



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 05:52 AM EST

PDB ID : 8GZ1  
EMDB ID : EMD-34387  
Title : Cryo-EM structure of human NaV1.6/beta1/beta2,apo state  
Authors : Li, Y.; Jiang, D.  
Deposited on : 2022-09-24  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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

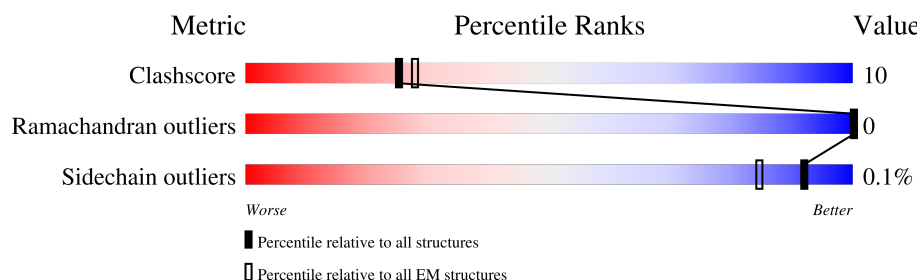
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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	D	218	
2	B	1980	
3	C	215	
4	A	3	
4	E	3	
4	F	3	
4	G	3	
4	H	3	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11912 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 Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	173	Total	C	N	O	S	0	0
			1409	897	231	271	10		

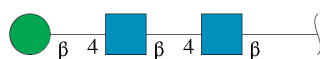
- Molecule 2 is a protein called Sodium channel protein type 8 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1152	Total	C	N	O	S	0	0
			9307	6188	1453	1586	80		

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	120	Total	C	N	O	S	0	0
			971	607	173	180	11		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(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	A	3	Total	C	N	O		0	0
			39	22	2	15			
4	E	3	Total	C	N	O		0	0
			39	22	2	15			
4	F	3	Total	C	N	O		0	0
			39	22	2	15			
4	G	3	Total	C	N	O		0	0
			39	22	2	15			
4	H	3	Total	C	N	O		0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

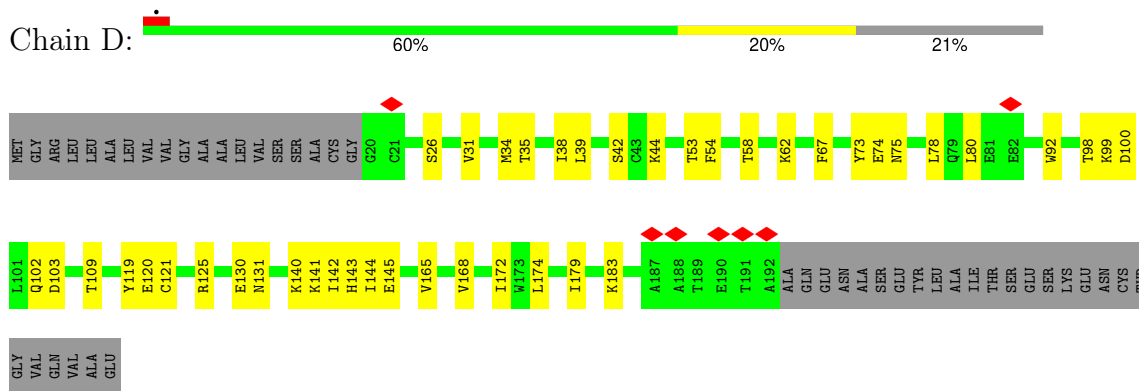
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	B	2	Total	Na	0
			2	2	

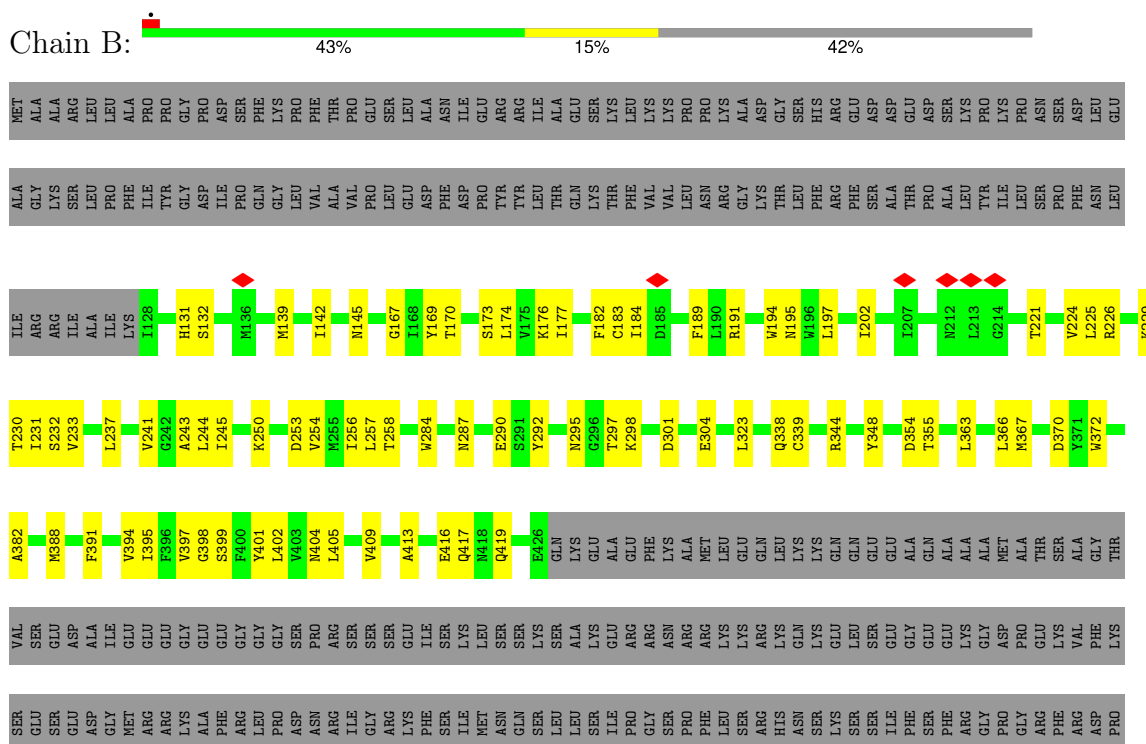
### 3 Residue-property plots

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: Sodium channel subunit beta-1



#### • Molecule 2: Sodium channel protein type 8 subunit alpha

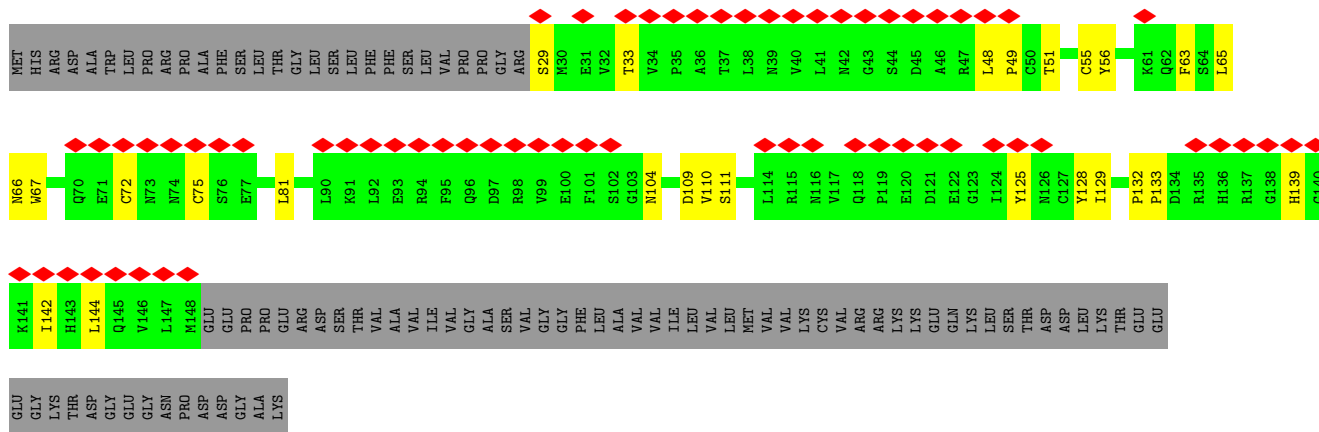


GLN	ARG	ALA	TYR	ASP	GLY	HIS	ASP	Y1675	T1566	F1459	I1340	F1200	SER	GLU	VAL	F926	I795	ASN	LYS	GLY
ALA	ALA	TYR	ASP	GLY	GLY	LEU	PHE	F1686	L1576	I1463	K1352	E1201	THR	LYS	HIS	F926	F796	SER	ARG	SER
ARG	ARG	ILE	THR	THR	LEU	ILE	THR	F1688	L1577	I1463	C1356	I1204	ILE	TYR	ALA	F929	T797	ILE	ASN	GLU
HIS	HIS	PHE	PHE	PHE	GLY	LEU	PHE	E1689	R1577	N1466	C1357	I1205	ILE	ILE	GLN	R931	L802	VAL	THR	PHE
LEU	LEU	ALA	TYR	TYR	GLY	ALA	GLY	G1692	I1583	K1471	N1358	I1208	PRO	GLY	ALA	W932	I805	ASP	ASP	ALA
ALA	ALA	PHE	ILE	ILE	GLY	GLY	GLY	G1696	W1584	K1472	E1362	L1215	VAL	ASP	HIS	W937	M807	ASN	ASP	ASP
ARG	ARG	THR	THR	THR	ARG	ARG	THR	C1697	W1585	K1473	V1370	I1220	GLY	MET	GLN	W945	Y810	GLY	GLY	HIS
GLY	GLY	ARG	ARG	ARG	GLY	ARG	GLY	G1701	F1590	F1474	V1370	I1220	VAL	PHE	ARG	M945	Y811	VAL	SER	SER
LEU	LEU	VAL	VAL	VAL	GLY	VAL	VAL	T1702	V1593	G1475	K1373	E1223	PRO	ILE	GLY	F946	Q814	GLY	THR	THR
VAL	VAL	LEU	LEU	LEU	GLY	VAL	VAL	G1706	I1594	G1476	T1374	Q1224	VAL	ASN	ALA	V947	E815	LEU	VAL	VAL
GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	G1707	G1598	G1477	E1375	K1225	GLY	ASN	ASP	Q950	G816	ILE	GLY	GLY
THR	THR	SER	SER	SER	GLY	GLY	GLY	G1708	W1598	K1494	E1376	K1226	GLN	PRO	VAL	F957	W817	GLY	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1709	W1599	G1496	E1377	R1229	GLY	LEU	LYS	V960	N818	PRO	GLY	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	L1710	L1602	S1497	E1381	T1230	TYR	VAL	LEU	V960	I819	GLN	GLY	GLY
ASP	ASP	LEU	LEU	LEU	LEU	LEU	LEU	I1714	A1603	K1498	E1382	I1231	LEU	ARG	LEU	G822	G822	LYS	ARG	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1717	D1604	K1499	R1388	L1245	ASP	VAL	GLY	F967	F823	ILE	ASP	ASP
ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	G1720	I1605	K1499	V1389	K1250	ALA	ALA	GLY	L975	V825	PRO	GLY	GLY
LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	G1721	Y1609	K1502	K1390	K1250	CYS	VAL	LYS	L829	L829	LEU	LEU	LEU
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1722	Y1609	P1503	M1391	Y1254	THR	GLY	LYS	S981	S833	ALA	PRO	PRO
THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	G1723	S1612	P1503	K1392	Y1254	THR	SER	ALA	W739	I740	GLY	GLY	GLY
ARG	ARG	GLY	GLY	GLY	GLY	GLY	GLY	D1724	S1612	I1504	E1393	K1258	GLY	PHE	ILE	K741	I741	ALA	ALA	ALA
GLY	GLY	PHE	PHE	PHE	PHE	PHE	PHE	K1725	F1616	I1504	M1395	K1258	CYS	GLY	ALA	K742	I742	THR	THR	THR
LYS	LYS	VAL	VAL	VAL	VAL	VAL	VAL	E1726	F1616	L1508	Q1408	L1267	VAL	GLY	ALA	K743	I743	GLY	GLY	GLY
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	H1727	I1619	K1509	Q1409	S1294	GLN	ASN	ASN	K835	E838	ARG	ARG	ARG
GLY	GLY	SER	SER	SER	SER	SER	SER	P1728	R1620	K1510	V1409	S1294	ARG	THR	THR	E839	I745	VAL	VAL	VAL
SER	SER	ASN	ASN	ASN	ASN	ASN	ASN	G1738	R1620	I1511	Q1409	S1294	PHE	ASN	GLY	G839	G839	GLY	SER	SER
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	N1738	Q1512	Q1512	K1413	T1297	LYS	THR	GLY	L840	L840	ILE	ILE	ILE
THR	THR	SER	SER	SER	SER	SER	SER	E1739	Q1513	Q1513	G1414	L1298	CYS	GLY	ALA	I749	I749	LYS	LYS	LYS
LYS	LYS	VAL	VAL	VAL	VAL	VAL	VAL	V1741	I1624	I1514	W1415	R1299	CYS	ASP	ASP	R847	R847	LYS	LYS	LYS
THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	G1742	G1625	I1515	W1415	R1299	GLN	ILE	ILE	L848	L848	GLY	GLY	GLY
ALA	ALA	SER	SER	SER	SER	SER	SER	F1745	R1626	F1516	D1424	A1300	VAL	SER	HIS	L849	L849	TYR	TYR	TYR
LEU	LEU	TYR	TYR	TYR	TYR	TYR	TYR	F1745	I1627	D1517	S1425	R1302	ILE	ARG	ARG	R850	R850	PRO	PRO	PRO
PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	Y1749	L1628	F1518	R1426	P1303	ILE	GLY	ASN	K853	K853	GLY	GLY	GLY
SER	SER	PRO	PRO	PRO	PRO	PRO	PRO	Y1749	I1631	V1519	K1427	L1304	GLY	SER	GLY	V764	V764	SER	SER	SER
SER	SER	ILE	ILE	ILE	ILE	ILE	ILE	Y1761	K1632	V1520	E1430	R1305	GLY	ASP	PHE	W858	W858	LEU	LEU	LEU
THR	THR	THR	THR	THR	THR	THR	THR	I1762	I1637	Q1521	E1430	A1306	GLY	PRO	GLN	I868	I868	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	L1766	L1640	D1525	E1430	A1306	GLY	GLY	ILE	T767	T767	SER	SER	SER
LYS	LYS	ARG	ARG	ARG	ARG	ARG	ARG	A1772	L1644	I1526	D1436	F1310	LEU	ASP	GLY	N870	N870	ASP	ASP	ASP
PRO	PRO	LYS	LYS	LYS	LYS	LYS	LYS	THR	F1652	A1523	K1433	R1309	GLY	LYS	LYS	V872	V872	GLN	GLN	GLN
GLY	GLY	GLN	GLN	GLN	GLN	GLN	GLN	GLY	F1652	F1524	Y1439	R1309	LEU	LEU	LEU	L765	L765	LEU	LEU	LEU
LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	F1652	F1525	Y1439	R1309	LEU	LEU	LEU	N766	N766	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	L1656	I1526	M1440	F1310	LEU	LEU	LEU	L768	L768	SER	SER	SER
LYS	LYS	VAL	VAL	VAL	VAL	VAL	VAL	GLY	M1536	I1526	Y1441	R1305	LEU	LEU	LEU	F769	F769	MET	MET	MET
PRO	PRO	VAL	VAL	VAL	VAL	VAL	VAL	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	H775	H775	ASP	ASP	ASP
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	P776	P776	GLY	GLY	GLY
PRO	PRO	ASP	ASP	ASP	ASP	ASP	ASP	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	F781	F781	ALA	ALA	ALA
LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	L785	L785	TYR	TYR	TYR
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	E903	E903	GLY	GLY	GLY
ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	C904	C904	ARG	ARG	ARG
ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	V791	V791	LYS	LYS	LYS
GLY	GLY	LEU	LEU	LEU	LEU	LEU	LEU	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	F792	F792	ASP	ASP	ASP
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	T793	T793	ARG	ARG	ARG
								GLY	T1538	I1526	Y1441	R1305	LEU	LEU	LEU	W917	W917	ILE	ILE	ILE

GLU  
GLY  
ARG  
ARG  
GLU  
ARG  
ARG  
ALA  
LYS  
GLN  
GLY  
VAL  
ARG  
GLU  
SER  
LYS  
CYS

• Molecule 3: Sodium channel subunit beta-2

Chain C: 



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

Chain A: 

MAG1  
MAG2  
BM43

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

Chain E: 

MAG1  
MAG2  
BM43

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

Chain F: 

MAG1  
MAG2  
BM43

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

Chain G: 



- Molecule 4: beta-D-mannopyranose-(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	41387	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	9.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.120	Depositor
Minimum map value	-1.549	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.4	Depositor
Map size ( $\text{\AA}$ )	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	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: BMA, NAG, NA

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	D	0.25	0/1435	0.50	0/1940
2	B	0.27	0/9550	0.47	0/12947
3	C	0.25	0/992	0.49	0/1341
All	All	0.26	0/11977	0.48	0/16228

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	D	1409	0	1368	26	0
2	B	9307	0	9393	204	0
3	C	971	0	934	27	0
4	A	39	0	34	0	0
4	E	39	0	34	1	0
4	F	39	0	34	0	0
4	G	39	0	34	0	0
4	H	39	0	34	0	0
5	B	14	0	13	0	0
5	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
All	All	11912	0	11891	243	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.

All (243) 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)
2:B:904:CYS:SG	3:C:55:CYS:SG	1.18	1.18
2:B:907:LYS:CA	3:C:56:TYR:OH	2.10	0.99
2:B:907:LYS:N	3:C:56:TYR:OH	2.03	0.92
2:B:945:MET:HG2	2:B:950:GLN:HA	1.64	0.79
2:B:907:LYS:HA	3:C:56:TYR:OH	1.85	0.77
2:B:1599:GLY:HA2	2:B:1619:ILE:HD12	1.69	0.75
2:B:904:CYS:HG	3:C:55:CYS:CB	1.95	0.75
2:B:416:GLU:OE1	2:B:419:GLN:NE2	2.26	0.68
2:B:907:LYS:CB	3:C:56:TYR:OH	2.43	0.67
2:B:907:LYS:NZ	3:C:55:CYS:HB3	2.10	0.66
2:B:736:HIS:HB3	2:B:739:TRP:HD1	1.60	0.66
2:B:1301:LEU:HD12	2:B:1304:LEU:HD11	1.78	0.66
2:B:1509:ASN:HB2	2:B:1512:GLN:HB2	1.78	0.66
2:B:284:TRP:HB2	2:B:338:GLN:HB2	1.77	0.66
1:D:103:ASP:HB2	2:B:1728:PRO:HB3	1.77	0.66
2:B:145:ASN:HD21	2:B:226:ARG:HD3	1.60	0.65
2:B:1566:THR:HG21	2:B:1597:ILE:HD11	1.77	0.65
2:B:1326:SER:OG	2:B:1466:ASN:ND2	2.29	0.65
2:B:1352:LYS:HB3	2:B:1425:SER:HB2	1.78	0.64
2:B:338:GLN:HG3	2:B:339:CYS:H	1.62	0.64
1:D:168:VAL:O	1:D:172:ILE:HG12	1.98	0.64
2:B:1517:ASP:O	2:B:1521:GLN:NE2	2.31	0.64
2:B:1602:LEU:HD13	2:B:1619:ILE:HD13	1.79	0.64
2:B:907:LYS:HA	3:C:56:TYR:HH	1.61	0.64
1:D:102:GLN:HG3	2:B:1728:PRO:HG3	1.80	0.64
1:D:42:SER:O	1:D:125:ARG:NH2	2.31	0.64
2:B:257:LEU:HD13	2:B:1637:ILE:HG23	1.79	0.63
2:B:1388:ARG:HH12	2:B:1720:ASP:HB2	1.64	0.63
1:D:44:LYS:NZ	1:D:100:ASP:OD2	2.31	0.63
3:C:104:ASN:H	3:C:109:ASP:HB2	1.63	0.63
3:C:66:ASN:N	3:C:128:TYR:O	2.28	0.62
2:B:767:THR:HG23	2:B:768:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1687:ASN:ND2	2:B:1689:GLU:OE1	2.32	0.62
1:D:35:THR:HG22	1:D:109:THR:HA	1.81	0.62
2:B:366:LEU:HD23	2:B:372:TRP:HB2	1.81	0.61
2:B:848:LEU:HB3	2:B:1340:ILE:HG23	1.82	0.61
2:B:817:TRP:CZ2	2:B:853:LYS:HA	2.35	0.61
2:B:1427:LYS:HB2	2:B:1430:GLU:HB2	1.82	0.61
2:B:1439:TYR:O	2:B:1442:ILE:HG12	2.00	0.61
2:B:1552:ASN:HB3	2:B:1556:TRP:HZ3	1.65	0.60
2:B:363:LEU:HD23	2:B:366:LEU:HD12	1.82	0.60
2:B:244:LEU:HD21	2:B:967:VAL:HG22	1.83	0.59
2:B:323:LEU:HD23	2:B:382:ALA:HB2	1.84	0.59
2:B:1186:ILE:HA	2:B:1189:LYS:NZ	2.18	0.59
2:B:1708:ASP:OD1	2:B:1709:GLY:N	2.35	0.59
3:C:66:ASN:HB2	3:C:128:TYR:HB2	1.84	0.59
2:B:797:THR:HG21	2:B:829:LEU:HD21	1.84	0.59
2:B:1320:LEU:O	2:B:1324:ILE:HG12	2.03	0.59
2:B:398:GLY:HA2	2:B:402:LEU:HD23	1.85	0.58
2:B:405:LEU:HD21	2:B:1640:LEU:HD13	1.85	0.58
2:B:1208:ILE:HD13	2:B:1305:ARG:HD2	1.86	0.58
2:B:1738:ASN:HB3	2:B:1741:VAL:HG12	1.84	0.58
2:B:287:ASN:ND2	2:B:290:GLU:OE2	2.37	0.57
1:D:143:HIS:NE2	1:D:145:GLU:OE2	2.37	0.57
2:B:243:ALA:HB2	2:B:417:GLN:HE22	1.70	0.57
2:B:189:PHE:HD2	2:B:195:ASN:HB3	1.70	0.57
1:D:174:LEU:HD22	2:B:1245:LEU:HD21	1.86	0.56
2:B:745:ILE:O	2:B:749:ILE:HG12	2.04	0.56
1:D:53:THR:O	1:D:75:ASN:ND2	2.38	0.56
2:B:904:CYS:CB	3:C:55:CYS:SG	2.77	0.56
2:B:194:TRP:CD1	2:B:232:SER:HB2	2.40	0.56
2:B:1186:ILE:HA	2:B:1189:LYS:HZ1	1.70	0.56
1:D:120:GLU:HG2	1:D:141:LYS:HG2	1.88	0.55
3:C:29:SER:HB2	3:C:139:HIS:H	1.71	0.55
2:B:1686:PHE:HD1	2:B:1696:ILE:HG21	1.70	0.55
2:B:807:MET:SD	2:B:811:TYR:HB2	2.47	0.55
2:B:231:ILE:HA	2:B:237:LEU:HD12	1.88	0.55
2:B:1697:CYS:O	2:B:1701:ILE:HG12	2.07	0.55
2:B:957:PHE:HA	2:B:960:VAL:HG12	1.87	0.54
2:B:1409:VAL:HA	2:B:1415:TRP:HB3	1.90	0.54
2:B:1623:ARG:O	2:B:1626:ARG:HG2	2.07	0.54
2:B:254:VAL:HG21	2:B:409:VAL:HG21	1.91	0.53
2:B:1380:MET:HE1	2:B:1388:ARG:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:THR:HA	2:B:233:VAL:HG12	1.90	0.53
2:B:769:PHE:HE2	2:B:785:LEU:HA	1.73	0.53
2:B:401:TYR:CZ	2:B:1644:LEU:HB2	2.43	0.53
1:D:78:LEU:HD13	1:D:92:TRP:HB2	1.91	0.53
2:B:1198:ASN:OD1	2:B:1199:TRP:N	2.42	0.52
1:D:121:CYS:SG	1:D:140:LYS:HB2	2.50	0.52
2:B:1267:LEU:HD21	2:B:1304:LEU:HB3	1.91	0.52
2:B:1433:LYS:HB3	2:B:1436:ASP:OD2	2.10	0.52
1:D:98:THR:HG23	1:D:100:ASP:H	1.73	0.52
1:D:130:GLU:HG2	1:D:131:ASN:H	1.75	0.52
2:B:907:LYS:CA	3:C:56:TYR:HH	2.15	0.52
2:B:907:LYS:HB2	3:C:56:TYR:OH	2.10	0.52
1:D:75:ASN:HB3	1:D:99:LYS:HD2	1.91	0.52
2:B:836:ASP:OD1	2:B:836:ASP:N	2.41	0.52
2:B:810:TYR:O	2:B:814:GLN:HG2	2.10	0.51
3:C:67:TRP:HZ3	3:C:125:TYR:HB3	1.75	0.51
2:B:1391:ASN:OD1	2:B:1392:VAL:N	2.43	0.51
2:B:1519:VAL:HA	2:B:1524:PHE:HD2	1.75	0.51
2:B:917:TRP:HZ3	2:B:931:ARG:HB2	1.74	0.51
2:B:250:LYS:HG2	2:B:413:ALA:HB2	1.93	0.51
2:B:1714:ILE:HG21	2:B:1742:GLY:HA3	1.92	0.51
2:B:816:GLY:HA2	2:B:819:ILE:HG22	1.93	0.50
2:B:1294:SER:O	2:B:1297:THR:HG22	2.12	0.50
2:B:1554:LEU:HA	2:B:1557:ILE:HG22	1.93	0.50
3:C:125:TYR:HB2	3:C:142:ILE:HB	1.92	0.50
2:B:1185:TRP:CZ2	2:B:1189:LYS:HD3	2.46	0.50
2:B:847:ARG:HD2	2:B:850:ARG:HH12	1.75	0.50
2:B:169:TYR:HB3	2:B:202:ILE:HD11	1.94	0.49
2:B:1426:ARG:HE	2:B:1430:GLU:HB3	1.78	0.49
2:B:1512:GLN:HA	2:B:1515:VAL:HG12	1.93	0.49
2:B:917:TRP:CZ3	2:B:931:ARG:HB2	2.47	0.49
2:B:1637:ILE:HD12	2:B:1637:ILE:H	1.76	0.49
2:B:1449:ILE:O	2:B:1453:PHE:HB3	2.12	0.49
2:B:1552:ASN:HB3	2:B:1556:TRP:CZ3	2.46	0.49
2:B:756:ASP:OD1	2:B:757:LEU:N	2.45	0.49
2:B:763:ILE:HD13	2:B:853:LYS:HB2	1.95	0.49
2:B:1197:HIS:CD2	2:B:1199:TRP:HB3	2.47	0.49
2:B:1388:ARG:HD3	2:B:1390:LYS:HD2	1.95	0.49
3:C:67:TRP:NE1	3:C:110:VAL:O	2.46	0.49
1:D:31:VAL:HG23	1:D:34:MET:HB2	1.95	0.48
2:B:817:TRP:CH2	2:B:853:LYS:HA	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1459:PHE:CZ	2:B:1463:ILE:HD11	2.48	0.48
3:C:72:CYS:SG	3:C:75:CYS:N	2.86	0.48
2:B:295:ASN:OD1	2:B:297:THR:OG1	2.29	0.48
2:B:405:LEU:HD11	2:B:1640:LEU:HD22	1.96	0.48
2:B:1583:ILE:HB	2:B:1586:ASN:ND2	2.29	0.48
2:B:1306:ALA:HB1	2:B:1310:PHE:HD2	1.79	0.47
2:B:241:VAL:O	2:B:245:ILE:HG12	2.15	0.47
2:B:131:HIS:CD2	2:B:132:SER:H	2.31	0.47
2:B:1516:PHE:HZ	2:B:1576:LEU:HB2	1.79	0.47
2:B:926:PHE:HA	2:B:929:VAL:HG12	1.96	0.47
2:B:197:LEU:HG	2:B:225:LEU:HD13	1.97	0.47
2:B:292:TYR:HD2	4:E:2:NAG:H5	1.80	0.47
2:B:1667:ILE:HA	2:B:1670:MET:HG3	1.96	0.47
2:B:367:MET:HG3	2:B:398:GLY:O	2.14	0.47
2:B:1215:LEU:HD21	2:B:1299:ARG:HG2	1.96	0.47
1:D:119:TYR:HB2	1:D:142:ILE:HG13	1.97	0.46
2:B:173:SER:HA	2:B:176:LYS:HG2	1.96	0.46
2:B:1538:THR:O	2:B:1541:VAL:HG12	2.15	0.46
2:B:868:ILE:O	2:B:871:SER:OG	2.22	0.46
2:B:1370:VAL:HG23	2:B:1375:GLU:HB3	1.97	0.46
2:B:1519:VAL:HA	2:B:1524:PHE:CD2	2.51	0.46
2:B:370:ASP:OD2	2:B:937:TRP:N	2.48	0.46
2:B:391:PHE:HA	2:B:394:VAL:HG12	1.97	0.46
2:B:1201:GLU:HA	2:B:1204:ILE:HG22	1.98	0.46
2:B:1356:CYS:SG	2:B:1389:TRP:HE3	2.39	0.46
1:D:58:THR:HB	1:D:67:PHE:HB3	1.97	0.46
2:B:1391:ASN:OD1	2:B:1395:ASN:ND2	2.46	0.46
2:B:1624:ILE:O	2:B:1627:ILE:HG12	2.16	0.46
2:B:1525:ASP:O	2:B:1529:MET:HG2	2.16	0.46
2:B:1585:TRP:CD1	2:B:1632:LYS:HE3	2.50	0.45
2:B:1762:ILE:HG23	2:B:1766:LEU:HD23	1.98	0.45
1:D:165:VAL:HA	1:D:168:VAL:HG22	1.97	0.45
2:B:344:ARG:HH12	2:B:348:TYR:C	2.20	0.45
2:B:899:LYS:O	2:B:903:GLU:HG2	2.17	0.45
2:B:1205:ILE:HG12	2:B:1309:ARG:HB3	1.98	0.45
2:B:1299:ARG:O	2:B:1302:ARG:HG3	2.16	0.45
2:B:869:GLY:O	2:B:873:GLY:N	2.49	0.45
2:B:775:HIS:HB3	2:B:776:PRO:HD3	1.98	0.45
2:B:167:GLY:HA2	2:B:170:THR:HG22	1.99	0.45
2:B:1191:CYS:HB3	2:B:1253:ALA:HB2	1.99	0.45
2:B:354:ASP:OD1	2:B:355:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:904:CYS:HB2	2:B:947:VAL:HG13	1.99	0.44
2:B:1516:PHE:HA	2:B:1519:VAL:HG22	2.00	0.44
1:D:26:SER:HB2	1:D:39:LEU:H	1.82	0.44
2:B:253:ASP:HA	2:B:256:ILE:HD12	2.00	0.44
2:B:781:PHE:O	2:B:785:LEU:HD23	2.16	0.44
2:B:1616:PHE:HZ	2:B:1620:ARG:HH21	1.65	0.44
2:B:1508:LEU:HD23	2:B:1508:LEU:H	1.82	0.44
2:B:741:LYS:O	2:B:745:ILE:HG12	2.16	0.44
2:B:1373:LYS:O	2:B:1377:GLU:HG2	2.18	0.44
2:B:858:TRP:HH2	2:B:1336:ILE:HG13	1.82	0.44
2:B:1191:CYS:O	2:B:1194:ILE:HG22	2.18	0.44
2:B:1441:TYR:O	2:B:1445:VAL:HG23	2.18	0.44
1:D:73:TYR:HD1	1:D:78:LEU:HB2	1.82	0.44
2:B:229:LYS:HE3	2:B:229:LYS:HB3	1.83	0.44
2:B:1590:PHE:O	2:B:1594:ILE:HG12	2.17	0.44
2:B:791:VAL:O	2:B:795:ILE:HG12	2.18	0.43
2:B:765:LEU:HB3	2:B:792:PHE:HZ	1.82	0.43
2:B:397:VAL:O	2:B:401:TYR:HB3	2.18	0.43
3:C:67:TRP:HB2	3:C:81:LEU:HB3	2.00	0.43
2:B:1358:ASN:O	2:B:1362:GLU:N	2.51	0.43
2:B:1692:GLY:O	2:B:1696:ILE:HG12	2.18	0.43
3:C:33:THR:O	3:C:51:THR:HG22	2.18	0.43
3:C:132:PRO:HB2	3:C:133:PRO:HD3	2.00	0.43
2:B:739:TRP:O	2:B:743:LYS:HG3	2.19	0.43
2:B:1628:LEU:O	2:B:1631:ILE:HG12	2.18	0.43
2:B:221:THR:O	2:B:224:VAL:HG13	2.18	0.43
2:B:1226:LYS:HA	2:B:1229:ARG:HG2	2.00	0.43
2:B:1394:ILE:HG21	2:B:1408:GLN:OE1	2.19	0.43
2:B:197:LEU:HD21	2:B:225:LEU:HB3	2.00	0.43
2:B:817:TRP:HZ2	2:B:853:LYS:HA	1.80	0.43
2:B:1250:LYS:HE2	2:B:1250:LYS:HB2	1.90	0.43
2:B:173:SER:HA	2:B:176:LYS:HE3	2.01	0.42
2:B:1205:ILE:HA	2:B:1208:ILE:HG22	2.01	0.42
2:B:1306:ALA:HB1	2:B:1310:PHE:CD2	2.53	0.42
2:B:1413:LYS:HG2	2:B:1706:GLY:H	1.84	0.42
1:D:38:ILE:HD11	1:D:144:ILE:HD13	2.01	0.42
2:B:297:THR:O	2:B:298:LYS:HB3	2.19	0.42
2:B:1254:TYR:HB3	2:B:1258:LYS:HB3	2.00	0.42
2:B:1423:VAL:HG11	2:B:1441:TYR:CE2	2.54	0.42
2:B:1652:PHE:O	2:B:1656:LEU:HD23	2.19	0.42
2:B:1675:TYR:HB3	2:B:1727:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:LEU:HB2	3:C:129:ILE:HG22	2.00	0.42
3:C:49:PRO:HA	3:C:111:SER:HB3	2.01	0.42
1:D:54:PHE:HB2	1:D:74:GLU:HA	2.01	0.42
2:B:388:MET:HG3	2:B:1696:ILE:HD13	2.00	0.42
2:B:746:VAL:HG21	2:B:805:ILE:HG13	2.01	0.42
2:B:1227:THR:O	2:B:1231:ILE:HG12	2.19	0.42
2:B:1717:ARG:O	2:B:1720:ASP:N	2.45	0.42
2:B:1724:ASP:OD1	2:B:1724:ASP:N	2.52	0.42
2:B:183:CYS:O	2:B:191:ARG:NH2	2.51	0.42
2:B:366:LEU:HD13	2:B:394:VAL:HG11	2.01	0.42
2:B:1223:GLU:OE1	2:B:1223:GLU:N	2.49	0.42
2:B:1702:THR:OG1	2:B:1749:TYR:OH	2.36	0.42
3:C:48:LEU:HD11	3:C:144:LEU:HB2	2.01	0.42
3:C:65:LEU:HA	3:C:129:ILE:HA	2.02	0.42
2:B:802:LEU:HA	2:B:805:ILE:HG12	2.01	0.42
2:B:395:ILE:HA	2:B:399:SER:HB3	2.02	0.42
2:B:131:HIS:CD2	2:B:132:SER:N	2.88	0.41
2:B:1258:LYS:HA	2:B:1258:LYS:HD3	1.77	0.41
2:B:404:ASN:HD21	2:B:1761:TYR:HD1	1.67	0.41
2:B:1226:LYS:O	2:B:1229:ARG:HG2	2.21	0.41
2:B:1220:ILE:HD13	2:B:1689:GLU:HB3	2.01	0.41
2:B:1701:ILE:HD11	2:B:1710:LEU:HG	2.02	0.41
2:B:871:SER:HA	2:B:975:LEU:HD21	2.01	0.41
1:D:80:LEU:H	1:D:80:LEU:HD23	1.85	0.41
2:B:1722:SER:OG	2:B:1725:LYS:HD3	2.21	0.41
2:B:822:GLY:HA2	2:B:825:VAL:HG12	2.02	0.41
2:B:1522:GLN:O	2:B:1526:ILE:HG12	2.21	0.41
2:B:1673:PHE:HE2	2:B:1745:PHE:CG	2.39	0.41
2:B:139:MET:O	2:B:142:ILE:HG22	2.21	0.41
2:B:182:PHE:CD2	2:B:184:ILE:HG22	2.56	0.41
2:B:243:ALA:CB	2:B:417:GLN:HE22	2.33	0.41
2:B:258:THR:OG1	2:B:402:LEU:HD12	2.20	0.41
2:B:793:THR:O	2:B:797:THR:HG23	2.21	0.41
2:B:1224:GLN:O	2:B:1225:ARG:HG2	2.21	0.41
2:B:174:LEU:HA	2:B:177:ILE:HG22	2.03	0.40
2:B:824:ILE:HG21	2:B:850:ARG:HG2	2.04	0.40
2:B:837:VAL:HB	2:B:840:LEU:HD12	2.03	0.40
2:B:933:LEU:HD12	2:B:968:VAL:HG21	2.02	0.40
1:D:62:LYS:HD3	1:D:62:LYS:HA	1.74	0.40
2:B:191:ARG:HA	2:B:191:ARG:HD3	2.00	0.40
2:B:301:ASP:O	2:B:304:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:929:VAL:O	2:B:933:LEU:HD23	2.22	0.40
2:B:1327:ILE:HG23	2:B:1331:LEU:HD23	2.03	0.40
3:C:63:PHE:HE2	3:C:65:LEU:HB3	1.86	0.40
1:D:179:ILE:O	1:D:183:LYS:HG2	2.22	0.40
2:B:1459:PHE:CE2	2:B:1463:ILE:HD11	2.56	0.40
2:B:1593:VAL:O	2:B:1597:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	171/218 (78%)	154 (90%)	17 (10%)	0	100	100
2	B	1146/1980 (58%)	1099 (96%)	47 (4%)	0	100	100
3	C	118/215 (55%)	110 (93%)	8 (7%)	0	100	100
All	All	1435/2413 (60%)	1363 (95%)	72 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	D	155/190 (82%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1015/1746 (58%)	1014 (100%)	1 (0%)	92	97
3	C	111/193 (58%)	111 (100%)	0	100	100
All	All	1281/2129 (60%)	1280 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1535	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	131	HIS
2	B	145	ASN
2	B	417	GLN
2	B	1466	ASN
2	B	1521	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

15 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	A	1	4,2	14,14,15	0.17	0	17,19,21	0.39	0
4	NAG	A	2	4	14,14,15	0.24	0	17,19,21	0.56	0
4	BMA	A	3	4	11,11,12	0.56	0	15,15,17	0.72	0
4	NAG	E	1	4,2	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	E	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	BMA	E	3	4	11,11,12	0.57	0	15,15,17	0.74	0
4	NAG	F	1	4,2	14,14,15	0.59	0	17,19,21	1.09	1 (5%)
4	NAG	F	2	4	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
4	BMA	F	3	4	11,11,12	0.51	0	15,15,17	0.84	0
4	NAG	G	1	4,2	14,14,15	0.40	0	17,19,21	0.48	0
4	NAG	G	2	4	14,14,15	0.19	0	17,19,21	0.50	0
4	BMA	G	3	4	11,11,12	0.56	0	15,15,17	0.71	0
4	NAG	H	1	4,2	14,14,15	0.26	0	17,19,21	0.59	0
4	NAG	H	2	4	14,14,15	0.23	0	17,19,21	0.44	0
4	BMA	H	3	4	11,11,12	0.56	0	15,15,17	0.68	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	A	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	1/2/19/22	0/1/1/1
4	NAG	E	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	3.37	116.70	112.19
4	F	2	NAG	C1-O5-C5	2.42	115.42	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

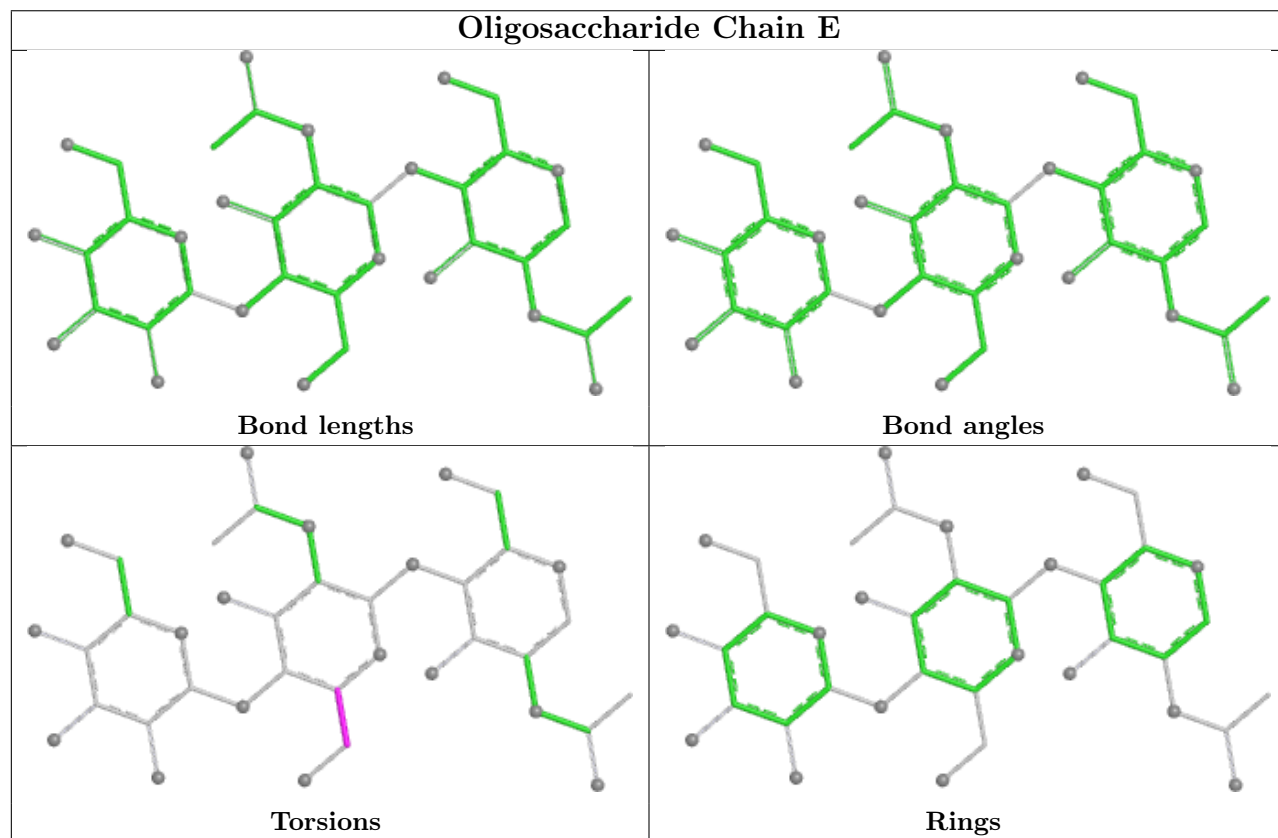
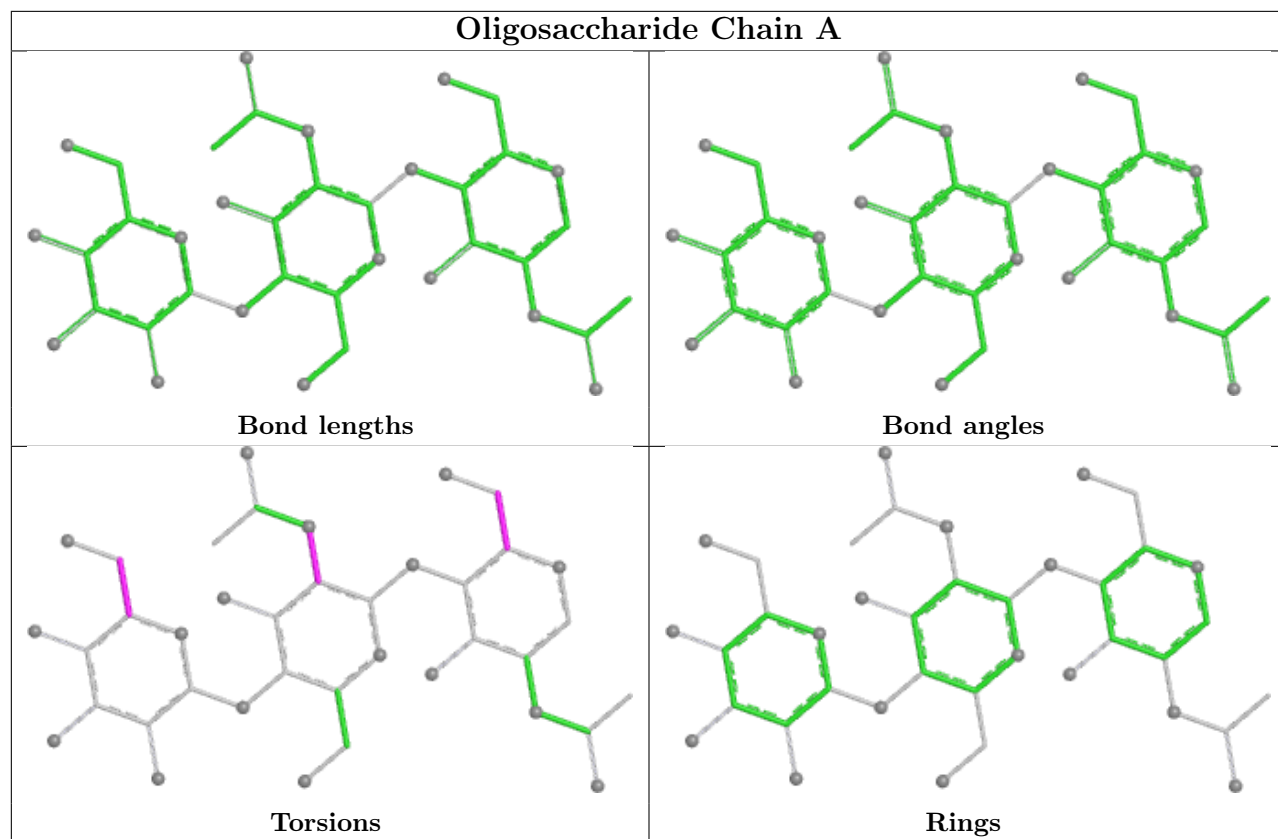
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	F	3	BMA	O5-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C1-C2-N2-C7
4	A	2	NAG	C3-C2-N2-C7

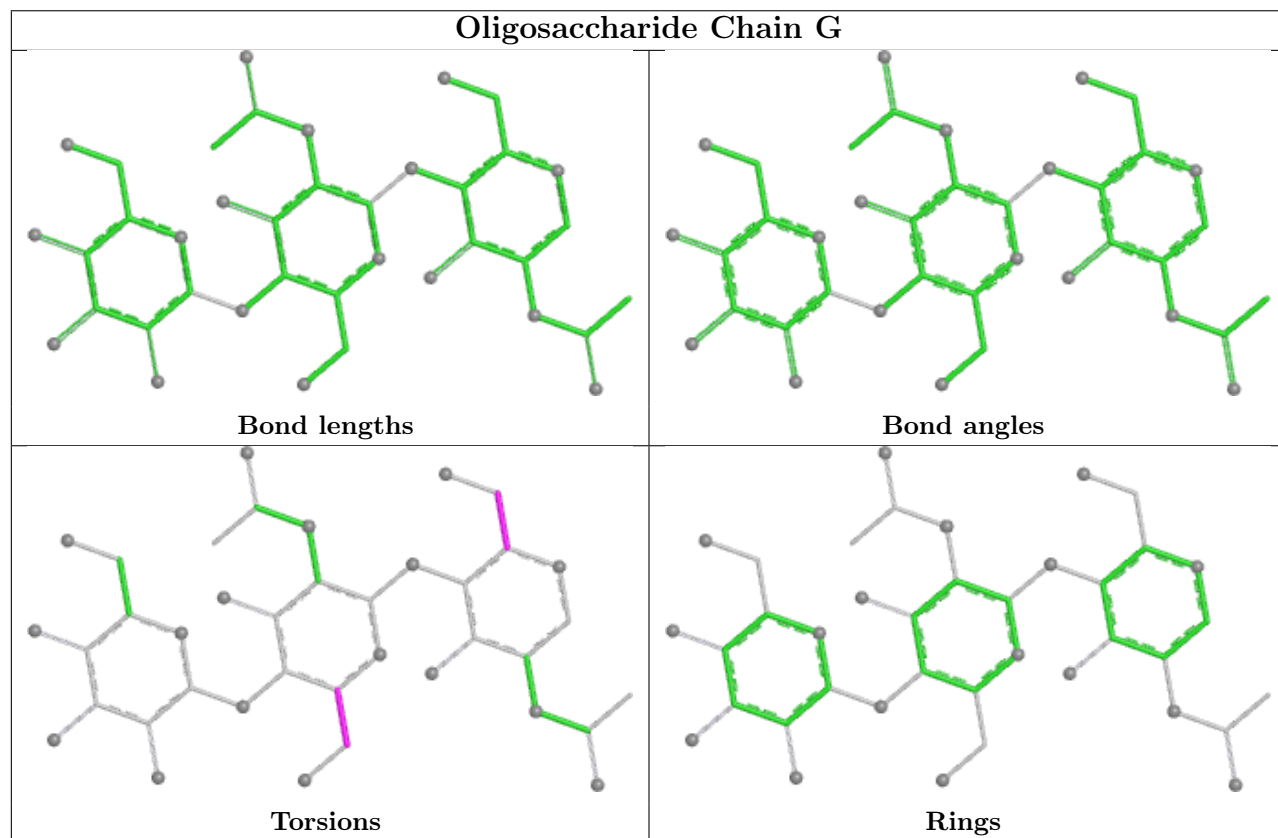
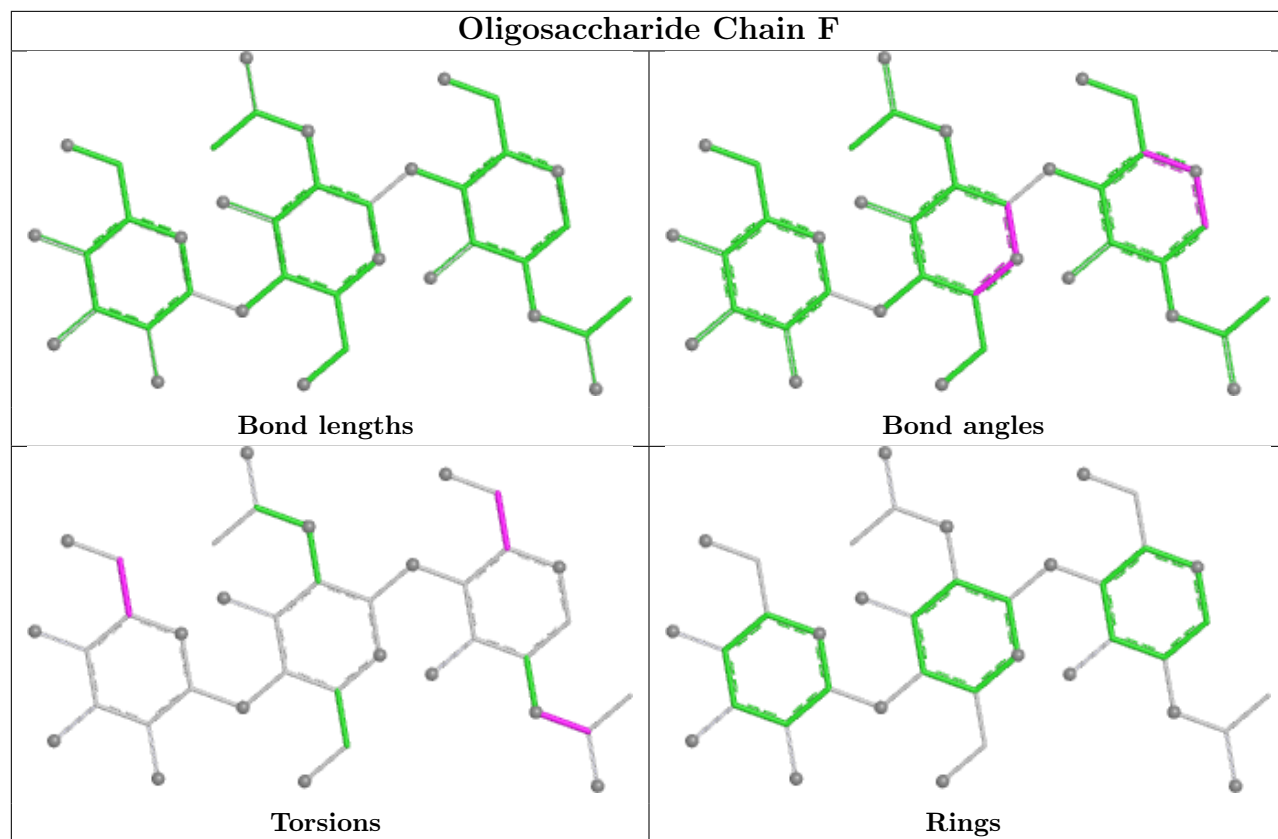
There are no ring outliers.

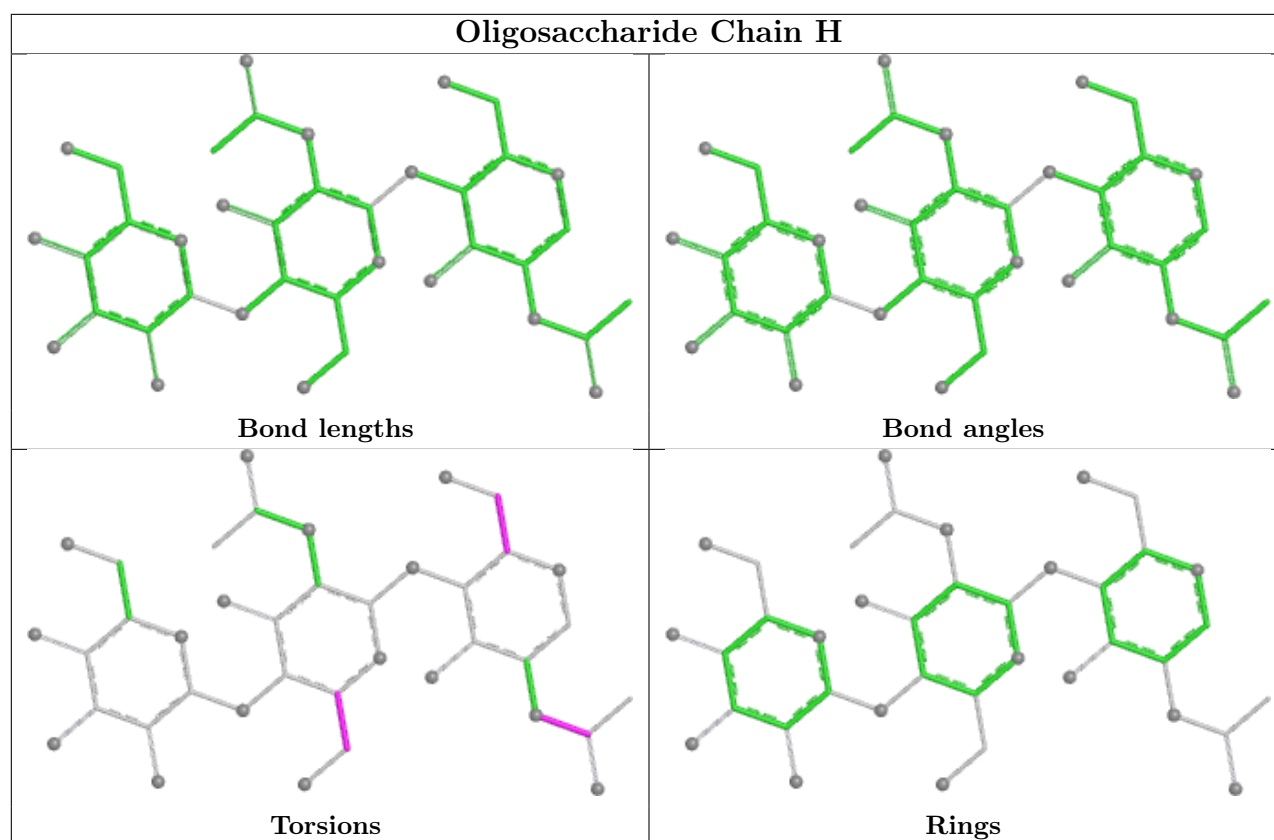
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
5	NAG	D	301	1	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	B	2001	2	14,14,15	0.24	0	17,19,21	0.42	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
5	NAG	D	301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2001	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

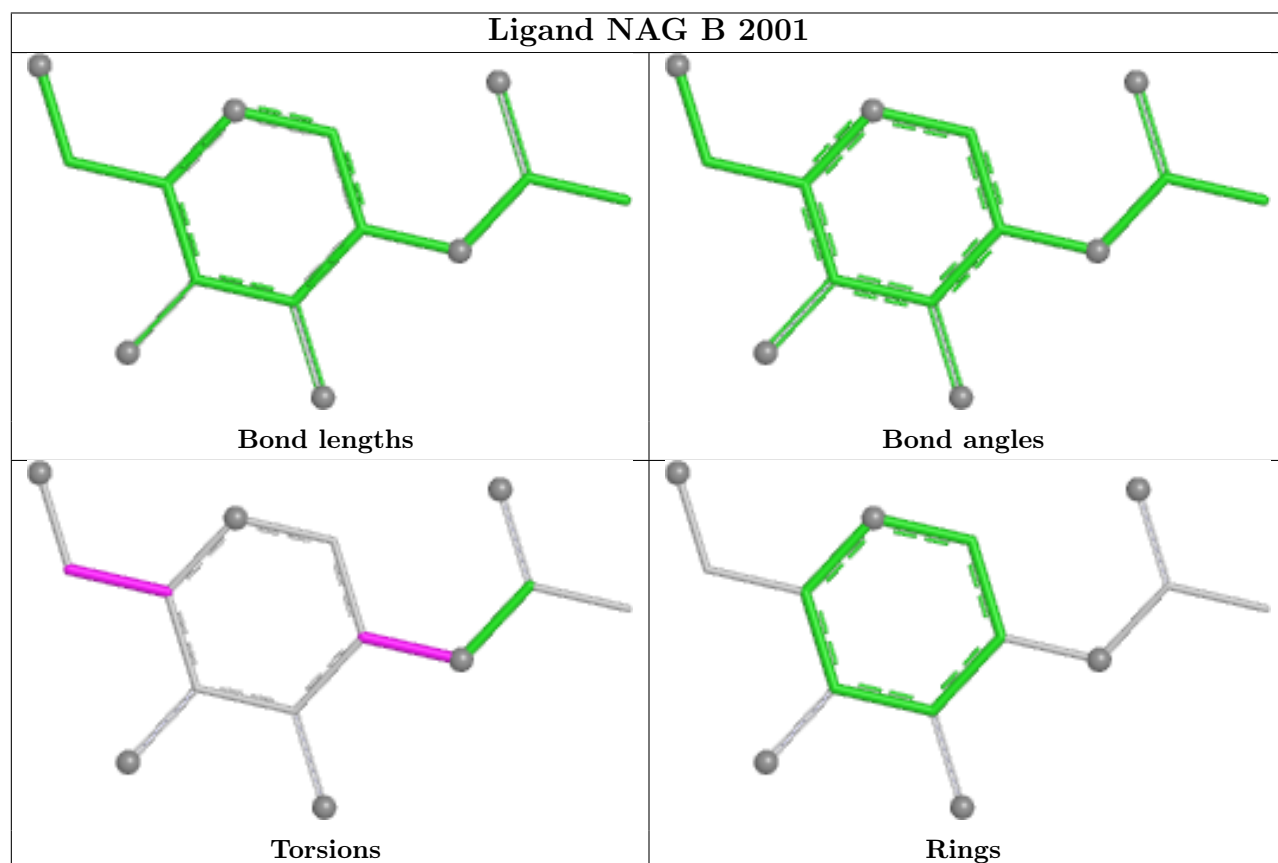
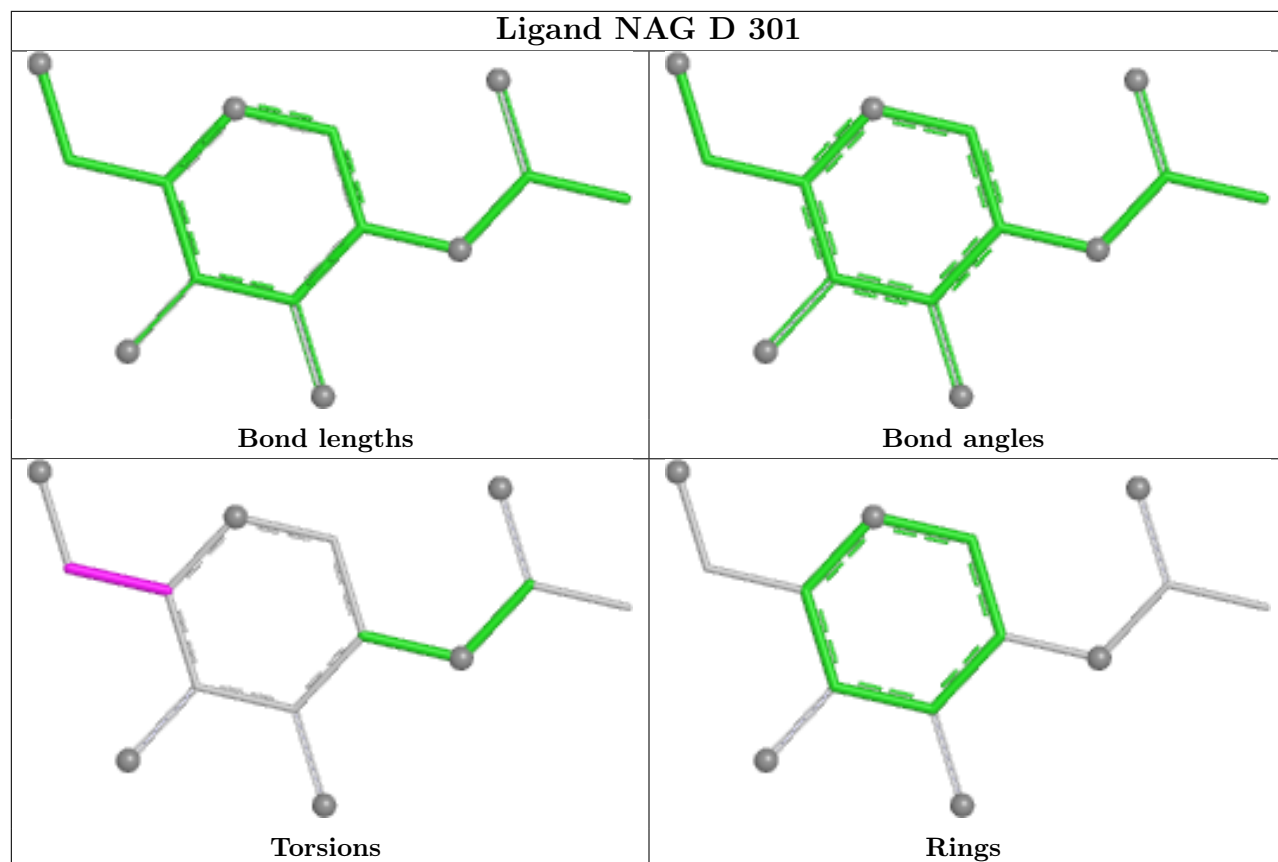
Mol	Chain	Res	Type	Atoms
5	D	301	NAG	C4-C5-C6-O6
5	D	301	NAG	O5-C5-C6-O6
5	B	2001	NAG	O5-C5-C6-O6
5	B	2001	NAG	C4-C5-C6-O6
5	B	2001	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.

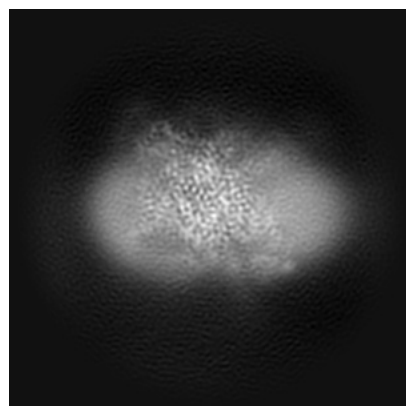
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34387. These allow visual inspection of the internal detail of the map and identification of artifacts.

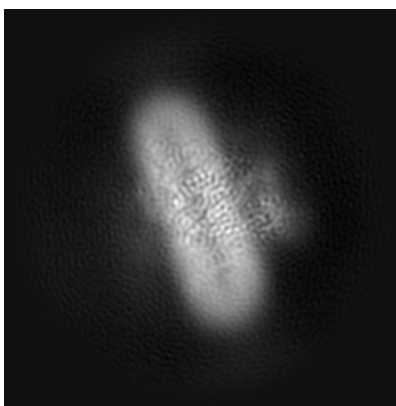
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

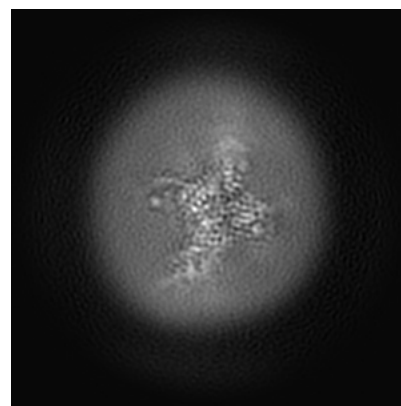
#### 6.1.1 Primary map



X

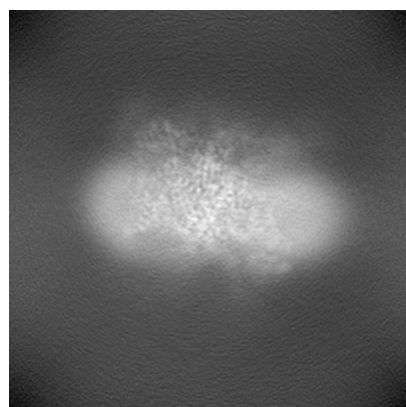


Y

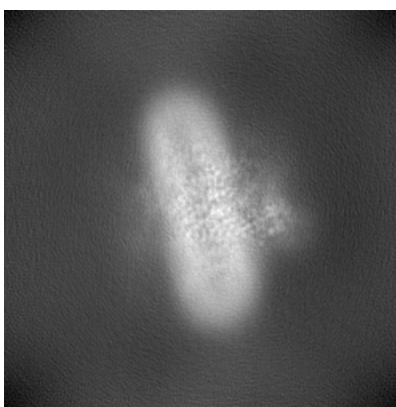


Z

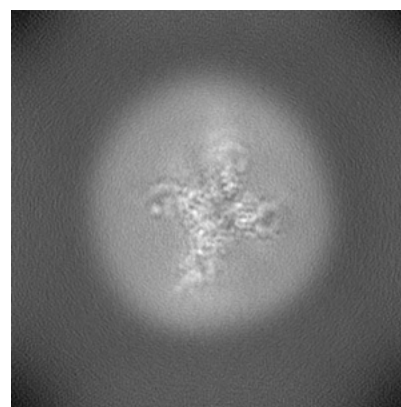
#### 6.1.2 Raw map



X



Y

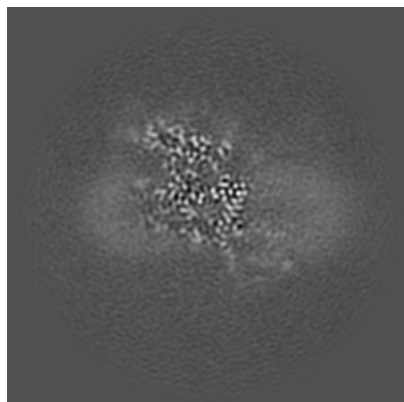


Z

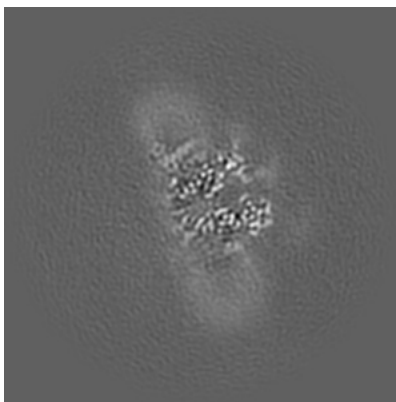
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

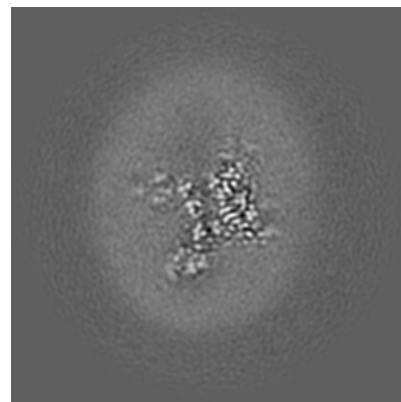
### 6.2.1 Primary map



X Index: 128

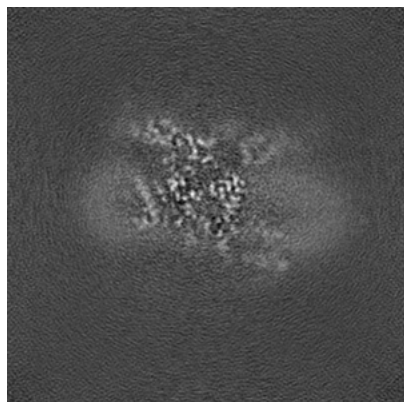


Y Index: 128

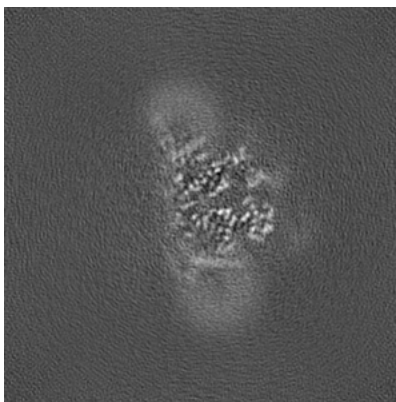


Z Index: 128

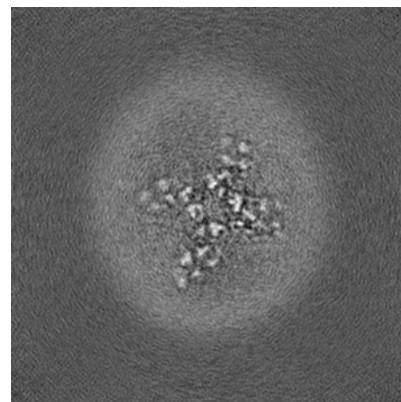
### 6.2.2 Raw map



X Index: 128



Y Index: 128

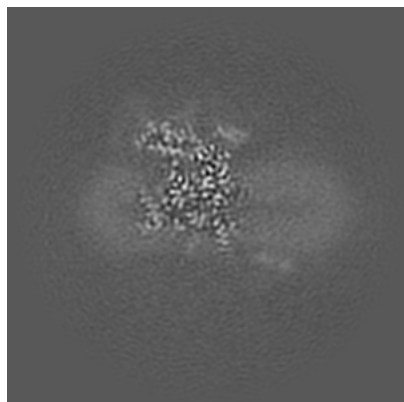


Z Index: 128

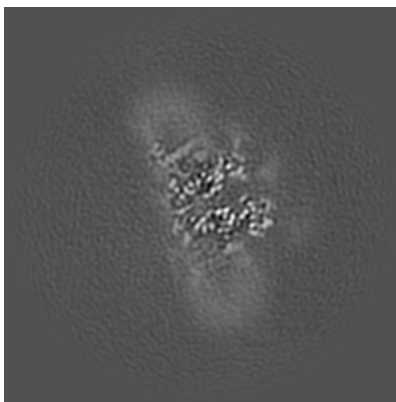
The images above show central slices of the map in three orthogonal directions.

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

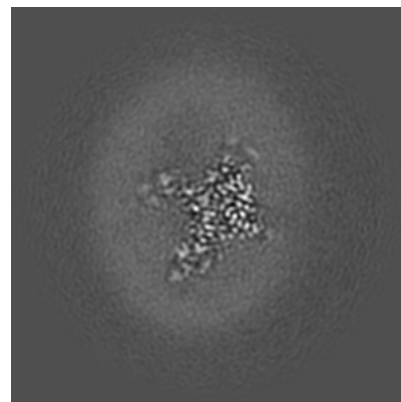
### 6.3.1 Primary map



X Index: 122

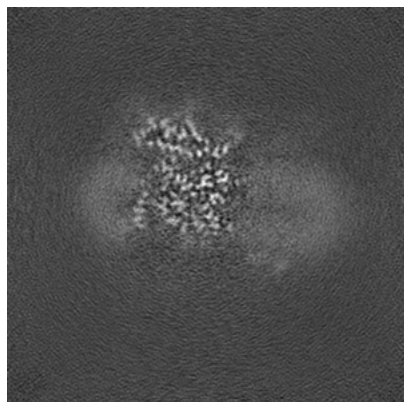


Y Index: 129

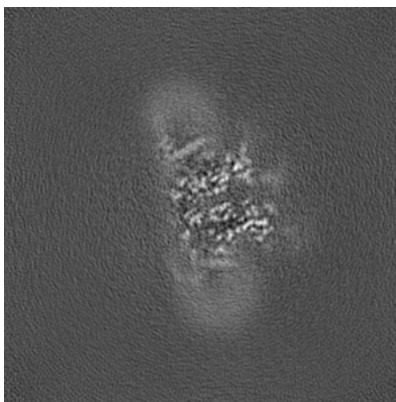


Z Index: 131

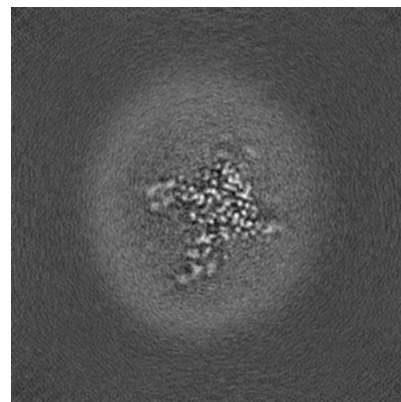
### 6.3.2 Raw map



X Index: 121



Y Index: 130

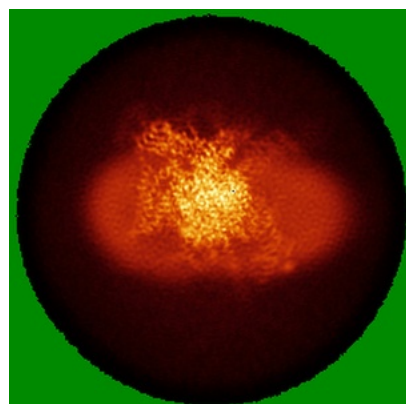


Z Index: 135

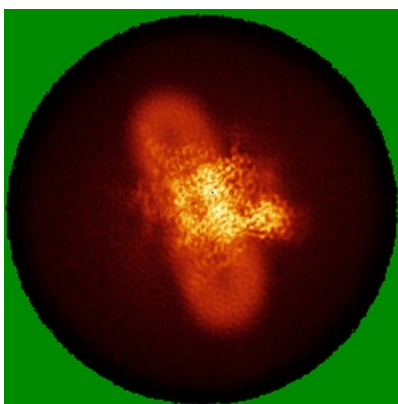
The images above show the largest variance slices of the map in three orthogonal directions.

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

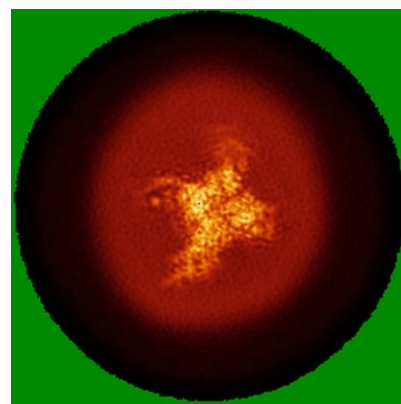
### 6.4.1 Primary map



X

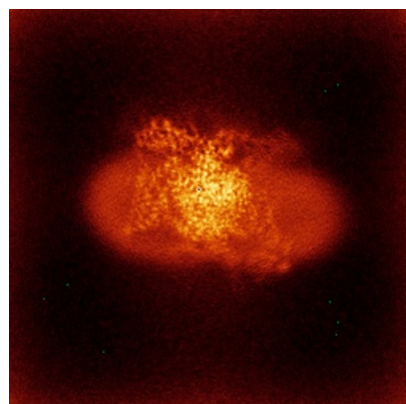


Y

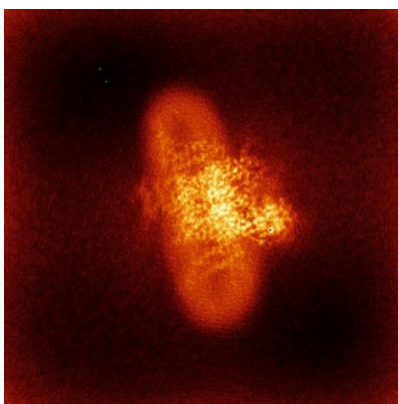


Z

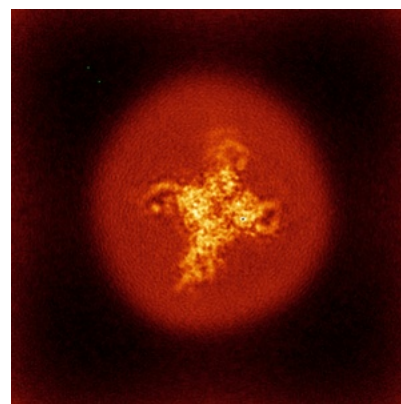
### 6.4.2 Raw map



X



Y



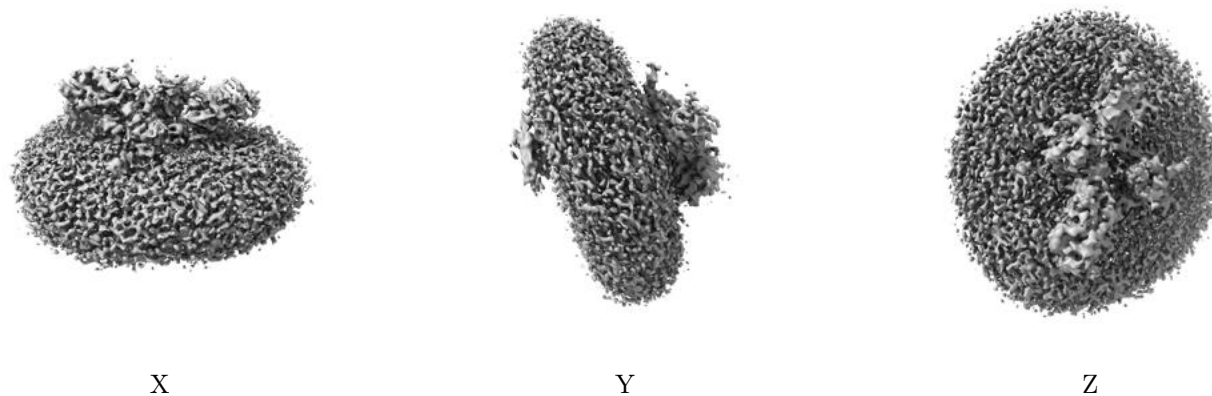
Z

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.



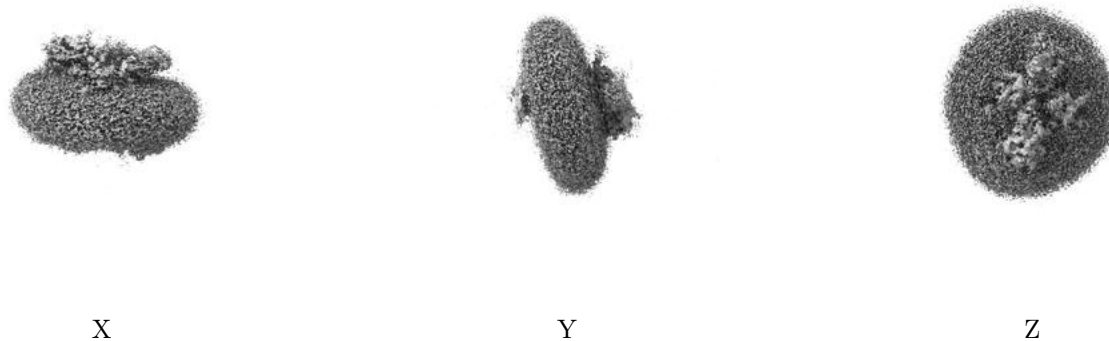
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

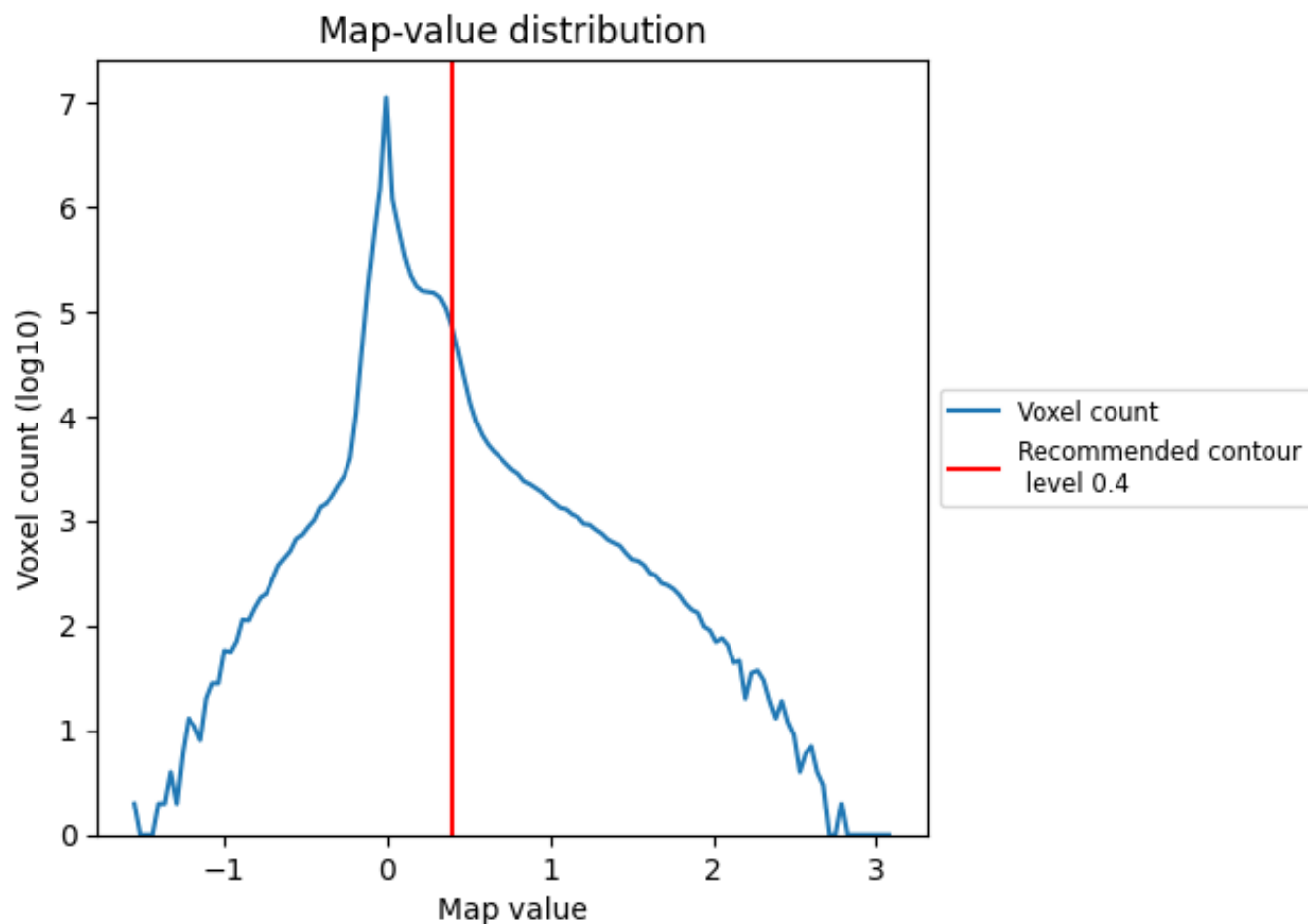
## 6.6 Mask visualisation [i](#)

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.

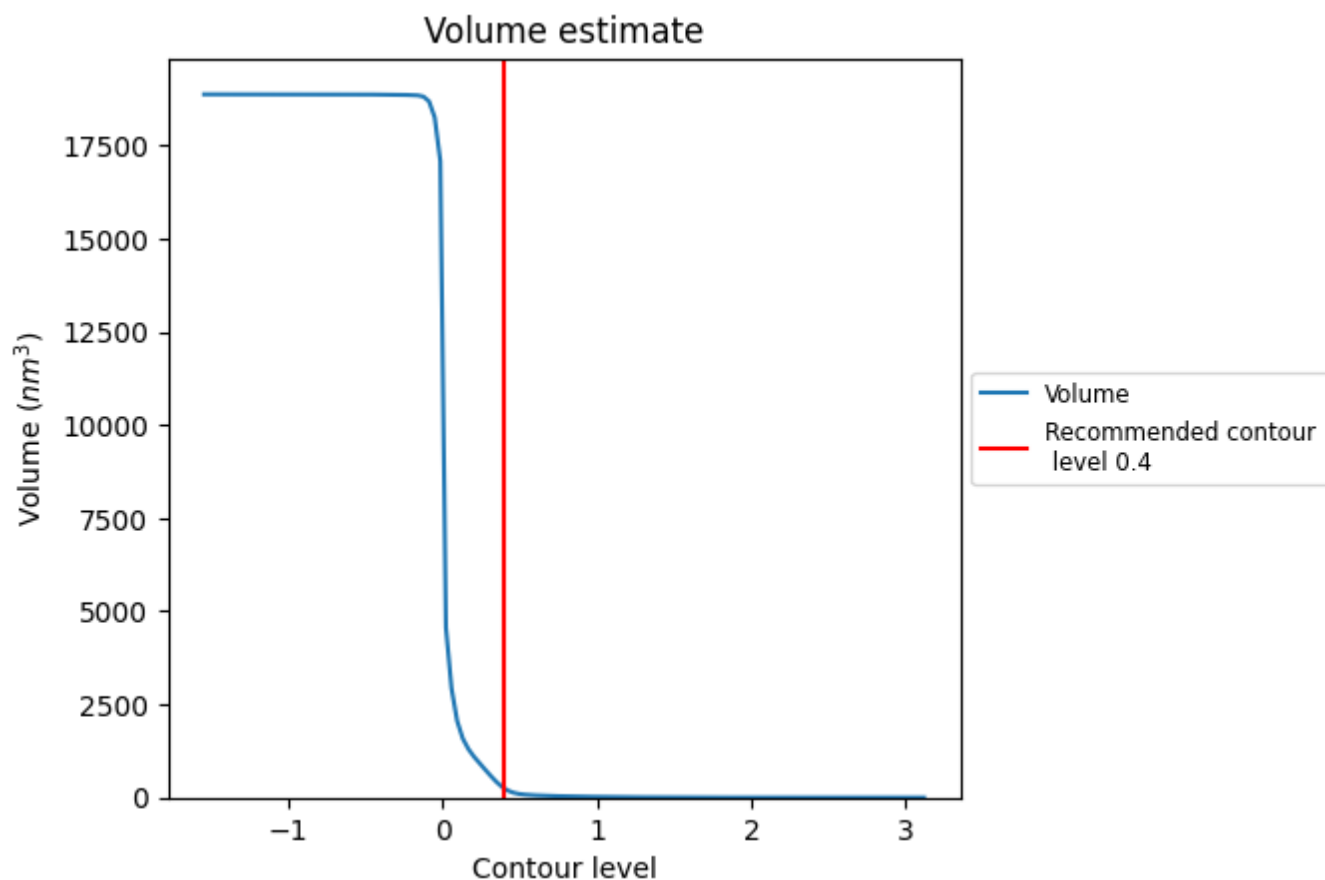
### 7.1 Map-value distribution [i](#)



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.



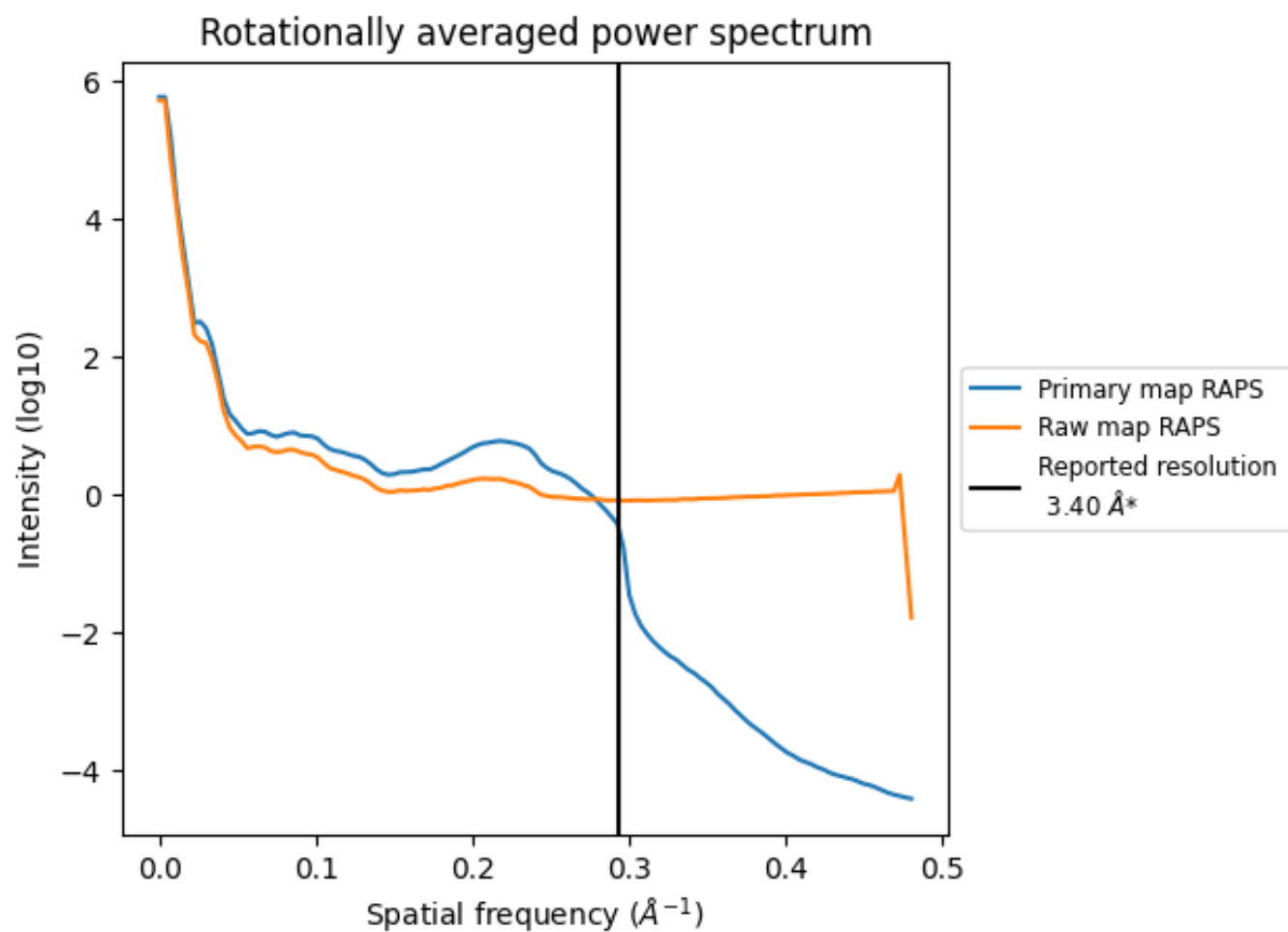
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm<sup>3</sup>; this corresponds to an approximate mass of 219 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 ⓘ

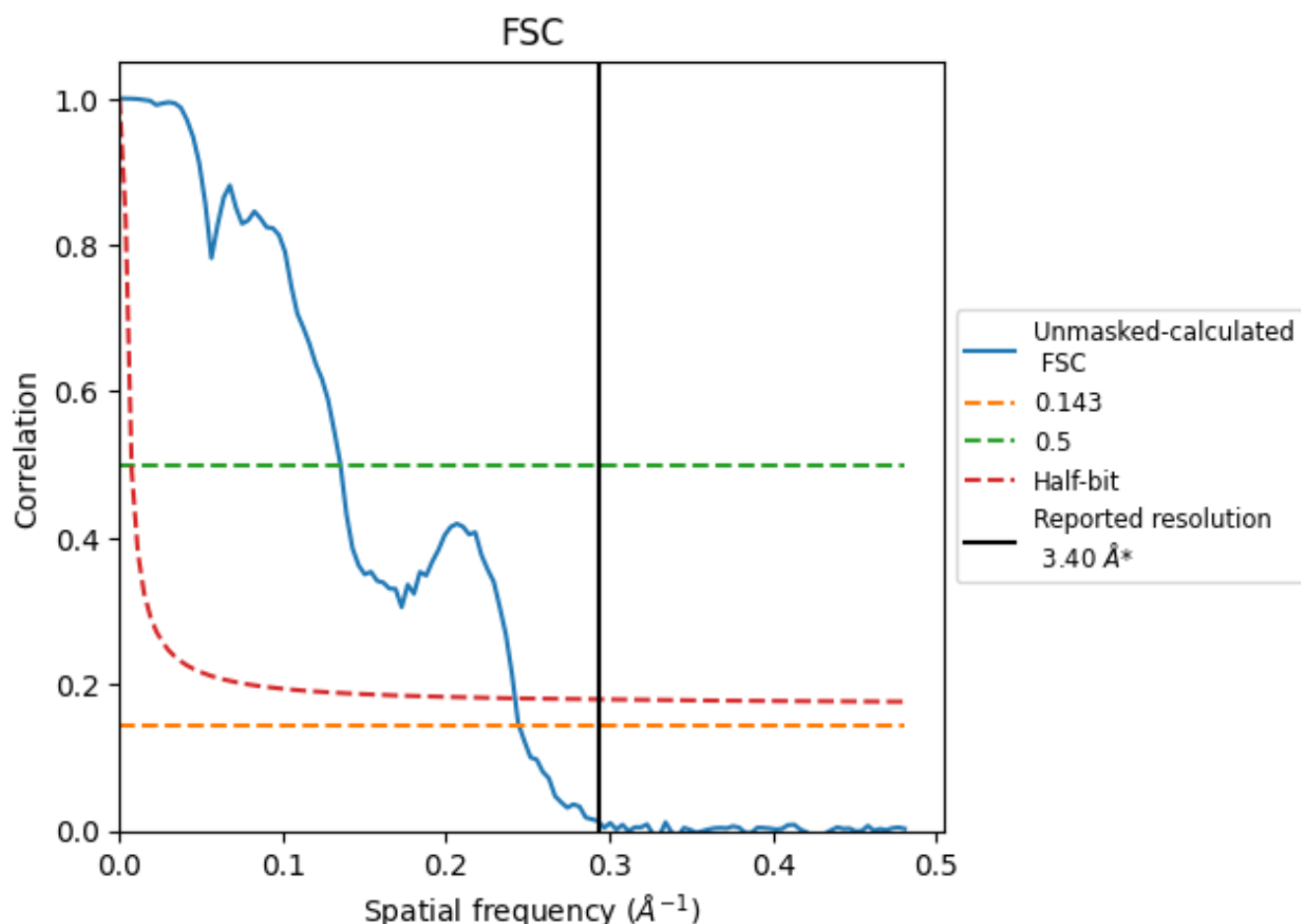


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

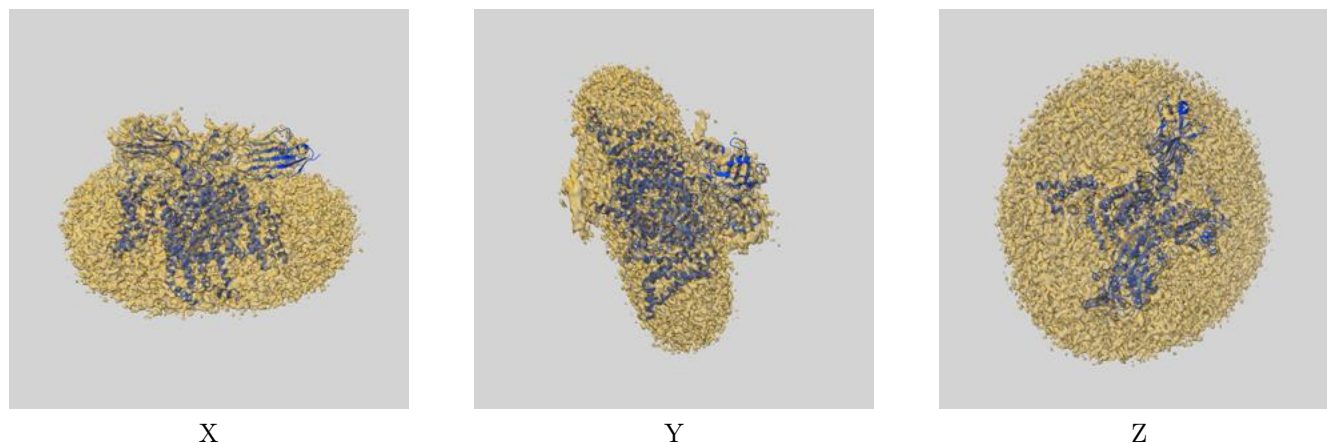
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	7.39	4.13

\*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 4.09 differs from the reported value 3.4 by more than 10 %

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

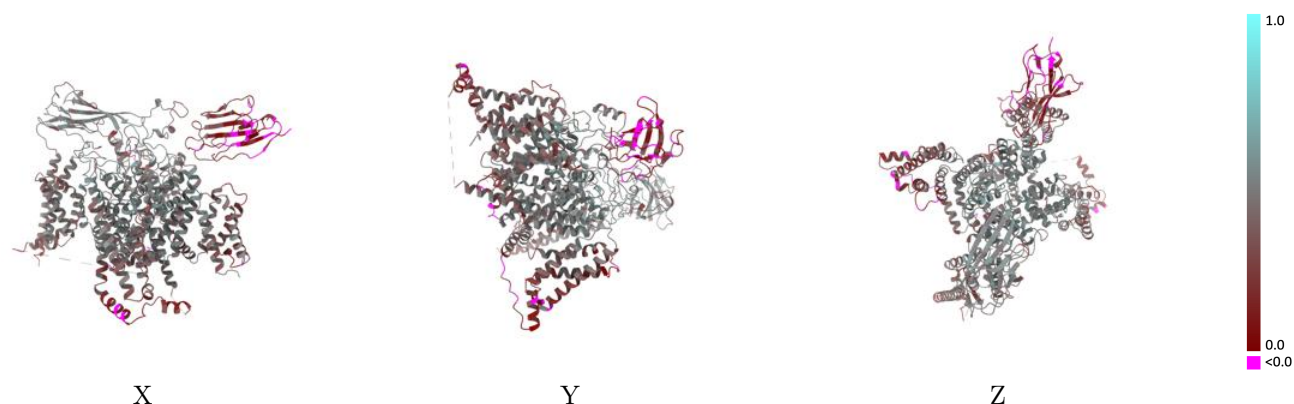
This section contains information regarding the fit between EMDB map EMD-34387 and PDB model 8GZ1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



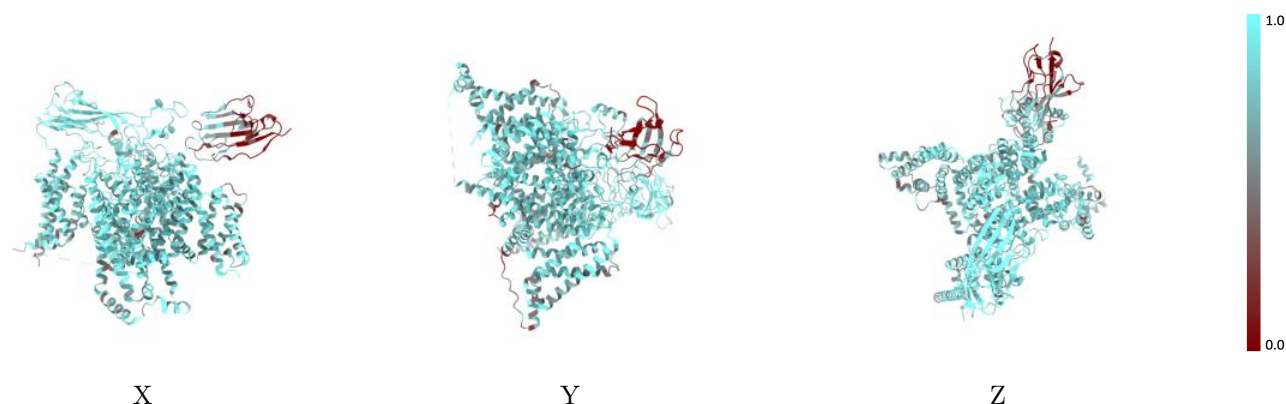
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



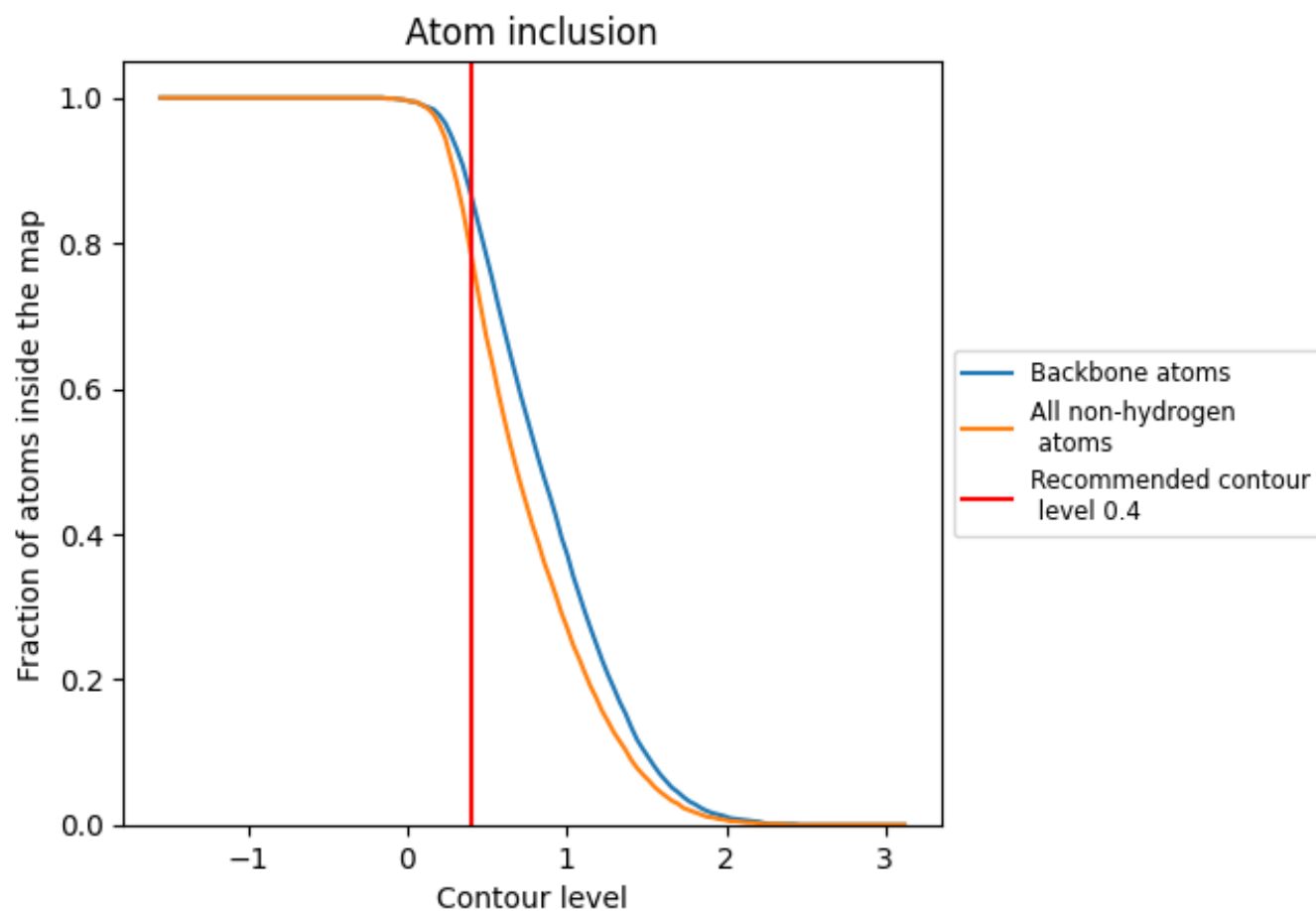
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7840	<div></div> 0.3910
A	<div></div> 0.4360	<div></div> 0.2640
B	<div></div> 0.8260	<div></div> 0.4130
C	<div></div> 0.3370	<div></div> 0.1240
D	<div></div> 0.8390	<div></div> 0.4350
E	<div></div> 0.6670	<div></div> 0.3880
F	<div></div> 0.8970	<div></div> 0.4400
G	<div></div> 0.6150	<div></div> 0.3110
H	<div></div> 0.5130	<div></div> 0.3000

1.0

0.0

<0.0