



## wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 08:37 AM EDT

PDB ID : 8CS9  
EMDB ID : EMD-26960  
Title : Composite reconstruction of Class 1 of the erythrocyte ankyrin-1 complex  
Authors : Vallese, F.; Kim, K.; Yen, L.Y.; Johnston, J.D.; Noble, A.J.; Cali, T.; Clarke, O.B.  
Deposited on : 2022-05-12  
Resolution : 2.74 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.39

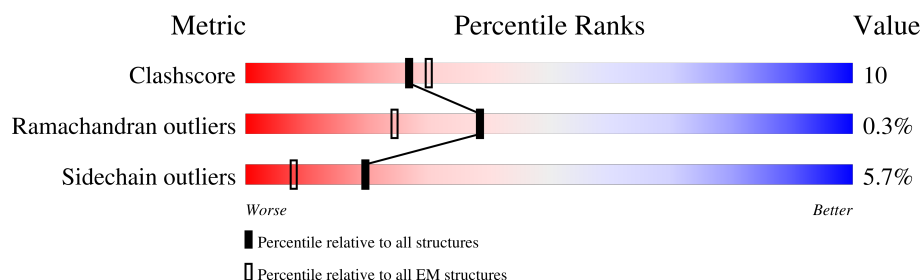
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.74 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  $\geq 3$ , 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	K	417	
3	L	409	
3	Q	409	
4	X	691	
5	P	91	
6	R	150	
6	S	150	

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Mol	Chain	Length	Quality of chain
6	T	150	
6	a	150	
6	b	150	
6	c	150	
7	V	911	
7	Y	911	
7	Z	911	
7	e	911	
7	f	911	
7	g	911	
8	B	2	
8	C	2	
8	D	2	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 60944 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	796	Total	C	N	O	S	0	0
			6017	3768	1116	1113	20		

- Molecule 2 is a protein called Blood group Rh(CE) polypeptide.

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

- Molecule 3 is a protein called Ammonium transporter Rh type A.

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

- Molecule 4 is a protein called Protein 4.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	656	Total	C	N	O	S	0	0
			5162	3276	914	949	23		

- Molecule 5 is a protein called Glycophorin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	33	Total	C	N	O	S	0	0
			248	168	40	38	2		

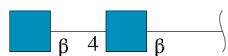
- Molecule 6 is a protein called Glycophorin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	36	Total	C	N	O	S	0	0
			277	183	47	46	1		
6	a	37	Total	C	N	O	S	0	0
			284	188	48	47	1		
6	S	33	Total	C	N	O	S	0	0
			255	169	43	42	1		
6	b	38	Total	C	N	O	S	0	0
			289	191	49	48	1		
6	T	37	Total	C	N	O	S	0	0
			284	188	48	47	1		
6	c	33	Total	C	N	O	S	0	0
			255	169	43	42	1		

- Molecule 7 is a protein called Band 3 anion transport protein.

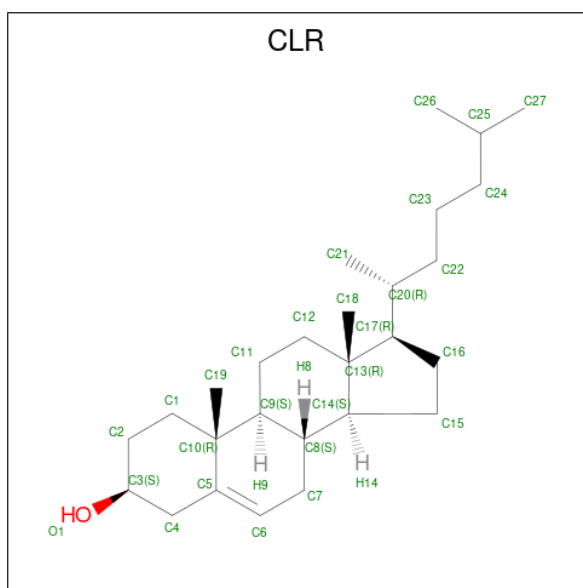
Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	810	Total	C	N	O	S	0	0
			6386	4195	1056	1111	24		
7	e	804	Total	C	N	O	S	0	0
			6339	4170	1047	1098	24		
7	Y	786	Total	C	N	O	S	0	0
			6226	4099	1028	1075	24		
7	f	802	Total	C	N	O	S	0	0
			6331	4164	1047	1096	24		
7	Z	786	Total	C	N	O	S	0	0
			6226	4099	1028	1075	24		
7	g	832	Total	C	N	O	S	0	0
			6556	4301	1079	1149	27		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	B	2	Total	C	N	O	0	0
			28	16	2	10		
8	C	2	Total	C	N	O	0	0
			28	16	2	10		
8	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			28	27	1	
9	L	1	Total	C	O	0
			28	27	1	
9	V	1	Total	C	O	0
			28	27	1	
9	e	1	Total	C	O	0
			28	27	1	
9	Y	1	Total	C	O	0
			28	27	1	
9	f	1	Total	C	O	0
			28	27	1	
9	c	1	Total	C	O	0
			28	27	1	
9	Z	1	Total	C	O	0
			28	27	1	

- Molecule 10 is Digitonin (three-letter code: AJP) (formula:  $C_{56}H_{92}O_{29}$ ).



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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\text{C}_8\text{H}_{15}\text{NO}_6$ ).



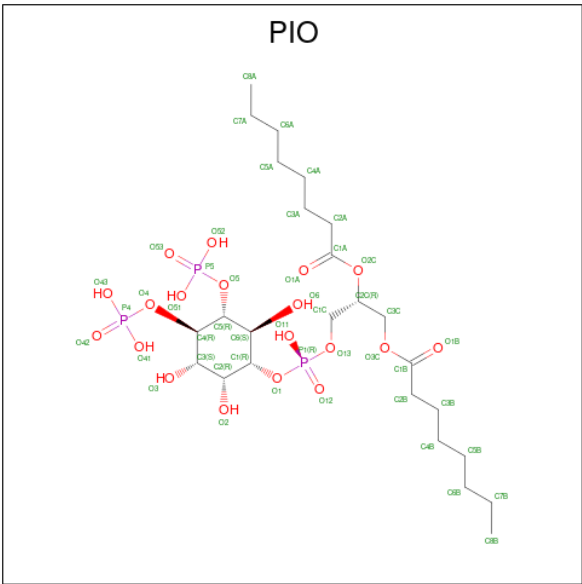
Mol	Chain	Residues	Atoms				AltConf
11	V	1	Total 14	C 8	N 1	O 5	0
11	V	1	Total 14	C 8	N 1	O 5	0

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Mol	Chain	Residues	Atoms				AltConf
11	Y	1	Total	C	N	O	0
			14	8	1	5	
11	Y	1	Total	C	N	O	0
			14	8	1	5	
11	Z	1	Total	C	N	O	0
			14	8	1	5	
11	Z	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 12 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 (three-letter code: PIO) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>19</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	V	1	Total	C	O	P	0
			47	25	19	3	
12	e	1	Total	C	O	P	0
			47	25	19	3	
12	Y	1	Total	C	O	P	0
			47	25	19	3	
12	f	1	Total	C	O	P	0
			47	25	19	3	
12	g	1	Total	C	O	P	0
			47	25	19	3	
12	g	1	Total	C	O	P	0
			47	25	19	3	



- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	32	Total 32	O 32	0
13	K	18	Total 18	O 18	0
13	L	46	Total 46	O 46	0
13	Q	34	Total 34	O 34	0
13	X	112	Total 112	O 112	0
13	V	17	Total 17	O 17	0
13	e	4	Total 4	O 4	0
13	f	2	Total 2	O 2	0
13	g	3	Total 3	O 3	0

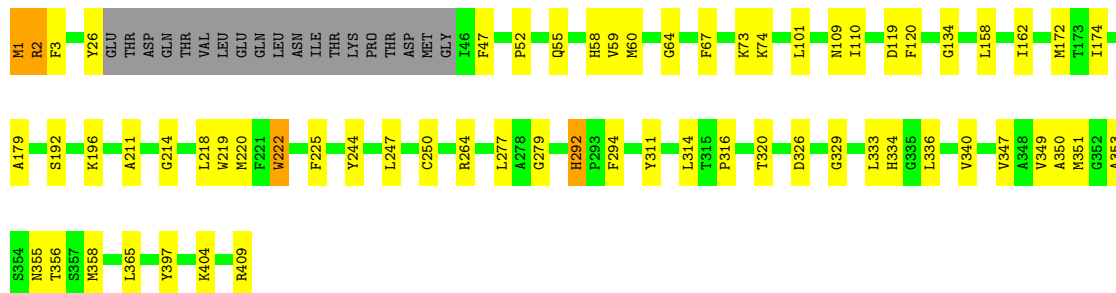






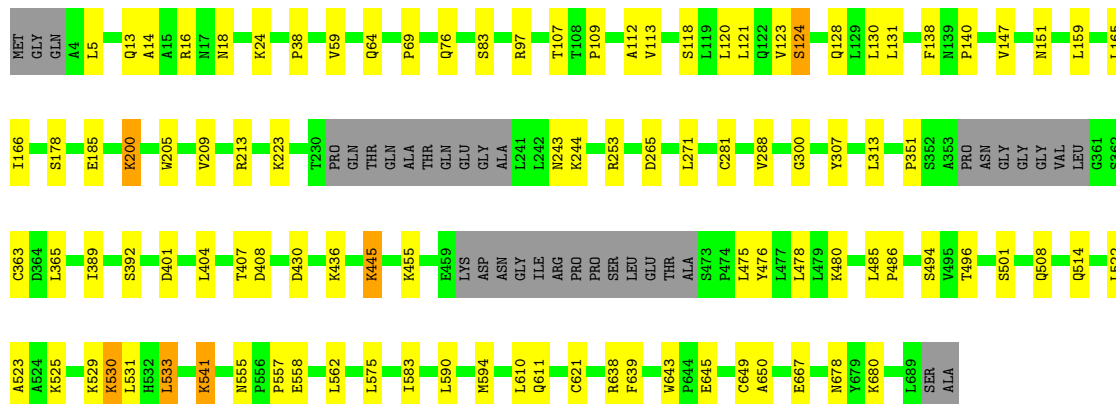
• Molecule 3: Ammonium transporter Rh type A

Chain Q: 80% 15% • 5%



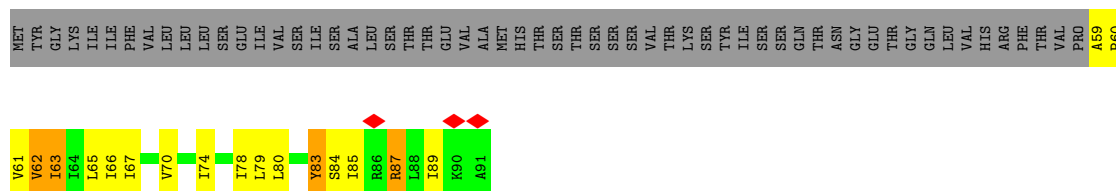
• Molecule 4: Protein 4.2

Chain X: 80% 14% • 5%



• Molecule 5: Glycophorin-B

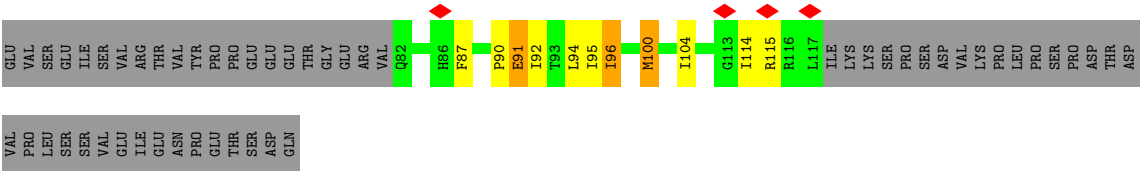
Chain P: 16% 15% • 64%



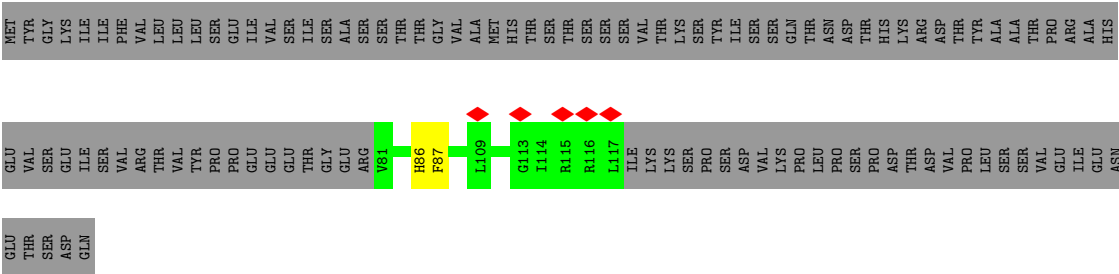
• Molecule 6: Glycophorin-A

Chain R: 17% 5% • 76%

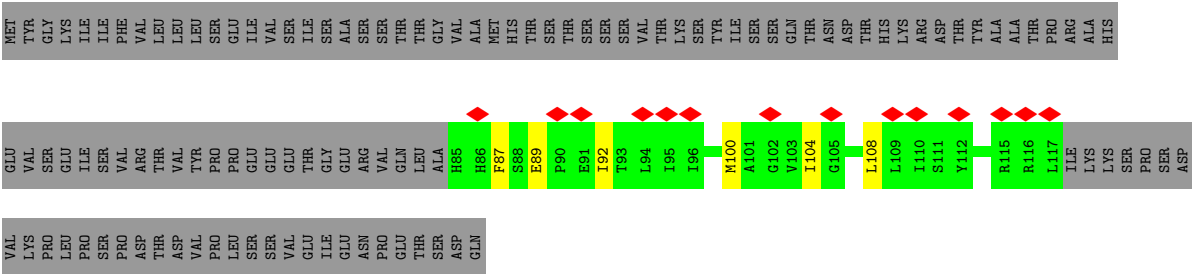




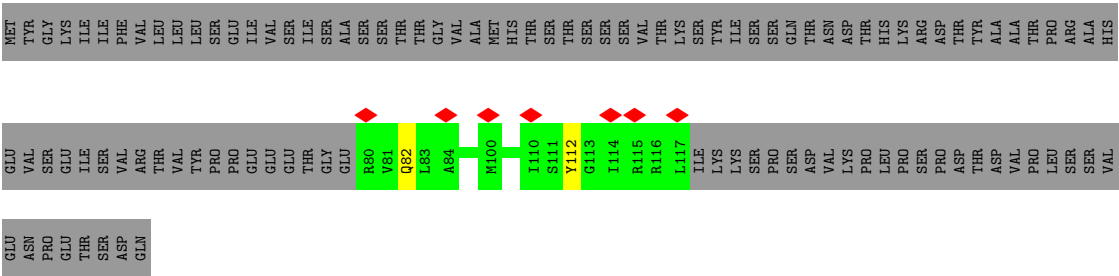
• Molecule 6: Glycophorin-A



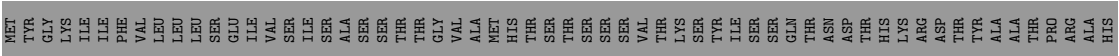
• Molecule 6: Glycophorin-A



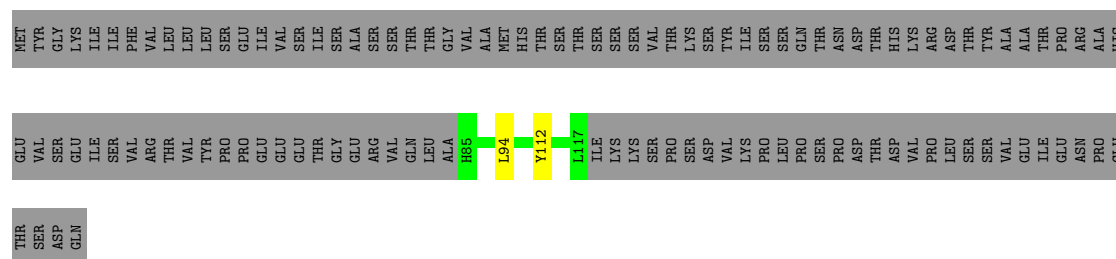
• Molecule 6: Glycophorin-A



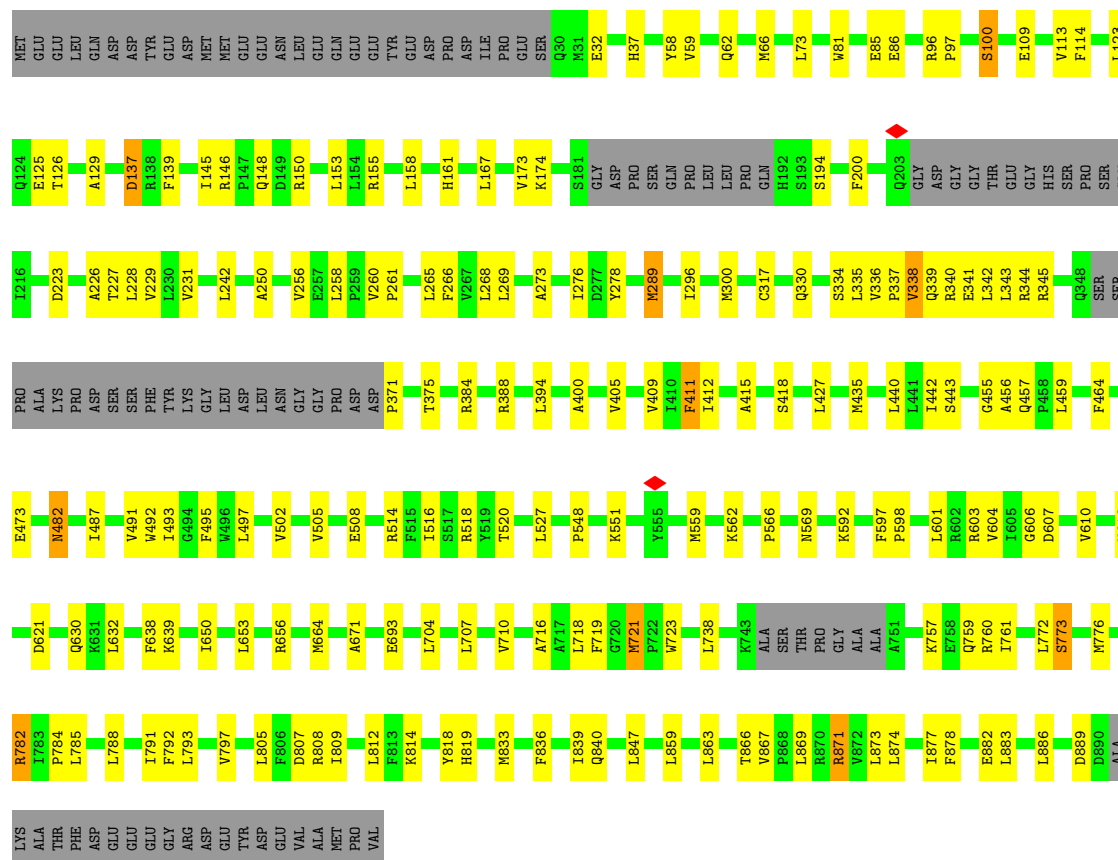
• Molecule 6: Glycophorin-A



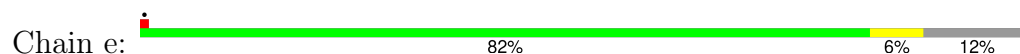
- Molecule 6: Glycophorin-A

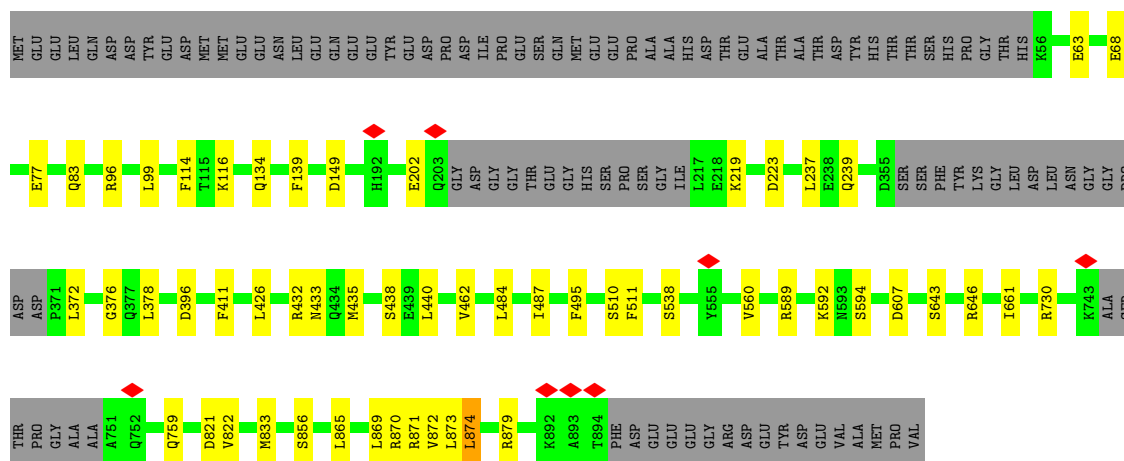


- Molecule 7: Band 3 anion transport protein

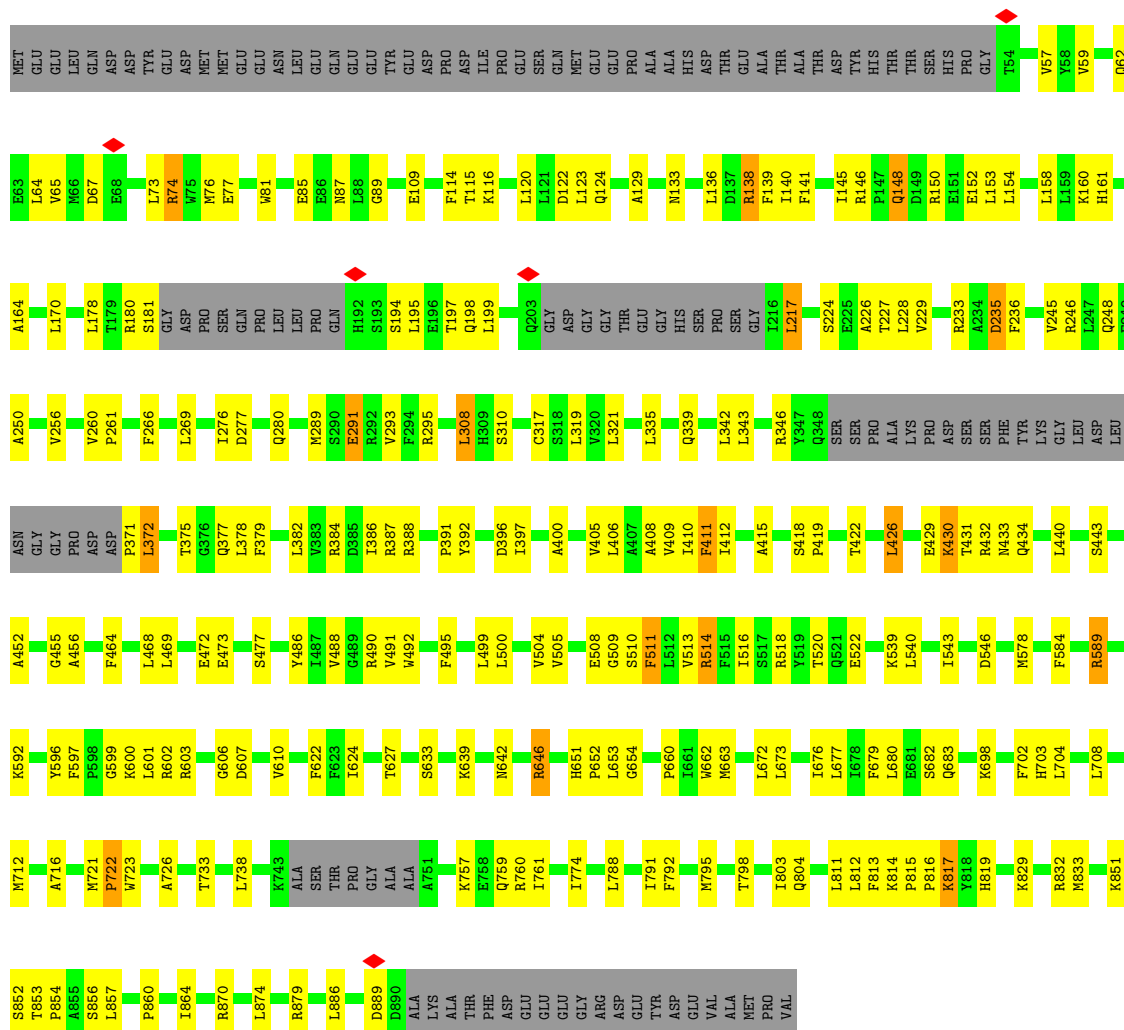


- Molecule 7: Band 3 anion transport protein





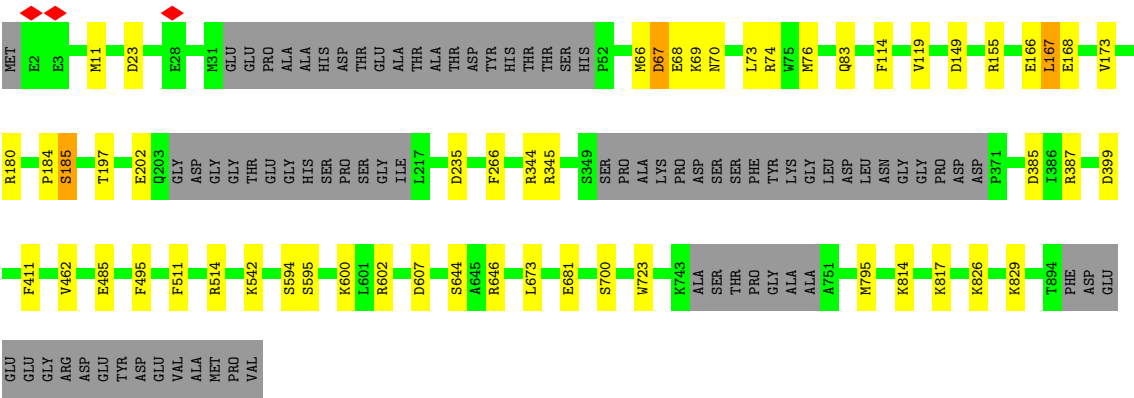
### • Molecule 7: Band 3 anion transport protein



### • Molecule 7: Band 3 anion transport protein







• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	126197	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	5.911	Depositor
Minimum map value	0.000	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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: CLR, NAG, PIO, AJP

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	0.31	0/6127	0.49	0/8331
2	K	0.31	0/3016	0.51	0/4105
3	L	0.29	0/3008	0.46	0/4075
3	Q	0.31	0/3025	0.50	0/4098
4	X	0.27	0/5269	0.51	0/7149
5	P	0.52	0/249	0.64	0/336
6	R	0.38	0/282	0.56	0/381
6	S	0.25	0/260	0.55	0/351
6	T	0.41	0/289	0.58	0/391
6	a	0.24	0/289	0.54	0/391
6	b	0.25	0/294	0.52	0/398
6	c	0.40	0/260	0.55	0/351
7	V	0.29	0/6536	0.52	0/8885
7	Y	0.33	0/6371	0.54	0/8655
7	Z	0.30	0/6371	0.51	0/8655
7	e	0.35	0/6489	0.54	0/8822
7	f	0.36	0/6481	0.56	0/8808
7	g	0.35	0/6709	0.55	0/9118
All	All	0.32	0/61325	0.52	0/83300

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	6017	0	6114	87	0
2	K	2943	0	3056	43	0
3	L	2938	0	2978	40	0
3	Q	2954	0	2989	40	0
4	X	5162	0	5173	52	0
5	P	248	0	298	18	0
6	R	277	0	289	15	0
6	S	255	0	265	5	0
6	T	284	0	298	9	0
6	a	284	0	298	0	0
6	b	289	0	300	0	0
6	c	255	0	265	0	0
7	V	6386	0	6558	107	0
7	Y	6226	0	6437	145	0
7	Z	6226	0	6437	102	0
7	e	6339	0	6541	0	0
7	f	6331	0	6536	0	0
7	g	6556	0	6703	0	0
8	B	28	0	25	0	0
8	C	28	0	25	0	0
8	D	28	0	25	0	0
9	L	56	0	92	4	0
9	V	28	0	46	9	0
9	Y	28	0	46	1	0
9	Z	28	0	46	4	0
9	c	28	0	46	0	0
9	e	28	0	46	0	0
9	f	28	0	46	0	0
10	Q	32	0	0	1	0
11	V	28	0	25	0	0
11	Y	28	0	25	0	0
11	Z	28	0	25	0	0
12	V	47	0	44	3	0
12	Y	47	0	44	3	0
12	e	47	0	44	0	0
12	f	47	0	44	0	0
12	g	94	0	88	0	0
13	A	32	0	0	0	0
13	K	18	0	0	0	0
13	L	46	0	0	0	0
13	Q	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	V	17	0	0	0	0
13	X	112	0	0	1	0
13	e	4	0	0	0	0
13	f	2	0	0	0	0
13	g	3	0	0	0	0
All	All	60944	0	62317	641	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 10.

The worst 5 of 641 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:57:VAL:HB	7:Y:295:ARG:HD3	1.62	0.82
7:V:495:PHE:HB3	9:V:1001:CLR:H261	1.62	0.79
3:Q:350:ALA:HB2	3:Q:358:MET:SD	2.23	0.79
4:X:59:VAL:HG22	4:X:123:VAL:HG22	1.65	0.78
7:Z:136:LEU:HD12	7:Z:154:LEU:HB2	1.64	0.77

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	792/1881 (42%)	772 (98%)	18 (2%)	2 (0%)	37	55
2	K	370/417 (89%)	362 (98%)	8 (2%)	0	100	100
3	L	384/409 (94%)	380 (99%)	4 (1%)	0	100	100
3	Q	386/409 (94%)	380 (98%)	4 (1%)	2 (0%)	25	41
4	X	648/691 (94%)	639 (99%)	8 (1%)	1 (0%)	44	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	31/91 (34%)	31 (100%)	0	0	100	100
6	R	34/150 (23%)	31 (91%)	2 (6%)	1 (3%)	3	5
6	S	31/150 (21%)	31 (100%)	0	0	100	100
6	T	35/150 (23%)	32 (91%)	1 (3%)	2 (6%)	1	1
6	a	35/150 (23%)	35 (100%)	0	0	100	100
6	b	36/150 (24%)	36 (100%)	0	0	100	100
6	c	31/150 (21%)	31 (100%)	0	0	100	100
7	V	800/911 (88%)	789 (99%)	11 (1%)	0	100	100
7	Y	776/911 (85%)	754 (97%)	20 (3%)	2 (0%)	37	55
7	Z	776/911 (85%)	761 (98%)	14 (2%)	1 (0%)	48	70
7	e	796/911 (87%)	765 (96%)	25 (3%)	6 (1%)	16	30
7	f	794/911 (87%)	766 (96%)	27 (3%)	1 (0%)	48	70
7	g	822/911 (90%)	792 (96%)	26 (3%)	4 (0%)	25	41
All	All	7577/10264 (74%)	7387 (98%)	168 (2%)	22 (0%)	38	55

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	e	873	LEU
7	e	874	LEU
7	f	181	SER
1	A	437	VAL
7	e	376	GLY

### 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	643/1594 (40%)	606 (94%)	37 (6%)	17	30
2	K	317/348 (91%)	299 (94%)	18 (6%)	17	31
3	L	307/328 (94%)	302 (98%)	5 (2%)	58	75

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	308/328 (94%)	296 (96%)	12 (4%)	27	47
4	X	558/588 (95%)	536 (96%)	22 (4%)	27	47
5	P	28/81 (35%)	23 (82%)	5 (18%)	1	2
6	R	29/136 (21%)	27 (93%)	2 (7%)	13	23
6	S	27/136 (20%)	26 (96%)	1 (4%)	29	49
6	T	30/136 (22%)	28 (93%)	2 (7%)	13	24
6	a	30/136 (22%)	28 (93%)	2 (7%)	13	24
6	b	30/136 (22%)	28 (93%)	2 (7%)	13	24
6	c	27/136 (20%)	25 (93%)	2 (7%)	11	20
7	V	692/786 (88%)	657 (95%)	35 (5%)	20	36
7	Y	679/786 (86%)	631 (93%)	48 (7%)	12	22
7	Z	679/786 (86%)	649 (96%)	30 (4%)	24	42
7	e	689/786 (88%)	638 (93%)	51 (7%)	11	20
7	f	689/786 (88%)	644 (94%)	45 (6%)	14	25
7	g	710/786 (90%)	657 (92%)	53 (8%)	11	20
All	All	6472/8799 (74%)	6100 (94%)	372 (6%)	20	31

5 of 372 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Y	723	TRP
6	T	100	MET
7	Y	856	SER
7	f	594	SER
7	Z	330	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
7	f	884	GLN
7	g	62	GLN
7	g	457	GLN
7	Z	433	ASN
7	V	630	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

6 monosaccharides 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	NAG	B	1	8,7	14,14,15	0.22	0	17,19,21	0.40	0
8	NAG	B	2	8	14,14,15	0.39	0	17,19,21	0.41	0
8	NAG	C	1	8,7	14,14,15	0.26	0	17,19,21	0.46	0
8	NAG	C	2	8	14,14,15	0.36	0	17,19,21	0.40	0
8	NAG	D	1	8,7	14,14,15	0.22	0	17,19,21	0.44	0
8	NAG	D	2	8	14,14,15	0.38	0	17,19,21	0.43	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	NAG	B	1	8,7	-	2/6/23/26	0/1/1/1
8	NAG	B	2	8	-	2/6/23/26	0/1/1/1
8	NAG	C	1	8,7	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1
8	NAG	D	1	8,7	-	1/6/23/26	0/1/1/1
8	NAG	D	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

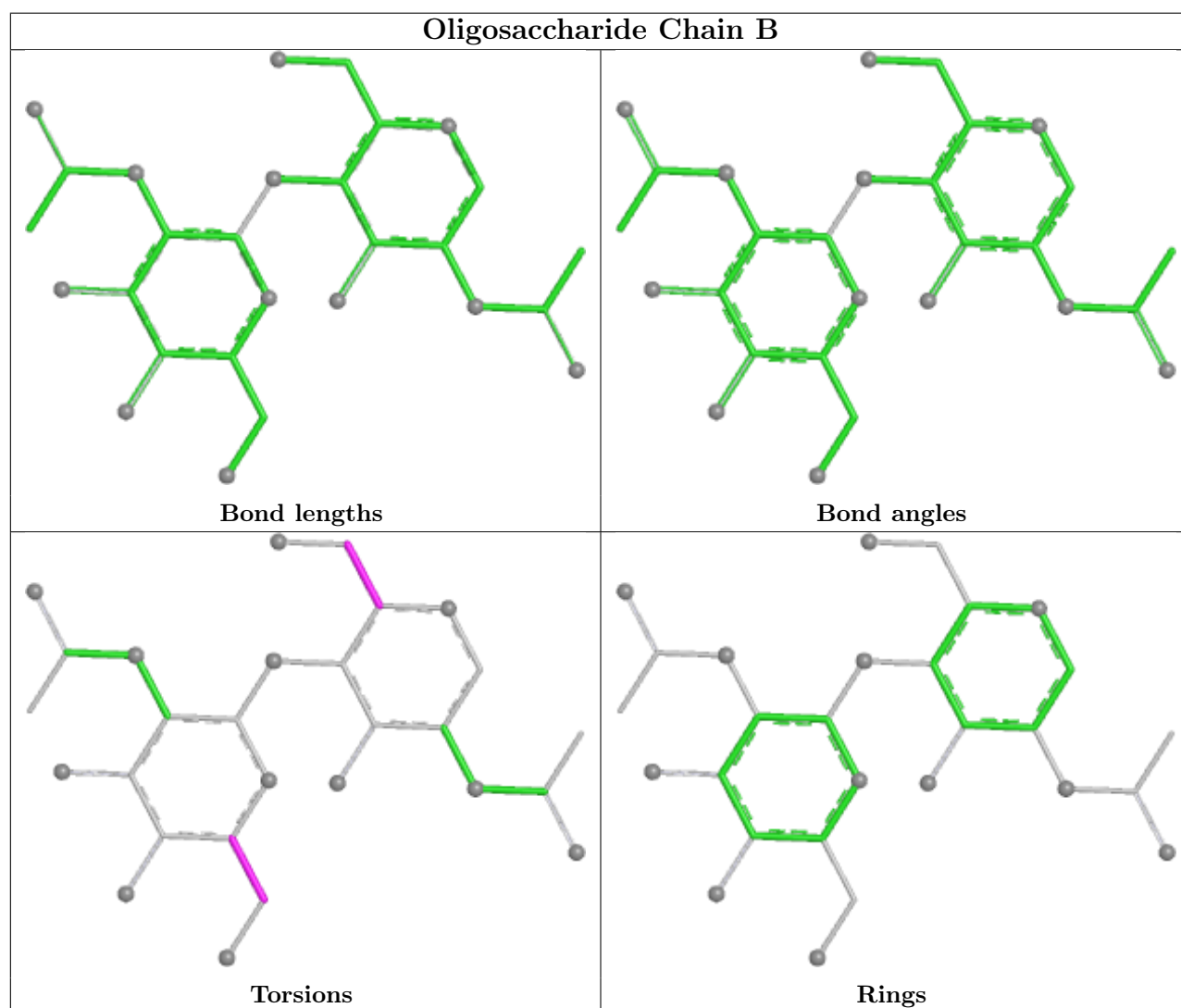
5 of 11 torsion outliers are listed below:

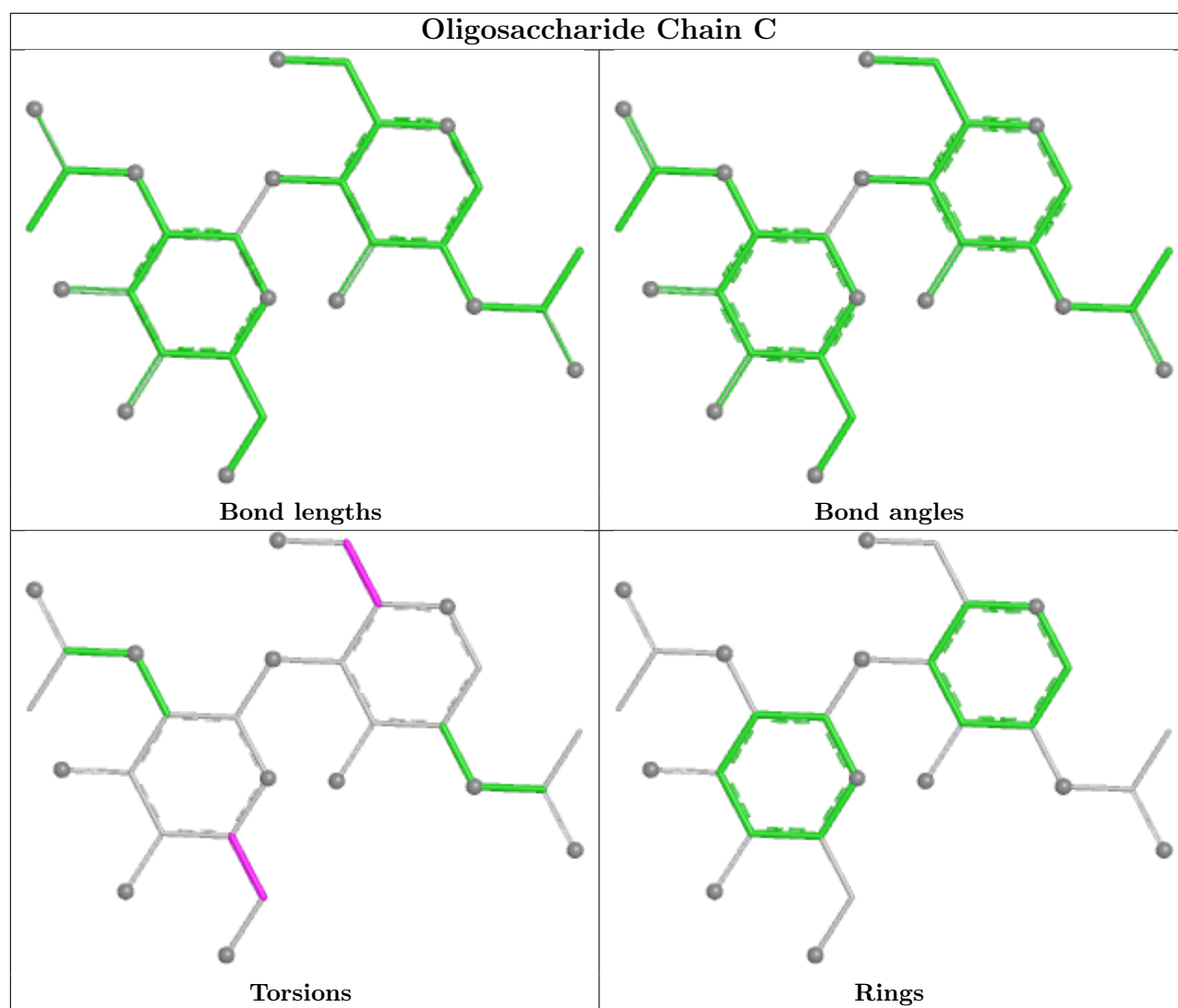
Mol	Chain	Res	Type	Atoms
8	B	1	NAG	O5-C5-C6-O6
8	B	1	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
8	D	2	NAG	C4-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6

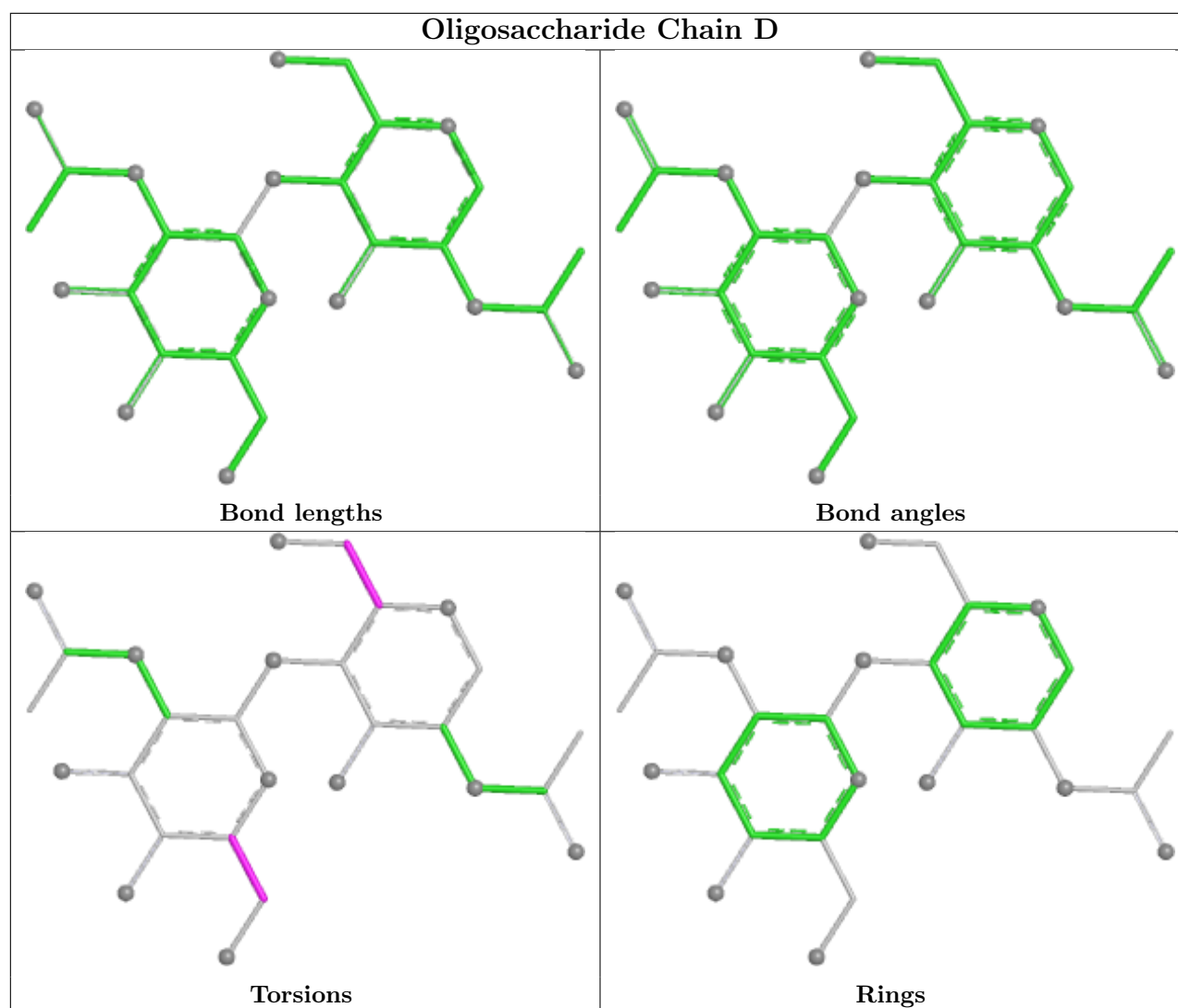
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

21 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	$\# Z  > 2$
11	NAG	V	1003	11	14,14,15	0.37	0	17,19,21	0.39	0
9	CLR	V	1001	-	31,31,31	0.33	0	48,48,48	0.54	0
9	CLR	c	201	-	31,31,31	0.36	0	48,48,48	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	CLR	L	502	-	31,31,31	0.44	0	48,48,48	0.94	2 (4%)
9	CLR	Z	1001	-	31,31,31	0.29	0	48,48,48	0.38	0
11	NAG	Y	1003	11	14,14,15	0.37	0	17,19,21	0.40	0
11	NAG	Y	1002	11,7	14,14,15	0.22	0	17,19,21	0.44	0
11	NAG	V	1002	11,7	14,14,15	0.24	0	17,19,21	0.43	0
12	PIO	V	1004	-	47,47,47	0.50	0	62,65,65	0.50	0
11	NAG	Z	1002	11,7	14,14,15	0.22	0	17,19,21	0.45	0
9	CLR	L	501	-	31,31,31	0.41	0	48,48,48	0.85	0
12	PIO	Y	1004	-	47,47,47	0.51	0	62,65,65	0.44	0
10	AJP	Q	501	-	37,37,95	0.47	0	58,62,149	0.63	1 (1%)
9	CLR	Y	1001	-	31,31,31	0.37	0	48,48,48	0.59	0
9	CLR	e	1001	-	31,31,31	0.36	0	48,48,48	0.60	0
12	PIO	g	1002	-	47,47,47	0.44	0	62,65,65	0.50	0
9	CLR	f	1001	-	31,31,31	0.28	0	48,48,48	0.49	0
12	PIO	e	1002	-	47,47,47	0.48	0	62,65,65	0.43	0
11	NAG	Z	1003	11	14,14,15	0.42	0	17,19,21	0.47	0
12	PIO	f	1002	-	47,47,47	0.50	0	62,65,65	0.42	0
12	PIO	g	1001	-	47,47,47	0.47	0	62,65,65	0.43	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
11	NAG	V	1003	11	-	0/6/23/26	0/1/1/1
9	CLR	V	1001	-	-	10/10/68/68	0/4/4/4
9	CLR	c	201	-	-	8/10/68/68	0/4/4/4
9	CLR	L	502	-	-	6/10/68/68	0/4/4/4
9	CLR	Z	1001	-	-	10/10/68/68	0/4/4/4
11	NAG	Y	1003	11	-	2/6/23/26	0/1/1/1
11	NAG	Y	1002	11,7	-	2/6/23/26	0/1/1/1
11	NAG	V	1002	11,7	-	0/6/23/26	0/1/1/1
12	PIO	V	1004	-	-	16/44/68/68	0/1/1/1
11	NAG	Z	1002	11,7	-	2/6/23/26	0/1/1/1
9	CLR	L	501	-	-	5/10/68/68	0/4/4/4
12	PIO	Y	1004	-	-	14/44/68/68	0/1/1/1
10	AJP	Q	501	-	-	-	0/6/6/11
9	CLR	Y	1001	-	-	8/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLR	e	1001	-	-	8/10/68/68	0/4/4/4
12	PIO	g	1002	-	-	24/44/68/68	0/1/1/1
9	CLR	f	1001	-	-	8/10/68/68	0/4/4/4
12	PIO	e	1002	-	-	28/44/68/68	0/1/1/1
11	NAG	Z	1003	11	-	3/6/23/26	0/1/1/1
12	PIO	f	1002	-	-	24/44/68/68	0/1/1/1
12	PIO	g	1001	-	-	11/44/68/68	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	502	CLR	C16-C15-C14	-3.89	97.53	105.14
10	Q	501	AJP	C19-C24-C23	-2.64	111.26	114.40
9	L	502	CLR	C7-C8-C9	2.22	112.29	109.72

There are no chirality outliers.

5 of 189 torsion outliers are listed below:

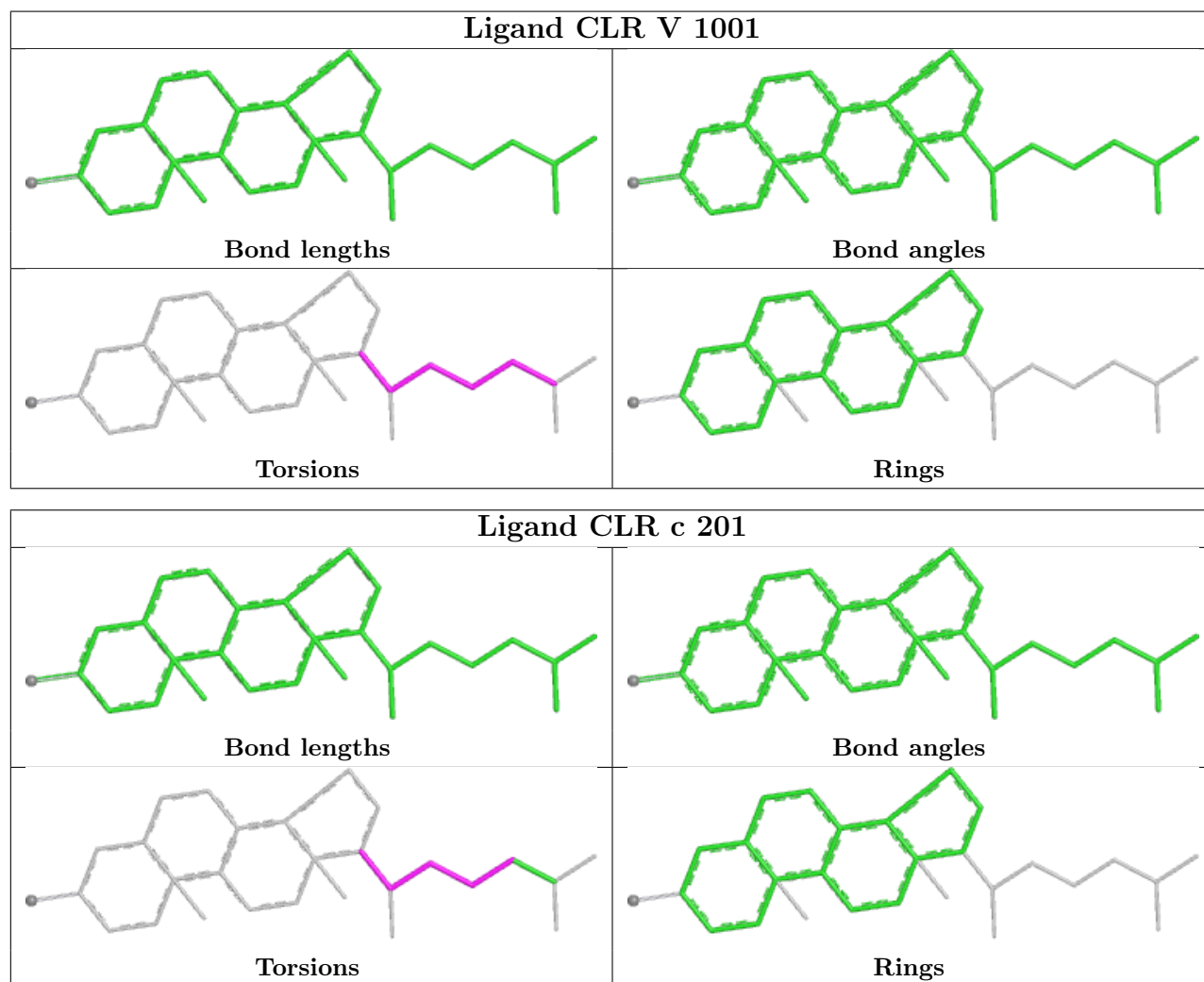
Mol	Chain	Res	Type	Atoms
12	V	1004	PIO	C1-O1-P1-O11
12	V	1004	PIO	C1-O1-P1-O13
12	V	1004	PIO	C4-C5-O5-P5
12	V	1004	PIO	C6-C5-O5-P5
12	V	1004	PIO	C2A-C1A-O2C-C2C

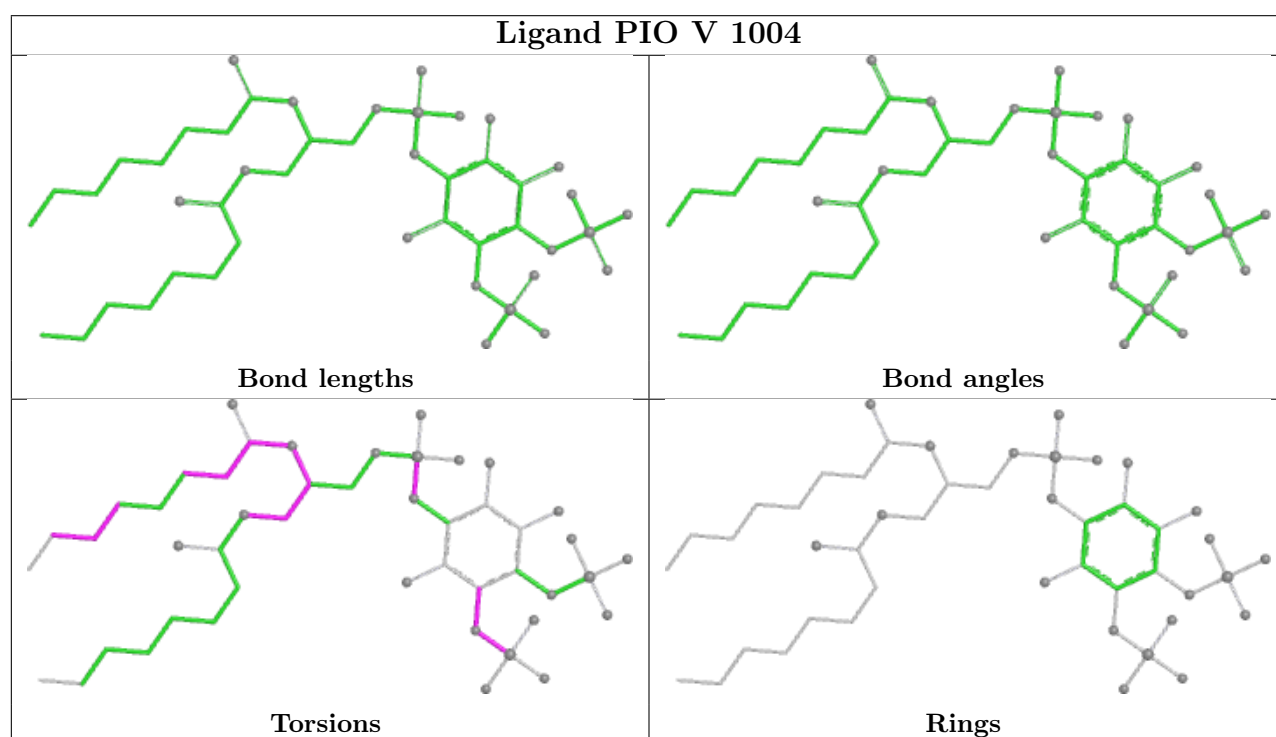
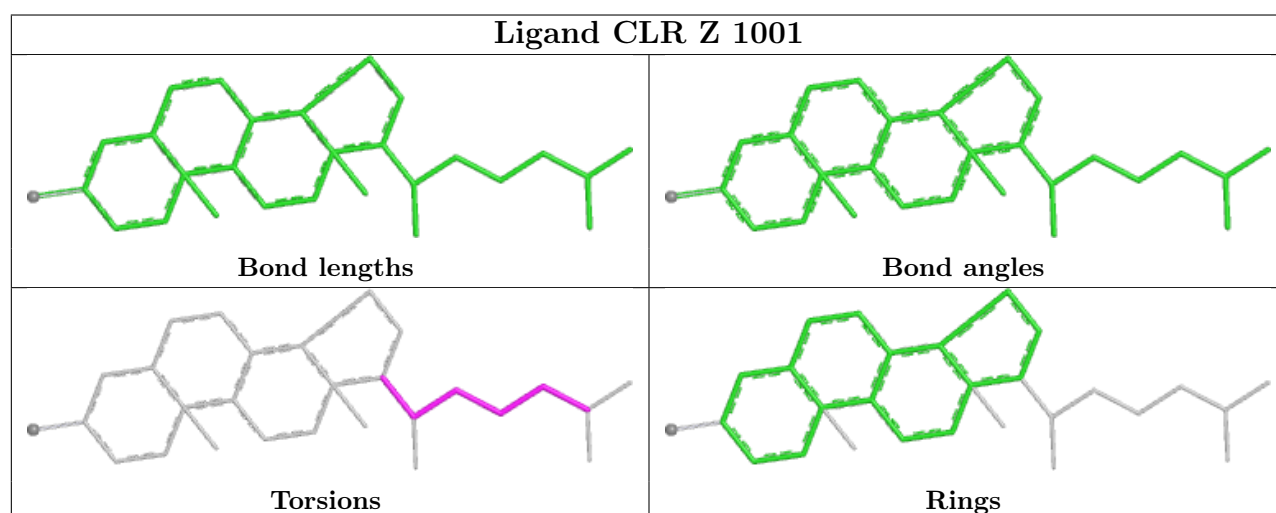
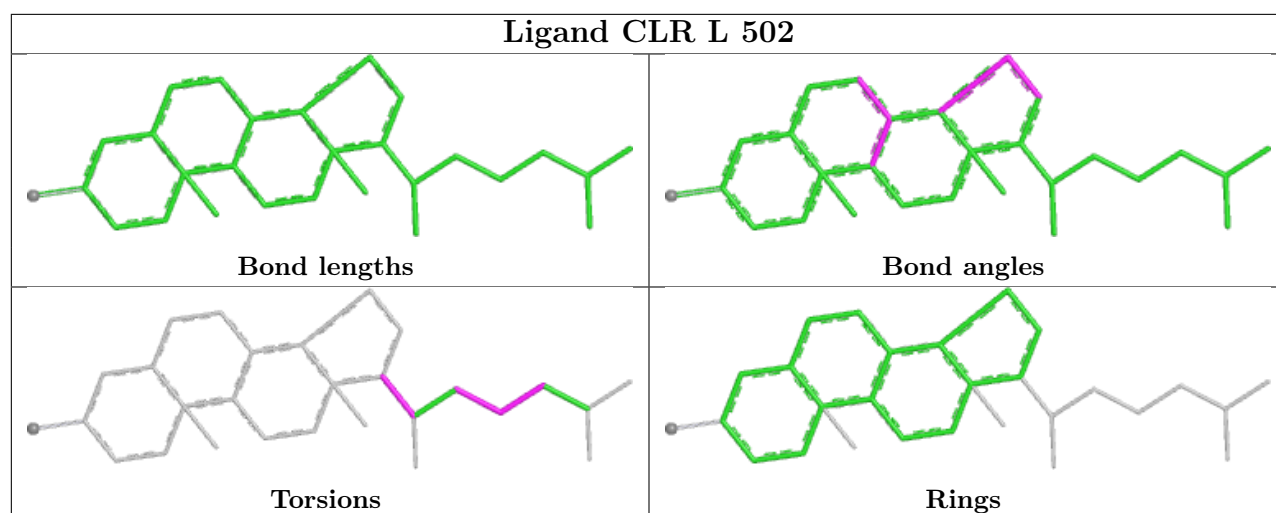
There are no ring outliers.

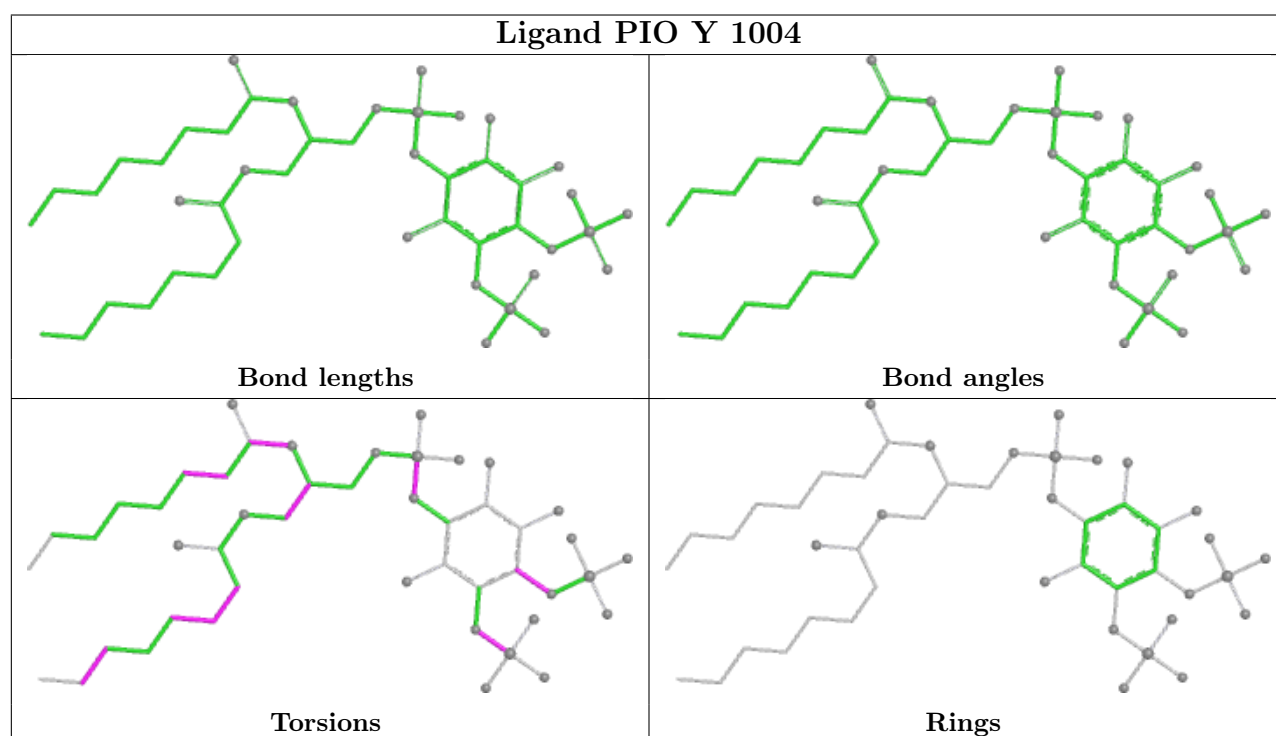
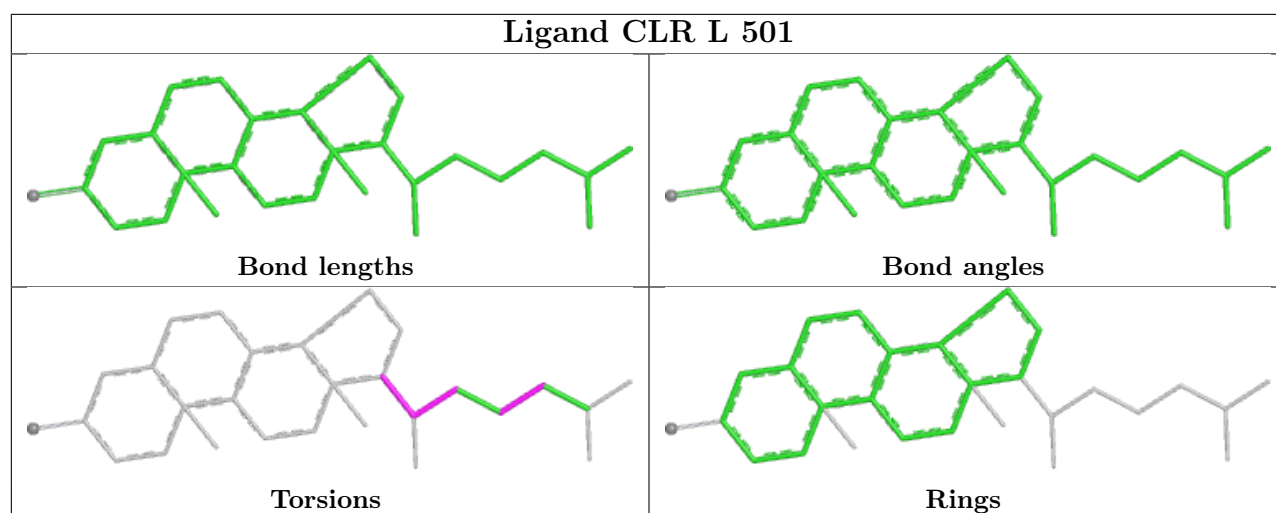
8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1001	CLR	9	0
9	L	502	CLR	3	0
9	Z	1001	CLR	4	0
12	V	1004	PIO	3	0
9	L	501	CLR	1	0
12	Y	1004	PIO	3	0
10	Q	501	AJP	1	0
9	Y	1001	CLR	1	0

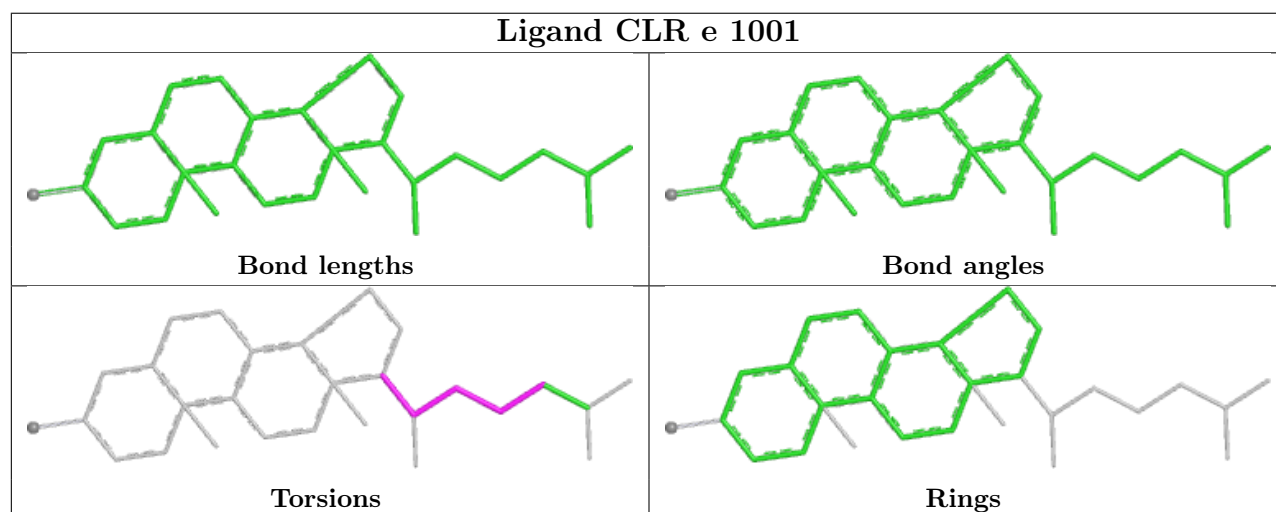
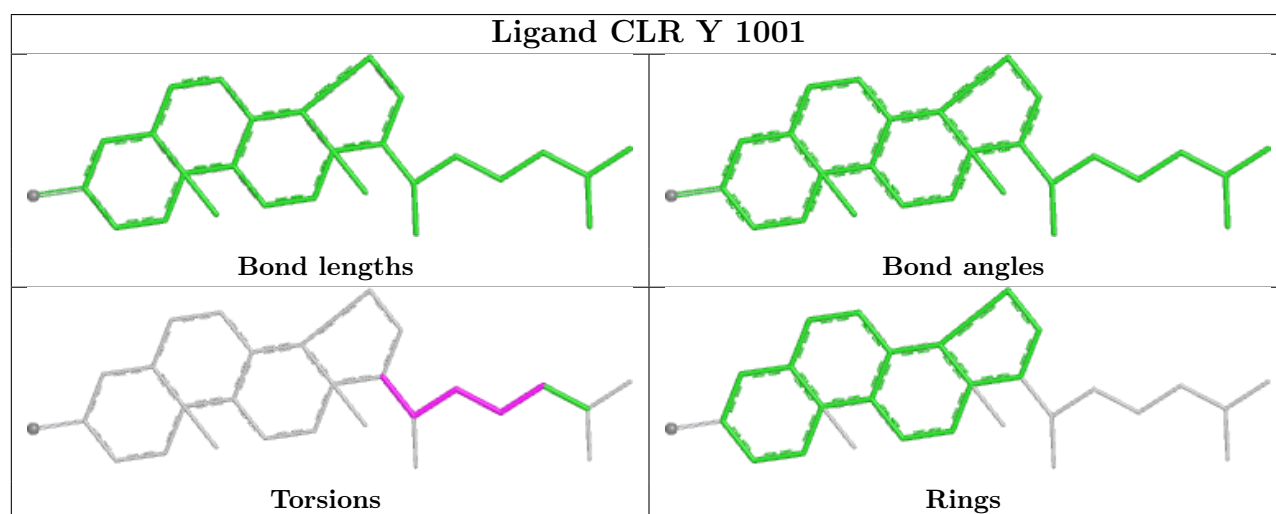
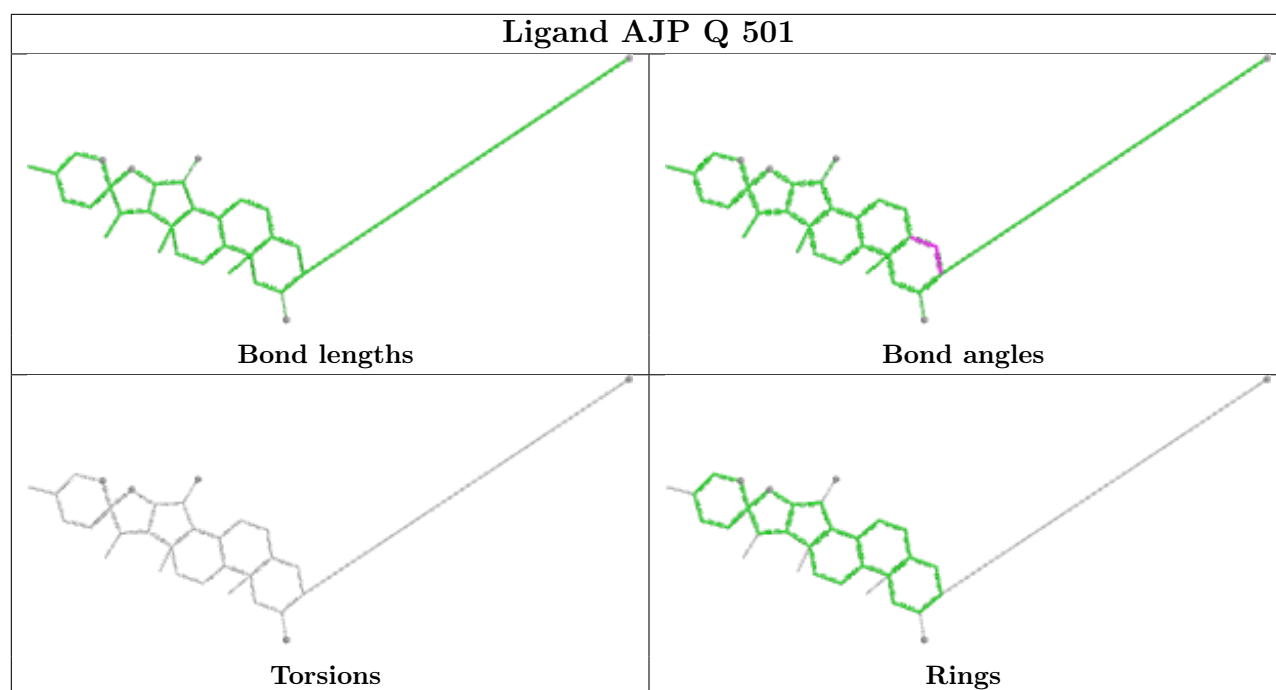
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

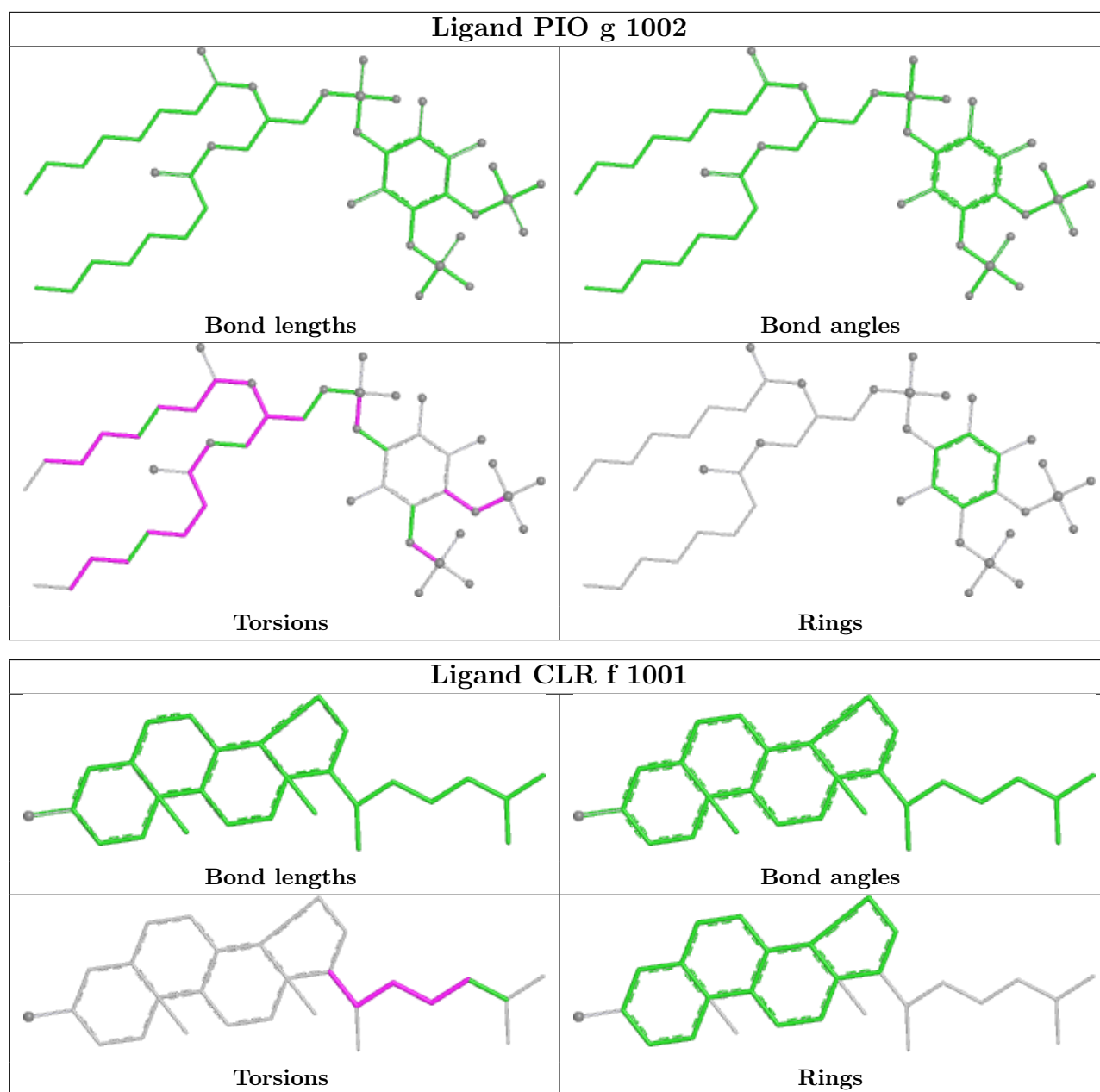


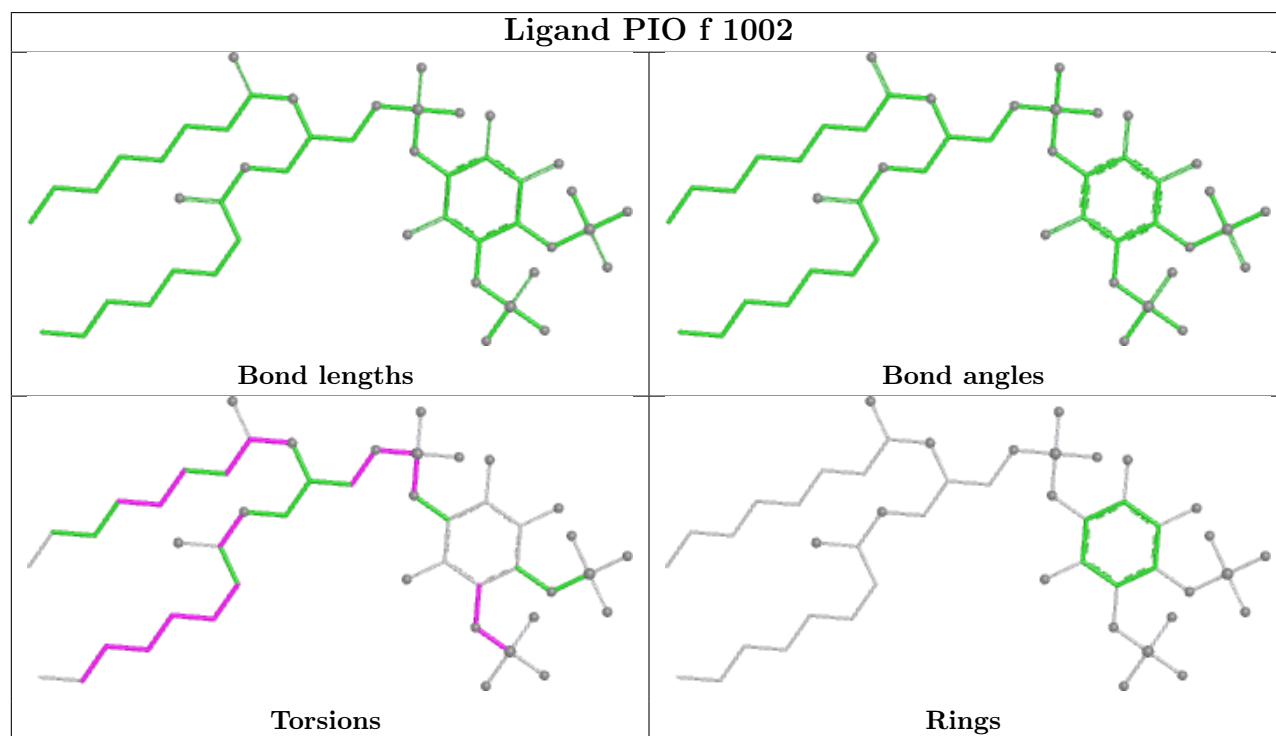
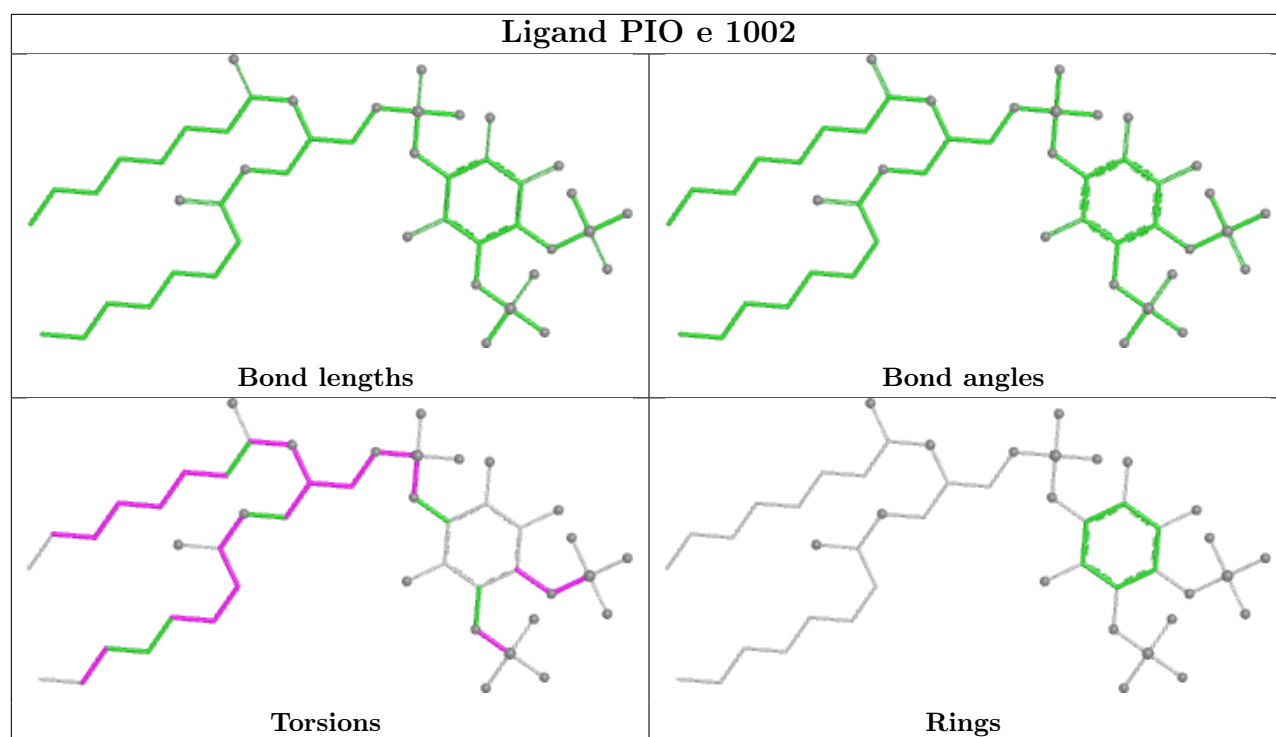


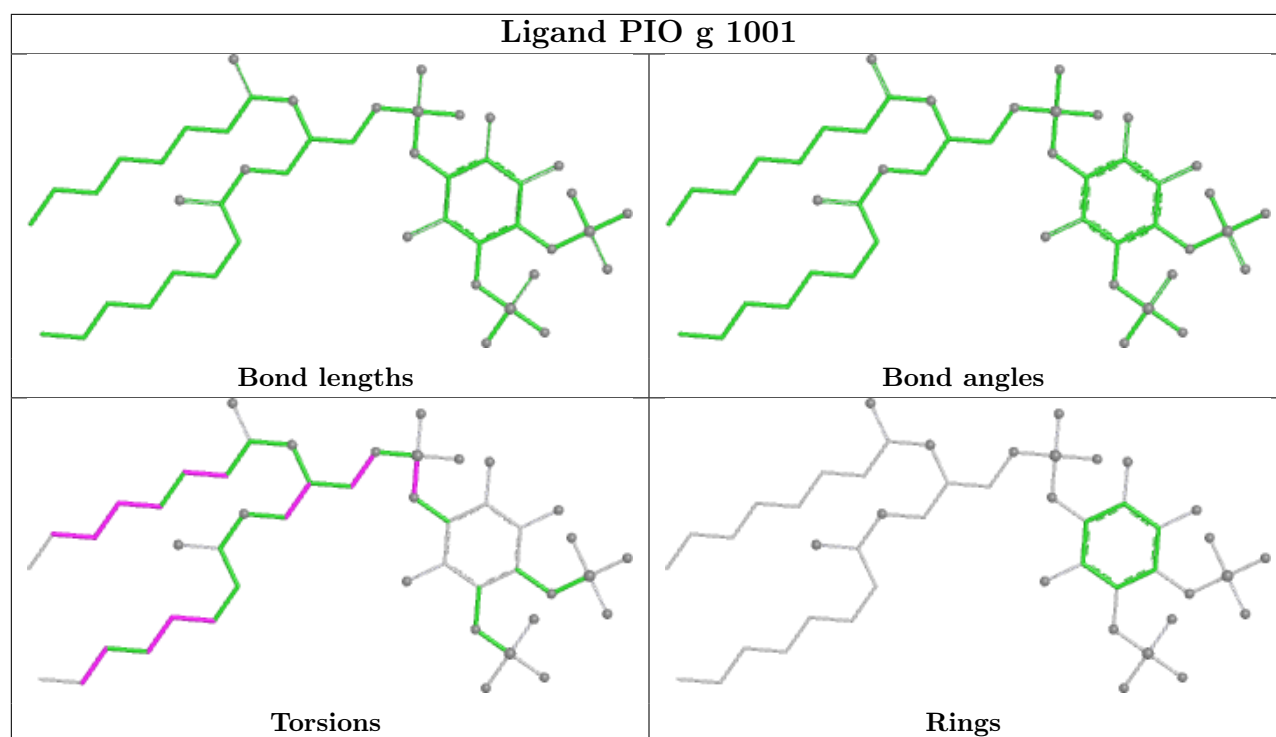












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

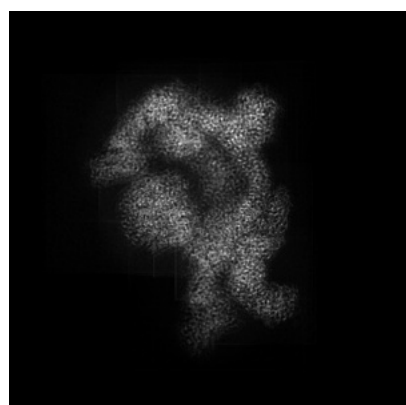
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26960. These allow visual inspection of the internal detail of the map and identification of artifacts.

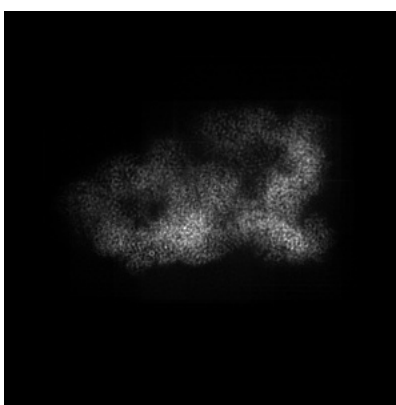
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

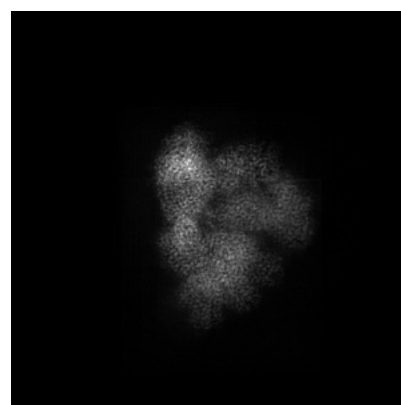
#### 6.1.1 Primary map



X



Y

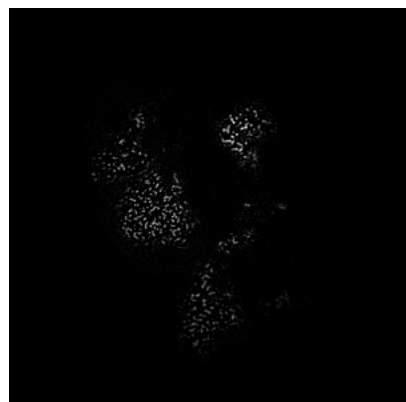


Z

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

### 6.2 Central slices [i](#)

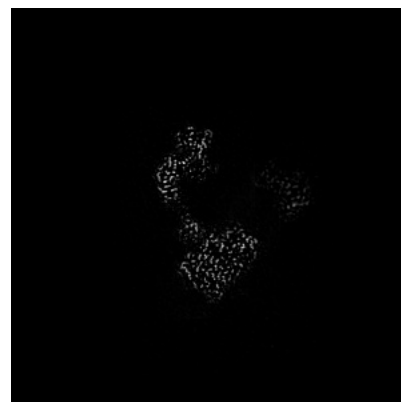
#### 6.2.1 Primary map



X Index: 225



Y Index: 225



Z Index: 225

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: 199



Y Index: 272

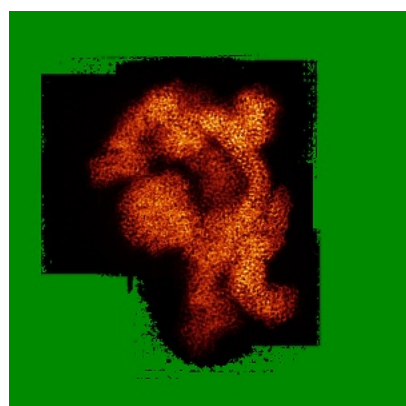


Z Index: 324

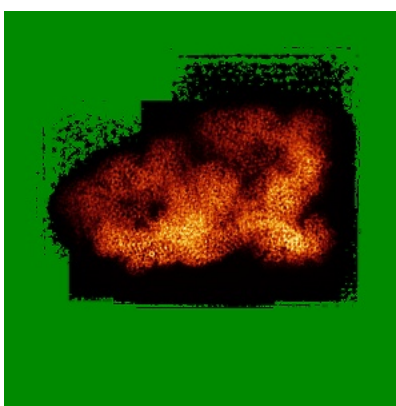
The images above show the largest variance slices of the map in three orthogonal directions.

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

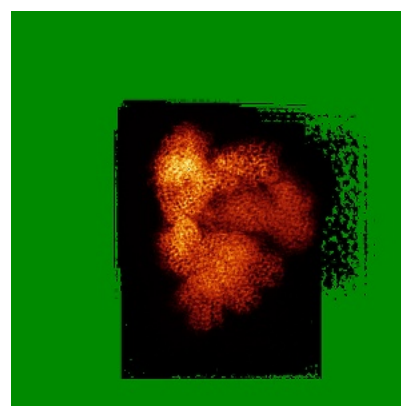
### 6.4.1 Primary map



X



Y

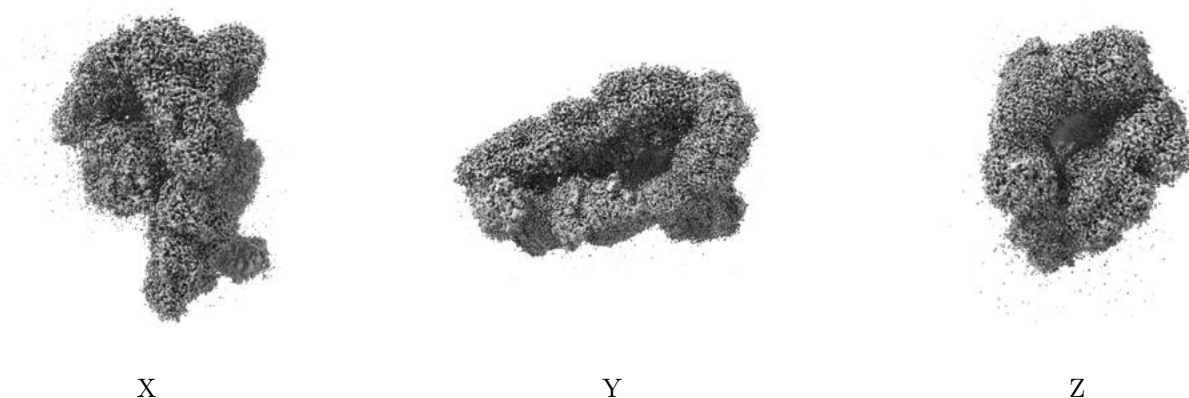


Z

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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

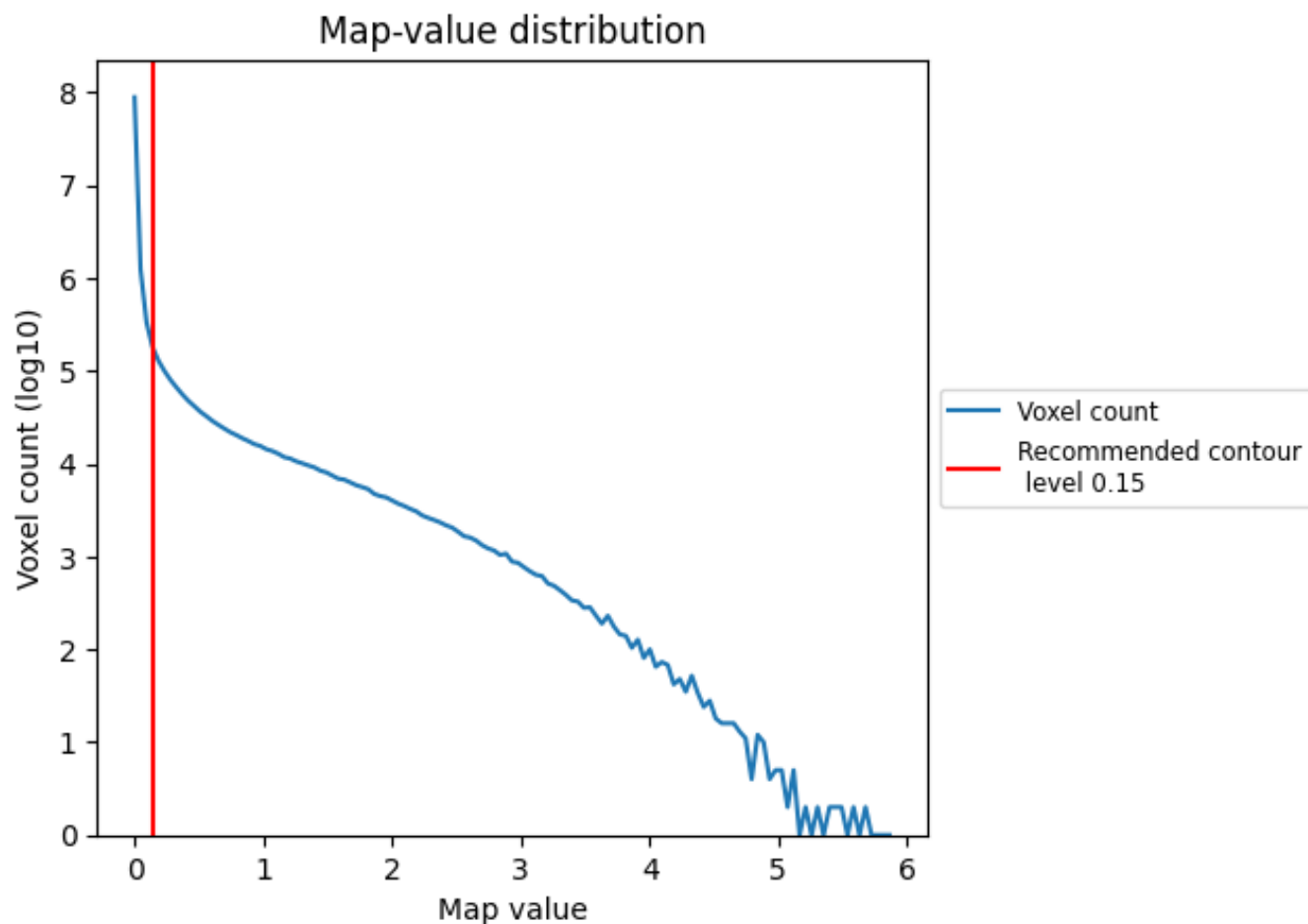
## 6.6 Mask visualisation [i](#)

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.

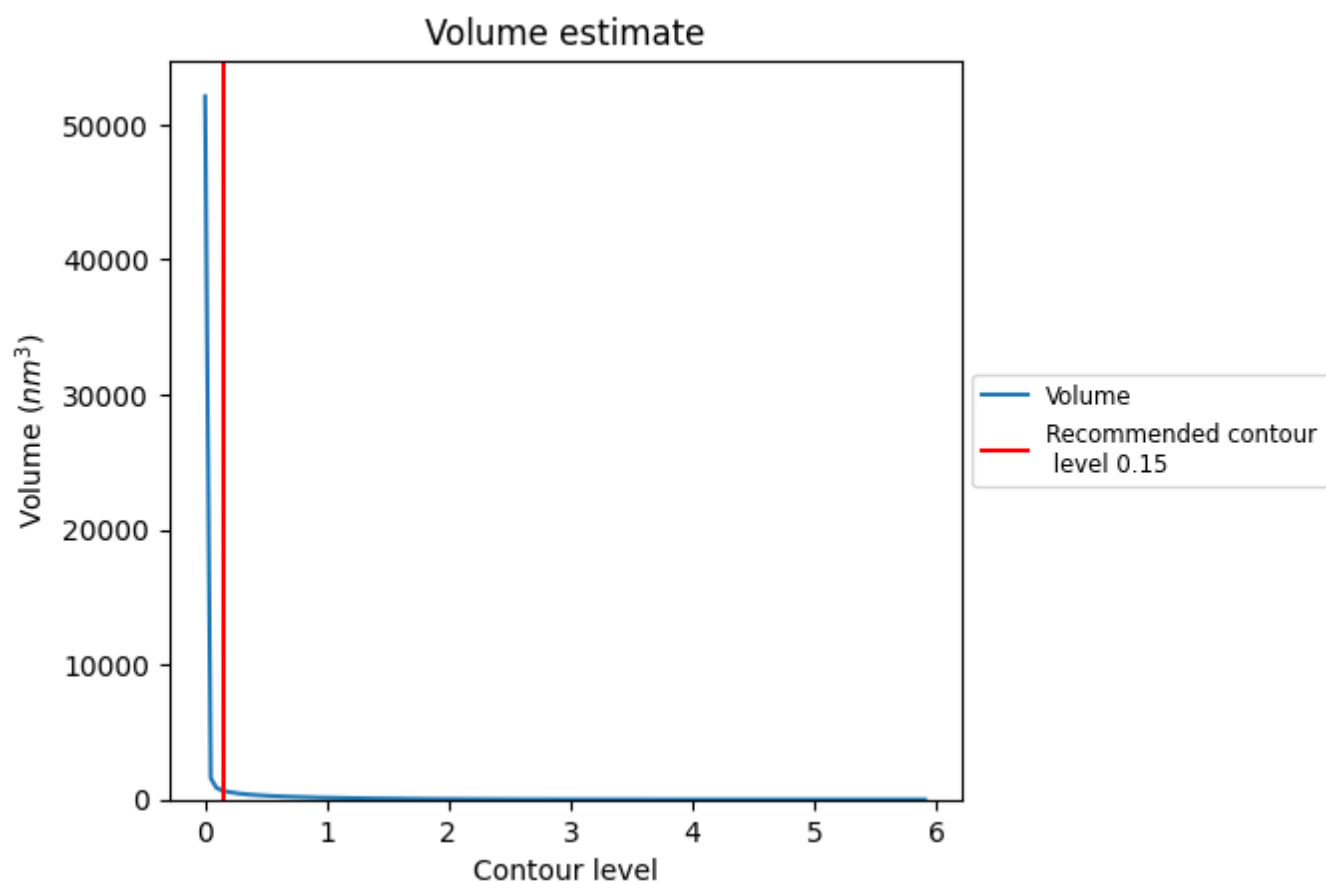
### 7.1 Map-value distribution [i](#)



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.



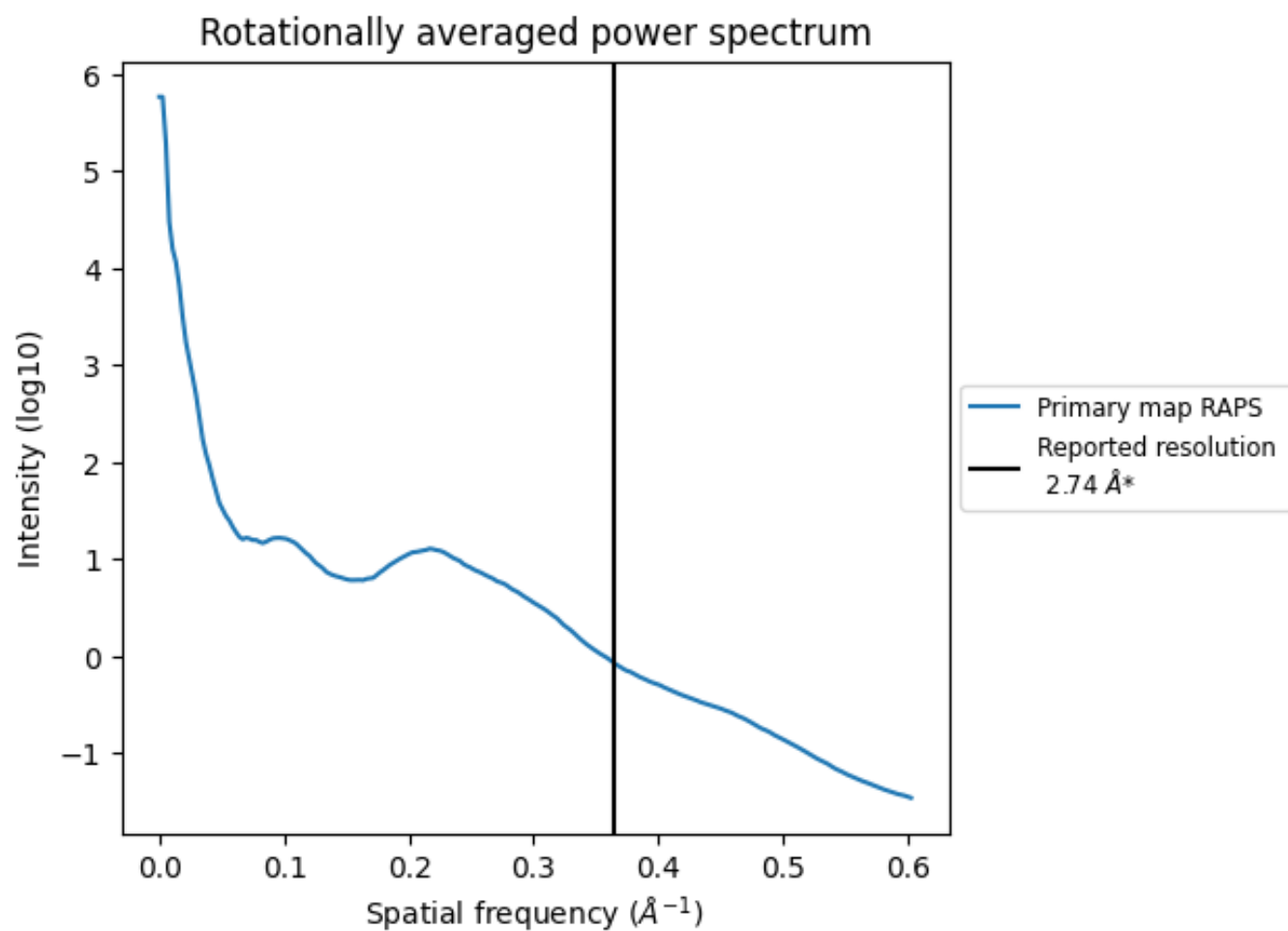
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 656  $\text{nm}^3$ ; this corresponds to an approximate mass of 592 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 ⓘ

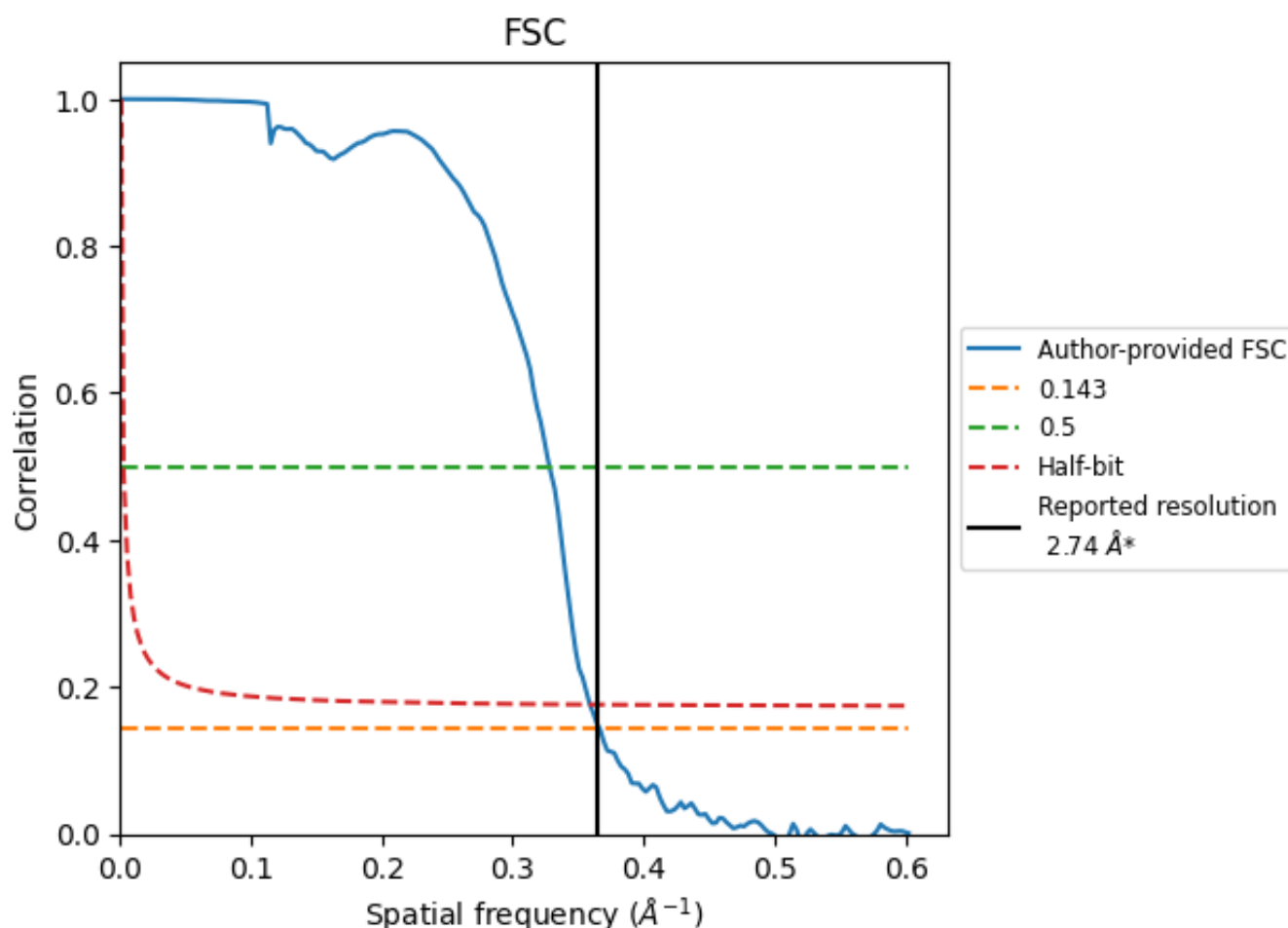


\*Reported resolution corresponds to spatial frequency of  $0.365 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.365 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

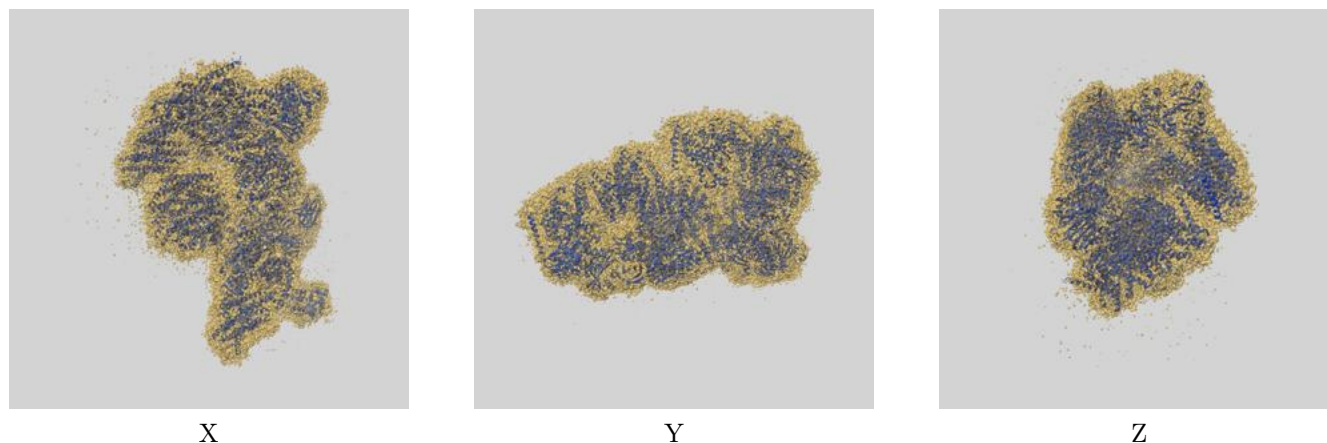
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.05	2.79
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26960 and PDB model 8CS9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

### 9.1 Map-model overlay [i](#)



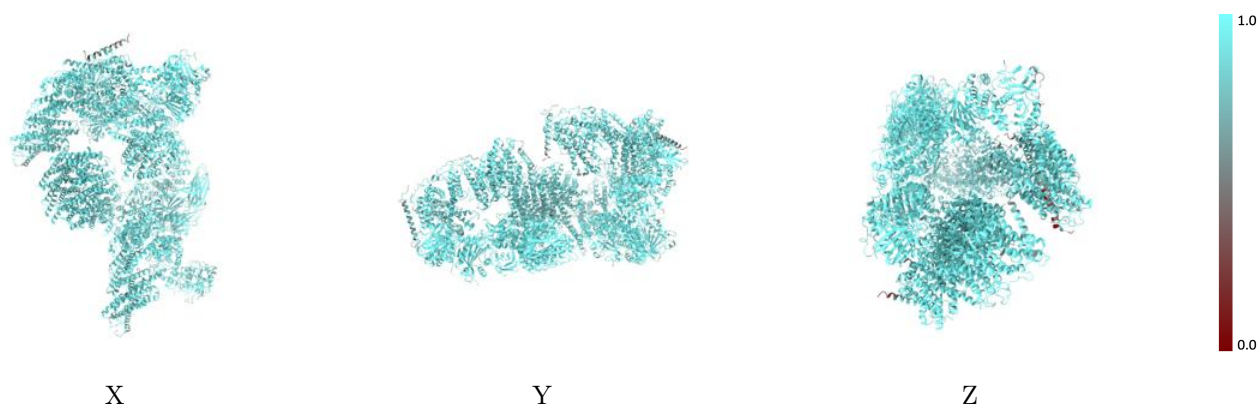
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



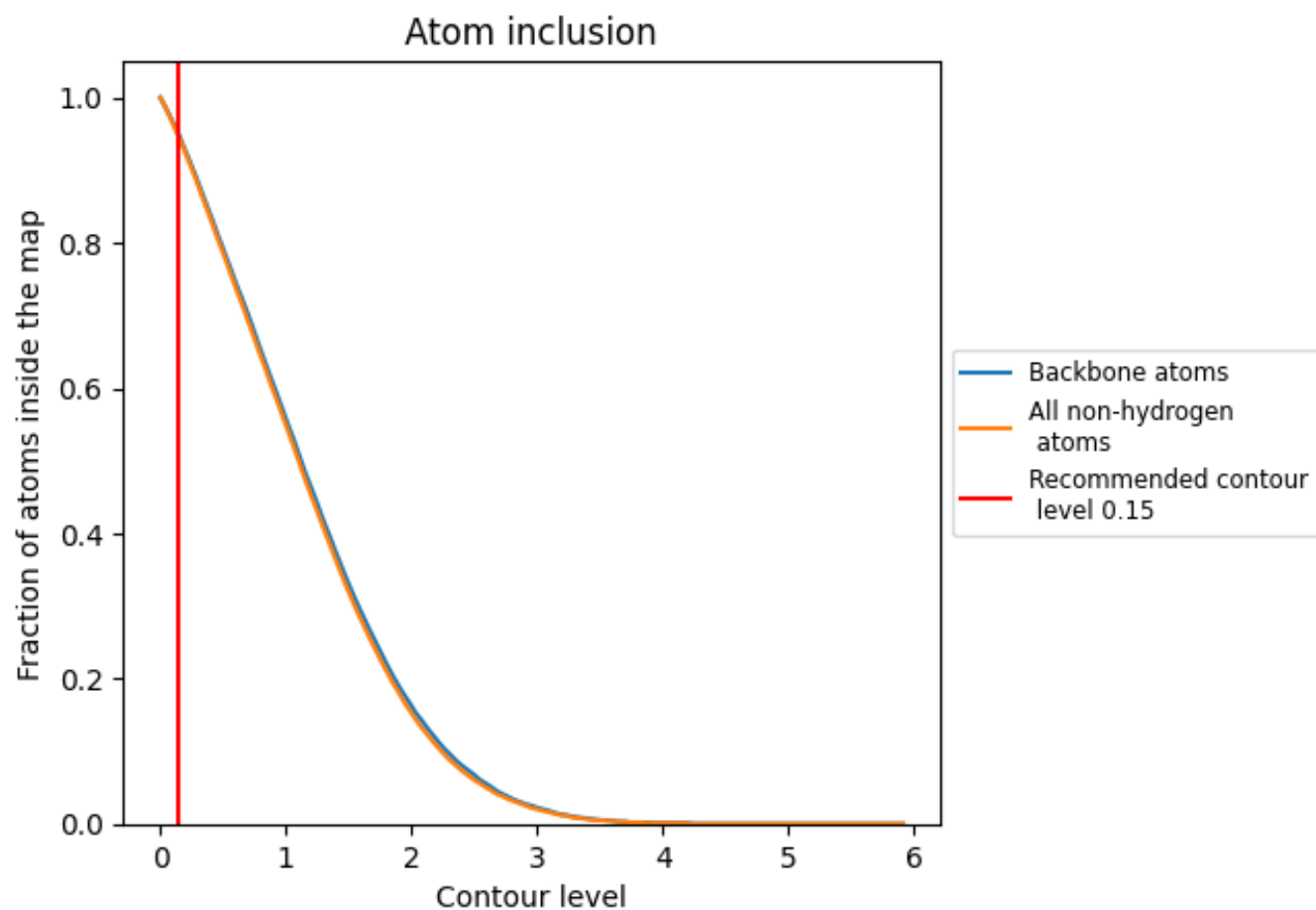
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.5880
A	 0.9930	 0.6630
B	 0.5360	 0.3070
C	 0.6790	 0.3330
D	 0.6790	 0.2980
K	 0.9820	 0.6590
L	 0.9960	 0.7190
P	 0.7650	 0.4020
Q	 0.9950	 0.7160
R	 0.7830	 0.3860
S	 0.4640	 0.2070
T	 0.6810	 0.3260
V	 0.9480	 0.5680
X	 0.9830	 0.7050
Y	 0.9230	 0.5200
Z	 0.9570	 0.5640
a	 0.6420	 0.2870
b	 0.6480	 0.2950
c	 0.8200	 0.4250
e	 0.9090	 0.5260
f	 0.9210	 0.5290
g	 0.9630	 0.5830

