



wwPDB EM Validation Summary Report ⓘ

May 12, 2025 – 07:14 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 wwPDB EM Validation Summary 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

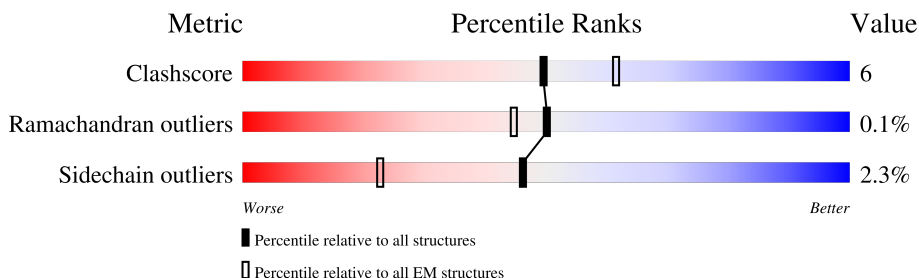
1 Overall quality at a glance

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

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		

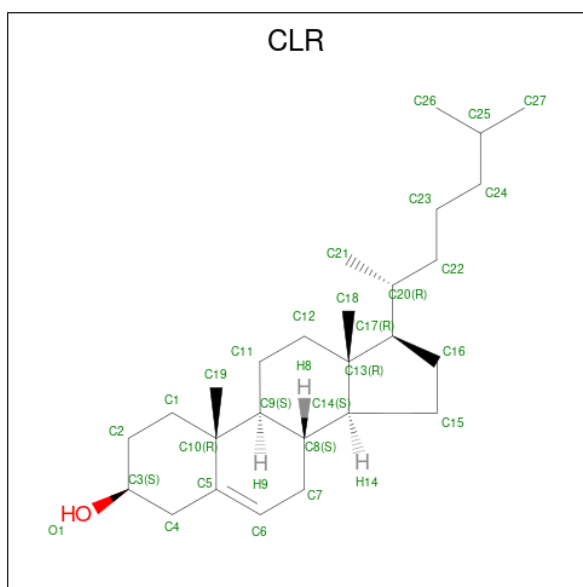
- Molecule 6 is a protein called Glycophorin-A.

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: C₂₇H₄₆O).



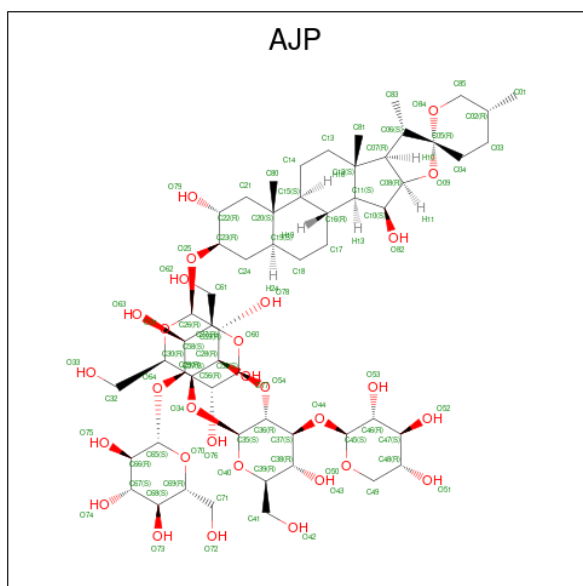
Mol	Chain	Residues	Atoms			AltConf
8	L	1	Total	C	O	0
			28	27	1	
8	L	1	Total	C	O	0
			28	27	1	
8	P	1	Total	C	O	0
			28	27	1	

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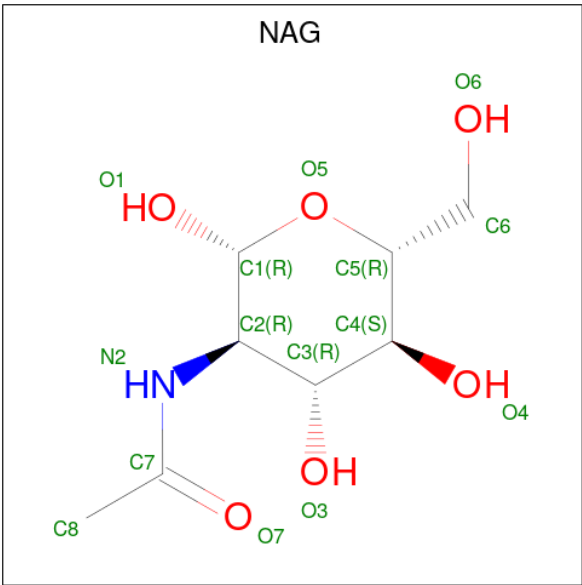
Mol	Chain	Residues	Atoms			AltConf
8	P	1	Total	C	O	0
			28	27	1	
8	T	1	Total	C	O	0
			28	27	1	
8	T	1	Total	C	O	0
			28	27	1	
8	S	1	Total	C	O	0
			28	27	1	
8	R	1	Total	C	O	0
			28	27	1	
8	M	1	Total	C	O	0
			28	27	1	
8	M	1	Total	C	O	0
			28	27	1	

- Molecule 9 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



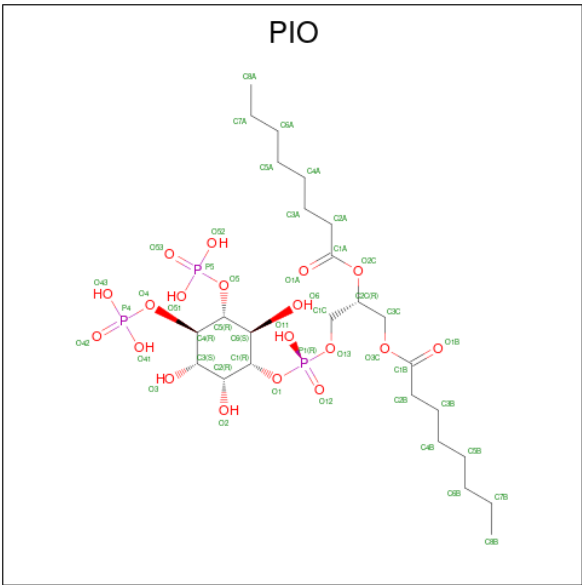
Mol	Chain	Residues	Atoms			AltConf
9	Q	1	Total	C	O	0
			32	27	5	
9	Q	1	Total	C	O	0
			43	33	10	

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

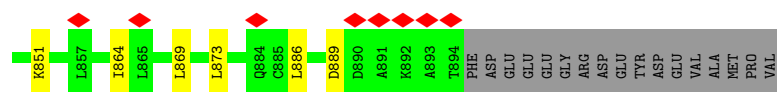
[illegible]

- Molecule 2: Band 3 anion transport protein

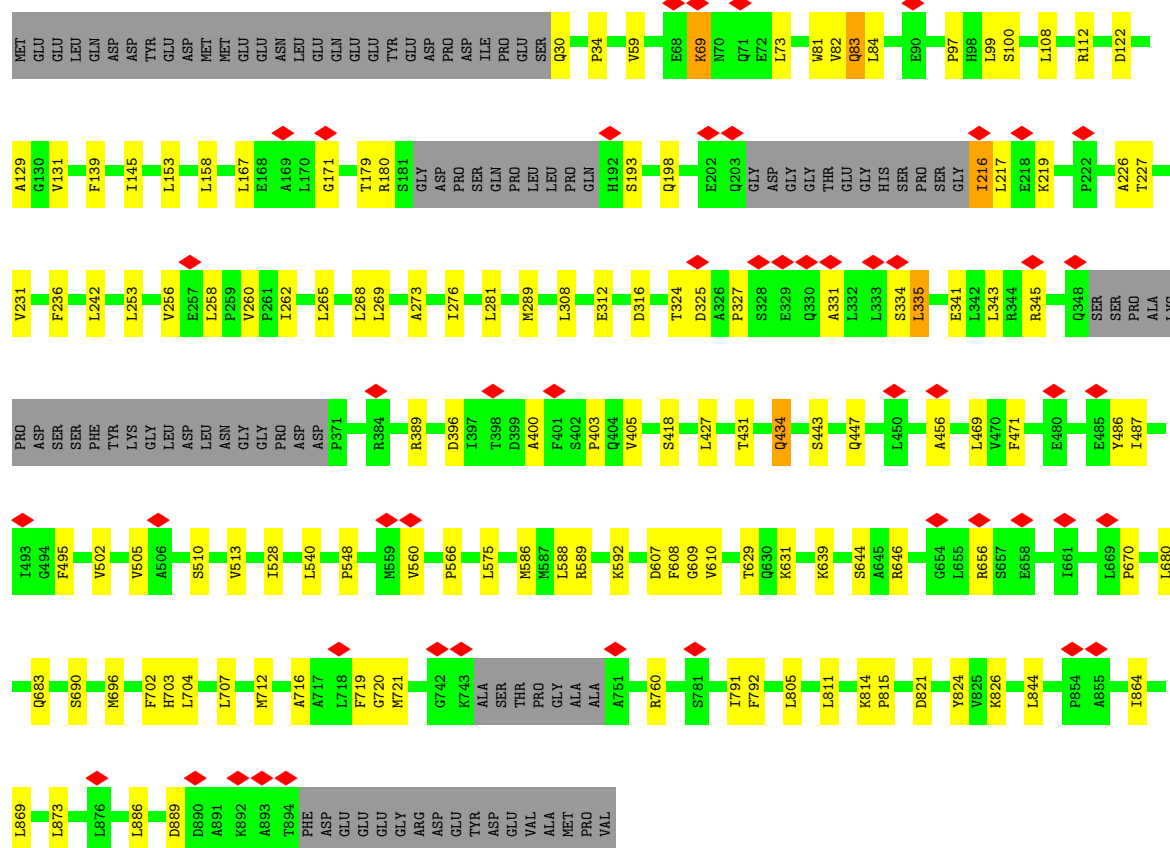
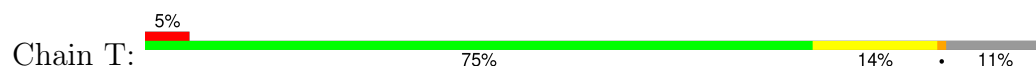
Chain P:



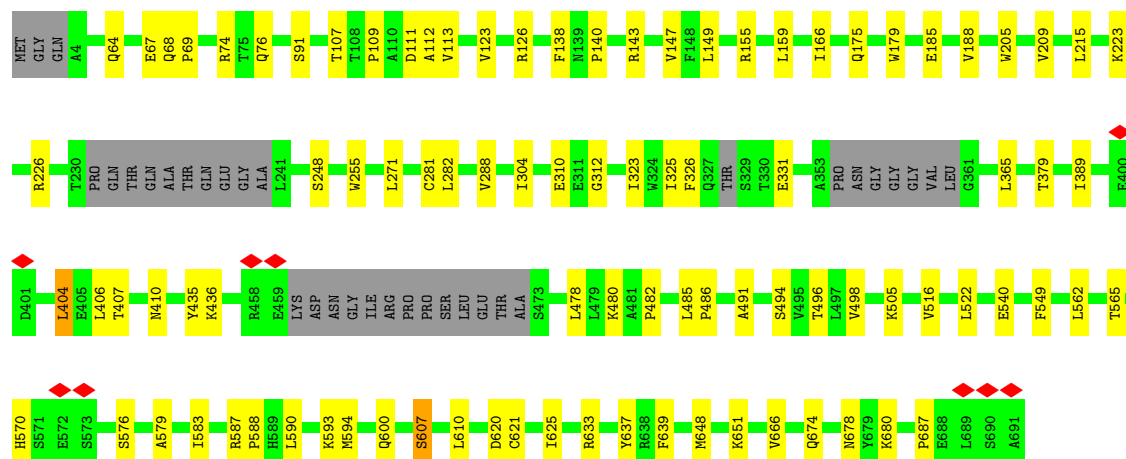
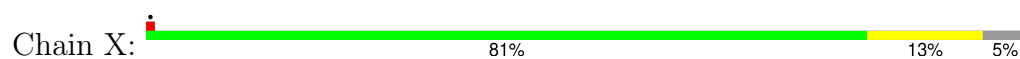
L672	L680	E681	S682	Q683	S690	M696	F702	H703	L704	L707	M712	A716	F719	G720	M721	R730	K743	ALA	SER	THR	PRO	GLY	ALA	A751	Q752	R760	E777	I791	F792	L805	L811	K814	D821	Y824	K826	K829	L844											
Q447	A456	L469	F470	F471	Y486	I487	F495	V502	V505	S510	V513	I528	P548	V560	P566	M586	R589	K592	D607	F608	G609	V610	T629	Q630	G631	K639	V640	S641	S644	K645	R646	R656	I661	L669	P670	A671												
R340	E341	L342	R344	R345	R346	Y347	K353	P354	D355	SER	PHE	TYR	LYS	GLY	LEU	ASP	ASN	GLY	PRO	ASP	P371	L372	Q373	G376	Q377	L378	R384	D385	R389	D396	A400	F401	S402	P403	Q404	Y405	A416	L417	S418	L427	T431	Q434	S443					
GLY	THR	GLY	GLY	HIS	SER	PRO	SER	GLY	ILE	L217	E218	A226	T227	V231	F236	L242	V245	L253	V256	E257	L258	F259	V260	P261	I262	L265	L268	L269	A273	P274	H275	I276	L281	W289	R292	L308	E312	D325	L335	Q339								
K69	L73	W81	V82	Q83	L84	P97	H98	L99	S100	H101	W105	L108	R112	L120	A129	G130	V131	F139	I145	R146	F147	Q148	L153	L158	L167	G171	T179	R180	S181	G182	D183	Q186	Q191	H192	S193	Q198	E202	Q203	GLY	ASP								
MET	GLU	LEU	GLN	ASP	THR	GLU	ASP	MET	MET	GLU	GLU	ASN	LEU	GLN	GLU	TYR	ASP	PRO	ASP	ILE	PRO	GLU	PRO	ALA	ALA	HIS	ASP	THR	GLU	THR	ALA	THR	THR	ASP	TYR	HIS	THR	THR	SER	SER	HIS	PRO	GLY	THR	HIS	K56	V69	E68



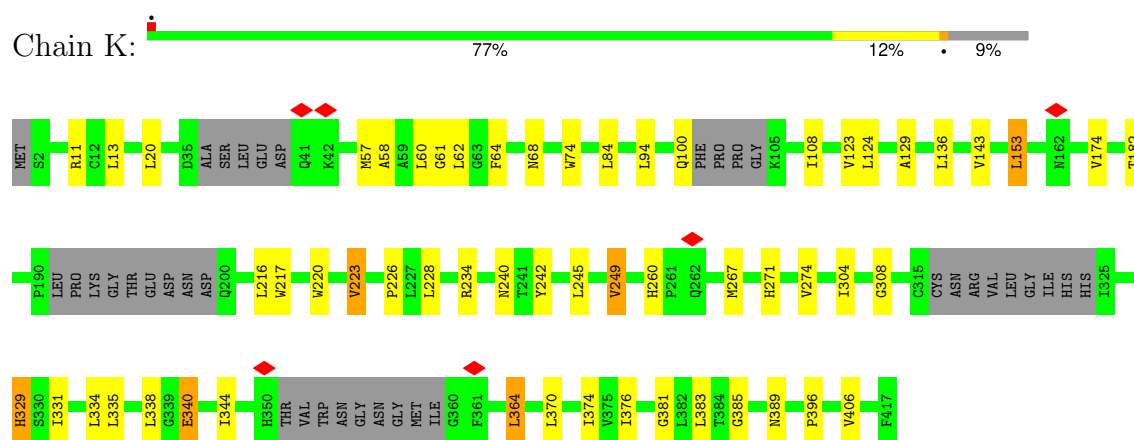
• Molecule 2: Band 3 anion transport protein



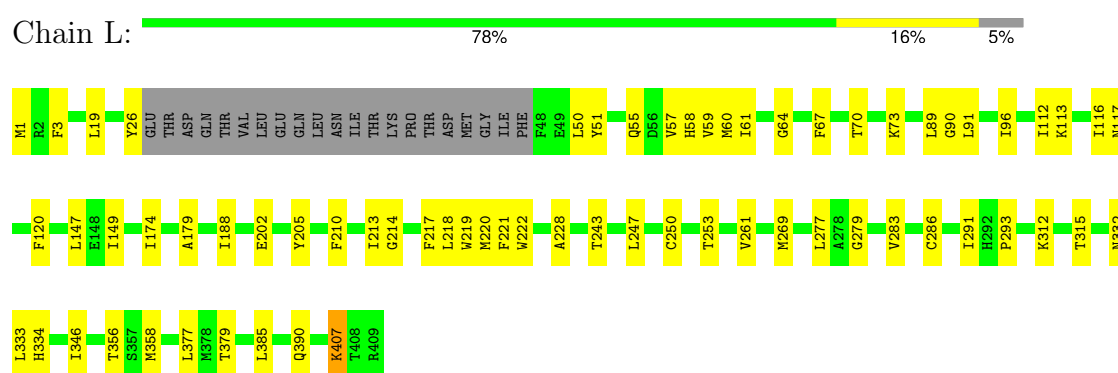
• Molecule 3: Protein 4.2



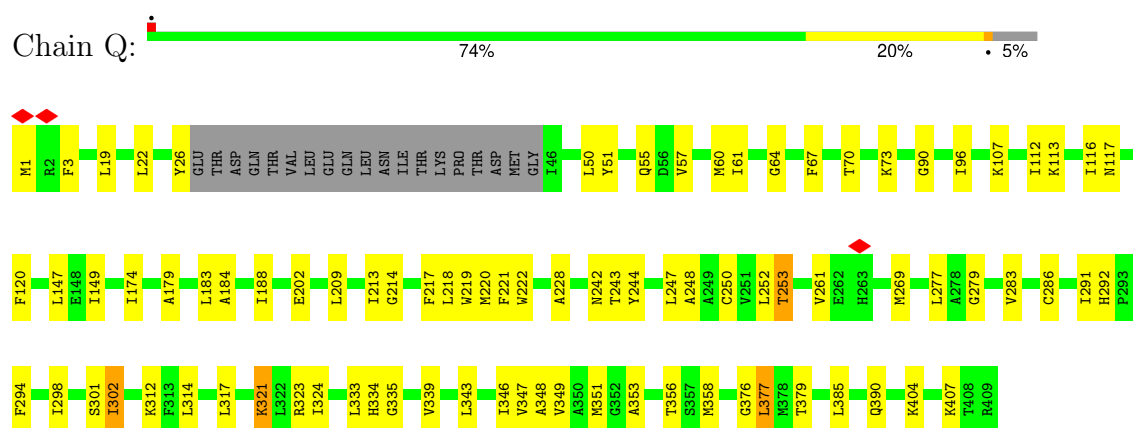
- Molecule 4: Blood group Rh(CE) polypeptide



- Molecule 5: Ammonium transporter Rh type A

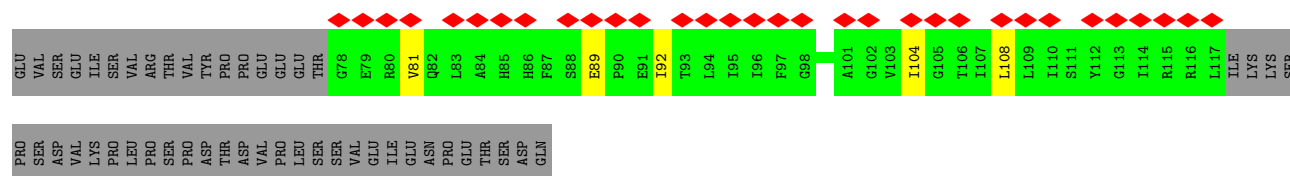


- Molecule 5: Ammonium transporter Rh type A

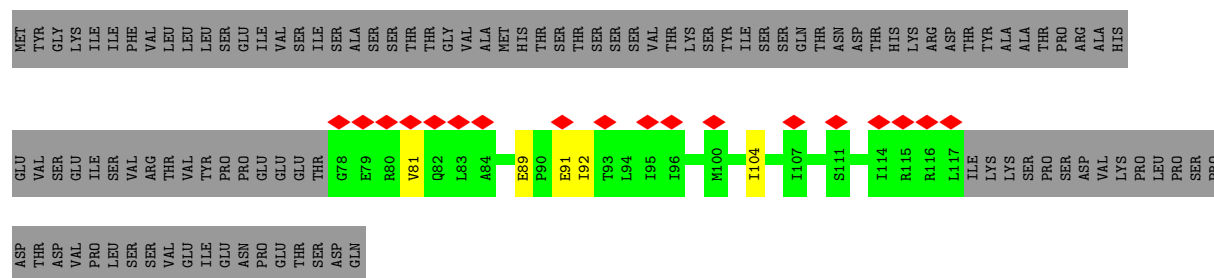


- Molecule 6: Glycophorin-A

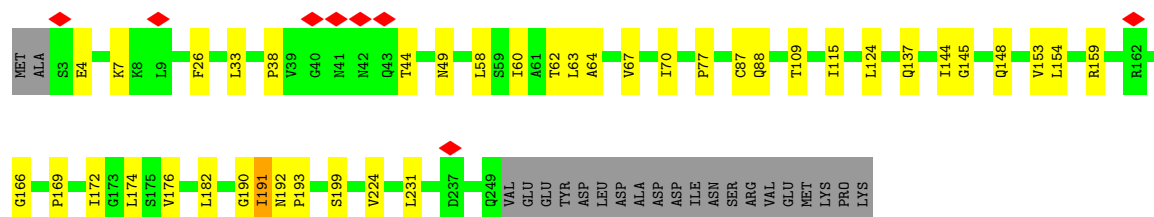
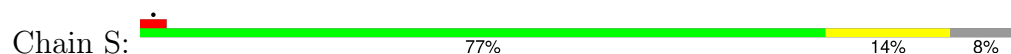




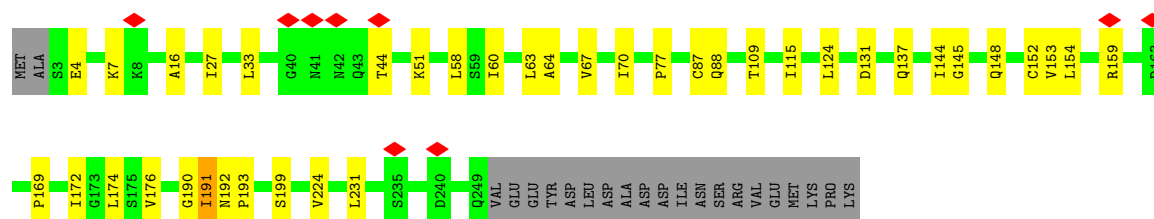
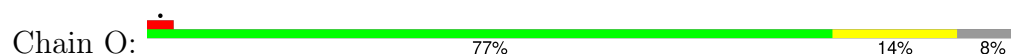
• Molecule 6: Glycophorin-A



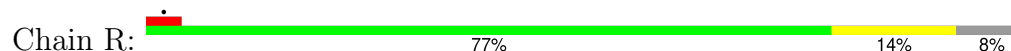
• Molecule 7: Aquaporin-1

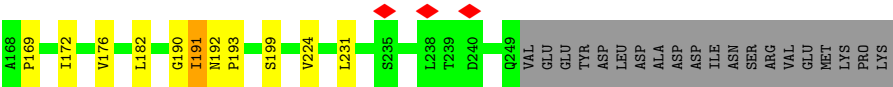


• Molecule 7: Aquaporin-1

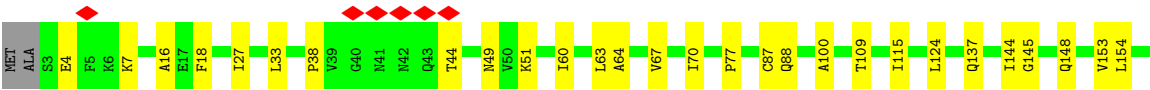
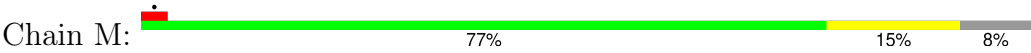


• Molecule 7: Aquaporin-1





• 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.

The worst 5 of 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

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	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
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

5 of 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

5.3.2 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
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

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	167	LEU
2	T	69	LYS
2	P	186	GLN
2	P	434	GLN
2	T	179	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
5	L	200	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	819	HIS
2	P	70	ASN
2	T	683	GLN
2	T	302	GLN

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.

The worst 5 of 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
7	M	87	P1L	C8-C7-SG	-3.67	109.03	113.40

There are no chirality outliers.

5 of 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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

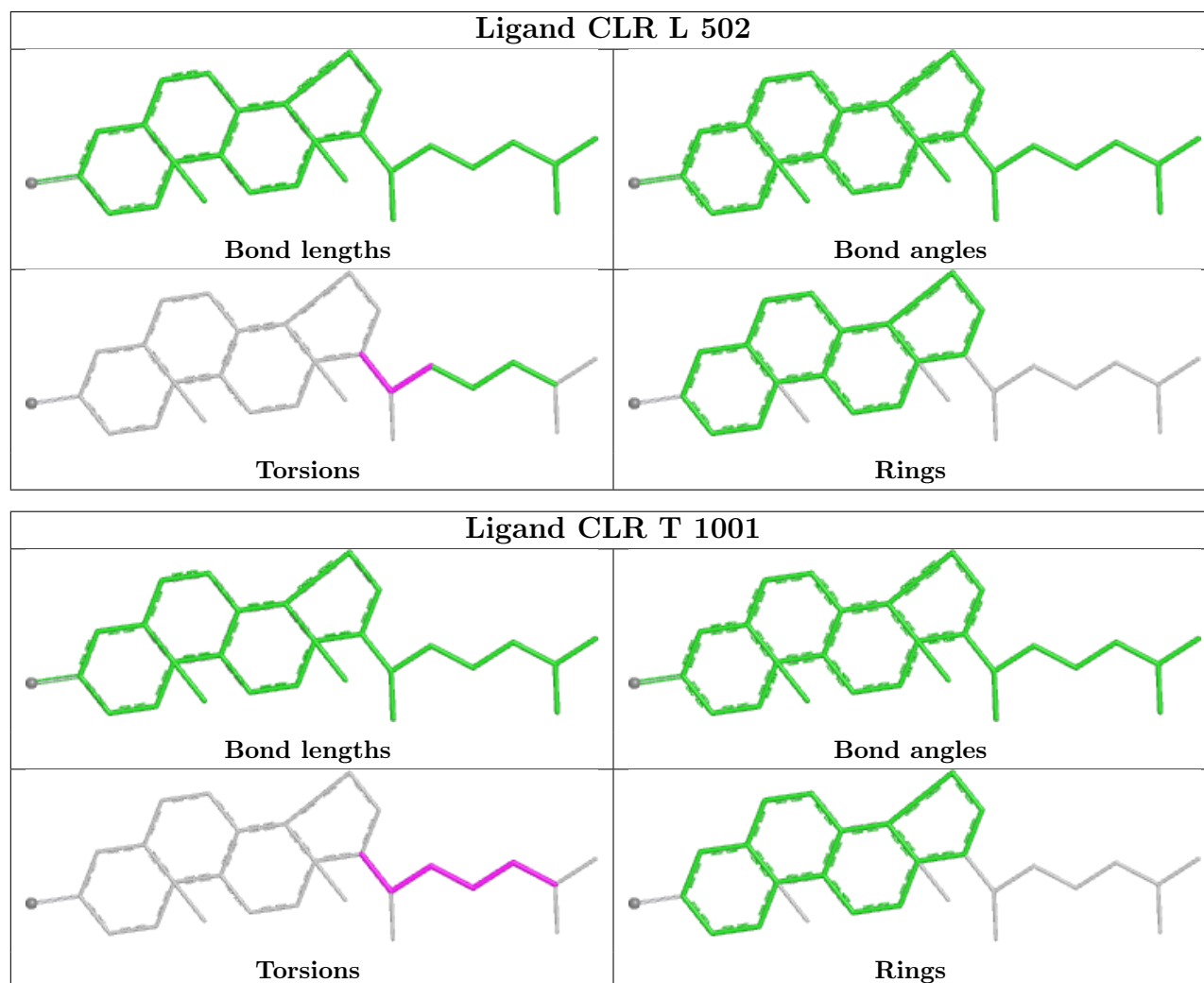
There are no ring outliers.

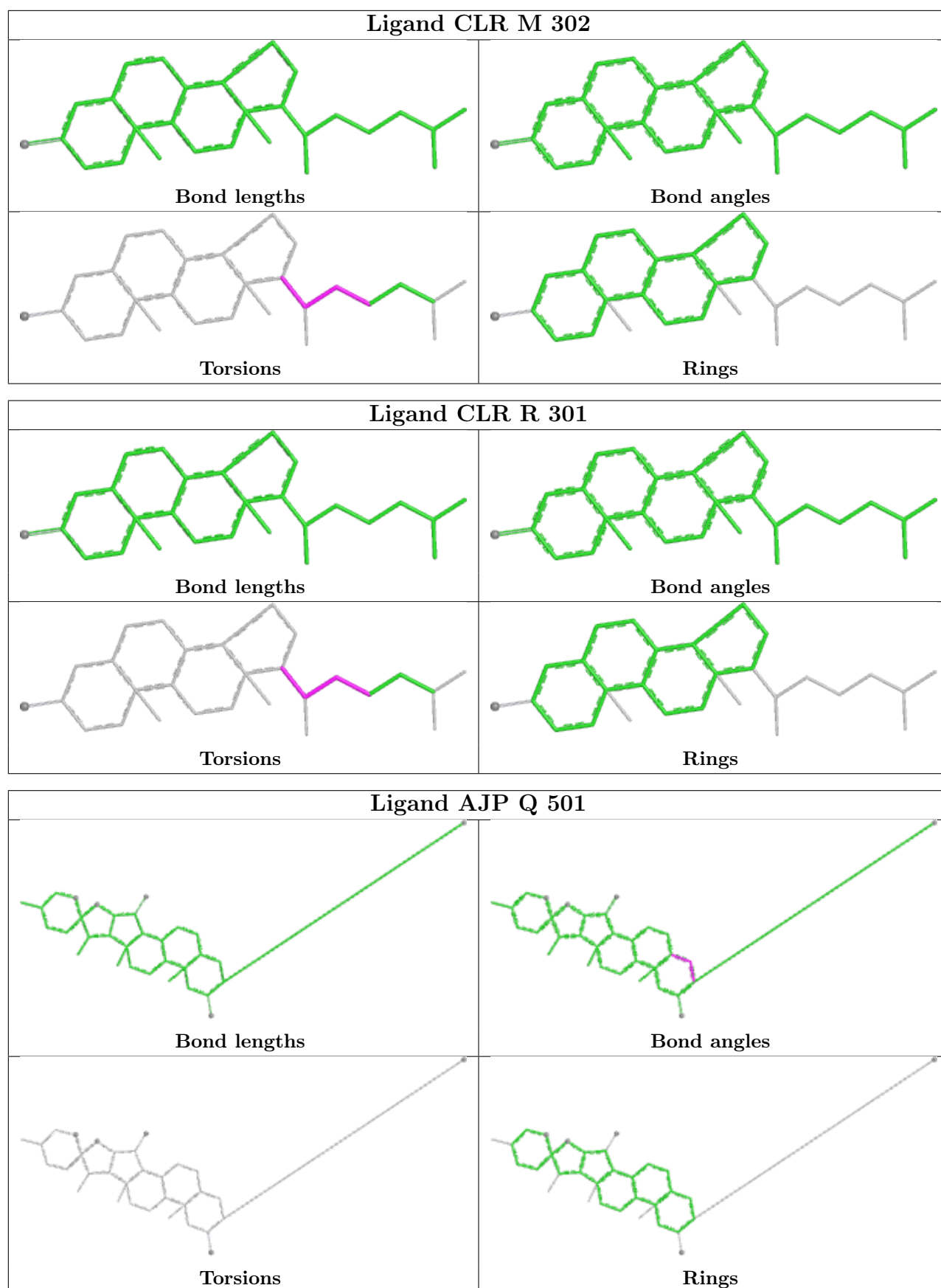
9 monomers are involved in 18 short contacts:

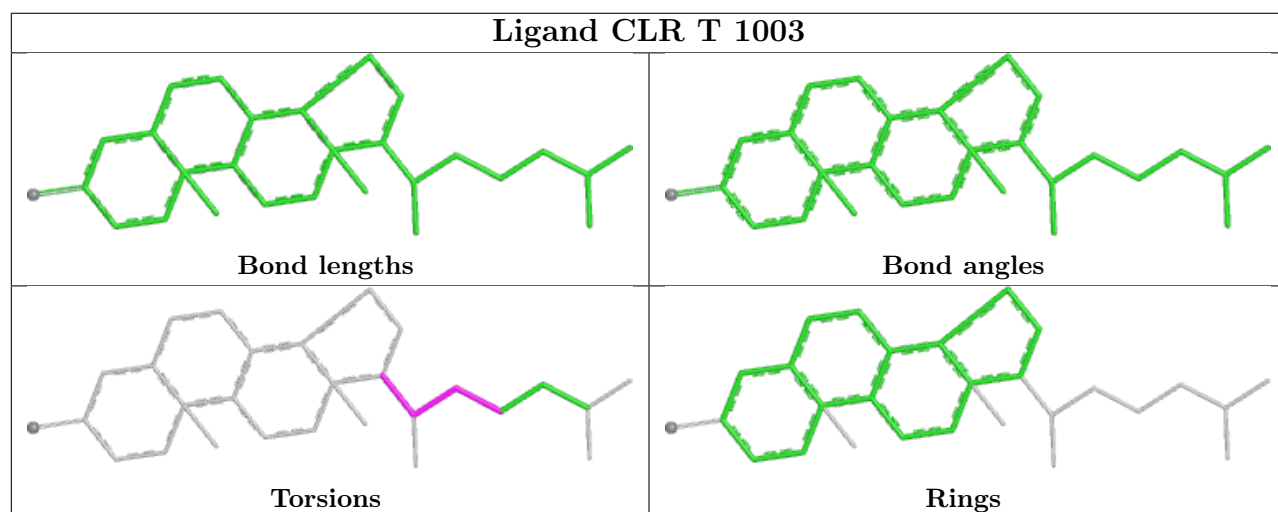
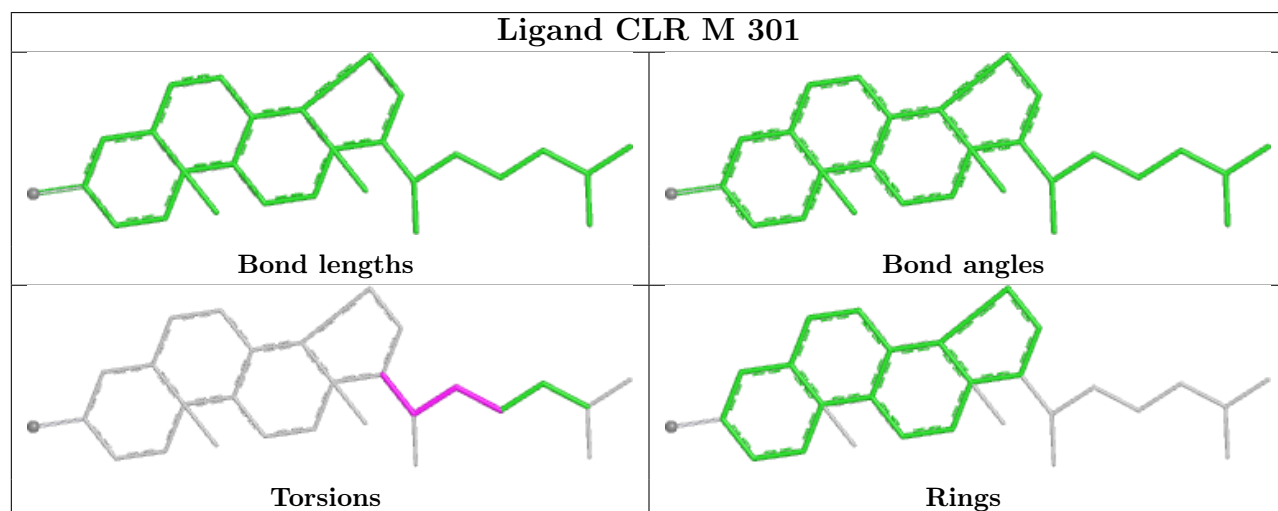
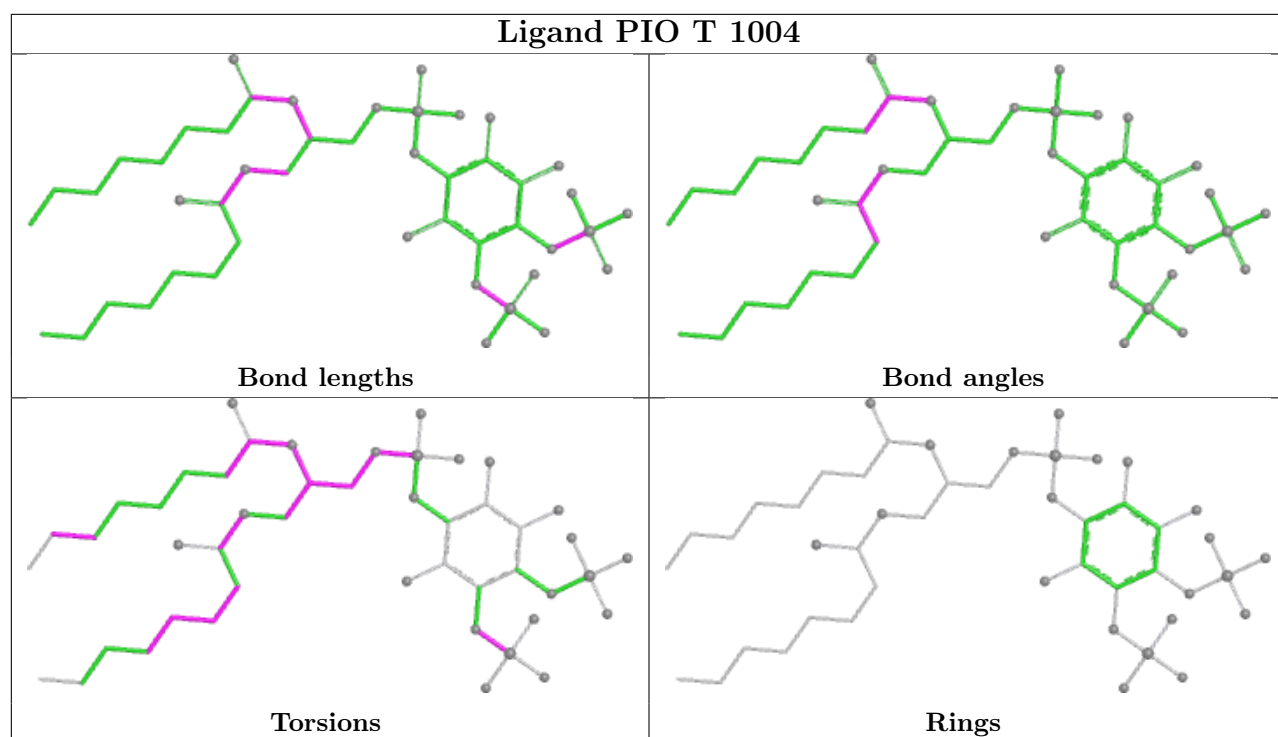
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	1001	CLR	2	0
8	M	302	CLR	2	0
8	R	301	CLR	2	0
11	T	1004	PIO	1	0
8	M	301	CLR	2	0
8	P	1001	CLR	3	0
8	S	301	CLR	1	0
8	L	501	CLR	1	0
9	Q	502	AJP	4	0

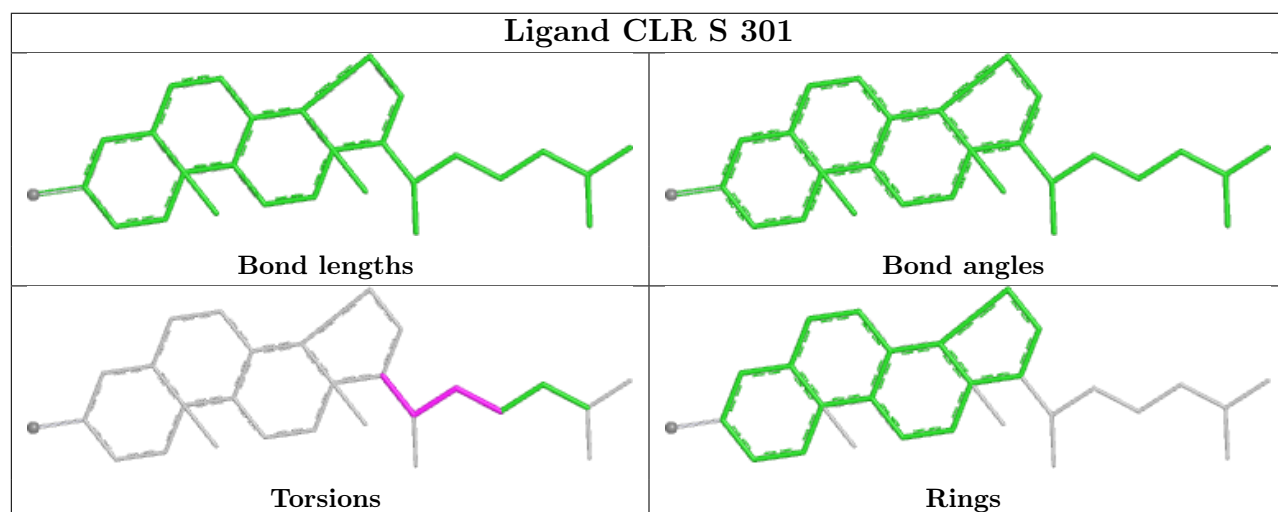
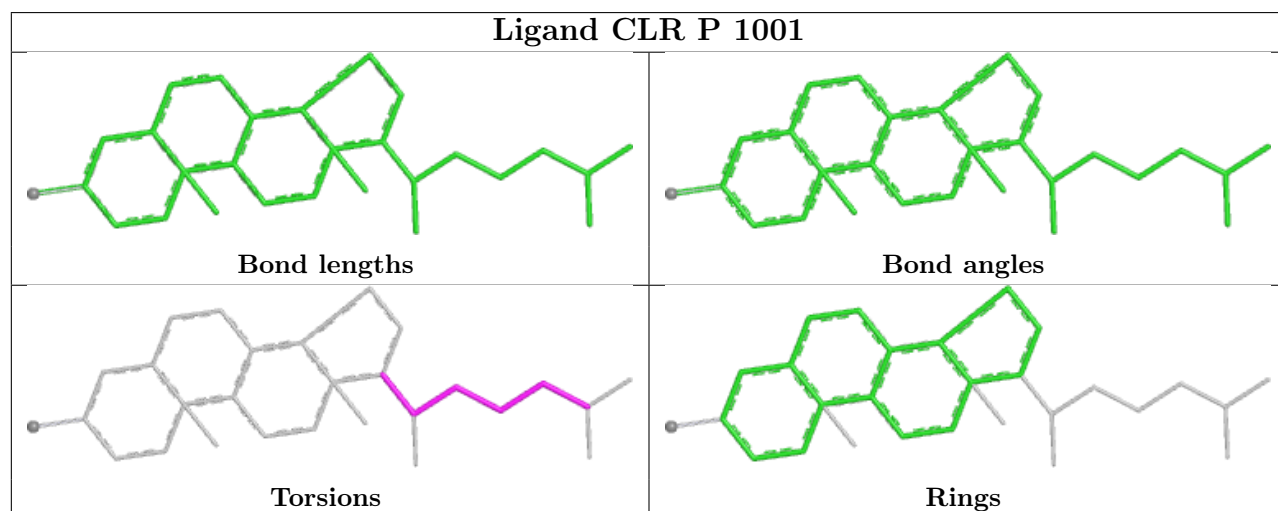
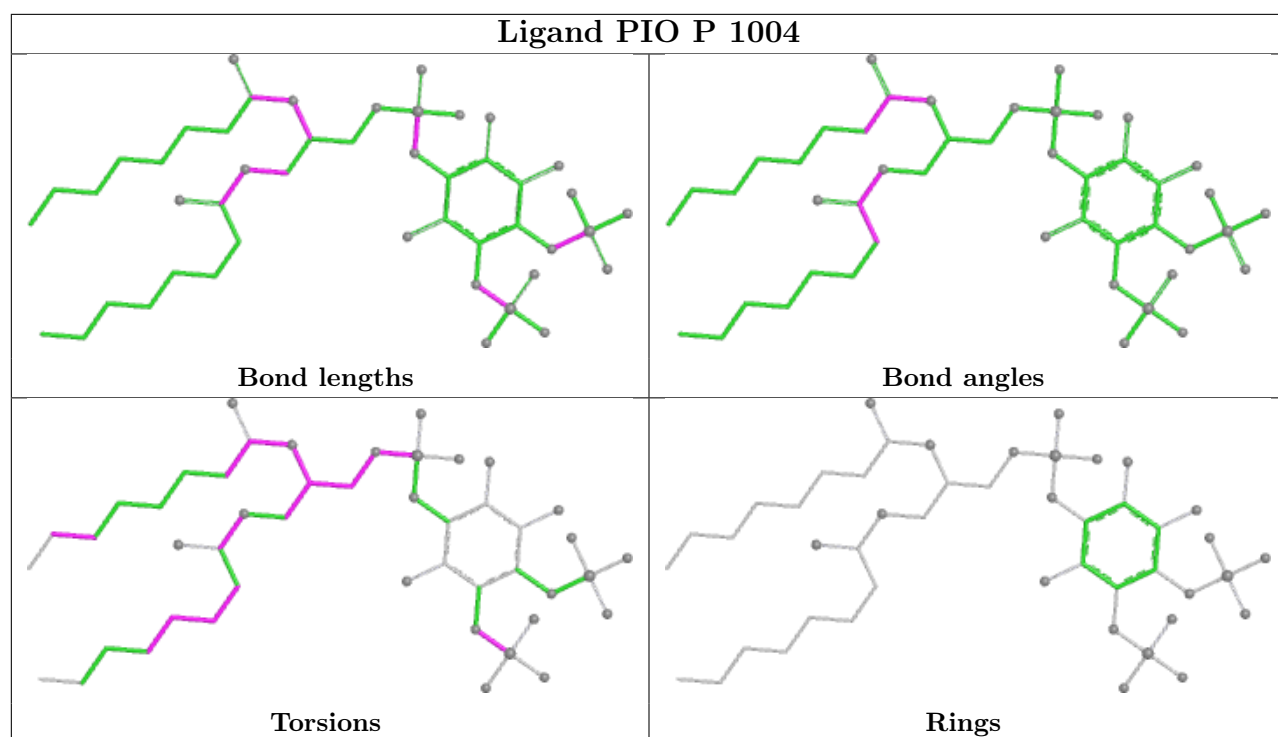
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

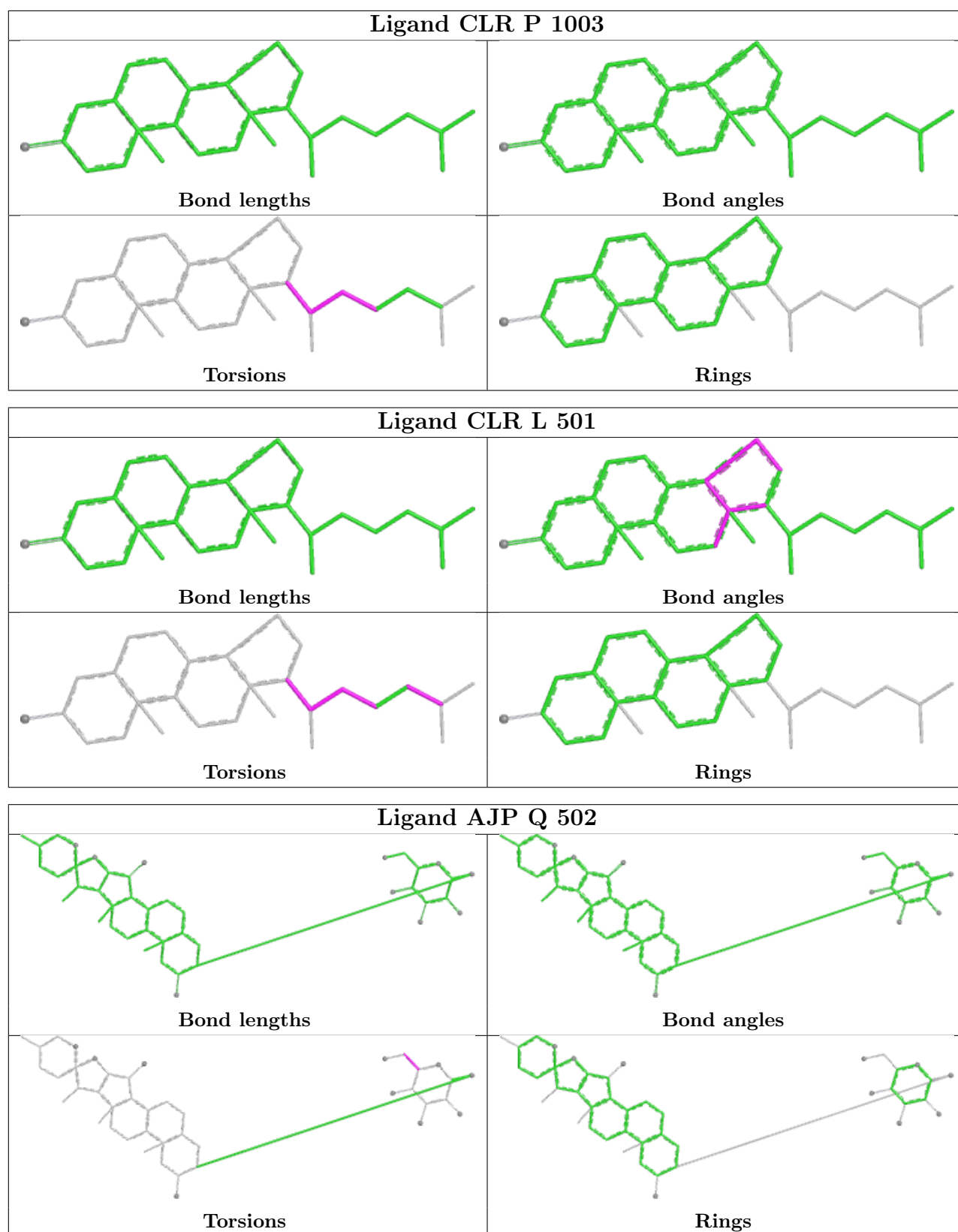
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

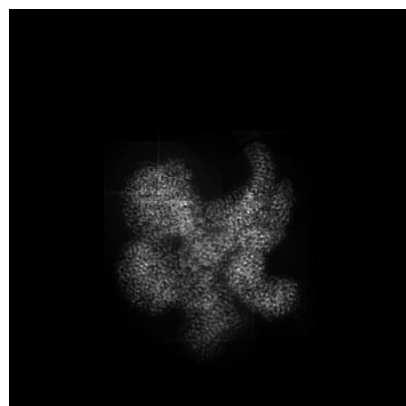
6 Map visualisation [i](#)

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

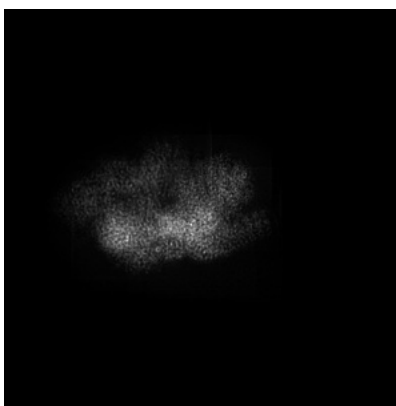
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

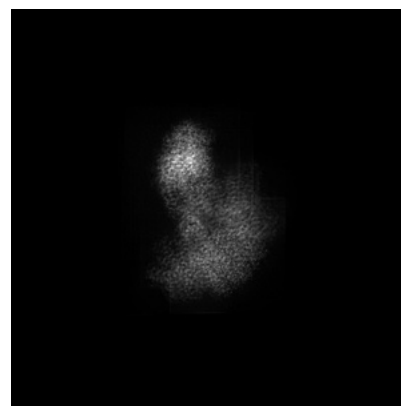
6.1.1 Primary map



X

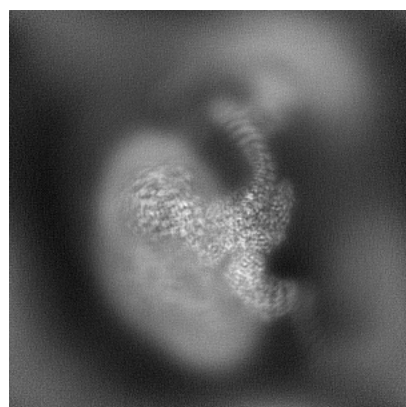


Y

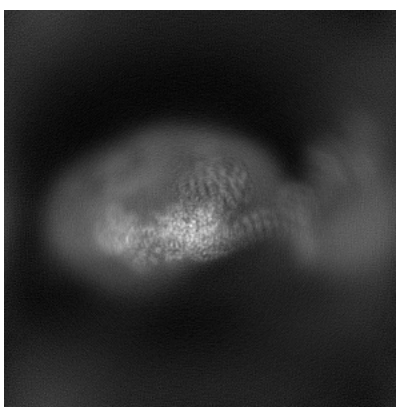


Z

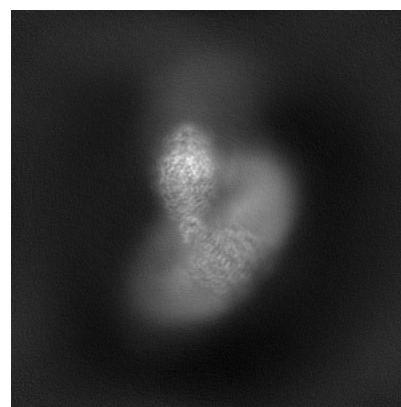
6.1.2 Raw map



X



Y

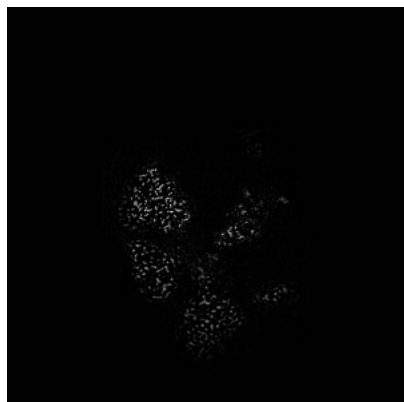


Z

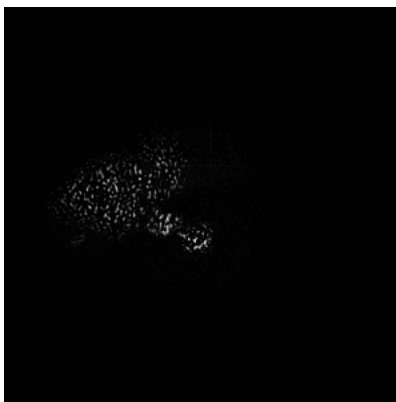
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225

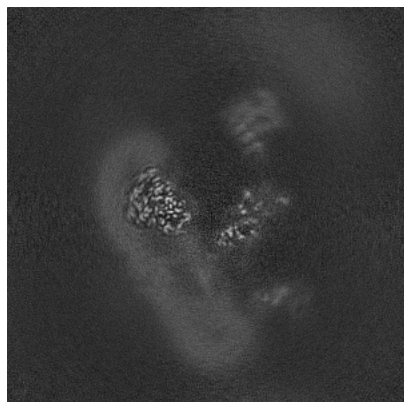


Y Index: 225

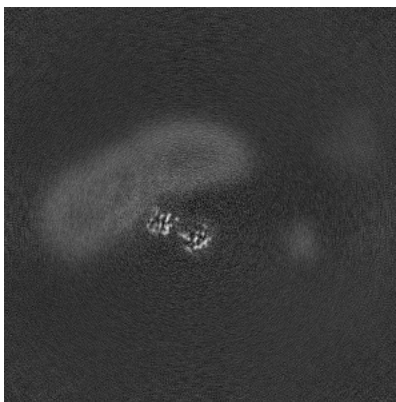


Z Index: 225

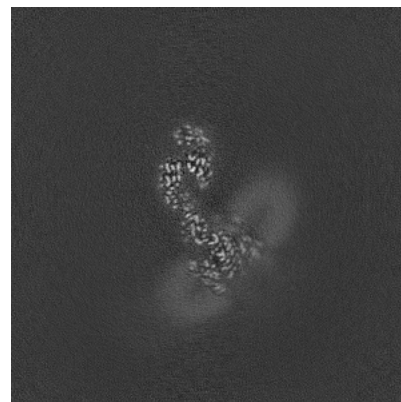
6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

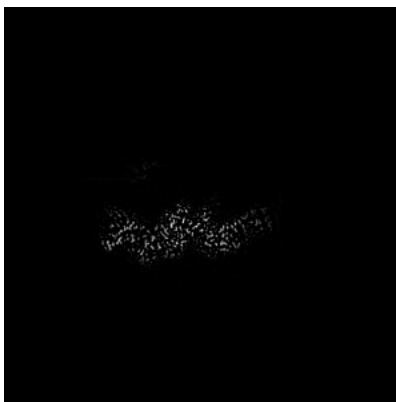
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

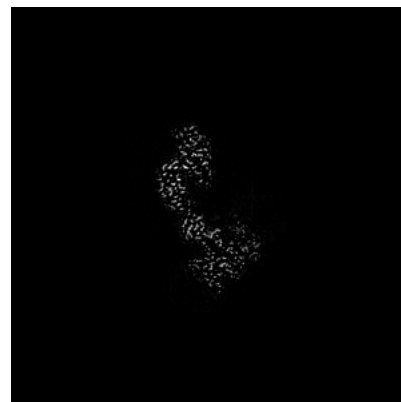
6.3.1 Primary map



X Index: 202

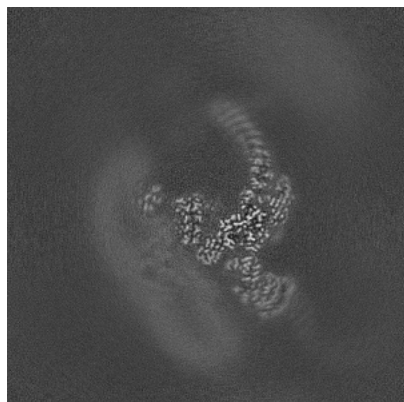


Y Index: 277

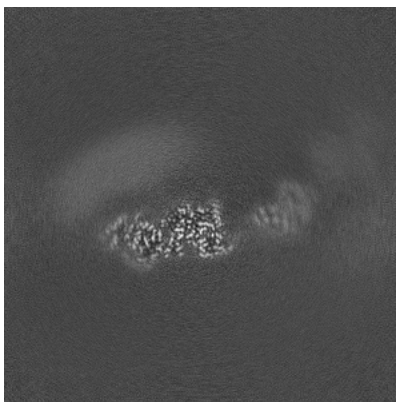


Z Index: 221

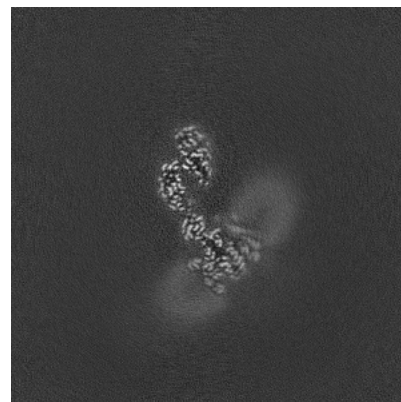
6.3.2 Raw map



X Index: 203



Y Index: 269

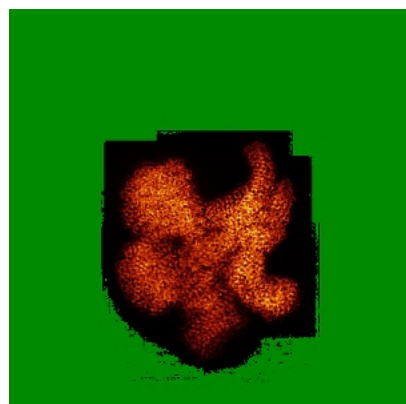


Z Index: 221

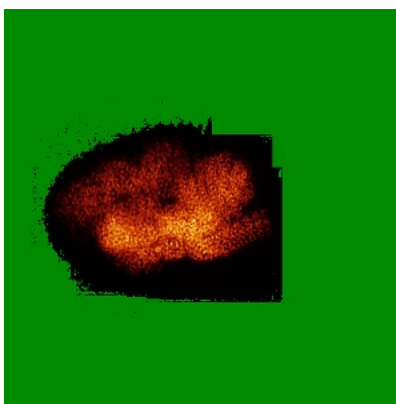
The images above show the largest variance slices of the map in three orthogonal directions.

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

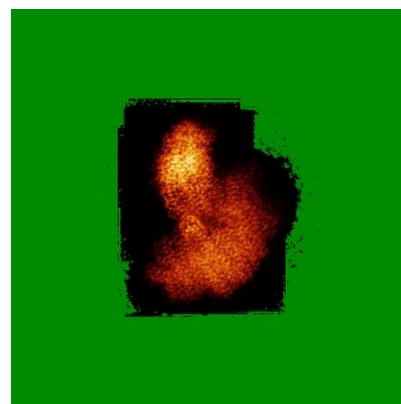
6.4.1 Primary map



X



Y

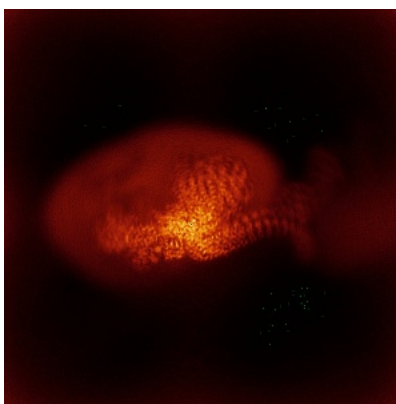


Z

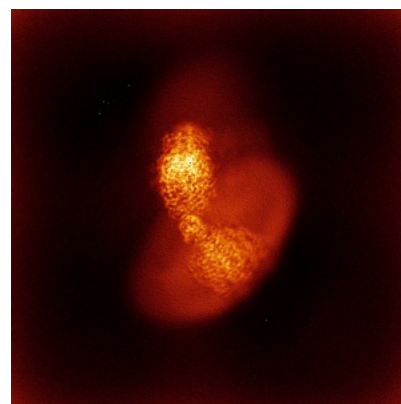
6.4.2 Raw map



X



Y

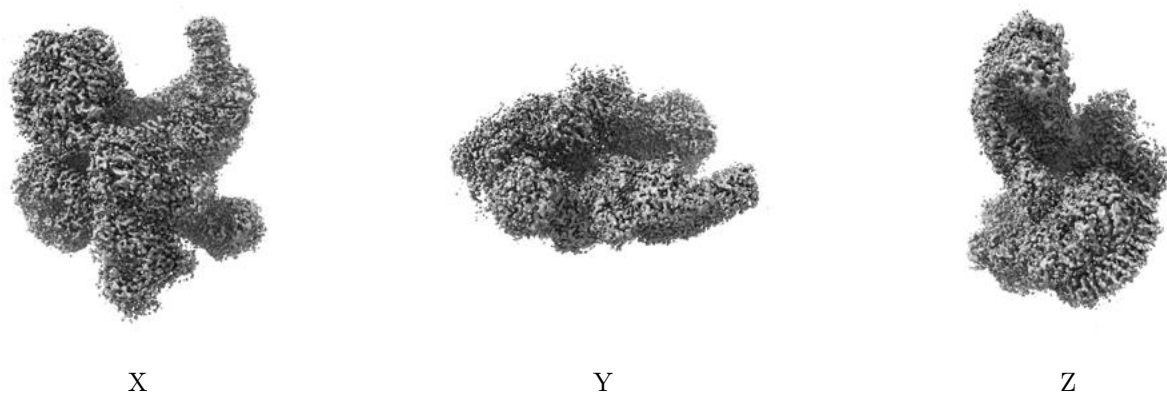


Z

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.

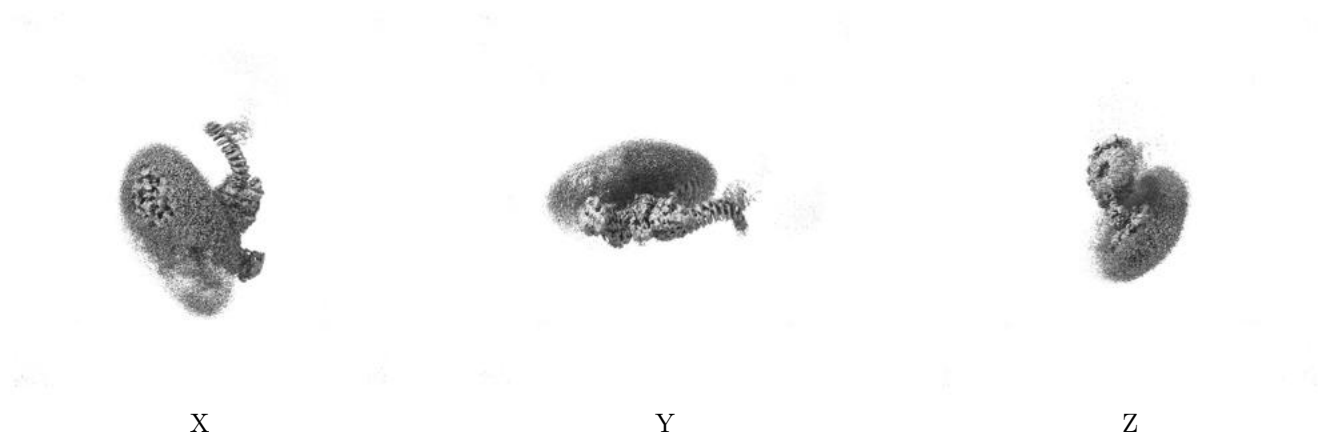
6.5 Orthogonal surface views [i](#)

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.

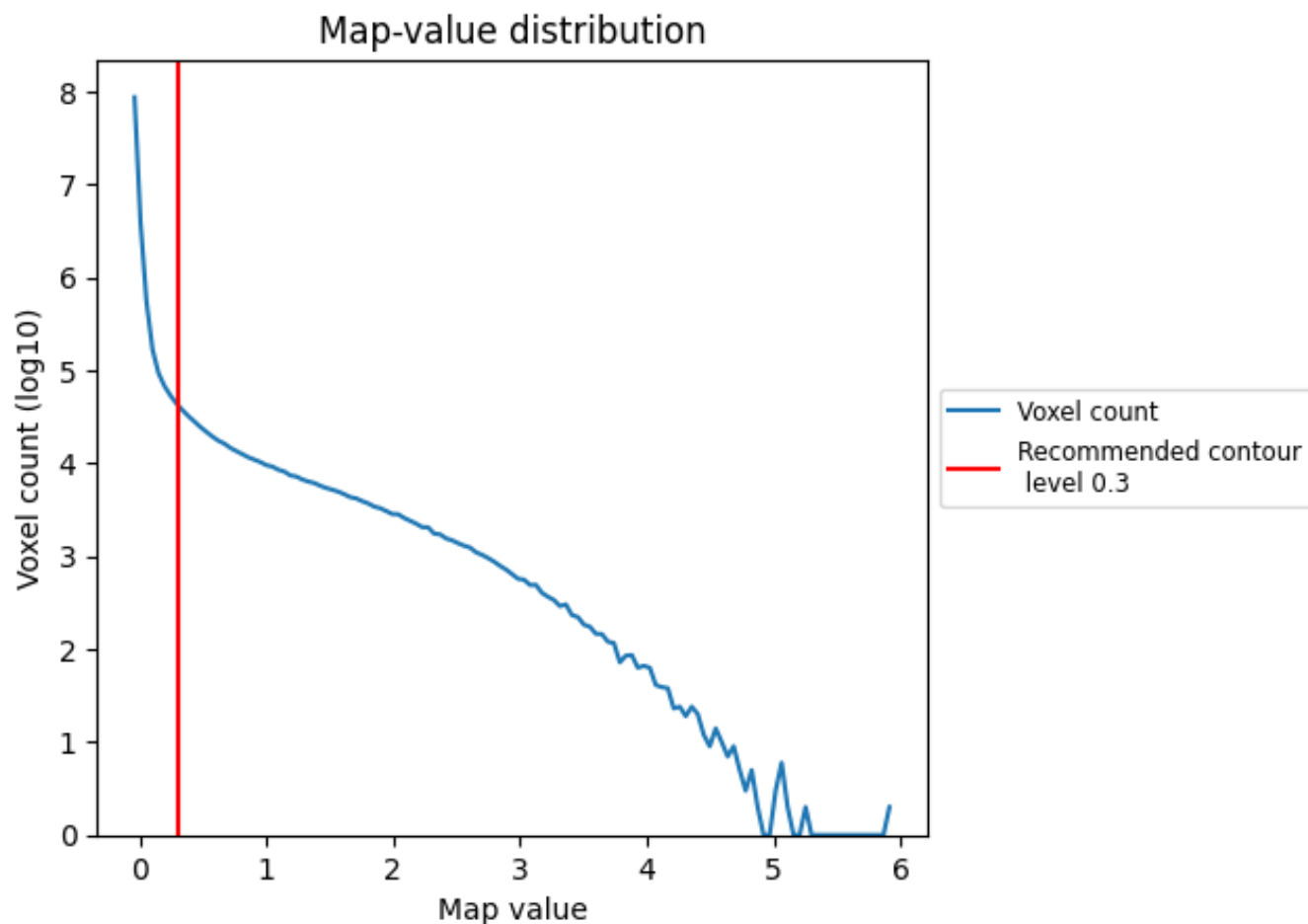
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

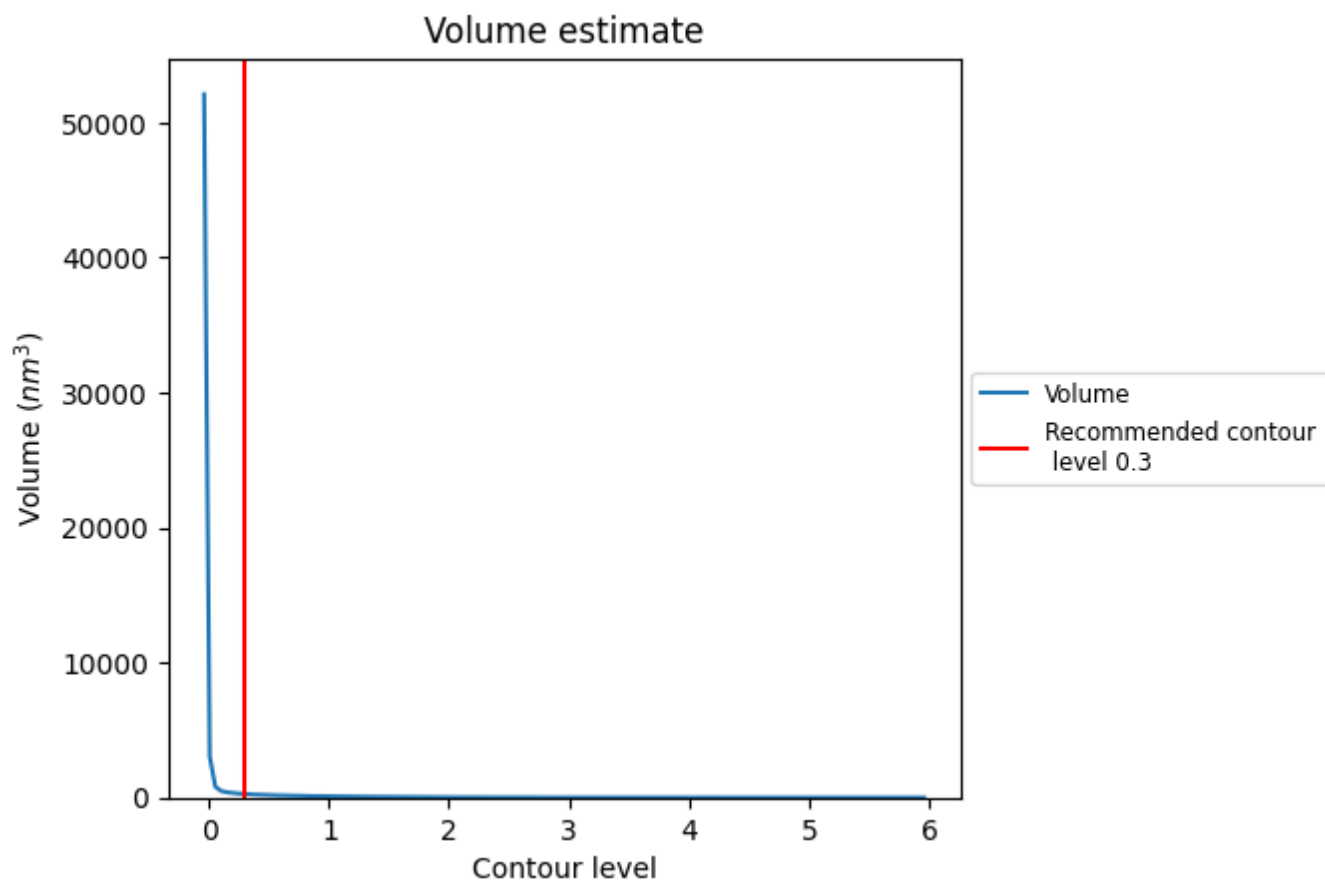
This section contains the results of statistical analysis of the map.

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.

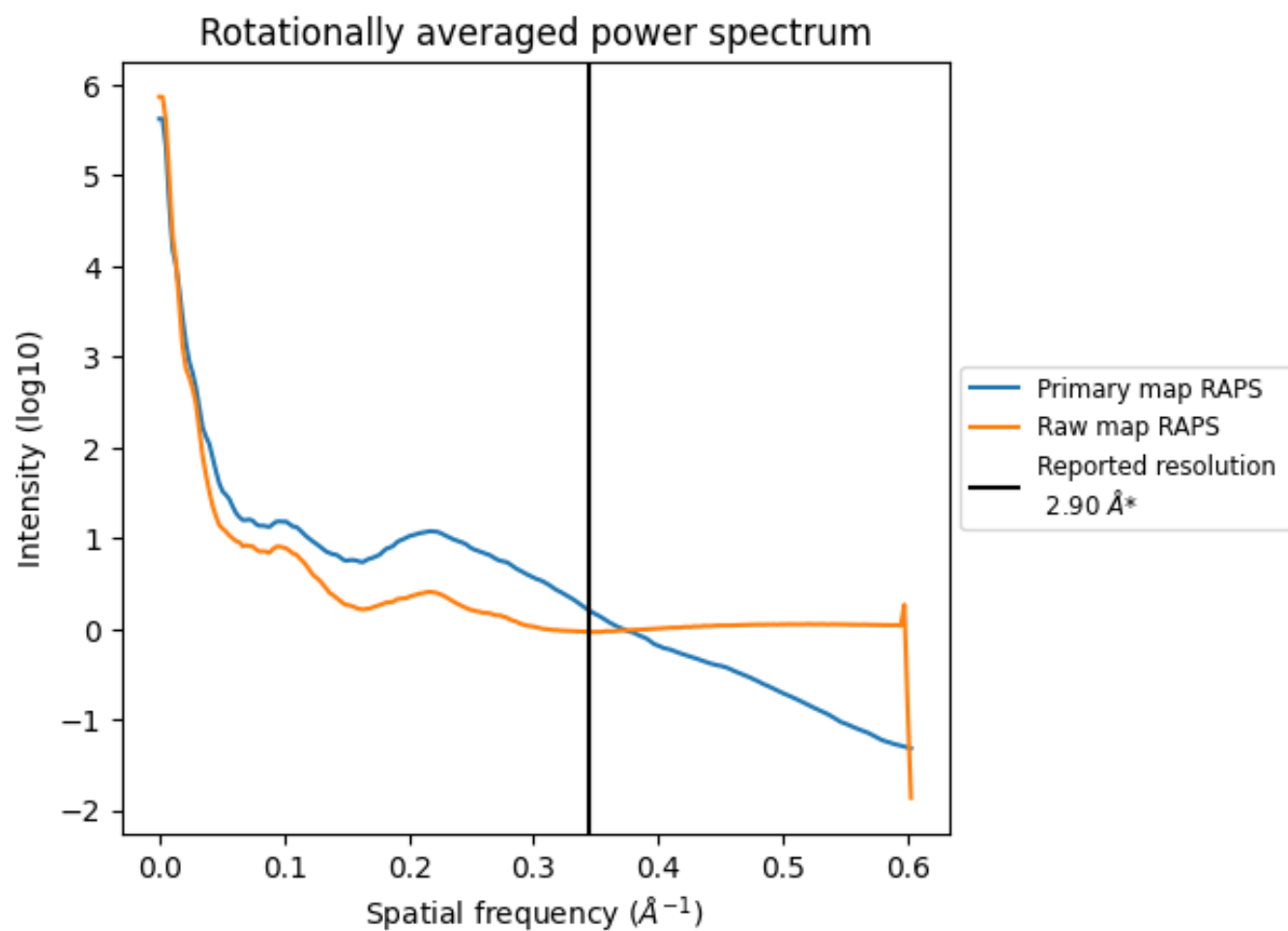
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm^3 ; 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 ⓘ

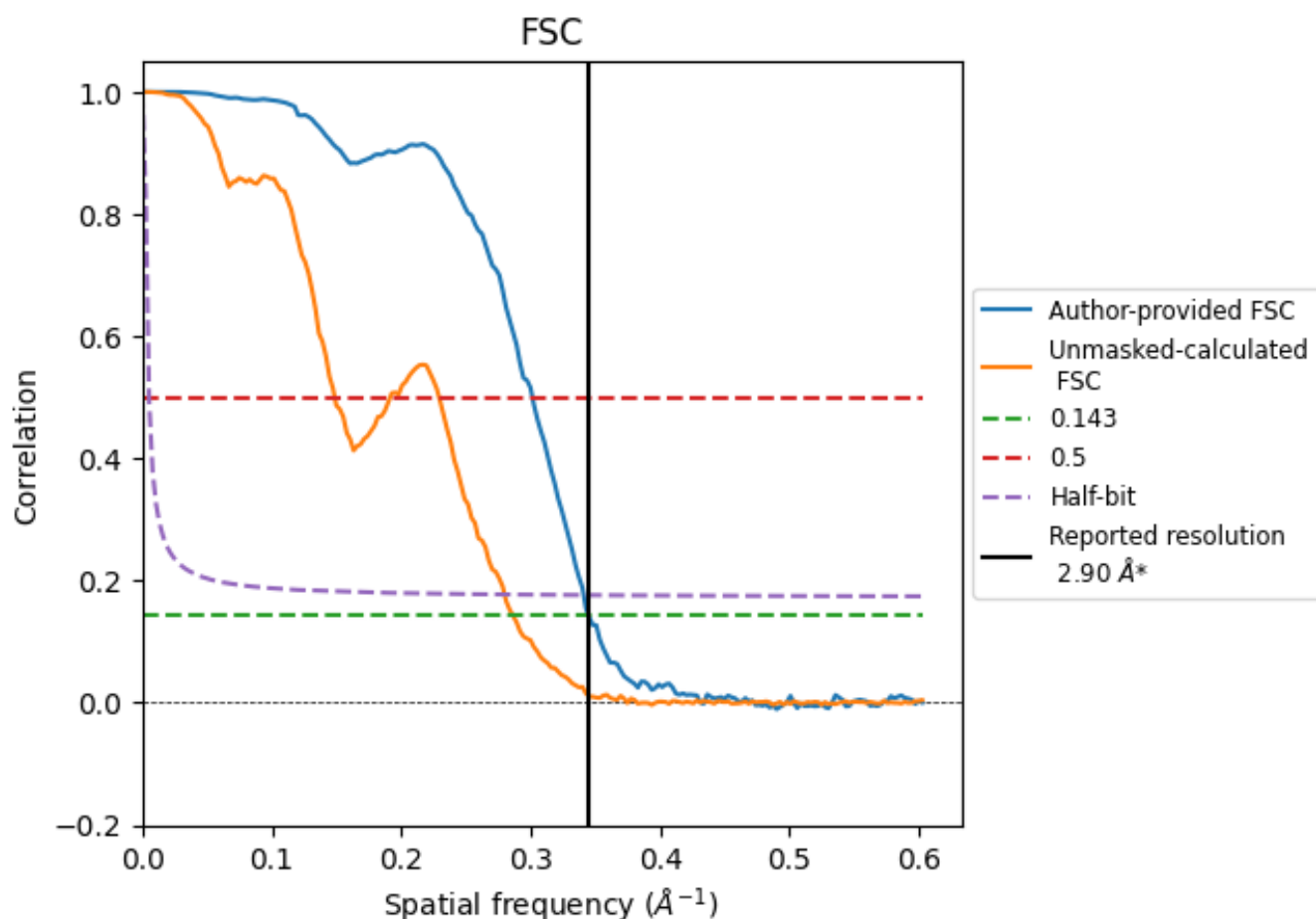


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

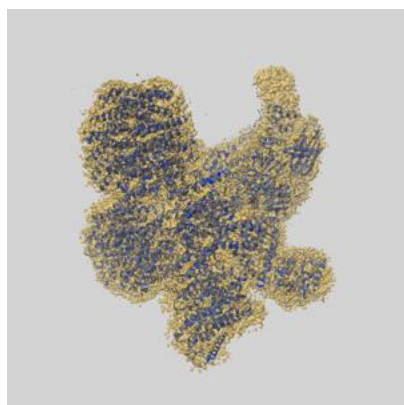
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.32	2.93
Unmasked-calculated*	3.49	6.72	3.57

*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 %

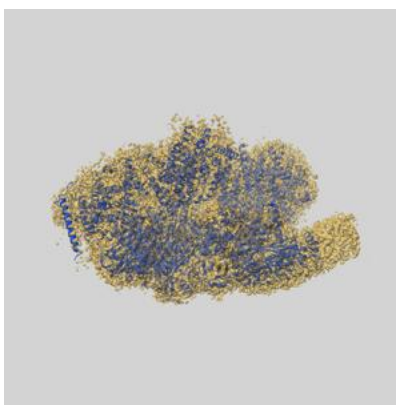
9 Map-model fit [i](#)

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](#).

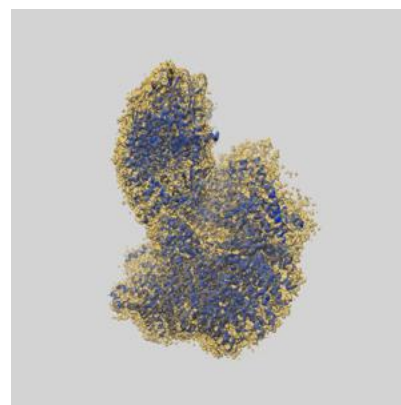
9.1 Map-model overlay [i](#)



X



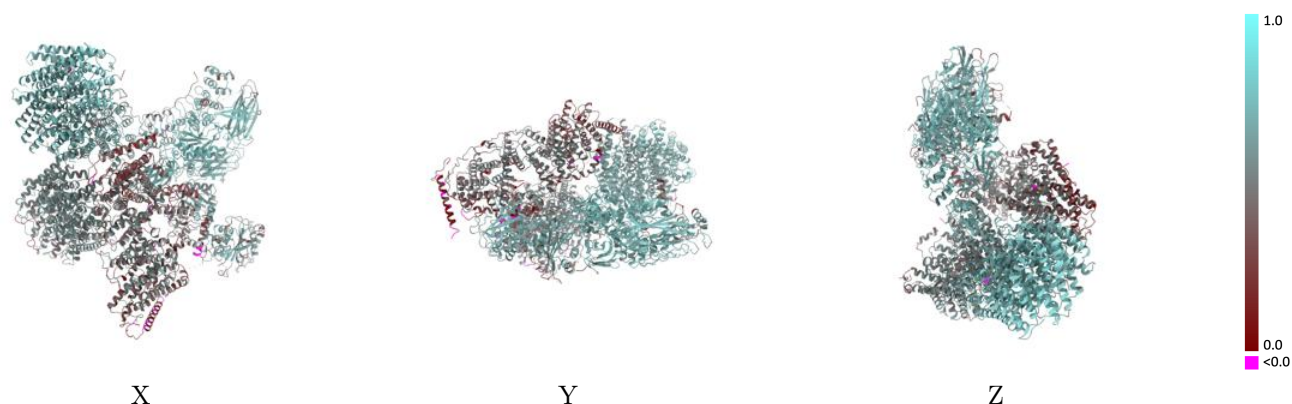
Y



Z

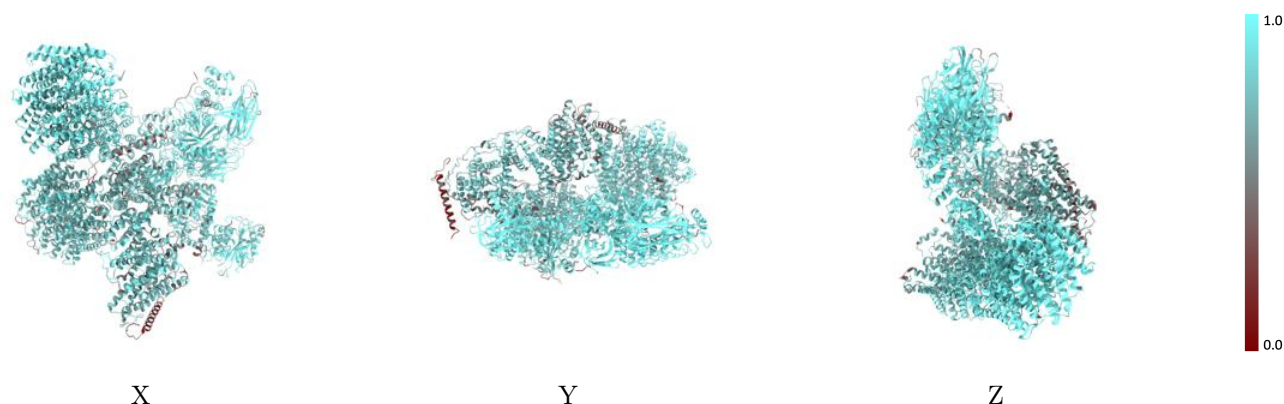
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



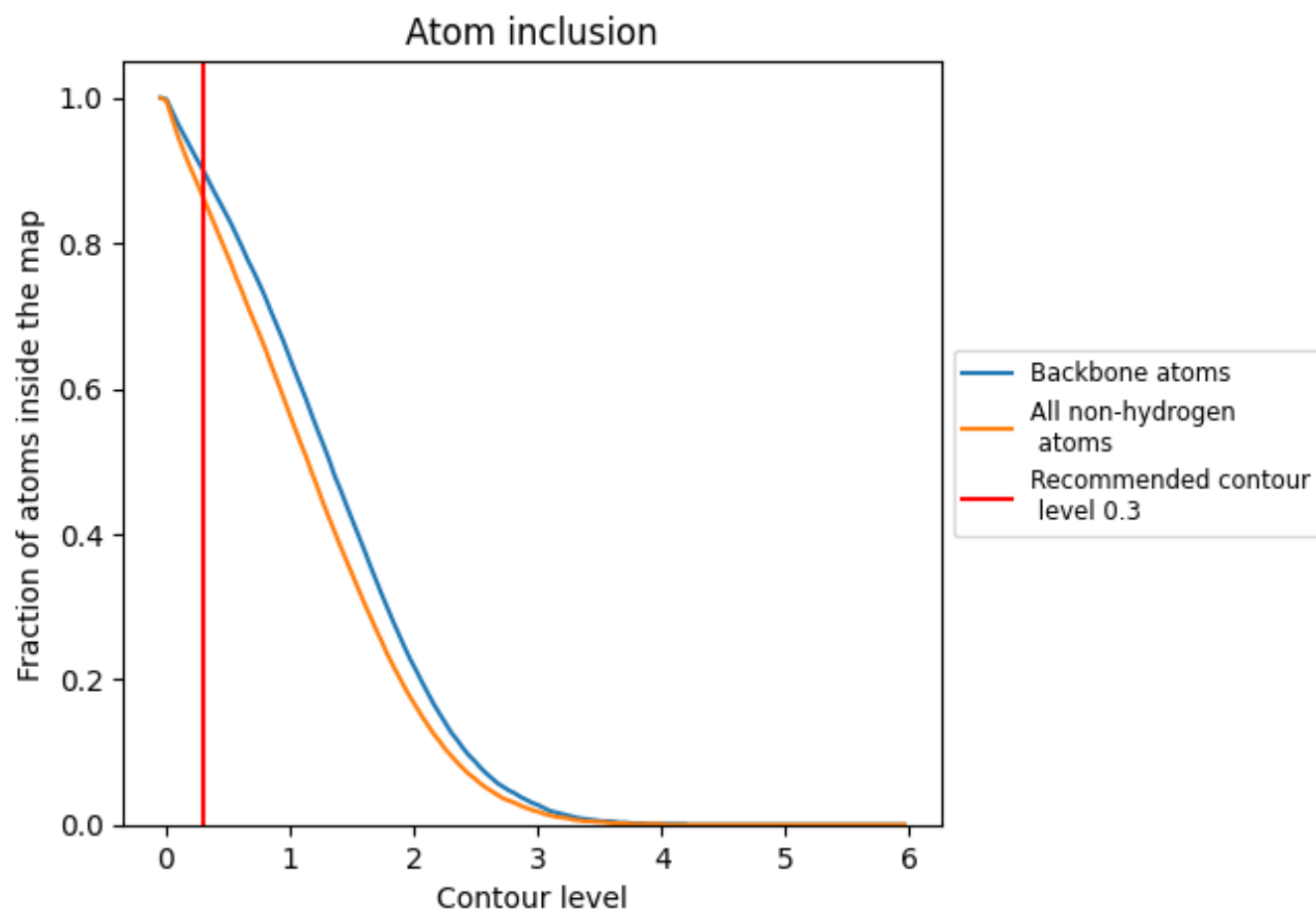
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

