



## wwPDB EM Validation Summary Report ⓘ

Nov 28, 2023 – 06:22 PM JST

PDB ID : 8WE9  
EMDB ID : EMD-37475  
Title : Human L-type voltage-gated calcium channel Cav1.2 (Class I) in the presence of pinaverium at 3.0 Angstrom resolution  
Authors : Gao, S.; Yao, X.; Fan, X.; Yan, N.  
Deposited on : 2023-09-17  
Resolution : 3.00 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.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

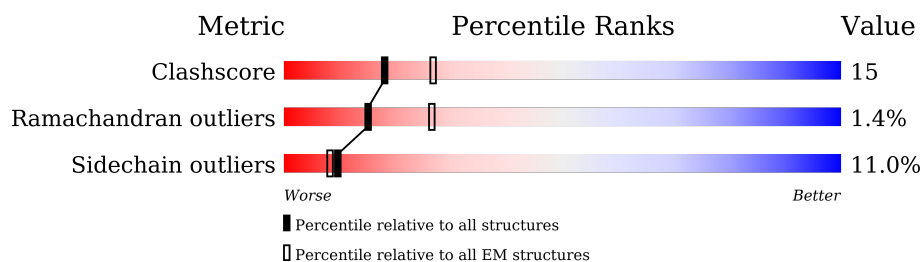
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2201	<p>7% 39% 15% • 43%</p>
2	D	1103	<p>61% 23% • 14%</p>
3	C	484	<p>62% 37% 25% 5% 33%</p>
4	B	3	<p>33% 67% 33%</p>
5	E	2	<p>50% 100%</p>
5	G	2	<p>50% 100%</p>
5	H	2	<p>100%</p>
6	F	4	<p>25% 25% 50%</p>

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20730 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 Voltage-dependent L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1260	Total	C	N	O	S	0	0
			10172	6686	1659	1764	63		

- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	948	Total	C	N	O	S	0	0
			7570	4803	1269	1467	31		

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2575	1619	467	479	10		

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



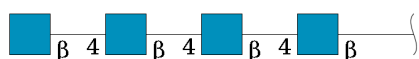
Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 5 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
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

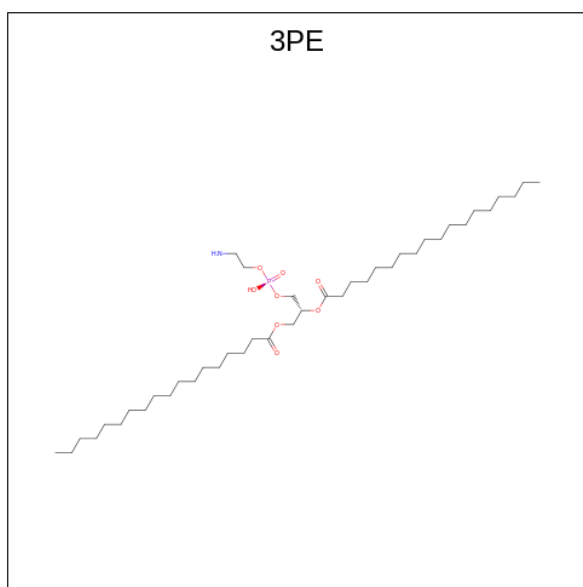


Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

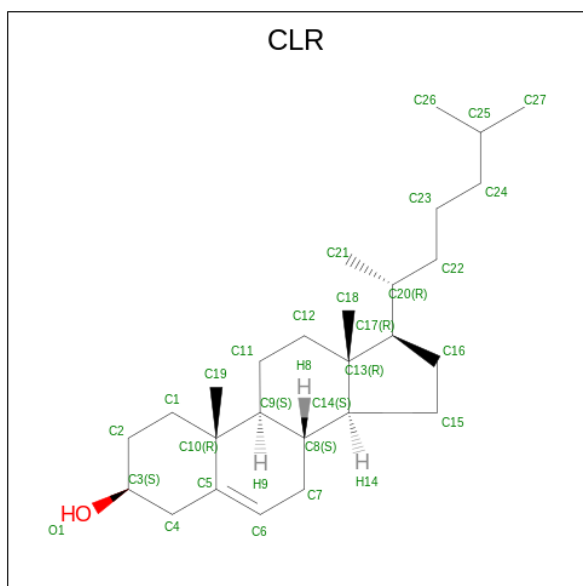
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	
7	D	1	Total	Ca	0
			1	1	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



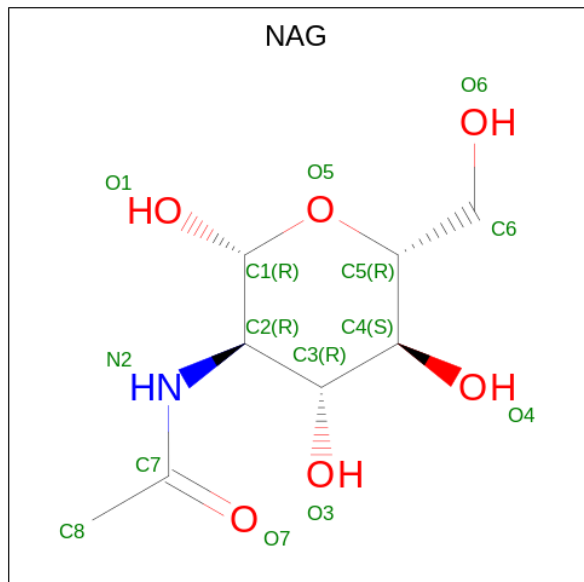
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			40	30	1	8	1	

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



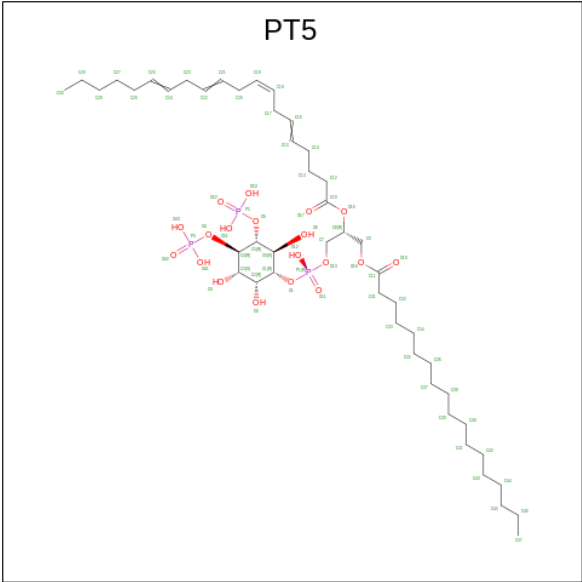
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	

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



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 11 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula:  $C_{47}H_{85}O_{19}P_3$ ).

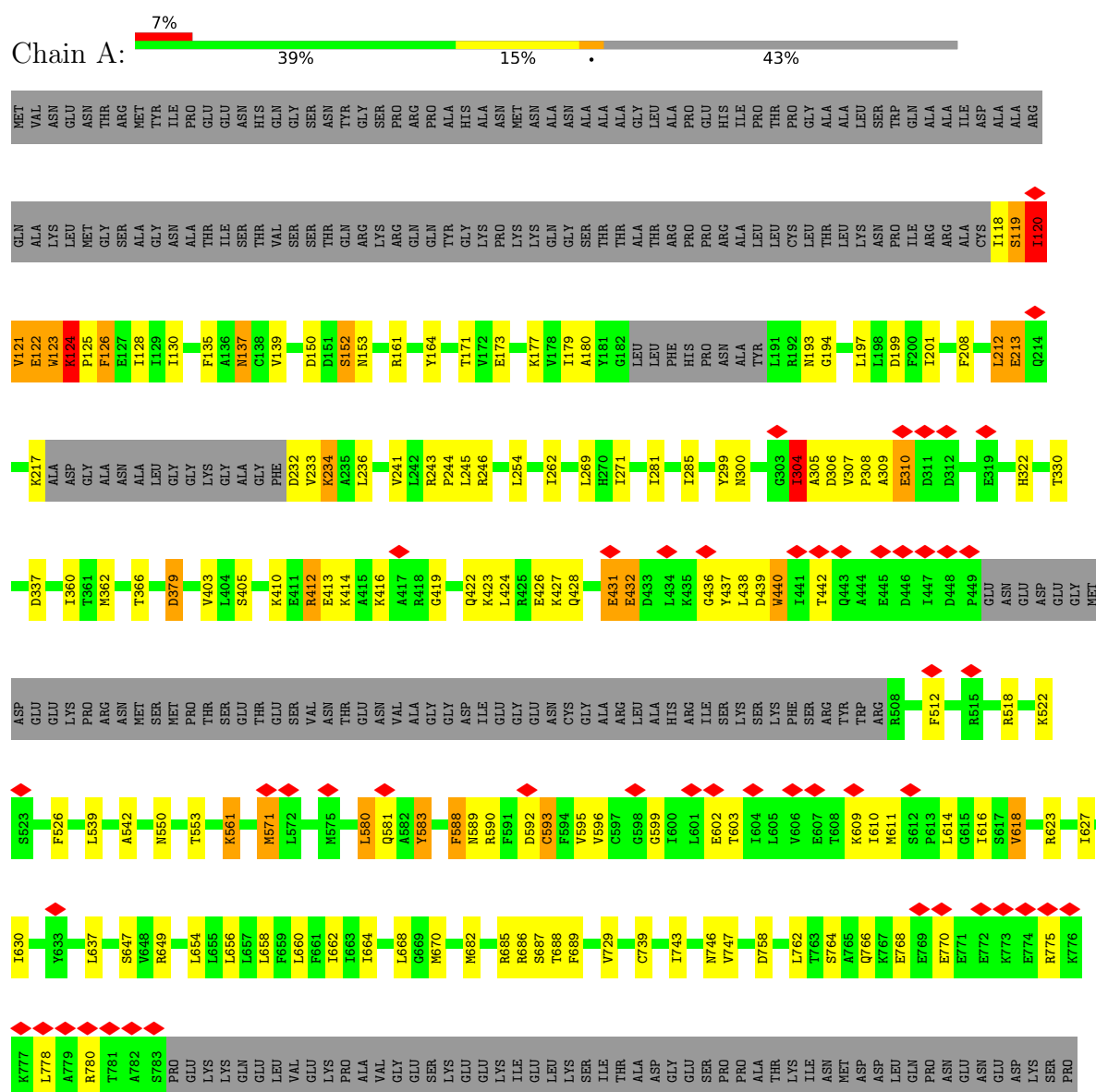


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	A	1	63	41	19	3	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1C







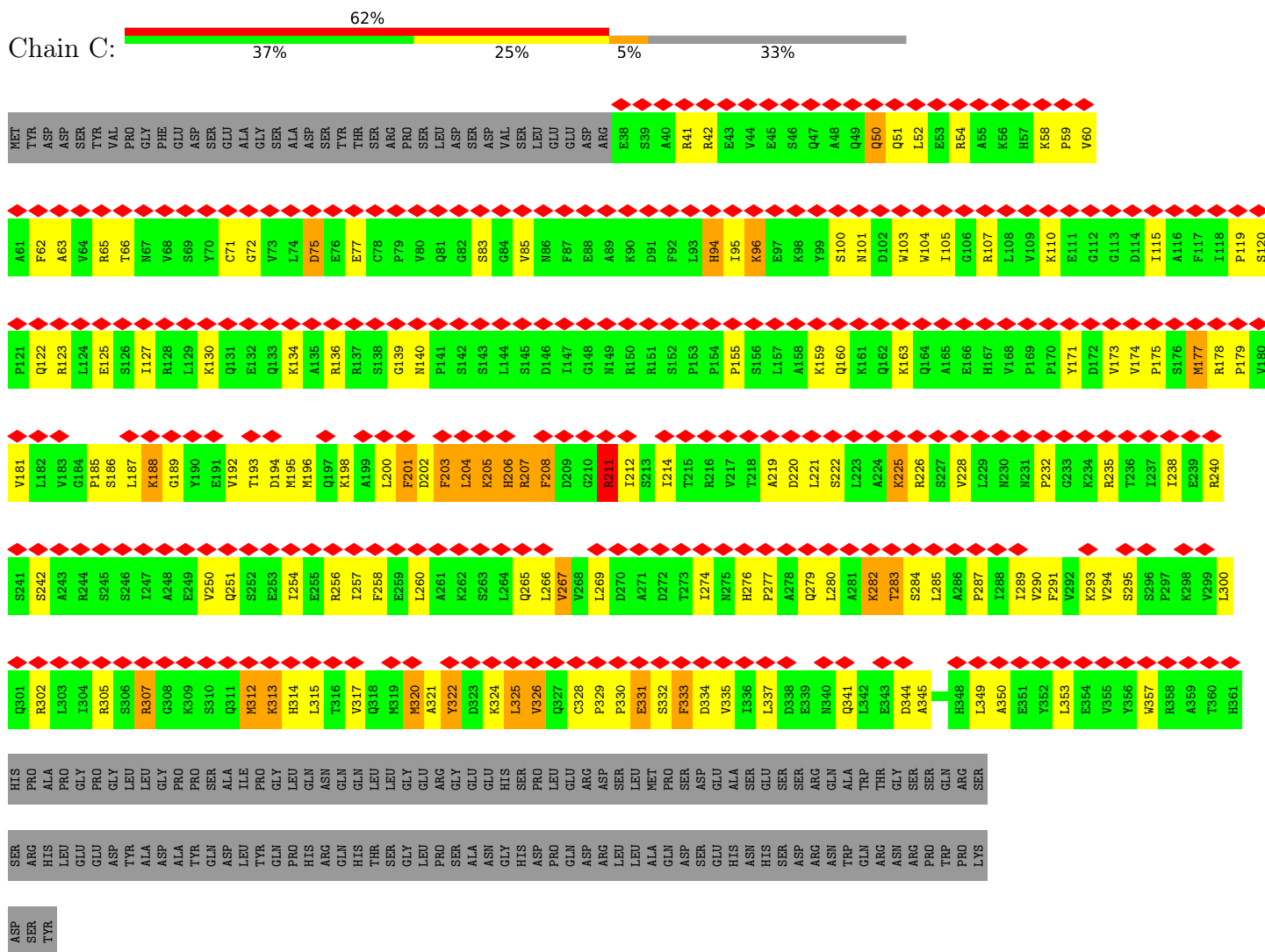
SER	LEU	MET	ALA	VAL	ASP	PRO	CYS	ASN	ILE	LEU	GLY	ALA	GLY	PRO	GLY	ALA	GLY	ARG	GLN	PHE	HIS	GLY	SER	GLY	ALA	ALA	SER	SER	LEU	PRO	VAL	GLU	ASN	CYS	ARG	LEU	ILE	ASP	ASP	GLY	GLN	ALA	GLY	PHE	GLY	ALA	GLY	ASP	PRO	LYS	ILE	VAL	ARG	VAL	THR	THR	GLN	GLY	ARG	PRO	LEU	ALA	ASP	GLY	ALA	CYS	ASP	LEU	GLN	MET	THR	ILE	GLY	ARG	VAL	TYR
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• Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1

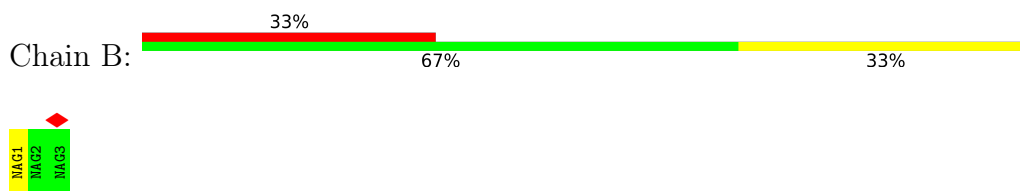
Chain D:  61% 23% 14%

S1020	K1021	G1022	T1023	C1024	P1025	C1026	D1027	T1028	L1029	L1030	T1037	S1038	D1039	R1053	D1057	D1061	M1062	E1066	D1067	Y1068	T1069	S1075	G1076	LEU	ASN	PRO	SER	LEU	TRP	TYR	ILE	ILE	GLY	ILE	GLN	PHE	LEU	LEU	LEU	LEU	TRP	LEU	VAL	LEU	GLY	SER	HIS	ARG	LEU	LEU				
E789	S790	S795	K796	E799	I800	L802	Q803	G804	K805	L806	L807	K808	V812	N819	I822	K827	THR	SER	ILE	ARG	ASP	PRO	ALA	GLY	CYS	PRO	VAL	ALA	CYS	VAL	PRO	SER	VAL	R843	N844	S845	D846	V847	M848	D849	C850	V851	D854	L859	L860	M861	A862	N863	T868	G872				
R873	F874	F875	K876	E877	P880	M883	S890	V891	Y892	S897	W898	D899	V903	C904	E905	A908	A909	PRO	LYS	GLN	GLY	ALA	GLY	CYS	ALA	HIS	ARG	SER	ALA	TYR	VAL	PRO	SER	VAL	ALA	ASP	ILE	LEU	GLN	ILE	GLY	TRP	ALA	THR	ALA	ALA	ALA	ALA	TRP	SER	ILE	LEU	GLN	PHE
LEU	LEU	SER	THR	PHE	PRO	ARG	LEU	LEU	GLU	ALA	VAL	GLU	MET	ASP	ASP	ASP	ASP	PRO	LYS	GLN	GLY	ASP	GLY	GLY	ALA	HIS	ARG	SER	ALA	TYR	VAL	PRO	SER	VAL	ALA	ASP	ILE	LEU	GLN	ILE	GLY	TRP	ALA	THR	ALA	ALA	ALA	ALA	TRP	SER	ILE	LEU	GLN	PHE
E769	S790	S795	K796	E799	I800	L802	Q803	G804	K805	L806	L807	K808	V812	N819	I822	K827	THR	SER	ILE	ARG	ASP	PRO	ALA	GLY	CYS	ALA	HIS	ARG	SER	ALA	TYR	VAL	PRO	SER	VAL	R843	N844	S845	D846	V847	M848	D849	C850	V851	D854	L859	L860	M861	A862	N863	T868	G872		
K690	T691	P692	M693	M694	S696	C697	I702	M703	R704	D708	E714	M717	Y719	W720	S721	K722	Q723	K724	K730	F733	W734	V735	I740	T741	R742	Y743	Y744	F745	K746	E747	E750	Q753	K765	L768	D769	N770	F780	M781	S783	G784	P785	Y788												
Q595	D601	R605	T608	M609	T610	T615	S618	P624	T625	Y626	S627	F628	Y629	Y630	I631	K634	L635	H524	E636	E637	T638	L639	T640	Q641	S645	K649	E654	F660	I661	A662	P663	Y666	C667	L670	K671	N675	M676	T677	N684	E685	F686	I687	D688	R689										
M478	L479	K480	M481	Q482	L485	M488	S493	T497	L500	T501	C507	P508	N509	P517	L522	L523	H524	P525	K530	P531	I532	T538	L539	N540	ARG	LYS	ARG	ARG	PRO	ASN	ILE	GLN	ASN	PRO	LYS	S553	L566	K577	M578	L579	E585	K586	T587	T590										
N311	K316	K319	N323	Y333	K334	G335	G336	F337	L357	L360	F361	T362	D363	G364	G365	E366	E371	D379	R383	N393	M406	K407	G408	T416	R420	R432	P433	D439	L456	V459	T460	T461	G462	T470	G471	E474	M475	K476	T477															
E182	V185	T186	S187	A188	L189	D190	F193	K194	E198	E199	L203	L204	W205	S210	Y218	P219	A220	S221	P222	W223	V224	ASP	ASN	SER	ARG	LEU	ASP	PRO	GLY	LYS	ASN	ASP	SER	E139	S142	Q143	R144	L147	T50	V54	D59	I60	Y61	E62	K63	Y64	Q65	D66	L67	Y68	S176			
P72	N74	A75	R76	Q77	L78	V79	K88	L89	L90	S91	S94	L100	A104	E105	K106	A109	D116	F117	K128	D129	D130	LEU	ASP	PRO	GLY	LYS	ASN	ASP	SER	E139	S142	Q143	R144	L147	T50	V54	D59	I60	Y61	E62	K63	Y64	Q65	D66	L67	Y68	S176							
MET	ALA	ALA	GLY	CYS	LEU	LEU	ALA	THR	THR	THR	LEU	PHE	GLN	SER	SER	LEU	LEU	LEU	LEU	LEU	LEU	PRO	F27	P28	S29	A30	V31	T32	T33	V37	D38	K39	R40	Q41	E42	D43	L44	L47	T50	V54	D59	I60	Y61	E62	K63	Y64	Q65	D66	L67	Y68				

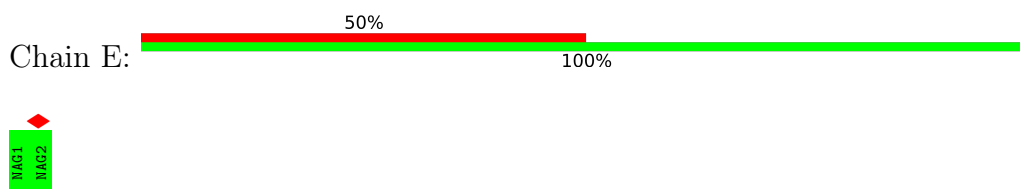
• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3



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



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



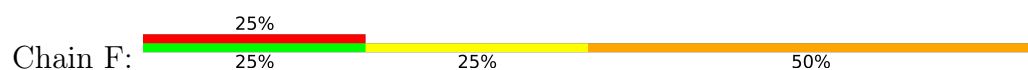
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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, Not provided	
Number of particles used	217938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.006	Depositor
Minimum map value	-1.886	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.35	Depositor
Map size ( $\text{\AA}$ )	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.114, 1.114, 1.114	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: 3PE, CA, PT5, NAG, CLR

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	0.34	0/10402	0.53	0/14093
2	D	0.32	0/7728	0.50	0/10477
3	C	0.28	0/2624	0.55	0/3544
All	All	0.32	0/20754	0.52	0/28114

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	10172	0	10395	329	0
2	D	7570	0	7369	171	0
3	C	2575	0	2619	118	0
4	B	42	0	37	0	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
6	F	56	0	49	3	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	40	0	54	1	0
9	A	84	0	138	5	0
10	A	14	0	13	0	0
10	D	28	0	26	0	0
11	A	63	0	66	2	0
All	All	20730	0	20841	617	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 15.

The worst 5 of 617 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)
3:C:203:PHE:CZ	3:C:350:ALA:HB2	1.61	1.32
1:A:1560:ILE:HG12	1:A:1603:THR:HA	1.33	1.11
3:C:203:PHE:HZ	3:C:350:ALA:HB2	0.96	1.06
3:C:203:PHE:HZ	3:C:350:ALA:CB	1.67	1.06
2:D:780:PHE:HB2	2:D:873:ARG:HG2	1.43	1.00

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	1244/2201 (56%)	1117 (90%)	103 (8%)	24 (2%)	8	36
2	D	936/1103 (85%)	857 (92%)	74 (8%)	5 (0%)	29	68
3	C	322/484 (66%)	263 (82%)	52 (16%)	7 (2%)	6	31
All	All	2502/3788 (66%)	2237 (89%)	229 (9%)	36 (1%)	15	43

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ILE
1	A	123	TRP
1	A	1007	GLN
1	A	1011	ILE
1	A	1013	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1117/1896 (59%)	977 (88%)	140 (12%)	4	20
2	D	837/971 (86%)	765 (91%)	72 (9%)	10	37
3	C	287/426 (67%)	252 (88%)	35 (12%)	5	21
All	All	2241/3293 (68%)	1994 (89%)	247 (11%)	10	25

5 of 247 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1565	VAL
3	C	110	LYS
2	D	44	LEU
3	C	96	LYS
3	C	282	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	50	GLN
3	C	206	HIS
3	C	276	HIS
3	C	265	GLN
2	D	717	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 ⓘ

13 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$
4	NAG	B	1	4,2	14,14,15	0.87	1 (7%)	17,19,21	1.37	1 (5%)
4	NAG	B	2	4	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	3	4	14,14,15	0.33	0	17,19,21	0.39	0
5	NAG	E	1	2,5	14,14,15	0.28	0	17,19,21	0.53	0
5	NAG	E	2	5	14,14,15	0.40	0	17,19,21	0.35	0
6	NAG	F	1	6,2	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	F	2	6	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	F	3	6	14,14,15	0.98	1 (7%)	17,19,21	1.64	2 (11%)
6	NAG	F	4	6	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
5	NAG	G	1	2,5	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.43	0
5	NAG	H	1	2,5	14,14,15	0.46	0	17,19,21	0.36	0
5	NAG	H	2	5	14,14,15	0.25	0	17,19,21	0.44	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
4	NAG	B	1	4,2	-	1/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	NAG	B	3	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	F	3	6	-	5/6/23/26	0/1/1/1
6	NAG	F	4	6	-	5/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	NAG	O5-C1	3.20	1.48	1.43
4	B	1	NAG	O5-C1	3.16	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C1-O5-C5	5.41	119.53	112.19
6	F	3	NAG	C1-O5-C5	4.42	118.18	112.19
6	F	3	NAG	C2-N2-C7	4.35	129.09	122.90
6	F	4	NAG	C2-N2-C7	4.32	129.05	122.90

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

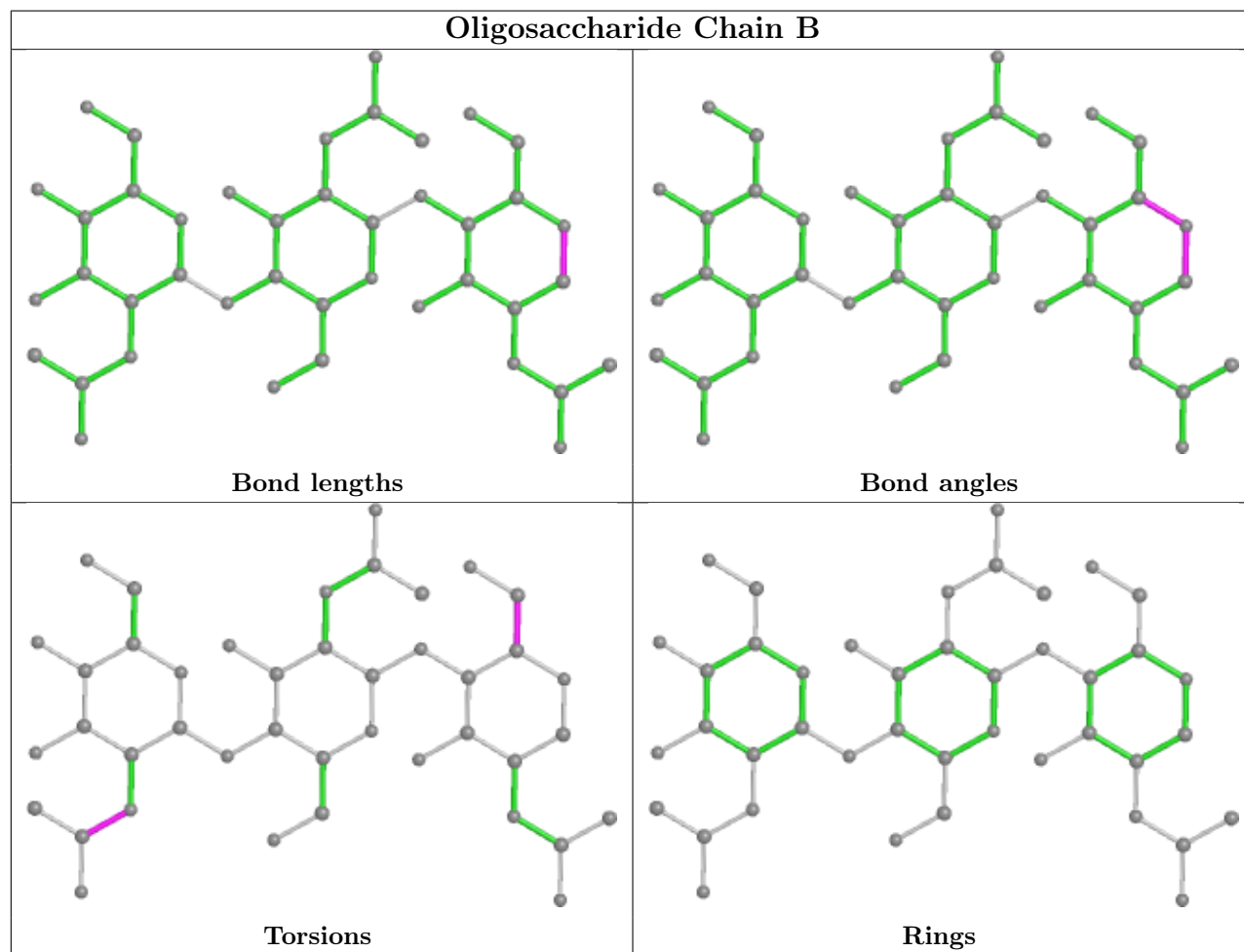
Mol	Chain	Res	Type	Atoms
6	F	3	NAG	C4-C5-C6-O6
6	F	3	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6

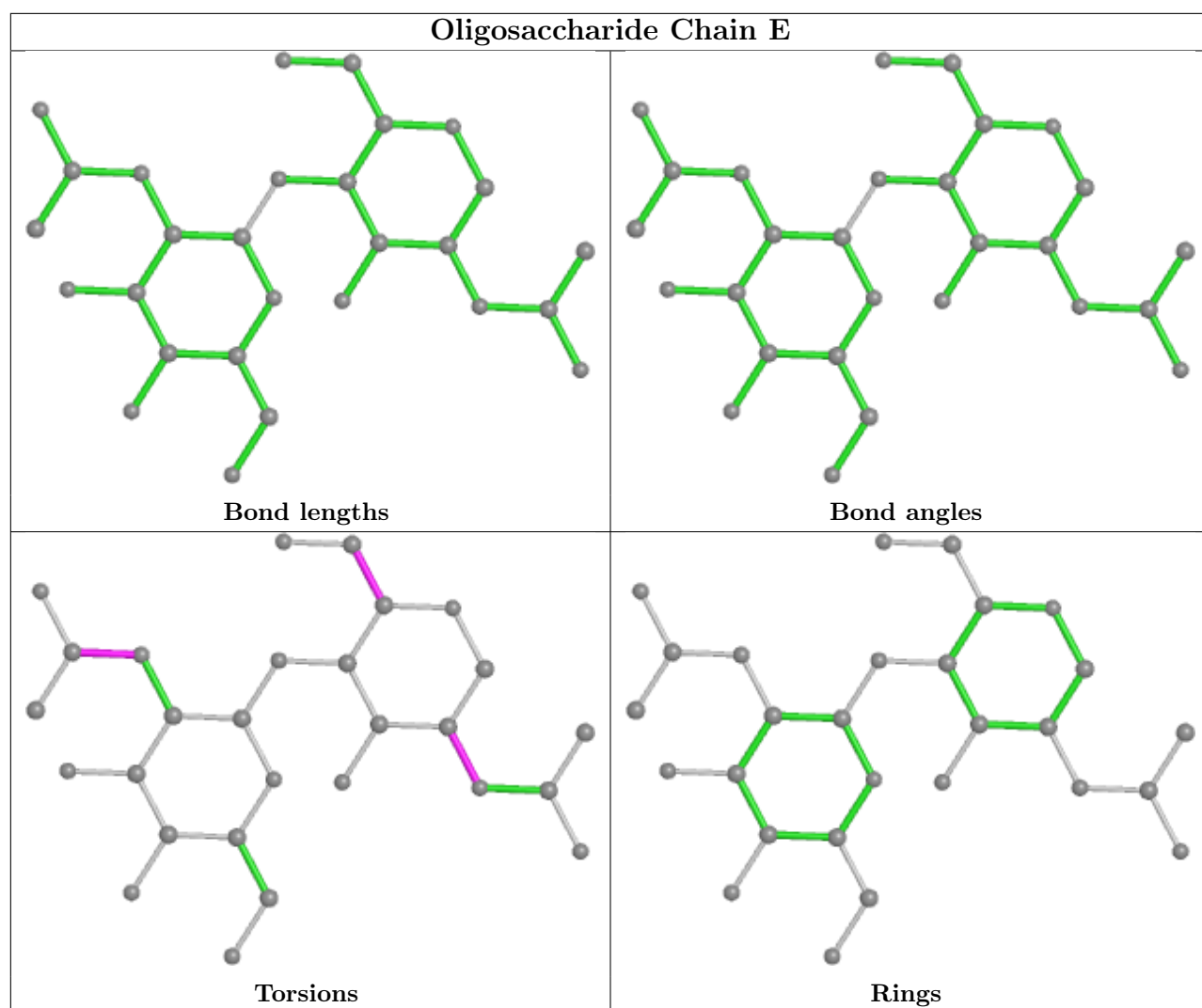
There are no ring outliers.

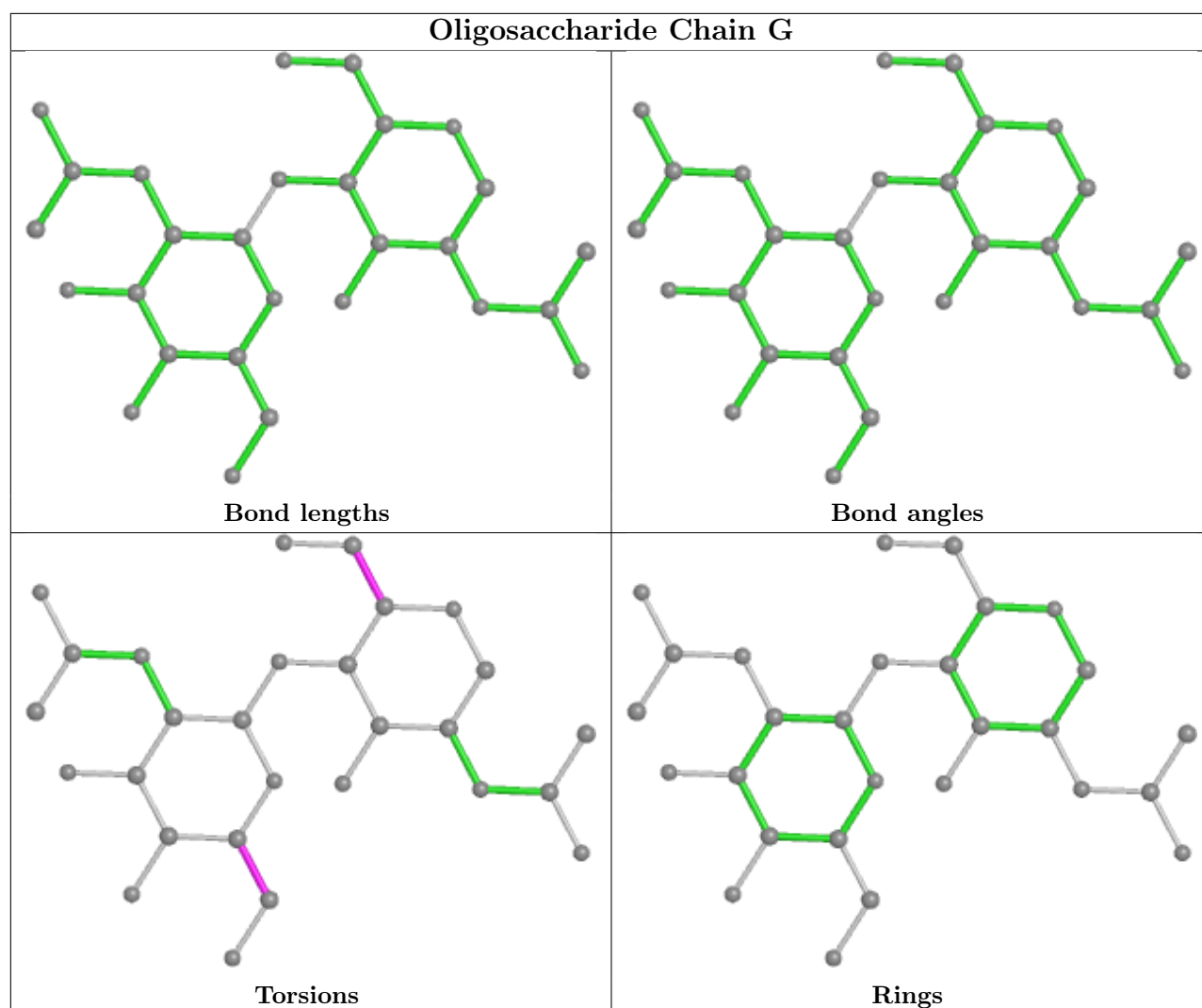
3 monomers are involved in 3 short contacts:

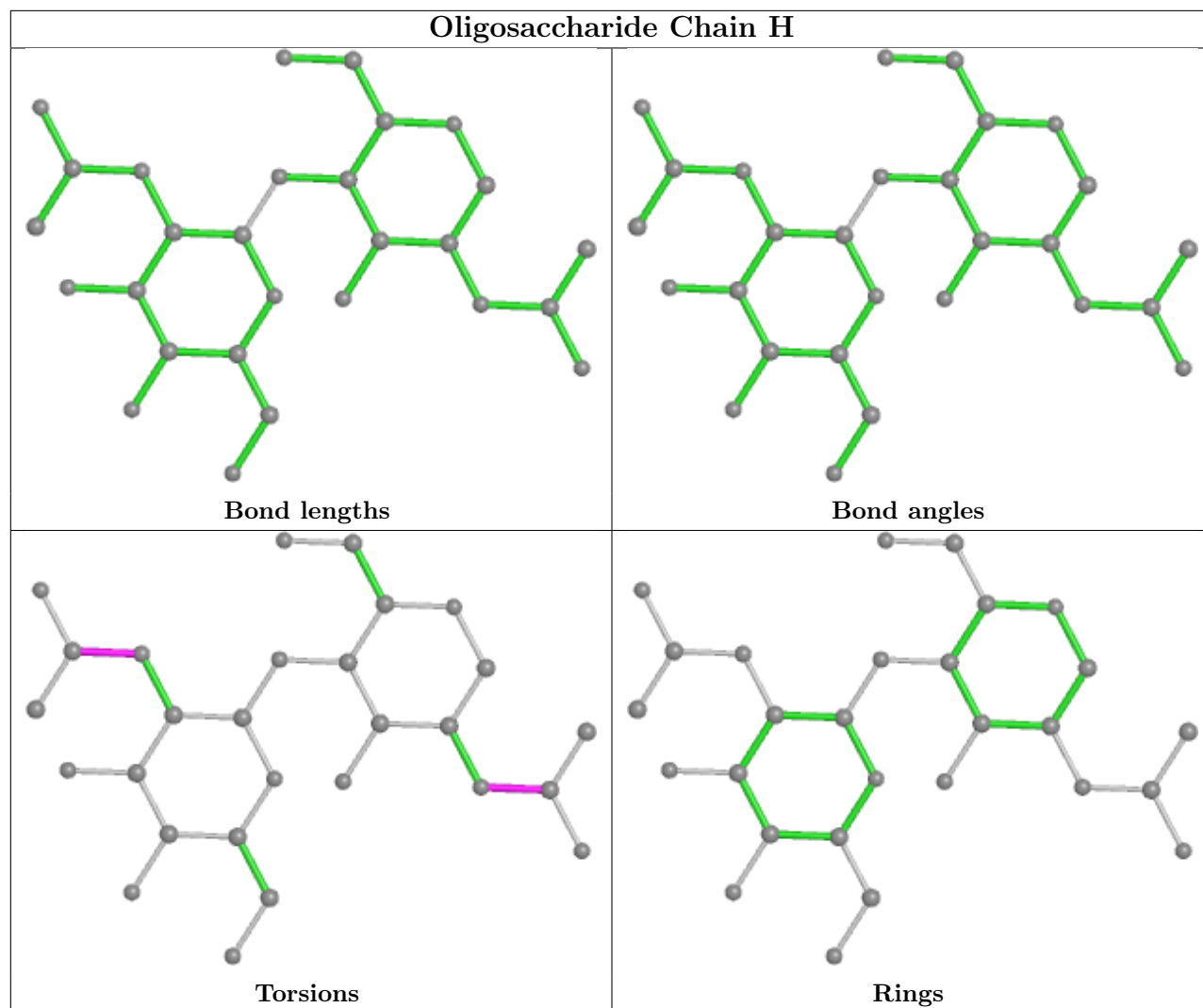
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	4	NAG	1	0
6	F	1	NAG	1	0
6	F	3	NAG	1	0

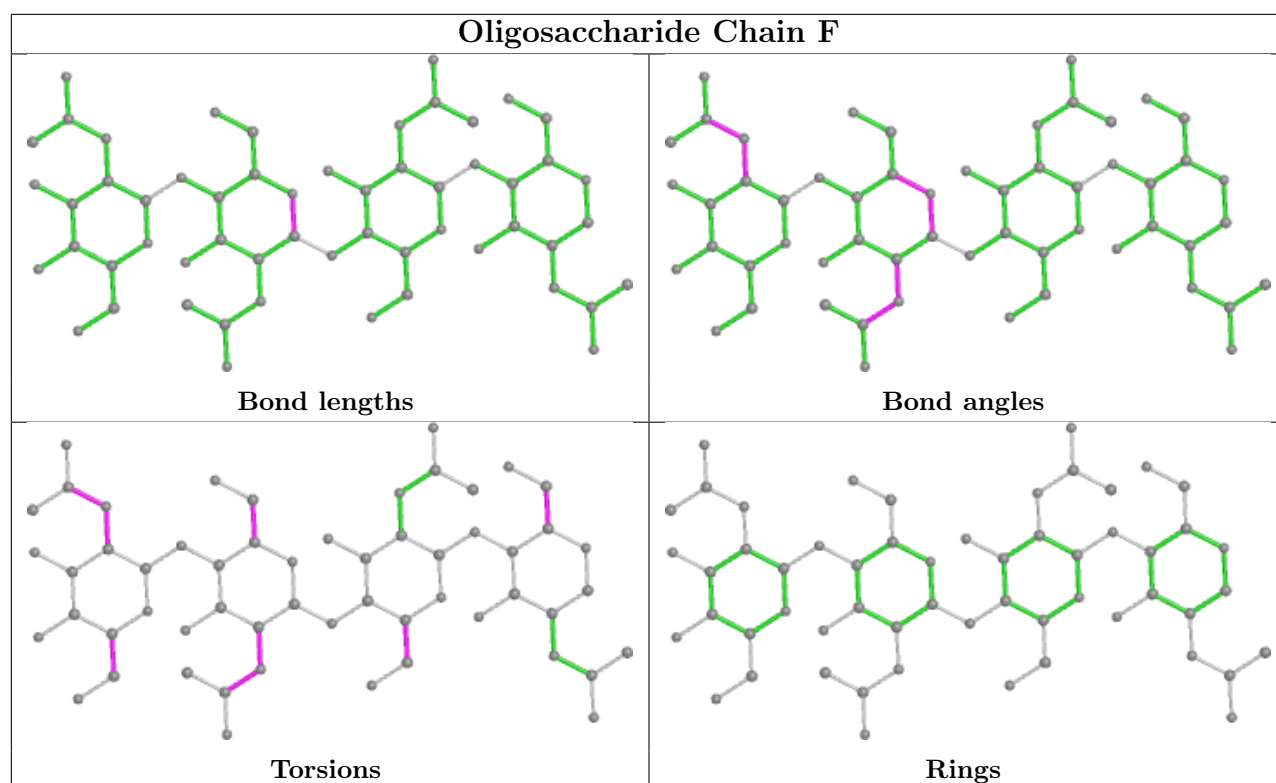
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z  > 2$
10	NAG	D	1203	2	14,14,15	0.79	1 (7%)	17,19,21	0.63	0
9	CLR	A	2303	-	31,31,31	0.36	0	48,48,48	0.66	0
9	CLR	A	2304	-	31,31,31	0.39	0	48,48,48	0.68	0
8	3PE	A	2302	-	39,39,50	0.57	0	42,44,55	0.68	2 (4%)
10	NAG	D	1202	2	14,14,15	0.46	0	17,19,21	0.39	0
11	PT5	A	2307	-	63,63,69	1.36	7 (11%)	76,81,87	1.16	5 (6%)
10	NAG	A	2306	1	14,14,15	0.38	0	17,19,21	1.27	1 (5%)
9	CLR	A	2305	-	31,31,31	0.36	0	48,48,48	0.51	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
10	NAG	D	1203	2	-	0/6/23/26	0/1/1/1
9	CLR	A	2303	-	-	7/10/68/68	0/4/4/4
9	CLR	A	2304	-	-	7/10/68/68	0/4/4/4
8	3PE	A	2302	-	-	15/43/43/54	-
10	NAG	D	1202	2	-	4/6/23/26	0/1/1/1
11	PT5	A	2307	-	-	23/60/84/90	0/1/1/1
10	NAG	A	2306	1	-	2/6/23/26	0/1/1/1
9	CLR	A	2305	-	-	8/10/68/68	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2307	PT5	P4-O4	3.85	1.66	1.59
11	A	2307	PT5	P5-O5	3.59	1.66	1.59
11	A	2307	PT5	O18-C11	3.51	1.43	1.33
11	A	2307	PT5	O16-C8	-2.81	1.39	1.46
11	A	2307	PT5	P1-O1	2.78	1.67	1.60

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2306	NAG	C1-O5-C5	4.76	118.64	112.19
11	A	2307	PT5	O16-C10-C12	3.65	119.37	111.50
11	A	2307	PT5	C20-C19-C18	3.46	152.74	123.57
11	A	2307	PT5	C17-C16-C15	3.41	152.31	123.57
11	A	2307	PT5	O18-C11-C31	2.62	120.12	111.91

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2302	3PE	O13-C11-C12-N
9	A	2303	CLR	C13-C17-C20-C21
9	A	2303	CLR	C16-C17-C20-C22
9	A	2304	CLR	C13-C17-C20-C21
9	A	2304	CLR	C13-C17-C20-C22

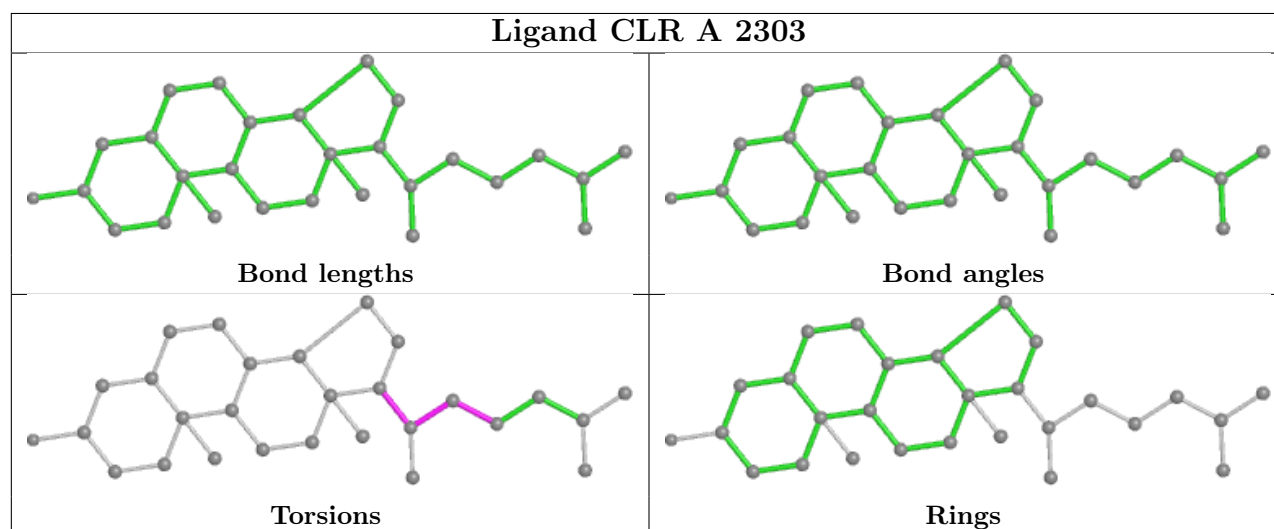


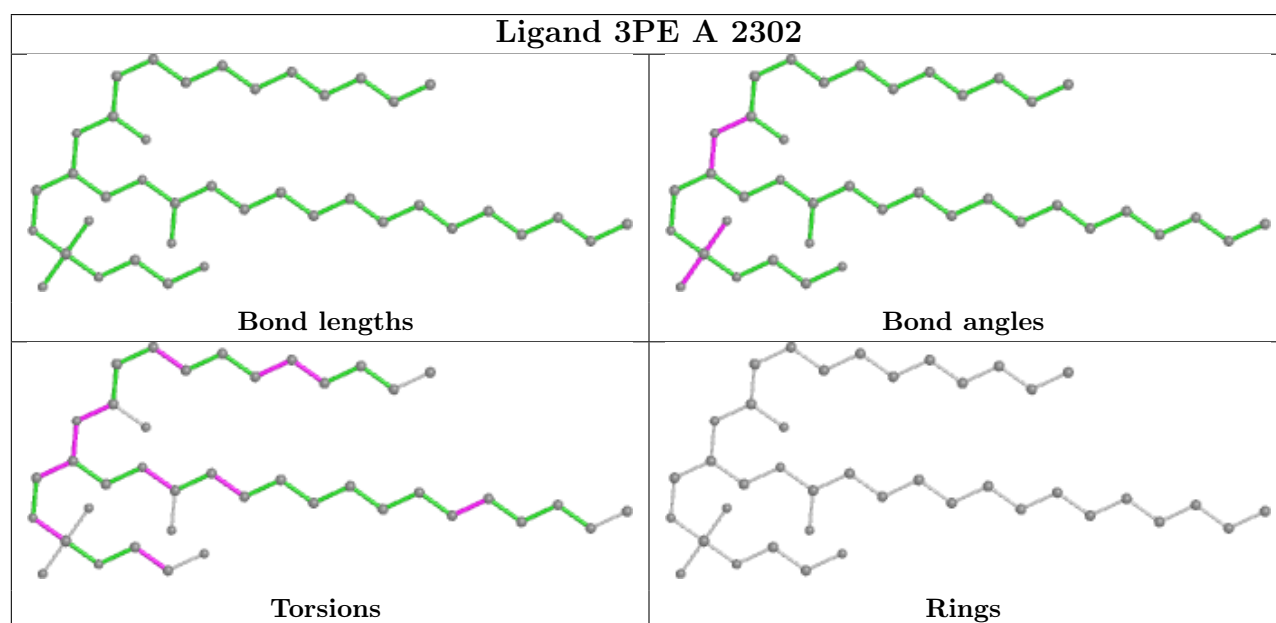
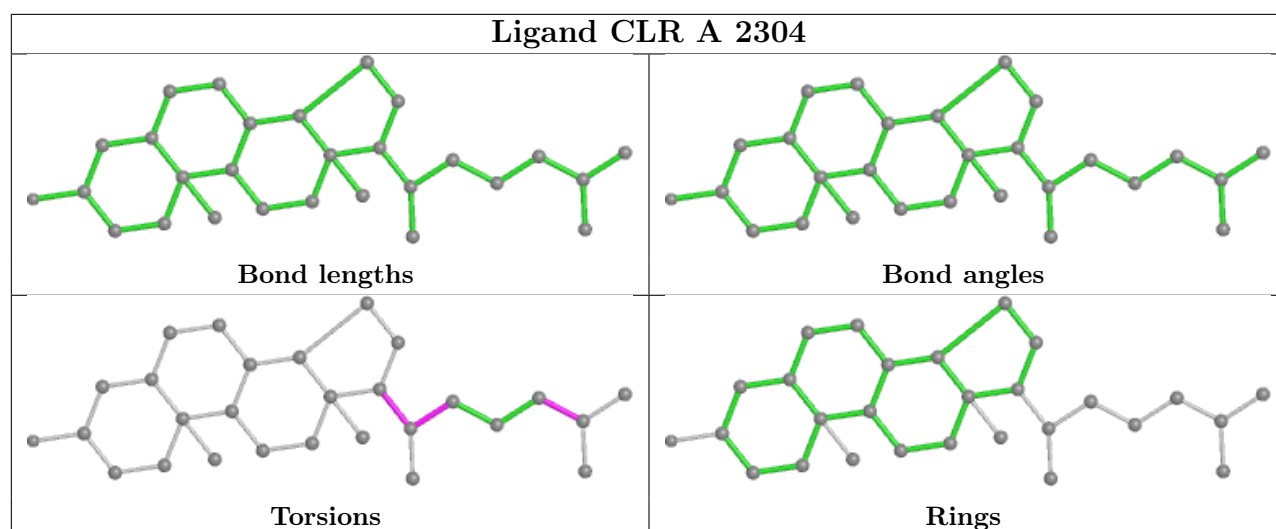
There are no ring outliers.

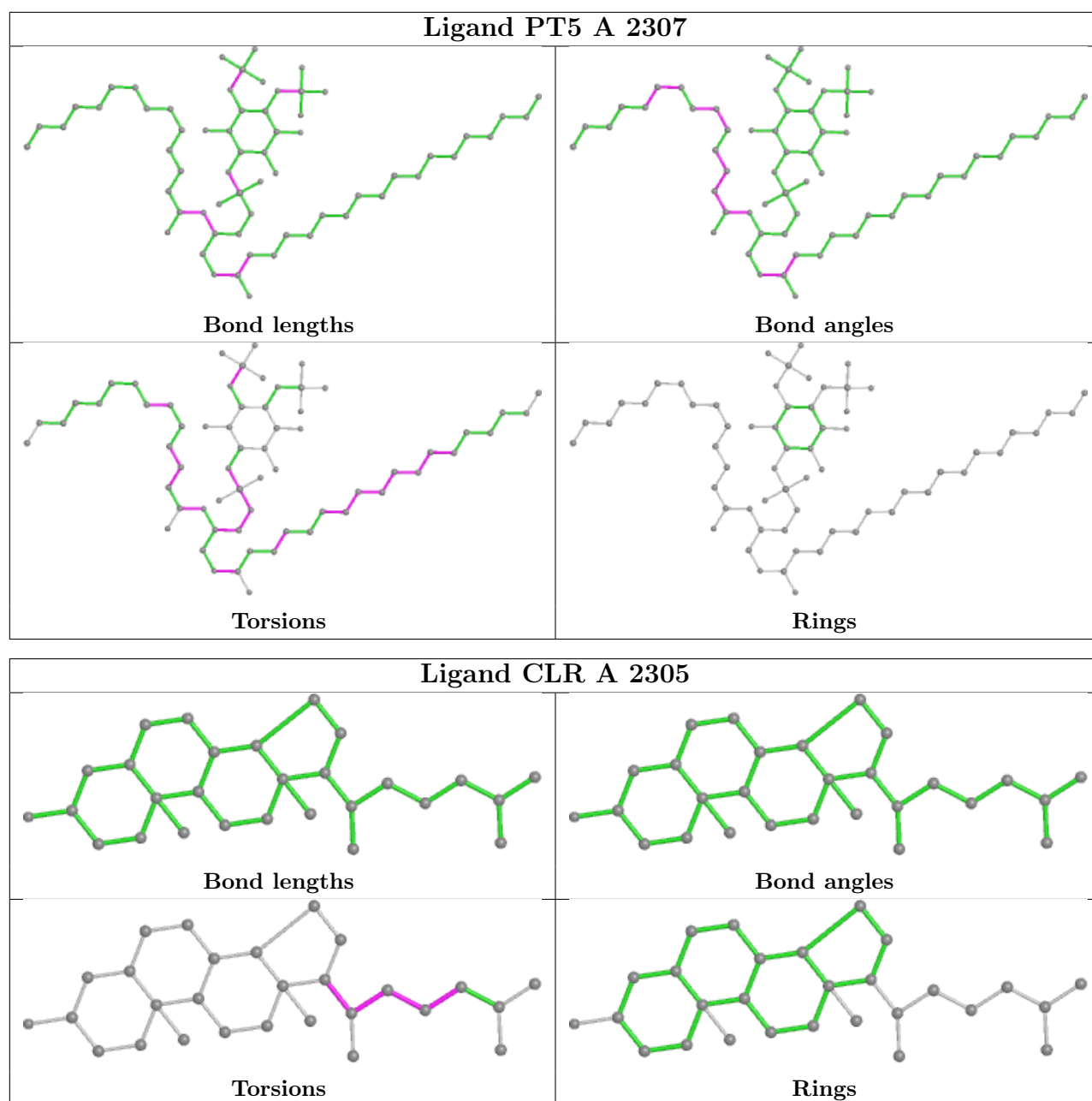
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2303	CLR	2	0
9	A	2304	CLR	3	0
8	A	2302	3PE	1	0
11	A	2307	PT5	2	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.

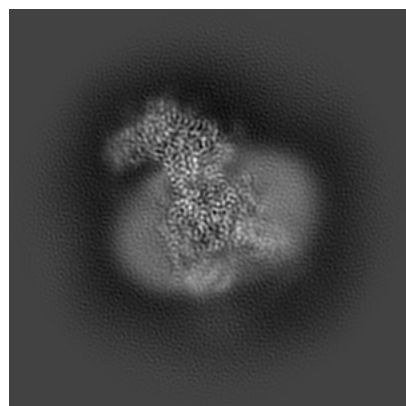
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37475. These allow visual inspection of the internal detail of the map and identification of artifacts.

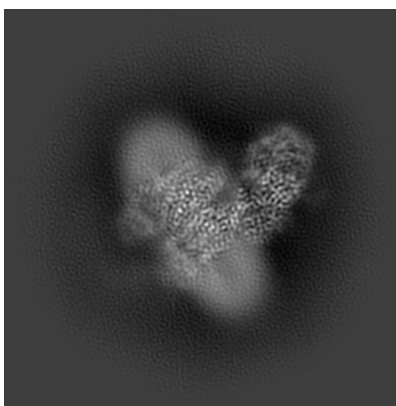
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

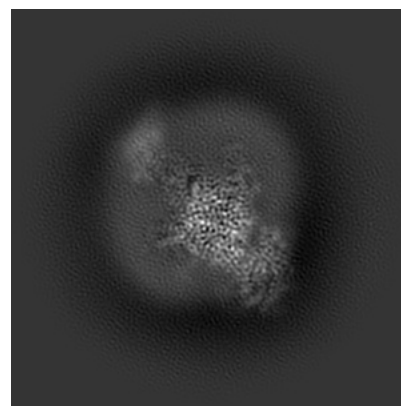
#### 6.1.1 Primary map



X

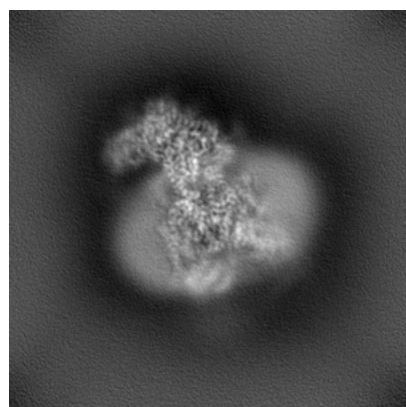


Y

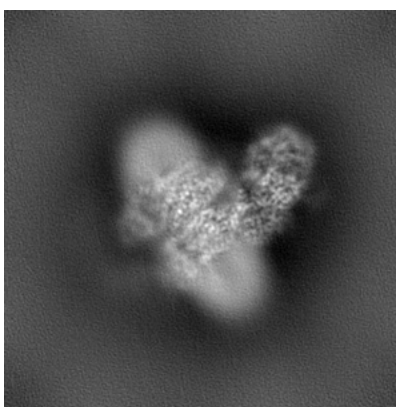


Z

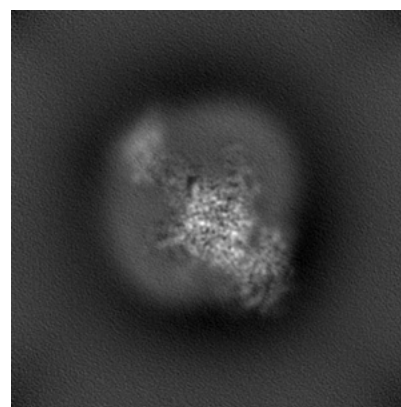
#### 6.1.2 Raw map



X



Y

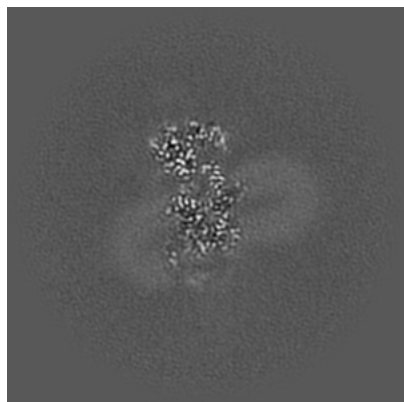


Z

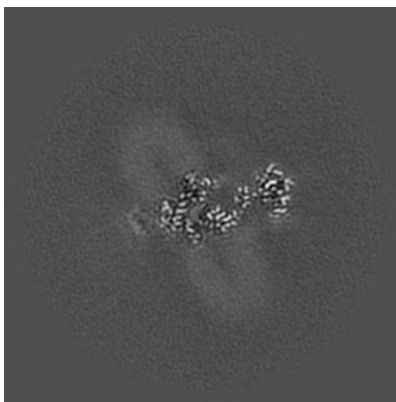
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

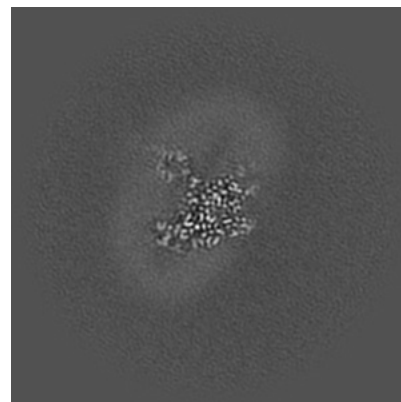
### 6.2.1 Primary map



X Index: 140

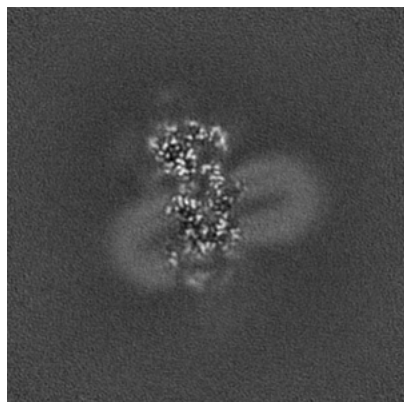


Y Index: 140

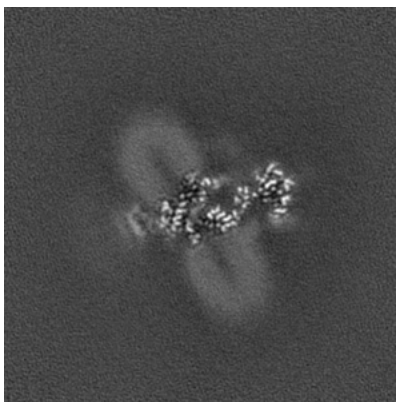


Z Index: 140

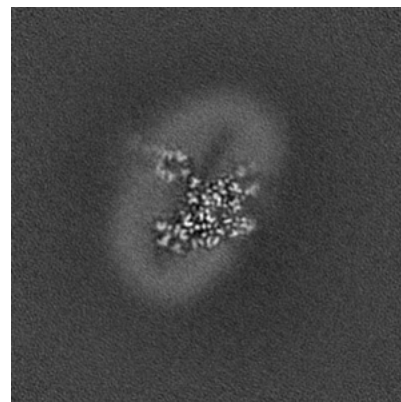
### 6.2.2 Raw map



X Index: 140



Y Index: 140

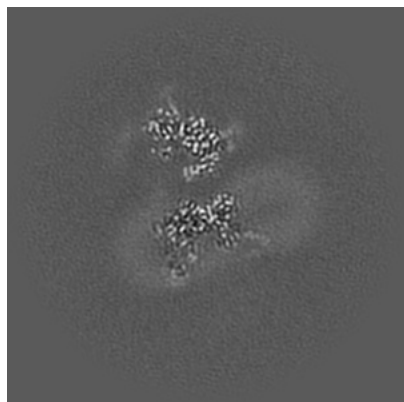


Z Index: 140

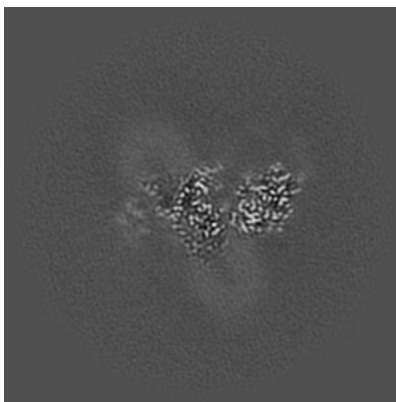
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

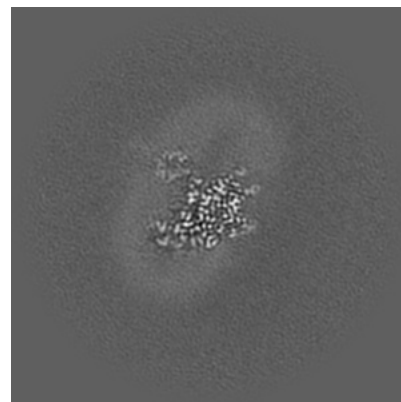
### 6.3.1 Primary map



X Index: 149

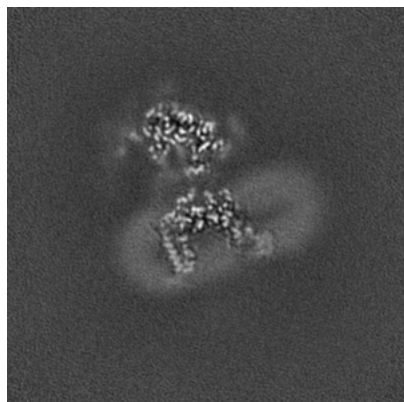


Y Index: 130

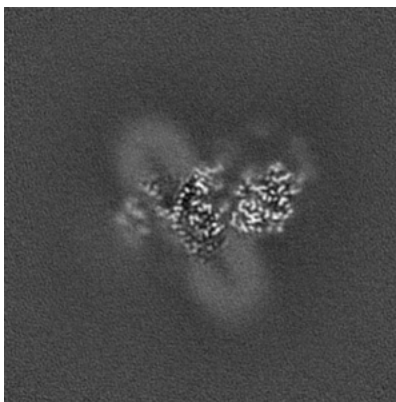


Z Index: 139

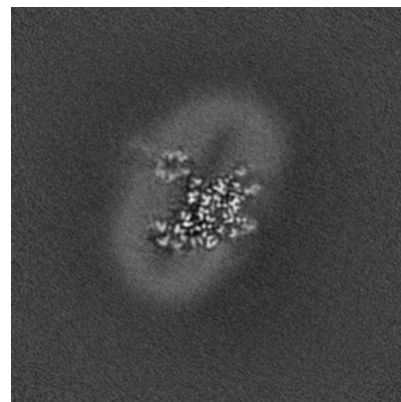
### 6.3.2 Raw map



X Index: 154



Y Index: 130



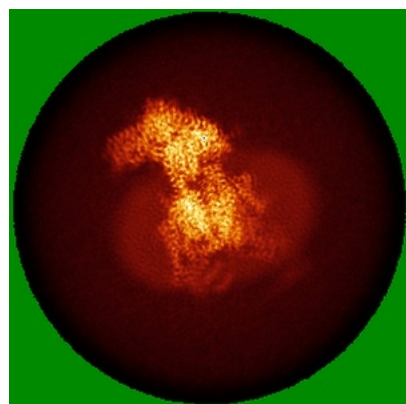
Z Index: 139

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

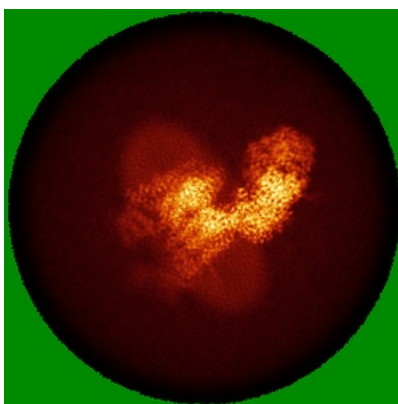


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

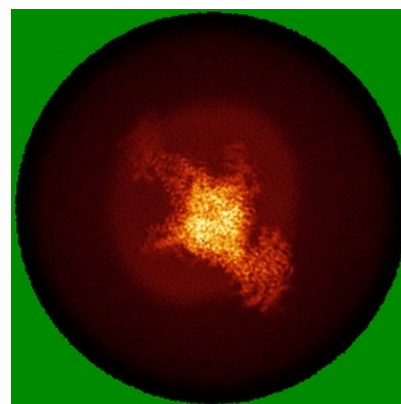
### 6.4.1 Primary map



X

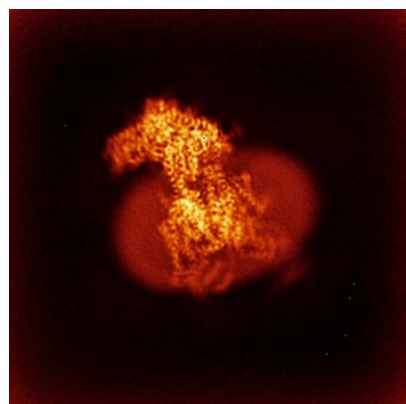


Y

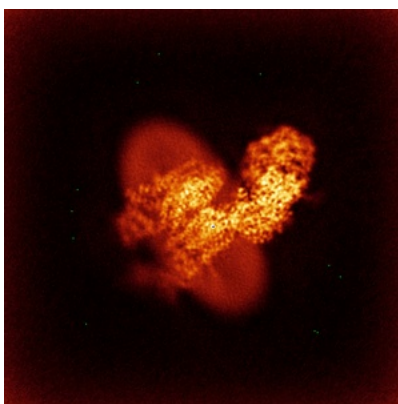


Z

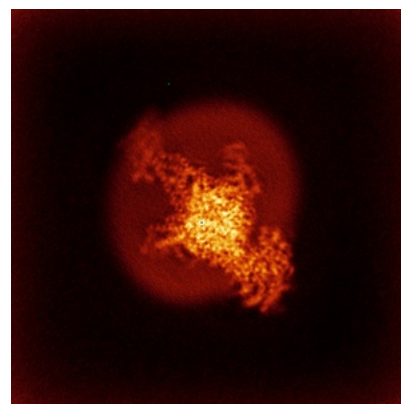
### 6.4.2 Raw map



X



Y

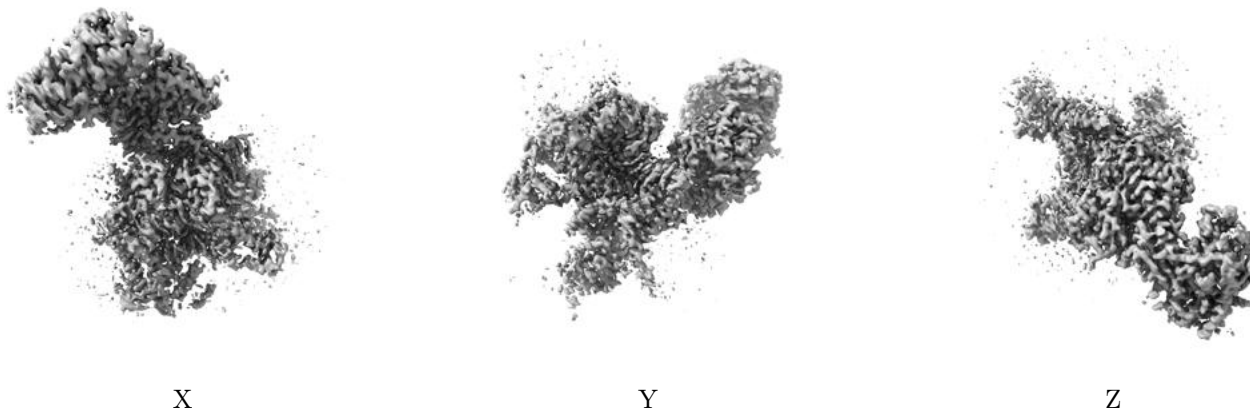


Z

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.

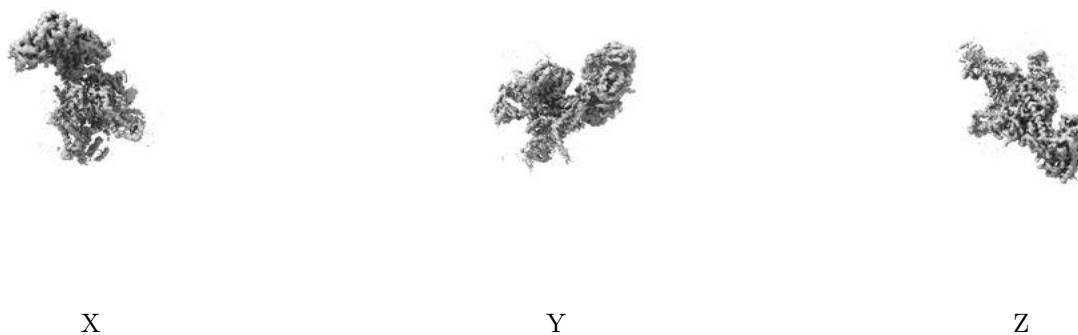
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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](#)

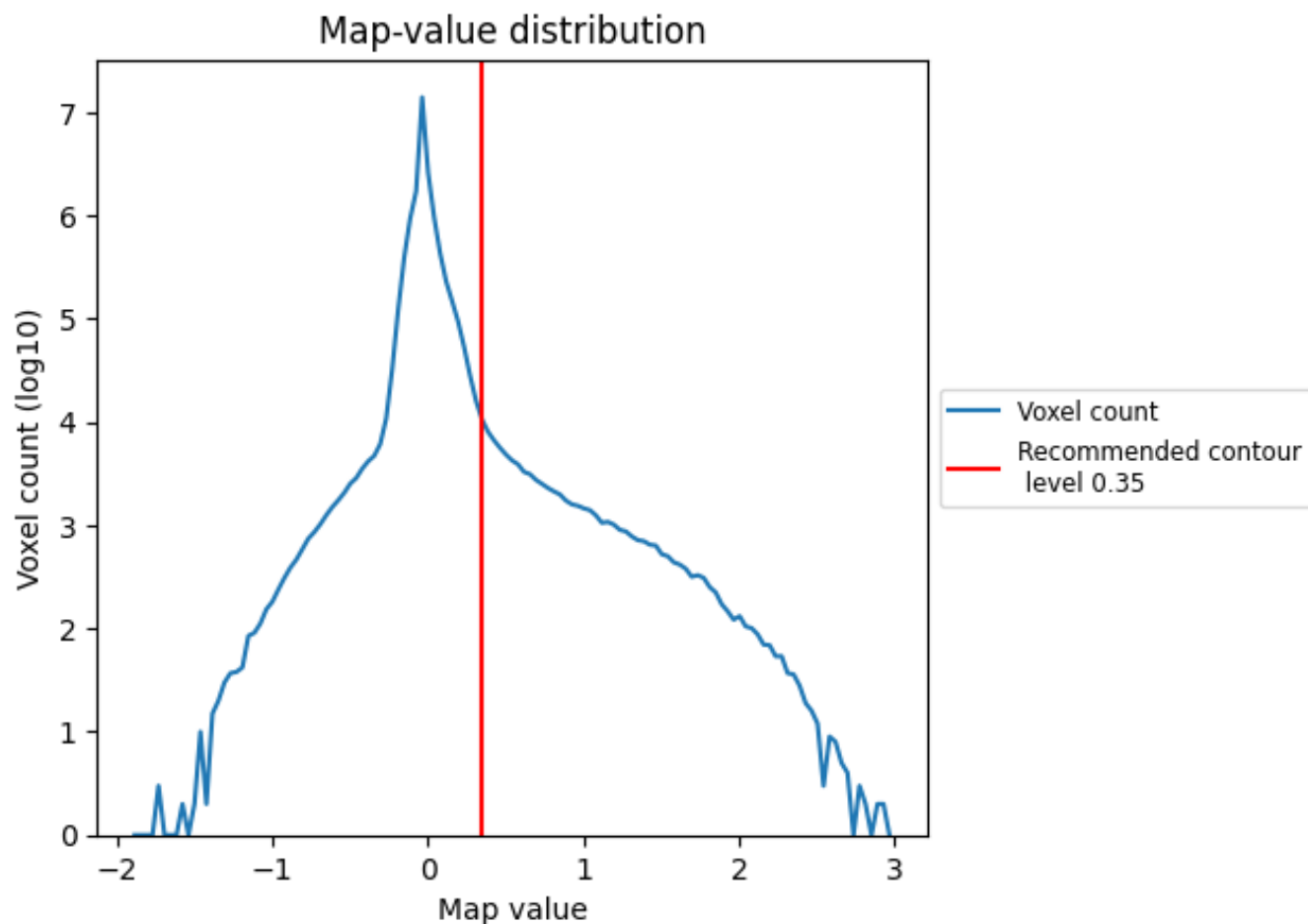
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

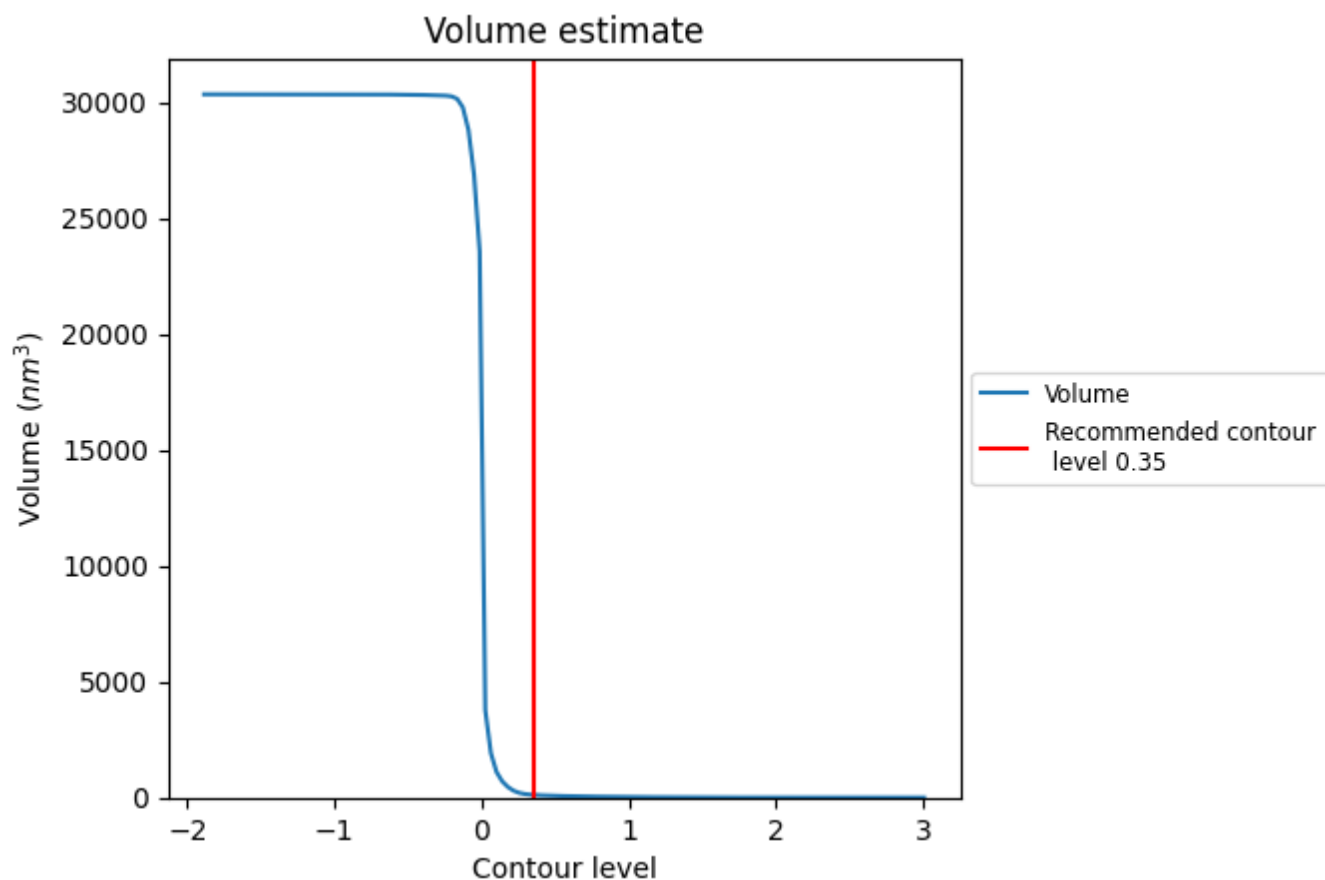
This section contains the results of statistical analysis of the map.

### 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.

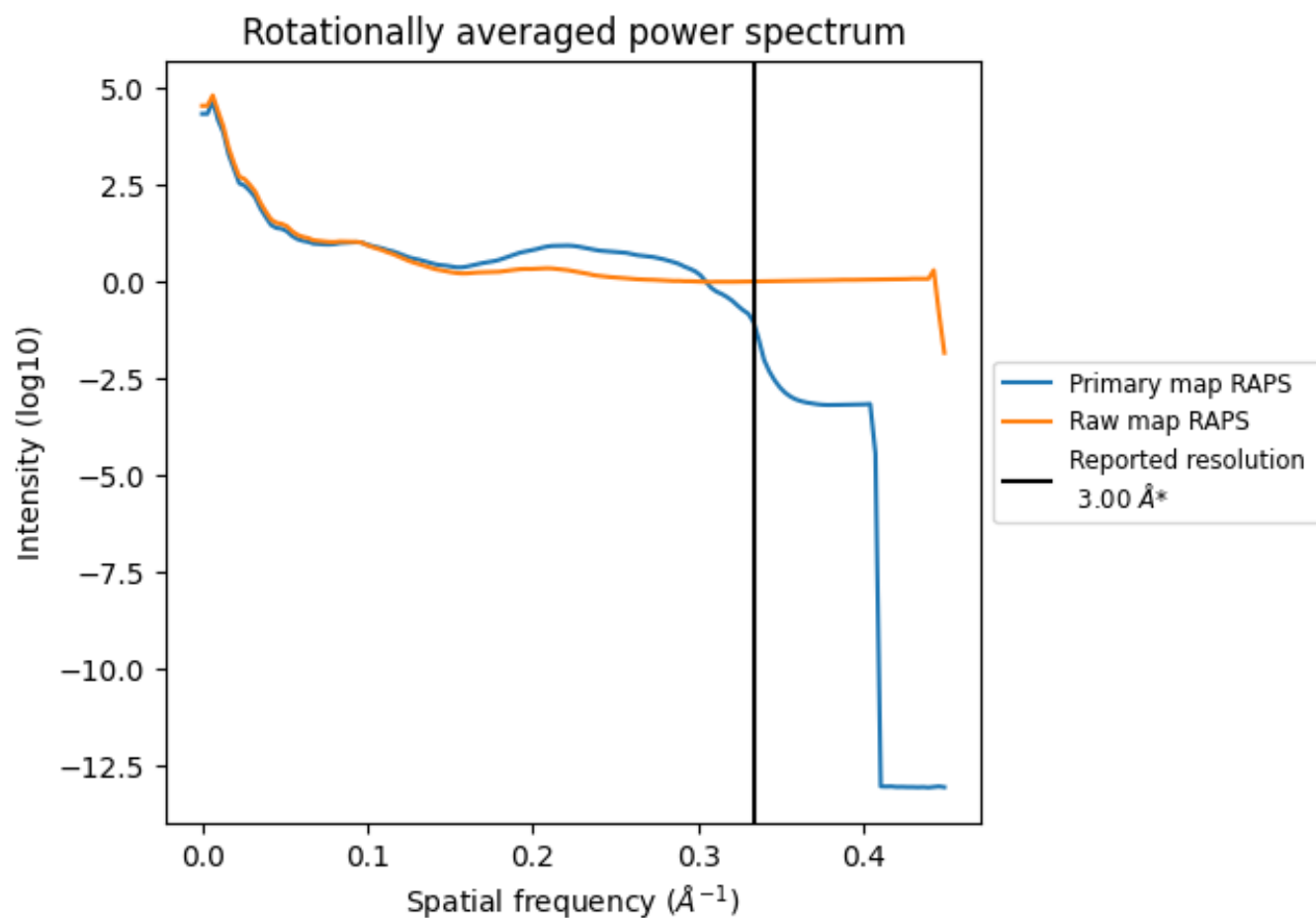
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm<sup>3</sup>; this corresponds to an approximate mass of 106 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

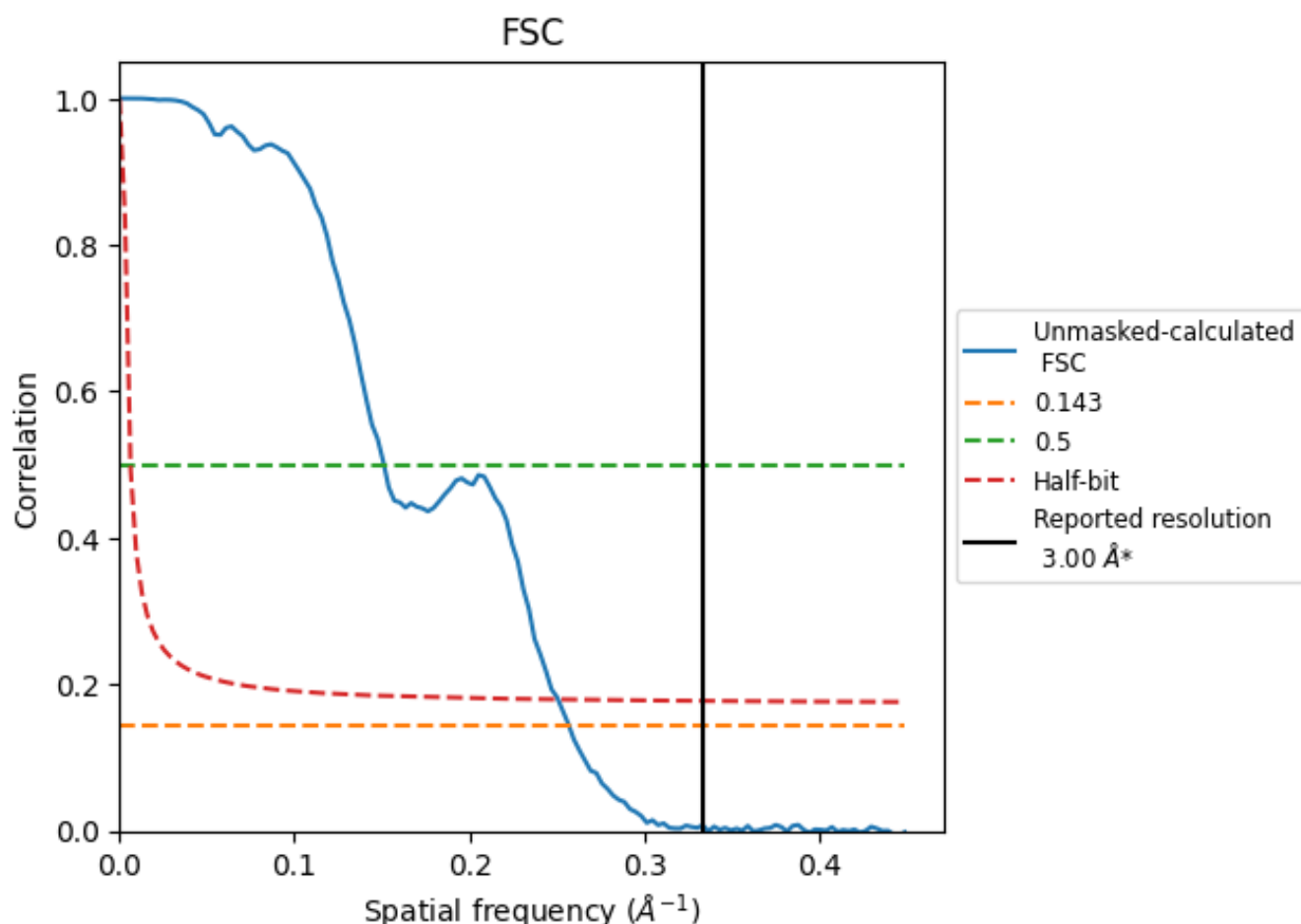


\*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

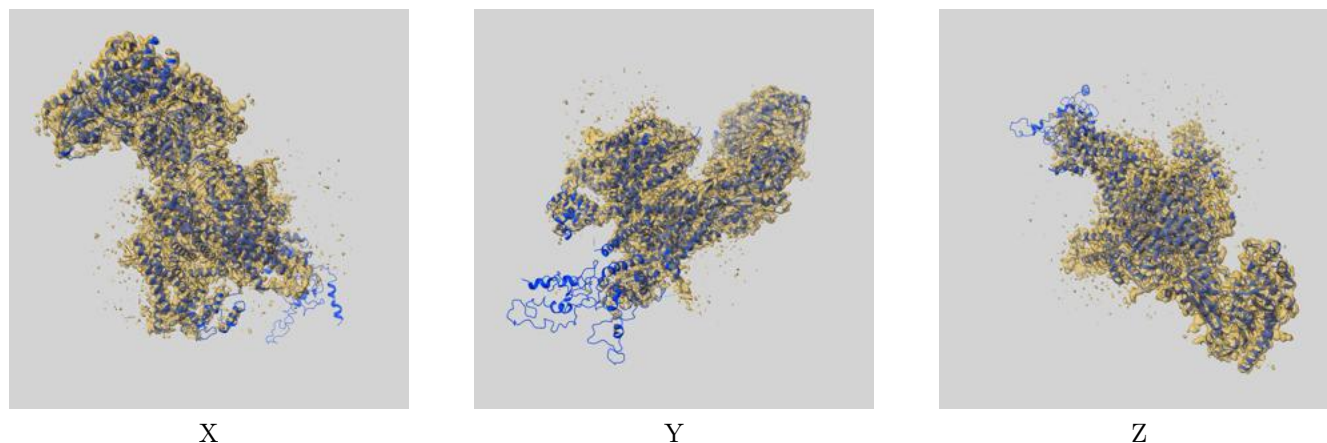
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.62	3.99

\*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 3.89 differs from the reported value 3.0 by more than 10 %

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

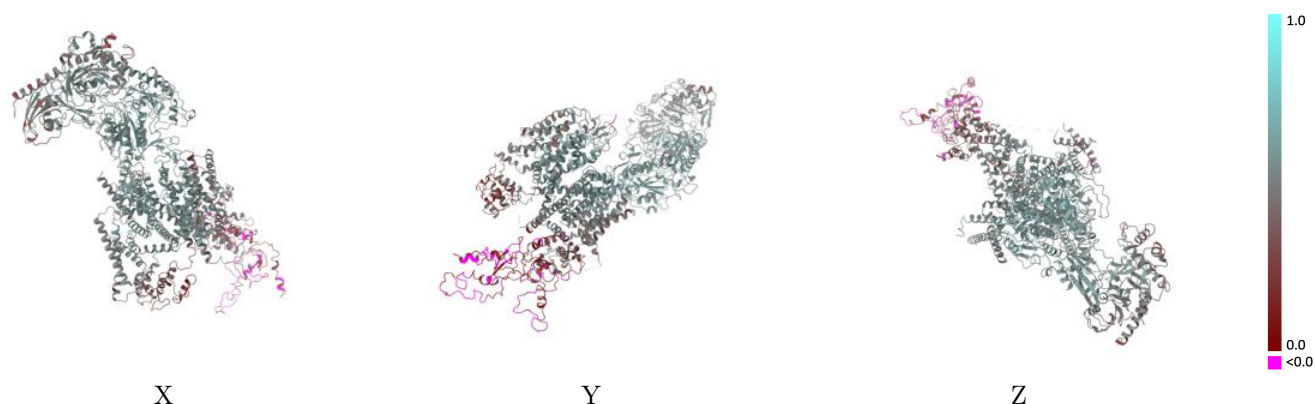
This section contains information regarding the fit between EMDB map EMD-37475 and PDB model 8WE9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



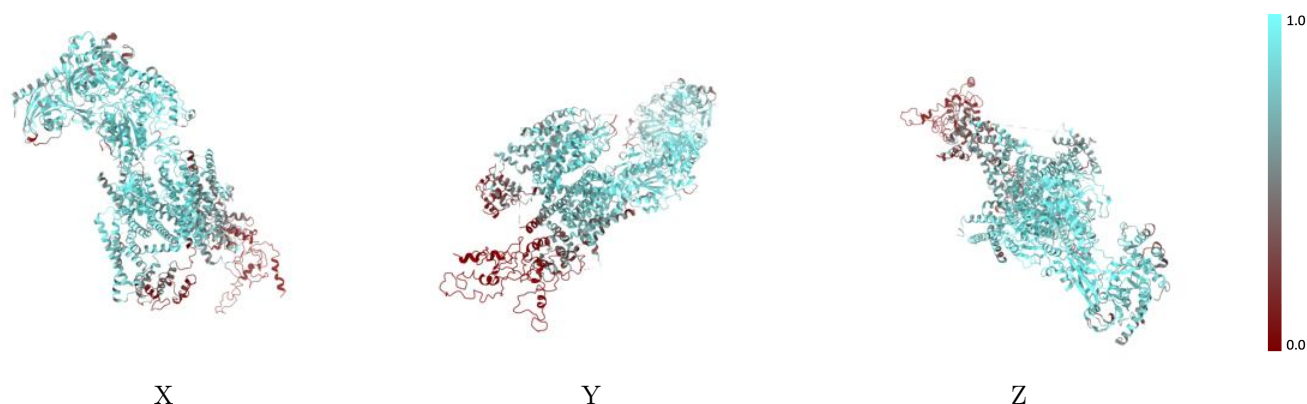
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



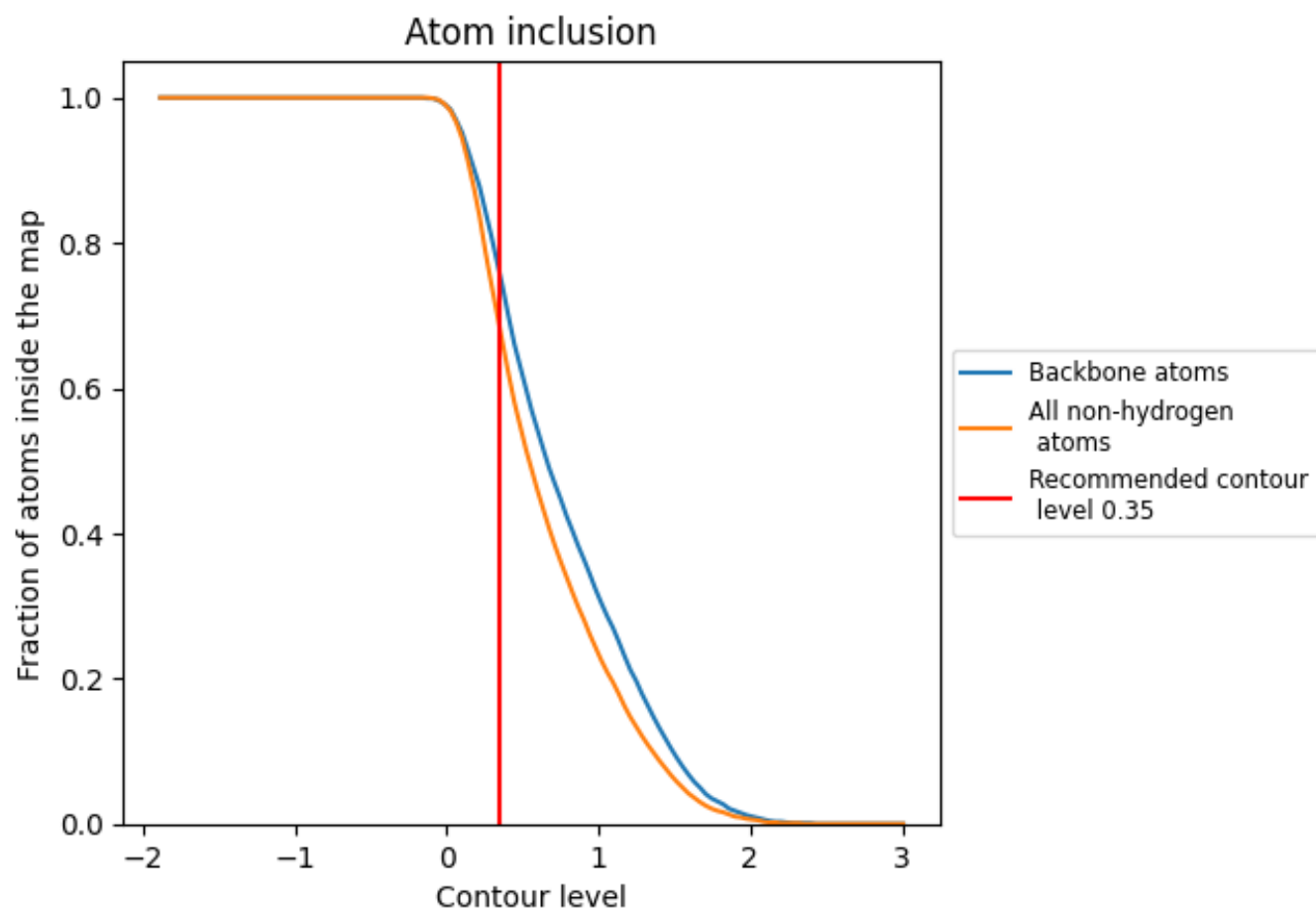
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6820	<div></div> 0.4700
A	<div></div> 0.7210	<div></div> 0.5040
B	<div></div> 0.5240	<div></div> 0.3740
C	<div></div> 0.0980	<div></div> 0.1590
D	<div></div> 0.8300	<div></div> 0.5300
E	<div></div> 0.2860	<div></div> 0.2910
F	<div></div> 0.6790	<div></div> 0.4340
G	<div></div> 0.4290	<div></div> 0.3510
H	<div></div> 0.6430	<div></div> 0.4270

1.0

0.0

<0.0