14	n	35	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	50	GLN
1	A	99	GLN
1	A	142	GLN
1	A	195	GLN
1	A	207	GLN
1	A	228	ASN
2	B	107	GLN
2	B	143	HIS

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Mol	Chain	Res	Type
2	B	223	GLN
3	C	103	HIS
3	C	186	HIS
3	C	231	GLN
3	C	239	HIS
3	C	257	HIS
4	D	18	GLN
5	E	252	GLN
5	E	314	ASN
6	F	190	ASN
6	F	195	ASN
6	F	225	GLN
6	F	259	ASN
6	F	284	HIS
6	F	331	GLN
6	F	355	HIS
7	G	147	GLN
7	G	201	HIS
8	H	63	ASN
8	H	107	GLN
8	H	264	GLN
8	H	266	GLN
9	I	64	HIS
9	I	86	ASN
9	I	115	HIS
9	I	174	ASN
10	J	26	ASN
10	J	46	ASN
10	J	61	GLN
10	J	169	GLN
11	K	38	GLN
11	K	72	GLN
11	K	104	ASN
11	K	136	GLN
12	L	279	HIS
13	M	180	ASN
13	M	280	ASN
13	M	282	GLN
14	N	62	GLN
14	N	66	ASN
14	N	205	HIS
1	a	21	GLN

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Mol	Chain	Res	Type
1	a	50	GLN
1	a	99	GLN
1	a	142	GLN
1	a	195	GLN
1	a	207	GLN
1	a	228	ASN
2	b	107	GLN
2	b	143	HIS
2	b	223	GLN
3	c	103	HIS
3	c	231	GLN
3	c	239	HIS
3	c	257	HIS
4	d	18	GLN
5	e	252	GLN
6	f	190	ASN
6	f	195	ASN
6	f	225	GLN
6	f	259	ASN
6	f	271	ASN
6	f	284	HIS
6	f	331	GLN
6	f	355	HIS
7	g	147	GLN
8	h	63	ASN
8	h	107	GLN
8	h	264	GLN
8	h	266	GLN
9	i	64	HIS
9	i	86	ASN
9	i	115	HIS
9	i	174	ASN
9	i	194	ASN
10	j	26	ASN
10	j	46	ASN
10	j	61	GLN
10	j	169	GLN
11	k	38	GLN
11	k	72	GLN
11	k	104	ASN
11	k	136	GLN
12	l	169	ASN

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Mol	Chain	Res	Type
12	l	222	GLN
12	l	279	HIS
13	m	180	ASN
13	m	280	ASN
13	m	282	GLN
14	n	62	GLN
14	n	66	ASN
14	n	205	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	N2E	L	401	-	35,37,37	2.22	11 (31%)	45,54,54	4.54	18 (40%)
15	N2E	l	401	-	35,37,37	2.23	11 (31%)	45,54,54	4.54	18 (40%)

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	N2E	L	401	-	-	2/14/16/16	0/5/5/5
15	N2E	l	401	-	-	2/14/16/16	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	l	401	N2E	C7-N6	-5.66	1.24	1.33
15	L	401	N2E	C7-N3	-5.63	1.29	1.38
15	L	401	N2E	C7-N6	-5.62	1.24	1.33
15	l	401	N2E	C7-N3	-5.59	1.29	1.38
15	l	401	N2E	C7-N8	4.99	1.43	1.35
15	L	401	N2E	C7-N8	4.96	1.43	1.35
15	L	401	N2E	C5-N4	-4.12	1.27	1.33
15	l	401	N2E	C5-N4	-4.07	1.28	1.33
15	l	401	N2E	C2-N3	-3.49	1.30	1.36
15	L	401	N2E	C2-N3	-3.47	1.30	1.36
15	L	401	N2E	C9-N8	-3.05	1.26	1.32
15	l	401	N2E	C9-N8	-3.03	1.26	1.32
15	l	401	N2E	C23-N22	-2.84	1.25	1.29
15	L	401	N2E	C23-N22	-2.76	1.25	1.29
15	l	401	N2E	O24-C23	-2.71	1.34	1.37
15	L	401	N2E	O24-C23	-2.70	1.34	1.37
15	l	401	N2E	C27-C1	2.69	1.51	1.48
15	L	401	N2E	C27-C1	2.68	1.50	1.48
15	l	401	N2E	C5-N6	2.61	1.42	1.37
15	L	401	N2E	C5-N6	2.61	1.42	1.37
15	l	401	N2E	C21-N22	2.34	1.42	1.38
15	L	401	N2E	C21-N22	2.26	1.42	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	401	N2E	C5-N4-N3	16.98	111.67	101.98
15	l	401	N2E	C5-N4-N3	16.93	111.65	101.98
15	l	401	N2E	C7-N3-N4	-12.06	104.98	110.04
15	L	401	N2E	C7-N3-N4	-11.99	105.01	110.04
15	L	401	N2E	N4-C5-N6	-11.88	102.93	114.71
15	l	401	N2E	N4-C5-N6	-11.87	102.94	114.71
15	l	401	N2E	C7-N6-C5	9.58	108.46	103.10
15	L	401	N2E	C7-N6-C5	9.57	108.45	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	l	401	N2E	C1-C9-N8	-9.52	116.74	125.38
15	L	401	N2E	C1-C9-N8	-9.49	116.77	125.38
15	L	401	N2E	C2-N3-N4	6.17	133.38	125.20
15	l	401	N2E	C2-N3-N4	6.16	133.38	125.20
15	L	401	N2E	O24-C23-N22	-4.40	109.60	114.87
15	l	401	N2E	O24-C23-N22	-4.34	109.67	114.87
15	l	401	N2E	C9-N8-C7	3.54	119.98	115.60
15	L	401	N2E	C9-N8-C7	3.50	119.93	115.60
15	L	401	N2E	C26-C21-N22	3.40	126.14	119.32
15	l	401	N2E	C26-C21-N22	3.39	126.12	119.32
15	L	401	N2E	C10-C5-N4	3.37	129.97	123.64
15	l	401	N2E	C10-C5-N4	3.35	129.94	123.64
15	l	401	N2E	C14-C15-C10	-3.20	119.62	123.07
15	L	401	N2E	C14-C15-C10	-3.19	119.63	123.07
15	L	401	N2E	C29-N28-C27	2.92	122.49	116.80
15	l	401	N2E	C29-N28-C27	2.89	122.43	116.80
15	l	401	N2E	C11-C10-C15	2.76	120.25	116.83
15	L	401	N2E	C11-C10-C15	2.72	120.21	116.83
15	L	401	N2E	C32-C27-N28	-2.67	120.46	123.12
15	l	401	N2E	C32-C27-N28	-2.65	120.48	123.12
15	l	401	N2E	N3-C7-N6	2.38	111.97	109.74
15	L	401	N2E	N3-C7-N6	2.34	111.93	109.74
15	l	401	N2E	C10-C5-N6	2.30	127.11	122.08
15	L	401	N2E	C10-C5-N6	2.29	127.09	122.08
15	L	401	N2E	C30-C29-N28	-2.29	119.80	123.42
15	l	401	N2E	C30-C29-N28	-2.27	119.82	123.42
15	l	401	N2E	O20-C18-C19	-2.17	118.50	121.51
15	L	401	N2E	O20-C18-C19	-2.11	118.58	121.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

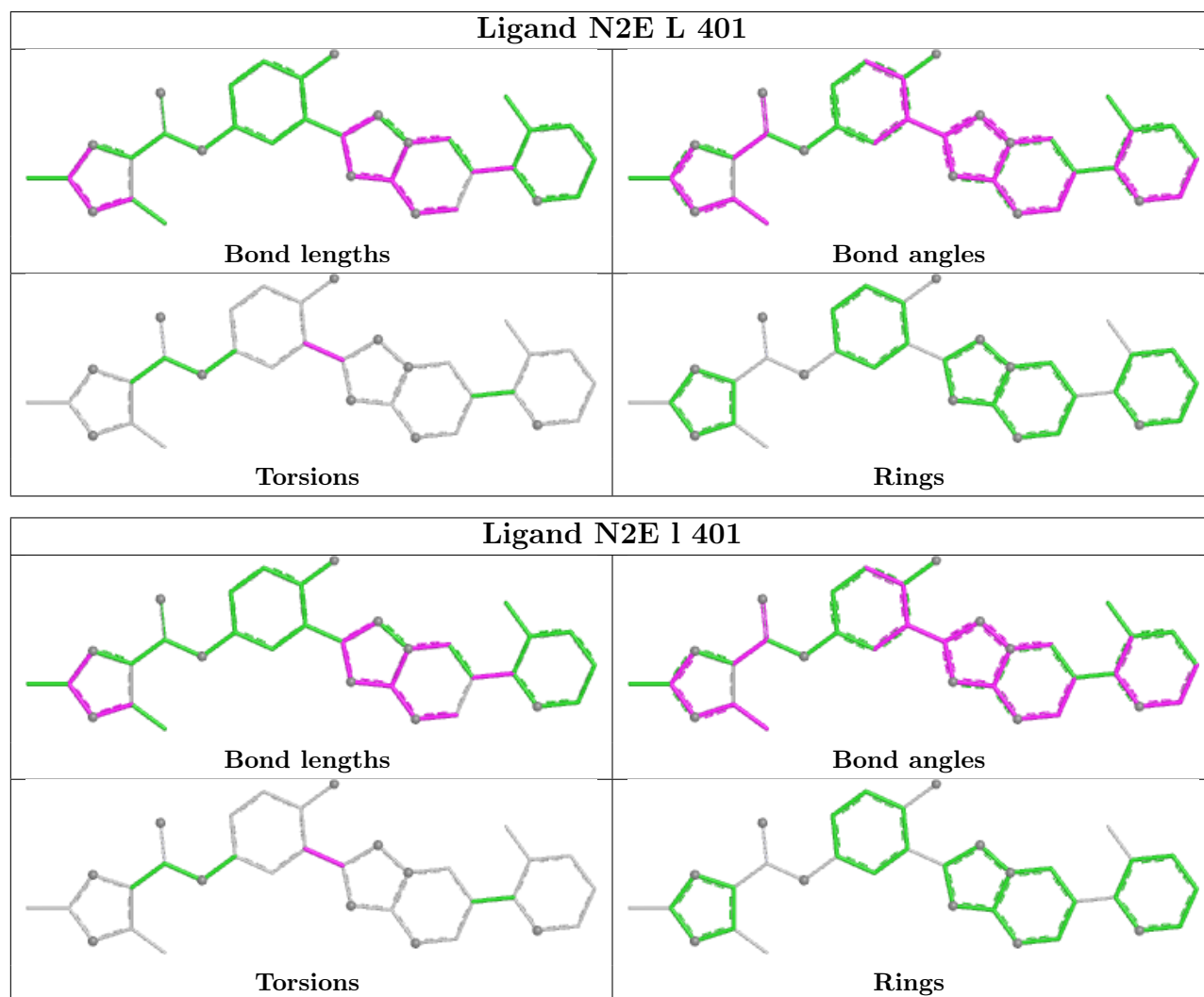
Mol	Chain	Res	Type	Atoms
15	L	401	N2E	C15-C10-C5-N6
15	l	401	N2E	C15-C10-C5-N6
15	L	401	N2E	C11-C10-C5-N6
15	l	401	N2E	C11-C10-C5-N6

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

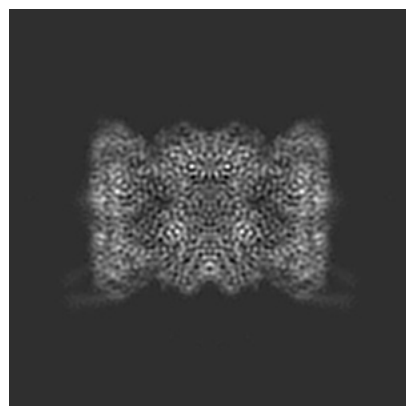
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10462. These allow visual inspection of the internal detail of the map and identification of artifacts.

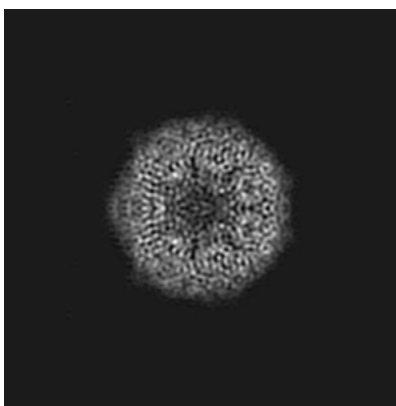
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

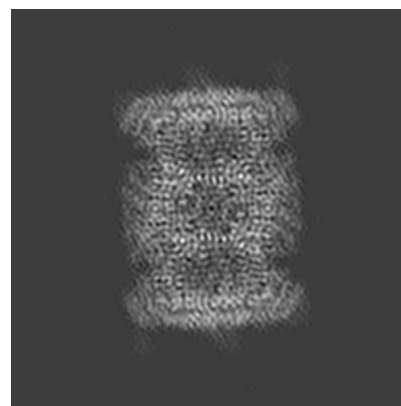
6.1.1 Primary map



X

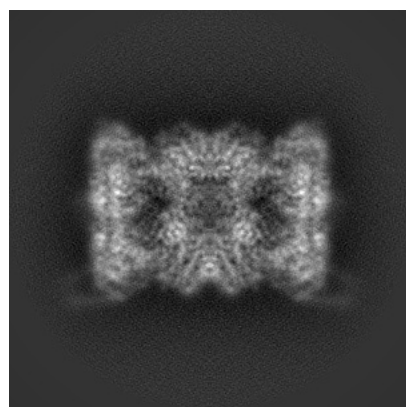


Y

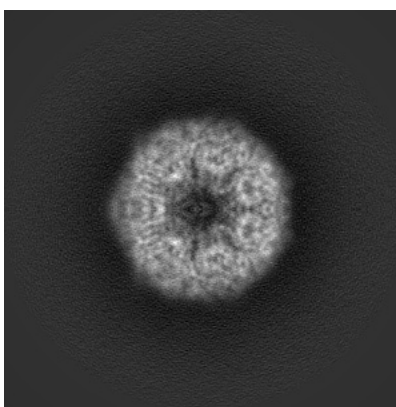


Z

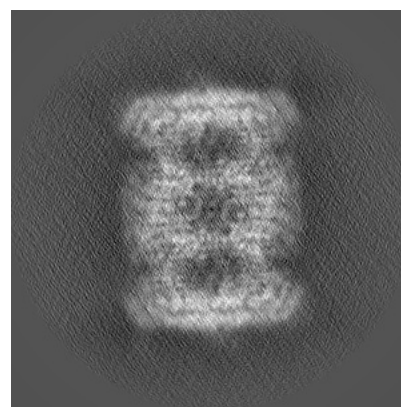
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

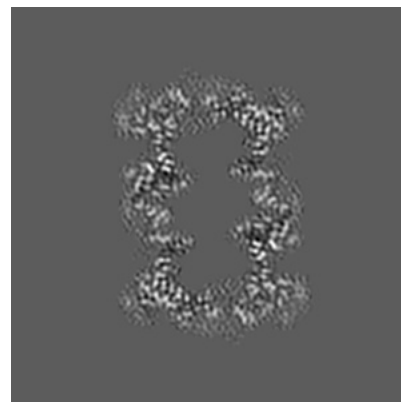
6.2.1 Primary map



X Index: 150

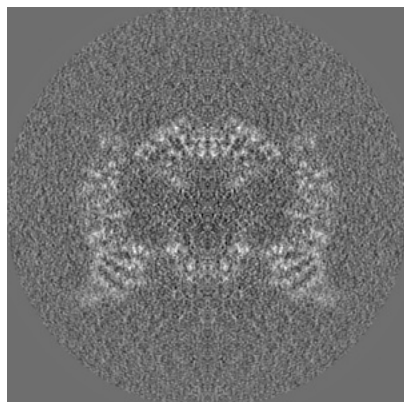


Y Index: 150

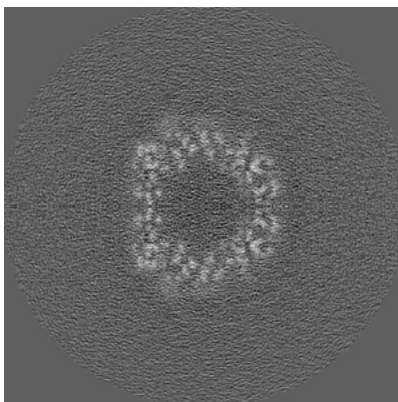


Z Index: 150

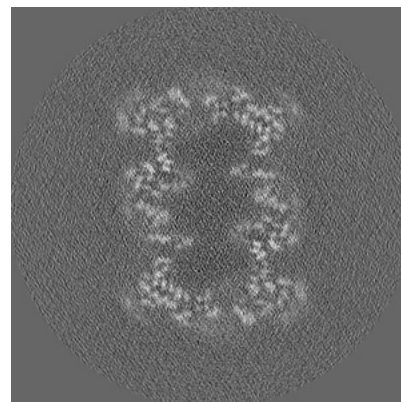
6.2.2 Raw map



X Index: 150



Y Index: 150

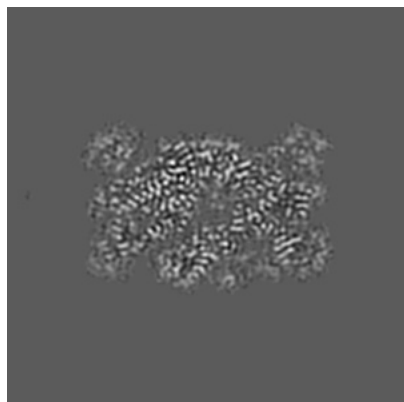


Z Index: 150

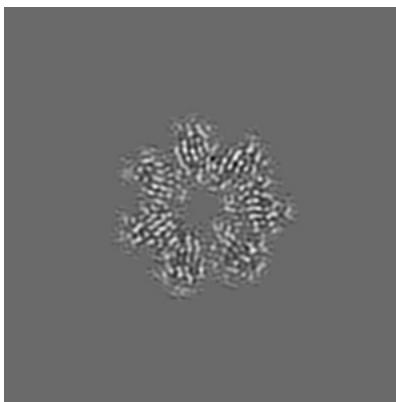
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

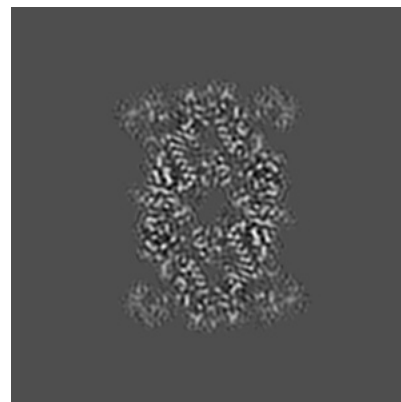
6.3.1 Primary map



X Index: 183

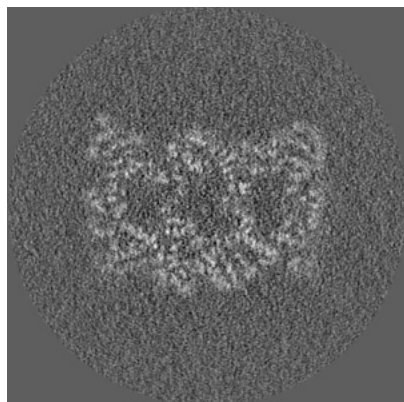


Y Index: 129

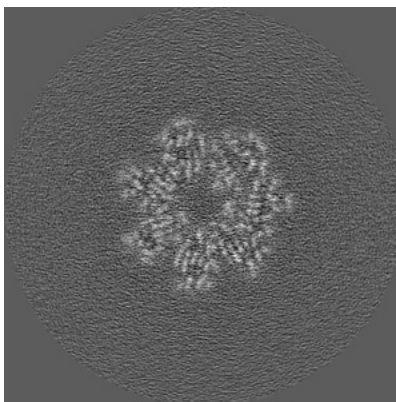


Z Index: 177

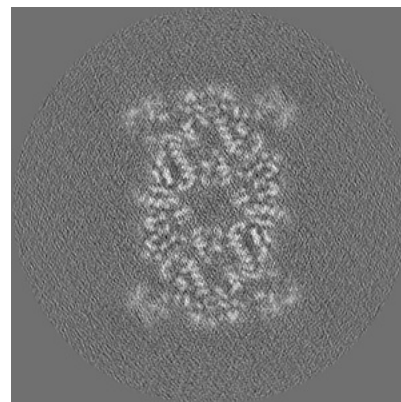
6.3.2 Raw map



X Index: 127



Y Index: 171

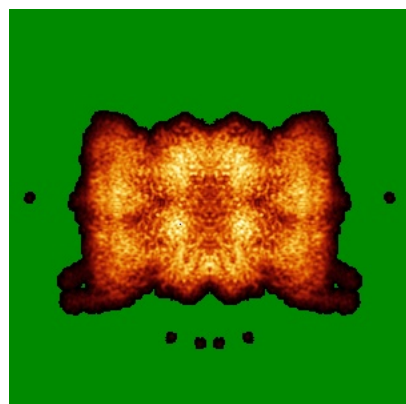


Z Index: 177

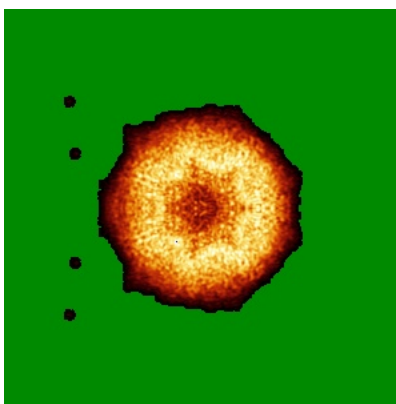
The images above show the largest variance slices of the map in three orthogonal directions.

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

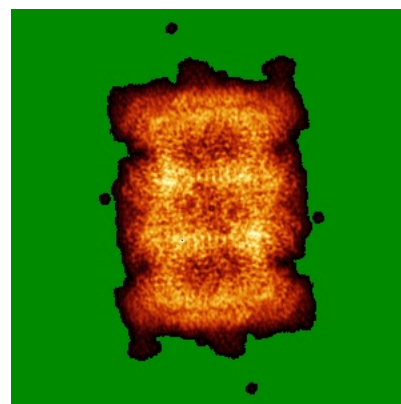
6.4.1 Primary map



X

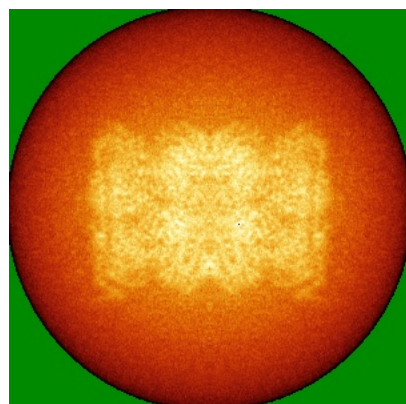


Y

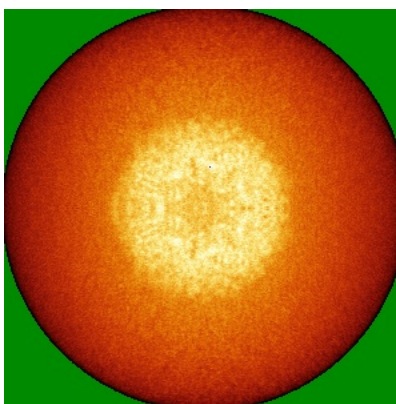


Z

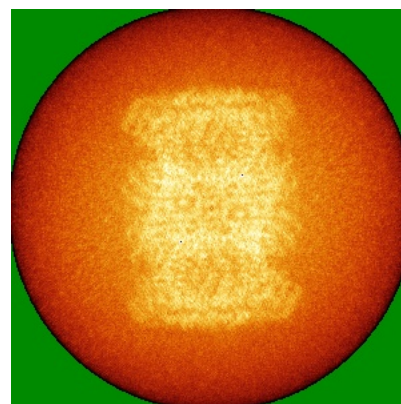
6.4.2 Raw map



X



Y

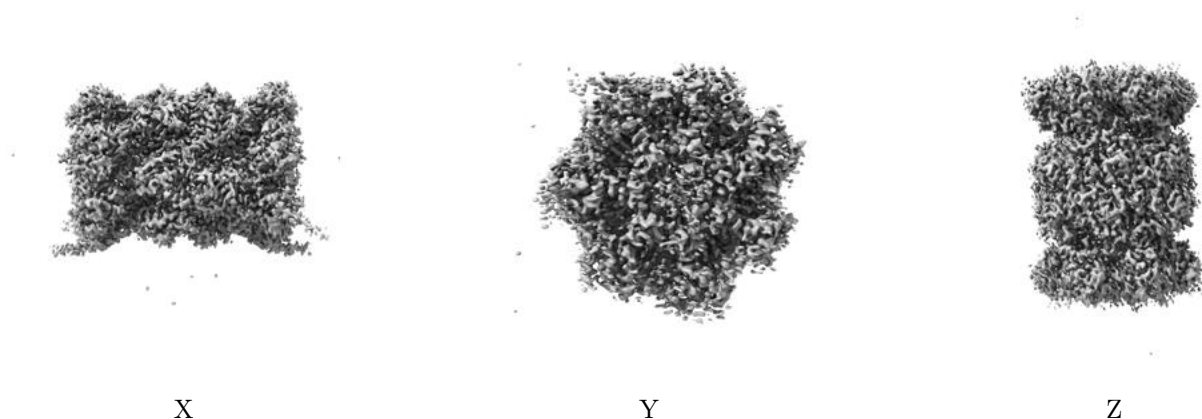


Z

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.

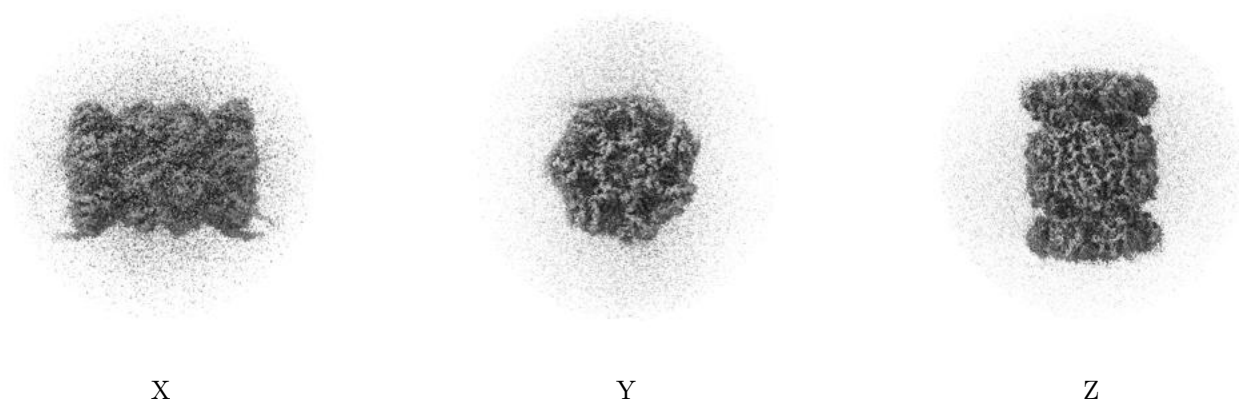
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0154. 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



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.

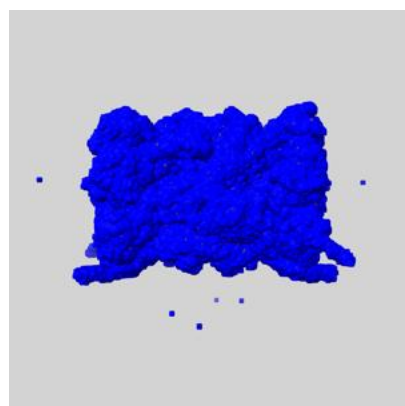
6.6 Mask visualisation [i](#)

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

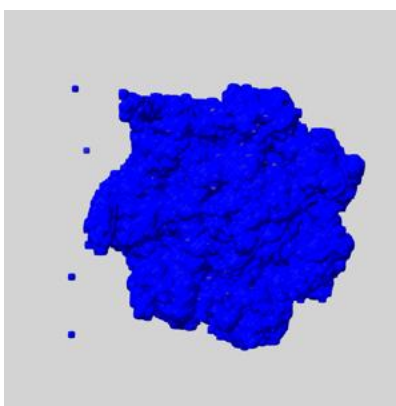
A mask typically either:

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

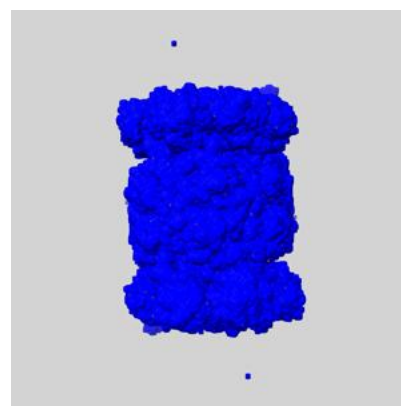
6.6.1 emd_10462_msk_1.map [i](#)



X



Y

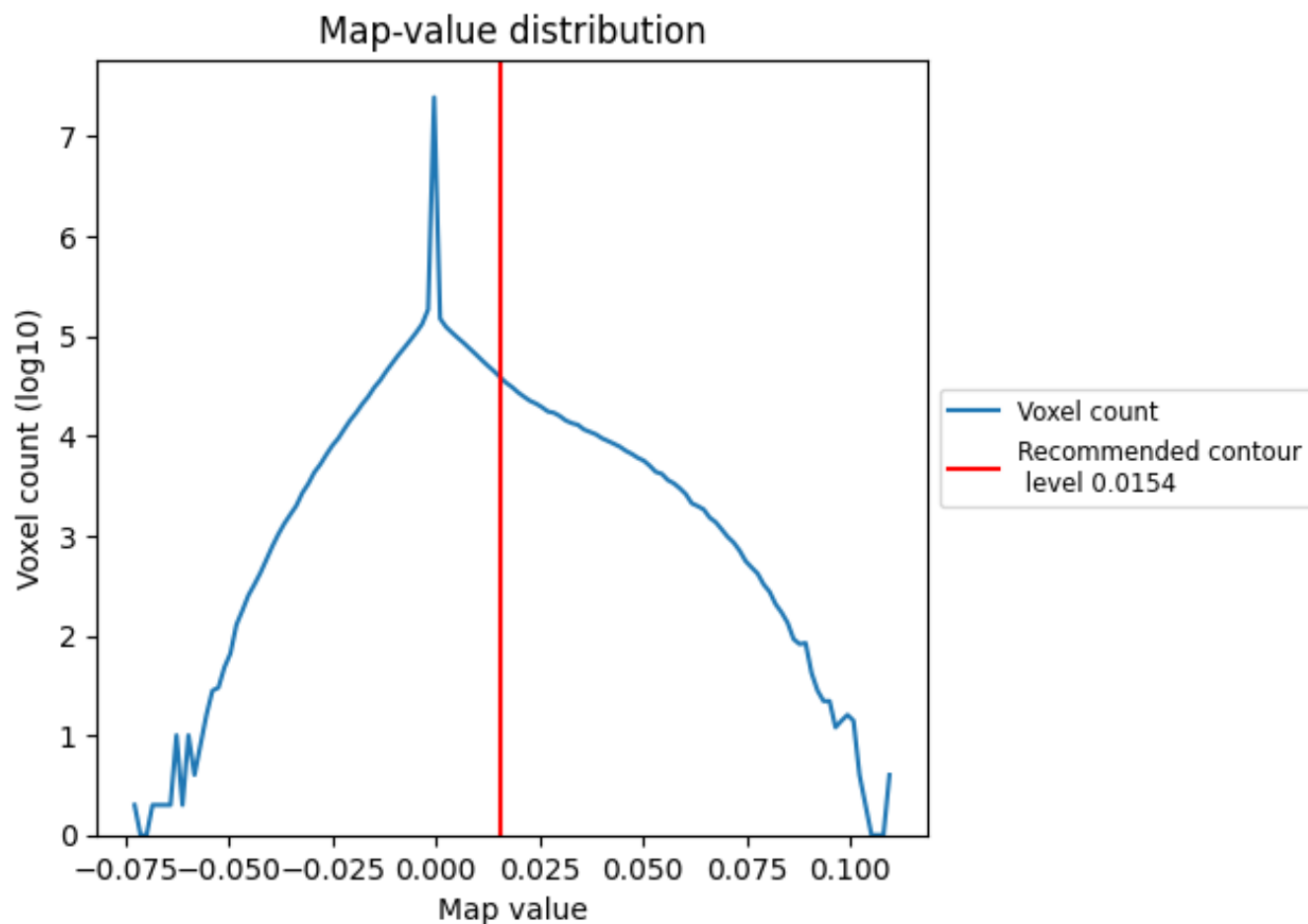


Z

7 Map analysis [i](#)

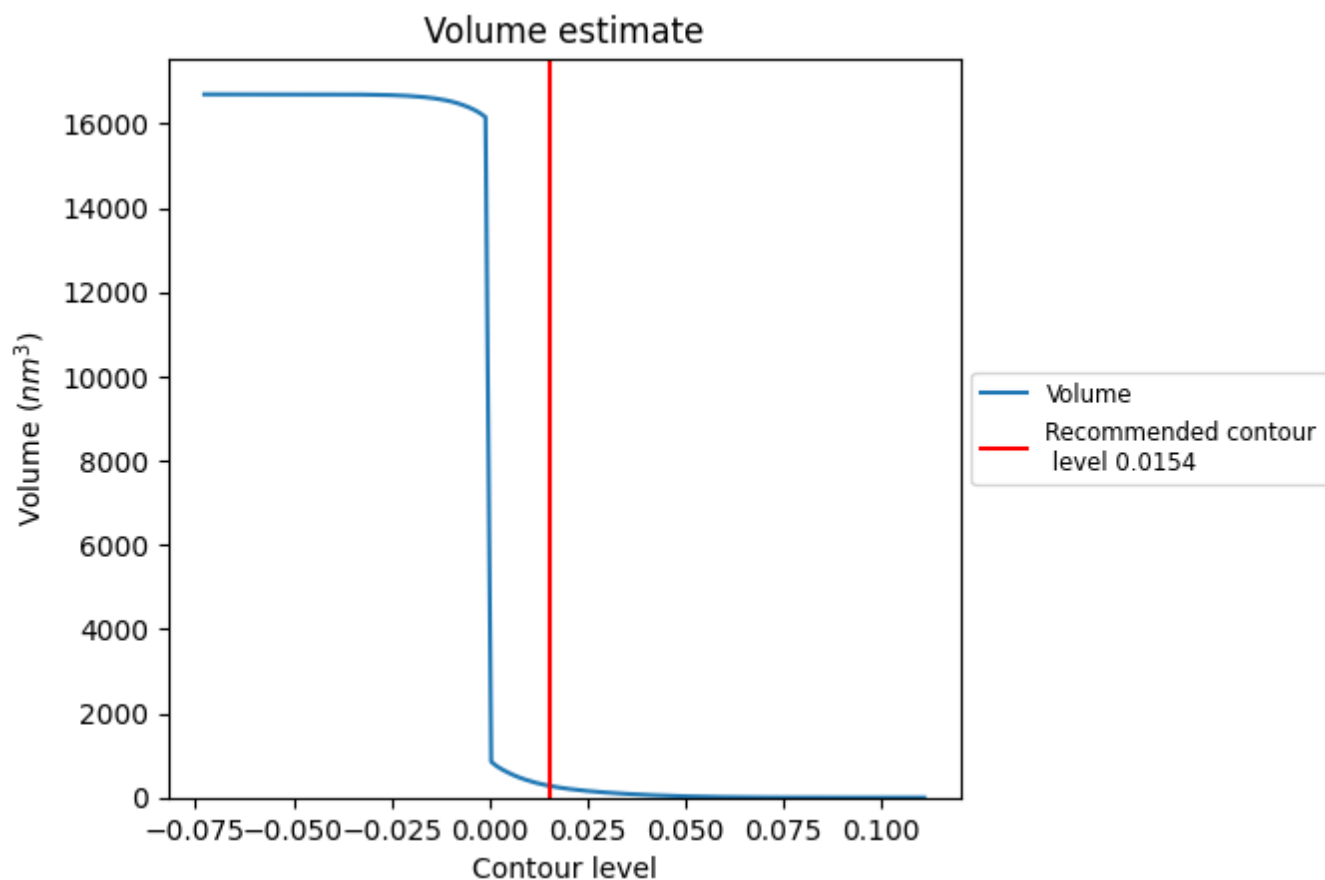
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

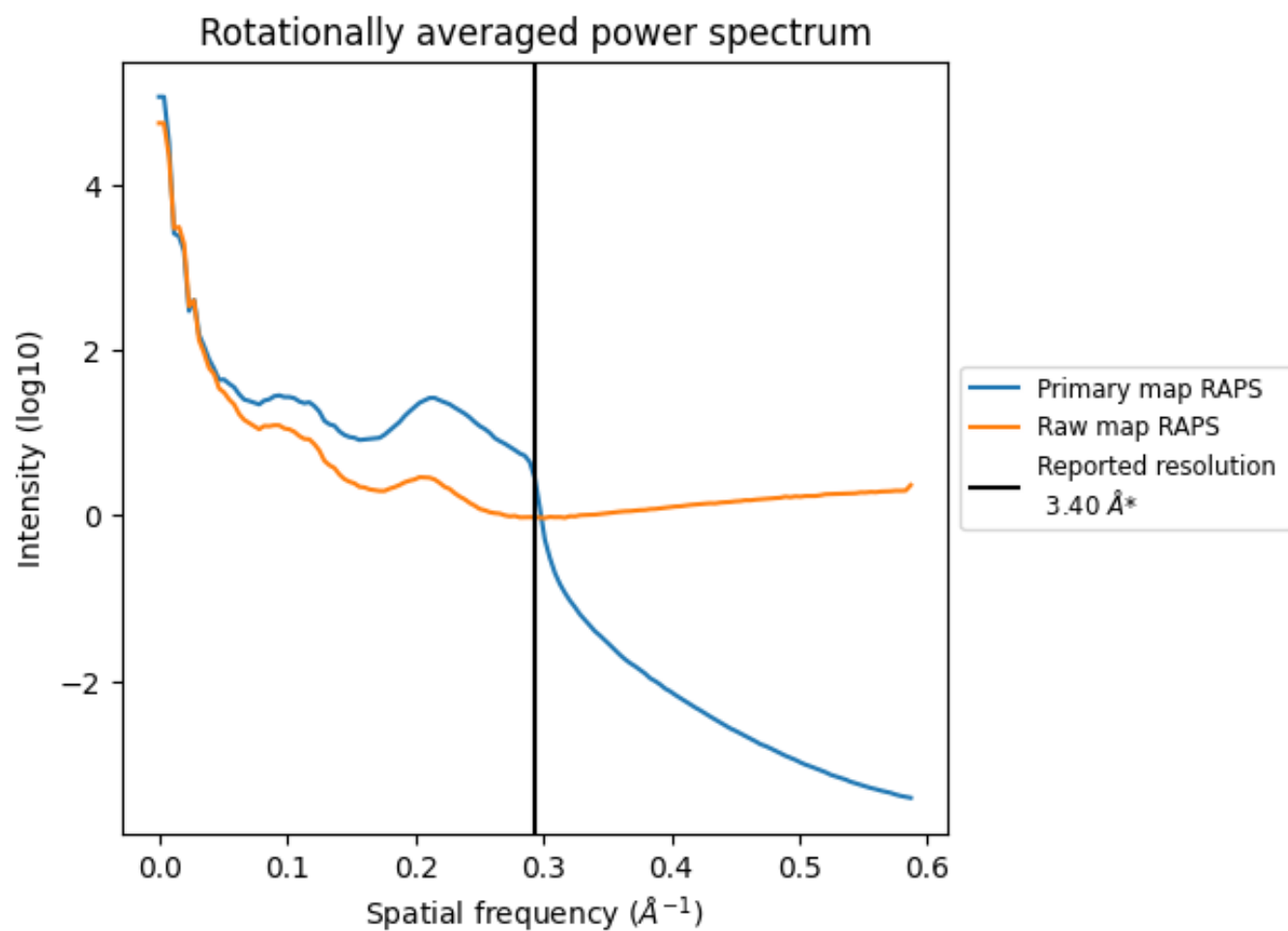
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 250 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](#)

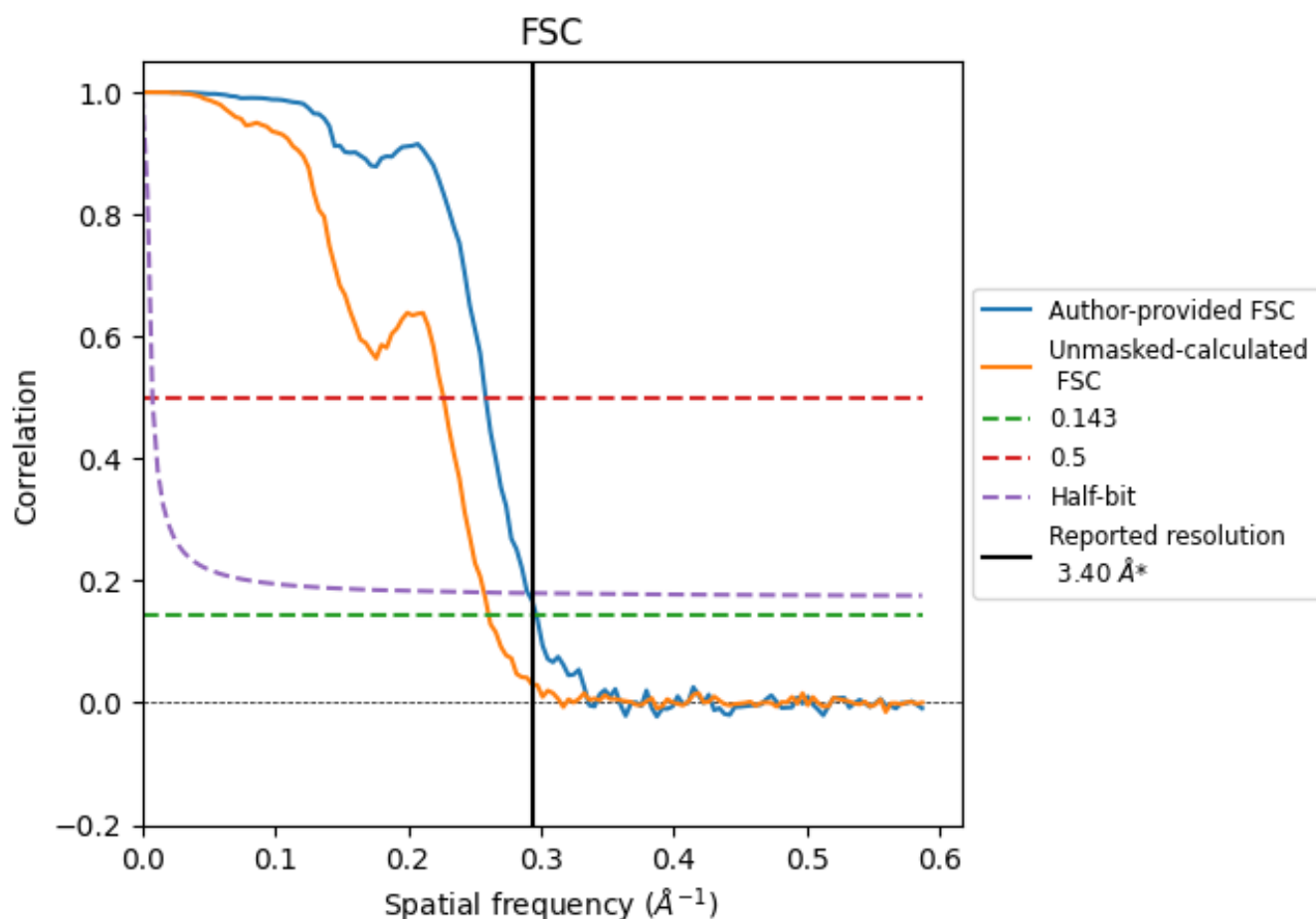


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

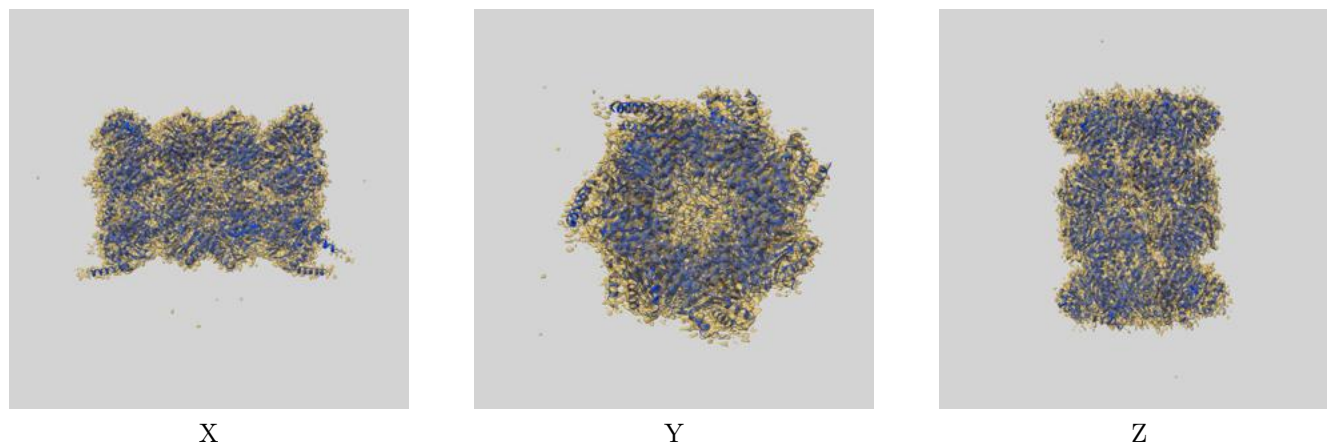
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	3.87	3.44
Unmasked-calculated*	3.83	4.41	3.89

*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 3.83 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

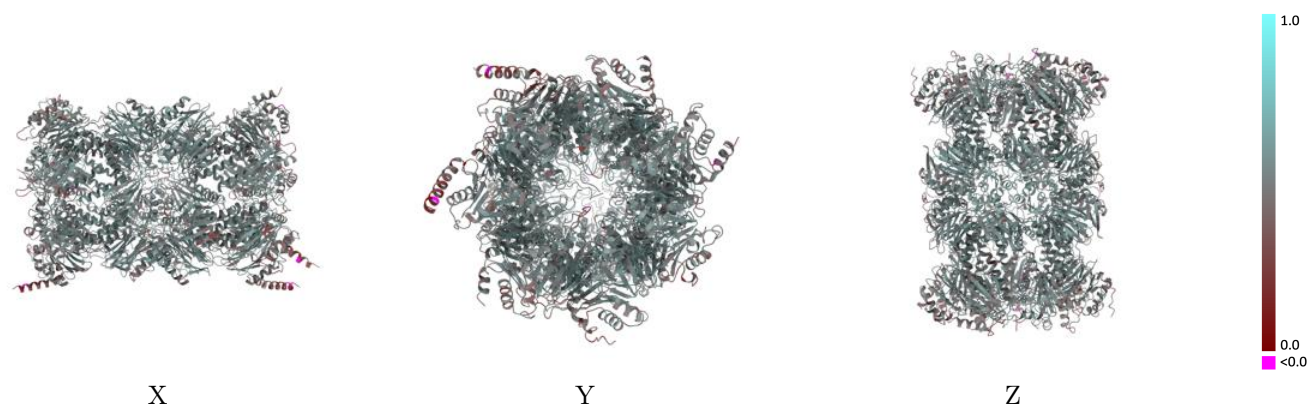
This section contains information regarding the fit between EMDB map EMD-10462 and PDB model 6TCZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



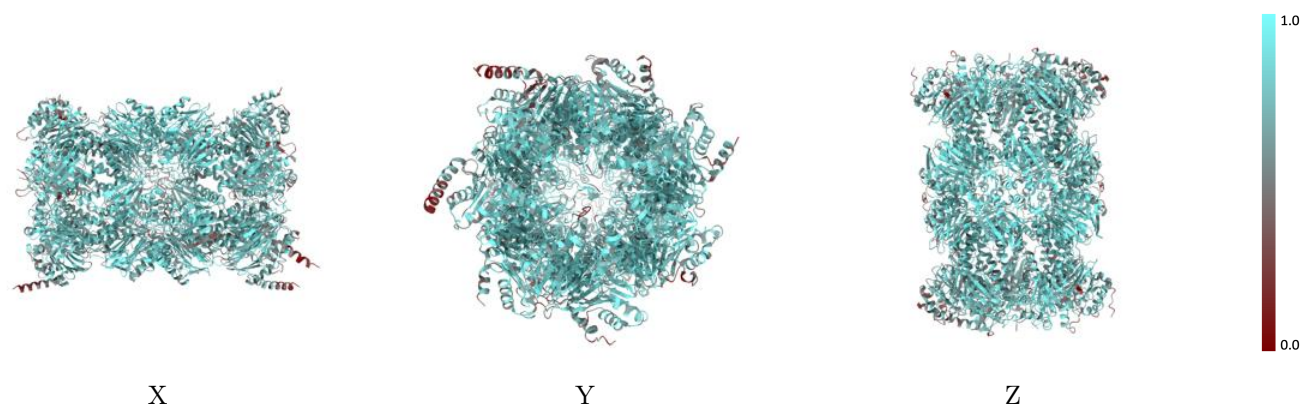
The images above show the 3D surface view of the map at the recommended contour level 0.0154 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



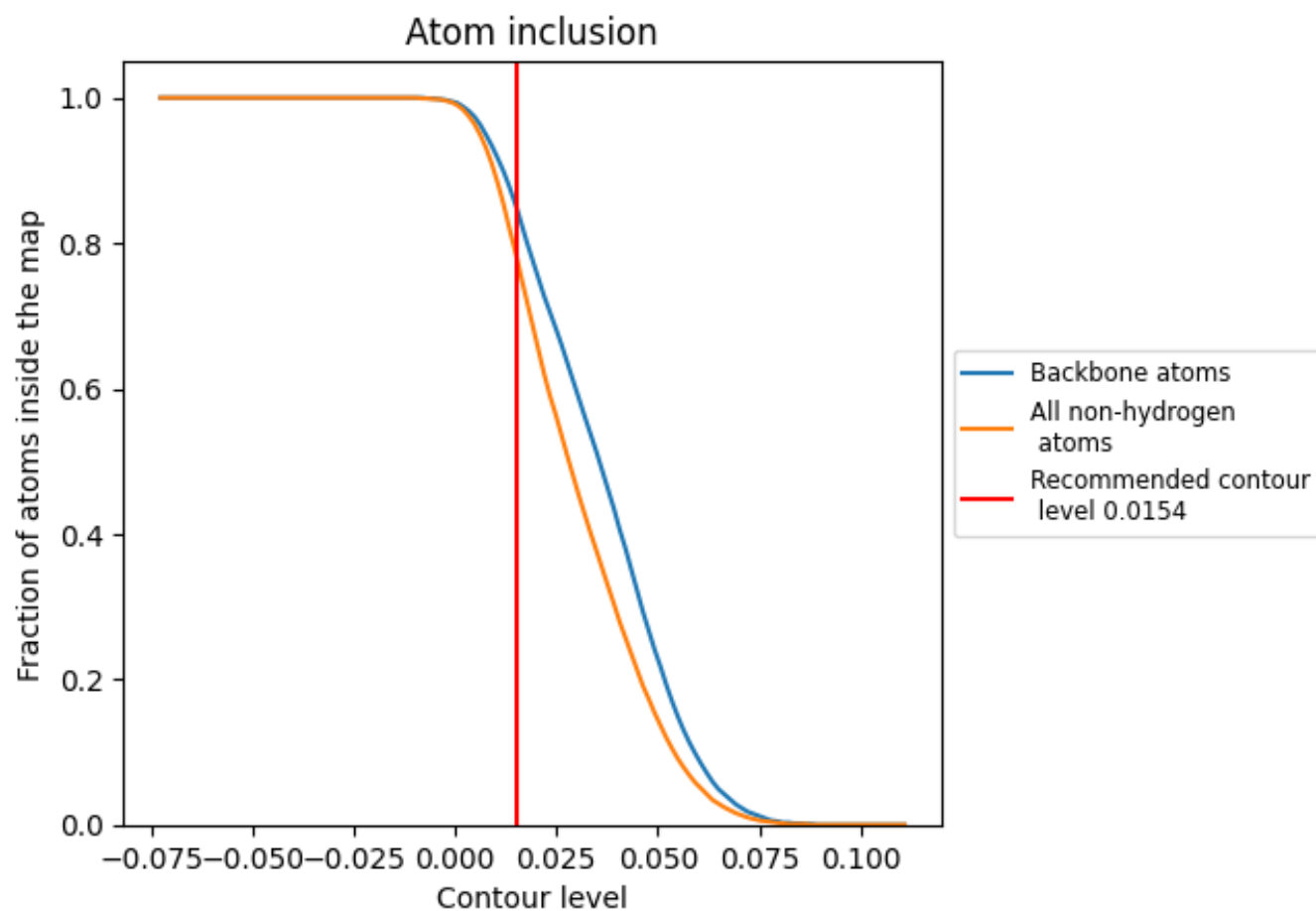
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0154).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.0154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.5140
A	 0.7350	 0.4980
B	 0.7390	 0.5050
C	 0.7160	 0.4910
D	 0.7210	 0.4820
E	 0.7410	 0.4920
F	 0.7560	 0.5090
G	 0.7620	 0.5040
H	 0.8390	 0.5470
I	 0.7540	 0.5100
J	 0.8270	 0.5330
K	 0.8140	 0.5310
L	 0.8370	 0.5410
M	 0.8040	 0.5320
N	 0.8490	 0.5440
a	 0.7420	 0.4980
b	 0.7420	 0.5040
c	 0.7180	 0.4900
d	 0.7250	 0.4830
e	 0.7450	 0.4900
f	 0.7600	 0.5070
g	 0.7640	 0.5040
h	 0.8410	 0.5460
i	 0.7540	 0.5080
j	 0.8210	 0.5340
k	 0.8070	 0.5300
l	 0.8410	 0.5390
m	 0.8060	 0.5320
n	 0.8490	 0.5470

