



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 01:30 PM EDT

PDB ID : 9Y0K / pdb_00009y0k
EMDB ID : EMD-72394
Title : Structure of Plasmodium falciparum 20S proteasome with bound J80
Authors : Zhang, H.; Zhao, J.; Fajtova, P.; O'Donoghue, A.J.
Deposited on : 2025-08-28
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

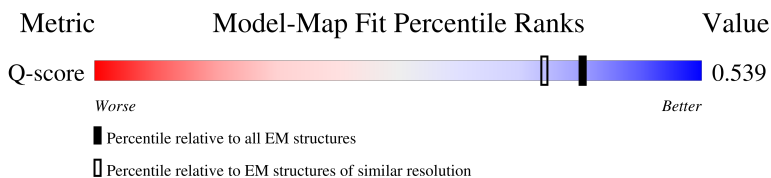
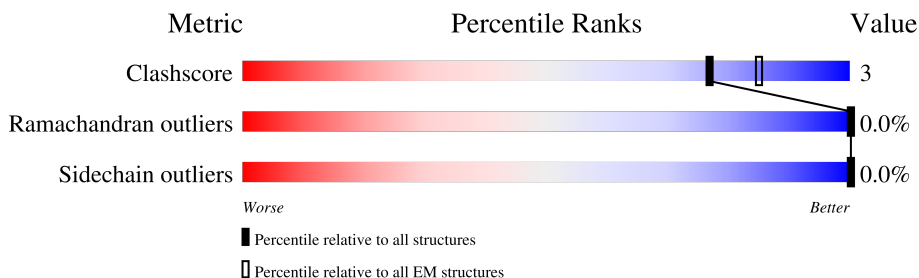
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	260	<div> <div>28%</div> <div>88%</div> <div>6%</div> <div>5%</div> </div>
1	O	260	<div> <div>22%</div> <div>88%</div> <div>6%</div> <div>5%</div> </div>
2	B	235	<div> <div>32%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
2	P	235	<div> <div>29%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	246	
3	Q	246	
4	D	241	
4	R	241	
5	E	256	
5	S	256	
6	F	254	
6	T	254	
7	G	252	
7	U	252	
8	H	252	
8	V	252	
9	I	229	
9	W	229	
10	J	218	
10	X	218	
11	K	195	
11	Y	195	
12	L	210	
12	Z	210	
13	M	240	
13	a	240	
14	N	302	
14	b	302	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 48226 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	246	Total	C	N	O	S	0	0
			1854	1171	313	358	12		
1	O	246	Total	C	N	O	S	0	0
			1854	1171	313	358	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	227	Total	C	N	O	S	0	0
			1692	1100	278	308	6		
2	P	227	Total	C	N	O	S	0	0
			1692	1100	278	308	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	240	Total	C	N	O	S	0	0
			1797	1156	296	342	3		
3	Q	240	Total	C	N	O	S	0	0
			1797	1156	296	342	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1757	1131	306	312	8		
4	R	233	Total	C	N	O	S	0	0
			1757	1131	306	312	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	231	Total	C	N	O	S	0	0
			1719	1085	288	336	10		
5	S	231	Total	C	N	O	S	0	0
			1719	1085	288	336	10		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	232	Total	C	N	O	S	0	0
			1758	1129	290	329	10		
6	T	232	Total	C	N	O	S	0	0
			1758	1129	290	329	10		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	245	Total	C	N	O	S	0	0
			1968	1257	331	368	12		
7	U	245	Total	C	N	O	S	0	0
			1968	1257	331	368	12		

- Molecule 8 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	204	Total	C	N	O	S	0	0
			1622	1038	280	294	10		
8	V	204	Total	C	N	O	S	0	0
			1622	1038	280	294	10		

- Molecule 9 is a protein called Proteasome subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	211	Total	C	N	O	S	0	0
			1545	980	271	281	13		
9	W	211	Total	C	N	O	S	0	0
			1545	980	271	281	13		

- Molecule 10 is a protein called Proteasome subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	208	Total	C	N	O	S	0	0
			1615	1035	264	304	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	208	Total	C	N	O	S	0	0
			1615	1035	264	304	12		

- Molecule 11 is a protein called Proteasome subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1582	1026	264	285	7		
11	Y	195	Total	C	N	O	S	0	0
			1582	1026	264	285	7		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	210	Total	C	N	O	S	0	0
			1636	1047	272	310	7		
12	Z	210	Total	C	N	O	S	0	0
			1636	1047	272	310	7		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1662	1064	276	316	6		
13	a	212	Total	C	N	O	S	0	0
			1662	1064	276	316	6		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	230	Total	C	N	O	S	0	0
			1851	1188	318	338	7		
14	b	230	Total	C	N	O	S	0	0
			1851	1188	318	338	7		

- Molecule 15 is N,N-diethyl-N 2 -hexanoyl-D-asparaginy-N-{(1S)-2-(2,4-difluorophenyl)-1-[(2S,3S,5S,6S)-5-formyl-2-hydroxy-3-(hydroxymethyl)-3,6-dimethylmorpholin-2-yl]ethyl}-4-fluoro-L-phenylalaninamide (CCD ID: A1CRO) (formula: C₃₉H₅₄F₃N₅O₈) (labeled as "Ligand of Interest" by depositor).

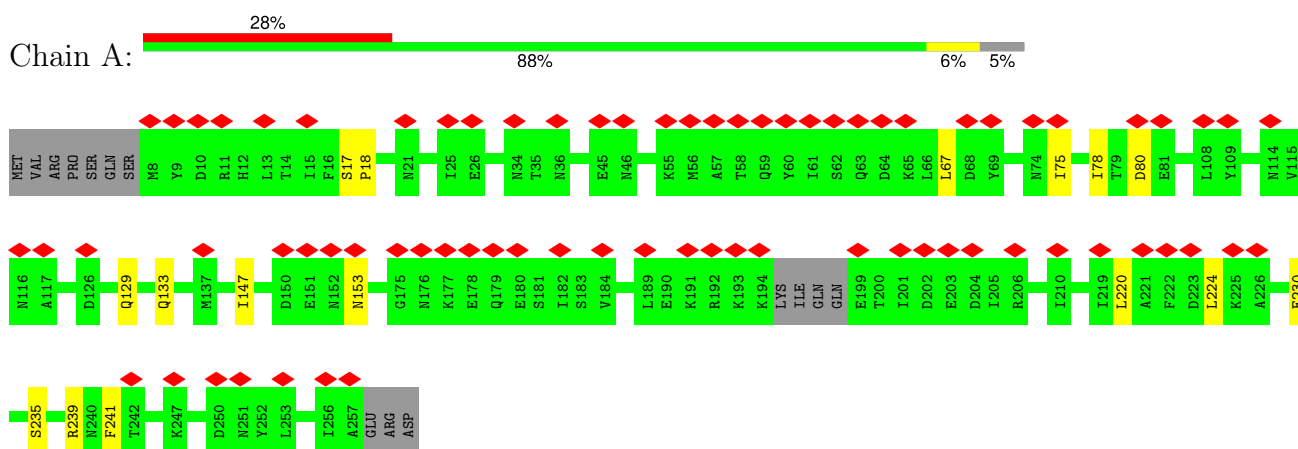


Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total 55	C 39	F 3	N 5	O 8	0
15	Z	1	Total 55	C 39	F 3	N 5	O 8	0

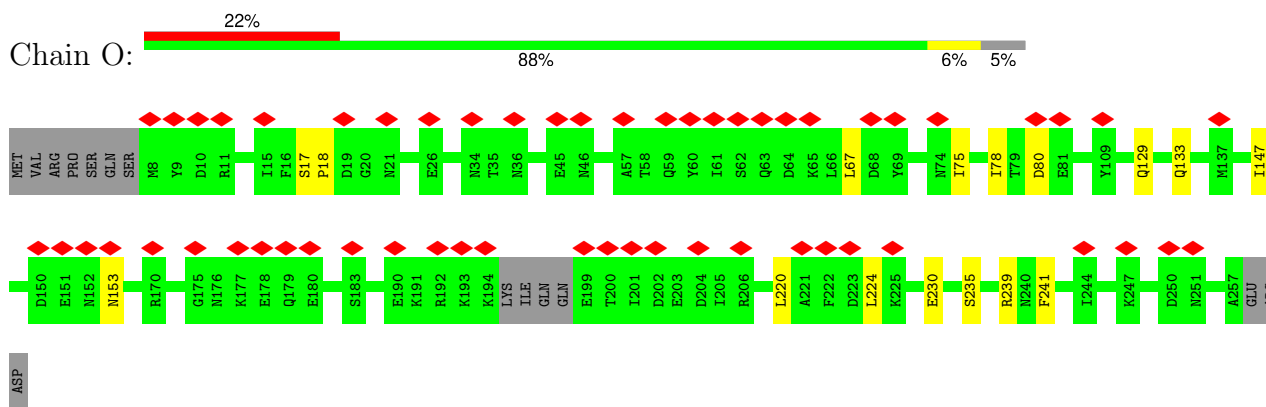
3 Residue-property plots

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.

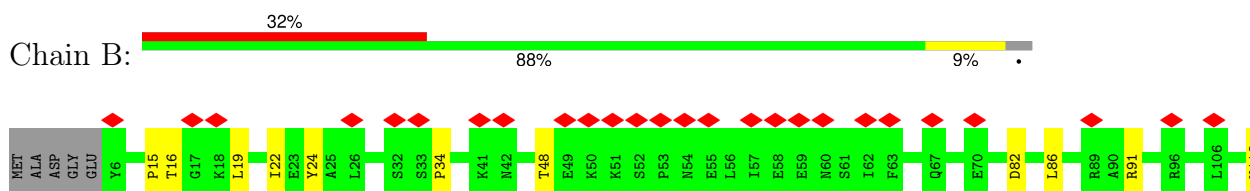
- Molecule 1: Proteasome subunit alpha type-6



- Molecule 1: Proteasome subunit alpha type-6

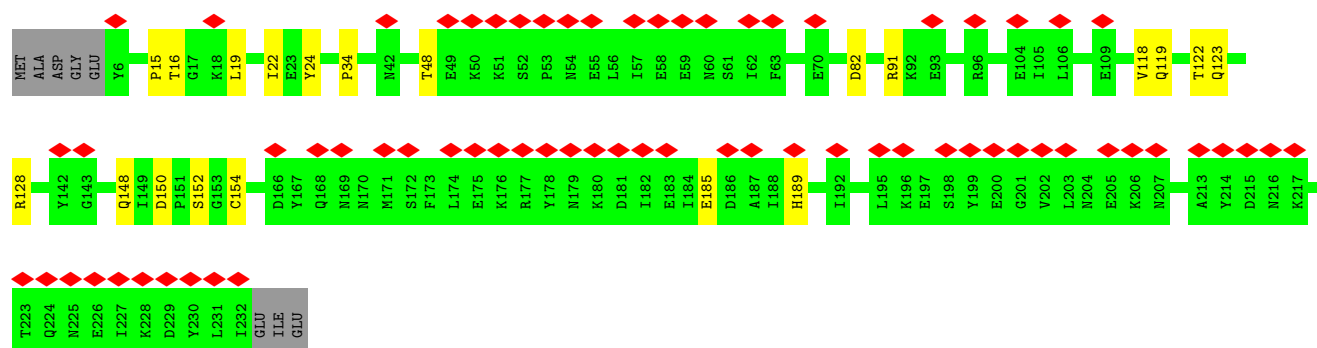
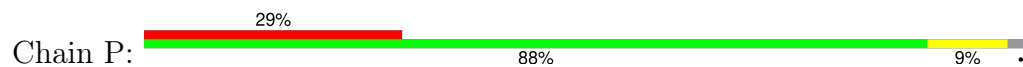


- Molecule 2: Proteasome subunit alpha type-2

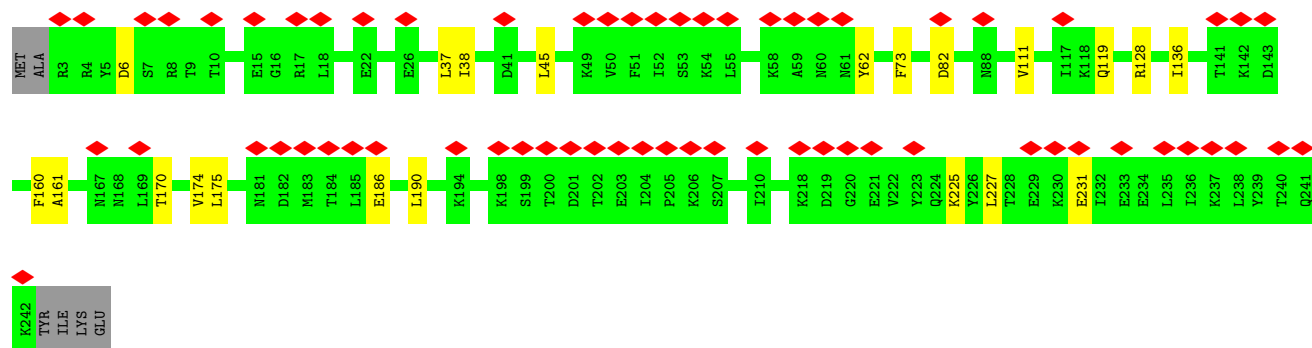
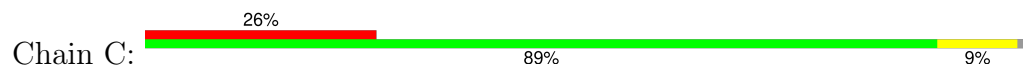




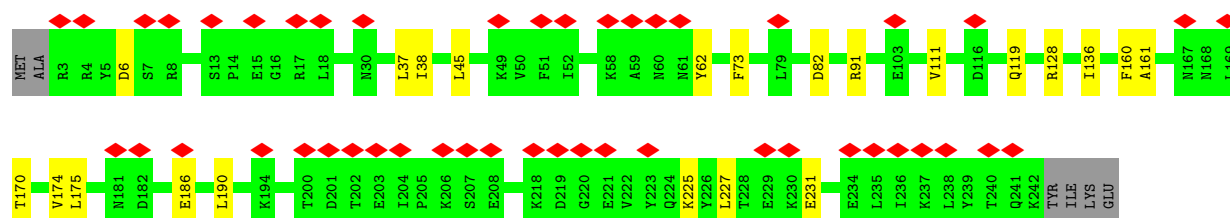
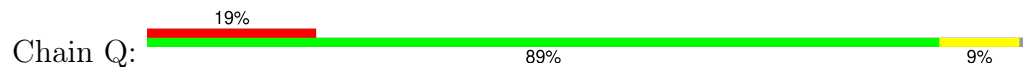
• Molecule 2: Proteasome subunit alpha type-2



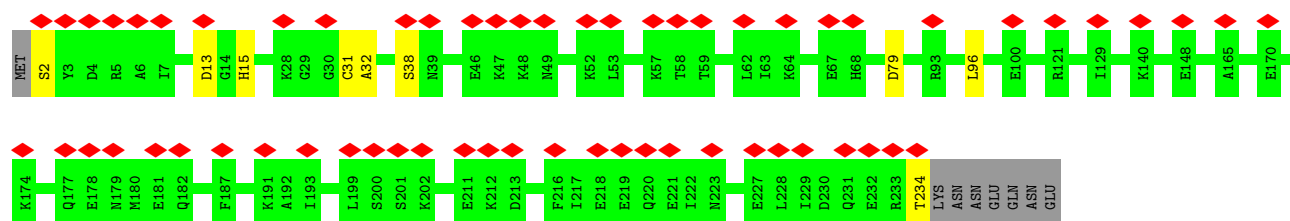
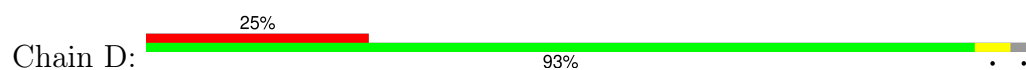
• Molecule 3: Proteasome subunit alpha type-3



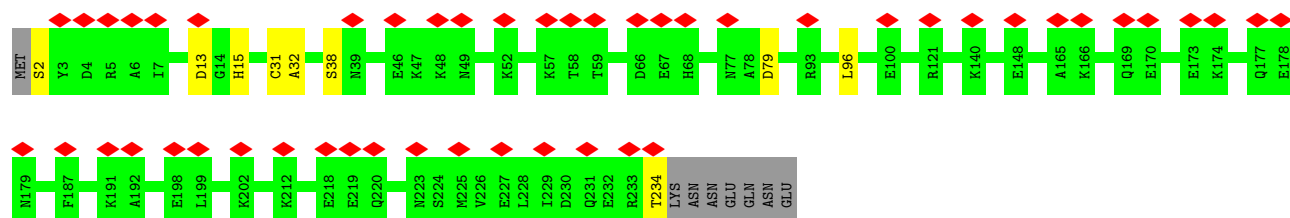
• Molecule 3: Proteasome subunit alpha type-3



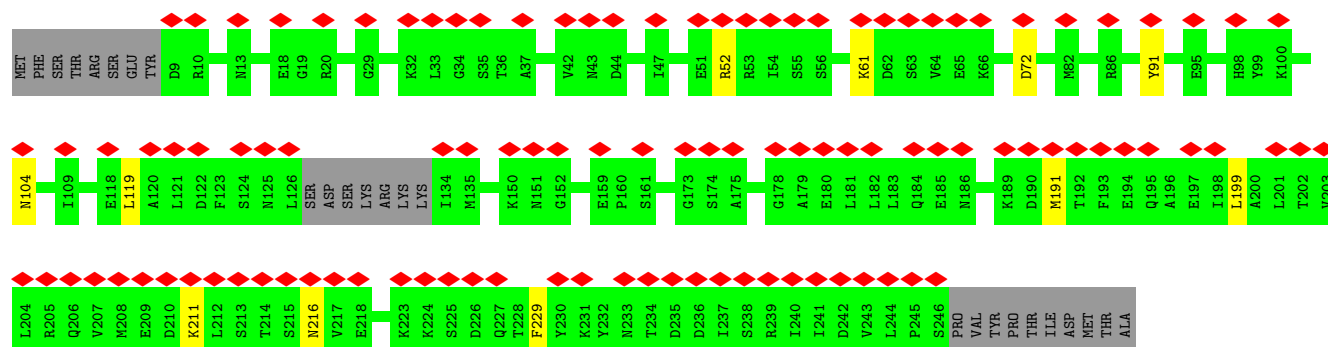
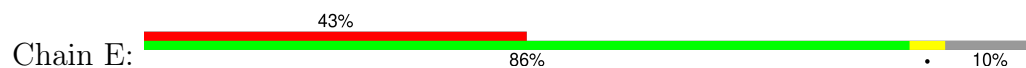
• Molecule 4: Proteasome subunit alpha type-4



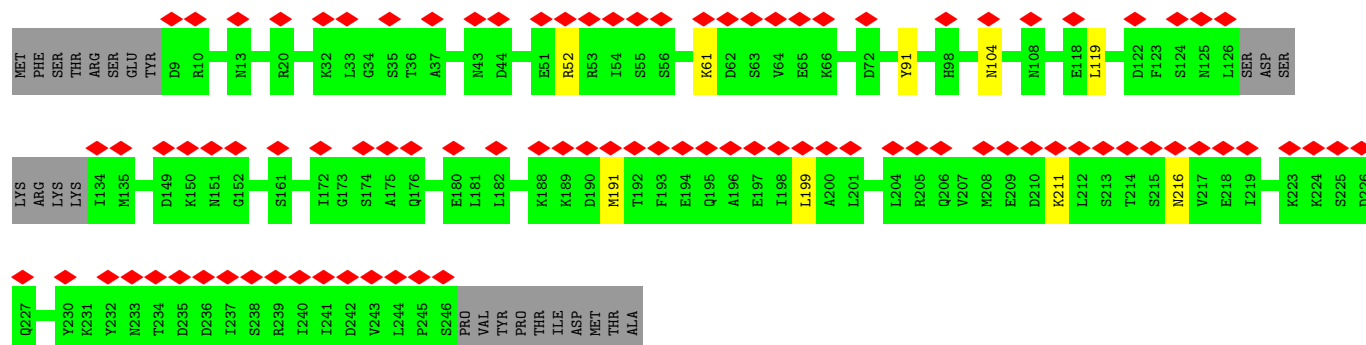
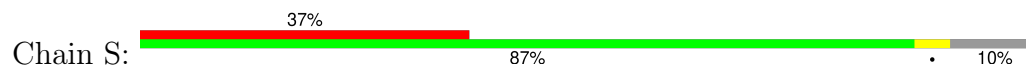
• Molecule 4: Proteasome subunit alpha type-4

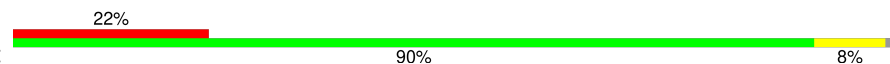


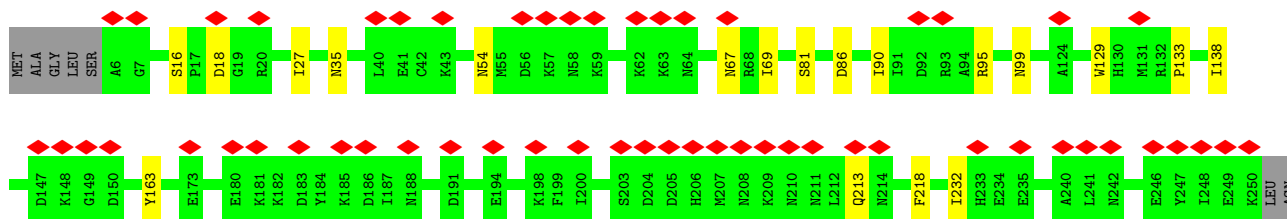
• Molecule 5: Proteasome subunit alpha type-5



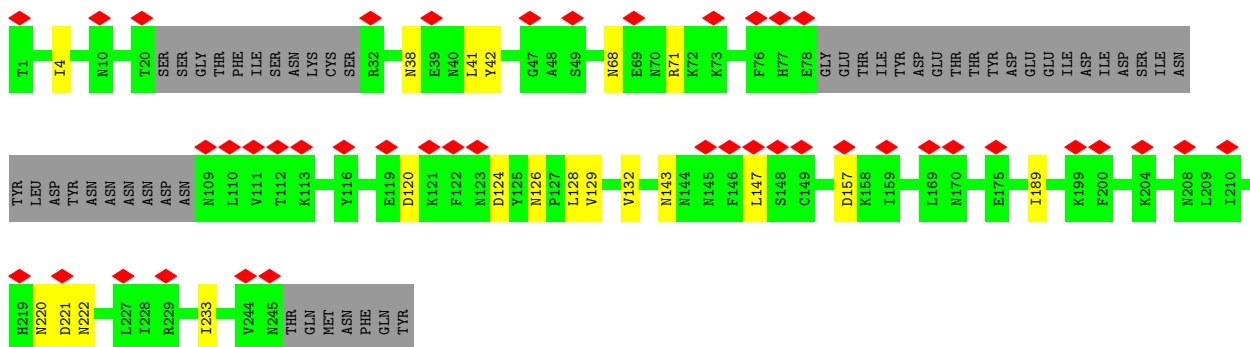
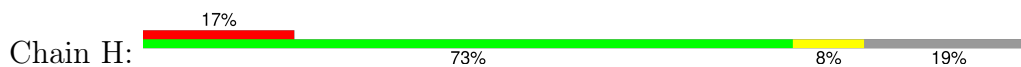
• Molecule 5: Proteasome subunit alpha type-5



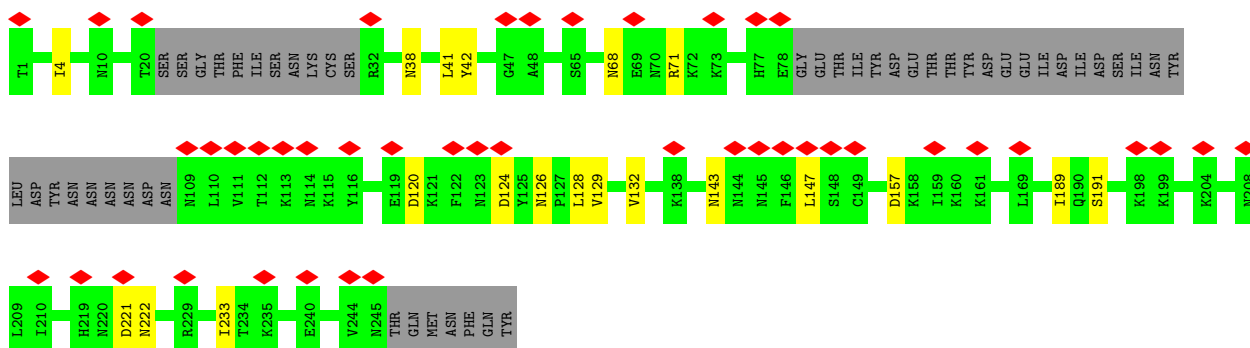
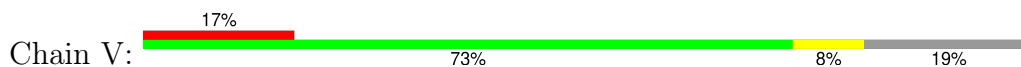




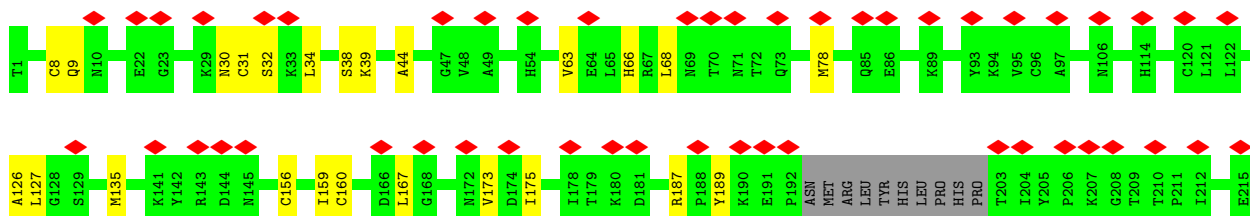
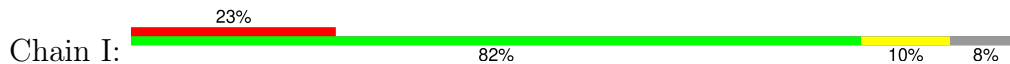
• Molecule 8: Proteasome endopeptidase complex

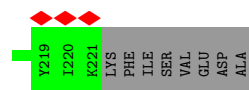


• Molecule 8: Proteasome endopeptidase complex

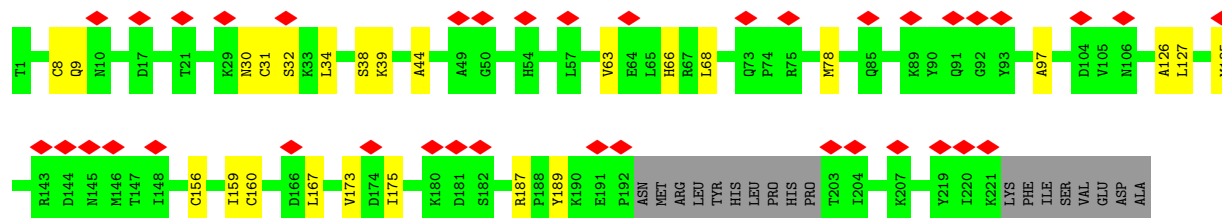
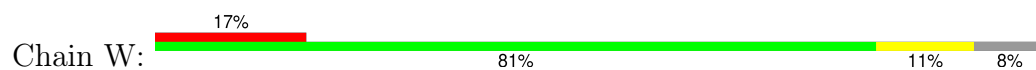


• Molecule 9: Proteasome subunit beta-2

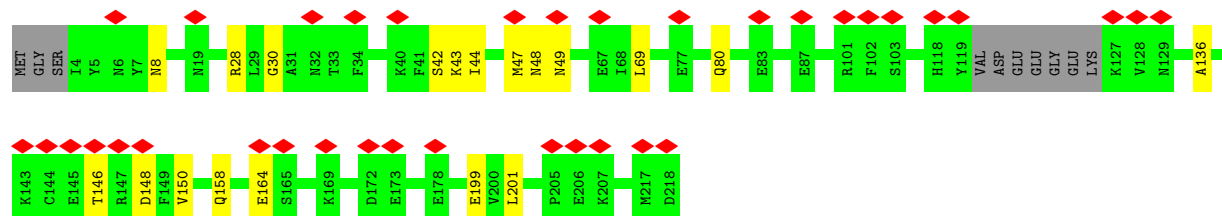
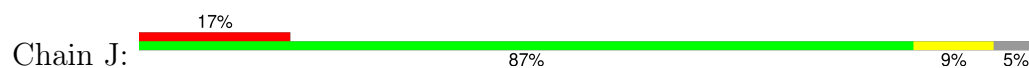




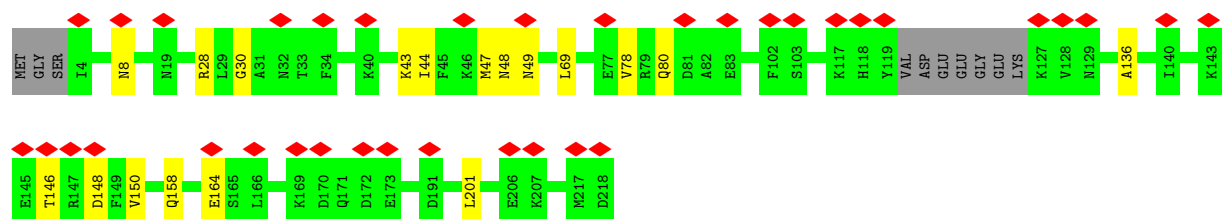
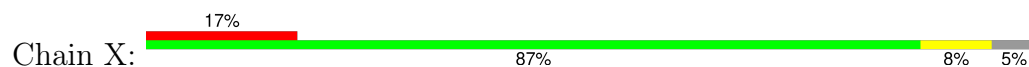
- Molecule 9: Proteasome subunit beta-2



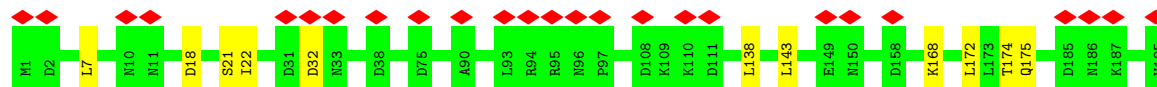
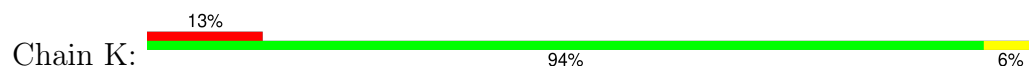
- Molecule 10: Proteasome subunit beta-3



- Molecule 10: Proteasome subunit beta-3

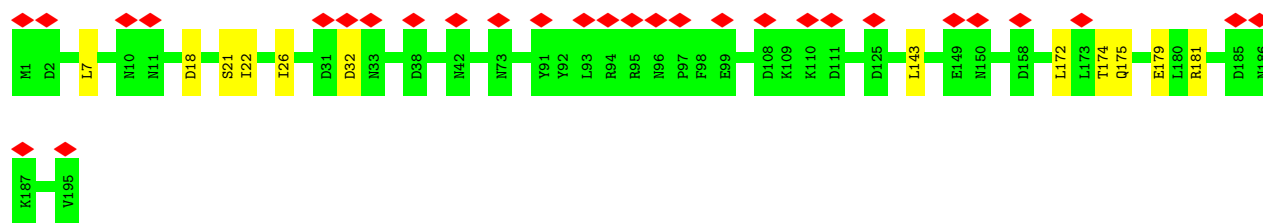


- Molecule 11: Proteasome subunit beta-4

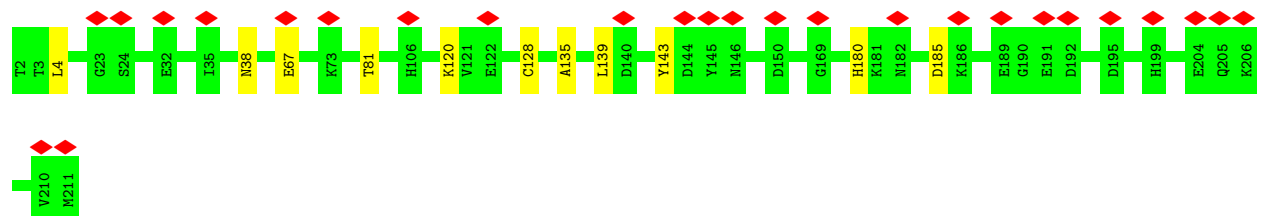


- Molecule 11: Proteasome subunit beta-4

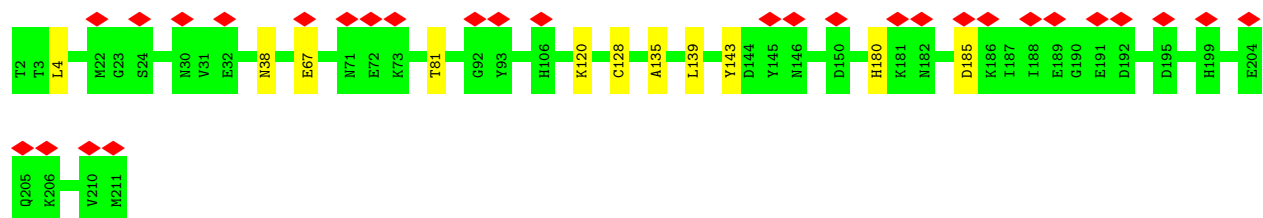




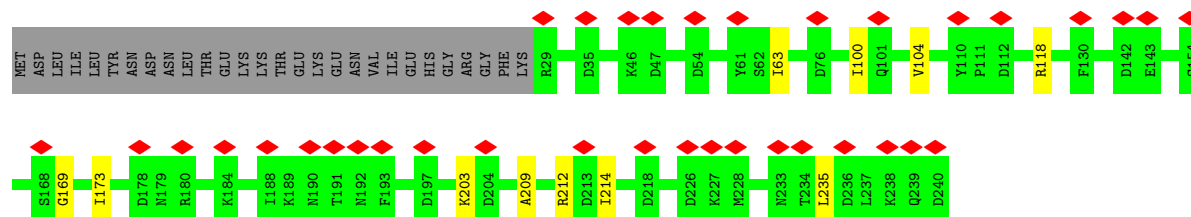
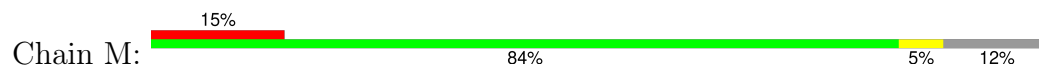
• Molecule 12: Proteasome subunit beta



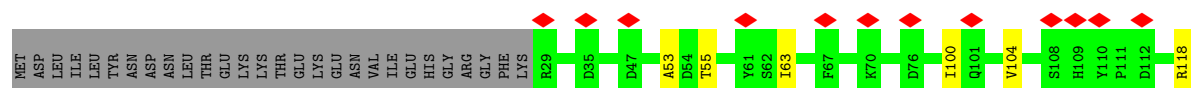
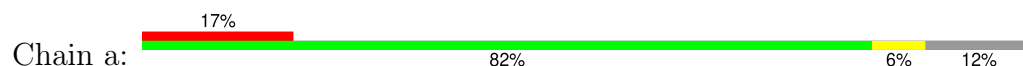
• Molecule 12: Proteasome subunit beta

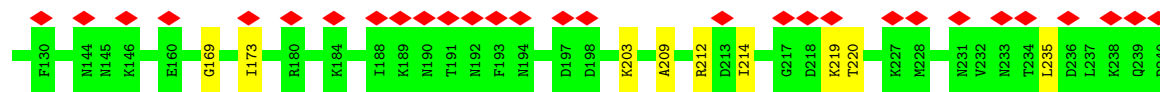


• Molecule 13: Proteasome subunit beta



• Molecule 13: Proteasome subunit beta

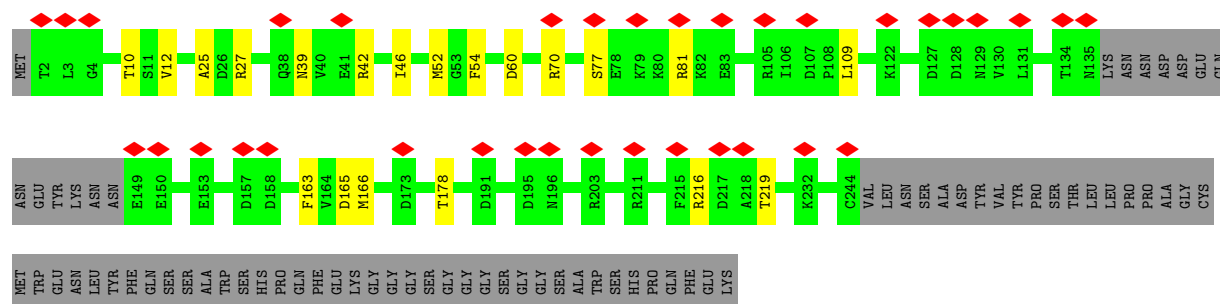




• Molecule 14: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133662	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	33.394	Depositor
Minimum map value	-21.165	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	10	Depositor
Map size (\AA)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1CRO

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	0.32	0/1880	0.62	0/2552
1	O	0.32	0/1880	0.62	0/2552
2	B	0.28	0/1726	0.56	0/2351
2	P	0.28	0/1726	0.56	0/2351
3	C	0.28	0/1832	0.59	0/2506
3	Q	0.28	0/1832	0.59	0/2506
4	D	0.28	0/1787	0.62	1/2423 (0.0%)
4	R	0.29	0/1787	0.62	1/2423 (0.0%)
5	E	0.27	0/1742	0.54	0/2364
5	S	0.27	0/1742	0.54	0/2364
6	F	0.30	0/1790	0.58	0/2424
6	T	0.30	0/1790	0.58	0/2424
7	G	0.34	0/2012	0.60	0/2727
7	U	0.34	0/2012	0.60	0/2727
8	H	0.31	0/1649	0.61	0/2215
8	V	0.31	0/1649	0.61	0/2215
9	I	0.31	0/1575	0.64	0/2147
9	W	0.31	0/1575	0.64	0/2147
10	J	0.30	0/1643	0.64	0/2223
10	X	0.30	0/1643	0.64	0/2223
11	K	0.28	0/1617	0.57	0/2184
11	Y	0.28	0/1617	0.57	0/2184
12	L	0.32	1/1670 (0.1%)	0.60	0/2253
12	Z	0.32	1/1670 (0.1%)	0.60	0/2253
13	M	0.27	0/1694	0.58	0/2300
13	a	0.28	0/1694	0.58	0/2300
14	N	0.27	0/1890	0.56	0/2555
14	b	0.27	0/1890	0.56	0/2555
All	All	0.30	2/49014 (0.0%)	0.59	2/66448 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	128	CYS	C-O	-6.57	1.16	1.23
12	Z	128	CYS	C-O	-6.49	1.16	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	234	THR	OG1-CB-CG2	6.00	121.30	109.30
4	R	234	THR	OG1-CB-CG2	5.97	121.25	109.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1854	0	1772	13	0
1	O	1854	0	1772	12	0
2	B	1692	0	1629	15	0
2	P	1692	0	1629	13	0
3	C	1797	0	1672	15	0
3	Q	1797	0	1672	15	0
4	D	1757	0	1745	4	0
4	R	1757	0	1745	4	0
5	E	1719	0	1656	7	0
5	S	1719	0	1656	6	0
6	F	1758	0	1696	14	0
6	T	1758	0	1696	14	0
7	G	1968	0	1881	14	0
7	U	1968	0	1881	13	0
8	H	1622	0	1613	13	0
8	V	1622	0	1613	13	0
9	I	1545	0	1515	17	0
9	W	1545	0	1515	18	0
10	J	1615	0	1586	11	0
10	X	1615	0	1586	11	0
11	K	1582	0	1536	8	0
11	Y	1582	0	1536	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1636	0	1580	6	0
12	Z	1636	0	1580	6	0
13	M	1662	0	1646	9	0
13	a	1662	0	1646	11	0
14	N	1851	0	1803	15	0
14	b	1851	0	1803	13	0
15	L	55	0	0	0	0
15	Z	55	0	0	0	0
All	All	48226	0	46660	267	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 3.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:4:LEU:HD11	12:L:139:LEU:HD11	1.59	0.85
12:Z:4:LEU:HD11	12:Z:139:LEU:HD11	1.59	0.84
10:J:164:GLU:OE2	13:a:212:ARG:NE	2.25	0.70
9:W:156:CYS:O	9:W:160:CYS:HB3	1.93	0.69
9:I:156:CYS:O	9:I:160:CYS:HB3	1.93	0.68
5:S:104:ASN:OD1	13:a:118:ARG:NH1	2.26	0.68
2:B:119:GLN:NE2	3:C:82:ASP:OD1	2.28	0.67
1:O:220:LEU:HD12	1:O:224:LEU:HD21	1.78	0.66
11:Y:18:ASP:OD2	11:Y:175:GLN:NE2	2.28	0.66
12:Z:139:LEU:O	12:Z:143:TYR:N	2.28	0.66
1:A:220:LEU:HD12	1:A:224:LEU:HD21	1.78	0.66
7:G:99:ASN:OD1	14:N:70:ARG:NH1	2.29	0.66
6:T:117:GLN:NE2	7:U:86:ASP:OD1	2.29	0.66
12:L:139:LEU:O	12:L:143:TYR:N	2.28	0.65
11:K:22:ILE:HD12	11:Y:172:LEU:HD13	1.77	0.65
11:K:18:ASP:OD2	11:K:175:GLN:NE2	2.28	0.65
3:Q:37:LEU:HD21	3:Q:175:LEU:HD22	1.78	0.64
1:A:133:GLN:NE2	2:B:128:ARG:O	2.29	0.64
3:C:37:LEU:HD21	3:C:175:LEU:HD22	1.78	0.64
2:P:119:GLN:NE2	3:Q:82:ASP:OD1	2.29	0.64
6:F:117:GLN:NE2	7:G:86:ASP:OD1	2.30	0.64
7:U:99:ASN:OD1	14:b:70:ARG:NH1	2.30	0.64
11:K:7:LEU:HD13	11:K:143:LEU:HD22	1.79	0.64
13:a:173:ILE:HD11	13:a:209:ALA:HB2	1.80	0.64
10:X:28:ARG:O	10:X:43:LYS:NZ	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:7:LEU:HD13	11:Y:143:LEU:HD22	1.79	0.64
13:M:212:ARG:NE	10:X:164:GLU:OE2	2.26	0.63
11:K:172:LEU:HD13	11:Y:22:ILE:HD12	1.81	0.63
13:M:173:ILE:HD11	13:M:209:ALA:HB2	1.80	0.63
1:O:133:GLN:NE2	2:P:128:ARG:O	2.32	0.63
12:L:180:HIS:NE2	12:L:185:ASP:OD2	2.30	0.63
5:E:104:ASN:OD1	13:M:118:ARG:NH1	2.32	0.62
10:X:8:ASN:ND2	10:X:30:GLY:O	2.32	0.62
12:L:38:ASN:ND2	12:L:67:GLU:OE2	2.32	0.62
12:Z:38:ASN:ND2	12:Z:67:GLU:OE2	2.32	0.62
1:A:80:ASP:OD1	8:H:71:ARG:NH2	2.32	0.62
12:Z:180:HIS:NE2	12:Z:185:ASP:OD2	2.30	0.62
10:J:28:ARG:O	10:J:43:LYS:NZ	2.31	0.62
10:J:8:ASN:ND2	10:J:30:GLY:O	2.32	0.62
6:T:139:ASN:OD1	14:b:81:ARG:NH2	2.33	0.62
7:U:218:PHE:HB3	7:U:232:ILE:HD12	1.83	0.61
7:G:218:PHE:HB3	7:G:232:ILE:HD12	1.83	0.60
1:O:80:ASP:OD1	8:V:71:ARG:NH2	2.35	0.60
8:H:4:ILE:HD11	8:H:189:ILE:HD11	1.83	0.60
7:U:95:ARG:NH2	14:b:77:SER:O	2.35	0.60
2:P:185:GLU:O	2:P:189:HIS:ND1	2.32	0.60
9:W:31:CYS:SG	9:W:32:SER:N	2.75	0.60
9:I:31:CYS:SG	9:I:32:SER:N	2.75	0.59
7:G:95:ARG:NH2	14:N:77:SER:O	2.36	0.59
1:A:129:GLN:NE2	2:B:82:ASP:OD1	2.36	0.58
8:V:4:ILE:HD11	8:V:189:ILE:HD11	1.83	0.58
6:F:116:TYR:O	6:F:120:THR:HG23	2.03	0.58
3:Q:225:LYS:NZ	3:Q:231:GLU:OE1	2.36	0.58
3:C:225:LYS:NZ	3:C:231:GLU:OE1	2.36	0.58
9:I:135:MET:HE1	14:b:216:ARG:NE	2.19	0.58
6:F:157:ALA:HB1	6:F:171:LEU:HD13	1.87	0.57
6:T:116:TYR:O	6:T:120:THR:HG23	2.03	0.57
1:A:78:ILE:O	8:H:68:ASN:ND2	2.38	0.57
14:N:216:ARG:NE	9:W:135:MET:HE1	2.20	0.57
2:P:152:SER:OG	2:P:154:CYS:SG	2.63	0.56
6:F:62:LYS:NZ	6:F:74:MET:O	2.36	0.56
6:F:11:ILE:HD13	6:F:123:SER:HB2	1.88	0.56
6:T:11:ILE:HD13	6:T:123:SER:HB2	1.88	0.55
6:T:157:ALA:HB1	6:T:171:LEU:HD13	1.87	0.55
2:B:185:GLU:O	2:B:189:HIS:ND1	2.32	0.55
3:Q:119:GLN:NE2	4:R:79:ASP:OD1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:211:LYS:O	5:S:216:ASN:ND2	2.40	0.55
6:F:139:ASN:OD1	14:N:81:ARG:NH2	2.40	0.54
14:b:46:ILE:HD11	14:b:52:MET:HB2	1.88	0.54
11:K:168:LYS:O	11:K:174:THR:OG1	2.20	0.54
14:N:46:ILE:HD11	14:N:52:MET:HB2	1.88	0.54
11:K:174:THR:HG23	11:Y:174:THR:HG23	1.90	0.54
14:N:42:ARG:NH1	14:N:54:PHE:O	2.41	0.54
5:E:211:LYS:O	5:E:216:ASN:ND2	2.40	0.54
4:R:13:ASP:OD2	4:R:15:HIS:ND1	2.41	0.54
3:Q:62:TYR:OH	3:Q:227:LEU:O	2.25	0.54
7:U:90:ILE:HG21	7:U:138:ILE:HD13	1.90	0.54
9:W:156:CYS:O	9:W:160:CYS:CB	2.56	0.54
4:D:13:ASP:OD2	4:D:15:HIS:ND1	2.41	0.53
14:b:42:ARG:NH1	14:b:54:PHE:O	2.41	0.53
8:H:41:LEU:HD21	8:H:132:VAL:HG11	1.89	0.53
8:V:41:LEU:HD21	8:V:132:VAL:HG11	1.90	0.53
14:N:216:ARG:CD	9:W:135:MET:HE1	2.39	0.53
9:I:63:VAL:HG22	9:I:78:MET:HE1	1.91	0.53
3:C:62:TYR:OH	3:C:227:LEU:O	2.25	0.52
3:C:119:GLN:NE2	4:D:79:ASP:OD1	2.43	0.52
9:I:156:CYS:O	9:I:160:CYS:CB	2.56	0.52
1:O:78:ILE:O	8:V:68:ASN:ND2	2.43	0.52
7:G:90:ILE:HG21	7:G:138:ILE:HD13	1.90	0.52
1:A:147:ILE:HD11	1:A:241:PHE:HE1	1.76	0.51
9:I:175:ILE:HD12	9:I:189:TYR:CD2	2.46	0.51
1:O:147:ILE:HD11	1:O:241:PHE:HE1	1.75	0.51
2:B:152:SER:HG	2:B:154:CYS:HG	1.55	0.51
10:J:146:THR:HG22	10:J:148:ASP:OD1	2.10	0.51
9:W:175:ILE:HD12	9:W:189:TYR:CD2	2.46	0.51
6:F:63:ILE:HD12	6:F:210:ALA:HB1	1.93	0.51
13:M:169:GLY:O	13:M:173:ILE:HD12	2.11	0.51
10:X:136:ALA:HB2	10:X:150:VAL:CG2	2.40	0.51
9:I:135:MET:HE1	14:b:216:ARG:CD	2.40	0.51
8:H:143:ASN:CB	8:H:147:LEU:HD23	2.41	0.51
1:O:129:GLN:NE2	2:P:82:ASP:OD1	2.42	0.51
10:X:146:THR:HG22	10:X:148:ASP:OD1	2.10	0.51
2:B:152:SER:OG	2:B:154:CYS:SG	2.63	0.51
10:J:136:ALA:HB2	10:J:150:VAL:CG2	2.40	0.51
9:W:63:VAL:HG22	9:W:78:MET:HE1	1.92	0.51
13:a:169:GLY:O	13:a:173:ILE:HD12	2.11	0.51
8:V:143:ASN:HB2	8:V:147:LEU:HD23	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:34:PRO:O	2:P:48:THR:OG1	2.25	0.50
8:V:143:ASN:CB	8:V:147:LEU:HD23	2.41	0.50
6:T:63:ILE:HD12	6:T:210:ALA:HB1	1.93	0.50
3:Q:6:ASP:OD2	4:R:2:SER:OG	2.26	0.50
6:F:72:ILE:HD11	6:F:85:THR:HG22	1.94	0.50
7:U:67:ASN:ND2	7:U:69:ILE:O	2.45	0.50
7:G:67:ASN:ND2	7:G:69:ILE:O	2.45	0.49
4:R:31:CYS:SG	4:R:32:ALA:N	2.85	0.49
8:H:143:ASN:HB2	8:H:147:LEU:HD23	1.93	0.49
4:D:31:CYS:SG	4:D:32:ALA:N	2.85	0.49
2:P:118:VAL:O	2:P:122:THR:HG23	2.12	0.49
14:b:163:PHE:HE1	14:b:178:THR:HG22	1.77	0.49
2:B:118:VAL:O	2:B:122:THR:HG23	2.12	0.48
3:C:38:ILE:HD12	3:C:160:PHE:HA	1.95	0.48
10:J:158:GLN:N	10:J:158:GLN:OE1	2.45	0.48
14:N:163:PHE:HE1	14:N:178:THR:HG22	1.77	0.48
9:W:8:CYS:SG	9:W:9:GLN:N	2.85	0.48
1:O:18:PRO:HA	2:P:24:TYR:CE1	2.49	0.48
9:I:30:ASN:OD1	9:I:187:ARG:NH1	2.46	0.48
6:T:72:ILE:HD11	6:T:85:THR:HG22	1.94	0.48
2:P:123:GLN:NE2	3:Q:128:ARG:O	2.46	0.48
8:V:128:LEU:HD22	8:V:157:ASP:OD2	2.14	0.48
10:X:158:GLN:OE1	10:X:158:GLN:N	2.45	0.48
9:I:159:ILE:HG21	9:I:173:VAL:HG23	1.96	0.48
10:J:48:ASN:OD1	10:J:49:ASN:N	2.47	0.48
9:W:159:ILE:HG21	9:W:173:VAL:HG23	1.96	0.48
3:Q:38:ILE:HD12	3:Q:160:PHE:HA	1.95	0.47
9:I:126:ALA:O	9:I:127:LEU:HD23	2.14	0.47
1:A:153:ASN:OD1	1:A:239:ARG:NH2	2.48	0.47
2:B:34:PRO:O	2:B:48:THR:OG1	2.25	0.47
6:T:34:CYS:SG	6:T:35:ALA:N	2.88	0.47
1:O:153:ASN:OD1	1:O:239:ARG:NH2	2.48	0.47
9:I:8:CYS:SG	9:I:9:GLN:N	2.85	0.47
10:J:80:GLN:N	10:J:80:GLN:OE1	2.48	0.47
3:Q:37:LEU:HD23	3:Q:161:ALA:HB1	1.97	0.47
9:W:126:ALA:O	9:W:127:LEU:HD23	2.14	0.47
8:H:128:LEU:HD22	8:H:157:ASP:OD2	2.14	0.47
3:Q:111:VAL:HG12	3:Q:136:ILE:CD1	2.45	0.47
10:X:80:GLN:OE1	10:X:80:GLN:N	2.48	0.47
3:C:111:VAL:HG12	3:C:136:ILE:CD1	2.45	0.47
13:M:173:ILE:HD11	13:M:209:ALA:CB	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:HA	2:B:24:TYR:CE1	2.50	0.47
3:C:37:LEU:HD23	3:C:161:ALA:HB1	1.97	0.47
7:G:35:ASN:OD1	7:G:54:ASN:ND2	2.48	0.47
9:W:30:ASN:OD1	9:W:187:ARG:NH1	2.46	0.47
6:F:34:CYS:SG	6:F:35:ALA:N	2.88	0.46
7:U:35:ASN:OD1	7:U:54:ASN:ND2	2.48	0.46
6:T:11:ILE:HD12	7:U:129:TRP:O	2.15	0.46
6:F:161:GLY:O	6:F:164:SER:OG	2.25	0.46
2:B:91:ARG:HD3	9:I:68:LEU:HD13	1.98	0.46
7:G:35:ASN:O	7:G:81:SER:OG	2.25	0.46
8:H:42:TYR:HB2	8:H:233:ILE:HD11	1.98	0.46
13:a:203:LYS:HD2	13:a:235:LEU:HD22	1.97	0.46
7:G:213:GLN:N	7:G:213:GLN:OE1	2.50	0.45
13:a:173:ILE:HD11	13:a:209:ALA:CB	2.45	0.45
11:Y:21:SER:OG	11:Y:32:ASP:OD1	2.35	0.45
13:a:55:THR:OG1	13:a:219:LYS:O	2.31	0.45
2:B:123:GLN:NE2	3:C:128:ARG:O	2.50	0.45
13:M:203:LYS:HD2	13:M:235:LEU:HD22	1.97	0.45
7:U:213:GLN:N	7:U:213:GLN:OE1	2.50	0.45
9:W:38:SER:OG	9:W:39:LYS:N	2.50	0.45
9:I:34:LEU:HD23	9:I:44:ALA:HB2	1.99	0.45
8:V:42:TYR:HB2	8:V:233:ILE:HD11	1.98	0.45
9:W:34:LEU:HD23	9:W:44:ALA:HB2	1.99	0.45
11:K:21:SER:OG	11:K:32:ASP:OD1	2.35	0.45
9:I:38:SER:OG	9:I:39:LYS:N	2.50	0.44
14:N:165:ASP:OD1	14:N:166:MET:N	2.50	0.44
12:L:81:THR:OG1	12:L:120:LYS:NZ	2.39	0.44
1:O:67:LEU:HD13	7:U:163:TYR:CE1	2.52	0.44
6:T:62:LYS:NZ	6:T:74:MET:O	2.36	0.44
12:Z:81:THR:OG1	12:Z:120:LYS:NZ	2.39	0.44
2:B:15:PRO:O	2:B:16:THR:OG1	2.29	0.44
3:C:111:VAL:HG12	3:C:136:ILE:HD13	2.00	0.44
3:C:6:ASP:OD2	4:D:2:SER:OG	2.30	0.44
8:H:129:VAL:HA	8:H:132:VAL:HG12	2.00	0.44
14:N:27:ARG:NH2	14:N:39:ASN:OD1	2.49	0.44
14:b:165:ASP:OD1	14:b:166:MET:N	2.50	0.44
14:N:12:VAL:HG12	14:N:25:ALA:HB2	1.99	0.44
3:Q:111:VAL:HG12	3:Q:136:ILE:HD13	2.00	0.44
8:V:129:VAL:HA	8:V:132:VAL:HG12	2.00	0.44
8:H:120:ASP:OD2	8:H:124:ASP:N	2.50	0.43
14:b:12:VAL:HG12	14:b:25:ALA:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:27:ARG:NH2	14:b:39:ASN:OD1	2.49	0.43
7:U:27:ILE:HD11	7:U:133:PRO:HG2	2.00	0.43
9:I:66:HIS:ND1	9:I:78:MET:HE2	2.33	0.43
8:V:120:ASP:OD2	8:V:124:ASP:N	2.50	0.43
8:H:38:ASN:ND2	8:H:126:ASN:OD1	2.49	0.43
10:J:42:SER:OG	10:J:199:GLU:OE2	2.32	0.43
10:X:48:ASN:OD1	10:X:49:ASN:N	2.47	0.43
13:a:53:ALA:O	13:a:220:THR:OG1	2.21	0.43
13:M:63:ILE:CG2	9:W:167:LEU:HD21	2.48	0.43
14:N:60:ASP:HB3	14:N:109:LEU:HD22	2.01	0.43
2:P:15:PRO:O	2:P:16:THR:OG1	2.29	0.43
6:T:161:GLY:O	6:T:164:SER:OG	2.25	0.43
5:E:91:TYR:CG	5:E:119:LEU:HD22	2.54	0.43
2:P:91:ARG:HD3	9:W:68:LEU:HD13	2.00	0.43
9:I:167:LEU:HD22	13:a:214:ILE:O	2.19	0.42
9:W:66:HIS:ND1	9:W:78:MET:HE2	2.33	0.42
14:b:60:ASP:HB3	14:b:109:LEU:HD22	2.01	0.42
10:J:44:ILE:HG21	10:J:201:LEU:HD22	2.01	0.42
7:G:27:ILE:HD11	7:G:133:PRO:HG2	2.00	0.42
3:Q:186:GLU:O	3:Q:190:LEU:HD23	2.20	0.42
5:S:52:ARG:NH2	5:S:61:LYS:O	2.53	0.42
7:U:16:SER:OG	7:U:18:ASP:OD1	2.31	0.42
3:Q:91:ARG:HG2	10:X:78:VAL:HG11	2.01	0.42
5:S:91:TYR:CG	5:S:119:LEU:HD22	2.54	0.42
8:V:221:ASP:OD1	8:V:222:ASN:N	2.52	0.42
1:A:67:LEU:HD13	7:G:163:TYR:CE1	2.55	0.42
5:E:91:TYR:CD2	5:E:119:LEU:HD22	2.54	0.42
8:H:221:ASP:OD1	8:H:222:ASN:N	2.52	0.42
1:O:75:ILE:HD12	1:O:230:GLU:HG3	2.01	0.42
5:S:91:TYR:CD2	5:S:119:LEU:HD22	2.54	0.42
11:K:138:LEU:HD11	11:Y:26:ILE:HG22	2.02	0.42
14:N:10:THR:OG1	14:N:219:THR:O	2.38	0.42
10:X:44:ILE:HG21	10:X:201:LEU:HD22	2.02	0.42
3:C:45:LEU:HD12	3:C:73:PHE:CE2	2.54	0.42
2:P:19:LEU:HB3	2:P:22:ILE:HD12	2.02	0.42
1:A:67:LEU:HD12	7:G:162:LYS:O	2.20	0.41
5:E:72:ASP:O	5:E:229:PHE:N	2.49	0.41
1:O:17:SER:HB3	1:O:18:PRO:HD2	2.02	0.41
1:A:75:ILE:HD12	1:A:230:GLU:HG3	2.01	0.41
2:B:19:LEU:HB3	2:B:22:ILE:HD12	2.02	0.41
3:C:186:GLU:O	3:C:190:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:52:ARG:NH2	5:E:61:LYS:O	2.53	0.41
6:F:70:ILE:HG12	6:F:105:ILE:HD13	2.01	0.41
9:I:167:LEU:HD21	13:a:63:ILE:CG2	2.50	0.41
3:Q:45:LEU:HD12	3:Q:73:PHE:CE2	2.54	0.41
8:V:38:ASN:ND2	8:V:126:ASN:OD1	2.49	0.41
12:L:4:LEU:HD13	12:L:135:ALA:HB1	2.03	0.41
1:O:235:SER:O	1:O:239:ARG:HA	2.19	0.41
8:H:220:ASN:ND2	8:V:191:SER:OG	2.53	0.41
5:S:191:MET:HE1	5:S:199:LEU:HD22	2.03	0.41
2:B:148:GLN:NE2	2:B:150:ASP:OD1	2.54	0.41
5:E:191:MET:HE1	5:E:199:LEU:HD22	2.03	0.41
6:F:184:GLU:O	6:F:188:LEU:HD23	2.20	0.41
7:G:16:SER:OG	7:G:18:ASP:OD1	2.31	0.41
6:T:70:ILE:HG12	6:T:105:ILE:HD13	2.01	0.41
1:A:17:SER:HB3	1:A:18:PRO:HD2	2.02	0.41
1:A:235:SER:O	1:A:239:ARG:HA	2.20	0.41
2:B:82:ASP:O	2:B:86:LEU:HD23	2.21	0.41
3:C:37:LEU:HD21	3:C:175:LEU:CD2	2.49	0.41
3:C:170:THR:O	3:C:174:VAL:HG23	2.21	0.41
6:F:205:THR:O	6:F:209:THR:HG22	2.21	0.41
10:X:47:MET:HE1	10:X:69:LEU:CB	2.51	0.41
11:Y:179:GLU:OE2	11:Y:181:ARG:NH2	2.52	0.41
13:M:214:ILE:O	9:W:167:LEU:HD22	2.21	0.40
6:T:184:GLU:O	6:T:188:LEU:HD23	2.20	0.40
13:a:100:ILE:O	13:a:104:VAL:HG23	2.20	0.40
6:F:11:ILE:HD12	7:G:129:TRP:O	2.21	0.40
14:N:61:ALA:HB2	14:N:111:ASN:HD21	1.86	0.40
10:J:47:MET:HE1	10:J:69:LEU:CB	2.51	0.40
2:P:148:GLN:NE2	2:P:150:ASP:OD1	2.54	0.40
3:Q:170:THR:O	3:Q:174:VAL:HG23	2.21	0.40
7:U:35:ASN:O	7:U:81:SER:OG	2.26	0.40
13:M:100:ILE:O	13:M:104:VAL:HG23	2.20	0.40
14:N:10:THR:HG21	14:N:220:SER:HB3	2.03	0.40
6:T:205:THR:O	6:T:209:THR:HG22	2.21	0.40
9:W:97:ALA:HB1	9:W:127:LEU:HD13	2.04	0.40
12:Z:4:LEU:HD13	12:Z:135:ALA:HB1	2.03	0.40
14:b:10:THR:OG1	14:b:219:THR:O	2.38	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	242/260 (93%)	235 (97%)	7 (3%)	0	100	100
1	O	242/260 (93%)	235 (97%)	7 (3%)	0	100	100
2	B	225/235 (96%)	215 (96%)	10 (4%)	0	100	100
2	P	225/235 (96%)	215 (96%)	10 (4%)	0	100	100
3	C	238/246 (97%)	230 (97%)	8 (3%)	0	100	100
3	Q	238/246 (97%)	230 (97%)	8 (3%)	0	100	100
4	D	231/241 (96%)	226 (98%)	4 (2%)	1 (0%)	30	66
4	R	231/241 (96%)	225 (97%)	5 (2%)	1 (0%)	30	66
5	E	227/256 (89%)	218 (96%)	9 (4%)	0	100	100
5	S	227/256 (89%)	218 (96%)	9 (4%)	0	100	100
6	F	228/254 (90%)	217 (95%)	11 (5%)	0	100	100
6	T	228/254 (90%)	218 (96%)	10 (4%)	0	100	100
7	G	243/252 (96%)	235 (97%)	8 (3%)	0	100	100
7	U	243/252 (96%)	235 (97%)	8 (3%)	0	100	100
8	H	198/252 (79%)	191 (96%)	7 (4%)	0	100	100
8	V	198/252 (79%)	191 (96%)	7 (4%)	0	100	100
9	I	207/229 (90%)	190 (92%)	17 (8%)	0	100	100
9	W	207/229 (90%)	190 (92%)	17 (8%)	0	100	100
10	J	204/218 (94%)	188 (92%)	16 (8%)	0	100	100
10	X	204/218 (94%)	188 (92%)	16 (8%)	0	100	100
11	K	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
11	Y	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
12	L	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
12	Z	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
13	M	210/240 (88%)	200 (95%)	10 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	210/240 (88%)	200 (95%)	10 (5%)	0	100	100
14	N	226/302 (75%)	217 (96%)	9 (4%)	0	100	100
14	b	226/302 (75%)	217 (96%)	9 (4%)	0	100	100
All	All	6160/6780 (91%)	5894 (96%)	264 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	38	SER
4	R	38	SER

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	191/231 (83%)	191 (100%)	0	100	100
1	O	191/231 (83%)	191 (100%)	0	100	100
2	B	167/205 (82%)	167 (100%)	0	100	100
2	P	167/205 (82%)	167 (100%)	0	100	100
3	C	171/213 (80%)	171 (100%)	0	100	100
3	Q	171/213 (80%)	171 (100%)	0	100	100
4	D	174/207 (84%)	173 (99%)	1 (1%)	84	93
4	R	174/207 (84%)	173 (99%)	1 (1%)	84	93
5	E	178/223 (80%)	178 (100%)	0	100	100
5	S	178/223 (80%)	178 (100%)	0	100	100
6	F	181/227 (80%)	181 (100%)	0	100	100
6	T	181/227 (80%)	181 (100%)	0	100	100
7	G	211/229 (92%)	211 (100%)	0	100	100
7	U	211/229 (92%)	211 (100%)	0	100	100
8	H	175/231 (76%)	175 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	175/231 (76%)	175 (100%)	0	100	100
9	I	160/194 (82%)	160 (100%)	0	100	100
9	W	160/194 (82%)	160 (100%)	0	100	100
10	J	174/191 (91%)	174 (100%)	0	100	100
10	X	174/191 (91%)	174 (100%)	0	100	100
11	K	164/174 (94%)	164 (100%)	0	100	100
11	Y	164/174 (94%)	164 (100%)	0	100	100
12	L	169/175 (97%)	169 (100%)	0	100	100
12	Z	169/175 (97%)	169 (100%)	0	100	100
13	M	184/216 (85%)	184 (100%)	0	100	100
13	a	184/216 (85%)	184 (100%)	0	100	100
14	N	194/266 (73%)	194 (100%)	0	100	100
14	b	194/266 (73%)	194 (100%)	0	100	100
All	All	4986/5964 (84%)	4984 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	96	LEU
4	R	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	21	GLN
2	B	148	GLN
4	D	92	GLN
4	D	97	ASN
6	F	174	ASN
6	F	189	HIS
7	G	54	ASN
7	G	112	HIS
7	G	210	ASN
8	H	10	ASN
8	H	162	GLN
9	I	114	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	63	GLN
10	J	118	HIS
11	K	123	ASN
11	K	186	ASN
12	L	202	ASN
2	P	21	GLN
2	P	148	GLN
3	Q	88	ASN
4	R	92	GLN
4	R	97	ASN
4	R	223	ASN
5	S	176	GLN
6	T	174	ASN
6	T	189	HIS
7	U	54	ASN
7	U	210	ASN
8	V	10	ASN
8	V	61	HIS
8	V	162	GLN
9	W	114	HIS
10	X	63	GLN
10	X	118	HIS
11	Y	123	ASN
11	Y	186	ASN
12	Z	202	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	A1CRO	L	301	12	53,57,57	3.43	21 (39%)	66,80,80	2.06	20 (30%)
15	A1CRO	Z	301	12	53,57,57	3.43	20 (37%)	66,80,80	2.06	20 (30%)

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	A1CRO	L	301	12	-	17/50/79/79	0/3/3/3
15	A1CRO	Z	301	12	-	17/50/79/79	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	301	A1CRO	C29-C28	9.65	1.54	1.38
15	Z	301	A1CRO	C29-C28	9.65	1.54	1.38
15	L	301	A1CRO	C14-N04	8.38	1.52	1.34
15	Z	301	A1CRO	C14-N04	8.34	1.51	1.34
15	L	301	A1CRO	C31-C30	8.16	1.53	1.37
15	Z	301	A1CRO	C31-C30	8.14	1.53	1.37
15	Z	301	A1CRO	C12-N03	7.83	1.50	1.34
15	L	301	A1CRO	C12-N03	7.81	1.50	1.34
15	L	301	A1CRO	C34-N05	7.55	1.49	1.35
15	Z	301	A1CRO	C34-N05	7.54	1.49	1.35
15	Z	301	A1CRO	C32-C27	7.51	1.53	1.38
15	L	301	A1CRO	C32-C27	7.49	1.53	1.38
15	Z	301	A1CRO	C10-N02	7.07	1.49	1.34
15	L	301	A1CRO	C10-N02	7.05	1.49	1.34
15	L	301	A1CRO	OG1-CB	-5.35	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Z	301	A1CRO	OG1-CB	-5.35	1.38	1.44
15	Z	301	A1CRO	C19-C20	4.75	1.59	1.51
15	L	301	A1CRO	C19-C20	4.74	1.59	1.51
15	L	301	A1CRO	C32-C31	-3.71	1.32	1.38
15	Z	301	A1CRO	C32-C31	-3.69	1.32	1.38
15	Z	301	A1CRO	C28-C27	-3.56	1.31	1.38
15	L	301	A1CRO	C28-C27	-3.56	1.31	1.38
15	L	301	A1CRO	C33-C34	3.38	1.57	1.51
15	Z	301	A1CRO	C33-C34	3.35	1.57	1.51
15	L	301	A1CRO	C09-C10	3.31	1.58	1.51
15	Z	301	A1CRO	C09-C10	3.30	1.57	1.51
15	Z	301	A1CRO	C17-C16	2.61	1.58	1.53
15	L	301	A1CRO	C17-C16	2.59	1.58	1.53
15	L	301	A1CRO	C29-C30	-2.51	1.32	1.37
15	Z	301	A1CRO	C29-C30	-2.50	1.32	1.37
15	Z	301	A1CRO	O06-C12	-2.35	1.18	1.23
15	L	301	A1CRO	O06-C12	-2.31	1.19	1.23
15	L	301	A1CRO	O05-C14	-2.30	1.19	1.23
15	Z	301	A1CRO	O05-C14	-2.25	1.19	1.23
15	L	301	A1CRO	C20-C21	2.17	1.41	1.38
15	Z	301	A1CRO	C20-C21	2.16	1.41	1.38
15	L	301	A1CRO	C19-C15	2.10	1.56	1.54
15	Z	301	A1CRO	C19-C15	2.09	1.56	1.54
15	L	301	A1CRO	C39-C17	2.09	1.55	1.52
15	Z	301	A1CRO	C39-C17	2.05	1.55	1.52
15	L	301	A1CRO	O08-C10	-2.00	1.19	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	301	A1CRO	O04-C16-C15	-4.77	102.36	110.70
15	Z	301	A1CRO	O04-C16-C15	-4.76	102.38	110.70
15	L	301	A1CRO	C24-C23-C22	-4.67	117.07	123.23
15	Z	301	A1CRO	C24-C23-C22	-4.62	117.13	123.23
15	L	301	A1CRO	C20-C19-C15	4.57	121.02	114.08
15	Z	301	A1CRO	C20-C19-C15	4.56	121.00	114.08
15	Z	301	A1CRO	OG1-C16-C15	4.42	111.17	104.29
15	L	301	A1CRO	OG1-CB-CG2	4.41	111.31	105.94
15	Z	301	A1CRO	OG1-CB-CG2	4.41	111.31	105.94
15	L	301	A1CRO	OG1-C16-C15	4.41	111.16	104.29
15	L	301	A1CRO	C21-C22-C23	4.13	121.07	116.67
15	Z	301	A1CRO	C21-C22-C23	4.08	121.02	116.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	A1CRO	C19-C20-C25	3.85	127.16	119.83
15	L	301	A1CRO	C19-C20-C25	3.83	127.13	119.83
15	Z	301	A1CRO	C33-C34-N05	3.21	124.28	118.37
15	L	301	A1CRO	C33-C34-N05	3.19	124.25	118.37
15	Z	301	A1CRO	C09-C10-N02	3.01	121.17	115.86
15	L	301	A1CRO	C09-C10-N02	3.00	121.16	115.86
15	Z	301	A1CRO	C24-C25-C20	2.77	125.02	121.39
15	Z	301	A1CRO	C13-C14-N04	2.77	122.53	116.63
15	L	301	A1CRO	C13-C14-N04	2.75	122.49	116.63
15	L	301	A1CRO	C24-C25-C20	2.75	124.98	121.39
15	L	301	A1CRO	C25-C24-C23	2.68	121.13	118.38
15	Z	301	A1CRO	C25-C24-C23	2.63	121.08	118.38
15	Z	301	A1CRO	OG1-C16-C17	-2.63	105.53	108.54
15	Z	301	A1CRO	C25-C20-C21	-2.62	112.11	116.62
15	L	301	A1CRO	C25-C20-C21	-2.61	112.14	116.62
15	L	301	A1CRO	OG1-C16-C17	-2.59	105.57	108.54
15	Z	301	A1CRO	O07-C34-C33	-2.54	117.32	122.07
15	L	301	A1CRO	O07-C34-C33	-2.54	117.32	122.07
15	L	301	A1CRO	C16-C15-N04	-2.43	107.27	110.53
15	Z	301	A1CRO	C16-C15-N04	-2.42	107.28	110.53
15	L	301	A1CRO	C14-C13-N03	-2.33	104.81	111.11
15	Z	301	A1CRO	C14-C13-N03	-2.32	104.84	111.11
15	Z	301	A1CRO	F01-C23-C22	2.29	121.54	118.28
15	L	301	A1CRO	F01-C23-C22	2.29	121.53	118.28
15	Z	301	A1CRO	C31-C30-C29	-2.21	119.90	122.80
15	L	301	A1CRO	C31-C30-C29	-2.18	119.94	122.80
15	Z	301	A1CRO	O07-C34-N05	-2.09	118.40	122.12
15	L	301	A1CRO	O07-C34-N05	-2.08	118.42	122.12

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	301	A1CRO	C12-C11-C33-C34
15	L	301	A1CRO	N04-C15-C16-OG1
15	L	301	A1CRO	N04-C15-C19-C20
15	L	301	A1CRO	C19-C15-N04-C14
15	L	301	A1CRO	C15-C19-C20-C21
15	Z	301	A1CRO	C12-C11-C33-C34
15	Z	301	A1CRO	N04-C15-C16-OG1
15	Z	301	A1CRO	N04-C15-C19-C20
15	Z	301	A1CRO	C19-C15-N04-C14

Continued on next page...

Continued from previous page...

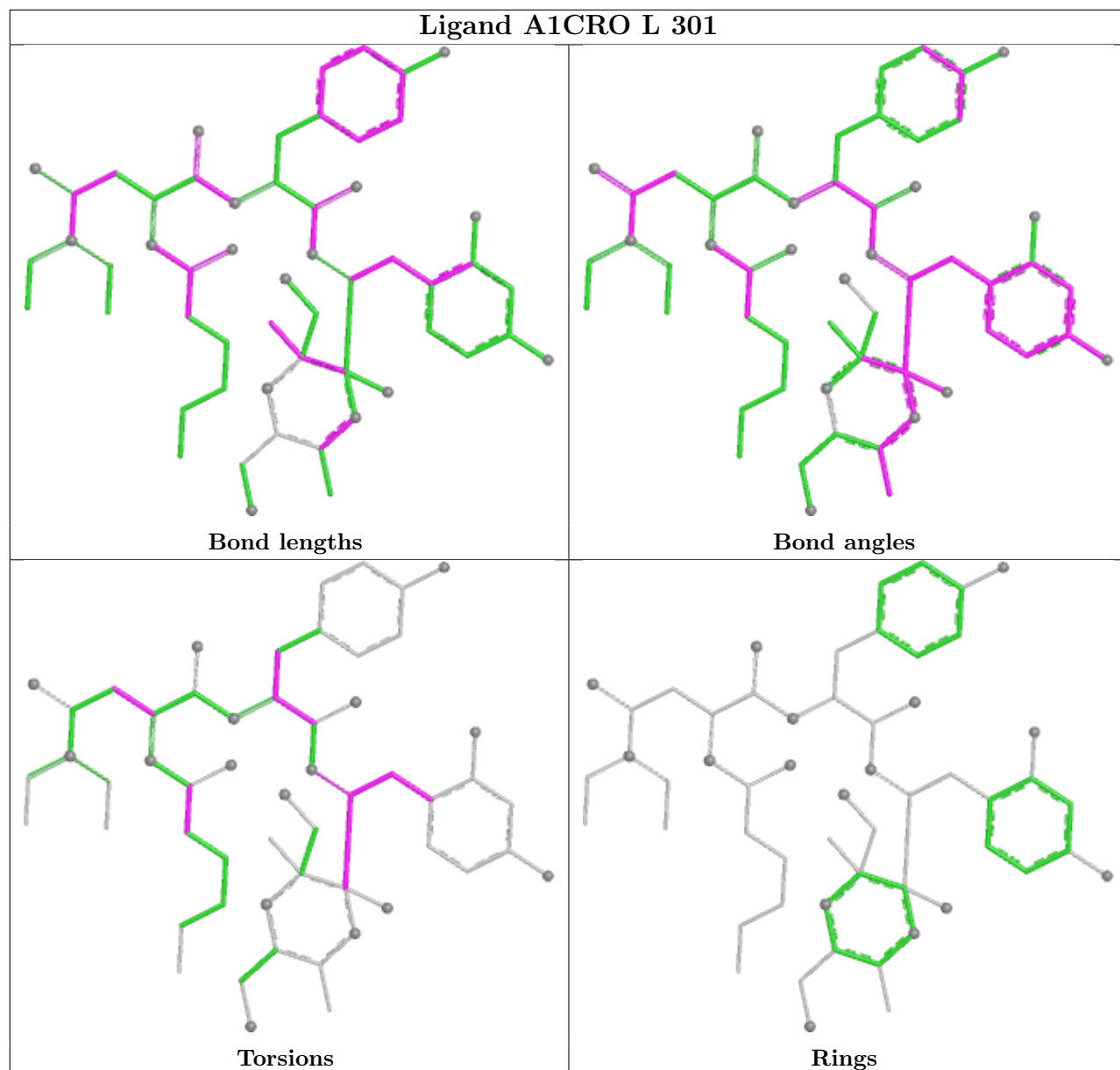
Mol	Chain	Res	Type	Atoms
15	Z	301	A1CRO	C15-C19-C20-C21
15	L	301	A1CRO	N03-C13-C26-C27
15	Z	301	A1CRO	N03-C13-C26-C27
15	L	301	A1CRO	C14-C13-C26-C27
15	Z	301	A1CRO	C14-C13-C26-C27
15	L	301	A1CRO	N02-C11-C33-C34
15	Z	301	A1CRO	N02-C11-C33-C34
15	L	301	A1CRO	C26-C13-C14-O05
15	Z	301	A1CRO	C26-C13-C14-O05
15	L	301	A1CRO	C08-C09-C10-N02
15	Z	301	A1CRO	C08-C09-C10-N02
15	L	301	A1CRO	C08-C09-C10-O08
15	Z	301	A1CRO	C08-C09-C10-O08
15	L	301	A1CRO	C26-C13-C14-N04
15	Z	301	A1CRO	C26-C13-C14-N04
15	L	301	A1CRO	C15-C19-C20-C25
15	Z	301	A1CRO	C15-C19-C20-C25
15	L	301	A1CRO	C16-C15-C19-C20
15	Z	301	A1CRO	C16-C15-C19-C20
15	L	301	A1CRO	N03-C13-C14-O05
15	Z	301	A1CRO	N03-C13-C14-O05
15	L	301	A1CRO	N03-C13-C14-N04
15	Z	301	A1CRO	N03-C13-C14-N04
15	L	301	A1CRO	C16-C15-N04-C14
15	Z	301	A1CRO	C16-C15-N04-C14

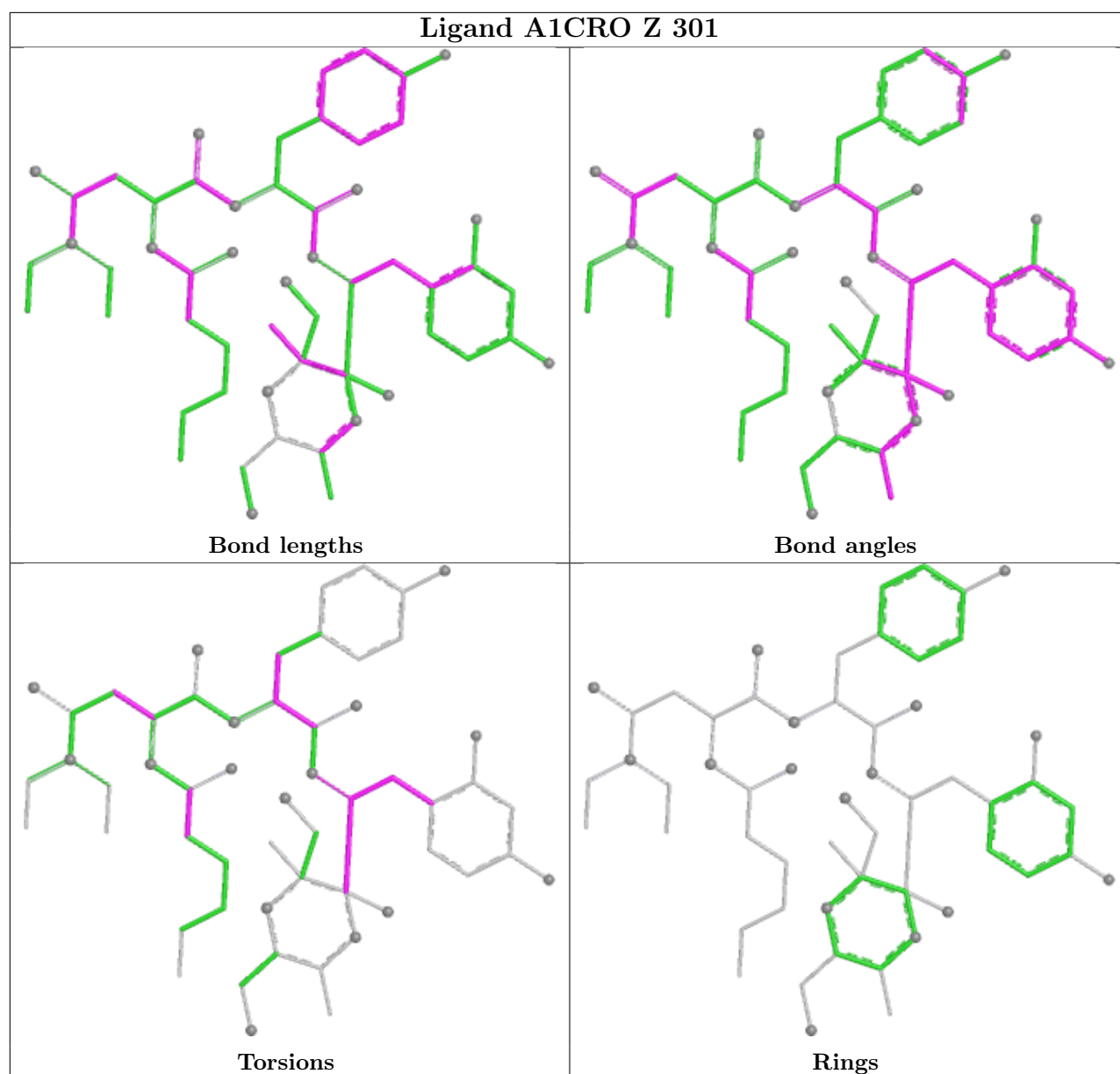
There are no ring outliers.

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.

Ligand A1CRO L 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

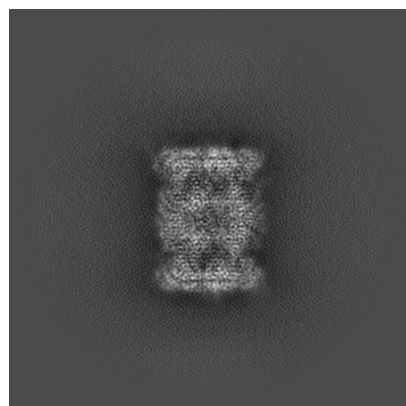
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72394. These allow visual inspection of the internal detail of the map and identification of artifacts.

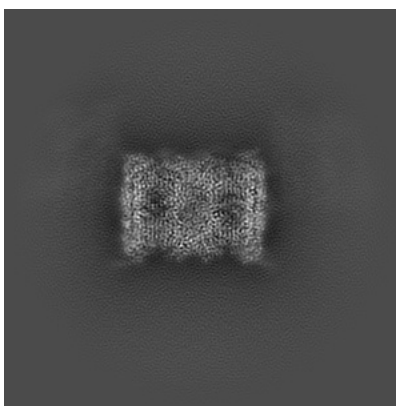
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

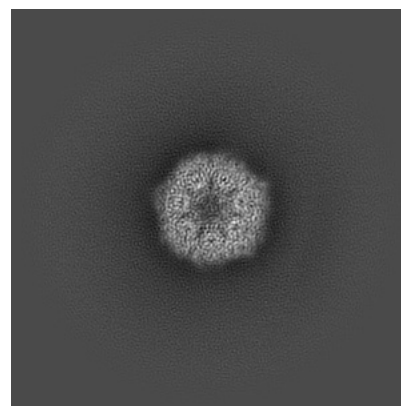
6.1.1 Primary map



X

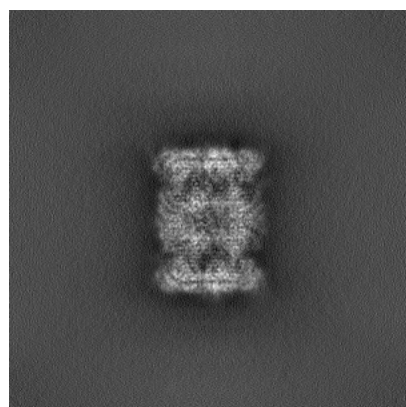


Y

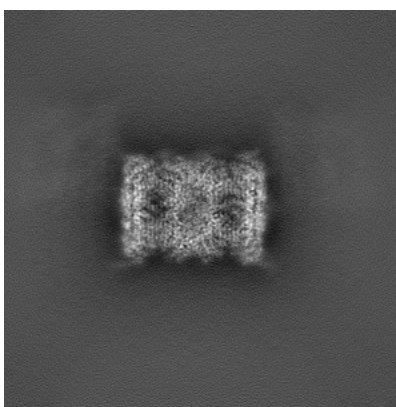


Z

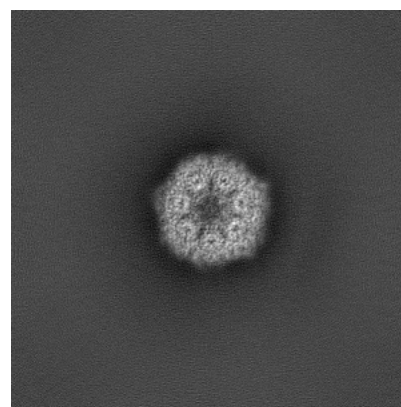
6.1.2 Raw map



X



Y

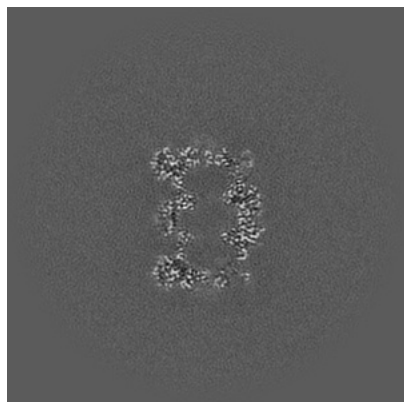


Z

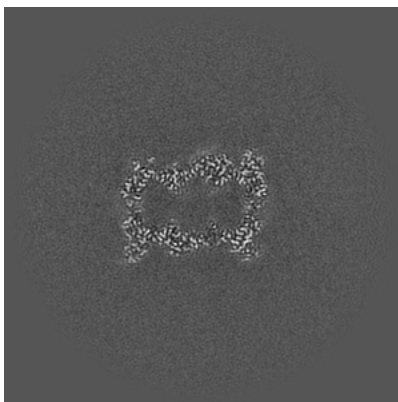
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

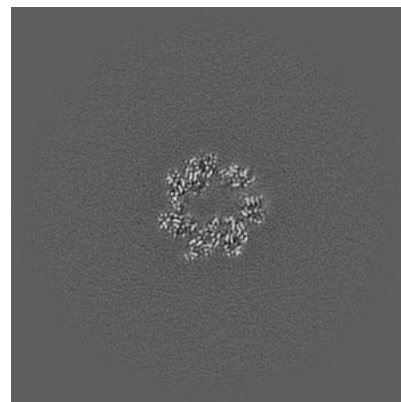
6.2.1 Primary map



X Index: 200

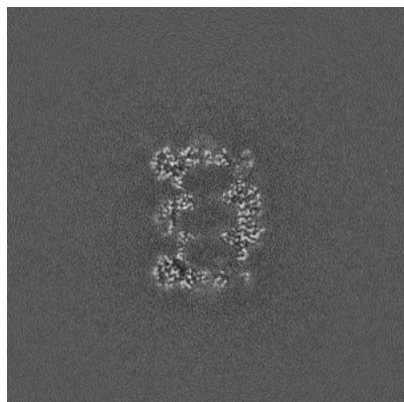


Y Index: 200

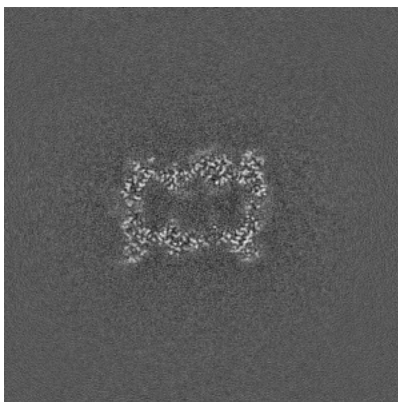


Z Index: 200

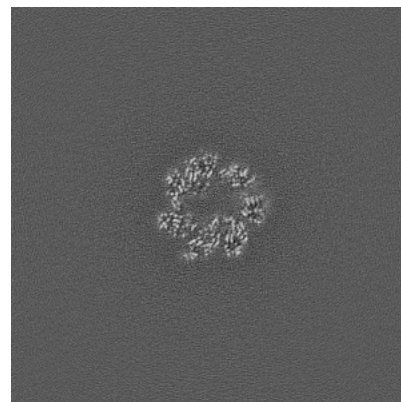
6.2.2 Raw map



X Index: 200



Y Index: 200

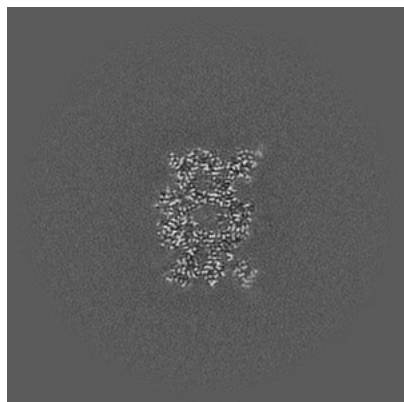


Z Index: 200

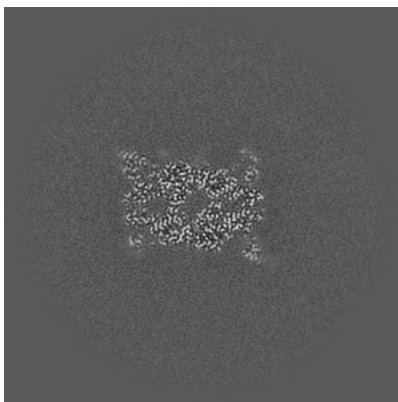
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

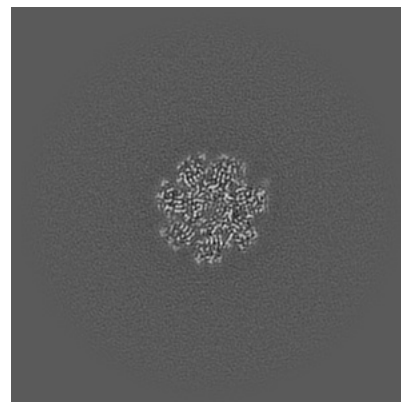
6.3.1 Primary map



X Index: 177

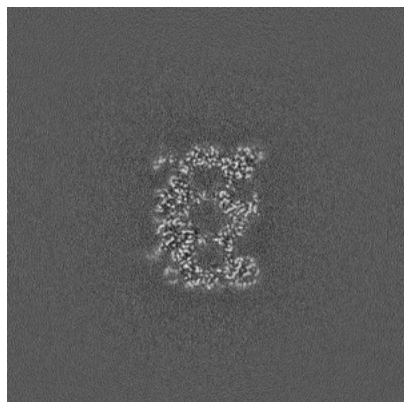


Y Index: 222

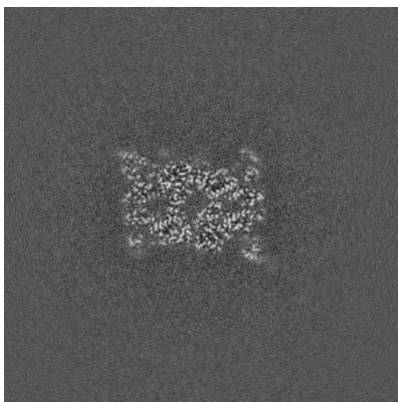


Z Index: 243

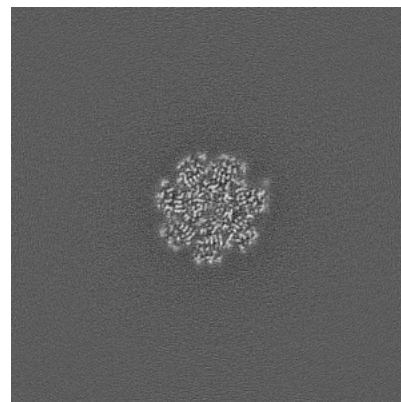
6.3.2 Raw map



X Index: 183



Y Index: 222

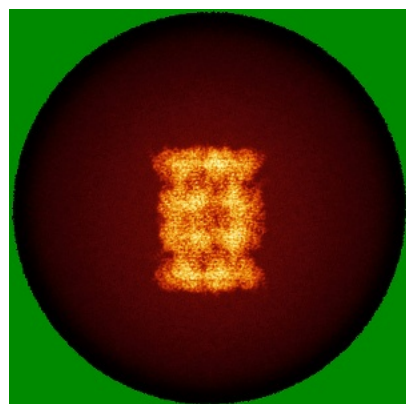


Z Index: 243

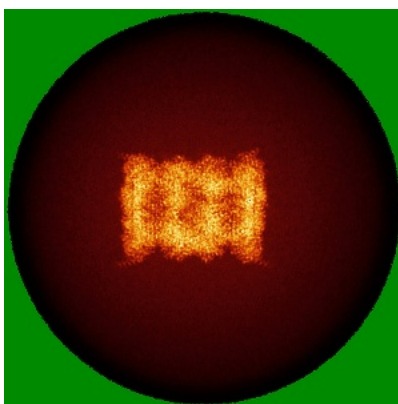
The images above show the largest variance slices of the map in three orthogonal directions.

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

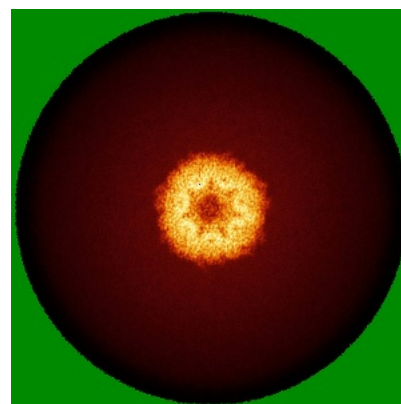
6.4.1 Primary map



X

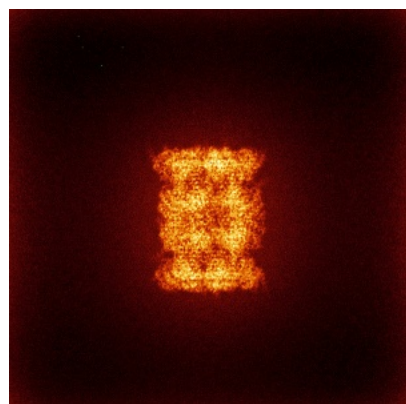


Y

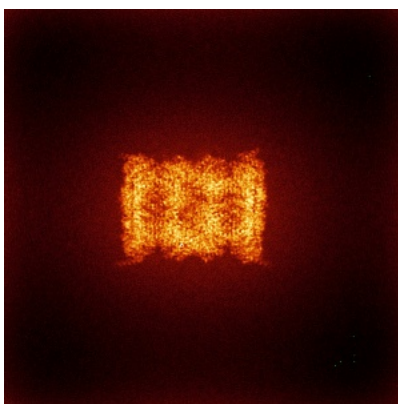


Z

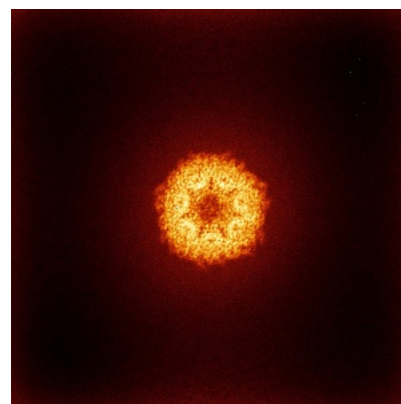
6.4.2 Raw map



X



Y

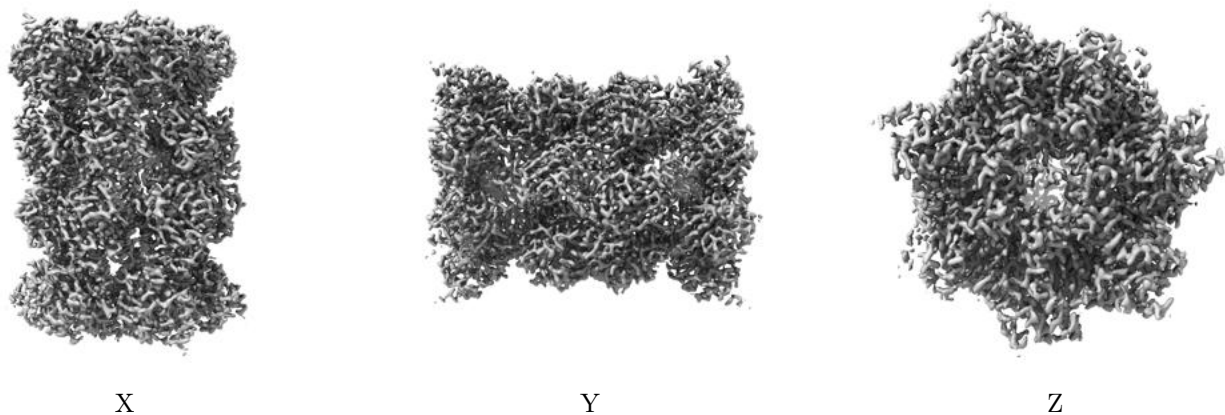


Z

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.

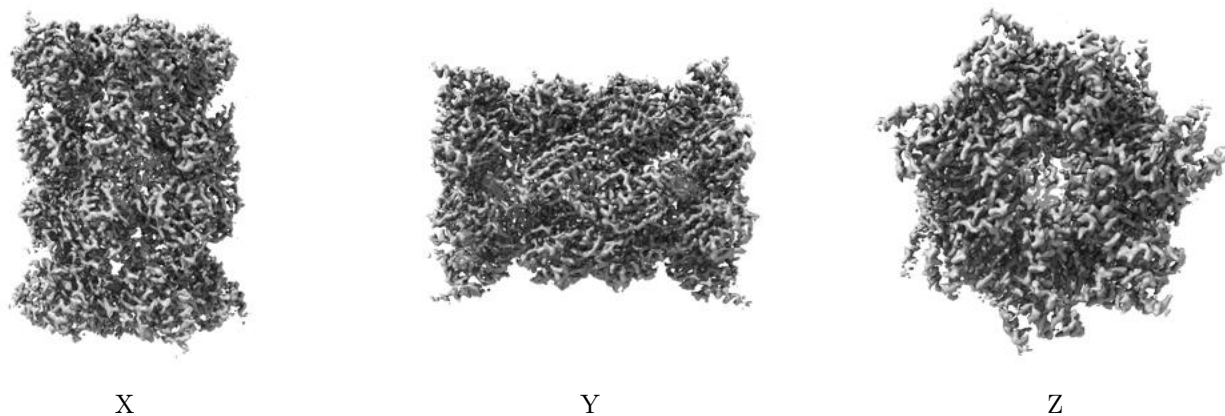
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. 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.

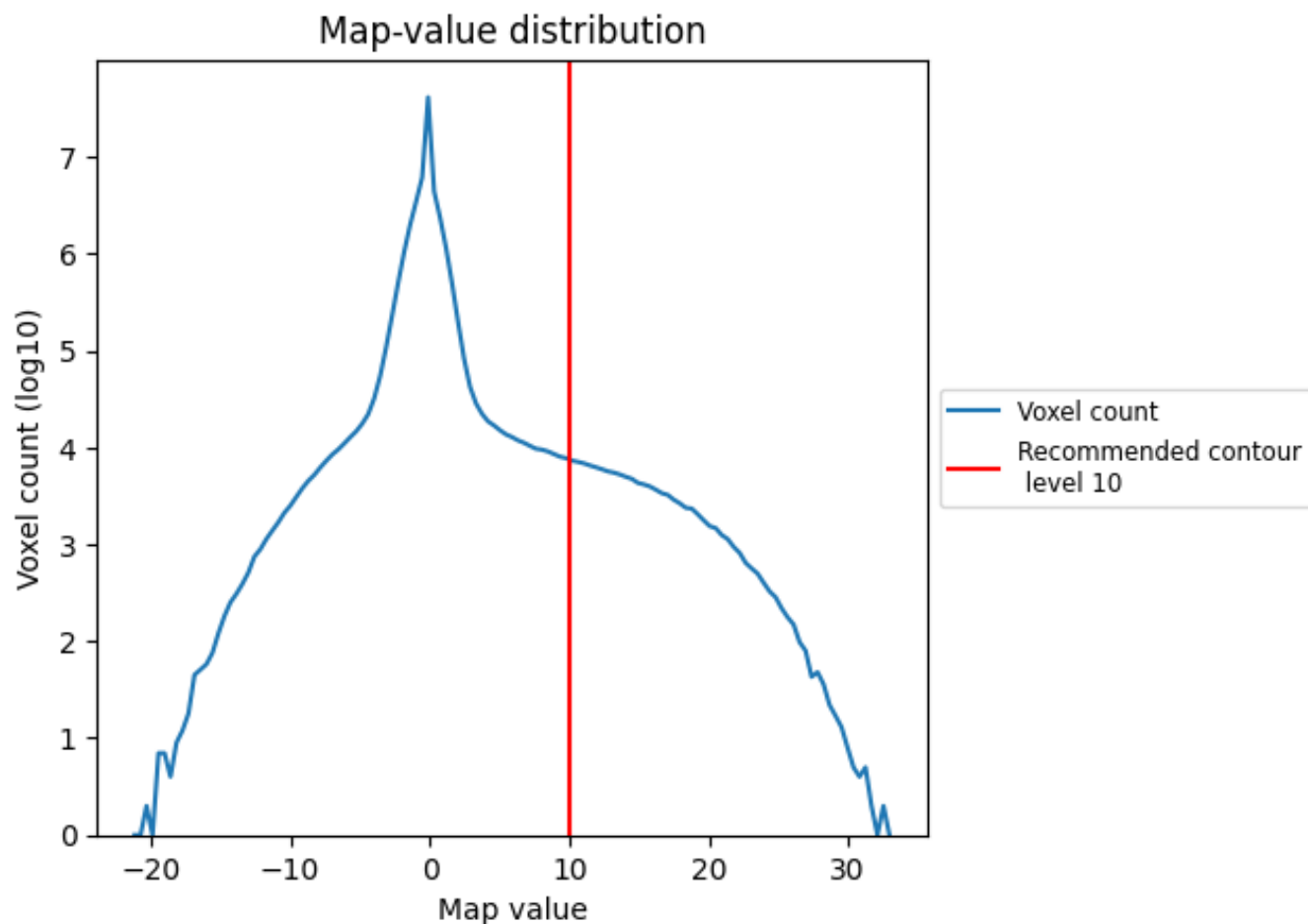
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

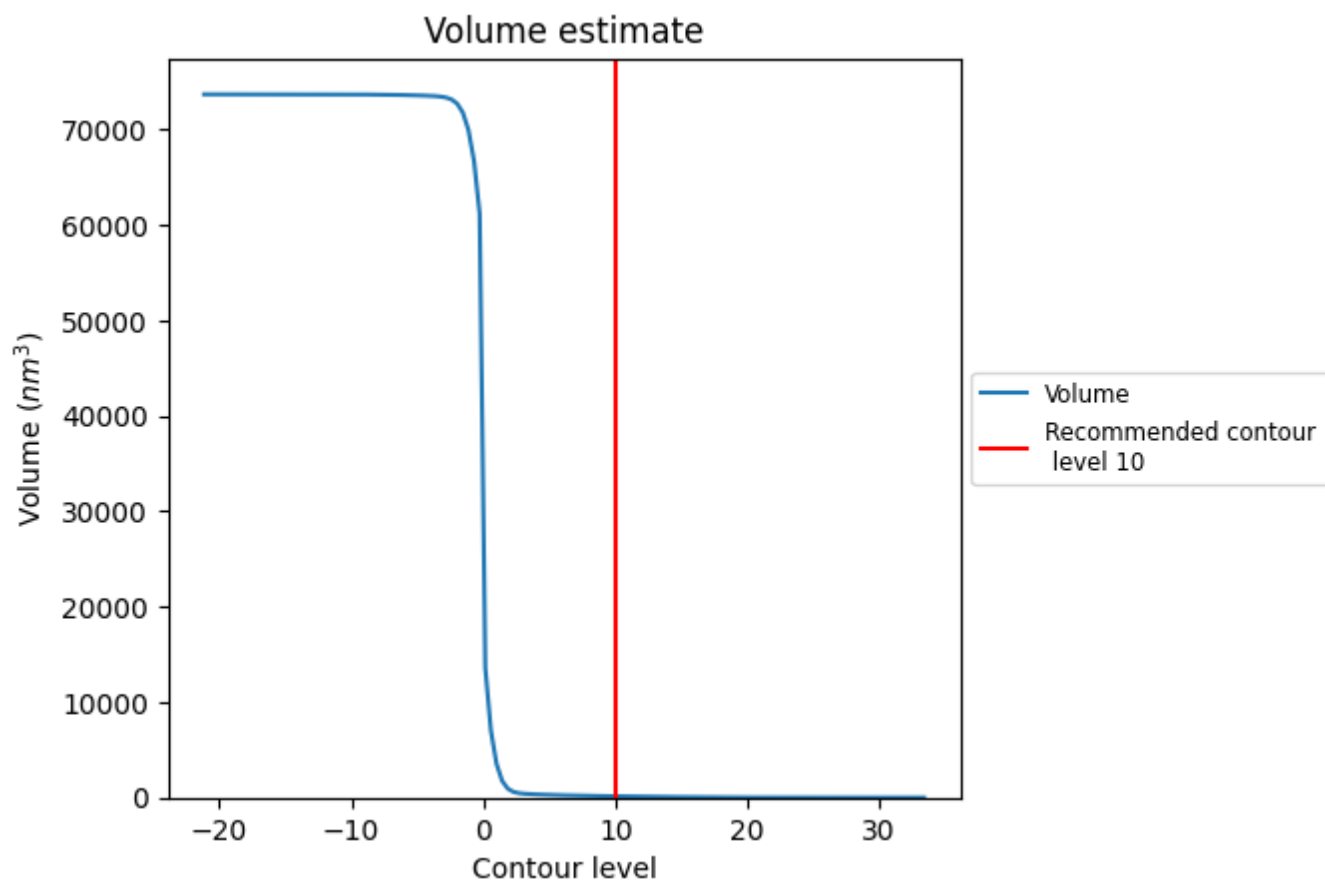
This section contains the results of statistical analysis of the map.

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.

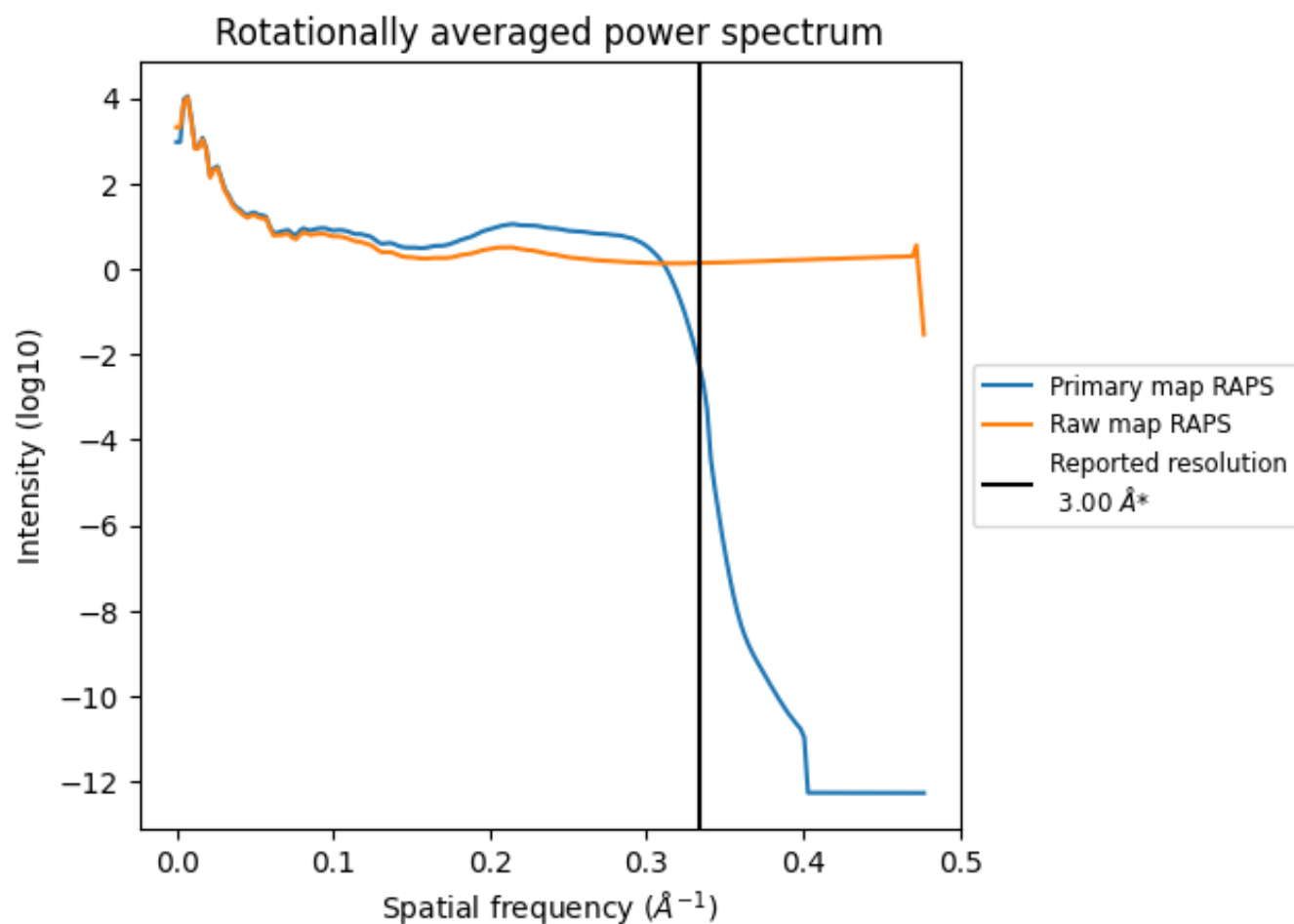
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 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 ⓘ

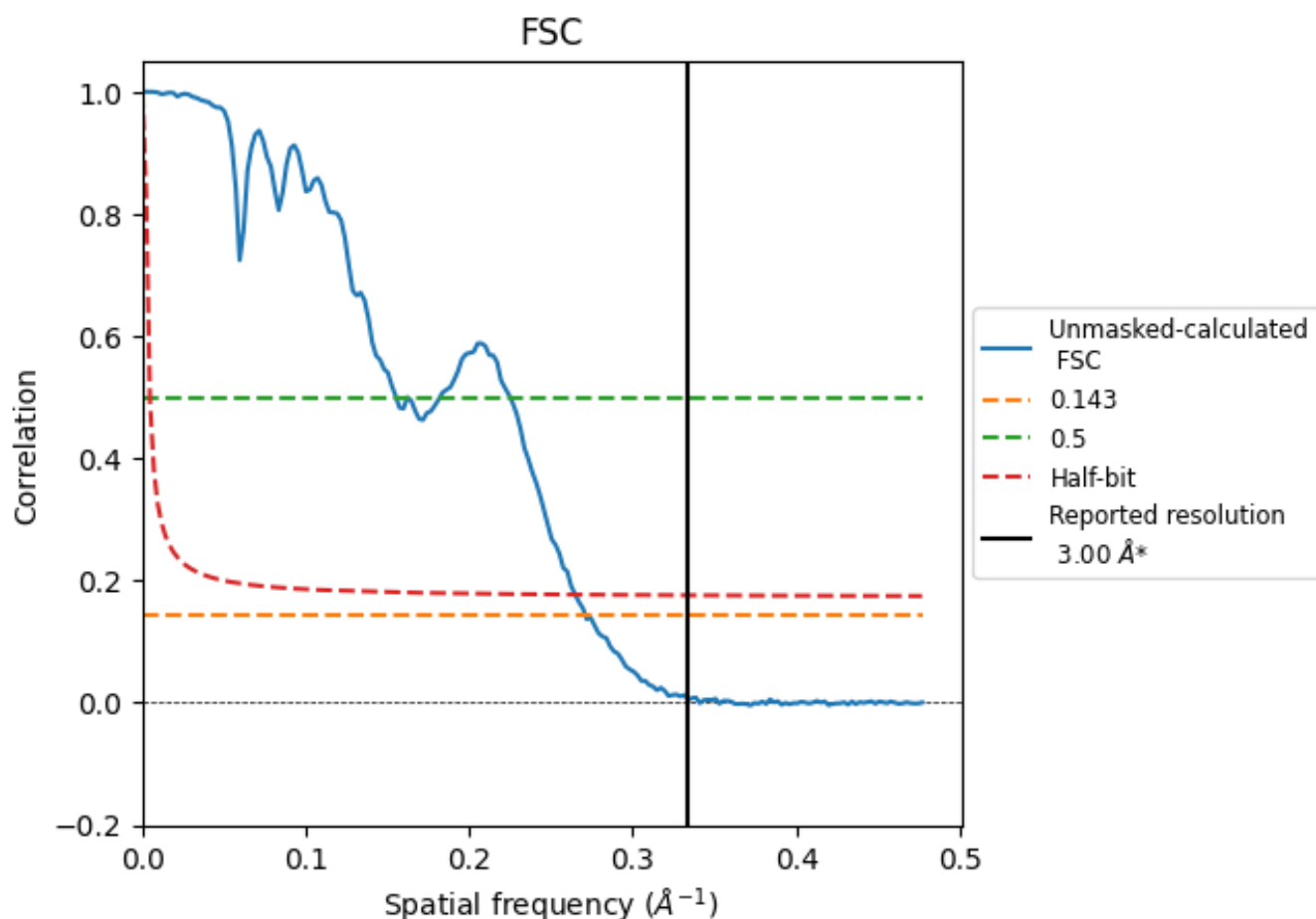


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

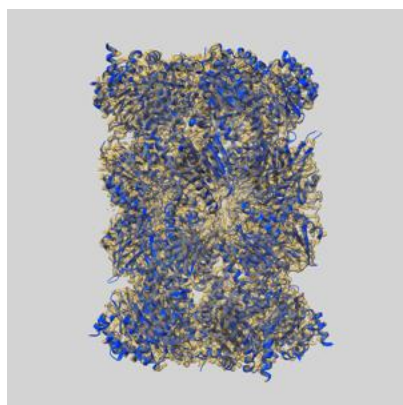
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	6.44	3.78

*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 3.69 differs from the reported value 3.0 by more than 10 %

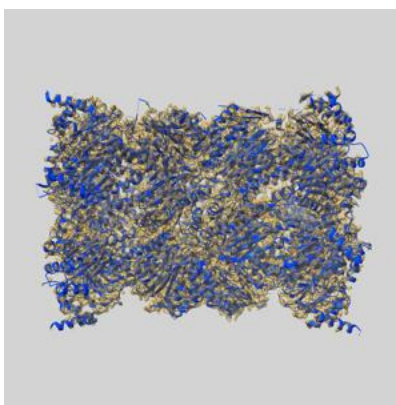
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72394 and PDB model 9Y0K. Per-residue inclusion information can be found in section [3](#) on page [8](#).

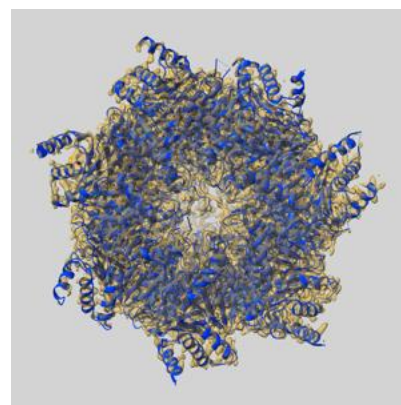
9.1 Map-model overlay [i](#)



X



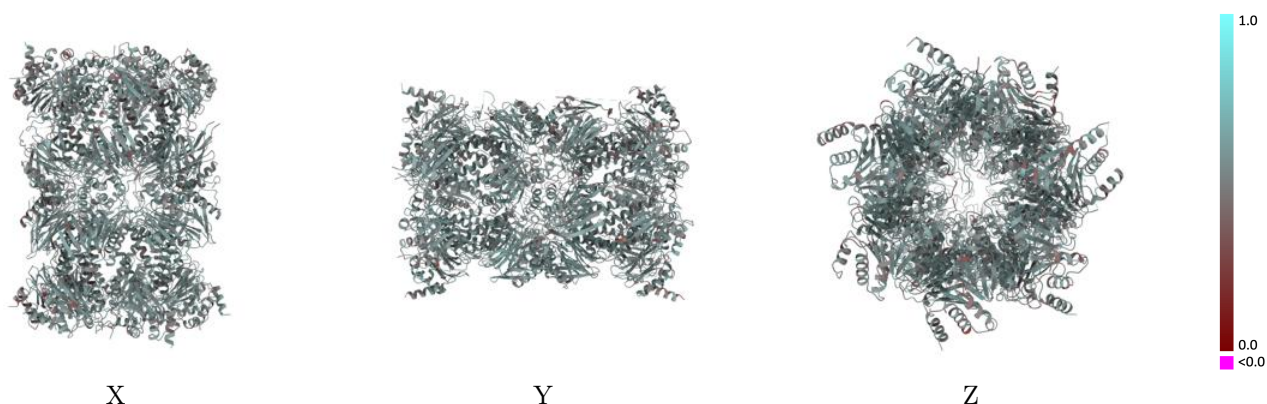
Y



Z

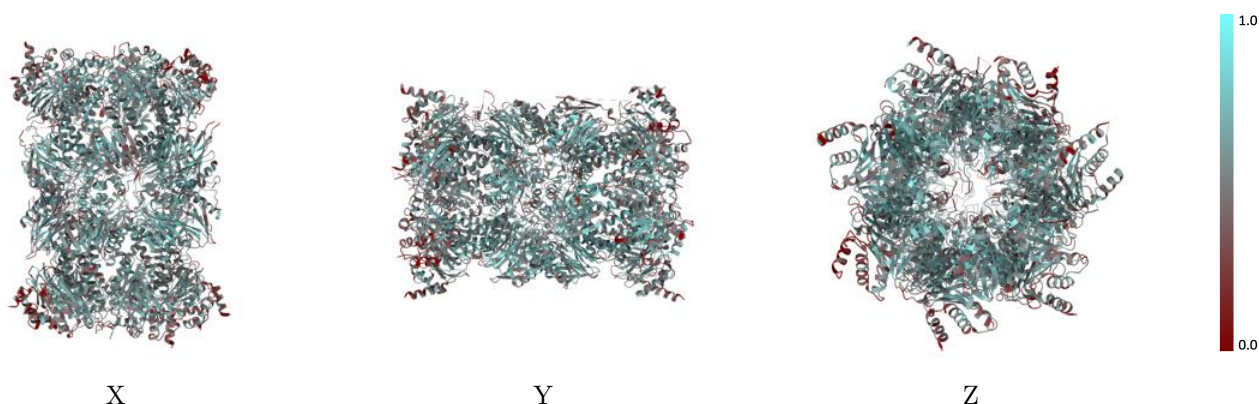
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



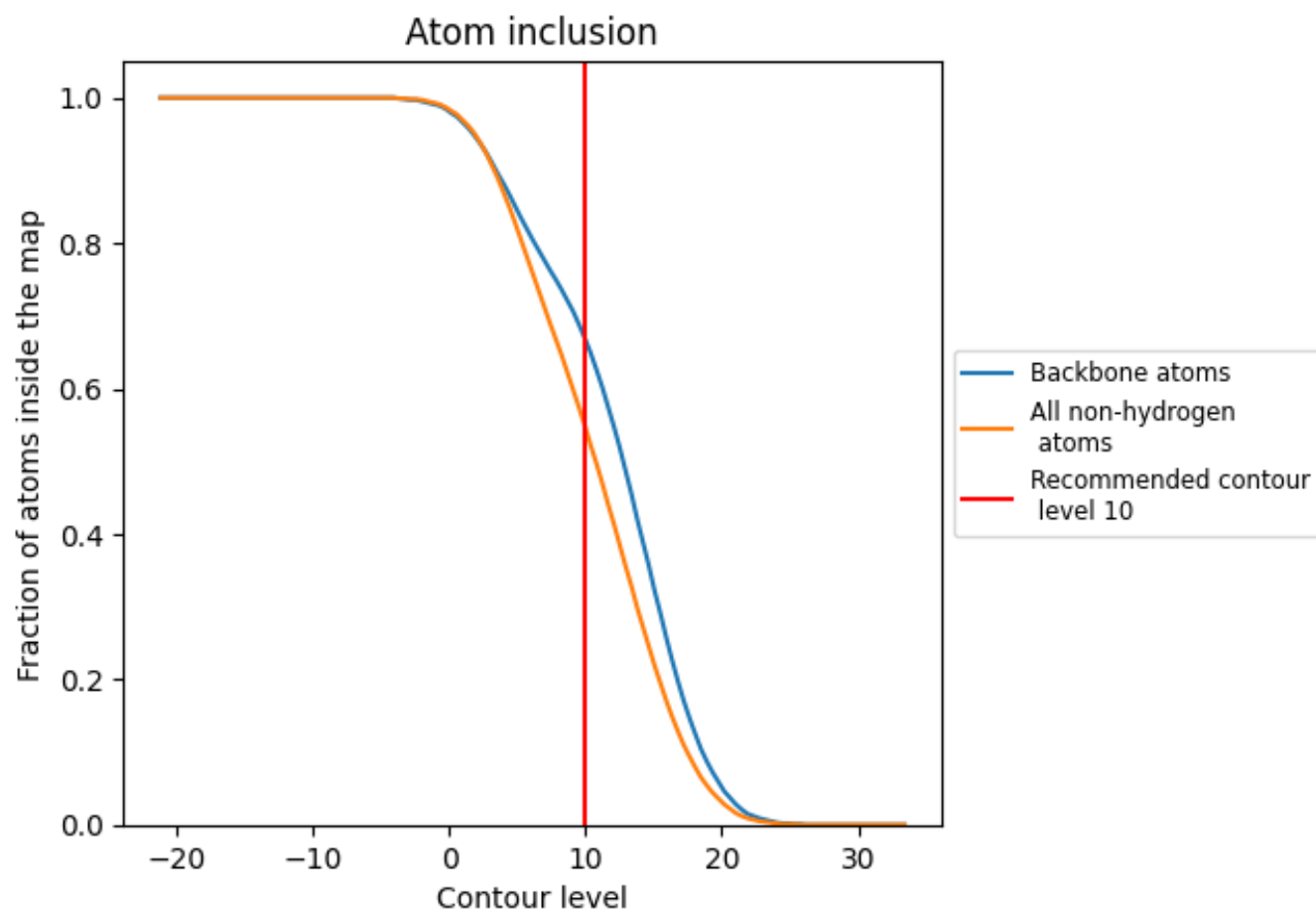
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 55% 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 (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5460	 0.5390
A	 0.5060	 0.5260
B	 0.4920	 0.5240
C	 0.5410	 0.5450
D	 0.5270	 0.5480
E	 0.4120	 0.5340
F	 0.5110	 0.5380
G	 0.5420	 0.5410
H	 0.5320	 0.5450
I	 0.5380	 0.5400
J	 0.5820	 0.5460
K	 0.6140	 0.5720
L	 0.6060	 0.5560
M	 0.5780	 0.5480
N	 0.5850	 0.5580
O	 0.5260	 0.5170
P	 0.5120	 0.5200
Q	 0.5700	 0.5400
R	 0.5470	 0.5330
S	 0.4420	 0.5130
T	 0.5350	 0.5180
U	 0.5470	 0.5260
V	 0.5290	 0.5360
W	 0.5560	 0.5380
X	 0.5830	 0.5410
Y	 0.6290	 0.5630
Z	 0.6010	 0.5470
a	 0.5710	 0.5360
b	 0.5810	 0.5400

