



Full wwPDB EM Validation Report ⓘ

May 12, 2025 – 07:15 PM EDT

PDB ID : 8CTE / pdb_00008cte
EMDB ID : EMD-26988
Title : Class 2 of erythrocyte ankyrin-1 complex (Composite map)
Authors : Vallese, F.; Kim, K.; Yen, L.Y.; Johnston, J.D.; Noble, A.J.; Cali, T.; Clarke, O.B.
Deposited on : 2022-05-14
Resolution : 2.90 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

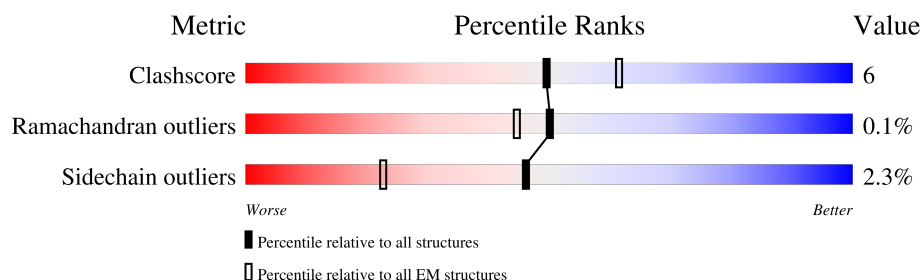
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1881	
2	P	911	
2	T	911	
2	W	911	
3	X	691	
4	K	417	
5	L	409	
5	Q	409	

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Mol	Chain	Length	Quality of chain
6	D	150	<div><div><div></div><div></div><div></div></div><div>12%23%73%</div><div></div></div>
6	N	150	<div><div><div></div><div></div><div></div></div><div>21%23%73%</div><div></div></div>
7	M	269	<div><div><div></div><div></div><div></div></div><div>77%15%8%</div><div></div></div>
7	O	269	<div><div><div></div><div></div><div></div></div><div>77%14%8%</div><div></div></div>
7	R	269	<div><div><div></div><div></div><div></div></div><div>77%14%8%</div><div></div></div>
7	S	269	<div><div><div></div><div></div><div></div></div><div>77%14%8%</div><div></div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 38844 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 Ankyrin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	451	Total	C	N	O	S	0	0
			3431	2144	643	632	12		

- Molecule 2 is a protein called Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	32	Total	C	N	O	S	0	0
			233	142	34	54	3		
2	P	804	Total	C	N	O	S	0	0
			6339	4170	1047	1098	24		
2	T	814	Total	C	N	O	S	0	0
			6406	4207	1060	1115	24		

- Molecule 3 is a protein called Protein 4.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	657	Total	C	N	O	S	0	0
			5167	3278	915	951	23		

- Molecule 4 is a protein called Blood group Rh(CE) polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	380	Total	C	N	O	S	2	0
			2943	1959	476	490	18		

- Molecule 5 is a protein called Ammonium transporter Rh type A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	388	Total	C	N	O	S	0	0
			2938	1928	473	513	24		
5	Q	390	Total	C	N	O	S	0	0
			2954	1940	475	515	24		

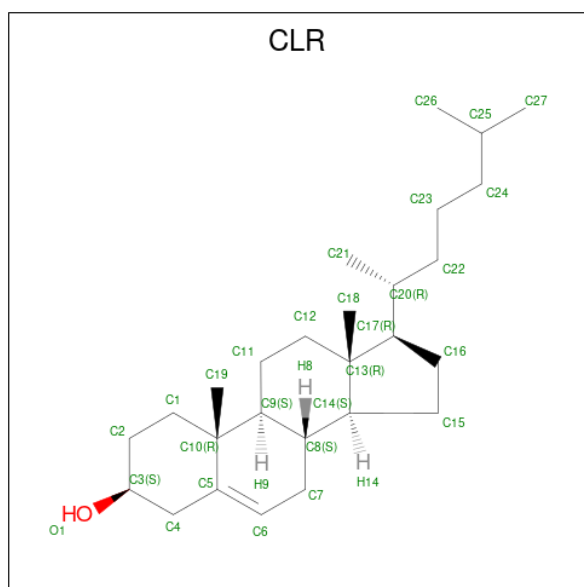
- Molecule 6 is a protein called Glycophorin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	40	Total	C	N	O	S	0	0
			302	198	51	52	1		
6	D	40	Total	C	N	O	S	0	0
			302	198	51	52	1		

- Molecule 7 is a protein called Aquaporin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	247	Total	C	N	O	S	1	0
			1838	1194	316	323	5		
7	O	247	Total	C	N	O	S	1	0
			1838	1194	316	323	5		
7	R	247	Total	C	N	O	S	1	0
			1838	1194	316	323	5		
7	M	247	Total	C	N	O	S	1	0
			1838	1194	316	323	5		

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



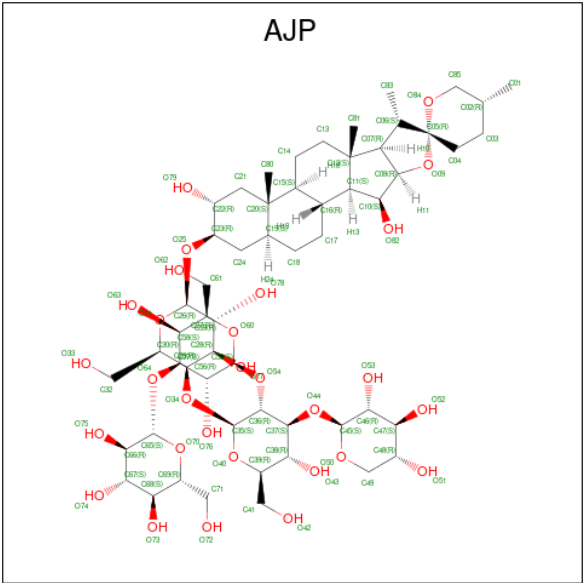
Mol	Chain	Residues	Atoms			AltConf
8	L	1	Total	C	O	0
			28	27	1	
8	L	1	Total	C	O	0
			28	27	1	
8	P	1	Total	C	O	0
			28	27	1	

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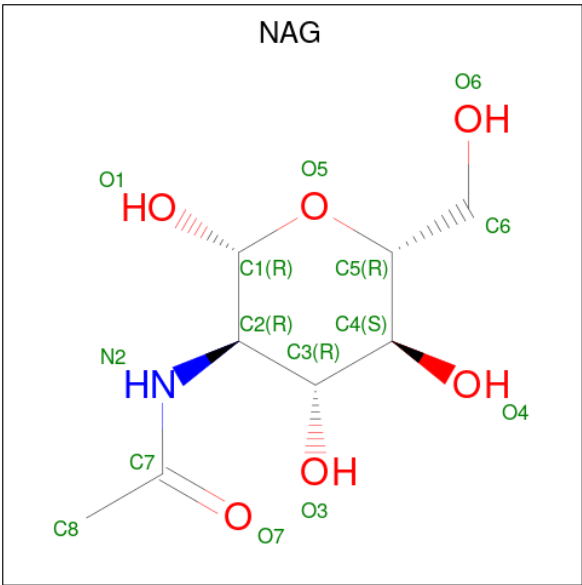
Mol	Chain	Residues	Atoms			AltConf
8	P	1	Total	C	O	0
			28	27	1	
8	T	1	Total	C	O	0
			28	27	1	
8	T	1	Total	C	O	0
			28	27	1	
8	S	1	Total	C	O	0
			28	27	1	
8	R	1	Total	C	O	0
			28	27	1	
8	M	1	Total	C	O	0
			28	27	1	
8	M	1	Total	C	O	0
			28	27	1	

- Molecule 9 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).



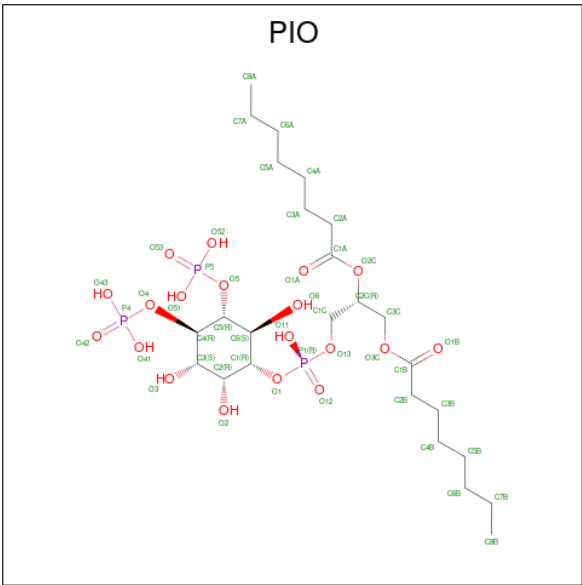
Mol	Chain	Residues	Atoms			AltConf
9	Q	1	Total	C	O	0
			32	27	5	
9	Q	1	Total	C	O	0
			43	33	10	

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
10	P	1	Total	C	N	O	0
			14	8	1	5	
10	T	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 11 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).

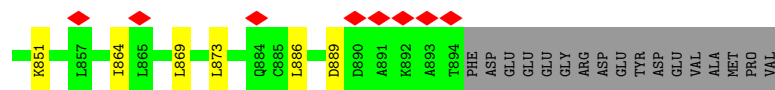


Mol	Chain	Residues	Atoms				AltConf
11	P	1	Total	C	O	P	0
			47	25	19	3	

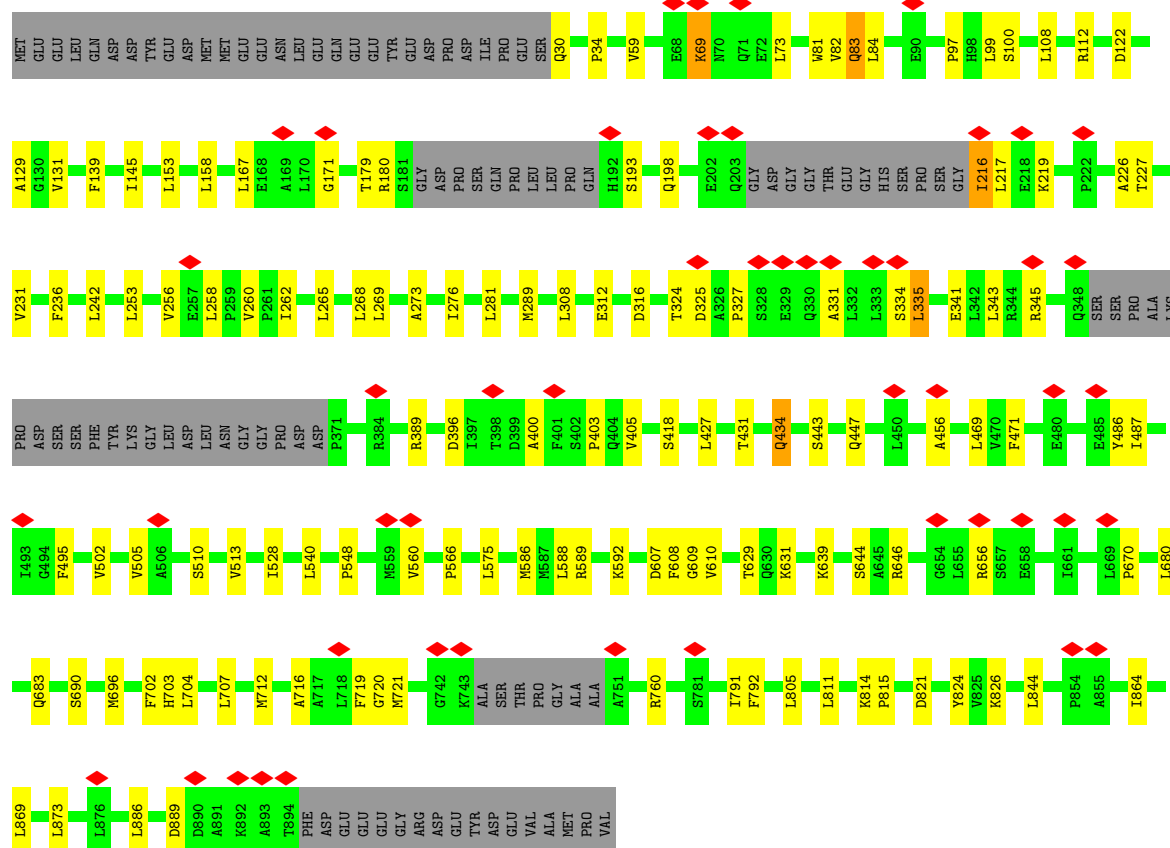
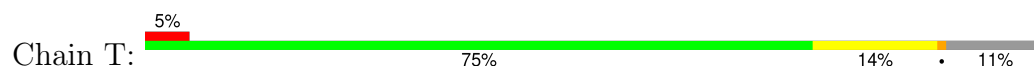
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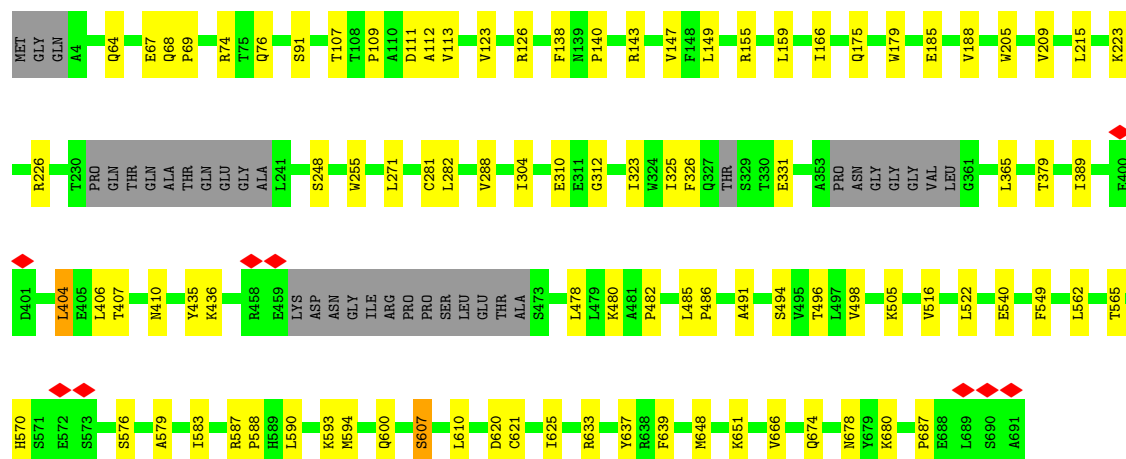
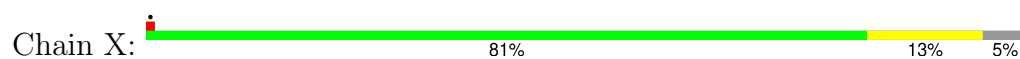
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	T	1	47	25	19	3	0

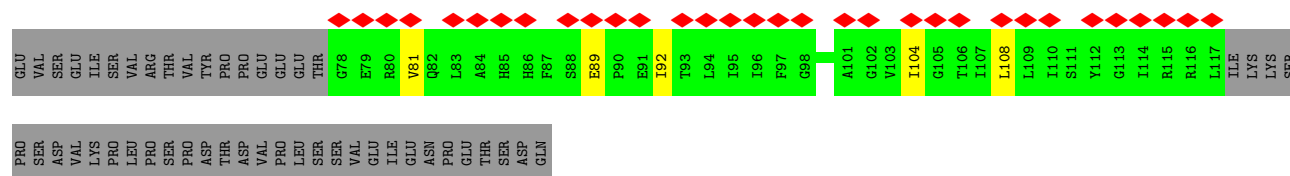


• Molecule 2: Band 3 anion transport protein

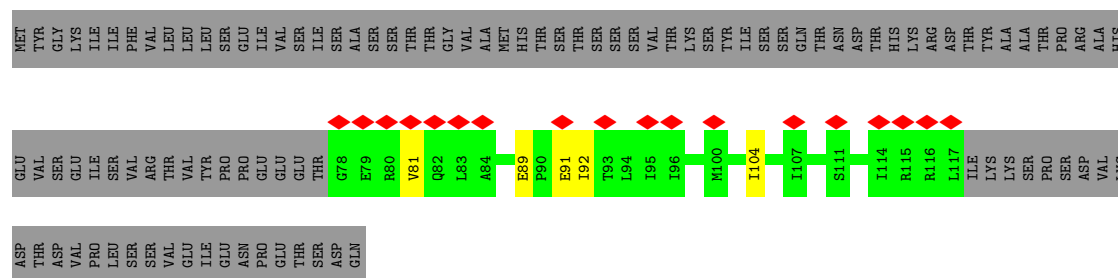


• Molecule 3: Protein 4.2

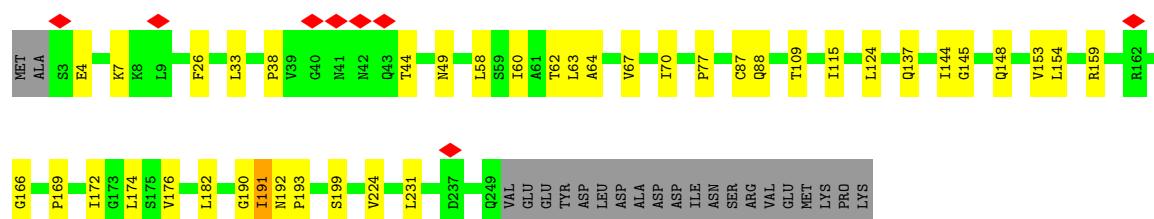
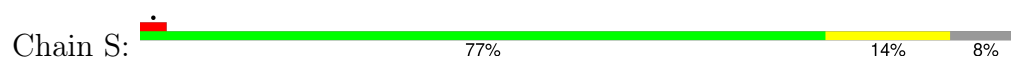




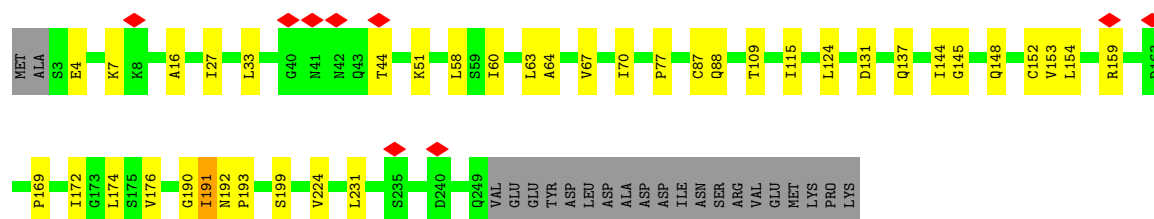
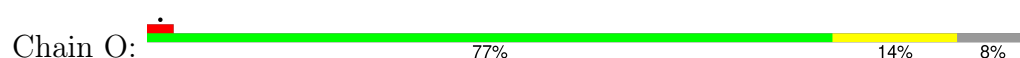
• Molecule 6: Glycophorin-A



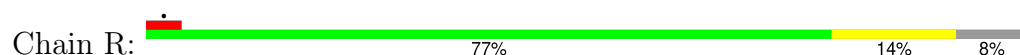
• Molecule 7: Aquaporin-1

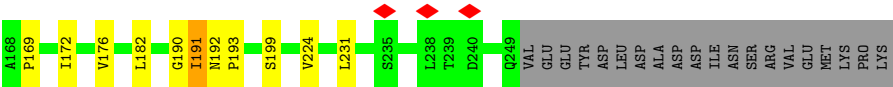


• Molecule 7: Aquaporin-1

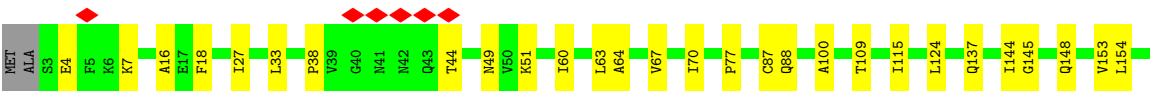
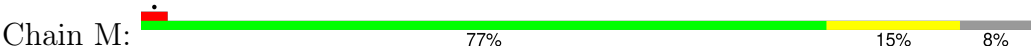


• Molecule 7: Aquaporin-1





• Molecule 7: Aquaporin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145465	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF (cryoSPARC v3) followed by per particle defocus refinement and refinement of higher order aberrations (cryoSPARC v3)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.959	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	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: AJP, P1L, CLR, NAG, PIO

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	0.10	0/3490	0.27	0/4740
2	P	0.11	0/6489	0.27	0/8822
2	T	0.11	0/6556	0.27	0/8913
2	W	0.11	0/236	0.26	0/321
3	X	0.16	0/5273	0.32	0/7151
4	K	0.13	0/3016	0.31	0/4105
5	L	0.13	0/3008	0.29	0/4075
5	Q	0.38	0/3025	0.63	0/4098
6	D	0.11	0/307	0.28	0/415
6	N	0.11	0/307	0.28	0/415
7	M	0.11	0/1849	0.27	0/2518
7	O	0.11	0/1849	0.27	0/2518
7	R	0.11	0/1849	0.27	0/2518
7	S	0.11	0/1849	0.27	0/2518
All	All	0.16	0/39103	0.32	0/53127

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3431	0	3489	30	0
2	P	6339	0	6541	74	0
2	T	6406	0	6572	76	0
2	W	233	0	166	0	0
3	X	5167	0	5175	49	0
4	K	2943	0	3056	28	0
5	L	2938	0	2978	46	0
5	Q	2954	0	2989	62	0
6	D	302	0	309	3	0
6	N	302	0	309	3	0
7	M	1838	0	1879	32	0
7	O	1838	0	1879	29	0
7	R	1838	0	1879	29	0
7	S	1838	0	1879	27	0
8	L	56	0	92	1	0
8	M	56	0	92	4	0
8	P	56	0	92	3	0
8	R	28	0	46	2	0
8	S	28	0	46	1	0
8	T	56	0	92	2	0
9	Q	75	0	0	4	0
10	P	14	0	13	0	0
10	T	14	0	13	0	0
11	P	47	0	44	0	0
11	T	47	0	44	1	0
All	All	38844	0	39674	433	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 6.

All (433) 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)
5:Q:377:LEU:HD11	9:Q:502:AJP:C83	1.80	1.11
5:Q:377:LEU:CD1	9:Q:502:AJP:C83	2.44	0.96
5:Q:188:ILE:HD11	5:Q:377:LEU:CD2	2.16	0.76
5:Q:188:ILE:HD11	5:Q:377:LEU:HD23	1.69	0.75
2:T:683:GLN:HE22	2:T:702:PHE:HB3	1.51	0.75
2:P:683:GLN:HE22	2:P:702:PHE:HB3	1.51	0.74
5:Q:286:CYS:HB3	5:Q:291:ILE:HG21	1.72	0.72
5:Q:346:ILE:HG23	5:Q:358:MET:HG3	1.71	0.70
4:K:340:GLU:HG2	4:K:370:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD13	1:A:261:ARG:HG3	1.75	0.67
4:K:153:LEU:HD23	4:K:376:ILE:HD12	1.77	0.65
4:K:364:LEU:HD23	6:D:91:GLU:HG3	1.78	0.65
2:T:227:THR:HG21	2:T:289:MET:HG2	1.78	0.65
2:P:227:THR:HG21	2:P:289:MET:HG2	1.78	0.64
1:A:183:ASN:HD22	3:X:143:ARG:HH12	1.46	0.64
1:A:193:LEU:HD13	1:A:228:ARG:HG3	1.80	0.64
2:T:513:VAL:HG21	2:T:683:GLN:HE21	1.63	0.64
2:P:513:VAL:HG21	2:P:683:GLN:HE21	1.63	0.62
7:O:70:ILE:HD13	7:M:231:LEU:HB3	1.82	0.62
4:K:385:GLY:O	4:K:389:ASN:ND2	2.33	0.62
5:L:217:PHE:HA	5:L:220:MET:HE2	1.82	0.62
2:P:443:SER:HB2	2:P:721:MET:HB3	1.80	0.62
2:T:443:SER:HB2	2:T:721:MET:HB3	1.80	0.61
4:K:123:VAL:HG11	4:K:143:VAL:HA	1.82	0.61
3:X:74:ARG:NH2	3:X:111:ASP:O	2.33	0.61
5:L:113:LYS:O	5:L:117:ASN:ND2	2.33	0.61
3:X:478:LEU:HB3	3:X:496:THR:HB	1.83	0.61
3:X:590:LEU:O	3:X:678:ASN:ND2	2.31	0.61
5:Q:217:PHE:HA	5:Q:220:MET:HE2	1.82	0.61
5:Q:314:LEU:HD12	5:Q:317:LEU:HD23	1.83	0.61
2:T:84:LEU:HD23	2:T:97:PRO:HB2	1.83	0.61
2:P:84:LEU:HD23	2:P:97:PRO:HB2	1.83	0.60
1:A:110:LYS:HE2	1:A:112:PHE:HE2	1.67	0.60
5:Q:113:LYS:O	5:Q:117:ASN:ND2	2.33	0.60
1:A:424:LEU:HD11	1:A:456:LEU:HD23	1.84	0.60
2:P:59:VAL:HB	2:P:81:TRP:HB2	1.84	0.60
7:O:115:ILE:HG23	7:M:137:GLN:HB3	1.84	0.59
2:P:487:ILE:HD11	2:P:720:GLY:HA2	1.84	0.59
2:T:59:VAL:HB	2:T:81:TRP:HB2	1.84	0.59
1:A:214:ALA:O	1:A:251:ASN:ND2	2.36	0.59
3:X:109:PRO:HG2	3:X:112:ALA:HB2	1.83	0.59
2:T:487:ILE:HD11	2:T:720:GLY:HA2	1.84	0.59
5:Q:377:LEU:HD12	9:Q:502:AJP:C83	2.33	0.58
1:A:268:LYS:HB3	1:A:272:GLU:HA	1.84	0.58
3:X:625:ILE:HG22	3:X:666:VAL:HG22	1.86	0.58
4:K:228:LEU:HB2	4:K:234:ARG:HG2	1.85	0.58
5:L:286:CYS:HB3	5:L:291:ILE:HG21	1.85	0.58
2:T:400:ALA:HA	2:T:405:VAL:HG21	1.86	0.58
7:R:137:GLN:HB3	7:M:115:ILE:HG23	1.84	0.58
3:X:637:TYR:HB3	2:T:34:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:273:ALA:HB3	2:P:276:ILE:HD12	1.86	0.58
4:K:57:MET:HE1	4:K:223:VAL:HB	1.85	0.57
1:A:25:LEU:HD21	1:A:63:GLU:HG3	1.85	0.57
2:T:273:ALA:HB3	2:T:276:ILE:HD12	1.86	0.57
3:X:140:PRO:HG2	3:X:159:LEU:HD22	1.87	0.57
5:L:407:LYS:NZ	5:Q:202:GLU:OE2	2.37	0.57
2:P:400:ALA:HA	2:P:405:VAL:HG21	1.86	0.57
2:P:389:ARG:NH1	2:P:456:ALA:O	2.38	0.57
4:K:61:GLY:HA3	4:K:216:LEU:HG	1.86	0.56
3:X:209:VAL:HG13	3:X:365:LEU:HD12	1.86	0.56
2:T:389:ARG:NH1	2:T:456:ALA:O	2.38	0.56
2:T:180:ARG:HH11	2:T:236:PHE:HB2	1.71	0.56
2:P:180:ARG:HH11	2:P:236:PHE:HB2	1.71	0.56
2:T:690:SER:HA	2:T:696:MET:HG3	1.88	0.56
7:S:144:ILE:HD11	8:R:301:CLR:H272	1.88	0.56
2:P:690:SER:HA	2:P:696:MET:HG3	1.88	0.56
7:R:144:ILE:HD11	8:M:301:CLR:H272	1.88	0.56
5:L:346:ILE:HG23	5:L:358:MET:HG3	1.87	0.56
2:P:811:LEU:HD23	2:P:814:LYS:HD2	1.88	0.56
8:S:301:CLR:H272	7:O:144:ILE:HD11	1.88	0.56
4:K:242[B]:TYR:OH	5:Q:55:GLN:NE2	2.39	0.55
5:L:59:VAL:HA	5:Q:220:MET:SD	2.45	0.55
7:R:231:LEU:HB3	7:M:70:ILE:HD13	1.88	0.55
1:A:358:LEU:HB3	1:A:393:THR:HG21	1.87	0.55
3:X:91:SER:OG	3:X:107:THR:OG1	2.24	0.55
2:T:811:LEU:HD23	2:T:814:LYS:HD2	1.88	0.55
5:Q:116:ILE:HD13	5:Q:228:ALA:HB1	1.89	0.55
2:T:505:VAL:HG21	2:T:707:LEU:HB2	1.88	0.55
5:L:116:ILE:HD13	5:L:228:ALA:HB1	1.89	0.55
4:K:308:GLY:HA3	4:K:331:ILE:HD13	1.89	0.54
5:L:243:THR:HA	5:L:283:VAL:HG11	1.89	0.54
5:L:407:LYS:H	5:L:407:LYS:HZ2	1.55	0.54
3:X:226:ARG:HG3	3:X:255:TRP:HA	1.89	0.54
2:T:456:ALA:HB2	2:T:704:LEU:HD23	1.90	0.54
2:T:824:TYR:HB2	2:T:886:LEU:HD23	1.90	0.54
7:S:137:GLN:HB3	7:R:115:ILE:HG23	1.89	0.54
2:P:231:VAL:HG12	2:P:268:LEU:HB2	1.90	0.53
5:L:89:LEU:HD13	5:Q:252:LEU:HD21	1.90	0.53
5:Q:243:THR:HA	5:Q:283:VAL:HG11	1.90	0.53
5:Q:343:LEU:O	5:Q:347:VAL:HG23	2.08	0.53
7:M:144:ILE:HD11	8:M:302:CLR:H272	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:505:VAL:HG21	2:P:707:LEU:HB2	1.88	0.53
4:K:220:TRP:HB3	4:K:245:LEU:HD11	1.91	0.53
2:P:824:TYR:HB2	2:P:886:LEU:HD23	1.90	0.53
3:X:651:LYS:HB2	2:T:30:GLN:HA	1.90	0.53
2:P:131:VAL:HG11	2:P:265:LEU:HD22	1.90	0.53
4:K:249:VAL:HG22	4:K:274:VAL:HG12	1.90	0.53
2:T:231:VAL:HG12	2:T:268:LEU:HB2	1.90	0.53
1:A:334:ILE:HB	1:A:338:HIS:HA	1.90	0.53
7:S:4:GLU:HA	7:S:7:LYS:HE2	1.91	0.53
1:A:181:ALA:O	1:A:218:ASN:ND2	2.41	0.53
2:T:131:VAL:HG11	2:T:265:LEU:HD22	1.90	0.53
3:X:633:ARG:NH2	2:T:122:ASP:OD1	2.40	0.52
5:L:222:TRP:HB3	5:L:247:LEU:HD11	1.92	0.52
2:T:644:SER:O	2:T:656:ARG:NH2	2.43	0.52
2:P:644:SER:O	2:P:656:ARG:NH2	2.43	0.52
3:X:91:SER:HG	3:X:107:THR:HG1	1.56	0.52
3:X:138:PHE:HB3	3:X:147:VAL:HG21	1.90	0.52
5:Q:324:ILE:HD11	9:Q:502:AJP:C10	2.39	0.52
7:O:4:GLU:HA	7:O:7:LYS:HE2	1.91	0.52
3:X:587:ARG:NH1	3:X:674:GLN:O	2.43	0.52
2:P:456:ALA:HB2	2:P:704:LEU:HD23	1.90	0.52
7:O:27:ILE:HG12	7:M:182:LEU:HD22	1.92	0.52
7:R:4:GLU:HA	7:R:7:LYS:HE2	1.91	0.52
3:X:149:LEU:O	3:X:155:ARG:NH1	2.43	0.51
3:X:223:LYS:HD3	3:X:271:LEU:HD22	1.91	0.51
2:P:343:LEU:HD11	2:P:354:PRO:HB3	1.92	0.51
2:T:805:LEU:HD21	2:T:844:LEU:HD11	1.92	0.51
1:A:325:LEU:HD13	1:A:360:LYS:HD2	1.92	0.51
5:Q:188:ILE:HD11	5:Q:377:LEU:HD21	1.91	0.51
2:T:586:MET:HE1	2:T:589:ARG:HH21	1.75	0.51
7:O:51:LYS:HE2	7:M:49:ASN:HB2	1.92	0.51
4:K:182:THR:HB	4:K:381:GLY:HA3	1.93	0.51
2:P:586:MET:HE1	2:P:589:ARG:HH21	1.75	0.51
2:P:805:LEU:HD21	2:P:844:LEU:HD11	1.92	0.51
7:M:4:GLU:HA	7:M:7:LYS:HE2	1.91	0.51
7:S:115:ILE:HG23	7:O:137:GLN:HB3	1.91	0.51
3:X:113:VAL:HG13	3:X:205:TRP:HB2	1.92	0.51
5:L:91:LEU:HD13	5:Q:244:TYR:CE1	2.45	0.51
2:T:431:THR:O	2:T:434:GLN:NE2	2.44	0.51
2:P:431:THR:O	2:P:434:GLN:NE2	2.44	0.51
7:O:27:ILE:HG23	7:M:182:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:SER:OG	1:A:310:HIS:ND1	2.40	0.51
2:T:193:SER:OG	2:T:198:GLN:NE2	2.43	0.51
5:Q:335:GLY:O	5:Q:339:VAL:HG23	2.10	0.51
2:P:193:SER:OG	2:P:198:GLN:NE2	2.43	0.51
5:Q:222:TRP:HB3	5:Q:247:LEU:HD11	1.92	0.51
2:T:216:ILE:HA	2:T:219:LYS:HE2	1.93	0.51
7:S:190:GLY:C	7:S:192:ASN:H	2.19	0.51
7:R:131:ASP:HB2	7:M:38:PRO:HB3	1.93	0.51
5:L:179:ALA:HB2	5:L:334:HIS:HB2	1.93	0.50
1:A:367:ARG:NH1	1:A:400:VAL:O	2.44	0.50
3:X:389:ILE:HB	3:X:436:LYS:HD2	1.92	0.50
5:L:60:MET:HG3	5:L:221:PHE:HB2	1.94	0.50
5:L:188:ILE:HD11	5:L:377:LEU:HD23	1.94	0.50
5:Q:179:ALA:HB2	5:Q:334:HIS:HB2	1.94	0.50
7:R:190:GLY:C	7:R:192:ASN:H	2.19	0.50
5:L:73:LYS:HE3	5:L:202:GLU:HB3	1.94	0.50
5:Q:120:PHE:HB3	5:Q:174:ILE:HD11	1.92	0.50
5:Q:298:ILE:O	5:Q:302:ILE:HG13	2.12	0.50
2:P:821:ASP:OD1	2:P:826:LYS:NZ	2.43	0.50
2:T:821:ASP:OD1	2:T:826:LYS:NZ	2.43	0.50
7:M:190:GLY:C	7:M:192:ASN:H	2.19	0.50
3:X:215:LEU:HD11	3:X:282:LEU:HD12	1.94	0.50
5:L:120:PHE:HB3	5:L:174:ILE:HD11	1.92	0.50
2:T:869:LEU:HD12	2:T:873:LEU:HB2	1.94	0.50
3:X:67:GLU:HG2	3:X:68:GLN:HG2	1.94	0.49
5:L:315:THR:HG1	5:L:332:ASN:HD21	1.59	0.49
2:T:139:PHE:HB3	2:T:145:ILE:HG12	1.94	0.49
7:S:70:ILE:HD13	7:O:231:LEU:HB3	1.93	0.49
7:R:182:LEU:HB2	7:M:27:ILE:HG23	1.93	0.49
5:Q:73:LYS:HE3	5:Q:202:GLU:HB3	1.94	0.49
7:O:190:GLY:C	7:O:192:ASN:H	2.19	0.49
7:O:33:LEU:HD11	7:O:124:LEU:HA	1.95	0.49
5:Q:60:MET:HG3	5:Q:221:PHE:HB2	1.94	0.49
7:R:190:GLY:O	7:R:192:ASN:N	2.45	0.49
7:M:190:GLY:O	7:M:192:ASN:N	2.45	0.49
3:X:498:VAL:HG22	3:X:540:GLU:HG3	1.94	0.49
2:T:447:GLN:HG2	2:T:712:MET:HB3	1.95	0.49
7:R:182:LEU:HD22	7:M:27:ILE:HG12	1.93	0.49
4:K:396:PRO:HB3	4:K:406:VAL:HG11	1.95	0.49
2:T:403:PRO:HB2	2:T:608:PHE:HE1	1.78	0.49
7:M:33:LEU:HD11	7:M:124:LEU:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:447:GLN:HG2	2:P:712:MET:HB3	1.95	0.49
7:S:33:LEU:HD11	7:S:124:LEU:HA	1.95	0.49
2:P:105:TRP:NE1	2:T:316:ASP:OD1	2.46	0.48
4:K:217:TRP:NE1	4:K:245:LEU:HB3	2.28	0.48
7:R:33:LEU:HD11	7:R:124:LEU:HA	1.95	0.48
2:P:101:HIS:NE2	2:T:335:LEU:HG	2.28	0.48
3:X:505:LYS:HD3	3:X:570:HIS:CD2	2.49	0.48
2:P:139:PHE:HB3	2:P:145:ILE:HG12	1.95	0.48
2:T:325:ASP:OD1	2:T:325:ASP:N	2.47	0.48
2:T:396:ASP:HB3	2:T:760:ARG:HG3	1.96	0.48
2:T:548:PRO:HD2	2:T:566:PRO:HB3	1.95	0.48
4:K:340:GLU:O	4:K:344:ILE:HG12	2.14	0.48
5:Q:250:CYS:SG	5:Q:279:GLY:N	2.84	0.48
2:P:403:PRO:HB2	2:P:608:PHE:HE1	1.78	0.48
1:A:76:LYS:O	1:A:109:GLN:NE2	2.47	0.48
4:K:84:LEU:HB2	4:K:124:LEU:HD11	1.96	0.48
5:L:250:CYS:SG	5:L:279:GLY:N	2.84	0.48
2:P:869:LEU:HD12	2:P:873:LEU:HB2	1.94	0.48
7:O:190:GLY:O	7:O:192:ASN:N	2.45	0.48
1:A:131:LEU:HD11	1:A:163:LEU:HD23	1.96	0.48
5:Q:1:MET:HG2	5:Q:3:PHE:H	1.79	0.48
2:P:325:ASP:OD1	2:P:325:ASP:N	2.47	0.48
2:P:418:SER:HB2	2:P:792:PHE:HZ	1.79	0.48
2:P:548:PRO:HD2	2:P:566:PRO:HB3	1.94	0.48
2:P:629:THR:O	2:P:631:LYS:NZ	2.45	0.48
7:S:49:ASN:HB2	7:R:51:LYS:HE2	1.94	0.48
7:S:190:GLY:O	7:S:192:ASN:N	2.45	0.48
5:L:210:PHE:HE1	5:Q:213:ILE:HD11	1.78	0.48
5:Q:385:LEU:O	5:Q:390:GLN:NE2	2.44	0.47
8:T:1001:CLR:H162	8:T:1001:CLR:H221	1.47	0.47
8:P:1001:CLR:H221	8:P:1001:CLR:H162	1.47	0.47
5:Q:19:LEU:HD13	5:Q:96:ILE:HG21	1.96	0.47
2:P:396:ASP:HB3	2:P:760:ARG:HG3	1.96	0.47
2:T:629:THR:O	2:T:631:LYS:NZ	2.45	0.47
3:X:331:GLU:OE2	3:X:435:TYR:OH	2.24	0.47
4:K:108:ILE:HD12	5:L:293:PRO:HG2	1.97	0.47
5:Q:348:ALA:HB1	5:Q:353:ALA:HB3	1.96	0.47
1:A:346:ALA:HA	1:A:386:VAL:HG11	1.96	0.47
3:X:485:LEU:HD12	3:X:486:PRO:HD2	1.97	0.47
5:Q:147:LEU:HD12	5:Q:379:THR:HG23	1.97	0.47
6:N:89:GLU:HA	6:N:92:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:89:GLU:HA	6:D:92:ILE:HG22	1.97	0.47
3:X:312:GLY:O	3:X:565:THR:OG1	2.31	0.47
5:L:91:LEU:HD11	5:Q:248:ALA:HB2	1.96	0.47
2:P:108:LEU:HD21	2:P:112:ARG:HH21	1.80	0.47
2:P:343:LEU:HD13	2:T:324:THR:O	2.15	0.47
2:T:592:LYS:NZ	2:T:607:ASP:OD1	2.46	0.47
5:L:64:GLY:HA3	5:L:218:LEU:HG	1.97	0.47
5:Q:64:GLY:HA2	5:Q:214:GLY:HA2	1.97	0.47
2:P:341:GLU:OE1	2:P:345:ARG:NE	2.48	0.47
2:T:418:SER:HB2	2:T:792:PHE:HZ	1.79	0.47
5:L:26:TYR:OH	5:Q:242:ASN:OD1	2.33	0.47
2:P:292:ARG:NH2	2:P:353:LYS:O	2.47	0.47
5:L:19:LEU:HD13	5:L:96:ILE:HG21	1.96	0.46
2:T:108:LEU:HD21	2:T:112:ARG:HH21	1.80	0.46
5:L:1:MET:HG2	5:L:3:PHE:H	1.79	0.46
5:L:90:GLY:HA2	5:L:149:ILE:HD11	1.97	0.46
5:Q:321:LYS:HA	5:Q:321:LYS:HD3	1.61	0.46
2:T:341:GLU:OE1	2:T:345:ARG:NE	2.48	0.46
3:X:480:LYS:HB3	3:X:494:SER:HB3	1.97	0.46
5:Q:22:LEU:O	5:Q:107:LYS:NZ	2.41	0.46
5:Q:277:LEU:HB2	5:Q:333:LEU:HD11	1.97	0.46
2:P:347:TYR:OH	2:T:325:ASP:HB3	2.16	0.46
5:L:67:PHE:O	5:L:70:THR:OG1	2.30	0.46
2:P:99:LEU:HG	2:T:331:ALA:HB1	1.97	0.46
2:T:242:LEU:HD12	2:T:268:LEU:HD21	1.98	0.46
7:S:109:THR:HG21	7:S:199:SER:HA	1.98	0.46
1:A:53:SER:HA	1:A:93:VAL:HG11	1.96	0.46
3:X:179:TRP:NE1	3:X:248:SER:OG	2.40	0.46
5:L:147:LEU:HD12	5:L:379:THR:HG23	1.97	0.46
5:L:385:LEU:O	5:L:390:GLN:NE2	2.44	0.46
7:O:109:THR:HG21	7:O:199:SER:HA	1.98	0.46
7:R:109:THR:HG21	7:R:199:SER:HA	1.98	0.46
7:S:231:LEU:HB3	7:R:70:ILE:HD13	1.98	0.46
5:Q:90:GLY:HA2	5:Q:149:ILE:HD11	1.97	0.46
2:P:242:LEU:HD12	2:P:268:LEU:HD21	1.98	0.46
7:S:145:GLY:O	7:S:148:GLN:HG3	2.16	0.46
3:X:610:LEU:HB3	3:X:648:MET:HE3	1.97	0.46
2:P:73:LEU:HD23	2:P:73:LEU:H	1.81	0.46
2:T:495:PHE:HB3	8:T:1001:CLR:H261	1.98	0.46
7:S:58:LEU:HD22	7:O:174:LEU:HB3	1.98	0.46
7:O:58:LEU:HD22	7:M:174:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:277:LEU:HB2	5:L:333:LEU:HD11	1.97	0.45
5:Q:261:VAL:HB	5:Q:312:LYS:HG2	1.99	0.45
2:T:226:ALA:HB3	2:T:262:ILE:HG13	1.98	0.45
4:K:129:ALA:HB2	4:K:329:HIS:CG	2.50	0.45
5:L:64:GLY:HA2	5:L:214:GLY:HA2	1.97	0.45
5:L:261:VAL:HB	5:L:312:LYS:HG2	1.98	0.45
2:P:592:LYS:NZ	2:P:607:ASP:OD1	2.46	0.45
2:T:73:LEU:H	2:T:73:LEU:HD23	1.81	0.45
7:O:145:GLY:O	7:O:148:GLN:HG3	2.16	0.45
7:R:145:GLY:O	7:R:148:GLN:HG3	2.16	0.45
8:R:301:CLR:H221	8:R:301:CLR:H162	1.72	0.45
7:M:145:GLY:O	7:M:148:GLN:HG3	2.16	0.45
1:A:400:VAL:HB	1:A:404:GLY:HA2	1.98	0.45
1:A:413:PHE:HB2	1:A:443:MET:HE3	1.99	0.45
5:Q:64:GLY:HA3	5:Q:218:LEU:HG	1.97	0.45
2:P:275:HIS:NE2	2:T:312:GLU:OE2	2.50	0.45
2:P:510:SER:HB2	2:P:703:HIS:CE1	2.52	0.45
7:M:88:GLN:OE1	7:M:159:ARG:NH2	2.50	0.45
5:L:219:TRP:CE2	5:L:247:LEU:HB3	2.51	0.45
7:S:88:GLN:OE1	7:S:159:ARG:NH2	2.50	0.45
7:M:109:THR:HG21	7:M:199:SER:HA	1.98	0.45
1:A:281:ARG:HB3	1:A:311:MET:HB3	1.98	0.45
5:Q:219:TRP:NE1	5:Q:247:LEU:HB3	2.32	0.45
7:S:182:LEU:HD22	7:R:27:ILE:HG12	1.98	0.45
8:M:301:CLR:H221	8:M:301:CLR:H162	1.72	0.45
2:P:226:ALA:HB3	2:P:262:ILE:HG13	1.98	0.45
1:A:358:LEU:HD11	1:A:390:LEU:HD23	1.99	0.45
3:X:410:ASN:OD1	3:X:579:ALA:HA	2.16	0.45
5:Q:188:ILE:CD1	5:Q:377:LEU:HD23	2.43	0.45
2:T:510:SER:HB2	2:T:703:HIS:CE1	2.52	0.45
7:O:88:GLN:OE1	7:O:159:ARG:NH2	2.50	0.45
8:L:501:CLR:H162	8:L:501:CLR:H221	1.35	0.45
5:Q:219:TRP:CE2	5:Q:247:LEU:HB3	2.51	0.45
4:K:74:TRP:HZ2	5:L:205:TYR:HA	1.82	0.45
2:T:815:PRO:HA	11:T:1004:PIO:H2A	1.99	0.45
7:R:64:ALA:HB3	7:R:169:PRO:HB3	1.99	0.45
3:X:594:MET:HB3	3:X:680:LYS:HD3	1.99	0.44
5:L:50:LEU:HB2	5:L:112:ILE:HG21	1.99	0.44
5:L:219:TRP:NE1	5:L:247:LEU:HB3	2.32	0.44
5:Q:50:LEU:HB2	5:Q:112:ILE:HG21	1.99	0.44
7:O:16:ALA:HB2	7:M:231:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:64:ALA:HB3	7:O:169:PRO:HB3	1.99	0.44
7:S:38:PRO:HB3	7:O:131:ASP:HB2	1.98	0.44
7:S:174:LEU:HB3	7:R:58:LEU:HD22	1.99	0.44
7:R:88:GLN:OE1	7:R:159:ARG:NH2	2.50	0.44
2:P:83:GLN:O	2:P:83:GLN:NE2	2.50	0.44
7:O:77:PRO:HD2	7:O:193:PRO:HD2	2.00	0.44
7:S:77:PRO:HD2	7:S:193:PRO:HD2	2.00	0.44
3:X:516:VAL:HG12	3:X:522:LEU:HD13	2.00	0.44
2:T:716:ALA:HB1	2:T:721:MET:HB2	2.00	0.44
1:A:120:GLN:HG3	1:A:121:GLU:HG2	2.00	0.44
5:L:60:MET:HG2	5:L:218:LEU:HD23	2.00	0.44
5:Q:60:MET:HG2	5:Q:218:LEU:HD23	2.00	0.44
2:T:83:GLN:O	2:T:83:GLN:NE2	2.50	0.44
3:X:600:GLN:HB3	3:X:687:PRO:HD3	1.99	0.43
2:T:471:PHE:HZ	2:T:670:PRO:HB3	1.83	0.43
7:S:182:LEU:HB2	7:R:27:ILE:HG23	1.99	0.43
2:P:719:PHE:HB2	2:P:721:MET:HE2	2.00	0.43
7:M:64:ALA:HB3	7:M:169:PRO:HB3	1.99	0.43
7:O:27:ILE:HA	7:M:182:LEU:HD13	2.00	0.43
7:M:77:PRO:HD2	7:M:193:PRO:HD2	2.00	0.43
3:X:69:PRO:HB2	3:X:76:GLN:HB2	1.99	0.43
3:X:185:GLU:HB3	3:X:188:VAL:HG23	1.99	0.43
3:X:562:LEU:HB2	3:X:583:ILE:HB	2.01	0.43
2:T:719:PHE:HB2	2:T:721:MET:HE2	2.00	0.43
4:K:64:PHE:CZ	5:L:213:ILE:HG12	2.53	0.43
5:L:210:PHE:CE1	5:Q:213:ILE:HD11	2.54	0.43
2:P:339:GLN:HE22	2:T:327:PRO:HB3	1.84	0.43
2:P:471:PHE:HZ	2:P:670:PRO:HB3	1.83	0.43
7:S:64:ALA:HB3	7:S:169:PRO:HB3	1.99	0.43
3:X:325:ILE:HG22	3:X:326:PHE:HD2	1.83	0.43
2:T:889:ASP:OD1	2:T:889:ASP:N	2.52	0.43
2:P:256:VAL:HG12	2:P:258:LEU:H	1.84	0.43
2:P:889:ASP:N	2:P:889:ASP:OD1	2.52	0.43
1:A:274:THR:OG1	1:A:277:HIS:ND1	2.41	0.43
3:X:64:GLN:HG2	3:X:76:GLN:HG3	2.01	0.43
5:Q:184:ALA:HB3	5:Q:376:GLY:HA3	2.01	0.43
2:T:129:ALA:HA	2:T:158:LEU:HD21	2.00	0.43
1:A:235:THR:HG22	1:A:239:GLY:HA2	2.01	0.43
3:X:639:PHE:CD2	3:X:648:MET:HG3	2.54	0.43
3:X:304:ILE:HG21	3:X:323:ILE:HG13	1.99	0.42
4:K:74:TRP:CZ2	5:L:205:TYR:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:240:ASN:OD1	5:Q:26:TYR:OH	2.36	0.42
2:P:69:LYS:HG2	2:P:171:GLY:H	1.84	0.42
7:O:153:VAL:HG22	7:O:172:ILE:HD12	2.01	0.42
5:L:51:TYR:OH	5:L:55:GLN:NE2	2.45	0.42
1:A:65:LEU:HD21	1:A:71:LEU:HD13	2.02	0.42
1:A:128:LYS:HG2	1:A:162:HIS:NE2	2.35	0.42
1:A:396:SER:HB2	1:A:399:ALA:HB2	2.01	0.42
2:P:129:ALA:HA	2:P:158:LEU:HD21	2.00	0.42
2:T:256:VAL:HG12	2:T:258:LEU:H	1.84	0.42
5:Q:60:MET:HG2	5:Q:218:LEU:HA	2.01	0.42
2:P:495:PHE:HB3	8:P:1001:CLR:H261	2.01	0.42
2:T:427:LEU:HD13	2:T:469:LEU:HD12	2.01	0.42
7:R:77:PRO:HD2	7:R:193:PRO:HD2	2.00	0.42
5:Q:209:LEU:HD12	5:Q:209:LEU:HA	1.86	0.42
6:N:108:LEU:HD22	2:P:378:LEU:HD13	2.01	0.42
2:P:716:ALA:HB1	2:P:721:MET:HB2	2.00	0.42
2:T:216:ILE:HD12	2:T:217:LEU:H	1.84	0.42
2:T:389:ARG:HD2	2:T:389:ARG:HA	1.84	0.42
7:S:153:VAL:HG22	7:S:172:ILE:HD12	2.01	0.42
2:T:69:LYS:HG2	2:T:171:GLY:H	1.84	0.42
7:M:153:VAL:HG22	7:M:172:ILE:HD12	2.01	0.42
6:N:104:ILE:HD13	2:P:502:VAL:HG11	2.01	0.42
7:S:154:LEU:HD11	7:S:224:VAL:HG22	2.01	0.42
5:L:58:HIS:CE1	5:Q:244:TYR:HE2	2.38	0.42
2:T:153:LEU:HD22	2:T:269:LEU:HD13	2.02	0.42
7:S:60:ILE:HG13	7:S:176:VAL:HG21	2.02	0.42
7:O:154:LEU:HD11	7:O:224:VAL:HG22	2.01	0.42
5:L:60:MET:HG2	5:L:218:LEU:HA	2.01	0.42
7:R:153:VAL:HG22	7:R:172:ILE:HD12	2.01	0.42
7:M:154:LEU:HD11	7:M:224:VAL:HG22	2.02	0.42
1:A:49:LEU:HB2	1:A:69:ILE:HD13	2.01	0.42
3:X:593:LYS:HB3	3:X:607:SER:HB3	2.00	0.42
5:Q:51:TYR:OH	5:Q:55:GLN:NE2	2.45	0.42
2:T:680:LEU:HD21	2:T:864:ILE:HD11	2.02	0.42
3:X:404:LEU:HD12	3:X:404:LEU:HA	1.81	0.41
3:X:621:CYS:HB3	3:X:639:PHE:CZ	2.55	0.41
5:Q:67:PHE:O	5:Q:70:THR:OG1	2.30	0.41
2:T:331:ALA:O	2:T:334:SER:OG	2.31	0.41
7:S:26:PHE:CD1	7:O:144:ILE:HG21	2.55	0.41
2:P:81:TRP:NE1	2:P:100:SER:OG	2.48	0.41
2:P:226:ALA:N	2:P:261:PRO:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:308:LEU:O	2:P:312:GLU:HG2	2.20	0.41
2:T:308:LEU:O	2:T:312:GLU:HG2	2.20	0.41
7:R:231:LEU:HD22	7:M:16:ALA:HB2	2.02	0.41
3:X:365:LEU:HD23	3:X:365:LEU:HA	1.94	0.41
5:L:57:VAL:O	5:L:61:ILE:HG12	2.20	0.41
5:Q:253:THR:HG21	5:Q:301:SER:HB3	2.02	0.41
6:D:104:ILE:HD13	2:T:502:VAL:HG11	2.02	0.41
2:P:146:ARG:HD2	2:P:148:GLN:HE21	1.86	0.41
7:M:60:ILE:HG13	7:M:176:VAL:HG21	2.02	0.41
3:X:166:ILE:HD12	3:X:288:VAL:HG11	2.02	0.41
5:Q:57:VAL:O	5:Q:61:ILE:HG12	2.20	0.41
3:X:123:VAL:HB	3:X:126:ARG:HE	1.85	0.41
4:K:223:VAL:HA	4:K:226:PRO:HG3	2.03	0.41
2:P:427:LEU:HD13	2:P:469:LEU:HD12	2.01	0.41
8:P:1001:CLR:H272	8:P:1001:CLR:H231	1.90	0.41
2:T:588:LEU:HD13	2:T:609:GLY:HA2	2.02	0.41
7:S:63:LEU:O	7:S:67:VAL:HG22	2.21	0.41
8:M:302:CLR:H162	8:M:302:CLR:H221	1.72	0.41
1:A:147:PRO:HA	1:A:150:VAL:HG12	2.02	0.41
3:X:482:PRO:HG3	3:X:491:ALA:HB1	2.03	0.41
5:Q:179:ALA:O	5:Q:183:LEU:HG	2.20	0.41
2:T:610:VAL:HG13	2:T:791:ILE:HD12	2.03	0.41
4:K:13:LEU:HD11	4:K:136:LEU:HD23	2.02	0.41
4:K:260:HIS:NE2	5:Q:404:LYS:HD3	2.36	0.41
7:R:154:LEU:HD11	7:R:224:VAL:HG22	2.02	0.41
2:P:610:VAL:HG13	2:P:791:ILE:HD12	2.03	0.41
7:O:60:ILE:HG13	7:O:176:VAL:HG21	2.02	0.41
4:K:58:ALA:HA	4:K:62:LEU:HD12	2.03	0.41
4:K:267:MET:HG3	4:K:271:HIS:CE1	2.56	0.41
5:Q:317:LEU:O	5:Q:321:LYS:HB2	2.21	0.41
2:P:680:LEU:HD21	2:P:864:ILE:HD11	2.02	0.41
2:T:81:TRP:NE1	2:T:100:SER:OG	2.48	0.41
2:T:389:ARG:HG2	2:T:456:ALA:HA	2.03	0.41
7:R:49:ASN:HB2	7:M:51:LYS:HE2	2.03	0.41
7:R:60:ILE:HG13	7:R:176:VAL:HG21	2.02	0.41
7:R:182:LEU:HD13	7:M:27:ILE:HA	2.02	0.41
7:M:18:PHE:HB2	7:M:100:ALA:HB1	2.03	0.41
5:L:210:PHE:CD2	5:Q:209:LEU:HD23	2.56	0.41
2:P:253:LEU:H	2:P:262:ILE:HD13	1.86	0.40
2:P:851:LYS:HE3	2:P:851:LYS:HB3	1.97	0.40
7:S:62:THR:HG23	7:O:152:CYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:166:GLY:HA3	7:R:167:SER:HB2	2.03	0.40
2:P:120:LEU:HB2	2:P:245:VAL:HG22	2.03	0.40
7:R:63:LEU:O	7:R:67:VAL:HG22	2.21	0.40
3:X:588:PRO:HB2	3:X:610:LEU:HD11	2.04	0.40
2:P:153:LEU:HD22	2:P:269:LEU:HD13	2.02	0.40
2:P:416:ALA:HA	2:P:730:ARG:HD3	2.04	0.40
2:T:540:LEU:HD21	2:T:575:LEU:HD13	2.03	0.40
7:M:63:LEU:O	7:M:67:VAL:HG22	2.21	0.40
2:T:99:LEU:HD23	2:T:99:LEU:HA	1.95	0.40
7:O:63:LEU:O	7:O:67:VAL:HG22	2.21	0.40
2:P:389:ARG:HG2	2:P:456:ALA:HA	2.03	0.40
2:P:669:LEU:HD23	2:P:672:LEU:HD12	2.04	0.40
2:T:253:LEU:H	2:T:262:ILE:HD13	1.86	0.40
7:O:115:ILE:HA	7:M:137:GLN:HG2	2.04	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	449/1881 (24%)	440 (98%)	8 (2%)	1 (0%)	44	73
2	P	796/911 (87%)	784 (98%)	12 (2%)	0	100	100
2	T	804/911 (88%)	792 (98%)	12 (2%)	0	100	100
2	W	30/911 (3%)	27 (90%)	3 (10%)	0	100	100
3	X	647/691 (94%)	639 (99%)	8 (1%)	0	100	100
4	K	370/417 (89%)	368 (100%)	2 (0%)	0	100	100
5	L	384/409 (94%)	381 (99%)	3 (1%)	0	100	100
5	Q	386/409 (94%)	384 (100%)	1 (0%)	1 (0%)	37	66
6	D	38/150 (25%)	37 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	N	38/150 (25%)	37 (97%)	1 (3%)	0	100	100
7	M	245/269 (91%)	237 (97%)	7 (3%)	1 (0%)	30	60
7	O	245/269 (91%)	237 (97%)	7 (3%)	1 (0%)	30	60
7	R	245/269 (91%)	237 (97%)	7 (3%)	1 (0%)	30	60
7	S	245/269 (91%)	237 (97%)	7 (3%)	1 (0%)	30	60
All	All	4922/7916 (62%)	4837 (98%)	79 (2%)	6 (0%)	50	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	S	191	ILE
7	O	191	ILE
7	R	191	ILE
7	M	191	ILE
1	A	437	VAL
5	Q	292	HIS

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	367/1594 (23%)	360 (98%)	7 (2%)	52	81
2	P	689/786 (88%)	672 (98%)	17 (2%)	42	75
2	T	692/786 (88%)	676 (98%)	16 (2%)	45	77
2	W	20/786 (2%)	20 (100%)	0	100	100
3	X	558/588 (95%)	547 (98%)	11 (2%)	50	79
4	K	317/348 (91%)	298 (94%)	19 (6%)	16	44
5	L	307/328 (94%)	303 (99%)	4 (1%)	65	88
5	Q	308/328 (94%)	297 (96%)	11 (4%)	30	65
6	D	31/136 (23%)	30 (97%)	1 (3%)	34	69
6	N	31/136 (23%)	30 (97%)	1 (3%)	34	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	M	185/213 (87%)	183 (99%)	2 (1%)	70	90
7	O	185/213 (87%)	183 (99%)	2 (1%)	70	90
7	R	185/213 (87%)	183 (99%)	2 (1%)	70	90
7	S	185/213 (87%)	183 (99%)	2 (1%)	70	90
All	All	4060/6668 (61%)	3965 (98%)	95 (2%)	46	77

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	187	ARG
1	A	235	THR
1	A	303	LYS
1	A	370	ASN
1	A	393	THR
1	A	437	VAL
3	X	175	GLN
3	X	281	CYS
3	X	310	GLU
3	X	379	THR
3	X	404	LEU
3	X	406	LEU
3	X	407	THR
3	X	549	PHE
3	X	576	SER
3	X	607	SER
3	X	620	ASP
4	K	11	ARG
4	K	20	LEU
4	K	60	LEU
4	K	68	ASN
4	K	94	LEU
4	K	100	GLN
4	K	153	LEU
4	K	174	VAL
4	K	223	VAL
4	K	249	VAL
4	K	304	ILE
4	K	329	HIS
4	K	334	LEU
4	K	335	LEU

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Mol	Chain	Res	Type
4	K	338	LEU
4	K	340	GLU
4	K	364	LEU
4	K	374	ILE
4	K	383	LEU
5	L	253	THR
5	L	269	MET
5	L	356	THR
5	L	407	LYS
5	Q	253	THR
5	Q	269	MET
5	Q	294	PHE
5	Q	302	ILE
5	Q	321	LYS
5	Q	323	ARG
5	Q	349	VAL
5	Q	351	MET
5	Q	356	THR
5	Q	377	LEU
5	Q	407	LYS
6	N	81	VAL
6	D	81	VAL
2	P	69	LYS
2	P	82	VAL
2	P	83	GLN
2	P	167	LEU
2	P	179	THR
2	P	186	GLN
2	P	191	GLN
2	P	260	VAL
2	P	281	LEU
2	P	335	LEU
2	P	343	LEU
2	P	434	GLN
2	P	486	TYR
2	P	528	ILE
2	P	560	VAL
2	P	639	LYS
2	P	646	ARG
2	T	69	LYS
2	T	82	VAL
2	T	83	GLN

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Mol	Chain	Res	Type
2	T	167	LEU
2	T	179	THR
2	T	216	ILE
2	T	260	VAL
2	T	281	LEU
2	T	335	LEU
2	T	343	LEU
2	T	434	GLN
2	T	486	TYR
2	T	528	ILE
2	T	560	VAL
2	T	639	LYS
2	T	646	ARG
7	S	44	THR
7	S	191	ILE
7	O	44	THR
7	O	191	ILE
7	R	44	THR
7	R	191	ILE
7	M	44	THR
7	M	191	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	123	HIS
1	A	137	GLN
1	A	153	GLN
1	A	154	GLN
1	A	183	ASN
1	A	237	GLN
1	A	347	HIS
1	A	449	HIS
2	W	18	GLN
3	X	64	GLN
3	X	76	GLN
3	X	100	GLN
3	X	154	GLN
3	X	175	GLN
3	X	220	HIS
3	X	225	GLN

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Mol	Chain	Res	Type
3	X	433	GLN
3	X	559	ASN
3	X	570	HIS
3	X	580	GLN
3	X	611	GLN
3	X	632	HIS
4	K	41	GLN
4	K	49	GLN
4	K	80	ASN
5	L	102	GLN
5	L	104	GLN
5	L	200	ASN
5	Q	55	GLN
5	Q	58	HIS
5	Q	102	GLN
5	Q	104	GLN
5	Q	200	ASN
6	D	82	GLN
2	P	70	ASN
2	P	83	GLN
2	P	133	ASN
2	P	192	HIS
2	P	198	GLN
2	P	330	GLN
2	P	377	GLN
2	P	457	GLN
2	P	630	GLN
2	P	683	GLN
2	P	819	HIS
2	T	37	HIS
2	T	83	GLN
2	T	198	GLN
2	T	302	GLN
2	T	330	GLN
2	T	377	GLN
2	T	457	GLN
2	T	630	GLN
2	T	683	GLN
2	T	819	HIS
7	S	42	ASN
7	M	42	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
7	P1L	O	87	7	21,22,23	0.65	0	19,23,25	1.58	3 (15%)
7	P1L	S	87	7	21,22,23	0.65	0	19,23,25	1.58	3 (15%)
7	P1L	M	87	7	21,22,23	0.65	0	19,23,25	1.58	3 (15%)
7	P1L	R	87	7	21,22,23	0.65	0	19,23,25	1.57	3 (15%)

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
7	P1L	O	87	7	-	2/20/22/24	-
7	P1L	S	87	7	-	2/20/22/24	-
7	P1L	M	87	7	-	2/20/22/24	-
7	P1L	R	87	7	-	2/20/22/24	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	87	P1L	CB-SG-C7	4.43	106.85	100.76
7	O	87	P1L	CB-SG-C7	4.41	106.83	100.76
7	M	87	P1L	CB-SG-C7	4.41	106.82	100.76
7	R	87	P1L	CB-SG-C7	4.41	106.82	100.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	87	P1L	C8-C7-SG	-3.67	109.03	113.40
7	O	87	P1L	C8-C7-SG	-3.67	109.03	113.40
7	R	87	P1L	C8-C7-SG	-3.66	109.04	113.40
7	S	87	P1L	C8-C7-SG	-3.64	109.06	113.40
7	M	87	P1L	O7-C7-SG	3.16	126.71	122.68
7	S	87	P1L	O7-C7-SG	3.16	126.70	122.68
7	O	87	P1L	O7-C7-SG	3.15	126.70	122.68
7	R	87	P1L	O7-C7-SG	3.15	126.69	122.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	87	P1L	C14-C15-C16-C17
7	O	87	P1L	C14-C15-C16-C17
7	R	87	P1L	C14-C15-C16-C17
7	M	87	P1L	C14-C15-C16-C17
7	O	87	P1L	C18-C19-C20-C21
7	M	87	P1L	C18-C19-C20-C21
7	S	87	P1L	C18-C19-C20-C21
7	R	87	P1L	C18-C19-C20-C21

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
8	CLR	L	502	-	31,31,31	0.40	0	48,48,48	0.59	0
8	CLR	T	1001	-	31,31,31	0.36	0	48,48,48	0.52	0
8	CLR	M	302	-	31,31,31	0.38	0	48,48,48	0.50	0
8	CLR	R	301	-	31,31,31	0.38	0	48,48,48	0.50	0
9	AJP	Q	501	-	37,37,95	0.49	0	58,62,149	0.68	1 (1%)
11	PIO	T	1004	-	47,47,47	1.21	6 (12%)	62,65,65	0.99	2 (3%)
8	CLR	M	301	-	31,31,31	0.38	0	48,48,48	0.50	0
8	CLR	T	1003	-	31,31,31	0.38	0	48,48,48	0.49	0
10	NAG	P	1002	2	14,14,15	0.25	0	17,19,21	0.46	0
11	PIO	P	1004	-	47,47,47	1.21	7 (14%)	62,65,65	0.99	2 (3%)
8	CLR	P	1001	-	31,31,31	0.36	0	48,48,48	0.51	0
8	CLR	S	301	-	31,31,31	0.37	0	48,48,48	0.50	0
8	CLR	P	1003	-	31,31,31	0.37	0	48,48,48	0.49	0
8	CLR	L	501	-	31,31,31	0.41	0	48,48,48	0.75	3 (6%)
9	AJP	Q	502	-	49,49,95	0.42	0	75,80,149	0.53	0
10	NAG	T	1002	2	14,14,15	0.24	0	17,19,21	0.45	0

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
8	CLR	L	502	-	-	5/10/68/68	0/4/4/4
8	CLR	T	1001	-	-	10/10/68/68	0/4/4/4
8	CLR	M	302	-	-	7/10/68/68	0/4/4/4
8	CLR	R	301	-	-	7/10/68/68	0/4/4/4
11	PIO	T	1004	-	-	19/44/68/68	0/1/1/1
9	AJP	Q	501	-	-	-	0/6/6/11
8	CLR	M	301	-	-	7/10/68/68	0/4/4/4
8	CLR	T	1003	-	-	7/10/68/68	0/4/4/4
10	NAG	P	1002	2	-	0/6/23/26	0/1/1/1
11	PIO	P	1004	-	-	19/44/68/68	0/1/1/1
8	CLR	P	1001	-	-	10/10/68/68	0/4/4/4
8	CLR	S	301	-	-	7/10/68/68	0/4/4/4
8	CLR	P	1003	-	-	7/10/68/68	0/4/4/4
8	CLR	L	501	-	-	9/10/68/68	0/4/4/4
9	AJP	Q	502	-	-	1/6/121/220	0/7/7/11
10	NAG	T	1002	2	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	1004	PIO	P5-O5	3.35	1.65	1.59
11	P	1004	PIO	P4-O4	3.29	1.65	1.59
11	P	1004	PIO	P5-O5	3.28	1.65	1.59
11	T	1004	PIO	P4-O4	3.28	1.65	1.59
11	T	1004	PIO	O2C-C2C	-2.66	1.40	1.46
11	P	1004	PIO	O2C-C2C	-2.64	1.40	1.46
11	T	1004	PIO	O3C-C1B	2.43	1.40	1.33
11	P	1004	PIO	O3C-C1B	2.42	1.40	1.33
11	T	1004	PIO	O3C-C3C	-2.21	1.40	1.45
11	P	1004	PIO	O3C-C3C	-2.18	1.40	1.45
11	P	1004	PIO	O2C-C1A	2.12	1.40	1.34
11	T	1004	PIO	O2C-C1A	2.11	1.40	1.34
11	P	1004	PIO	P1-O1	2.00	1.65	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	1004	PIO	O2C-C1A-C2A	3.89	119.89	111.48
11	T	1004	PIO	O2C-C1A-C2A	3.88	119.88	111.48
11	T	1004	PIO	O3C-C1B-C2B	2.81	120.39	111.83
11	P	1004	PIO	O3C-C1B-C2B	2.80	120.37	111.83
8	L	501	CLR	C16-C15-C14	-2.67	99.93	105.14
9	Q	501	AJP	C19-C24-C23	-2.36	111.59	114.40
8	L	501	CLR	C17-C13-C14	2.05	102.45	100.10
8	L	501	CLR	C12-C13-C14	-2.02	104.23	107.25

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	502	CLR	C13-C17-C20-C21
8	L	502	CLR	C16-C17-C20-C22
11	P	1004	PIO	C1C-O13-P1-O11
11	T	1004	PIO	C1C-O13-P1-O11
8	L	502	CLR	C16-C17-C20-C21
8	P	1001	CLR	C13-C17-C20-C21
8	T	1001	CLR	C13-C17-C20-C21
8	L	502	CLR	C13-C17-C20-C22
8	P	1003	CLR	C21-C20-C22-C23
8	T	1003	CLR	C21-C20-C22-C23
8	L	501	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
8	P	1001	CLR	C16-C17-C20-C21
8	T	1001	CLR	C16-C17-C20-C21
8	L	501	CLR	C13-C17-C20-C22
8	P	1001	CLR	C21-C20-C22-C23
8	T	1001	CLR	C21-C20-C22-C23
8	L	501	CLR	C13-C17-C20-C21
8	P	1001	CLR	C16-C17-C20-C22
8	T	1001	CLR	C16-C17-C20-C22
8	P	1001	CLR	C13-C17-C20-C22
8	T	1001	CLR	C13-C17-C20-C22
8	P	1003	CLR	C17-C20-C22-C23
8	T	1003	CLR	C17-C20-C22-C23
8	L	501	CLR	C21-C20-C22-C23
8	L	501	CLR	C17-C20-C22-C23
8	P	1001	CLR	C17-C20-C22-C23
8	T	1001	CLR	C17-C20-C22-C23
8	S	301	CLR	C17-C20-C22-C23
8	R	301	CLR	C17-C20-C22-C23
8	M	301	CLR	C17-C20-C22-C23
8	M	302	CLR	C17-C20-C22-C23
11	P	1004	PIO	C2A-C1A-O2C-C2C
11	T	1004	PIO	C2A-C1A-O2C-C2C
11	P	1004	PIO	C2B-C1B-O3C-C3C
11	T	1004	PIO	C2B-C1B-O3C-C3C
8	L	501	CLR	C16-C17-C20-C22
8	P	1003	CLR	C20-C22-C23-C24
8	T	1003	CLR	C20-C22-C23-C24
8	P	1001	CLR	C20-C22-C23-C24
8	T	1001	CLR	C20-C22-C23-C24
11	P	1004	PIO	O1A-C1A-O2C-C2C
11	T	1004	PIO	O1A-C1A-O2C-C2C
11	P	1004	PIO	O1B-C1B-O3C-C3C
11	T	1004	PIO	O1B-C1B-O3C-C3C
8	S	301	CLR	C20-C22-C23-C24
8	R	301	CLR	C20-C22-C23-C24
8	M	301	CLR	C20-C22-C23-C24
8	M	302	CLR	C20-C22-C23-C24
8	L	501	CLR	C20-C22-C23-C24
8	L	501	CLR	C23-C24-C25-C27
11	P	1004	PIO	C3B-C4B-C5B-C6B
11	T	1004	PIO	C3B-C4B-C5B-C6B
8	L	502	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
8	L	501	CLR	C23-C24-C25-C26
8	P	1001	CLR	C22-C23-C24-C25
8	T	1001	CLR	C22-C23-C24-C25
11	P	1004	PIO	O13-C1C-C2C-C3C
11	T	1004	PIO	O13-C1C-C2C-C3C
11	P	1004	PIO	C1B-C2B-C3B-C4B
11	T	1004	PIO	C1B-C2B-C3B-C4B
11	P	1004	PIO	C2B-C3B-C4B-C5B
11	T	1004	PIO	C2B-C3B-C4B-C5B
8	S	301	CLR	C21-C20-C22-C23
8	R	301	CLR	C21-C20-C22-C23
8	M	301	CLR	C21-C20-C22-C23
8	M	302	CLR	C21-C20-C22-C23
8	S	301	CLR	C13-C17-C20-C22
8	R	301	CLR	C13-C17-C20-C22
8	M	301	CLR	C13-C17-C20-C22
8	M	302	CLR	C13-C17-C20-C22
8	S	301	CLR	C16-C17-C20-C22
8	R	301	CLR	C16-C17-C20-C22
8	M	301	CLR	C16-C17-C20-C22
8	M	302	CLR	C16-C17-C20-C22
8	S	301	CLR	C13-C17-C20-C21
8	R	301	CLR	C13-C17-C20-C21
8	M	301	CLR	C13-C17-C20-C21
8	M	302	CLR	C13-C17-C20-C21
9	Q	502	AJP	C29-C30-C32-O33
8	T	1001	CLR	C23-C24-C25-C27
8	S	301	CLR	C16-C17-C20-C21
8	R	301	CLR	C16-C17-C20-C21
8	M	301	CLR	C16-C17-C20-C21
8	M	302	CLR	C16-C17-C20-C21
8	P	1001	CLR	C23-C24-C25-C27
8	P	1001	CLR	C23-C24-C25-C26
8	T	1001	CLR	C23-C24-C25-C26
8	P	1003	CLR	C13-C17-C20-C22
8	T	1003	CLR	C13-C17-C20-C22
11	P	1004	PIO	O13-C1C-C2C-O2C
11	T	1004	PIO	O13-C1C-C2C-O2C
8	P	1003	CLR	C16-C17-C20-C22
8	T	1003	CLR	C16-C17-C20-C22
11	P	1004	PIO	C1C-O13-P1-O1
11	P	1004	PIO	C1C-O13-P1-O12

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Mol	Chain	Res	Type	Atoms
11	T	1004	PIO	C1C-O13-P1-O1
11	T	1004	PIO	C1C-O13-P1-O12
11	P	1004	PIO	C2C-C1C-O13-P1
11	T	1004	PIO	C2C-C1C-O13-P1
11	P	1004	PIO	C5A-C6A-C7A-C8A
11	T	1004	PIO	C5A-C6A-C7A-C8A
8	P	1003	CLR	C13-C17-C20-C21
8	T	1003	CLR	C13-C17-C20-C21
11	P	1004	PIO	C1C-C2C-O2C-C1A
11	T	1004	PIO	C1C-C2C-O2C-C1A
11	P	1004	PIO	C5-O5-P5-O53
11	T	1004	PIO	C5-O5-P5-O53
11	T	1004	PIO	O2C-C1A-C2A-C3A
11	P	1004	PIO	O2C-C1A-C2A-C3A
8	P	1003	CLR	C16-C17-C20-C21
8	T	1003	CLR	C16-C17-C20-C21
11	P	1004	PIO	O2C-C2C-C3C-O3C
11	T	1004	PIO	O2C-C2C-C3C-O3C
11	P	1004	PIO	O1A-C1A-C2A-C3A
11	T	1004	PIO	O1A-C1A-C2A-C3A

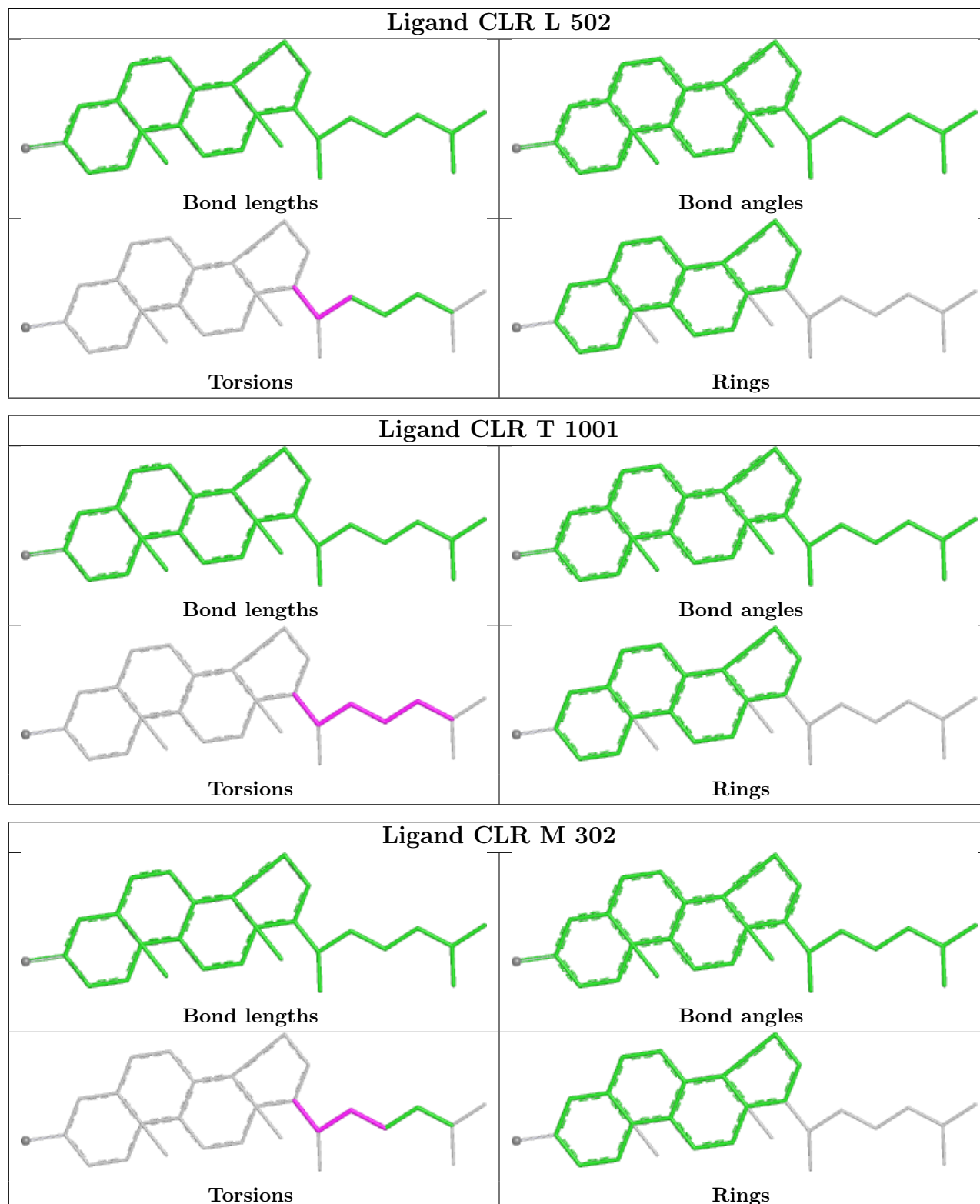
There are no ring outliers.

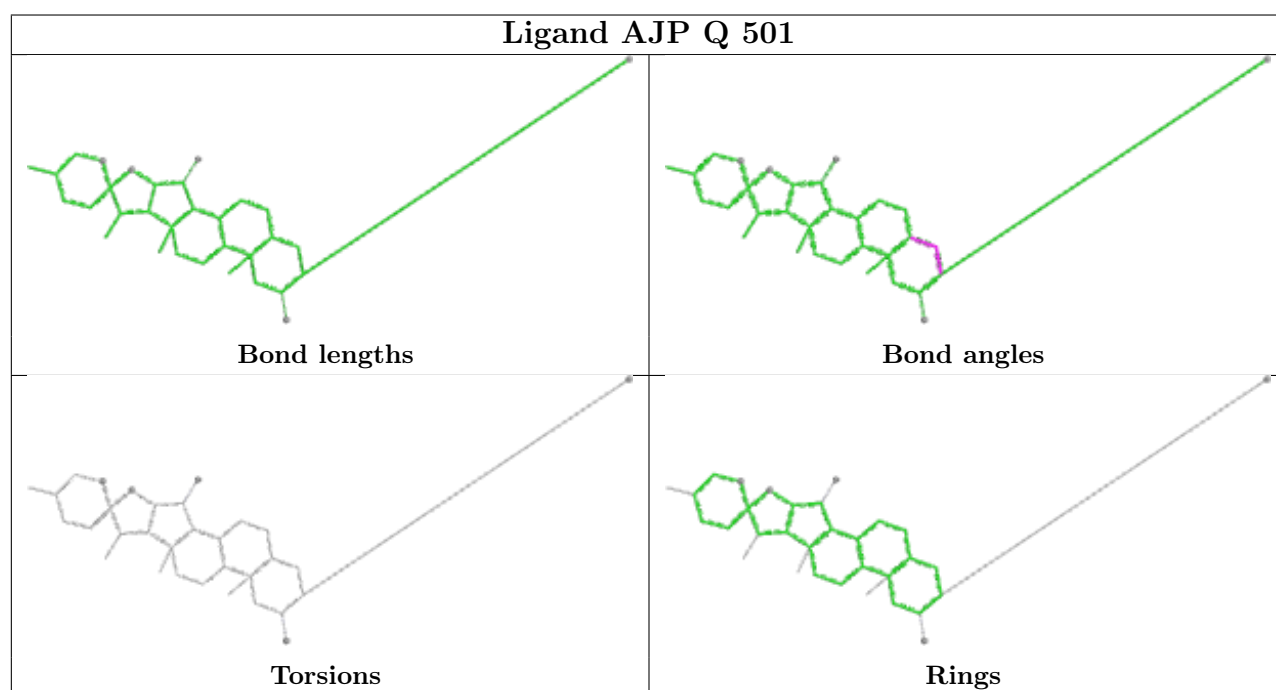
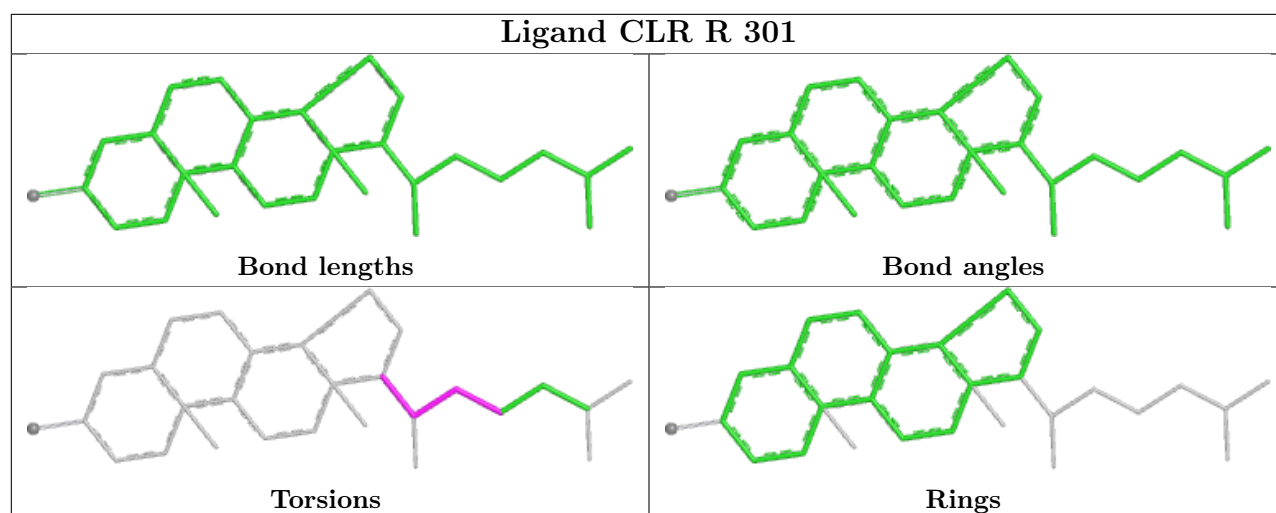
9 monomers are involved in 18 short contacts:

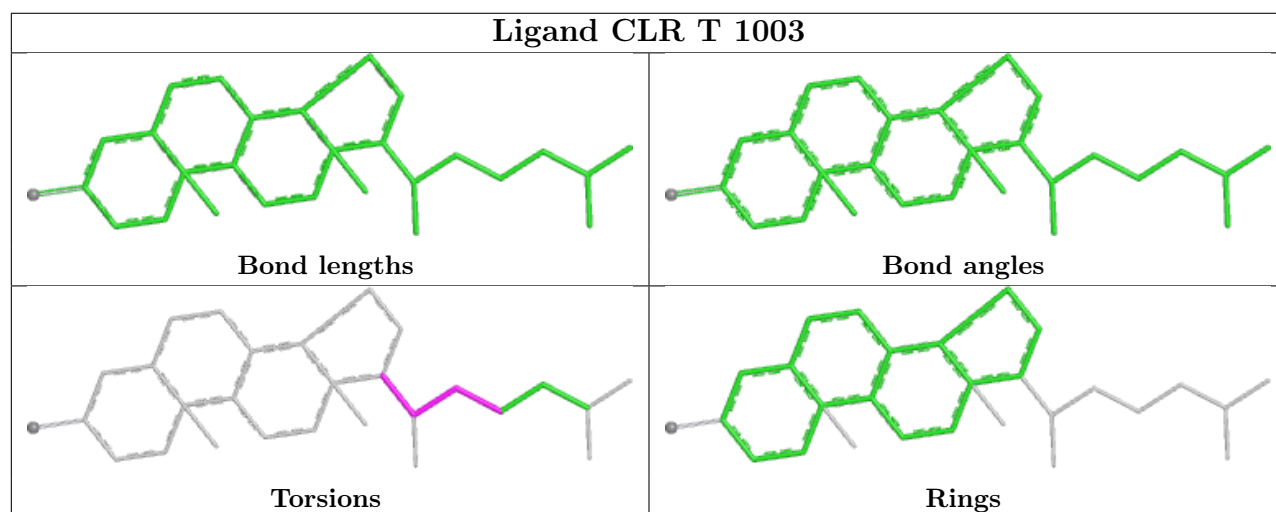
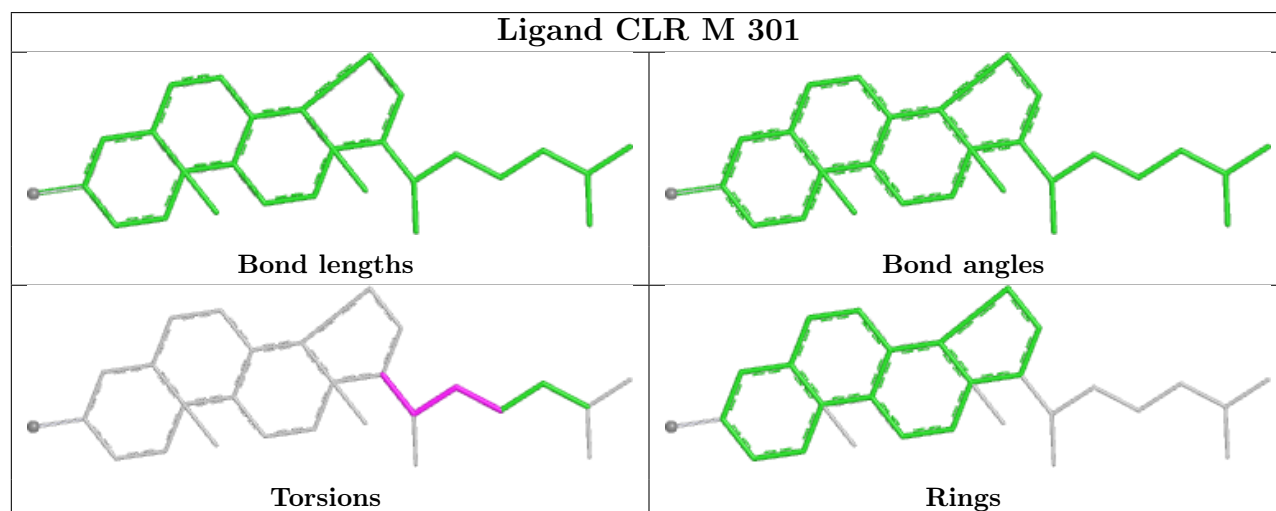
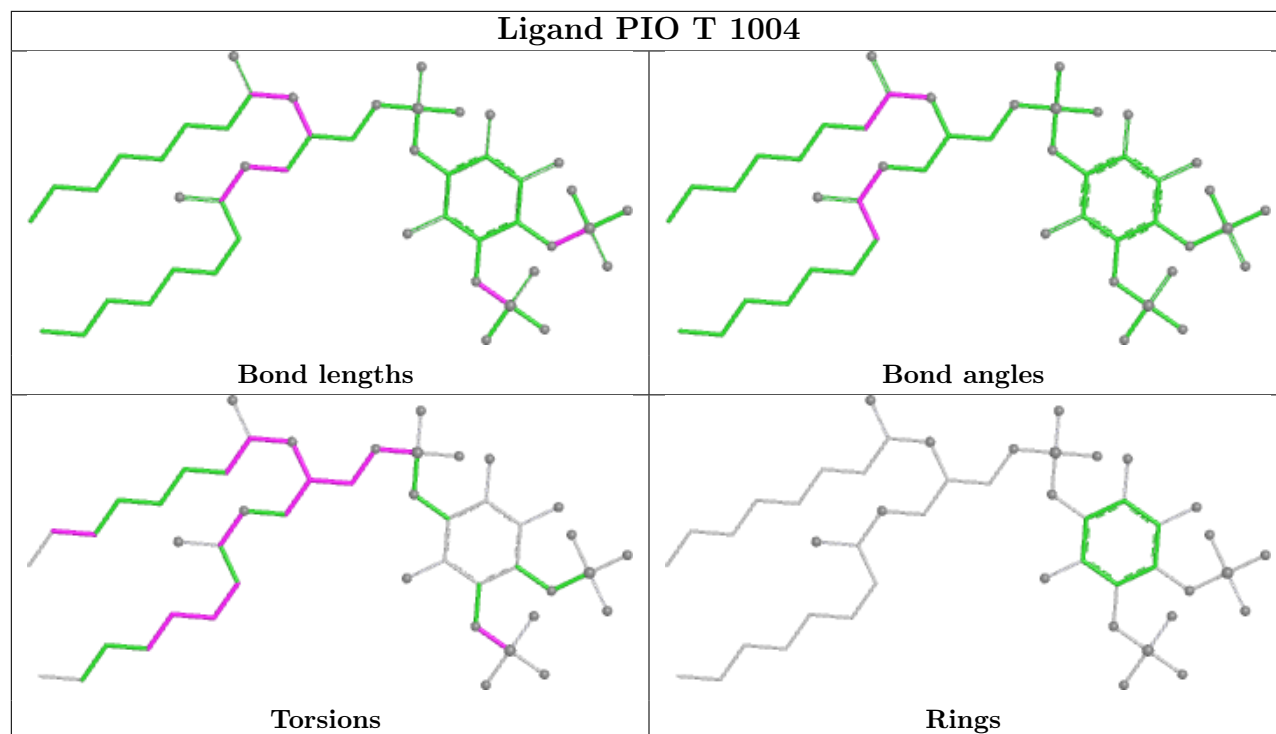
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	1001	CLR	2	0
8	M	302	CLR	2	0
8	R	301	CLR	2	0
11	T	1004	PIO	1	0
8	M	301	CLR	2	0
8	P	1001	CLR	3	0
8	S	301	CLR	1	0
8	L	501	CLR	1	0
9	Q	502	AJP	4	0

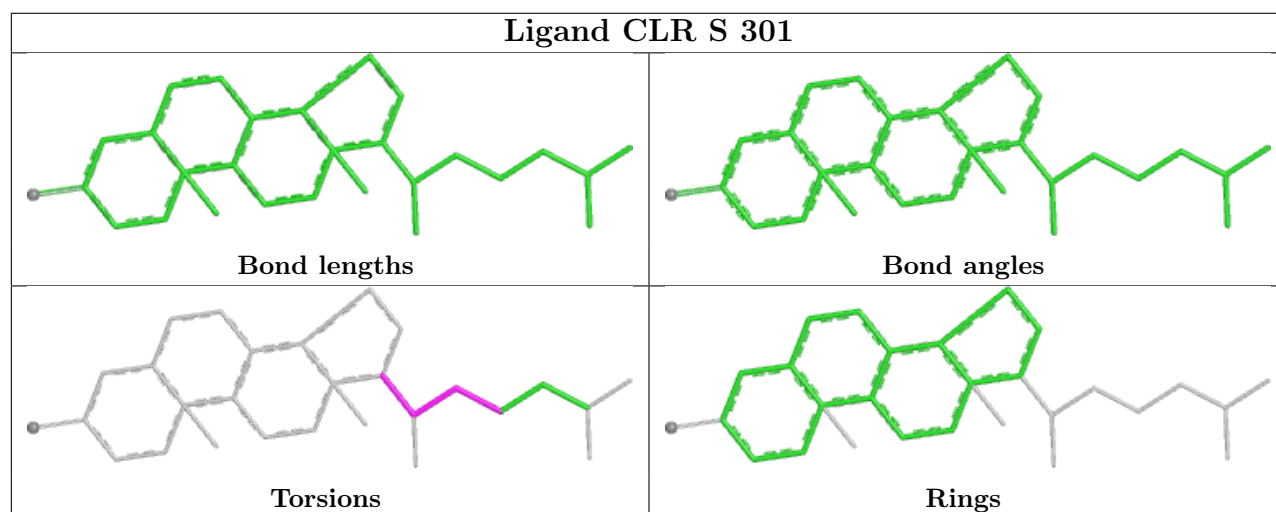
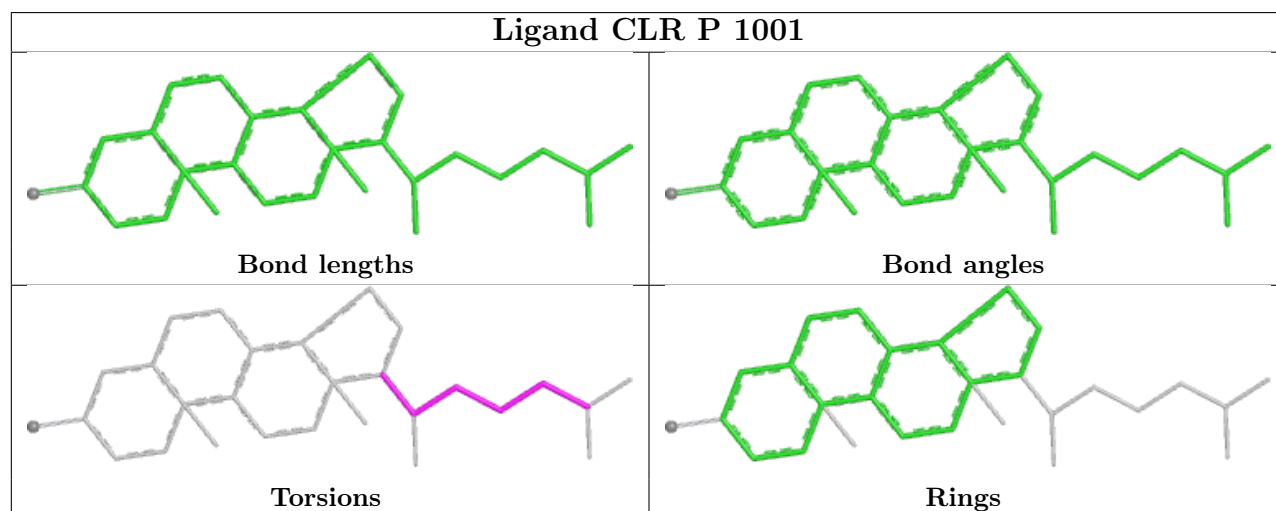
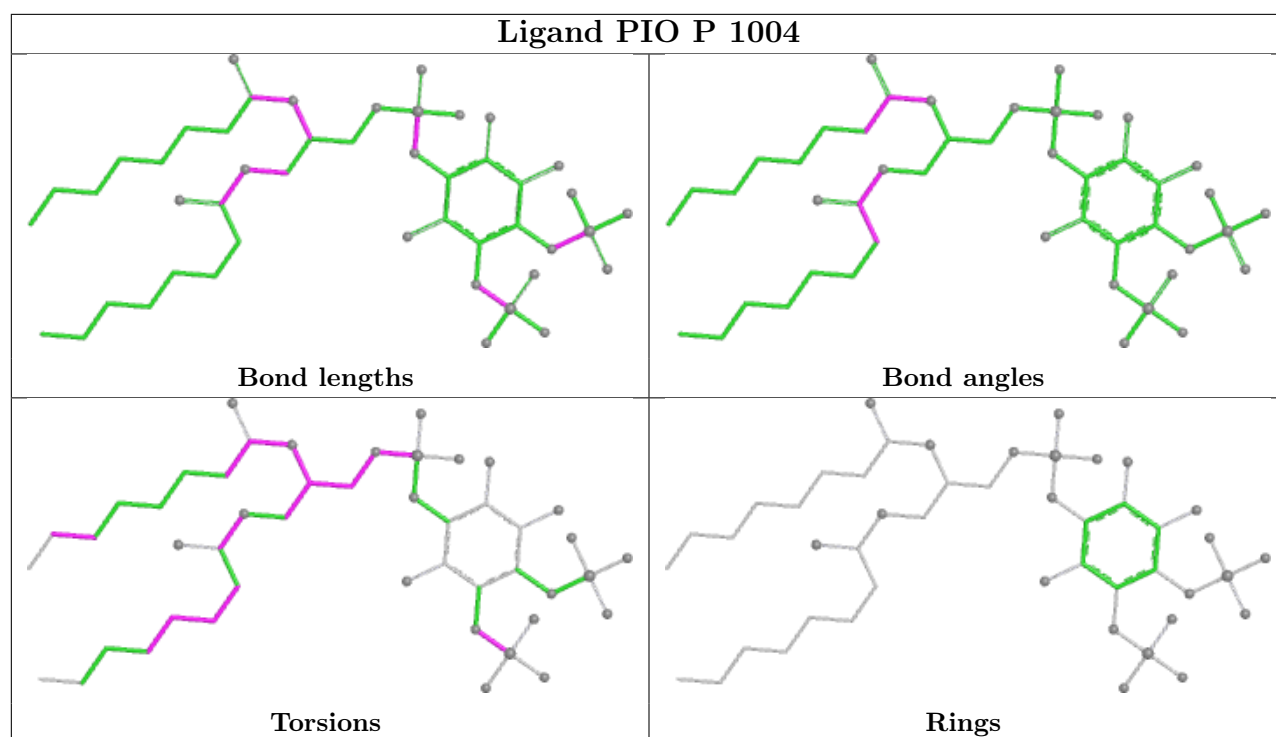
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

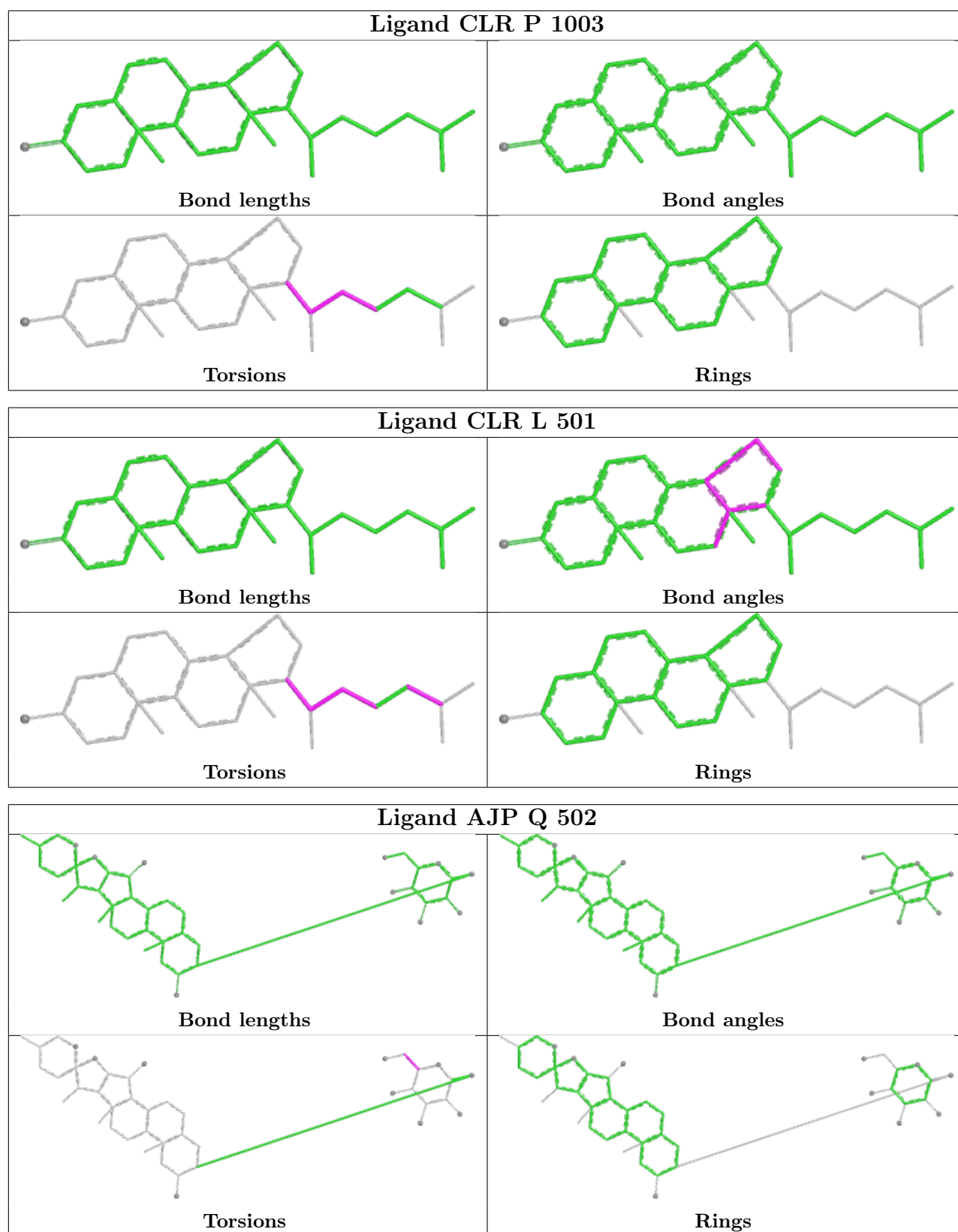
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

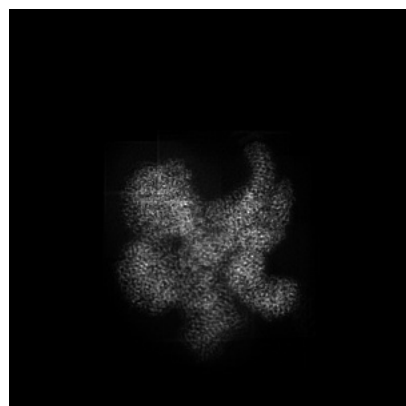
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26988. These allow visual inspection of the internal detail of the map and identification of artifacts.

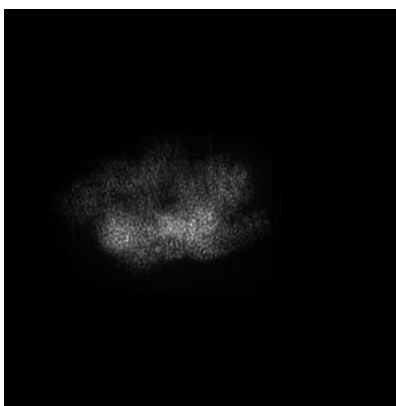
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

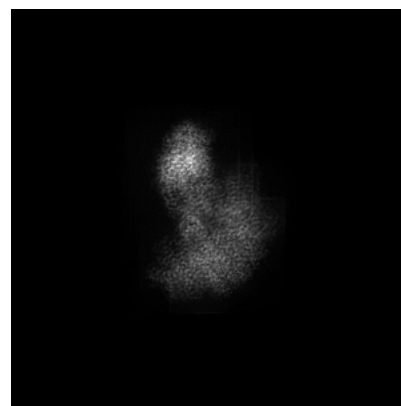
6.1.1 Primary map



X

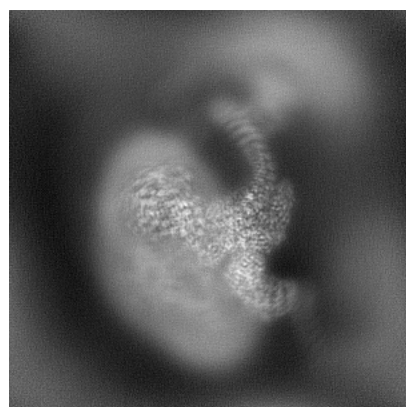


Y

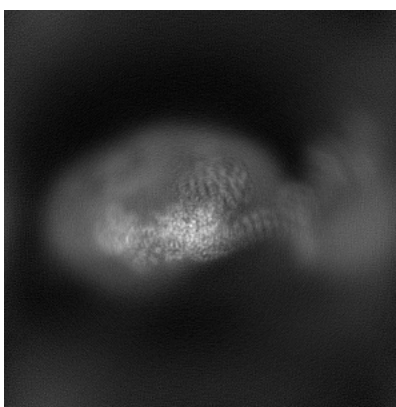


Z

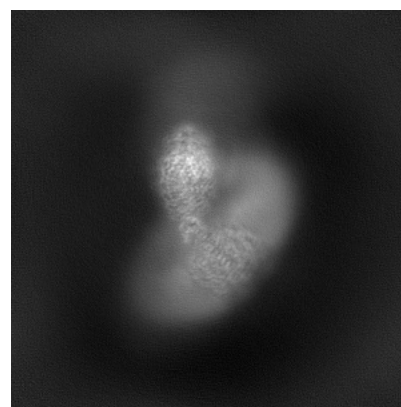
6.1.2 Raw map



X



Y

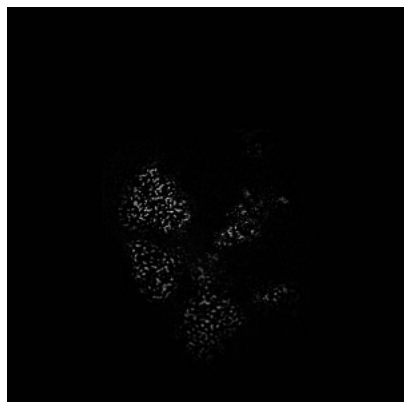


Z

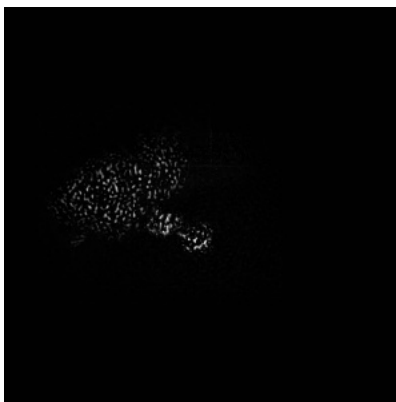
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225

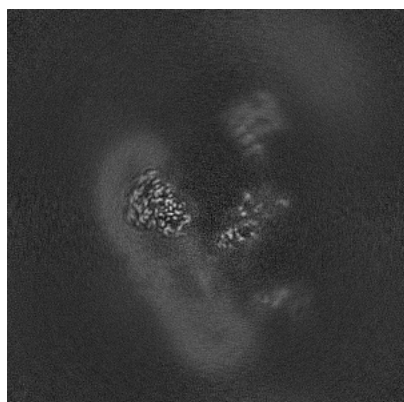


Y Index: 225

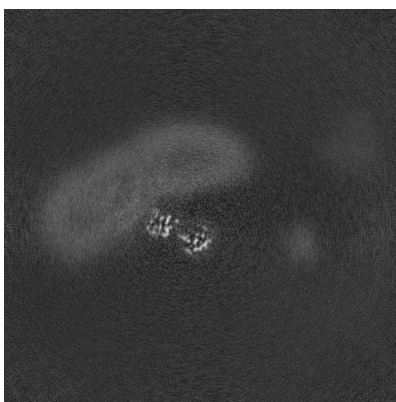


Z Index: 225

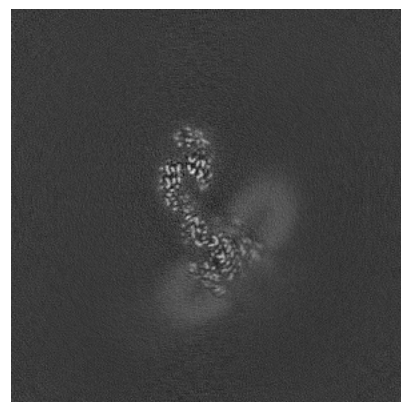
6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

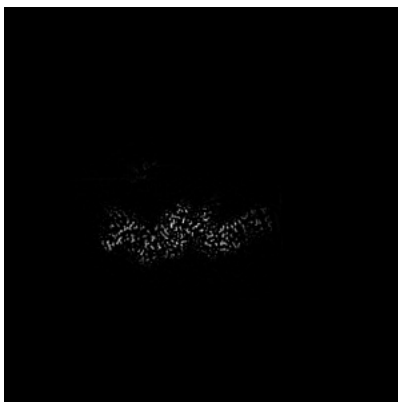
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

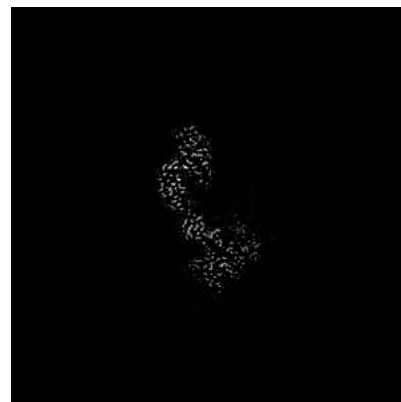
6.3.1 Primary map



X Index: 202

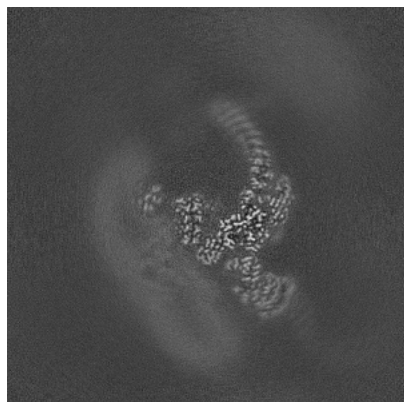


Y Index: 277

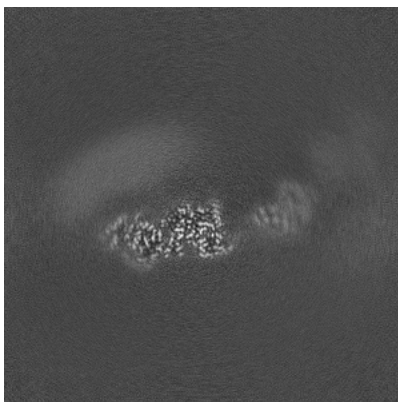


Z Index: 221

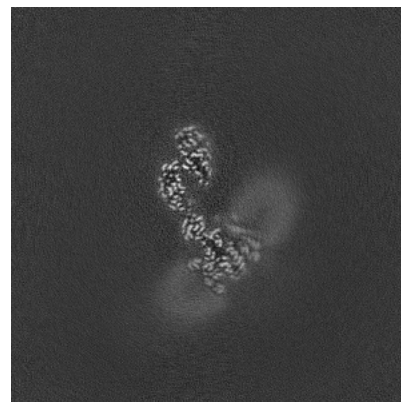
6.3.2 Raw map



X Index: 203



Y Index: 269

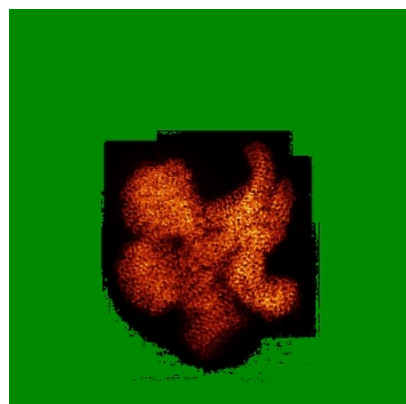


Z Index: 221

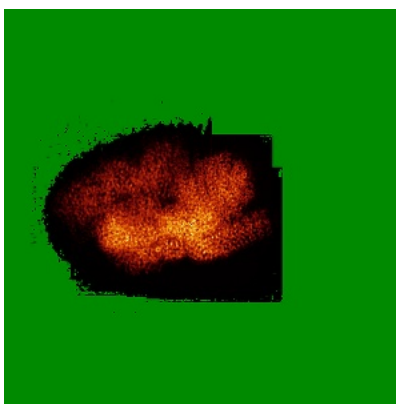
The images above show the largest variance slices of the map in three orthogonal directions.

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

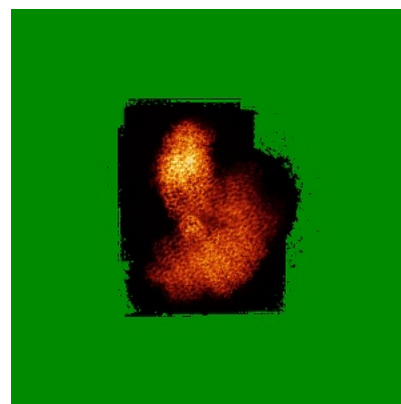
6.4.1 Primary map



X



Y

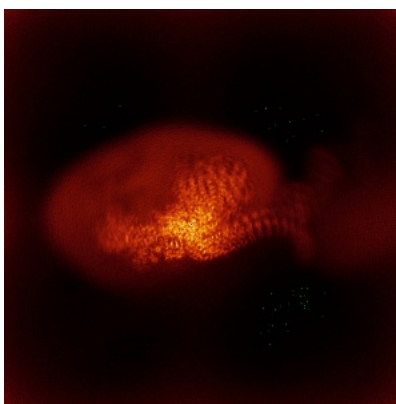


Z

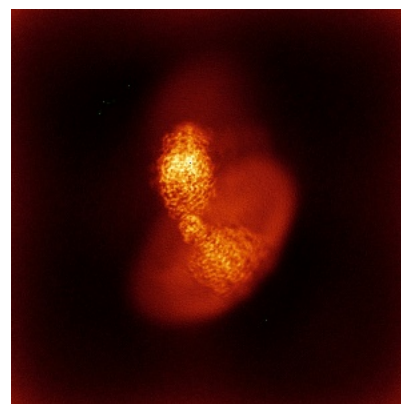
6.4.2 Raw map



X



Y

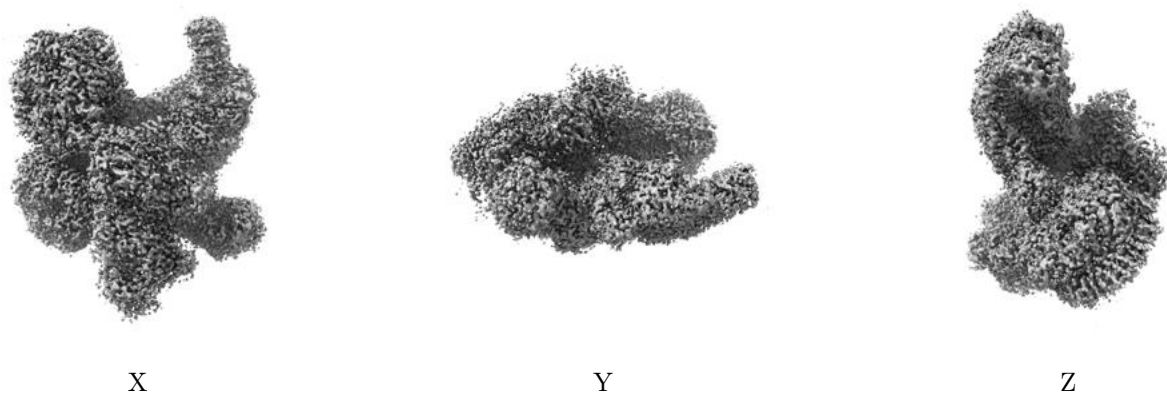


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

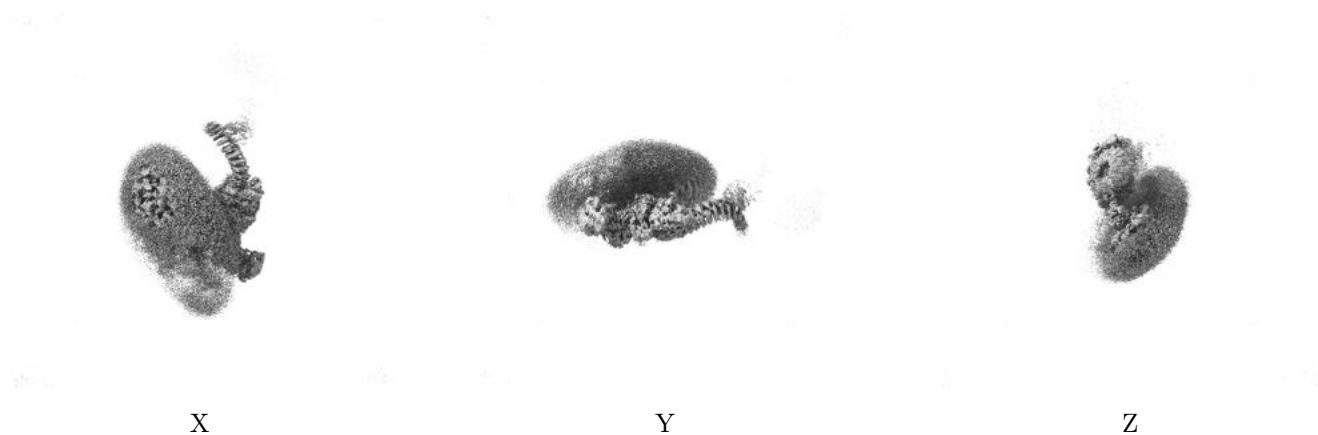
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

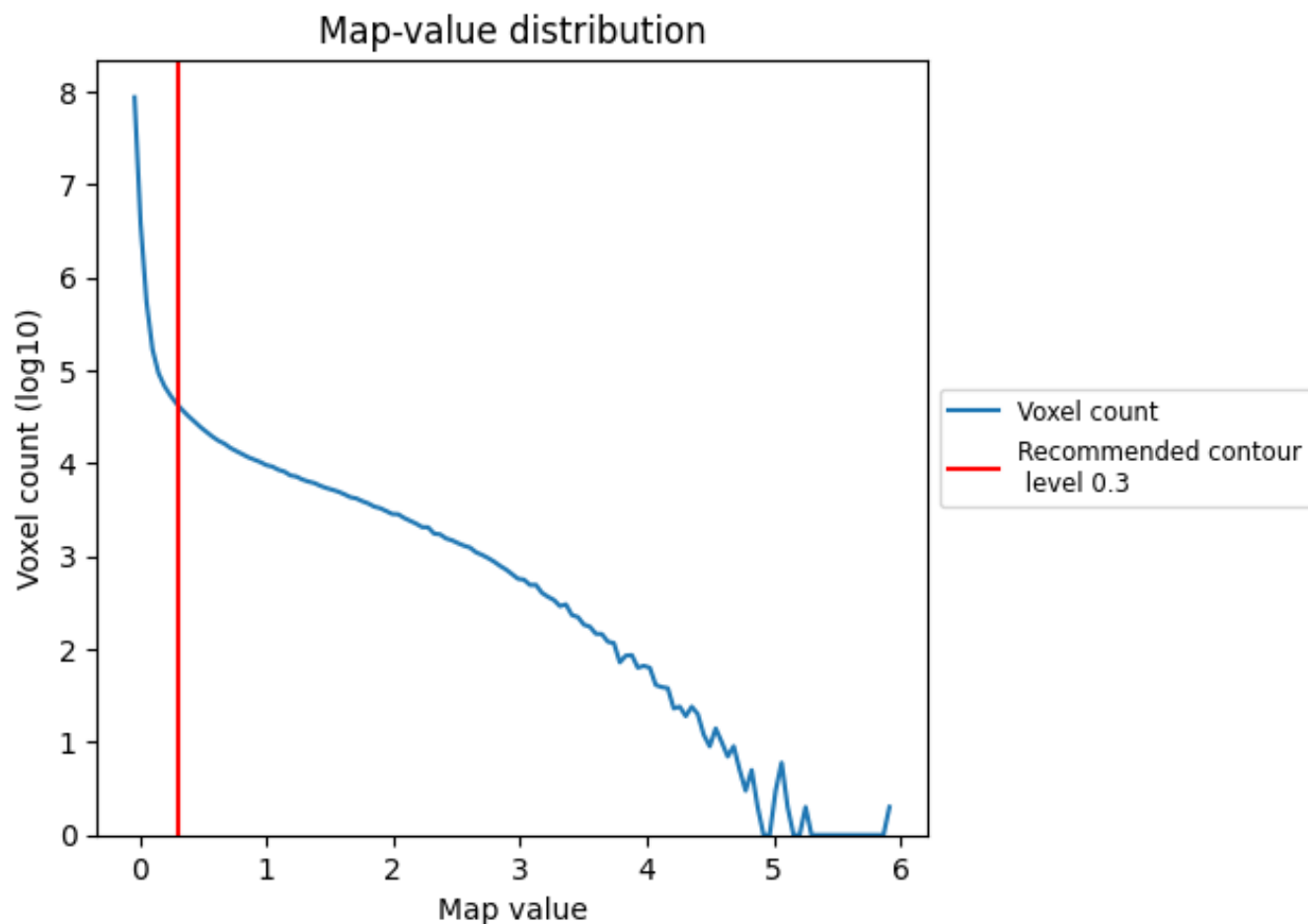
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

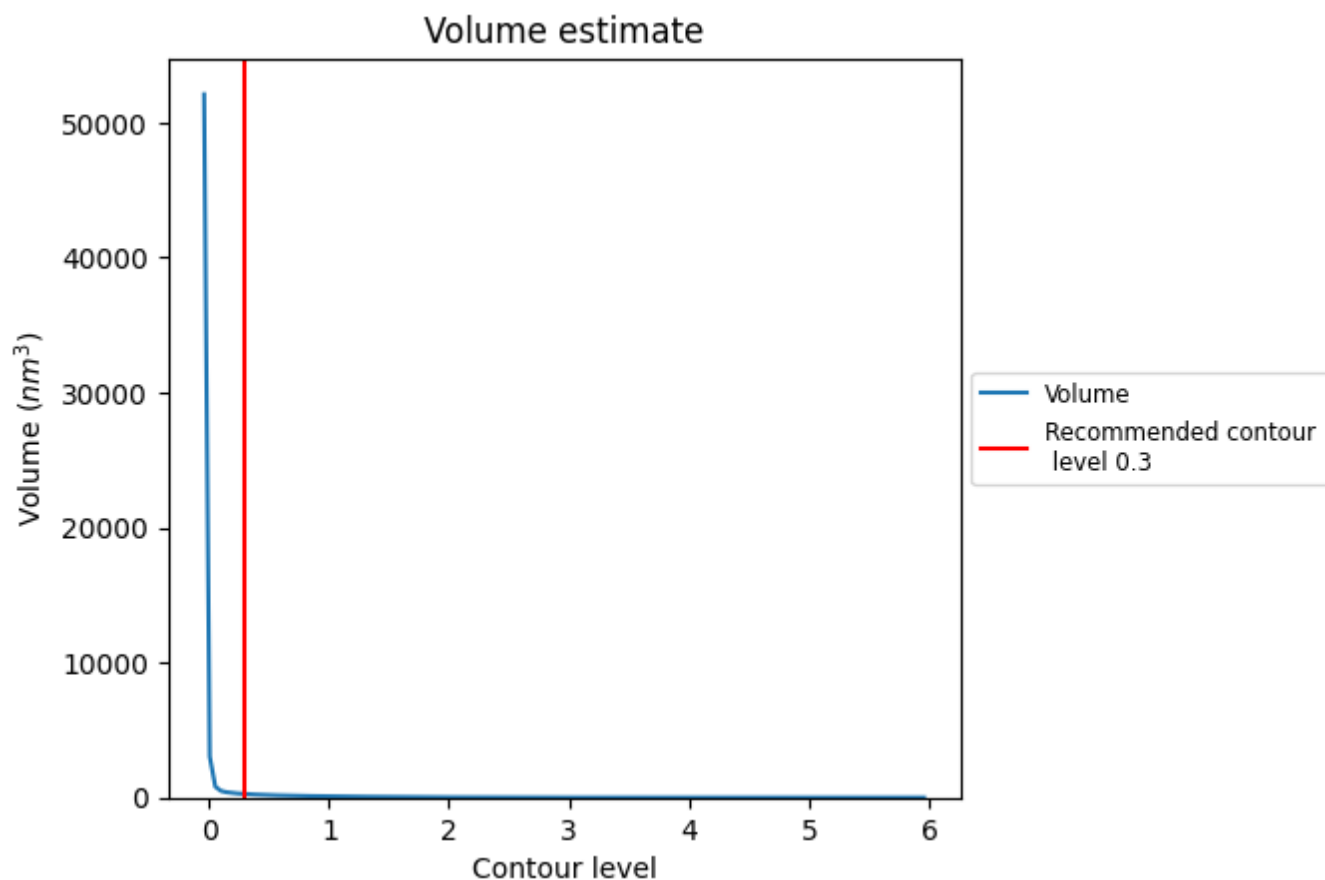
This section contains the results of statistical analysis of the map.

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.

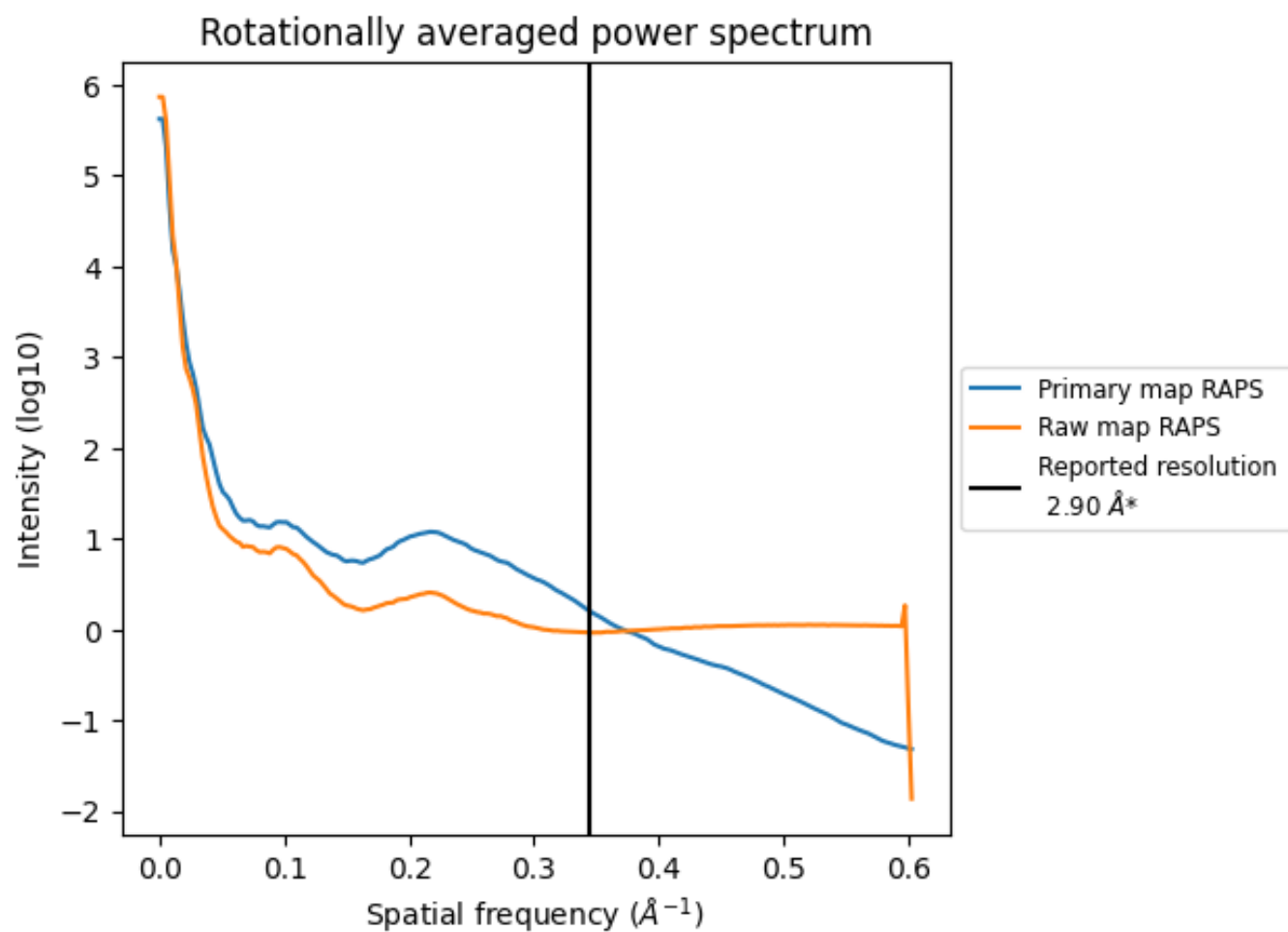
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm³; this corresponds to an approximate mass of 239 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 ⓘ

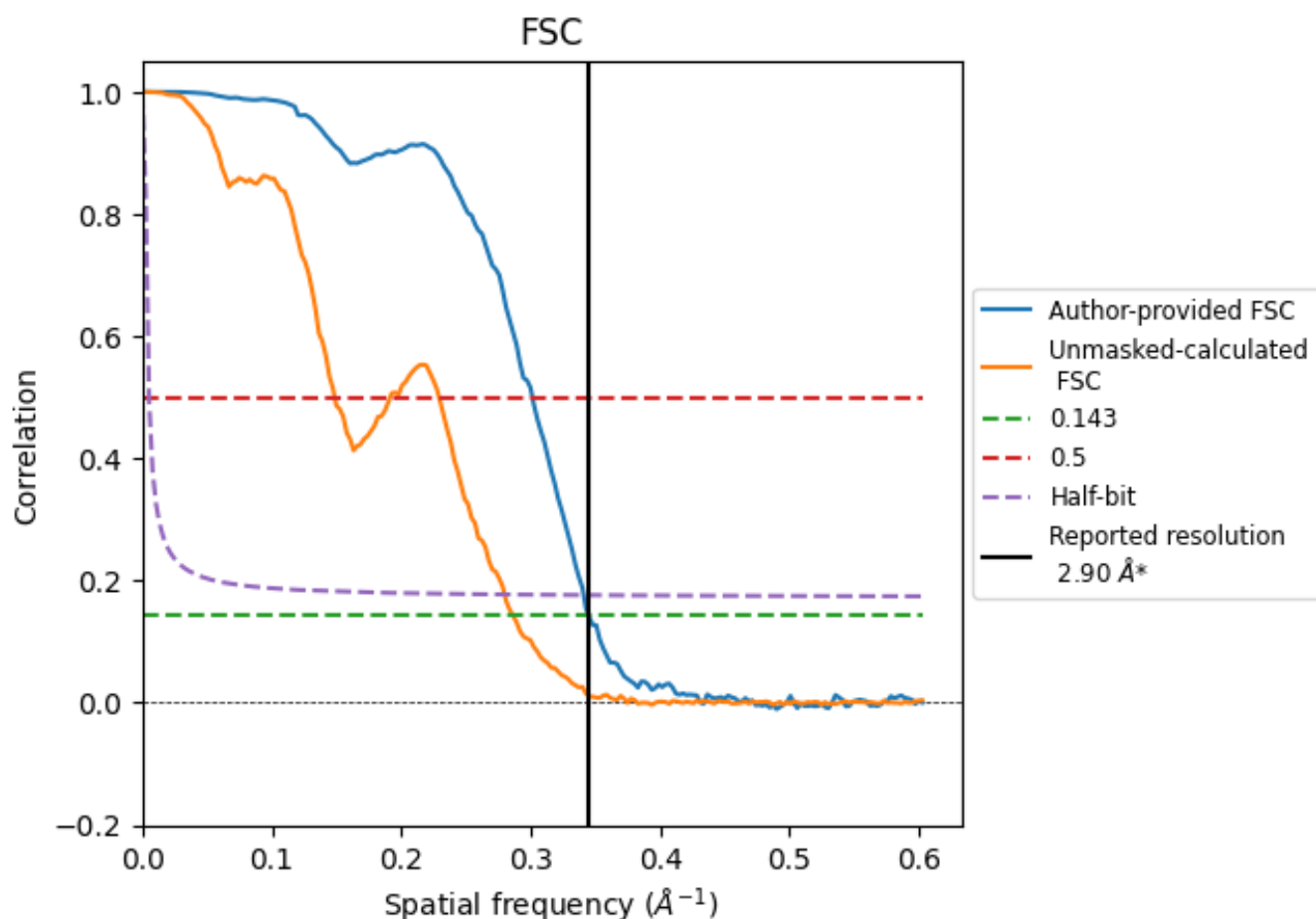


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

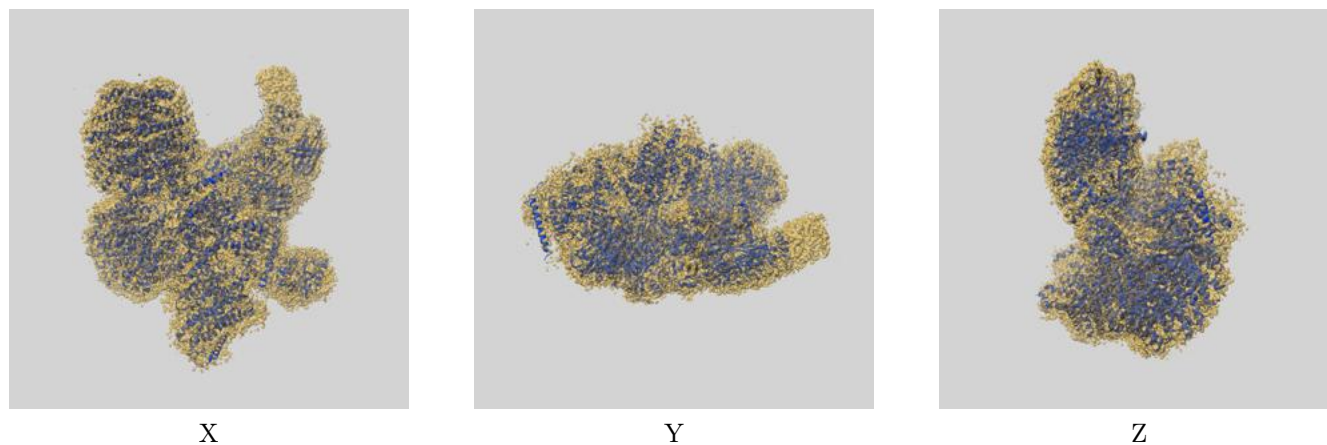
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.32	2.93
Unmasked-calculated*	3.49	6.72	3.57

*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 3.49 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

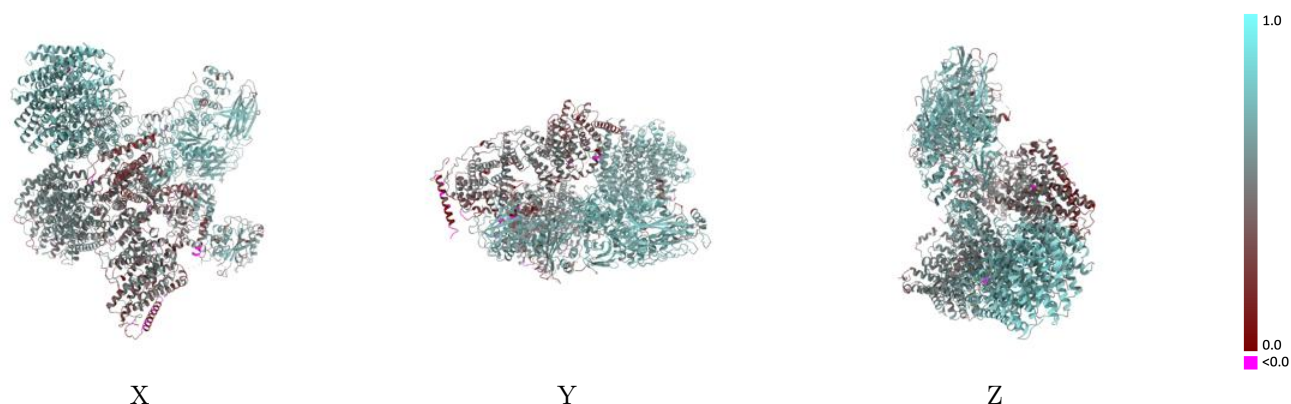
This section contains information regarding the fit between EMDB map EMD-26988 and PDB model 8CTE. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



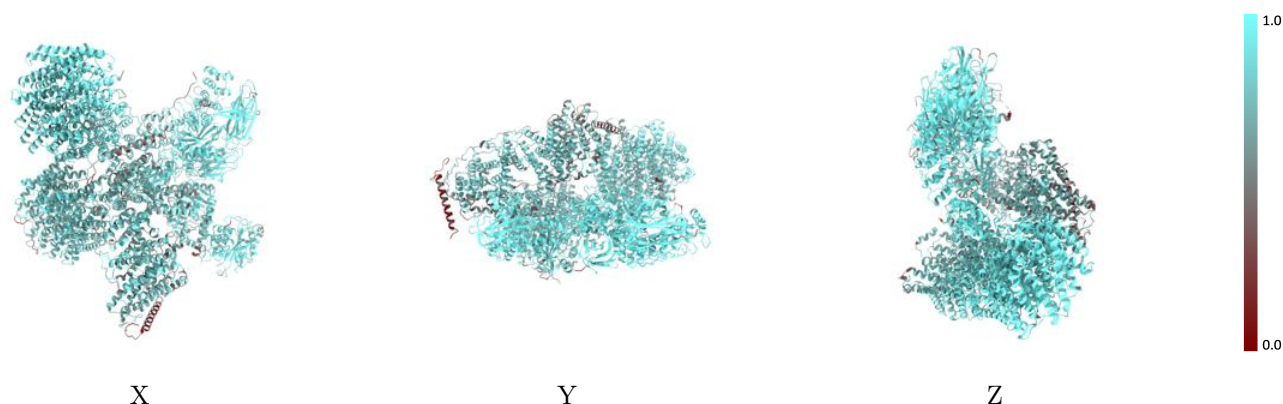
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



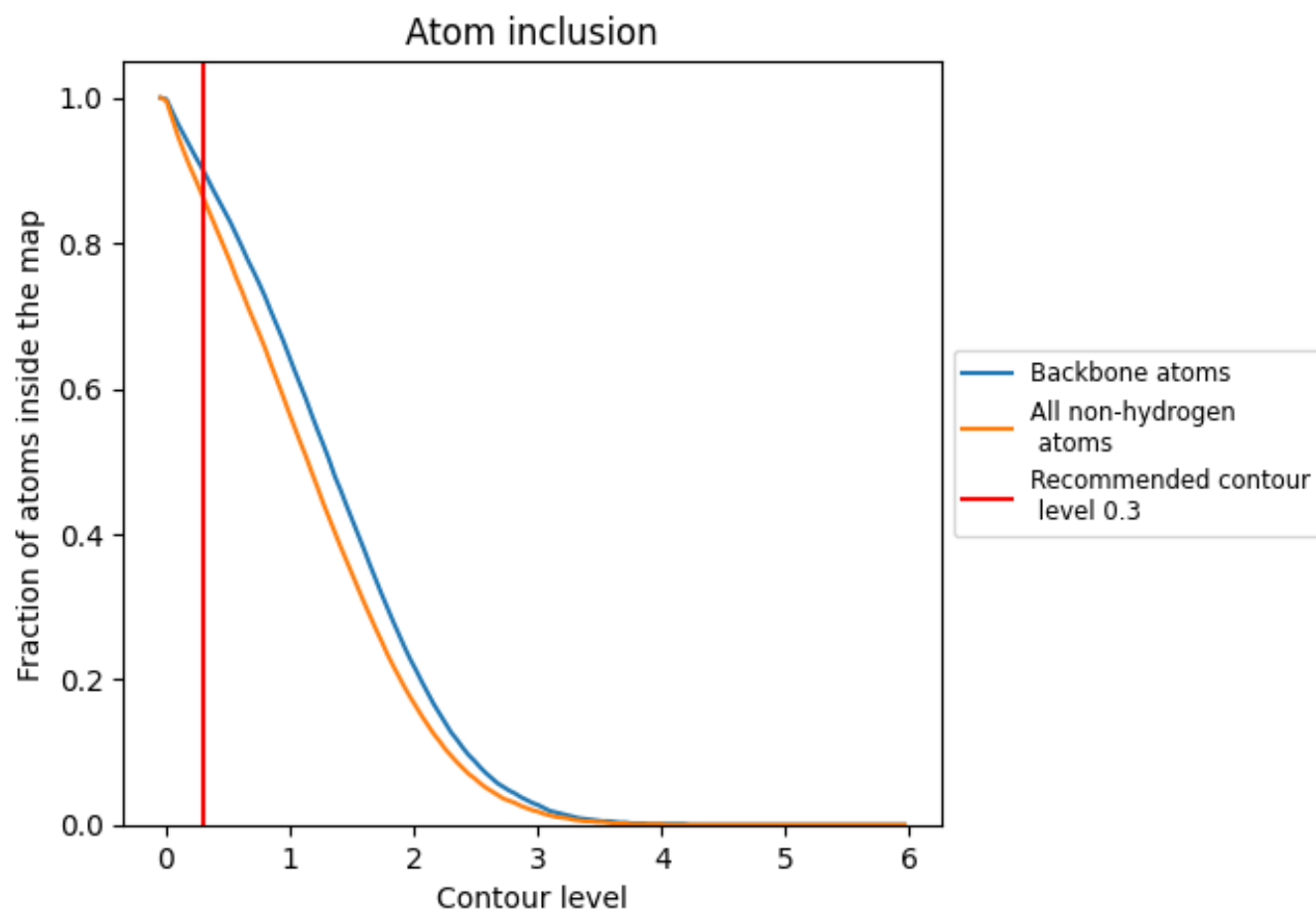
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.5620
A	 0.9610	 0.6450
D	 0.4410	 0.2290
K	 0.9220	 0.6600
L	 0.9700	 0.7010
M	 0.8570	 0.5400
N	 0.2390	 0.1260
O	 0.8480	 0.5250
P	 0.7910	 0.4630
Q	 0.9560	 0.6880
R	 0.8360	 0.5250
S	 0.8550	 0.5240
T	 0.7750	 0.4390
W	 0.5970	 0.4490
X	 0.9470	 0.6770

