Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 11:43 am GMT

PDB ID	:	6QM8
EMDB ID	:	EMD-4591
Title	:	Leishmania tarentolae proteasome 20S subunit apo structure
Authors	:	Rowland, P.; Goswami, P.
Deposited on	:	2019-02-01
Resolution	:	3.30 Å(reported)
Based on initial model	:	4R3O

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:

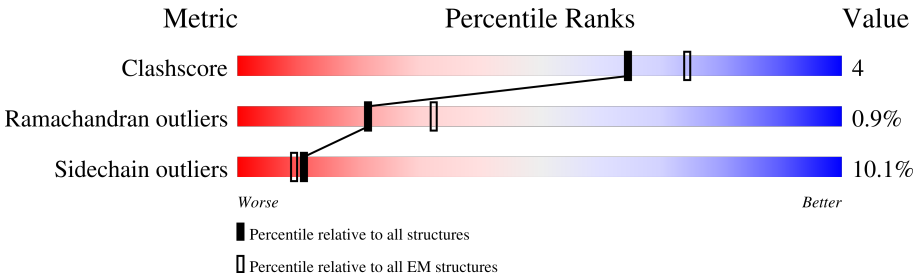
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	A	250	80% 17%
1	O	250	78% 18%
2	B	231	81% 16%
2	P	231	84% 13%
3	C	285	80% 16%
3	Q	285	80% 16%
4	D	248	74% 21%
4	R	248	74% 21%

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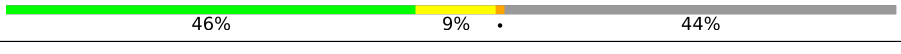
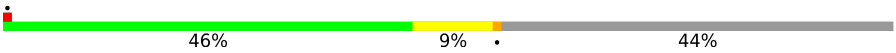
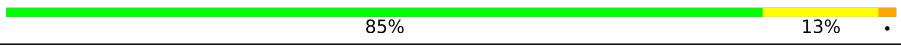
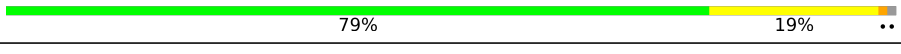
Mol	Chain	Length	Quality of chain
5	E	344	
5	S	344	
6	F	428	
6	T	428	
7	G	238	
7	U	238	
8	H	283	
8	V	283	
9	I	254	
9	W	254	
10	J	205	
10	X	205	
11	K	206	
11	Y	206	
12	L	302	
12	Z	302	
13	M	339	
13	a	339	
14	N	220	
14	b	220	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 49124 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 alpha1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		
1	O	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		

- Molecule 2 is a protein called Proteasome alpha2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		
2	P	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		

- Molecule 3 is a protein called Proteasome alpha3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	276	Total	C	N	O	S	0	0
			2195	1379	382	422	12		
3	Q	276	Total	C	N	O	S	0	0
			2195	1379	382	422	12		

- Molecule 4 is a protein called Proteasome alpha4 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	239	Total	C	N	O	S	0	0
			1873	1180	322	363	8		
4	R	239	Total	C	N	O	S	0	0
			1873	1180	322	363	8		

- Molecule 5 is a protein called Proteasome alpha5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		
5	S	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		

- Molecule 6 is a protein called Proteasome alpha6 chain.

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

- Molecule 7 is a protein called Proteasome alpha7 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	228	Total	C	N	O	S	0	0
			1727	1077	306	334	10		
7	U	228	Total	C	N	O	S	0	0
			1727	1077	306	334	10		

- Molecule 8 is a protein called Proteasome beta1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total	C	N	O	S	0	0
			1710	1062	295	341	12		
8	V	229	Total	C	N	O	S	0	0
			1710	1062	295	341	12		

- Molecule 9 is a protein called Proteasome beta2 chain.

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

- Molecule 10 is a protein called Proteasome beta3 chain.

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	X	204	Total 1557	C 980	N 259	O 302	S 16	0	0

- Molecule 11 is a protein called Proteasome beta4 chain.

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

- Molecule 12 is a protein called Proteasome beta5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	202	Total 1579	C 998	N 277	O 297	S 7	0	0
12	Z	202	Total 1579	C 998	N 277	O 297	S 7	0	0

- Molecule 13 is a protein called Proteasome beta6 chain.

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

- Molecule 14 is a protein called Proteasome beta7 chain.

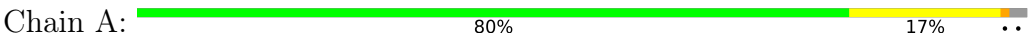
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total 1712	C 1083	N 292	O 323	S 14	0	0
14	b	218	Total 1712	C 1083	N 292	O 323	S 14	0	0

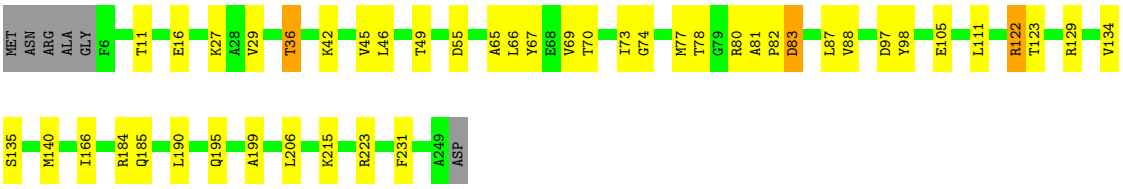
3 Residue-property plots (i)

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 alpha1 chain

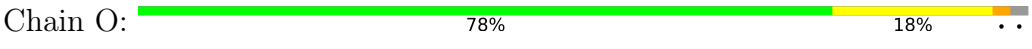
Chain A:

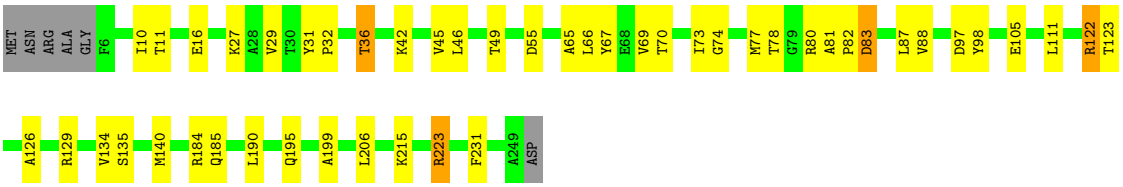




• Molecule 1: Proteasome alpha1 chain

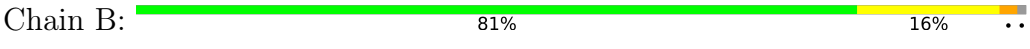
Chain O:

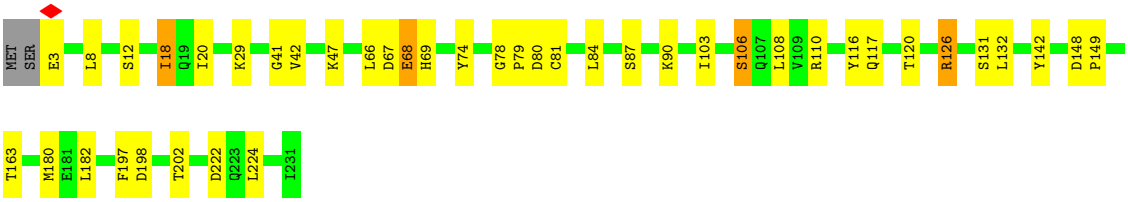




• Molecule 2: Proteasome alpha2 chain

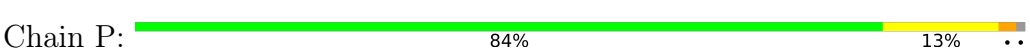
Chain B:

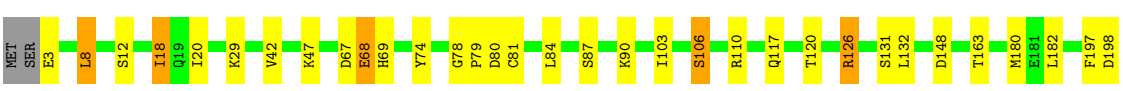


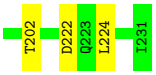


• Molecule 2: Proteasome alpha2 chain

Chain P:

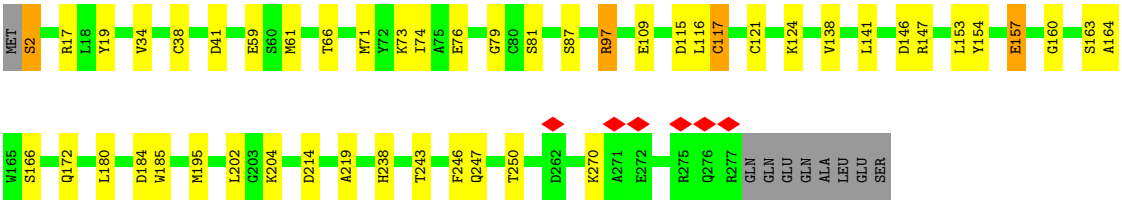






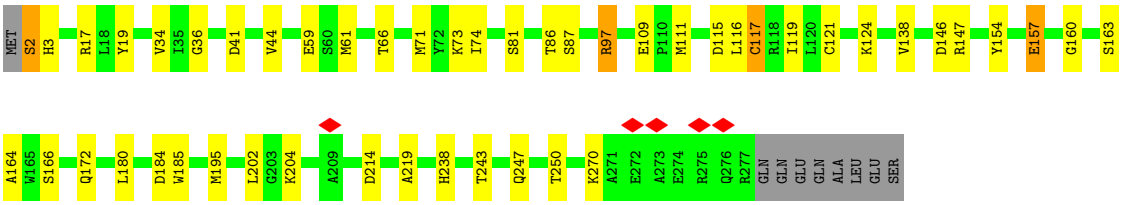
• Molecule 3: Proteasome alpha3 chain

Chain C:



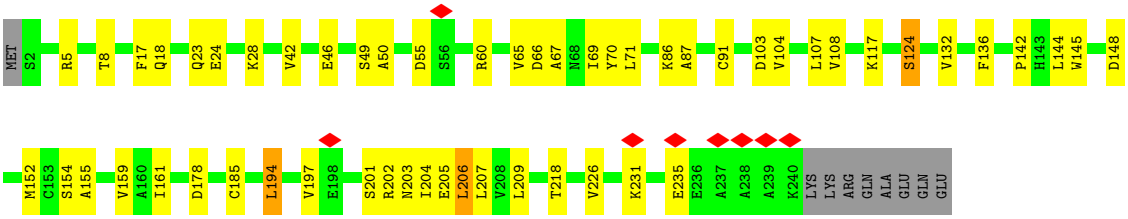
• Molecule 3: Proteasome alpha3 chain

Chain Q:



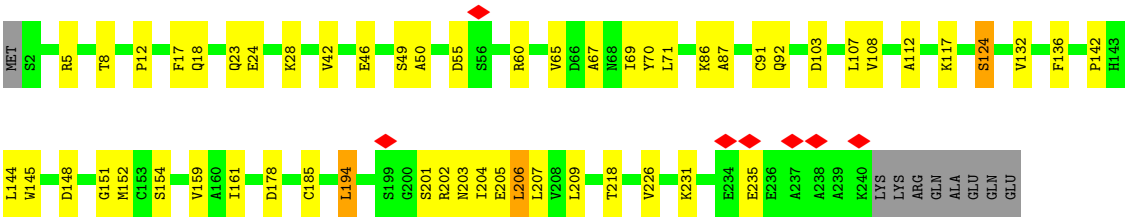
• Molecule 4: Proteasome alpha4 chain

Chain D:



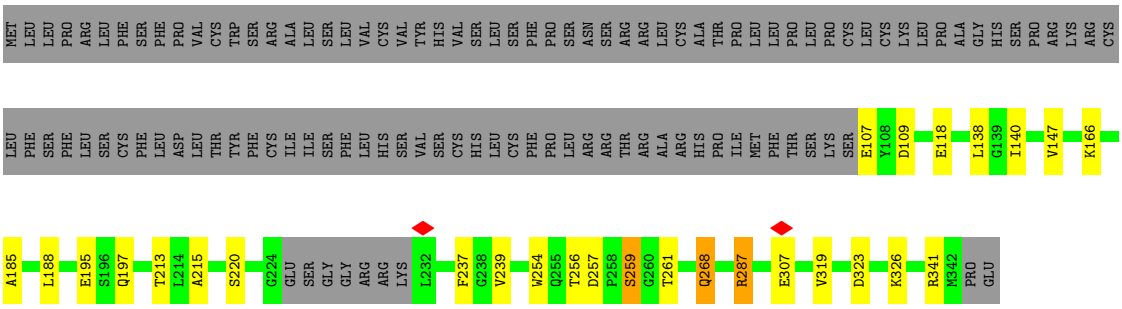
• Molecule 4: Proteasome alpha4 chain

Chain R:

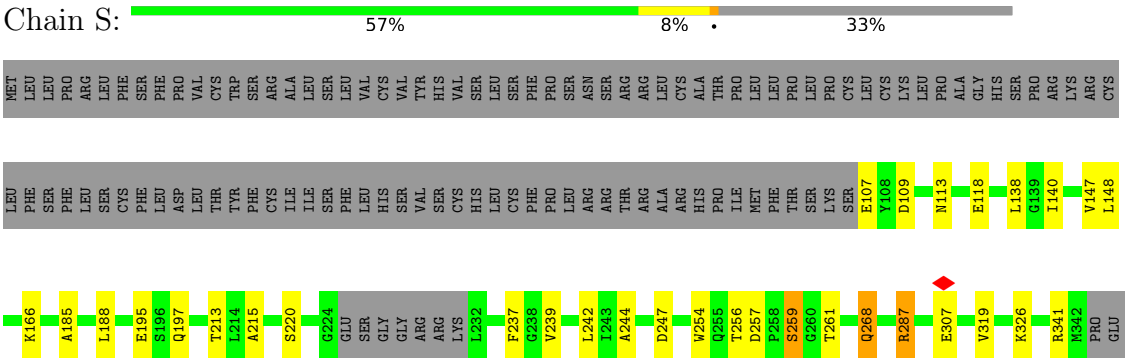


• Molecule 5: Proteasome alpha5 chain

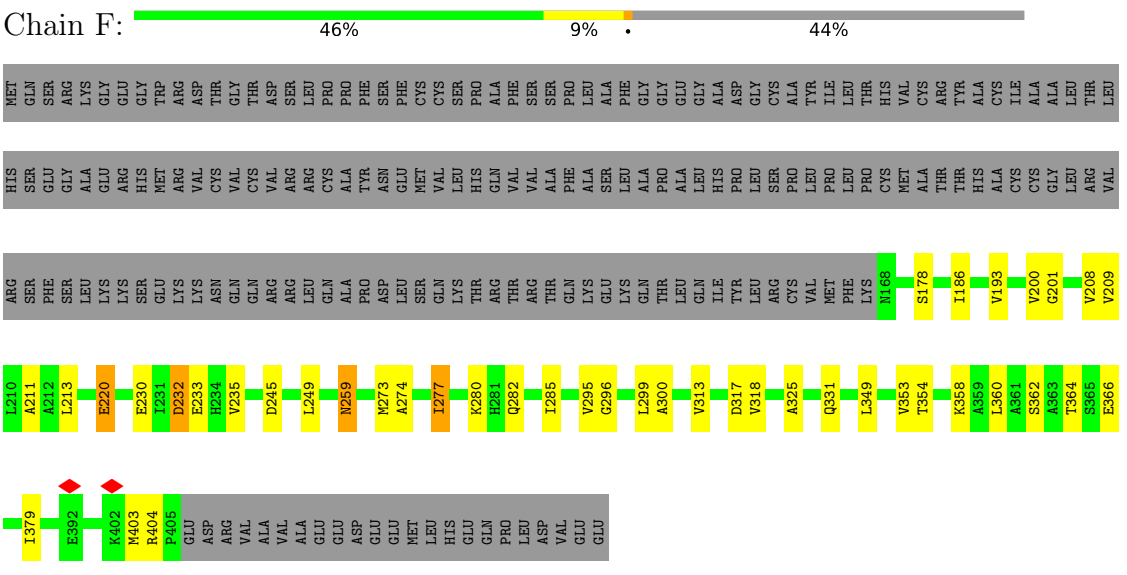
Chain E:



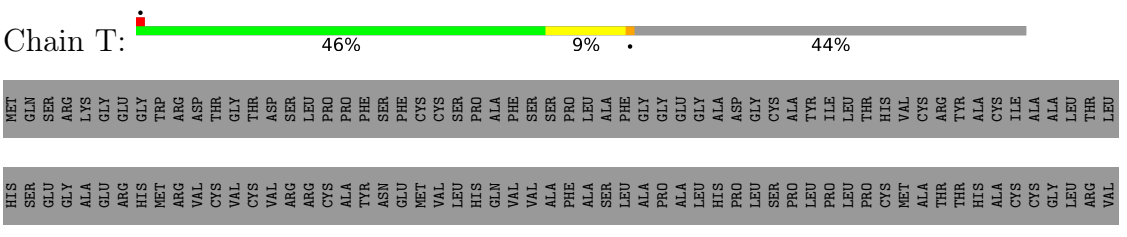
• Molecule 5: Proteasome alpha5 chain

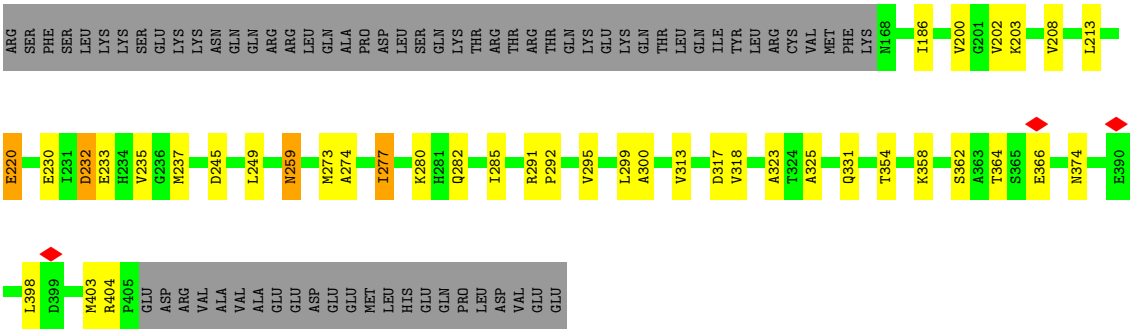


• Molecule 6: Proteasome alpha6 chain

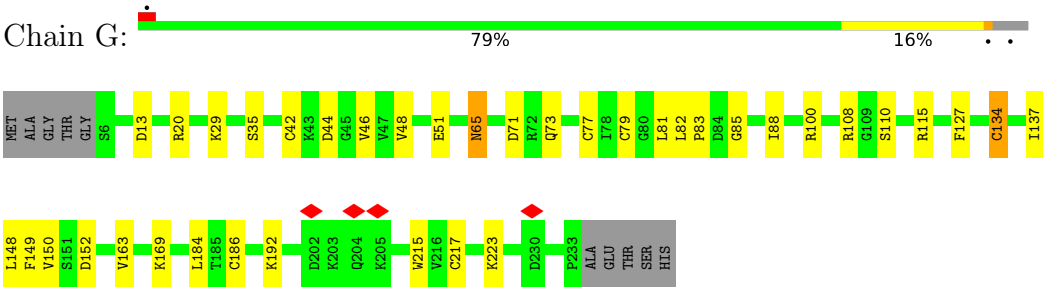


• Molecule 6: Proteasome alpha6 chain

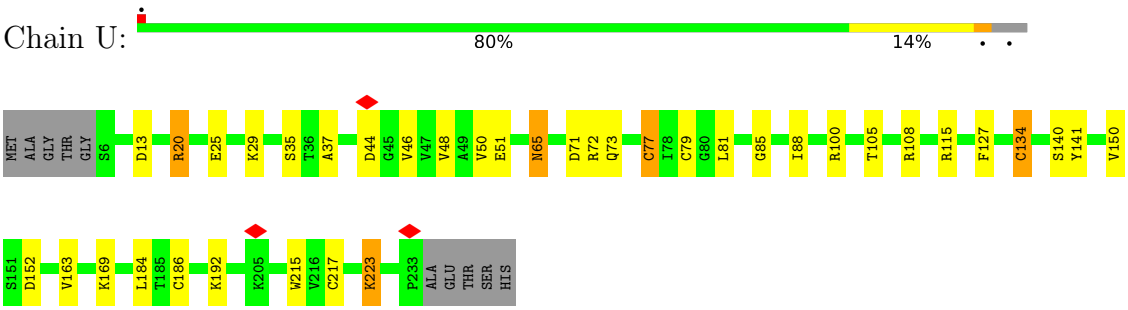




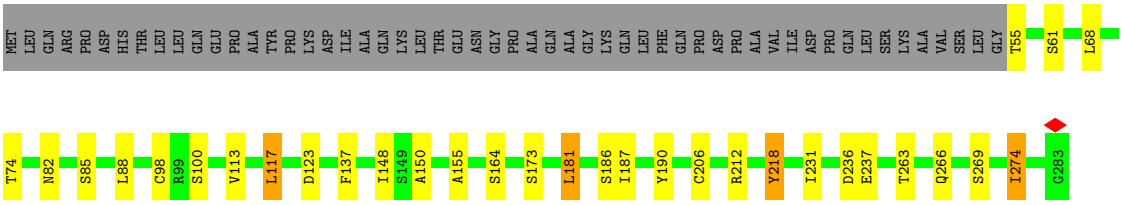
• Molecule 7: Proteasome alpha7 chain



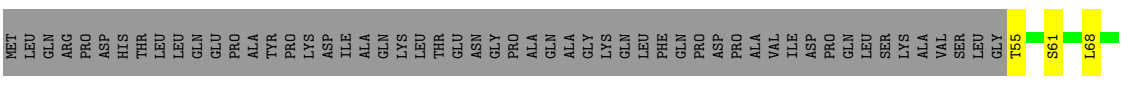
• Molecule 7: Proteasome alpha7 chain

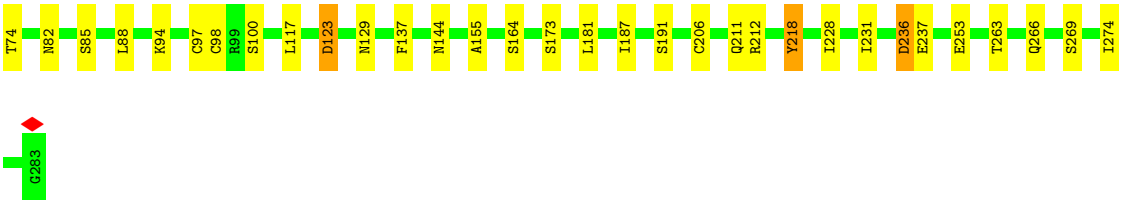


• Molecule 8: Proteasome beta1 chain



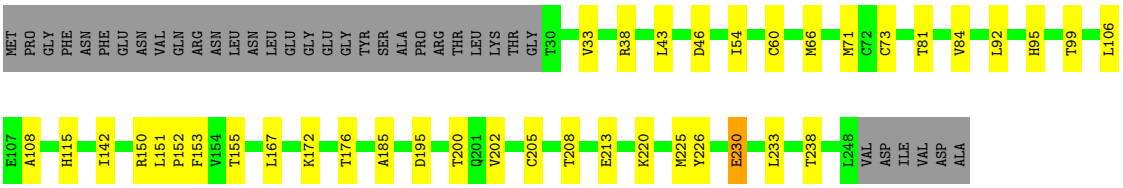
• Molecule 8: Proteasome beta1 chain





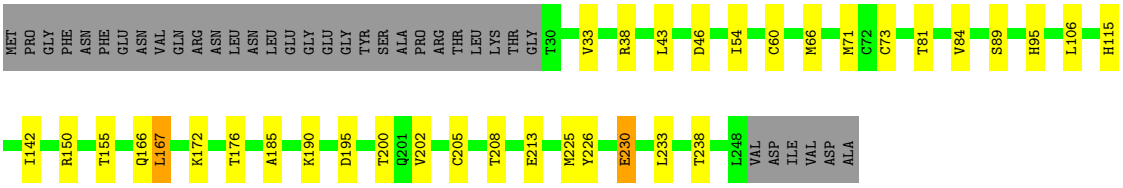
• Molecule 9: Proteasome beta2 chain

Chain I:



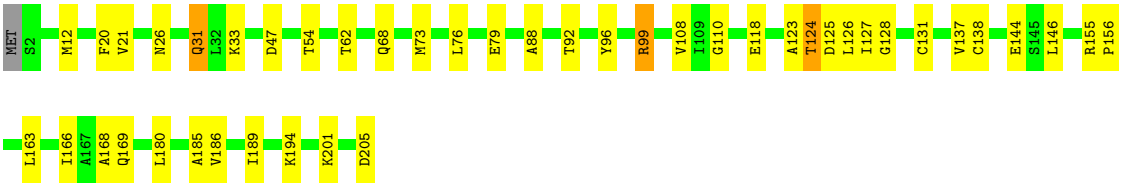
• Molecule 9: Proteasome beta2 chain

Chain W:



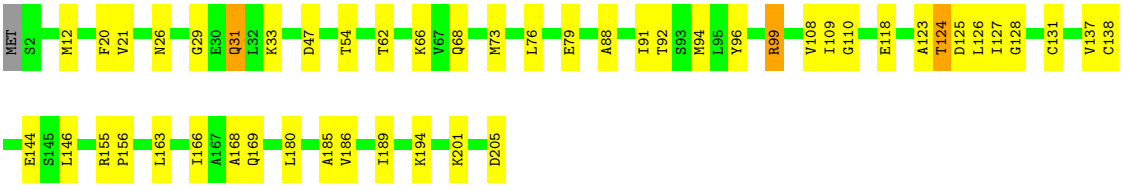
• Molecule 10: Proteasome beta3 chain

Chain J:



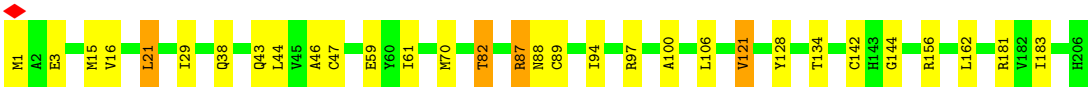
• Molecule 10: Proteasome beta3 chain

Chain X:



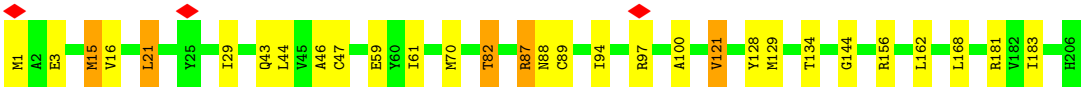
• Molecule 11: Proteasome beta4 chain

Chain K:



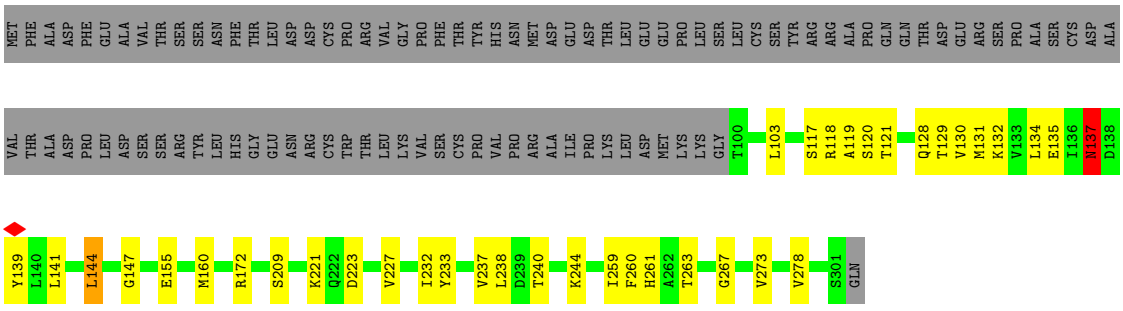
• Molecule 11: Proteasome beta4 chain

Chain Y:



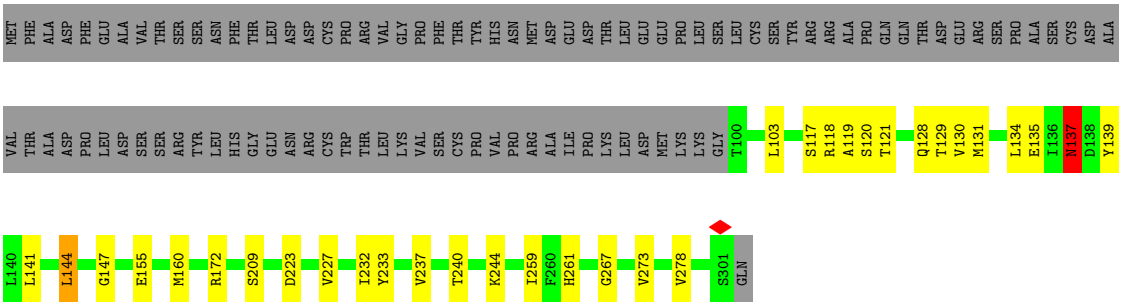
• Molecule 12: Proteasome beta5 chain

Chain L:



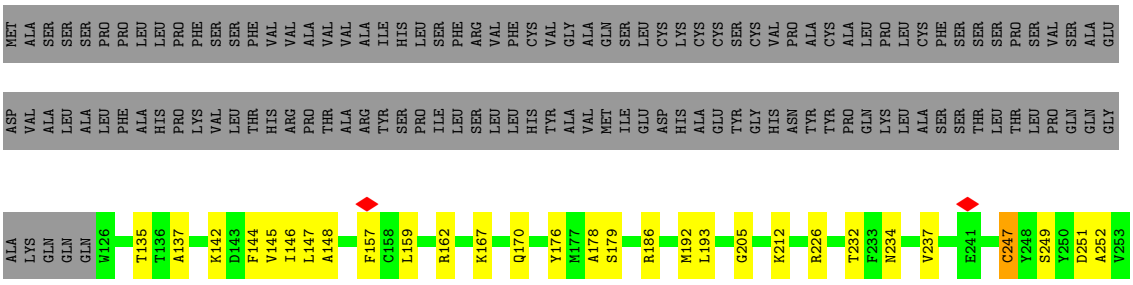
• Molecule 12: Proteasome beta5 chain

Chain Z:

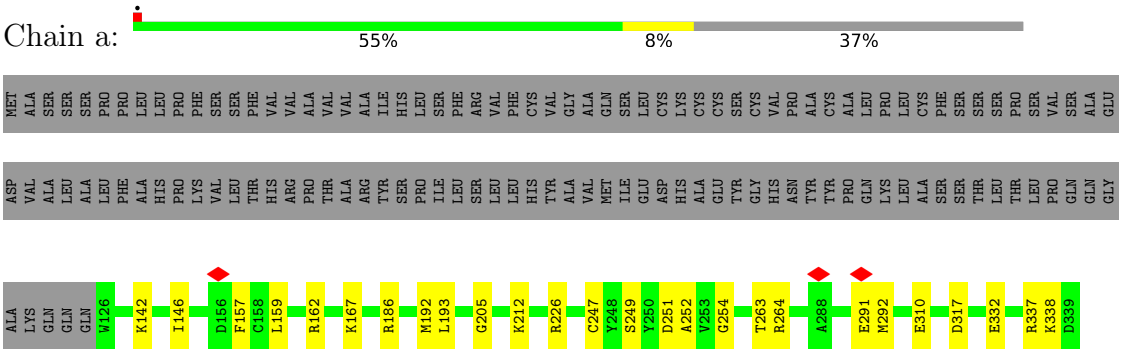


• Molecule 13: Proteasome beta6 chain

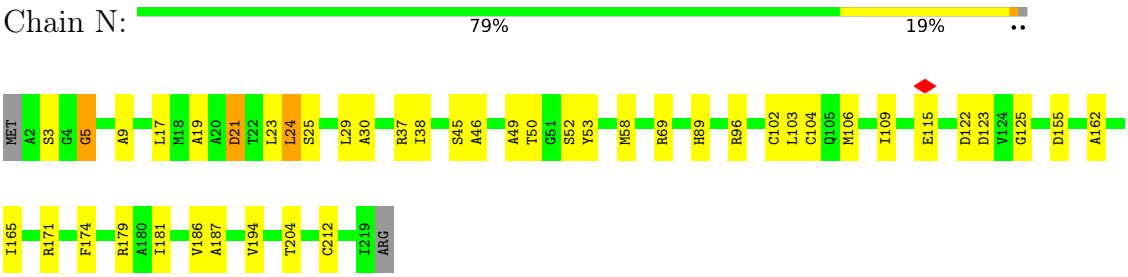
Chain M:



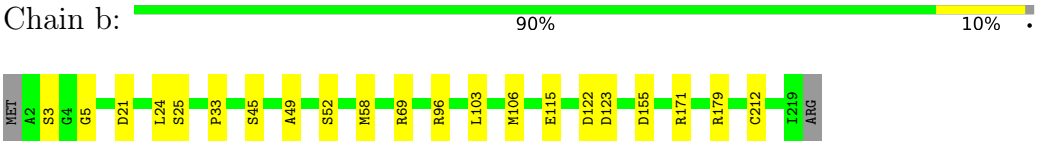
• Molecule 13: Proteasome beta6 chain



• Molecule 14: Proteasome beta7 chain



• Molecule 14: Proteasome beta7 chain



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97438	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.515	Depositor
Minimum map value	-0.311	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0545	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.65	0/1889	0.87	0/2562
1	O	0.64	0/1889	0.88	0/2562
2	B	0.65	0/1787	0.86	0/2421
2	P	0.64	0/1787	0.85	0/2421
3	C	0.65	0/2242	0.85	0/3034
3	Q	0.64	0/2242	0.86	0/3034
4	D	0.67	0/1902	0.86	0/2562
4	R	0.67	0/1902	0.87	0/2562
5	E	0.67	0/1784	0.85	0/2414
5	S	0.66	0/1784	0.85	0/2414
6	F	0.65	0/1907	0.85	0/2575
6	T	0.64	0/1907	0.84	0/2575
7	G	0.65	0/1759	0.86	0/2379
7	U	0.64	0/1759	0.85	0/2379
8	H	0.64	0/1742	0.89	1/2359 (0.0%)
8	V	0.63	0/1742	0.89	1/2359 (0.0%)
9	I	0.63	0/1685	0.87	0/2284
9	W	0.63	0/1685	0.88	0/2284
10	J	0.63	0/1583	0.87	0/2135
10	X	0.62	0/1583	0.87	0/2135
11	K	0.63	0/1643	0.87	0/2222
11	Y	0.63	0/1643	0.88	0/2222
12	L	0.63	0/1613	0.88	1/2183 (0.0%)
12	Z	0.63	0/1613	0.89	1/2183 (0.0%)
13	M	0.64	0/1743	0.92	4/2354 (0.2%)
13	a	0.64	0/1743	0.91	3/2354 (0.1%)
14	N	0.63	0/1748	0.85	0/2363
14	b	0.63	0/1748	0.86	0/2363
All	All	0.64	0/50054	0.87	11/67694 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	R	0	1
7	G	0	1
7	U	0	1
10	X	0	1
14	N	0	1
14	b	0	1
All	All	0	7

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	137	ASN	CB-CA-C	9.28	128.96	110.40
12	L	137	ASN	CB-CA-C	8.66	127.72	110.40
13	M	264	ARG	NE-CZ-NH1	7.40	124.00	120.30
13	a	162	ARG	NE-CZ-NH2	6.81	123.71	120.30
8	V	218	TYR	CB-CG-CD1	6.64	124.98	121.00
13	a	162	ARG	NE-CZ-NH1	-6.08	117.26	120.30
13	a	264	ARG	NE-CZ-NH2	6.08	123.34	120.30
13	M	162	ARG	NE-CZ-NH1	5.98	123.29	120.30
13	M	162	ARG	NE-CZ-NH2	-5.78	117.41	120.30
13	M	264	ARG	NE-CZ-NH2	-5.77	117.42	120.30
8	H	218	TYR	CB-CG-CD1	5.32	124.19	121.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	124	SER	Peptide
7	G	134	CYS	Peptide
14	N	49	ALA	Peptide
4	R	124	SER	Peptide
7	U	134	CYS	Peptide
10	X	29	GLY	Peptide
14	b	49	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1857	0	1871	19	0
1	O	1857	0	1871	21	0
2	B	1754	0	1741	13	0
2	P	1754	0	1741	12	0
3	C	2195	0	2142	21	0
3	Q	2195	0	2142	20	0
4	D	1873	0	1868	20	0
4	R	1873	0	1868	17	0
5	E	1756	0	1736	9	0
5	S	1756	0	1736	13	0
6	F	1869	0	1823	18	0
6	T	1869	0	1823	17	0
7	G	1727	0	1691	15	0
7	U	1727	0	1691	15	0
8	H	1710	0	1665	12	0
8	V	1710	0	1665	14	0
9	I	1659	0	1684	17	0
9	W	1659	0	1684	14	0
10	J	1557	0	1552	21	0
10	X	1557	0	1552	23	0
11	K	1612	0	1571	11	0
11	Y	1612	0	1571	11	0
12	L	1579	0	1538	15	0
12	Z	1579	0	1538	13	0
13	M	1702	0	1638	17	0
13	a	1702	0	1638	0	0
14	N	1712	0	1668	16	0
14	b	1712	0	1668	0	0
All	All	49124	0	48376	374	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 4.

All (374) 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)
7:U:150:VAL:HG21	7:U:163:VAL:HG21	1.60	0.82
1:A:36:THR:HG22	1:A:49:THR:HG23	1.61	0.80
8:V:68:LEU:HD23	8:V:98:CYS:SG	2.21	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:150:VAL:HG21	7:G:163:VAL:HG21	1.65	0.77
1:O:36:THR:HG22	1:O:49:THR:HG23	1.66	0.76
4:R:70:TYR:CD2	4:R:209:LEU:HD21	2.21	0.75
8:H:68:LEU:HD23	8:H:98:CYS:SG	2.28	0.73
4:D:70:TYR:CD2	4:D:209:LEU:HD21	2.23	0.72
13:M:237:VAL:HG22	13:M:247:CYS:HB3	1.70	0.71
9:I:238:THR:HG21	10:J:168:ALA:HB1	1.73	0.71
6:F:200:VAL:HG22	6:F:325:ALA:HB2	1.73	0.70
9:W:33:VAL:HG22	9:W:155:THR:HG22	1.73	0.69
8:H:88:LEU:HD13	8:H:231:ILE:HG22	1.75	0.69
1:A:123:THR:O	2:B:126:ARG:NH1	2.26	0.68
9:I:71:MET:HG3	9:I:205:CYS:SG	2.34	0.68
1:O:67:TYR:CD2	1:O:88:VAL:HG21	2.28	0.68
5:E:185:ALA:HB2	5:E:239:VAL:HG21	1.76	0.68
1:A:67:TYR:CD2	1:A:88:VAL:HG21	2.28	0.67
7:G:88:ILE:HD12	7:G:134:CYS:SG	2.34	0.67
1:O:69:VAL:HG11	1:O:111:LEU:HD21	1.77	0.66
1:A:49:THR:HG21	1:A:65:ALA:CB	2.26	0.65
7:G:100:ARG:NH1	8:V:269:SER:O	2.28	0.65
5:S:185:ALA:HB2	5:S:239:VAL:HG21	1.78	0.65
9:W:238:THR:HG21	10:X:168:ALA:HB1	1.78	0.65
6:T:200:VAL:HG22	6:T:325:ALA:HB2	1.76	0.65
13:M:147:LEU:HD11	13:M:178:ALA:HB2	1.78	0.64
13:M:137:ALA:HB2	13:M:263:THR:HG23	1.80	0.64
3:C:97:ARG:HD2	10:J:76:LEU:HD13	1.79	0.64
11:Y:43:GLN:OE1	11:Y:82:THR:HG21	1.98	0.64
13:M:232:THR:HG23	13:M:234:ASN:HD21	1.61	0.64
9:I:33:VAL:HG22	9:I:155:THR:HG22	1.81	0.63
1:O:123:THR:O	2:P:126:ARG:NH1	2.32	0.62
1:O:49:THR:HG21	1:O:65:ALA:CB	2.29	0.62
7:U:88:ILE:HD12	7:U:134:CYS:SG	2.40	0.62
8:V:88:LEU:HD13	8:V:231:ILE:HG22	1.82	0.62
11:K:183:ILE:HG22	11:Y:21:LEU:HD11	1.82	0.62
3:Q:124:LYS:NZ	3:Q:157:GLU:O	2.33	0.62
13:M:145:VAL:HG11	13:M:237:VAL:HG13	1.81	0.62
8:H:269:SER:O	7:U:100:ARG:NH1	2.34	0.61
9:W:71:MET:HG3	9:W:205:CYS:SG	2.40	0.61
14:N:38:ILE:HG21	14:N:187:ALA:HB2	1.82	0.60
3:Q:66:THR:OG1	10:X:79:GLU:HG2	2.01	0.60
3:Q:97:ARG:HD2	10:X:76:LEU:HD13	1.83	0.59
3:C:34:VAL:HG11	3:C:81:SER:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:VAL:HG11	3:C:81:SER:CB	2.33	0.59
3:Q:34:VAL:HG11	3:Q:81:SER:HB3	1.85	0.59
1:O:77:MET:HE3	1:O:87:LEU:CB	2.33	0.58
6:T:274:ALA:HB1	6:T:318:VAL:HG11	1.84	0.58
9:W:185:ALA:HA	9:W:202:VAL:HG11	1.85	0.58
3:Q:73:LYS:O	3:Q:97:ARG:NH1	2.32	0.58
6:T:235:VAL:HG21	6:T:273:MET:HE1	1.85	0.58
3:C:66:THR:OG1	10:J:79:GLU:HG2	2.03	0.58
2:P:80:ASP:OD2	2:P:126:ARG:NH2	2.37	0.58
8:V:68:LEU:HD11	8:V:155:ALA:HB3	1.86	0.58
11:K:21:LEU:HD11	11:Y:183:ILE:HG22	1.85	0.58
8:H:68:LEU:N	8:H:68:LEU:HD12	2.19	0.58
9:I:185:ALA:HA	9:I:202:VAL:HG11	1.86	0.57
13:M:146:ILE:CG2	13:M:301:LEU:HD12	2.34	0.57
9:I:92:LEU:HD11	9:I:108:ALA:HB2	1.85	0.57
8:V:263:THR:HG21	8:V:274:ILE:HG23	1.86	0.57
8:H:68:LEU:HD11	8:H:155:ALA:HB3	1.87	0.56
3:Q:154:TYR:CE1	3:Q:164:ALA:HB2	2.39	0.56
9:W:142:ILE:N	9:W:142:ILE:HD12	2.20	0.56
10:J:123:ALA:HB2	10:J:137:VAL:HB	1.86	0.56
1:A:69:VAL:HG11	1:A:111:LEU:HD21	1.86	0.56
3:Q:34:VAL:HG11	3:Q:81:SER:CB	2.35	0.56
3:C:71:MET:HG3	3:C:219:ALA:HB2	1.87	0.56
3:C:124:LYS:NZ	3:C:157:GLU:O	2.36	0.56
9:I:142:ILE:N	9:I:142:ILE:HD12	2.21	0.55
1:O:122:ARG:NH1	1:O:129:ARG:O	2.39	0.55
1:O:195:GLN:OE1	1:O:223:ARG:NH1	2.38	0.55
1:A:122:ARG:NH1	1:A:129:ARG:O	2.39	0.54
7:G:48:VAL:HG11	7:G:77:CYS:CB	2.37	0.54
1:A:195:GLN:OE1	1:A:223:ARG:NH1	2.40	0.54
3:Q:71:MET:HG3	3:Q:219:ALA:HB2	1.89	0.54
12:Z:141:LEU:HD12	12:Z:278:VAL:HG22	1.89	0.54
3:C:117:CYS:O	3:C:121:CYS:SG	2.66	0.54
5:E:147:VAL:HG22	5:E:319:VAL:HG12	1.89	0.54
9:W:84:VAL:HG22	9:W:115:HIS:CD2	2.43	0.54
10:X:62:THR:OG1	11:Y:87:ARG:NH2	2.41	0.54
8:V:94:LYS:NZ	8:V:236:ASP:O	2.41	0.54
14:N:102:CYS:SG	14:N:104:CYS:SG	3.03	0.53
1:A:74:GLY:HA3	1:A:231:PHE:CD1	2.43	0.53
11:K:94:ILE:HG22	11:K:100:ALA:HB2	1.89	0.53
10:X:124:THR:HG22	10:X:128:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:123:ALA:HB2	10:X:137:VAL:HB	1.90	0.53
5:S:147:VAL:HG22	5:S:319:VAL:HG12	1.91	0.53
4:D:194:LEU:HD13	4:D:204:ILE:HD11	1.90	0.53
3:C:121:CYS:HB3	3:C:160:GLY:O	2.09	0.53
4:D:91:CYS:SG	4:D:107:LEU:HD13	2.48	0.53
11:Y:16:VAL:CG1	11:Y:46:ALA:HB2	2.38	0.53
2:P:67:ASP:O	2:P:69:HIS:N	2.42	0.53
4:D:201:SER:HB3	4:D:226:VAL:HG11	1.90	0.53
12:L:260:PHE:O	12:L:263:THR:OG1	2.27	0.53
3:C:166:SER:HB3	3:C:185:TRP:CZ2	2.45	0.52
6:F:277:ILE:HD11	6:F:299:LEU:HD12	1.92	0.52
11:K:43:GLN:OE1	11:K:82:THR:HG21	2.09	0.52
2:P:20:ILE:HD11	2:P:120:THR:HB	1.92	0.52
4:R:201:SER:HB3	4:R:226:VAL:HG11	1.92	0.52
1:A:73:ILE:HG21	1:A:111:LEU:HD23	1.91	0.52
2:B:67:ASP:O	2:B:69:HIS:N	2.43	0.52
12:L:119:ALA:HB2	12:L:130:VAL:HG21	1.92	0.52
1:O:77:MET:HE3	1:O:87:LEU:HB3	1.92	0.52
3:C:154:TYR:CE1	3:C:164:ALA:HB2	2.45	0.51
8:H:263:THR:HG21	8:H:274:ILE:HG23	1.92	0.51
1:O:73:ILE:HG21	1:O:111:LEU:HD23	1.92	0.51
8:V:55:THR:HG21	8:V:100:SER:HA	1.91	0.51
4:D:65:VAL:HG21	4:D:71:LEU:HD23	1.93	0.51
10:J:124:THR:HG22	10:J:128:GLY:HA2	1.92	0.51
4:D:132:VAL:HG23	4:D:161:ILE:HD13	1.91	0.51
3:C:73:LYS:O	3:C:97:ARG:NH1	2.40	0.51
4:D:87:ALA:HB1	4:D:107:LEU:HD11	1.93	0.51
1:O:46:LEU:HD21	1:O:199:ALA:HB2	1.91	0.51
2:B:80:ASP:OD2	2:B:126:ARG:NH2	2.44	0.51
10:J:26:ASN:HD21	10:J:186:VAL:HG23	1.75	0.51
9:I:233:LEU:HD13	10:J:169:GLN:HG3	1.93	0.51
10:J:62:THR:OG1	11:K:87:ARG:NH2	2.44	0.51
4:R:91:CYS:SG	4:R:107:LEU:HD13	2.51	0.51
7:U:20:ARG:NH1	7:U:25:GLU:OE2	2.44	0.51
10:X:31:GLN:HA	10:X:31:GLN:HE21	1.75	0.51
10:X:88:ALA:O	10:X:92:THR:HG23	2.10	0.51
1:O:77:MET:HE3	1:O:87:LEU:HB2	1.92	0.51
4:R:144:LEU:HD21	4:R:159:VAL:HG12	1.93	0.50
10:X:126:LEU:HD12	10:X:127:ILE:HG23	1.93	0.50
12:L:237:VAL:HG21	12:L:261:HIS:HB2	1.93	0.50
4:D:42:VAL:HG13	4:D:206:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:235:VAL:HG21	6:F:273:MET:HE1	1.92	0.50
1:A:77:MET:HE3	1:A:87:LEU:CB	2.41	0.50
3:Q:121:CYS:HB3	3:Q:160:GLY:O	2.11	0.50
1:A:46:LEU:HD21	1:A:199:ALA:HB2	1.94	0.50
4:R:65:VAL:HG11	4:R:107:LEU:HD21	1.94	0.50
4:R:71:LEU:HD12	4:R:71:LEU:C	2.31	0.50
7:U:35:SER:O	7:U:79:CYS:SG	2.69	0.50
5:S:197:GLN:HB3	12:Z:160:MET:HG3	1.92	0.50
7:U:186:CYS:SG	7:U:217:CYS:HB3	2.52	0.50
6:F:186:ILE:HD11	6:F:285:ILE:HB	1.94	0.50
9:I:54:ILE:HD11	10:J:144:GLU:HG2	1.94	0.50
1:A:185:GLN:HG3	1:A:190:LEU:HD22	1.94	0.49
14:N:21:ASP:O	14:N:37:ARG:HD3	2.11	0.49
6:F:282:GLN:HA	6:F:285:ILE:HG12	1.94	0.49
11:K:16:VAL:CG1	11:K:46:ALA:HB2	2.42	0.49
1:O:83:ASP:OD2	1:O:129:ARG:NH1	2.46	0.49
4:R:194:LEU:HD13	4:R:204:ILE:HD11	1.95	0.49
1:A:77:MET:HE3	1:A:87:LEU:HB2	1.93	0.49
13:M:170:GLN:NE2	13:M:176:TYR:OH	2.45	0.49
4:R:65:VAL:HG21	4:R:71:LEU:HD23	1.95	0.49
5:E:197:GLN:HB3	12:L:160:MET:HG3	1.94	0.49
9:I:238:THR:HG21	10:J:168:ALA:CB	2.42	0.49
6:T:277:ILE:HD11	6:T:299:LEU:CD1	2.43	0.49
12:Z:103:LEU:C	12:Z:103:LEU:HD12	2.33	0.49
3:C:141:LEU:HG	3:C:153:LEU:HD11	1.95	0.49
7:U:48:VAL:HG11	7:U:77:CYS:HB3	1.94	0.49
1:A:98:TYR:HH	9:I:95:HIS:CE1	2.31	0.48
12:L:103:LEU:HD12	12:L:103:LEU:C	2.33	0.48
3:Q:166:SER:HB3	3:Q:185:TRP:CZ2	2.49	0.48
7:U:88:ILE:CD1	7:U:134:CYS:SG	3.00	0.48
8:V:68:LEU:HD12	8:V:68:LEU:N	2.28	0.48
6:T:213:LEU:HD11	6:T:364:THR:HG22	1.94	0.48
12:L:118:ARG:O	12:L:132:LYS:NZ	2.45	0.48
12:L:118:ARG:NH1	12:L:267:GLY:O	2.47	0.48
4:R:206:LEU:C	4:R:206:LEU:HD12	2.33	0.48
9:I:84:VAL:HG22	9:I:115:HIS:CD2	2.49	0.48
11:K:16:VAL:HG21	11:K:44:LEU:HD11	1.96	0.48
4:R:132:VAL:HG23	4:R:161:ILE:HD13	1.96	0.48
7:G:48:VAL:HG11	7:G:77:CYS:HB3	1.95	0.48
13:M:135:THR:HG21	13:M:267:ALA:HB3	1.96	0.48
14:N:24:LEU:HD21	14:N:53:TYR:CG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:ILE:HG21	3:C:116:LEU:HD21	1.96	0.47
7:G:35:SER:O	7:G:79:CYS:SG	2.71	0.47
9:W:233:LEU:HD13	10:X:169:GLN:HG3	1.95	0.47
4:D:108:VAL:HG21	4:D:145:TRP:CG	2.50	0.47
11:K:1:MET:HA	11:K:144:GLY:HA2	1.95	0.47
11:Y:94:ILE:HG22	11:Y:100:ALA:HB2	1.95	0.47
3:C:238:HIS:HB2	11:K:121:VAL:HG13	1.96	0.47
13:M:144:PHE:HB3	13:M:325:THR:HG22	1.97	0.47
10:J:88:ALA:O	10:J:92:THR:HG23	2.15	0.47
14:N:19:ALA:HB2	14:N:186:VAL:HG22	1.97	0.47
4:R:206:LEU:HD12	4:R:207:LEU:N	2.29	0.47
12:Z:237:VAL:HG21	12:Z:261:HIS:HB2	1.96	0.47
4:D:145:TRP:CE2	4:D:155:ALA:HB2	2.49	0.47
6:F:249:LEU:HD12	6:F:295:VAL:HG11	1.96	0.47
2:B:20:ILE:HD11	2:B:120:THR:HB	1.97	0.47
8:H:55:THR:HG21	8:H:100:SER:HA	1.97	0.47
10:J:96:TYR:CE1	10:J:99:ARG:HG3	2.49	0.47
14:N:46:ALA:HB2	14:N:194:VAL:HG11	1.97	0.47
14:N:174:PHE:CE2	14:N:204:THR:HG21	2.49	0.47
8:H:82:ASN:ND2	8:H:85:SER:HB3	2.30	0.47
10:J:92:THR:HG22	10:J:124:THR:HG21	1.97	0.47
4:R:108:VAL:HG21	4:R:145:TRP:CG	2.50	0.47
10:X:26:ASN:HD21	10:X:186:VAL:HG23	1.80	0.47
5:E:287:ARG:NH2	6:F:220:GLU:O	2.48	0.47
14:N:5:GLY:O	14:N:50:THR:HG23	2.14	0.47
8:V:68:LEU:HD23	8:V:98:CYS:HG	1.77	0.47
10:X:92:THR:HG22	10:X:124:THR:HG21	1.97	0.46
9:I:43:LEU:HB3	9:I:73:CYS:SG	2.55	0.46
12:L:259:ILE:HG21	12:L:273:VAL:HG13	1.97	0.46
7:G:85:GLY:O	7:G:88:ILE:HB	2.16	0.46
11:Y:16:VAL:HG21	11:Y:44:LEU:HD11	1.98	0.46
5:E:268:GLN:HE21	5:E:268:GLN:HA	1.80	0.46
9:W:43:LEU:HB3	9:W:73:CYS:SG	2.55	0.46
14:N:21:ASP:OD1	14:N:21:ASP:N	2.47	0.46
10:X:91:ILE:HD12	10:X:109:ILE:HD11	1.98	0.46
3:C:180:LEU:HD21	3:C:204:LYS:HG2	1.98	0.46
5:E:259:SER:HB2	5:E:261:THR:HG23	1.98	0.46
6:F:211:ALA:HB1	6:F:360:LEU:HD22	1.98	0.46
1:O:74:GLY:HA3	1:O:231:PHE:CD1	2.51	0.46
4:D:144:LEU:HD21	4:D:159:VAL:HG12	1.97	0.46
4:D:206:LEU:HD12	4:D:207:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:238:HIS:HB2	11:Y:121:VAL:HG13	1.97	0.46
4:R:136:PHE:CE1	4:R:142:PRO:HB3	2.50	0.46
4:R:42:VAL:HG13	4:R:206:LEU:HD13	1.98	0.46
4:R:112:ALA:HB1	4:R:151:GLY:O	2.15	0.46
10:J:20:PHE:CE1	10:J:110:GLY:HA3	2.50	0.46
10:J:33:LYS:HB2	12:Z:233:TYR:OH	2.16	0.46
9:W:38:ARG:NH1	9:W:176:THR:HG22	2.31	0.46
13:M:146:ILE:HG22	13:M:301:LEU:HD12	1.97	0.45
6:F:349:LEU:HD11	6:F:379:ILE:HD13	1.99	0.45
2:P:67:ASP:O	2:P:68:GLU:C	2.53	0.45
12:Z:119:ALA:HB2	12:Z:130:VAL:HG21	1.98	0.45
4:D:69:ILE:HG12	4:D:104:VAL:HG22	1.98	0.45
4:D:136:PHE:CE1	4:D:142:PRO:HB3	2.50	0.45
6:T:186:ILE:HD11	6:T:285:ILE:HB	1.98	0.45
6:T:202:VAL:HG12	6:T:323:ALA:HB1	1.98	0.45
1:A:29:VAL:HG21	1:A:134:VAL:HG23	1.99	0.45
3:Q:2:SER:HB2	7:U:127:PHE:CD1	2.51	0.45
2:P:78:GLY:N	2:P:79:PRO:CD	2.80	0.45
3:Q:238:HIS:CB	11:Y:121:VAL:HG13	2.46	0.45
6:T:277:ILE:HD11	6:T:299:LEU:HD12	1.99	0.45
6:F:274:ALA:HB1	6:F:318:VAL:HG11	1.98	0.45
2:B:41:GLY:HA2	2:B:142:TYR:CD1	2.51	0.45
5:E:195:GLU:HG3	5:E:215:ALA:HB1	1.99	0.45
10:J:31:GLN:HE21	10:J:31:GLN:HA	1.82	0.45
14:N:23:LEU:HD11	14:N:30:ALA:HB1	1.98	0.45
10:X:108:VAL:HG13	10:X:137:VAL:HG23	1.99	0.45
2:B:116:TYR:CD1	2:B:149:PRO:HA	2.52	0.45
9:I:151:LEU:HB3	9:I:152:PRO:HD2	1.99	0.45
3:C:146:ASP:OD1	3:C:146:ASP:N	2.50	0.45
7:U:65:ASN:HD22	7:U:65:ASN:HA	1.68	0.45
11:Y:1:MET:HA	11:Y:144:GLY:HA2	1.99	0.45
4:D:71:LEU:C	4:D:71:LEU:HD12	2.37	0.44
13:M:148:ALA:HB2	13:M:321:PHE:CD1	2.51	0.44
2:P:106:SER:HB3	3:Q:61:MET:HE2	1.98	0.44
5:S:268:GLN:HE21	5:S:268:GLN:HA	1.81	0.44
12:Z:259:ILE:HG21	12:Z:273:VAL:HG13	1.99	0.44
12:L:141:LEU:HD12	12:L:278:VAL:HG22	1.98	0.44
5:S:113:ASN:HB3	6:T:291:ARG:HB3	1.99	0.44
6:T:285:ILE:HG22	6:T:292:PRO:HB3	1.99	0.44
7:U:48:VAL:HG11	7:U:77:CYS:CB	2.47	0.44
1:A:83:ASP:OD2	1:A:129:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:144:LEU:C	12:L:144:LEU:HD12	2.38	0.44
3:Q:117:CYS:O	3:Q:121:CYS:SG	2.72	0.44
12:Z:118:ARG:NH1	12:Z:267:GLY:O	2.49	0.44
12:L:259:ILE:CG2	12:L:273:VAL:HG13	2.48	0.44
4:R:87:ALA:HB1	4:R:107:LEU:HD11	2.00	0.44
13:M:148:ALA:HB2	13:M:321:PHE:CE1	2.52	0.44
5:S:148:LEU:HD11	5:S:244:ALA:HB3	1.99	0.44
4:D:66:ASP:O	4:D:69:ILE:N	2.50	0.44
5:E:213:THR:HG21	5:E:254:TRP:HB3	2.00	0.44
12:L:233:TYR:OH	10:X:33:LYS:HB2	2.16	0.44
10:X:21:VAL:HG22	10:X:189:ILE:HG12	1.99	0.44
4:D:194:LEU:HA	4:D:197:VAL:HG12	2.00	0.44
6:F:277:ILE:HD11	6:F:299:LEU:CD1	2.48	0.44
6:T:249:LEU:HD12	6:T:295:VAL:HG11	1.98	0.44
7:G:88:ILE:CD1	7:G:134:CYS:SG	3.05	0.44
1:O:185:GLN:HG3	1:O:190:LEU:HD22	2.00	0.44
1:O:98:TYR:HH	9:W:95:HIS:CE1	2.34	0.44
10:J:21:VAL:HG22	10:J:189:ILE:HG12	1.99	0.43
12:L:103:LEU:HD22	12:L:238:LEU:HD22	2.00	0.43
13:M:311:ARG:HD3	13:M:311:ARG:HA	1.89	0.43
1:O:81:ALA:N	1:O:82:PRO:HD2	2.33	0.43
7:U:85:GLY:O	7:U:88:ILE:HB	2.18	0.43
12:Z:144:LEU:C	12:Z:144:LEU:HD12	2.38	0.43
6:F:213:LEU:HD11	6:F:364:THR:HG22	2.00	0.43
11:Y:15:MET:HE1	11:Y:168:LEU:HD23	2.00	0.43
9:I:95:HIS:O	9:I:99:THR:HG23	2.17	0.43
4:R:69:ILE:HG21	4:R:107:LEU:CD2	2.48	0.43
5:S:213:THR:HG21	5:S:254:TRP:HB3	2.00	0.43
9:W:54:ILE:HD11	10:X:144:GLU:HG2	1.99	0.43
12:Z:259:ILE:CG2	12:Z:273:VAL:HG13	2.48	0.43
2:B:18:ILE:HD13	2:B:18:ILE:HA	1.93	0.43
6:T:208:VAL:HG11	6:T:300:ALA:HB1	1.99	0.43
1:A:81:ALA:N	1:A:82:PRO:HD2	2.33	0.43
4:D:206:LEU:HD12	4:D:206:LEU:C	2.38	0.43
7:G:110:SER:HA	7:G:149:PHE:CE2	2.53	0.43
3:Q:146:ASP:OD1	3:Q:146:ASP:N	2.51	0.43
8:V:82:ASN:ND2	8:V:85:SER:HB3	2.34	0.43
7:G:186:CYS:SG	7:G:217:CYS:HB3	2.59	0.43
6:T:232:ASP:O	6:T:233:GLU:C	2.57	0.43
2:B:66:LEU:HD12	2:B:108:LEU:HD21	2.00	0.43
2:P:18:ILE:HD13	2:P:18:ILE:HA	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:36:GLY:HA2	3:Q:44:VAL:O	2.19	0.43
8:V:123:ASP:OD1	8:V:123:ASP:C	2.57	0.43
8:H:113:VAL:HG12	8:H:117:LEU:HD22	2.00	0.42
1:O:29:VAL:HG21	1:O:134:VAL:HG23	2.01	0.42
7:U:72:ARG:HG2	7:U:223:LYS:HG2	2.01	0.42
7:U:105:THR:HG21	8:V:129:ASN:HD22	1.84	0.42
8:H:190:TYR:CE2	14:N:29:LEU:HD21	2.53	0.42
9:I:43:LEU:HD12	9:I:71:MET:HB2	2.02	0.42
6:T:398:LEU:HD12	6:T:398:LEU:HA	1.93	0.42
2:B:78:GLY:N	2:B:79:PRO:CD	2.82	0.42
3:C:238:HIS:CB	11:K:121:VAL:HG13	2.49	0.42
2:P:74:TYR:HB3	2:P:81:CYS:SG	2.59	0.42
9:I:152:PRO:HG2	9:I:153:PHE:CD2	2.54	0.42
5:S:287:ARG:NH2	6:T:220:GLU:O	2.52	0.42
2:B:67:ASP:O	2:B:68:GLU:C	2.58	0.42
6:F:208:VAL:HG11	6:F:300:ALA:HB1	2.02	0.42
7:G:137:ILE:CG2	7:G:148:LEU:HD11	2.50	0.42
11:K:106:LEU:HD11	11:K:142:CYS:HA	2.02	0.42
6:T:299:LEU:HD23	6:T:299:LEU:HA	1.91	0.42
9:W:238:THR:HG21	10:X:168:ALA:CB	2.47	0.42
2:B:69:HIS:NE2	2:B:103:ILE:O	2.51	0.42
12:L:137:ASN:OD1	12:L:139:TYR:N	2.48	0.42
13:M:309:ALA:HB2	13:M:336:LEU:HD13	2.02	0.42
3:Q:180:LEU:HD21	3:Q:204:LYS:HG2	2.00	0.42
1:A:166:ILE:HG22	1:A:190:LEU:HD23	2.02	0.42
3:C:2:SER:HB2	7:G:127:PHE:CD1	2.55	0.42
1:O:31:TYR:N	1:O:32:PRO:HD2	2.35	0.42
10:X:20:PHE:CE1	10:X:110:GLY:HA3	2.55	0.42
7:G:110:SER:HA	7:G:149:PHE:CZ	2.55	0.41
12:L:137:ASN:HD21	12:L:172:ARG:CD	2.33	0.41
13:M:263:THR:HG21	13:M:271:VAL:HB	2.02	0.41
1:O:126:ALA:HB2	2:P:8:LEU:HD21	2.02	0.41
3:C:38:CYS:N	3:C:166:SER:O	2.49	0.41
9:I:38:ARG:NH1	9:I:176:THR:HG22	2.35	0.41
10:J:92:THR:HG22	10:J:124:THR:CG2	2.50	0.41
3:Q:111:MET:CE	3:Q:119:ILE:HD12	2.50	0.41
5:S:259:SER:HB2	5:S:261:THR:HG23	2.02	0.41
6:T:282:GLN:HA	6:T:285:ILE:HG12	2.02	0.41
5:E:188:LEU:HD21	5:E:237:PHE:CD2	2.56	0.41
6:F:193:VAL:HG22	6:F:296:GLY:N	2.36	0.41
14:N:162:ALA:HA	14:N:165:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:69:HIS:NE2	2:P:103:ILE:O	2.52	0.41
10:X:96:TYR:CE1	10:X:99:ARG:HG3	2.54	0.41
12:Z:137:ASN:HD21	12:Z:172:ARG:CD	2.33	0.41
6:F:232:ASP:O	6:F:233:GLU:C	2.58	0.41
8:H:181:LEU:HB3	8:H:186:SER:HB2	2.03	0.41
10:J:126:LEU:HD12	10:J:127:ILE:HG23	2.01	0.41
14:N:9:ALA:HA	14:N:17:LEU:O	2.21	0.41
1:O:11:THR:HG23	1:O:11:THR:O	2.19	0.41
10:X:92:THR:HG22	10:X:124:THR:CG2	2.50	0.41
10:J:108:VAL:HG13	10:J:137:VAL:HG23	2.03	0.41
13:M:146:ILE:HG21	13:M:301:LEU:HD12	2.02	0.41
2:B:106:SER:HB3	3:C:61:MET:HE2	2.01	0.41
5:S:195:GLU:HG3	5:S:215:ALA:HB1	2.03	0.41
7:G:65:ASN:HD22	7:G:65:ASN:HA	1.66	0.41
8:H:148:ILE:HD12	8:H:150:ALA:HB3	2.01	0.41
13:M:301:LEU:HD23	13:M:301:LEU:HA	1.88	0.41
3:Q:74:ILE:HG21	3:Q:116:LEU:HD21	2.02	0.41
3:C:79:GLY:HA3	3:C:246:PHE:CE1	2.56	0.41
4:D:69:ILE:HG21	4:D:107:LEU:HD22	2.03	0.41
9:W:167:LEU:HD12	9:W:167:LEU:HA	1.88	0.41
2:B:74:TYR:HB3	2:B:81:CYS:SG	2.61	0.41
10:J:12:MET:HG3	10:J:146:LEU:HD22	2.03	0.41
14:N:89:HIS:CD2	14:N:125:GLY:O	2.74	0.41
4:D:65:VAL:HG11	4:D:107:LEU:HD21	2.02	0.40
6:F:201:GLY:HA2	6:F:209:VAL:O	2.20	0.40
2:P:74:TYR:CB	2:P:81:CYS:SG	3.10	0.40
5:S:188:LEU:HD21	5:S:237:PHE:CD2	2.56	0.40
1:A:11:THR:HG23	1:A:11:THR:O	2.21	0.40
7:G:82:LEU:N	7:G:83:PRO:CD	2.84	0.40
7:U:37:ALA:HB2	7:U:50:VAL:HG23	2.02	0.40
5:S:242:LEU:HD23	5:S:242:LEU:HA	1.88	0.40
5:S:247:ASP:OD1	5:S:247:ASP:N	2.55	0.40
8:V:253:GLU:OE1	8:V:253:GLU:N	2.54	0.40
9:W:166:GLN:HE21	9:W:190:LYS:HE2	1.86	0.40
12:Z:141:LEU:HD12	12:Z:278:VAL:CG2	2.52	0.40
6:F:299:LEU:HD23	6:F:299:LEU:HA	1.91	0.40
6:F:349:LEU:O	6:F:353:VAL:HG23	2.22	0.40
14:N:23:LEU:HB2	14:N:181:ILE:HG12	2.02	0.40
10:X:12:MET:HG3	10:X:146:LEU:HD22	2.02	0.40
12:Z:137:ASN:OD1	12:Z:139:TYR:N	2.50	0.40
14:N:46:ALA:HB3	14:N:109:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:211:GLN:HA	8:V:228:ILE:HG21	2.03	0.40
10:X:66:LYS:HB3	10:X:94:MET:CE	2.51	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	A	242/250 (97%)	226 (93%)	15 (6%)	1 (0%)	34	66
1	O	242/250 (97%)	227 (94%)	14 (6%)	1 (0%)	34	66
2	B	227/231 (98%)	208 (92%)	17 (8%)	2 (1%)	17	48
2	P	227/231 (98%)	208 (92%)	17 (8%)	2 (1%)	17	48
3	C	274/285 (96%)	254 (93%)	18 (7%)	2 (1%)	22	54
3	Q	274/285 (96%)	257 (94%)	16 (6%)	1 (0%)	34	66
4	D	237/248 (96%)	226 (95%)	8 (3%)	3 (1%)	12	40
4	R	237/248 (96%)	225 (95%)	9 (4%)	3 (1%)	12	40
5	E	225/344 (65%)	215 (96%)	10 (4%)	0	100	100
5	S	225/344 (65%)	213 (95%)	12 (5%)	0	100	100
6	F	236/428 (55%)	218 (92%)	16 (7%)	2 (1%)	19	51
6	T	236/428 (55%)	216 (92%)	18 (8%)	2 (1%)	19	51
7	G	226/238 (95%)	213 (94%)	12 (5%)	1 (0%)	34	66
7	U	226/238 (95%)	211 (93%)	14 (6%)	1 (0%)	34	66
8	H	227/283 (80%)	203 (89%)	23 (10%)	1 (0%)	34	66
8	V	227/283 (80%)	204 (90%)	22 (10%)	1 (0%)	34	66
9	I	217/254 (85%)	194 (89%)	19 (9%)	4 (2%)	8	35
9	W	217/254 (85%)	197 (91%)	16 (7%)	4 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	202/205 (98%)	183 (91%)	17 (8%)	2 (1%)	15	46
10	X	202/205 (98%)	184 (91%)	16 (8%)	2 (1%)	15	46
11	K	204/206 (99%)	186 (91%)	17 (8%)	1 (0%)	29	61
11	Y	204/206 (99%)	185 (91%)	18 (9%)	1 (0%)	29	61
12	L	200/302 (66%)	175 (88%)	23 (12%)	2 (1%)	15	46
12	Z	200/302 (66%)	171 (86%)	27 (14%)	2 (1%)	15	46
13	M	212/339 (62%)	195 (92%)	11 (5%)	6 (3%)	5	25
13	a	212/339 (62%)	195 (92%)	11 (5%)	6 (3%)	5	25
14	N	216/220 (98%)	190 (88%)	23 (11%)	3 (1%)	11	38
14	b	216/220 (98%)	191 (88%)	22 (10%)	3 (1%)	11	38
All	All	6290/7666 (82%)	5770 (92%)	461 (7%)	59 (1%)	21	48

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	68	GLU
4	D	49	SER
10	J	156	PRO
2	P	68	GLU
4	R	49	SER
10	X	156	PRO
11	Y	134	THR
7	G	169	LYS
11	K	134	THR
12	L	147	GLY
13	M	205	GLY
13	M	292	MET
14	N	52	SER
14	N	115	GLU
4	R	67	ALA
9	W	46	ASP
12	Z	147	GLY
13	a	205	GLY
13	a	291	GLU
13	a	292	MET
14	b	5	GLY
14	b	52	SER
14	b	115	GLU

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Mol	Chain	Res	Type
2	B	180	MET
3	C	59	GLU
4	D	67	ALA
9	I	200	THR
10	J	185	ALA
12	L	232	ILE
13	M	291	GLU
14	N	5	GLY
2	P	180	MET
3	Q	59	GLU
7	U	169	LYS
9	W	200	THR
10	X	185	ALA
1	A	80	ARG
3	C	76	GLU
6	F	366	GLU
8	H	266	GLN
9	I	46	ASP
9	I	226	TYR
9	I	230	GLU
13	M	317	ASP
1	O	80	ARG
4	R	50	ALA
6	T	366	GLU
8	V	266	GLN
9	W	226	TYR
9	W	230	GLU
13	a	252	ALA
13	a	317	ASP
4	D	50	ALA
6	F	259	ASN
13	M	252	ALA
12	Z	232	ILE
6	T	259	ASN
13	a	254	GLY
13	M	254	GLY

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	A	193/197 (98%)	175 (91%)	18 (9%)	9	30
1	O	193/197 (98%)	173 (90%)	20 (10%)	7	25
2	B	188/190 (99%)	164 (87%)	24 (13%)	4	18
2	P	188/190 (99%)	164 (87%)	24 (13%)	4	18
3	C	233/241 (97%)	211 (91%)	22 (9%)	8	30
3	Q	233/241 (97%)	209 (90%)	24 (10%)	7	26
4	D	200/208 (96%)	173 (86%)	27 (14%)	4	16
4	R	200/208 (96%)	171 (86%)	29 (14%)	3	14
5	E	193/301 (64%)	177 (92%)	16 (8%)	11	36
5	S	193/301 (64%)	178 (92%)	15 (8%)	12	38
6	F	200/363 (55%)	184 (92%)	16 (8%)	12	37
6	T	200/363 (55%)	182 (91%)	18 (9%)	9	32
7	G	184/190 (97%)	164 (89%)	20 (11%)	6	24
7	U	184/190 (97%)	164 (89%)	20 (11%)	6	24
8	H	184/229 (80%)	169 (92%)	15 (8%)	11	36
8	V	184/229 (80%)	167 (91%)	17 (9%)	9	31
9	I	180/209 (86%)	167 (93%)	13 (7%)	14	41
9	W	180/209 (86%)	167 (93%)	13 (7%)	14	41
10	J	167/168 (99%)	149 (89%)	18 (11%)	6	24
10	X	167/168 (99%)	149 (89%)	18 (11%)	6	24
11	K	172/172 (100%)	153 (89%)	19 (11%)	6	24
11	Y	172/172 (100%)	153 (89%)	19 (11%)	6	24
12	L	163/253 (64%)	146 (90%)	17 (10%)	7	25
12	Z	163/253 (64%)	147 (90%)	16 (10%)	8	29
13	M	181/288 (63%)	163 (90%)	18 (10%)	8	28
13	a	181/288 (63%)	163 (90%)	18 (10%)	8	28
14	N	181/183 (99%)	165 (91%)	16 (9%)	10	33
14	b	181/183 (99%)	164 (91%)	17 (9%)	8	30
All	All	5238/6384 (82%)	4711 (90%)	527 (10%)	11	27

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	27	LYS
1	A	36	THR
1	A	42	LYS
1	A	45	VAL
1	A	55	ASP
1	A	66	LEU
1	A	70	THR
1	A	78	THR
1	A	83	ASP
1	A	97	ASP
1	A	105	GLU
1	A	122	ARG
1	A	135	SER
1	A	140	MET
1	A	184	ARG
1	A	206	LEU
1	A	215	LYS
2	B	3	GLU
2	B	8	LEU
2	B	12	SER
2	B	18	ILE
2	B	29	LYS
2	B	42	VAL
2	B	47	LYS
2	B	84	LEU
2	B	87	SER
2	B	90	LYS
2	B	106	SER
2	B	110	ARG
2	B	117	GLN
2	B	126	ARG
2	B	131	SER
2	B	132	LEU
2	B	148	ASP
2	B	163	THR
2	B	182	LEU
2	B	197	PHE
2	B	198	ASP
2	B	202	THR
2	B	222	ASP
2	B	224	LEU
3	C	2	SER

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Mol	Chain	Res	Type
3	C	17	ARG
3	C	19	TYR
3	C	41	ASP
3	C	87	SER
3	C	97	ARG
3	C	109	GLU
3	C	115	ASP
3	C	117	CYS
3	C	138	VAL
3	C	147	ARG
3	C	157	GLU
3	C	163	SER
3	C	172	GLN
3	C	184	ASP
3	C	195	MET
3	C	202	LEU
3	C	214	ASP
3	C	243	THR
3	C	247	GLN
3	C	250	THR
3	C	270	LYS
4	D	5	ARG
4	D	8	THR
4	D	17	PHE
4	D	18	GLN
4	D	23	GLN
4	D	24	GLU
4	D	28	LYS
4	D	46	GLU
4	D	55	ASP
4	D	60	ARG
4	D	86	LYS
4	D	103	ASP
4	D	117	LYS
4	D	124	SER
4	D	148	ASP
4	D	152	MET
4	D	154	SER
4	D	178	ASP
4	D	185	CYS
4	D	194	LEU
4	D	202	ARG

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Mol	Chain	Res	Type
4	D	203	ASN
4	D	205	GLU
4	D	206	LEU
4	D	218	THR
4	D	231	LYS
4	D	235	GLU
5	E	107	GLU
5	E	109	ASP
5	E	118	GLU
5	E	138	LEU
5	E	140	ILE
5	E	166	LYS
5	E	220	SER
5	E	256	THR
5	E	257	ASP
5	E	259	SER
5	E	268	GLN
5	E	287	ARG
5	E	307	GLU
5	E	323	ASP
5	E	326	LYS
5	E	341	ARG
6	F	178	SER
6	F	220	GLU
6	F	230	GLU
6	F	232	ASP
6	F	245	ASP
6	F	259	ASN
6	F	277	ILE
6	F	280	LYS
6	F	313	VAL
6	F	317	ASP
6	F	331	GLN
6	F	354	THR
6	F	358	LYS
6	F	362	SER
6	F	403	MET
6	F	404	ARG
7	G	13	ASP
7	G	20	ARG
7	G	29	LYS
7	G	42	CYS

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Mol	Chain	Res	Type
7	G	44	ASP
7	G	46	VAL
7	G	51	GLU
7	G	65	ASN
7	G	71	ASP
7	G	73	GLN
7	G	81	LEU
7	G	108	ARG
7	G	115	ARG
7	G	140	SER
7	G	141	TYR
7	G	152	ASP
7	G	184	LEU
7	G	192	LYS
7	G	215	TRP
7	G	223	LYS
8	H	61	SER
8	H	74	THR
8	H	117	LEU
8	H	123	ASP
8	H	137	PHE
8	H	164	SER
8	H	173	SER
8	H	181	LEU
8	H	187	ILE
8	H	206	CYS
8	H	212	ARG
8	H	218	TYR
8	H	236	ASP
8	H	237	GLU
8	H	274	ILE
9	I	60	CYS
9	I	66	MET
9	I	81	THR
9	I	106	LEU
9	I	150	ARG
9	I	167	LEU
9	I	172	LYS
9	I	195	ASP
9	I	208	THR
9	I	213	GLU
9	I	220	LYS

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Mol	Chain	Res	Type
9	I	225	MET
9	I	230	GLU
10	J	31	GLN
10	J	47	ASP
10	J	54	THR
10	J	68	GLN
10	J	73	MET
10	J	99	ARG
10	J	118	GLU
10	J	124	THR
10	J	125	ASP
10	J	131	CYS
10	J	138	CYS
10	J	155	ARG
10	J	163	LEU
10	J	166	ILE
10	J	180	LEU
10	J	194	LYS
10	J	201	LYS
10	J	205	ASP
11	K	3	GLU
11	K	15	MET
11	K	21	LEU
11	K	29	ILE
11	K	38	GLN
11	K	47	CYS
11	K	59	GLU
11	K	61	ILE
11	K	70	MET
11	K	82	THR
11	K	87	ARG
11	K	88	ASN
11	K	89	CYS
11	K	97	ARG
11	K	121	VAL
11	K	128	TYR
11	K	156	ARG
11	K	162	LEU
11	K	181	ARG
12	L	117	SER
12	L	120	SER
12	L	121	THR

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Mol	Chain	Res	Type
12	L	128	GLN
12	L	129	THR
12	L	131	MET
12	L	134	LEU
12	L	135	GLU
12	L	137	ASN
12	L	144	LEU
12	L	155	GLU
12	L	209	SER
12	L	221	LYS
12	L	223	ASP
12	L	227	VAL
12	L	240	THR
12	L	244	LYS
13	M	142	LYS
13	M	157	PHE
13	M	159	LEU
13	M	167	LYS
13	M	179	SER
13	M	186	ARG
13	M	192	MET
13	M	193	LEU
13	M	212	LYS
13	M	226	ARG
13	M	247	CYS
13	M	249	SER
13	M	251	ASP
13	M	263	THR
13	M	310	GLU
13	M	311	ARG
13	M	332	GLU
13	M	338	LYS
14	N	3	SER
14	N	21	ASP
14	N	24	LEU
14	N	25	SER
14	N	45	SER
14	N	58	MET
14	N	69	ARG
14	N	96	ARG
14	N	103	LEU
14	N	106	MET

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Mol	Chain	Res	Type
14	N	122	ASP
14	N	123	ASP
14	N	155	ASP
14	N	171	ARG
14	N	179	ARG
14	N	212	CYS
1	O	10	ILE
1	O	16	GLU
1	O	27	LYS
1	O	36	THR
1	O	42	LYS
1	O	45	VAL
1	O	55	ASP
1	O	66	LEU
1	O	70	THR
1	O	78	THR
1	O	83	ASP
1	O	97	ASP
1	O	105	GLU
1	O	122	ARG
1	O	135	SER
1	O	140	MET
1	O	184	ARG
1	O	206	LEU
1	O	215	LYS
1	O	223	ARG
2	P	3	GLU
2	P	8	LEU
2	P	12	SER
2	P	18	ILE
2	P	29	LYS
2	P	42	VAL
2	P	47	LYS
2	P	84	LEU
2	P	87	SER
2	P	90	LYS
2	P	106	SER
2	P	110	ARG
2	P	117	GLN
2	P	126	ARG
2	P	131	SER
2	P	132	LEU

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Mol	Chain	Res	Type
2	P	148	ASP
2	P	163	THR
2	P	182	LEU
2	P	197	PHE
2	P	198	ASP
2	P	202	THR
2	P	222	ASP
2	P	224	LEU
3	Q	2	SER
3	Q	3	HIS
3	Q	17	ARG
3	Q	19	TYR
3	Q	41	ASP
3	Q	86	THR
3	Q	87	SER
3	Q	97	ARG
3	Q	109	GLU
3	Q	115	ASP
3	Q	117	CYS
3	Q	138	VAL
3	Q	147	ARG
3	Q	157	GLU
3	Q	163	SER
3	Q	172	GLN
3	Q	184	ASP
3	Q	195	MET
3	Q	202	LEU
3	Q	214	ASP
3	Q	243	THR
3	Q	247	GLN
3	Q	250	THR
3	Q	270	LYS
4	R	5	ARG
4	R	8	THR
4	R	12	PRO
4	R	17	PHE
4	R	18	GLN
4	R	23	GLN
4	R	24	GLU
4	R	28	LYS
4	R	46	GLU
4	R	55	ASP

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Mol	Chain	Res	Type
4	R	60	ARG
4	R	86	LYS
4	R	92	GLN
4	R	103	ASP
4	R	117	LYS
4	R	124	SER
4	R	148	ASP
4	R	152	MET
4	R	154	SER
4	R	178	ASP
4	R	185	CYS
4	R	194	LEU
4	R	202	ARG
4	R	203	ASN
4	R	205	GLU
4	R	206	LEU
4	R	218	THR
4	R	231	LYS
4	R	235	GLU
5	S	107	GLU
5	S	109	ASP
5	S	118	GLU
5	S	138	LEU
5	S	140	ILE
5	S	166	LYS
5	S	220	SER
5	S	256	THR
5	S	257	ASP
5	S	259	SER
5	S	268	GLN
5	S	287	ARG
5	S	307	GLU
5	S	326	LYS
5	S	341	ARG
6	T	203	LYS
6	T	220	GLU
6	T	230	GLU
6	T	232	ASP
6	T	237	MET
6	T	245	ASP
6	T	259	ASN
6	T	277	ILE

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Mol	Chain	Res	Type
6	T	280	LYS
6	T	313	VAL
6	T	317	ASP
6	T	331	GLN
6	T	354	THR
6	T	358	LYS
6	T	362	SER
6	T	374	ASN
6	T	403	MET
6	T	404	ARG
7	U	13	ASP
7	U	20	ARG
7	U	29	LYS
7	U	44	ASP
7	U	46	VAL
7	U	51	GLU
7	U	65	ASN
7	U	71	ASP
7	U	73	GLN
7	U	77	CYS
7	U	81	LEU
7	U	108	ARG
7	U	115	ARG
7	U	140	SER
7	U	141	TYR
7	U	152	ASP
7	U	184	LEU
7	U	192	LYS
7	U	215	TRP
7	U	223	LYS
8	V	61	SER
8	V	74	THR
8	V	97	CYS
8	V	117	LEU
8	V	123	ASP
8	V	137	PHE
8	V	144	ASN
8	V	164	SER
8	V	173	SER
8	V	181	LEU
8	V	187	ILE
8	V	191	SER

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Mol	Chain	Res	Type
8	V	206	CYS
8	V	212	ARG
8	V	218	TYR
8	V	236	ASP
8	V	237	GLU
9	W	60	CYS
9	W	66	MET
9	W	81	THR
9	W	89	SER
9	W	106	LEU
9	W	150	ARG
9	W	167	LEU
9	W	172	LYS
9	W	195	ASP
9	W	208	THR
9	W	213	GLU
9	W	225	MET
9	W	230	GLU
10	X	31	GLN
10	X	47	ASP
10	X	54	THR
10	X	68	GLN
10	X	73	MET
10	X	99	ARG
10	X	118	GLU
10	X	124	THR
10	X	125	ASP
10	X	131	CYS
10	X	138	CYS
10	X	155	ARG
10	X	163	LEU
10	X	166	ILE
10	X	180	LEU
10	X	194	LYS
10	X	201	LYS
10	X	205	ASP
11	Y	3	GLU
11	Y	15	MET
11	Y	21	LEU
11	Y	29	ILE
11	Y	47	CYS
11	Y	59	GLU

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Mol	Chain	Res	Type
11	Y	61	ILE
11	Y	70	MET
11	Y	82	THR
11	Y	87	ARG
11	Y	88	ASN
11	Y	89	CYS
11	Y	97	ARG
11	Y	121	VAL
11	Y	128	TYR
11	Y	129	MET
11	Y	156	ARG
11	Y	162	LEU
11	Y	181	ARG
12	Z	117	SER
12	Z	120	SER
12	Z	121	THR
12	Z	128	GLN
12	Z	129	THR
12	Z	131	MET
12	Z	134	LEU
12	Z	135	GLU
12	Z	137	ASN
12	Z	144	LEU
12	Z	155	GLU
12	Z	209	SER
12	Z	223	ASP
12	Z	227	VAL
12	Z	240	THR
12	Z	244	LYS
13	a	142	LYS
13	a	146	ILE
13	a	157	PHE
13	a	159	LEU
13	a	167	LYS
13	a	186	ARG
13	a	192	MET
13	a	193	LEU
13	a	212	LYS
13	a	226	ARG
13	a	247	CYS
13	a	249	SER
13	a	251	ASP

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Mol	Chain	Res	Type
13	a	263	THR
13	a	310	GLU
13	a	332	GLU
13	a	337	ARG
13	a	338	LYS
14	b	3	SER
14	b	21	ASP
14	b	24	LEU
14	b	25	SER
14	b	33	PRO
14	b	45	SER
14	b	58	MET
14	b	69	ARG
14	b	96	ARG
14	b	103	LEU
14	b	106	MET
14	b	122	ASP
14	b	123	ASP
14	b	155	ASP
14	b	171	ARG
14	b	179	ARG
14	b	212	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	232	GLN
1	A	236	ASN
2	B	117	GLN
2	B	121	GLN
3	C	104	GLN
3	C	108	GLN
3	C	175	GLN
3	C	263	GLN
4	D	115	GLN
5	E	191	HIS
6	F	225	GLN
6	F	331	GLN
7	G	54	HIS
7	G	64	ASN
7	G	65	ASN

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Mol	Chain	Res	Type
8	H	129	ASN
8	H	135	ASN
9	I	115	HIS
9	I	166	GLN
9	I	201	GLN
9	I	247	GLN
10	J	26	ASN
10	J	31	GLN
10	J	65	ASN
11	K	22	ASN
12	L	184	ASN
12	L	291	GLN
13	M	170	GLN
13	M	180	ASN
13	M	188	GLN
14	N	70	GLN
14	N	75	ASN
14	N	153	ASN
14	N	185	GLN
1	O	207	GLN
1	O	236	ASN
2	P	117	GLN
2	P	121	GLN
3	Q	175	GLN
3	Q	263	GLN
4	R	115	GLN
5	S	288	ASN
6	T	225	GLN
7	U	65	ASN
8	V	129	ASN
8	V	135	ASN
9	W	102	GLN
9	W	115	HIS
9	W	166	GLN
9	W	247	GLN
10	X	26	ASN
10	X	31	GLN
10	X	65	ASN
11	Y	22	ASN
11	Y	64	ASN
12	Z	184	ASN
12	Z	291	GLN

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Mol	Chain	Res	Type
13	a	170	GLN
13	a	180	ASN
13	a	188	GLN
14	b	70	GLN
14	b	148	GLN
14	b	185	GLN
14	b	205	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

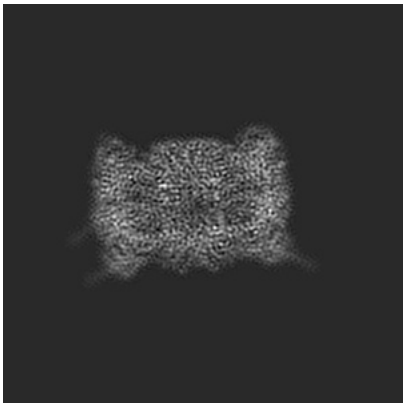
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4591. These allow visual inspection of the internal detail of the map and identification of artifacts.

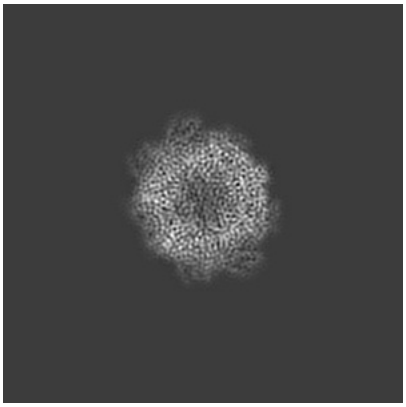
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

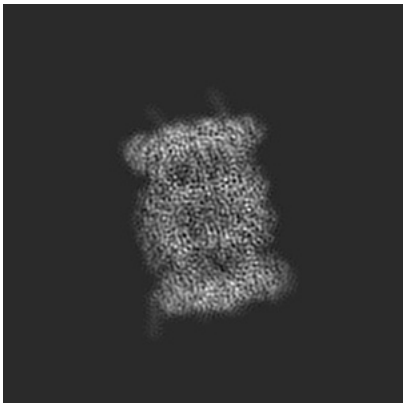
6.1.1 Primary map



X



Y



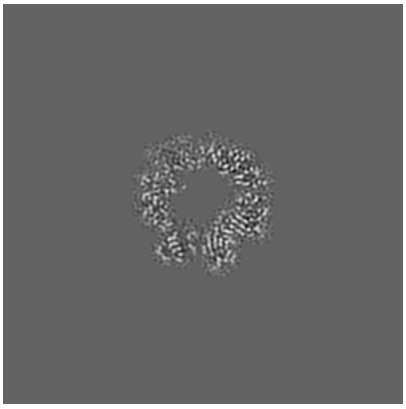
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 150



Y Index: 150

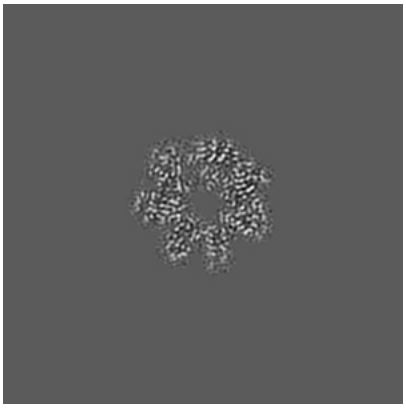
Z Index: 150

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: 167



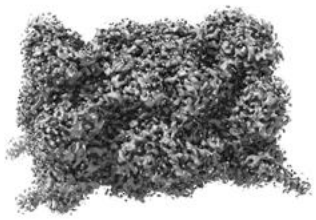
Y Index: 159

Z Index: 178

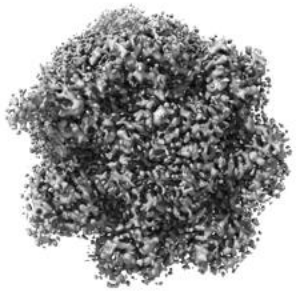
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

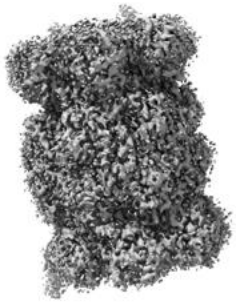
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0545. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

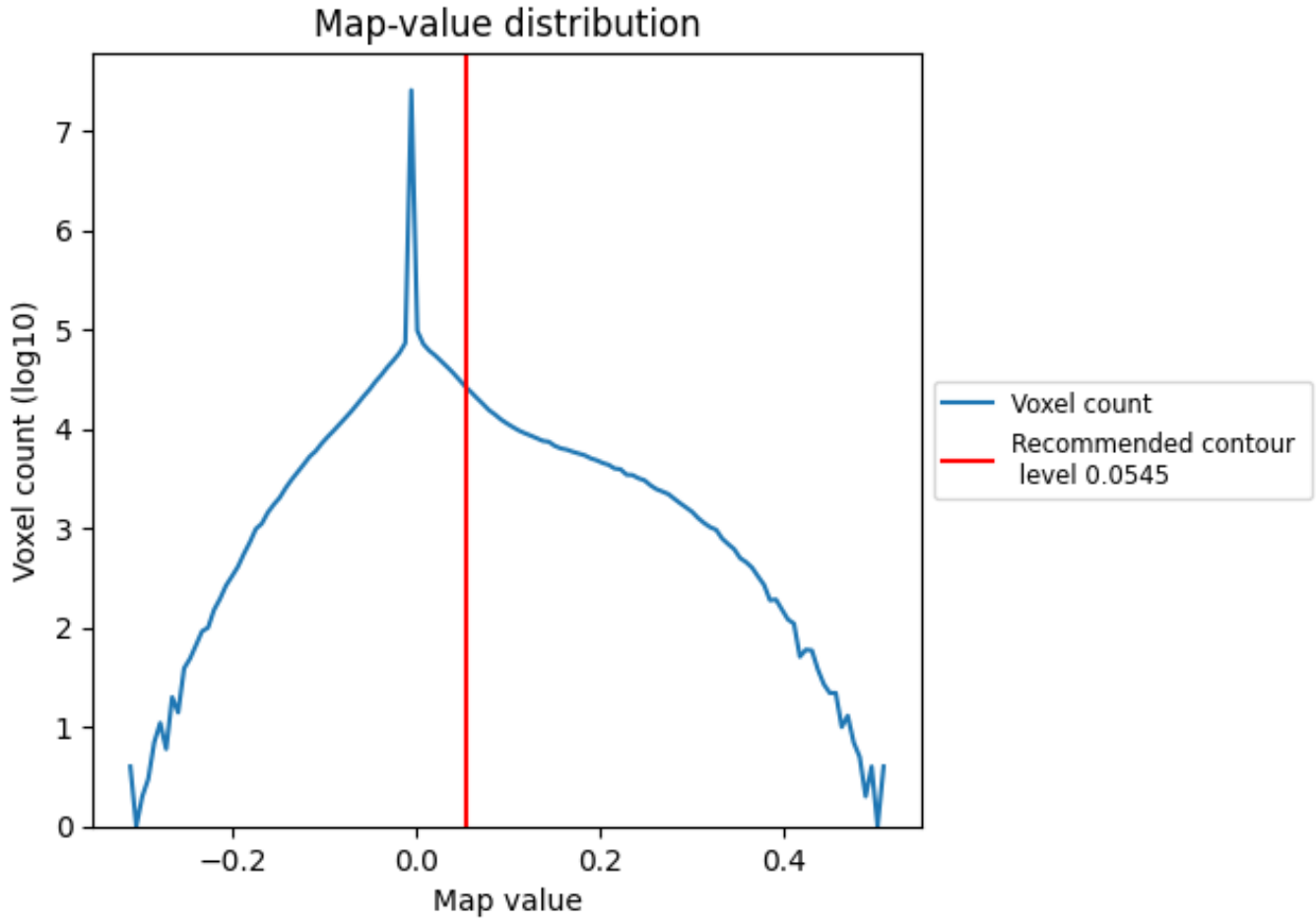
6.5 Mask visualisation (i)

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

7 Map analysis

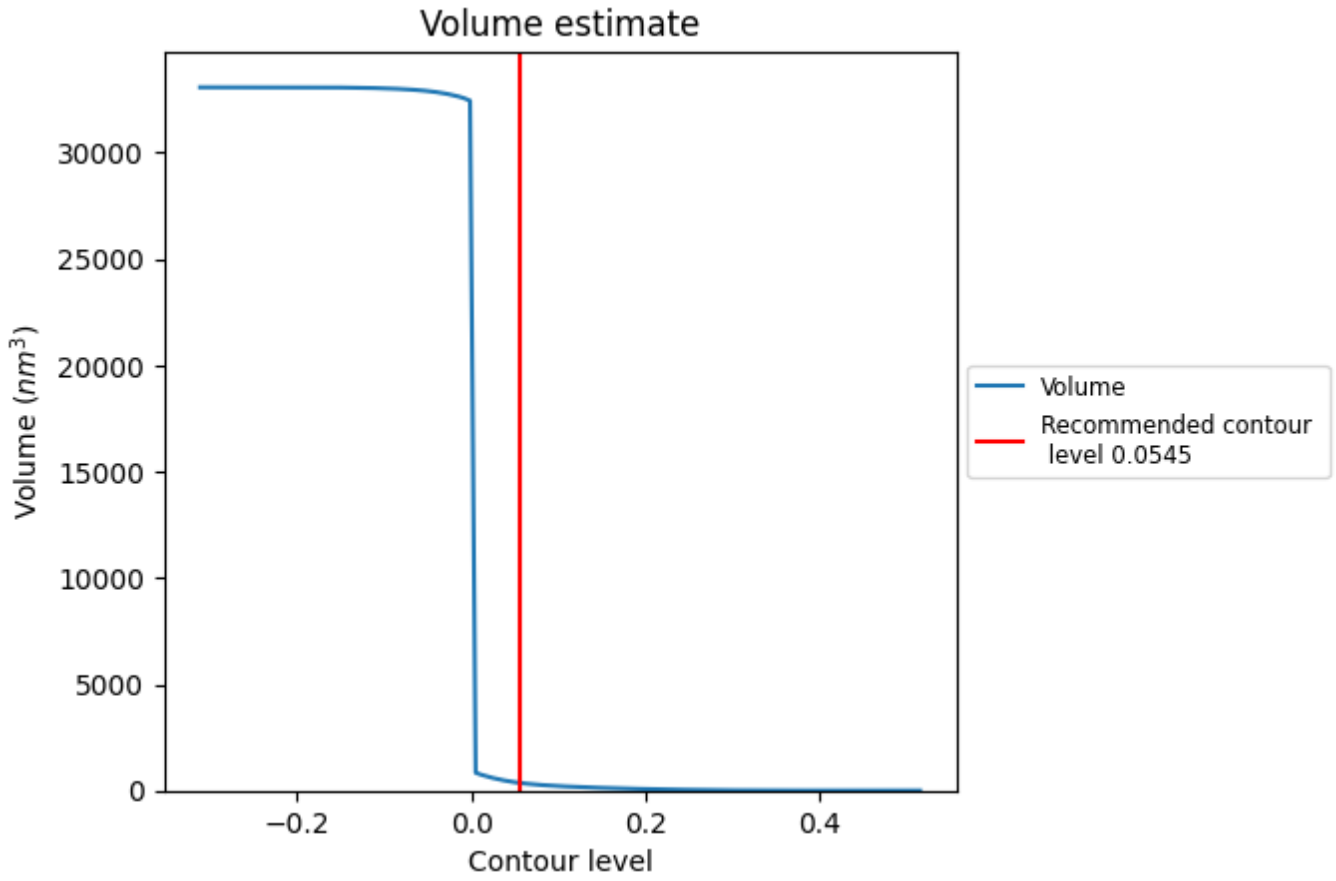
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

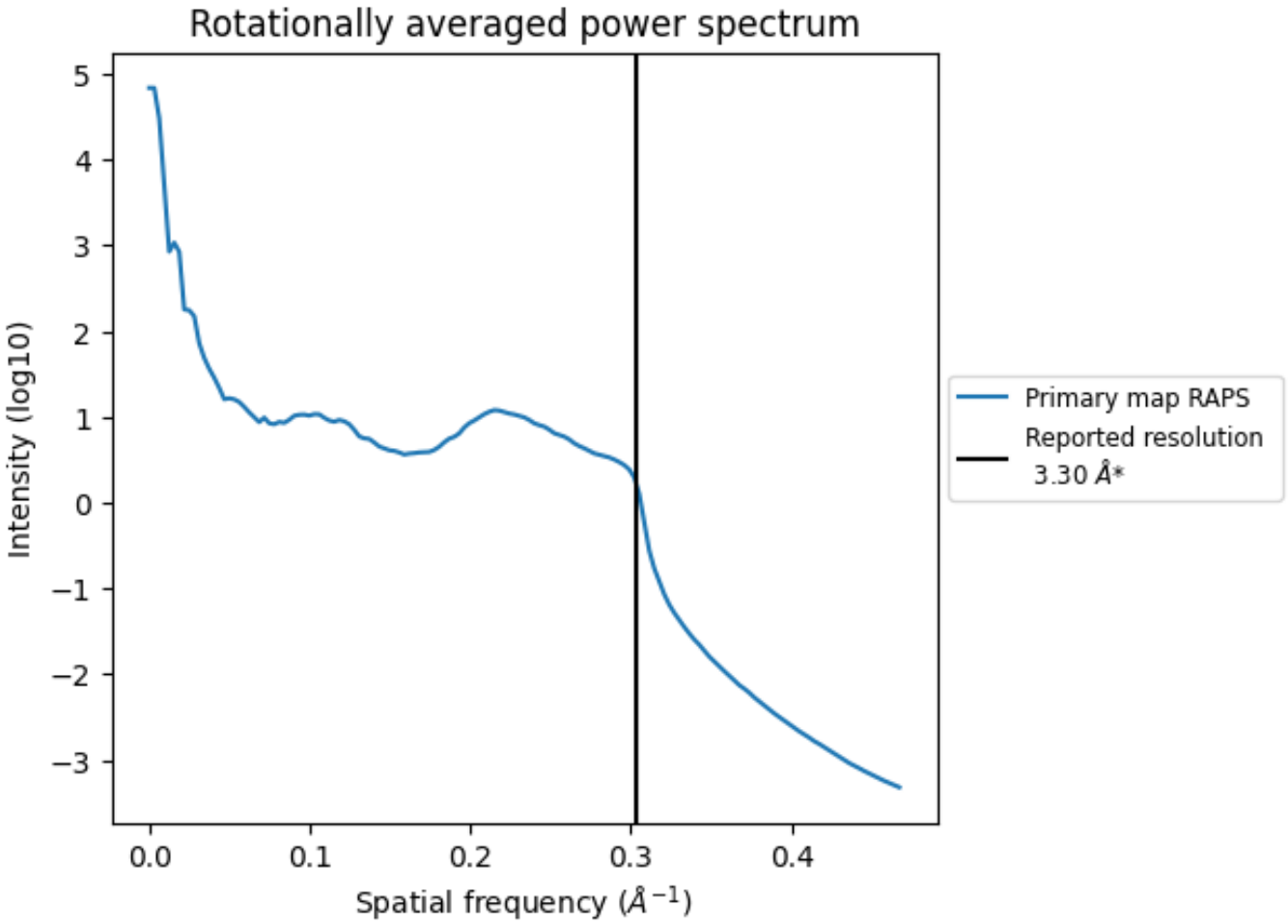
7.2 Volume estimate



The volume at the recommended contour level is 365 nm^3; this corresponds to an approximate mass of 330 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 0.303 Å^{-1}

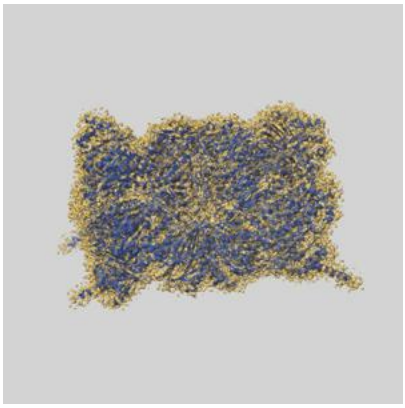
8 Fourier-Shell correlation

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

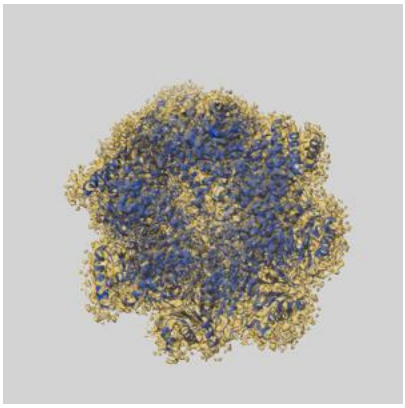
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4591 and PDB model 6QM8. Per-residue inclusion information can be found in section 3 on page 7.

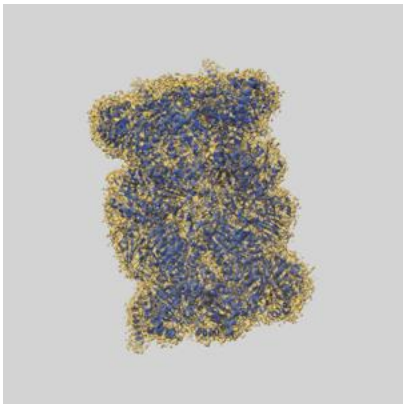
9.1 Map-model overlay



X



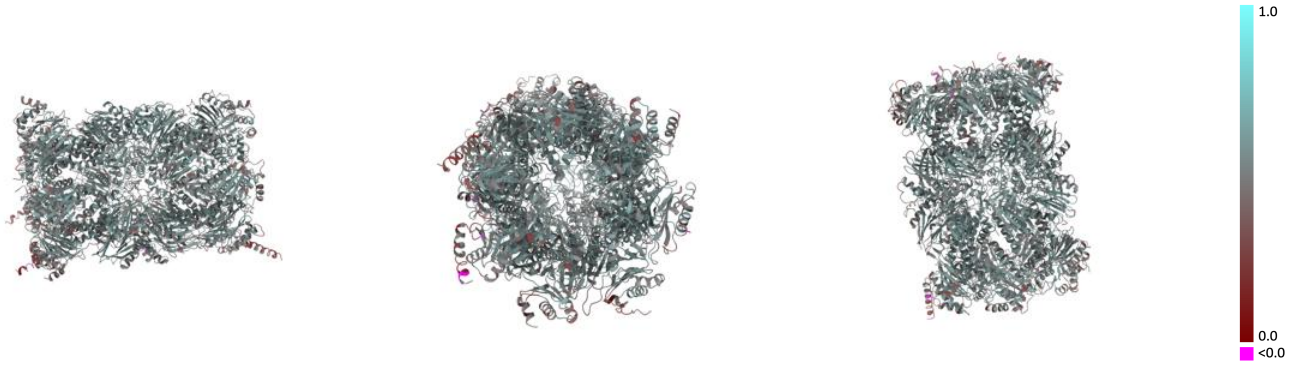
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0545 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.

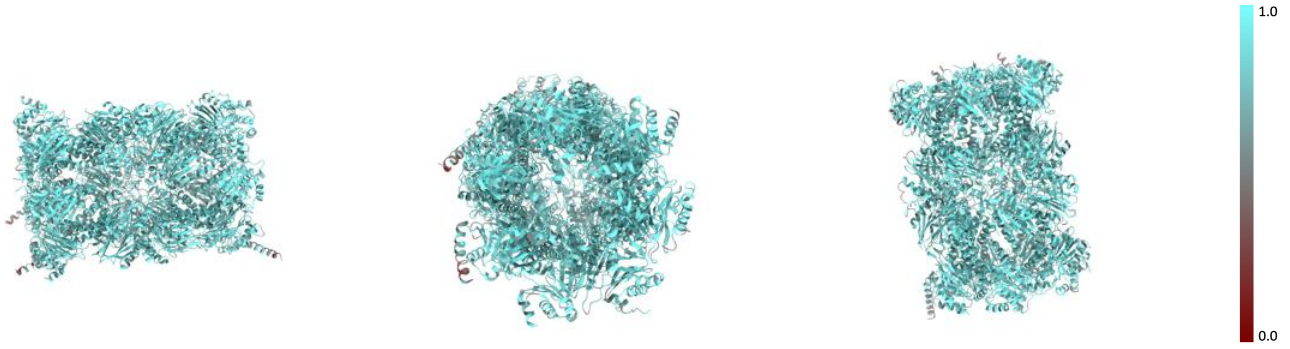
9.2 Q-score mapped to coordinate model (i)



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.

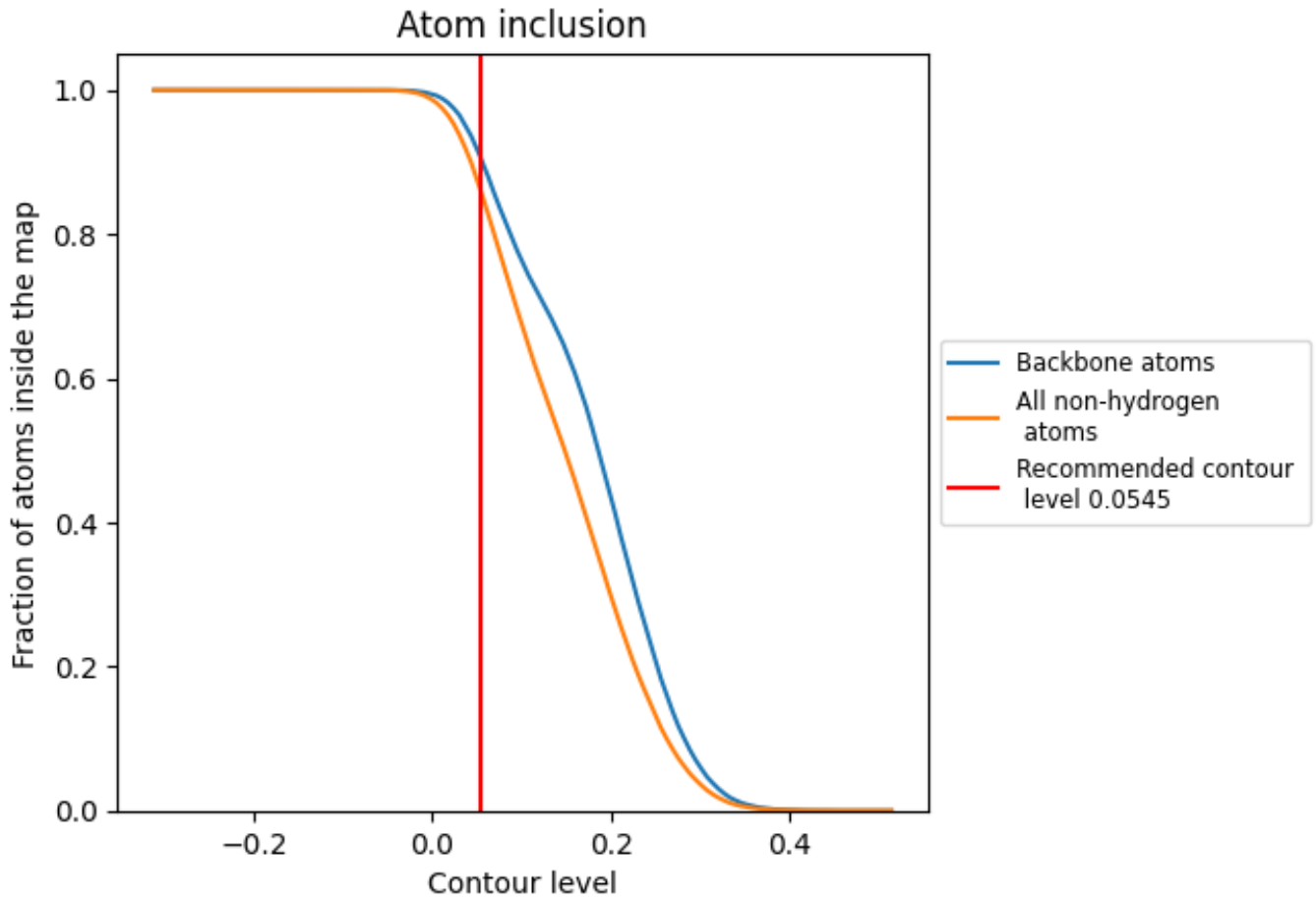
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0545).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.0545) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.5160
A	0.8636	0.5160
B	0.8627	0.5230
C	0.8310	0.4880
D	0.8131	0.4750
E	0.8334	0.4920
F	0.8500	0.5060
G	0.8507	0.5050
H	0.9014	0.5480
I	0.8640	0.5260
J	0.8685	0.5310
K	0.8579	0.5230
L	0.8598	0.5270
M	0.8518	0.5140
N	0.8784	0.5420
O	0.8702	0.5190
P	0.8795	0.5240
Q	0.8501	0.4960
R	0.8098	0.4740
S	0.8503	0.4930
T	0.8588	0.5130
U	0.8655	0.5140
V	0.9044	0.5480
W	0.8609	0.5190
X	0.8815	0.5360
Y	0.8617	0.5220
Z	0.8826	0.5290
a	0.8494	0.5220
b	0.8946	0.5410