



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:08 PM UTC

PDB ID : 7KWO / pdb_00007kwo
EMDB ID : EMD-23057
Title : rFVIIIIFc-VWF-XTEN (BIVV001)
Authors : Fuller, J.R.; Batchelor, J.D.
Deposited on : 2020-12-01
Resolution : 2.90 Å (reported)
Based on initial models : 6N29, 6MF2

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

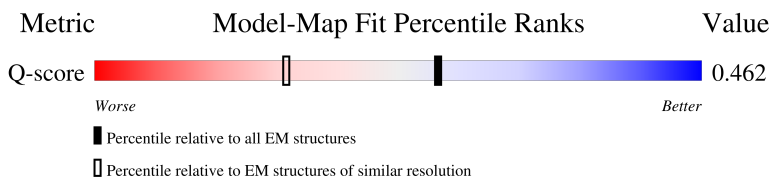
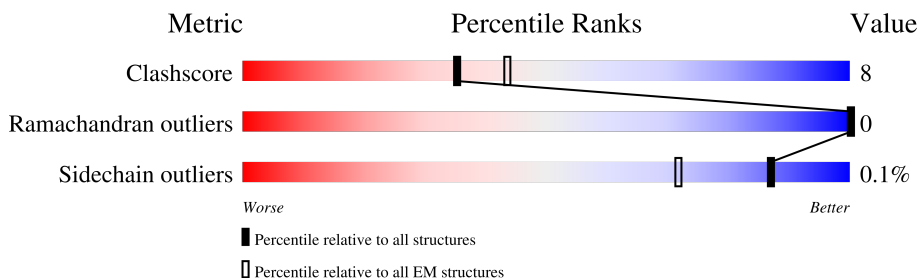
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1965	 13% 48% 13% 39%
2	V	1646	 23% 6% 71%
3	B	3	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13469 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.

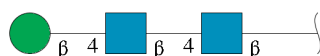
- Molecule 1 is a protein called Coagulation factor FVIII-Fc-XTEN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1200	Total	C	N	O	S	0	0
			9743	6288	1640	1759	56		

- Molecule 2 is a protein called von Willebrand factor-XTEN-Fc.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	478	Total	C	N	O	S	0	0
			3641	2244	632	707	58		

- Molecule 3 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
3	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	V	1	Total	Ca	0
			1	1	

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	

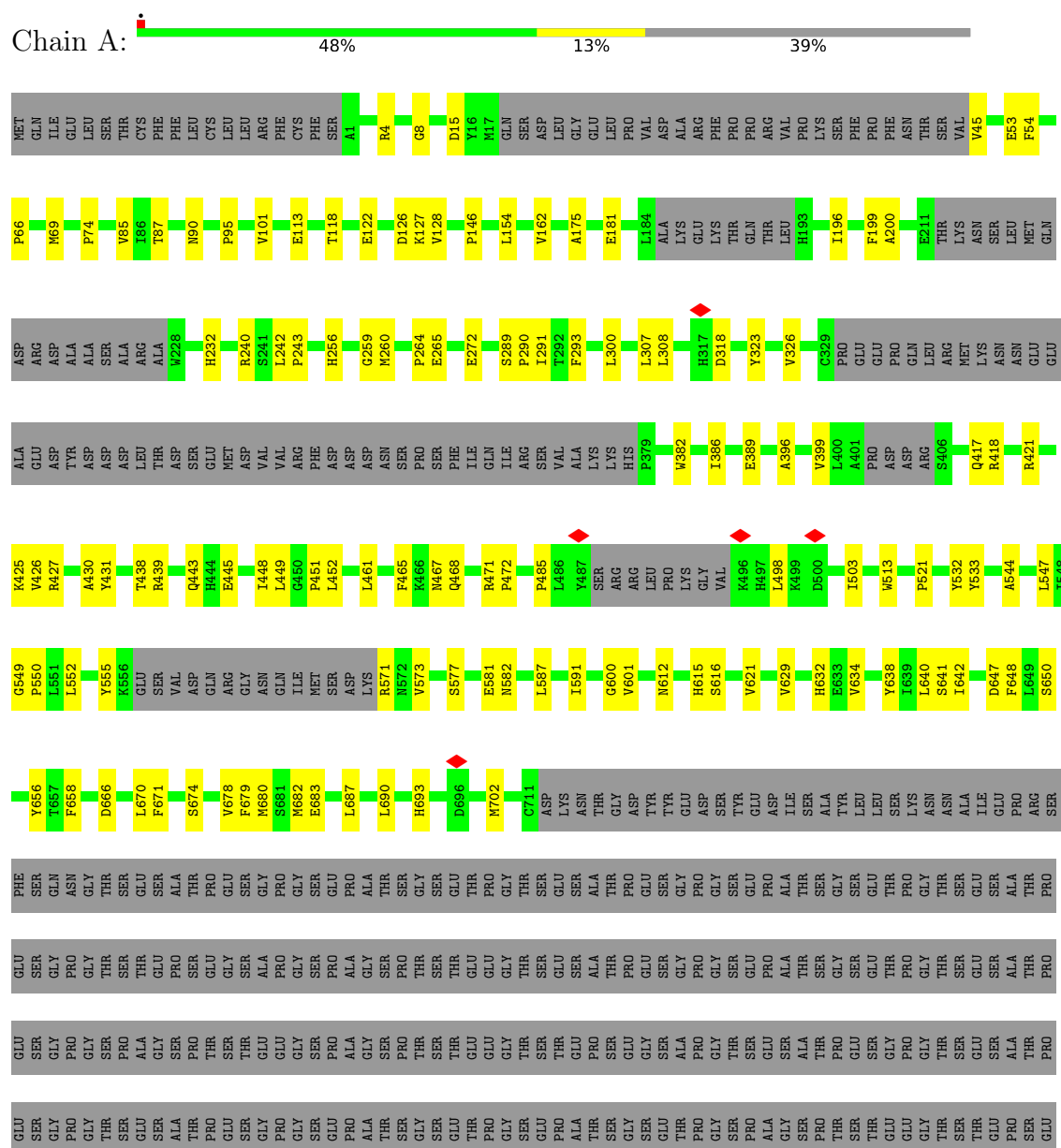
- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Cu	0
			1	1	

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: Coagulation factor FVIII-Fc-XTEN



GLY	THR	P1746	F1983	C2169	S2264	LEU	THR	THR	LYS
SER	LEU	W1889	F1986	C2173	D2267	THR	VAL	CYS	PRO
ALA	GLN	Y1890	V1986	S2173	D2267	VAL	GLY	LEU	ASP
PRO	SER	F1891	S1990	C2174	S2175	GLY	GLY	VAL	THR
GLY	GLN	N1894	S1991	S2175	S2175	ASP	THR	GLY	THR
THR	GLU	L1769	V1998	G2179	F2276	THR	PHE	GLY	THR
SER	THR	G1760	V1998	M2180	Q2276	ASP	ASP	THR	THR
THR	ILE	P1761	L2001	M2180	W2277	THR	THR	THR	THR
GLU	ASP	P1761	L2001	A2184	G2278	GLY	THR	THR	THR
PRO	TYR	R1764	R1900	I2185	K2279	THR	THR	THR	THR
SER	ASP	R1764	R1900	I2185	V2280	THR	THR	THR	THR
GLY	ASP	V1767	ALA	S2186	F2280	THR	THR	THR	THR
GLY	THR	V1767	PRO	Q2189	F2280	THR	THR	THR	THR
SER	THR	F1775	CYS	Q2189	D2298	THR	THR	THR	THR
ALA	ILE	F1775	ASN	S2194	D2298	THR	THR	THR	THR
PRO	SER	F1785	ILE	S2194	L2301	THR	THR	THR	THR
GLY	VAL	F1785	GLN	T2196	L2301	THR	THR	THR	THR
SER	GLU	F1785	MET	T2196	L2301	THR	THR	THR	THR
GLU	GLU	L1789	GLU	T2197	R2304	THR	THR	THR	THR
PRO	LYS	E1793	ASP	N2198	R2304	THR	THR	THR	THR
ALA	LYS	E1793	P1910	M2199	Q2313	THR	THR	THR	THR
THR	GLU	ASP	Y1916	F2200	Q2313	THR	THR	THR	THR
SER	GLN	ARG	H1919	A2201	Q2313	THR	THR	THR	THR
GLY	GLN	GLN	H1919	A2201	Q2313	THR	THR	THR	THR
GLU	GLY	GLY	D1927	P2205	Q2313	THR	THR	THR	THR
THR	ASP	ALA	T1928	S2206	Q2313	THR	THR	THR	THR
GLY	GLU	GLU	L1929	K2207	Q2313	THR	THR	THR	THR
THR	GLU	GLU	P1930	A2208	E2322	THR	THR	THR	THR
SER	ASN	ASN	P1802	R2209	Q2325	THR	THR	THR	THR
GLU	GLN	GLN	K1808	R2215	Q2329	THR	THR	THR	THR
SER	SER	SER	D1937	R2215	Q2329	THR	THR	THR	THR
ALA	PRO	ARG	Q1938	W2219	Q2329	THR	THR	THR	THR
THR	THR	SER	R1941	R2220	Q2329	THR	THR	THR	THR
GLY	PHE	GLN	Y1815	P2221	Q2329	THR	THR	THR	THR
SER	GLY	GLY	M1823	Q2222	Q2329	THR	THR	THR	THR
GLY	GLY	GLY	W1835	Q2222	Q2329	THR	THR	THR	THR
THR	THR	THR	A1836	Q2223	Q2329	THR	THR	THR	THR
GLY	GLY	GLY	Y1700	Q2223	Q2329	THR	THR	THR	THR
THR	THR	THR	S1713	Q2225	Q2329	THR	THR	THR	THR
SER	SER	SER	D1846	W2229	Q2329	THR	THR	THR	THR
THR	THR	THR	D1846	W2229	Q2329	THR	THR	THR	THR
GLU	PRO	HIS	I1852	T2237	Q2329	THR	THR	THR	THR
PRO	VAL	VAL	G1853	W2238	Q2329	THR	THR	THR	THR
GLY	LEU	LEU	L1856	K2239	Q2329	THR	THR	THR	THR
SER	ASN	ASN	H1859	V2240	Q2329	THR	THR	THR	THR
ALA	ARG	ARG	T1860	T2241	Q2329	THR	THR	THR	THR
PRO	GLN	GLN	A1974	T2244	Q2329	THR	THR	THR	THR
ALA	GLN	GLN	L1975	T2244	Q2329	THR	THR	THR	THR
SER	SER	SER	T1862	Q2246	Q2329	THR	THR	THR	THR
GLY	GLY	GLY	Y1976	Q2246	Q2329	THR	THR	THR	THR
SER	GLY	GLY	Q1870	K2249	Q2329	THR	THR	THR	THR
ILE	THR	THR	T1881	S2250	Q2329	THR	THR	THR	THR
THR	ARG	ARG	F1738	L2251	Q2329	THR	THR	THR	THR
THR	THR	THR	F1738	L2252	Q2329	THR	THR	THR	THR
THR	THR	THR	F1738	T2253	Q2329	THR	THR	THR	THR
THR	THR	THR	F1738	S2254	Q2329	THR	THR	THR	THR
THR	THR	THR	F1738	M2255	Q2329	THR	THR	THR	THR

• Molecule 2: von Willebrand factor-XTEN-Fc



VAL	THR	GLU	LEU	MET
ASP	SER	THR	ALA	ILE
PRO	ASP	GLU	GLY	ALA
GLU	PRO	ALA	GLY	ALA
PRO	THR	GLY	CYS	PHE
PHE	ASP	TYR	GLN	ALA
VAL	PHE	TYR	LYS	ALA
GLY	ALA	LYS	ARG	GLY
LEU	ASN	LEU	SER	VAL
CYS	SER	SER	PHE	LEU
GLU	TRP	GLY	SER	LEU
LYS	ALA	GLU	ILE	ALA
THR	LEU	ALA	ILE	LEU
LEU	SER	TYR	GLY	ALA
CYS	SER	GLY	ASP	LEU
GLU	GLY	PHE	PHE	ILE
CYS	GLU	VAL	GLN	LEU
ALA	GLN	ALA	ASN	PRO
GLY	TRP	ARG	GLY	GLY
GLY	CYS	ILE	LYS	THR
LEU	GLU	ASP	ARG	LEU
GLU	ARG	GLY	VAL	CYS
CYS	ALA	SER	SER	ALA
ALA	SER	GLY	LEU	GLU
CYS	PRO	ASN	SER	GLY
PRO	PRO	PHE	VAL	THR
ALA	SER	GLN	THR	ARG
ARG	SER	ASP	ILE	ALA
THR	SER	TYR	ILE	ARG
CYS	GLY	PHE	HIS	CYS
ALA	GLU	ASN	LEU	SER
GLN	MET	LYS	PHE	LEU
GLU	LYS	THR	VAL	GLY
GLY	LYS	CYS	GLY	GLY
MET	LEU	GLY	GLY	SER
VAL	LEU	THR	VAL	ASP
LEU	TRP	CYS	VAL	ASP
TYR	GLU	GLY	THR	PHE
GLY	GLN	ASN	GLN	VAL
TRP	CYS	PHE	GLY	ASN
THR	GLN	ASN	ASP	PHE
ASP	LEU	ILE	ARG	GLY
HIS	LEU	PHE	VAL	SER
SER	LYS	ALA	SER	THR
ALA	SER	GLU	GLU	TYR
CYS	THR	ASP	MET	SER
PRO	SER	SER	PRO	PHE
VAL	PHE	MET	ALA	ALA
CYS	ALA	THR	SER	GLY
PRO	ARG	GLN	LYS	TYR
ALA	GLY	GLU	GLY	CYS
GLY	HIS	GLY	LEU	SER
MET	PRO	THR	TYR	THR



HIS ASN HIS TYR THR GLN LYS SER LEU SER LEU SER PRO GLY

NAG1
NAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116200	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.036	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0145	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: CA, ZN, TYS, CU, BMA, NAG

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	0.16	0/10002	0.35	0/13549
2	V	0.16	0/3717	0.36	0/5052
All	All	0.16	0/13719	0.35	0/18601

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	9743	0	9487	156	0
2	V	3641	0	3445	58	0
3	B	39	0	34	0	0
4	A	28	0	26	0	0
4	V	14	0	13	0	0
5	A	1	0	0	0	0
5	V	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
All	All	13469	0	13005	210	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 8.

All (210) 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:V:870:ILE:O	2:V:874:HIS:HB2	1.78	0.82
1:A:265:GLU:H	1:A:290:PRO:HG3	1.47	0.79
1:A:1678:ASP:OD1	2:V:820:ARG:NH1	2.17	0.78
1:A:615:HIS:HB3	1:A:702:MET:HE3	1.70	0.73
1:A:113:GLU:HB2	1:A:126:ASP:HB3	1.71	0.72
1:A:1936:GLN:NE2	1:A:1991:SER:O	2.22	0.71
2:V:1225:CYS:HB3	2:V:1232:LEU:HD11	1.74	0.69
1:A:658:PHE:HB3	1:A:680:MET:HE2	1.74	0.68
1:A:2063:SER:OG	1:A:2159:ARG:NH1	2.27	0.67
2:V:870:ILE:HG22	2:V:1083:VAL:HG11	1.76	0.67
1:A:1965:VAL:HG12	1:A:1986:VAL:HG12	1.75	0.67
1:A:425:LYS:NZ	1:A:544:ALA:O	2.27	0.67
2:V:971:SER:HB2	2:V:983:VAL:HB	1.79	0.65
1:A:389:GLU:OE1	1:A:439:ARG:NH1	2.30	0.65
1:A:2246:GLN:NE2	1:A:2290:PHE:O	2.30	0.64
1:A:300:LEU:HD13	1:A:326:VAL:HG22	1.80	0.64
1:A:2264:SER:HB3	1:A:2301:LEU:HD21	1.80	0.64
1:A:389:GLU:OE2	1:A:431:TYR:OH	2.16	0.63
2:V:965:LEU:HD21	2:V:1166:PRO:HD3	1.81	0.62
1:A:1894:ASN:OD1	1:A:1897:ARG:NH2	2.32	0.62
2:V:1045:THR:OG1	2:V:1089:CYS:O	2.17	0.62
1:A:259:GLY:O	1:A:291:ILE:HA	2.00	0.62
1:A:532:TYR:HB3	1:A:640:LEU:HD21	1.80	0.62
1:A:1680:TYS:O1	1:A:1680:TYS:HE1	1.98	0.62
1:A:1962:VAL:HG12	1:A:1974:ALA:HB2	1.82	0.61
1:A:2255:MET:HA	1:A:2314:VAL:O	2.01	0.61
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.84	0.60
1:A:272:GLU:HG2	1:A:307:LEU:H	1.65	0.60
2:V:844:ILE:O	2:V:847:ASN:ND2	2.35	0.59
2:V:788:CYS:SG	2:V:801:SER:OG	2.59	0.59
1:A:2025:LEU:HD12	1:A:2166:LEU:HB3	1.84	0.59
1:A:2206:SER:O	1:A:2209:ARG:NH1	2.34	0.59
2:V:1143:GLU:OE1	2:V:1145:ARG:NH2	2.36	0.59
1:A:293:PHE:CE2	1:A:1975:LEU:HD12	2.39	0.58
1:A:399:VAL:O	1:A:421:ARG:NH2	2.34	0.58
1:A:2185:ILE:O	1:A:2209:ARG:NH2	2.35	0.58
1:A:471:ARG:HG2	1:A:472:PRO:HD2	1.86	0.57
2:V:1229:VAL:HG12	2:V:1230:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HD2	1:A:85:VAL:HB	1.85	0.57
1:A:53:GLU:HB2	1:A:74:PRO:HG3	1.87	0.56
1:A:2196:PHE:N	1:A:2220:ARG:O	2.31	0.56
2:V:1123:ALA:HA	2:V:1127:PRO:HB3	1.88	0.56
1:A:1975:LEU:HD11	1:A:2001:LEU:HD12	1.87	0.56
1:A:66:PRO:HG2	1:A:69:MET:HG3	1.87	0.56
1:A:2076:LEU:O	1:A:2147:ARG:NH1	2.38	0.56
1:A:616:SER:HB3	1:A:621:VAL:HG22	1.89	0.55
1:A:687:LEU:HB3	1:A:1802:PRO:HB3	1.88	0.55
1:A:196:ILE:HD13	1:A:256:HIS:HB2	1.88	0.55
2:V:1206:PHE:HD2	2:V:1210:LYS:HB3	1.71	0.55
2:V:1208:SER:OG	2:V:1228:ASP:O	2.22	0.55
2:V:1148:SER:HA	2:V:1171:GLU:HG3	1.89	0.55
1:A:417:GLN:NE2	1:A:600:GLY:O	2.40	0.55
1:A:2169:CYS:SG	1:A:2173:SER:HA	2.46	0.55
1:A:2205:PRO:HA	1:A:2219:TRP:HB2	1.87	0.55
1:A:648:PHE:CZ	1:A:1953:ILE:HD11	2.42	0.54
1:A:650:SER:HB2	1:A:693:HIS:HB2	1.90	0.54
1:A:200:ALA:HB1	1:A:260:MET:HE2	1.88	0.54
1:A:399:VAL:HB	1:A:421:ARG:HH12	1.72	0.54
1:A:658:PHE:HB2	1:A:678:VAL:CG1	2.37	0.54
1:A:2093:PHE:HZ	2:V:989:GLN:OE1	1.91	0.54
2:V:960:ARG:HE	2:V:1128:GLN:HE22	1.55	0.54
1:A:2198:ASN:OD1	1:A:2201:ALA:N	2.34	0.54
2:V:889:CYS:HB2	2:V:891:TYR:CZ	2.42	0.54
1:A:2249:LYS:NZ	2:V:1078:GLU:OE2	2.40	0.54
1:A:15:ASP:HB3	1:A:45:VAL:HG22	1.88	0.54
2:V:1056:VAL:HG13	2:V:1088:THR:HB	1.89	0.53
2:V:791:THR:HG22	2:V:793:GLN:H	1.73	0.53
1:A:113:GLU:OE1	1:A:127:LYS:NZ	2.32	0.53
1:A:629:VAL:HG21	1:A:682:MET:HE2	1.89	0.53
1:A:2117:GLY:HA2	1:A:2142:PRO:HD2	1.90	0.53
1:A:467:ASN:ND2	1:A:503:ILE:O	2.42	0.52
2:V:977:HIS:ND1	2:V:1102:ASP:OD2	2.42	0.52
2:V:1158:GLN:HE21	2:V:1186:LEU:HG	1.73	0.52
1:A:449:LEU:HD22	1:A:550:PRO:HD3	1.91	0.52
1:A:4:ARG:NH2	1:A:87:THR:OG1	2.42	0.52
1:A:632:HIS:ND1	1:A:683:GLU:OE1	2.40	0.51
1:A:1881:THR:OG1	1:A:1947:MET:O	2.20	0.51
1:A:1767:VAL:CG2	1:A:1860:THR:HG23	2.40	0.51
1:A:2180:MET:HG2	1:A:2185:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PRO:HA	1:A:290:PRO:HG2	1.92	0.51
1:A:426:VAL:HG22	1:A:547:LEU:HD21	1.93	0.51
2:V:881:LEU:HD23	2:V:1006:ASP:HB2	1.92	0.50
2:V:1214:LEU:O	2:V:1222:CYS:HA	2.10	0.50
1:A:1759:LEU:HD23	1:A:1852:ILE:HG23	1.92	0.50
1:A:1789:LEU:HD11	1:A:1835:TRP:CD1	2.47	0.50
2:V:1211:LYS:HE3	2:V:1226:HIS:HE1	1.76	0.50
1:A:2237:THR:HA	1:A:2304:ARG:HG2	1.94	0.50
1:A:1859:HIS:O	1:A:1862:THR:OG1	2.27	0.50
1:A:382:TRP:HB2	1:A:461:LEU:HD23	1.92	0.50
1:A:2070:TRP:HA	1:A:2151:LEU:O	2.12	0.50
1:A:1919:HIS:HB3	1:A:2010:MET:HE3	1.94	0.49
1:A:386:ILE:O	1:A:465:PHE:HA	2.13	0.49
2:V:1215:ASN:HB3	2:V:1218:ASP:HB3	1.94	0.49
1:A:199:PHE:HZ	1:A:308:LEU:HD21	1.78	0.49
1:A:90:ASN:ND2	1:A:128:VAL:O	2.30	0.49
1:A:2093:PHE:HZ	2:V:989:GLN:CD	2.21	0.48
1:A:1749:ARG:HG3	1:A:1753:ASN:HB2	1.95	0.48
1:A:1944:LEU:HB3	1:A:1978:LEU:HD21	1.94	0.48
1:A:2244:THR:HB	1:A:2322:GLU:HB3	1.94	0.48
1:A:2229:TRP:HA	1:A:2308:ILE:O	2.14	0.48
1:A:656:TYR:HE1	1:A:682:MET:HA	1.77	0.48
1:A:396:ALA:O	1:A:421:ARG:NH1	2.47	0.48
2:V:1158:GLN:NE2	2:V:1184:ASP:OD1	2.45	0.48
1:A:581:GLU:HB2	1:A:612:ASN:HB3	1.95	0.48
1:A:550:PRO:HB3	1:A:573:VAL:HG11	1.95	0.48
2:V:1008:THR:HA	2:V:1014:VAL:HA	1.96	0.48
1:A:2048:PRO:HA	1:A:2062:TRP:HB2	1.96	0.47
1:A:1927:ASP:HB3	1:A:2013:LEU:HG	1.96	0.47
1:A:122:GLU:OE2	1:A:2239:LYS:NZ	2.36	0.47
1:A:443:GLN:HG2	1:A:445:GLU:H	1.79	0.47
1:A:2089:ALA:HB3	1:A:2161:THR:HG21	1.95	0.47
2:V:872:MET:HE2	2:V:1099:ALA:HB2	1.95	0.47
1:A:2223:VAL:O	1:A:2225:ASN:ND2	2.48	0.47
1:A:467:ASN:HD21	1:A:472:PRO:HA	1.80	0.47
1:A:2186:SER:HB3	1:A:2189:GLN:HG3	1.96	0.47
1:A:571:ARG:HA	1:A:638:TYR:HE2	1.80	0.47
1:A:2241:THR:HG22	1:A:2325:GLY:HA2	1.95	0.47
1:A:1886:THR:HA	1:A:1891:PHE:CD1	2.50	0.46
2:V:1146:TYR:OH	2:V:1171:GLU:OE2	2.28	0.46
1:A:671:PHE:O	1:A:674:SER:OG	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:960:ARG:NE	2:V:1128:GLN:HE22	2.13	0.46
2:V:973:VAL:HB	2:V:981:SER:HB2	1.98	0.46
2:V:1046:CYS:O	2:V:1053:GLN:NE2	2.48	0.46
2:V:1122:THR:HG23	2:V:1125:LEU:H	1.79	0.46
1:A:417:GLN:O	1:A:418:ARG:NH1	2.44	0.46
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.51	0.46
1:A:582:ASN:HA	1:A:587:LEU:HD22	1.98	0.46
1:A:2207:LYS:NZ	1:A:2215:ARG:O	2.46	0.46
2:V:1208:SER:HA	2:V:1227:CYS:HB3	1.97	0.46
1:A:1899:CYS:SG	1:A:1916:TYR:OH	2.73	0.46
1:A:2313:TRP:HB2	1:A:2316:GLN:O	2.15	0.46
1:A:2026:GLY:HA3	1:A:2031:HIS:HB3	1.98	0.46
1:A:2179:GLY:HA3	1:A:2184:ALA:HB3	1.96	0.46
1:A:2194:SER:HB3	1:A:2222:GLN:HG2	1.97	0.46
1:A:666:ASP:HB2	1:A:1835:TRP:HZ3	1.81	0.45
1:A:2275:PHE:HA	1:A:2280:VAL:HA	1.98	0.45
1:A:260:MET:HA	1:A:291:ILE:HD13	1.98	0.45
1:A:427:ARG:HD2	1:A:448:ILE:HA	1.98	0.45
2:V:1184:ASP:O	2:V:1188:GLN:N	2.50	0.45
1:A:175:ALA:HB2	1:A:196:ILE:HG21	1.98	0.45
1:A:452:LEU:HD11	1:A:552:LEU:HG	1.98	0.45
1:A:577:SER:HA	1:A:642:ILE:O	2.17	0.45
1:A:430:ALA:HB2	1:A:451:PRO:HB3	1.99	0.45
2:V:829:CYS:SG	2:V:836:TYR:HB2	2.57	0.45
2:V:925:VAL:HB	2:V:936:LEU:HB2	1.99	0.45
1:A:1929:LEU:HD12	1:A:1930:PRO:HD2	1.99	0.44
1:A:2021:CYS:SG	1:A:2175:SER:HB2	2.58	0.44
2:V:1043:PRO:O	2:V:1047:HIS:N	2.50	0.44
1:A:242:LEU:HD12	1:A:243:PRO:HD2	1.98	0.44
1:A:2071:ILE:HG21	1:A:2162:LEU:HD23	1.98	0.44
1:A:641:SER:HB2	1:A:670:LEU:HD13	1.99	0.44
2:V:907:ILE:HG12	2:V:927:ILE:HG23	1.98	0.44
1:A:438:THR:O	1:A:438:THR:HG23	2.17	0.44
1:A:634:VAL:CG1	1:A:679:PHE:CE2	3.01	0.44
1:A:647:ASP:HB2	1:A:1950:ASN:ND2	2.32	0.43
2:V:897:TYR:HE1	2:V:906:ARG:HB2	1.83	0.43
2:V:1109:HIS:O	2:V:1113:GLN:HG2	2.18	0.43
1:A:1700:ILE:O	1:A:1775:PHE:HA	2.18	0.43
1:A:389:GLU:OE2	1:A:468:GLN:NE2	2.51	0.43
1:A:1737:GLU:HB2	1:A:1761:PRO:CG	2.49	0.43
1:A:591:ILE:HG23	1:A:601:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1870:GLN:OE1	1:A:1941:ARG:NH1	2.43	0.43
1:A:1837:TYR:CZ	1:A:1853:GLY:HA3	2.53	0.43
1:A:521:PRO:HG2	1:A:555:TYR:HB2	2.01	0.43
1:A:1929:LEU:HB3	1:A:2012:THR:OG1	2.18	0.43
1:A:1946:SER:O	1:A:1980:PRO:HA	2.19	0.43
2:V:791:THR:HG23	2:V:816:ARG:O	2.19	0.43
1:A:8:GLY:HA3	1:A:54:PHE:HE2	1.82	0.42
1:A:1738:PHE:HA	1:A:1746:PRO:HA	2.00	0.42
1:A:1789:LEU:HD13	1:A:1823:MET:HB3	2.01	0.42
2:V:1150:ALA:HB3	2:V:1174:HIS:CE1	2.54	0.42
1:A:452:LEU:HA	1:A:550:PRO:HG2	2.02	0.42
1:A:2174:CYS:O	1:A:2241:THR:HG21	2.19	0.42
2:V:844:ILE:HG13	2:V:847:ASN:HD21	1.85	0.42
2:V:874:HIS:CG	2:V:1083:VAL:HG22	2.54	0.42
1:A:1945:LEU:HB2	1:A:1983:PHE:CE1	2.55	0.42
2:V:988:TYR:HB3	2:V:992:VAL:HG13	2.01	0.42
1:A:118:THR:HB	1:A:122:GLU:HB2	2.00	0.42
1:A:461:LEU:HB2	1:A:513:TRP:HB2	2.01	0.42
1:A:1846:ASP:OD1	1:A:1889:TRP:NE1	2.44	0.41
2:V:817:HIS:O	2:V:820:ARG:HG2	2.20	0.41
2:V:831:HIS:CG	2:V:832:GLN:H	2.38	0.41
2:V:879:ASP:HB2	2:V:1006:ASP:OD2	2.20	0.41
1:A:1785:PHE:HB3	1:A:1815:TYR:CE1	2.56	0.41
1:A:2105:TYR:HD2	1:A:2146:ALA:HB2	1.85	0.41
1:A:1764:ARG:HG2	1:A:1856:LEU:HB2	2.01	0.41
1:A:95:PRO:HG2	1:A:162:VAL:HG11	2.03	0.41
1:A:2054:HIS:NE2	1:A:2135:ILE:HD11	2.36	0.41
1:A:2150:ARG:HD3	1:A:2152:HIS:NE2	2.35	0.41
1:A:240:ARG:HD3	1:A:323:TYR:CZ	2.56	0.41
2:V:846:CYS:SG	2:V:863:CYS:N	2.93	0.41
1:A:264:PRO:HA	1:A:290:PRO:CG	2.51	0.41
1:A:1965:VAL:HG11	1:A:1976:TYR:CE1	2.56	0.41
2:V:1198:VAL:HG22	2:V:1207:ALA:HA	2.01	0.41
1:A:656:TYR:CE1	1:A:682:MET:HA	2.56	0.41
1:A:101:VAL:HG13	1:A:1957:HIS:CE1	2.56	0.41
1:A:634:VAL:HG13	1:A:679:PHE:CZ	2.55	0.41
1:A:1938:GLN:O	1:A:1990:PRO:HD2	2.20	0.41
2:V:831:HIS:HB3	2:V:836:TYR:HE2	1.86	0.41
2:V:849:CYS:HA	2:V:858:CYS:HA	2.03	0.41
1:A:289:SER:OG	1:A:1979:TYR:OH	2.33	0.41
1:A:1808:LYS:HB2	1:A:1811:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PRO:HB3	1:A:154:LEU:HG	2.03	0.40
1:A:232:HIS:CG	1:A:318:ASP:HB3	2.56	0.40
1:A:485:PRO:HD3	1:A:498:LEU:HD11	2.03	0.40
2:V:954:GLU:OE2	2:V:1210:LYS:NZ	2.54	0.40
1:A:181:GLU:OE1	1:A:181:GLU:N	2.36	0.40
1:A:1946:SER:HB2	1:A:1978:LEU:HB3	2.02	0.40
2:V:1100:PHE:HE2	2:V:1125:LEU:HD11	1.85	0.40
1:A:1998:VAL:O	1:A:1998:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	935/1965 (48%)	909 (97%)	26 (3%)	0	100	100
2	V	476/1646 (29%)	457 (96%)	19 (4%)	0	100	100
All	All	1411/3611 (39%)	1366 (97%)	45 (3%)	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	A	1066/1722 (62%)	1065 (100%)	1 (0%)	88	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	420/1415 (30%)	419 (100%)	1 (0%)	87	96
All	All	1486/3137 (47%)	1484 (100%)	2 (0%)	87	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	LEU
2	V	1165	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	HIS
1	A	468	GLN
1	A	693	HIS
1	A	1820	GLN
1	A	1915	ASN
1	A	1954	HIS
1	A	2266	GLN
2	V	847	ASN
2	V	1011	ASN
2	V	1072	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	TYS	A	1680	1	15,16,17	0.64	0	15,22,24	0.89	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
1	TYS	A	1680	1	-	2/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1680	TYS	CE1-CZ-OH-S
1	A	1680	TYS	CE2-CZ-OH-S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1680	TYS	1	0

5.5 Carbohydrates ⓘ

3 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
3	NAG	B	1	1,3	14,14,15	0.40	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	2	3	14,14,15	0.17	0	17,19,21	0.45	0
3	BMA	B	3	3	11,11,12	0.49	0	15,15,17	0.77	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
3	NAG	B	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

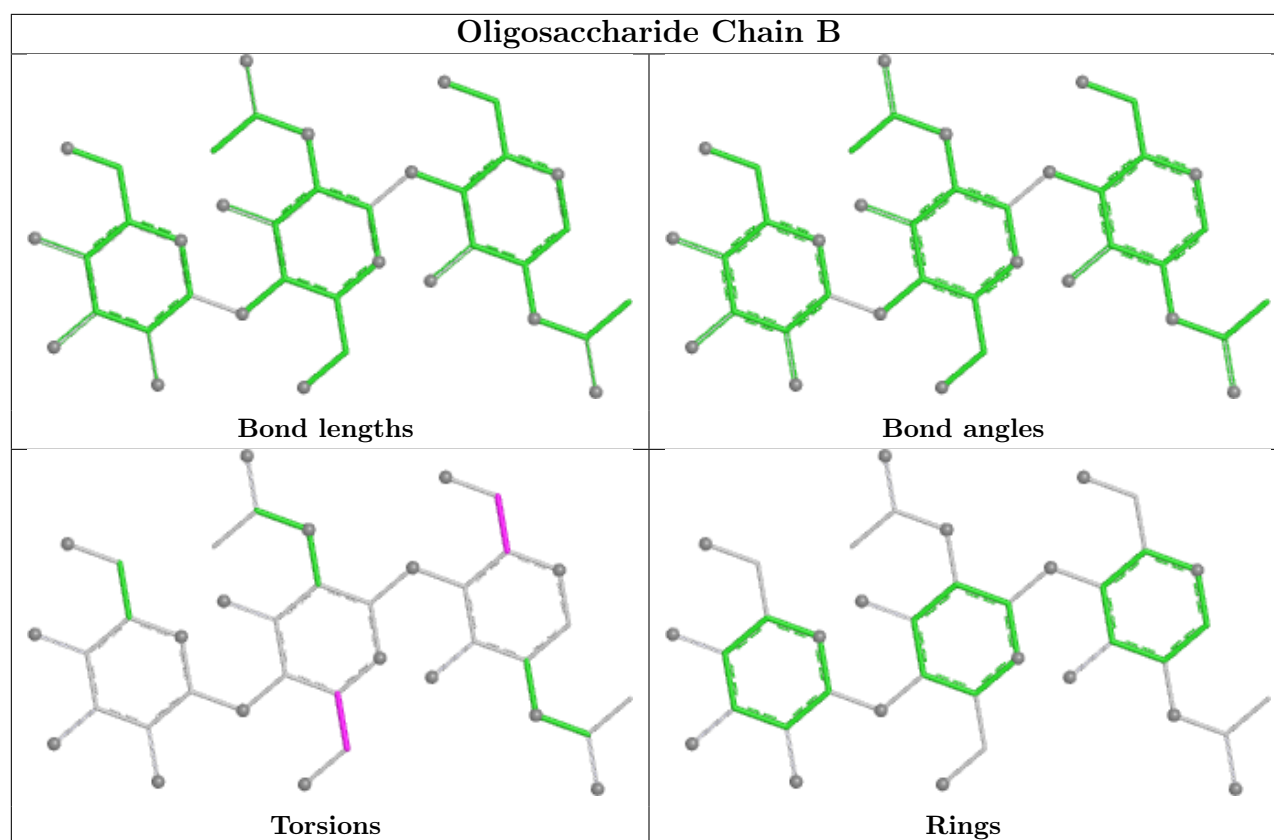
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-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](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
4	NAG	A	2602	1	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	A	2601	1	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	V	1701	2	14,14,15	0.27	0	17,19,21	0.57	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	2602	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2601	1	-	4/6/23/26	0/1/1/1
4	NAG	V	1701	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2601	NAG	O5-C5-C6-O6
4	A	2601	NAG	C4-C5-C6-O6
4	A	2602	NAG	C8-C7-N2-C2
4	A	2602	NAG	O7-C7-N2-C2
4	A	2602	NAG	O5-C5-C6-O6
4	A	2602	NAG	C4-C5-C6-O6
4	V	1701	NAG	C4-C5-C6-O6
4	V	1701	NAG	O5-C5-C6-O6
4	A	2601	NAG	C3-C2-N2-C7
4	V	1701	NAG	C3-C2-N2-C7
4	A	2601	NAG	C1-C2-N2-C7
4	V	1701	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

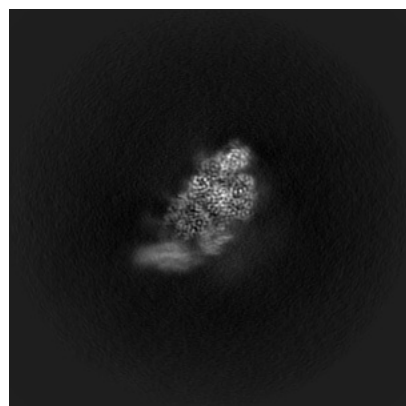
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23057. These allow visual inspection of the internal detail of the map and identification of artifacts.

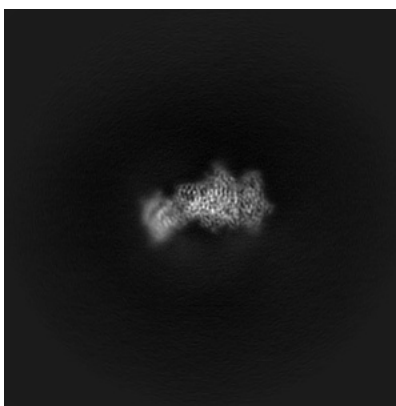
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

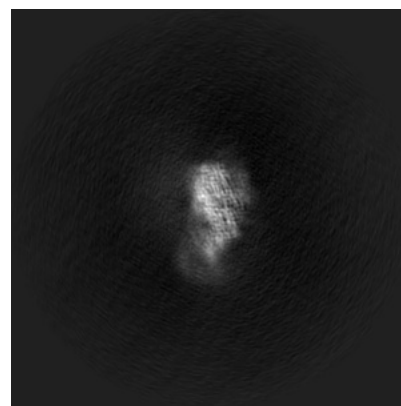
6.1.1 Primary map



X

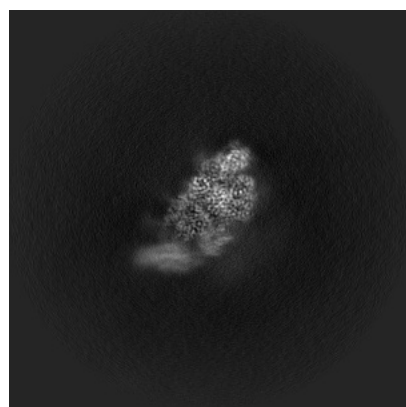


Y

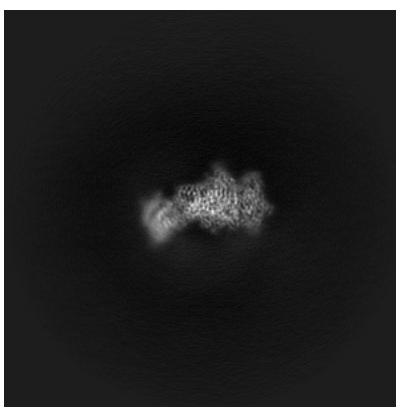


Z

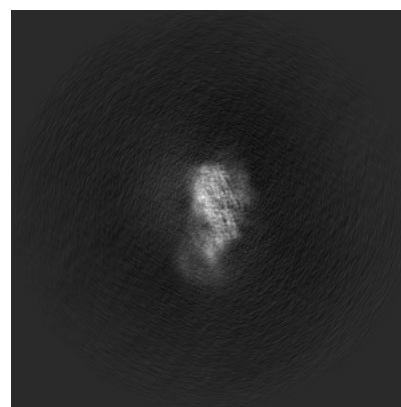
6.1.2 Raw map



X



Y

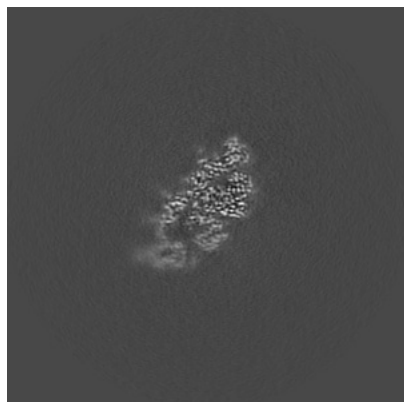


Z

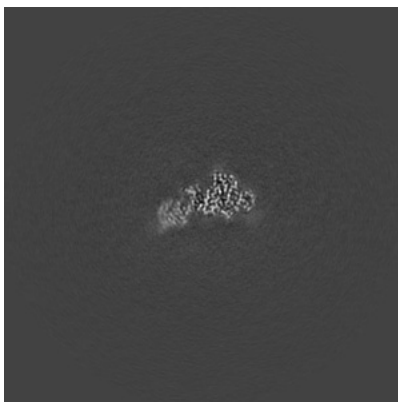
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

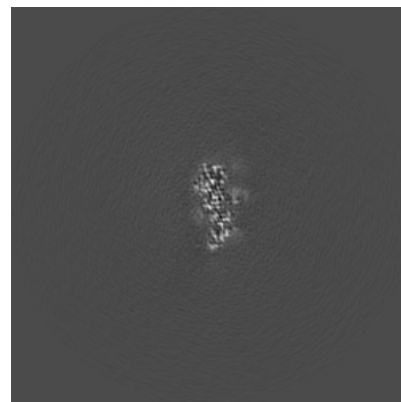
6.2.1 Primary map



X Index: 192

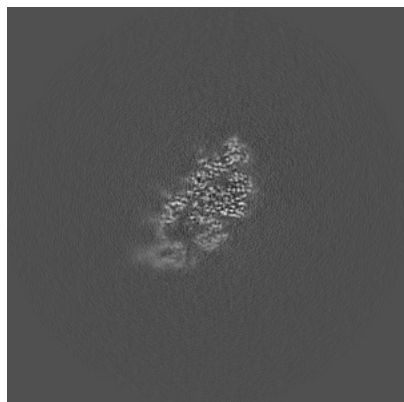


Y Index: 192

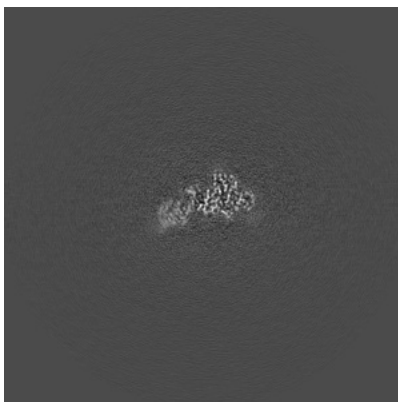


Z Index: 192

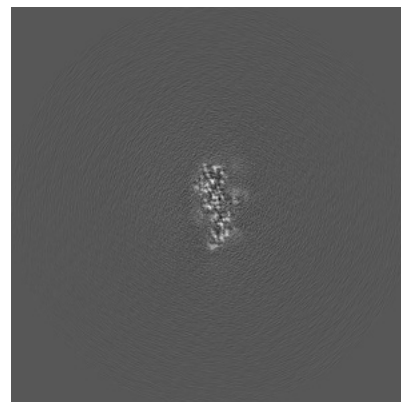
6.2.2 Raw map



X Index: 192



Y Index: 192

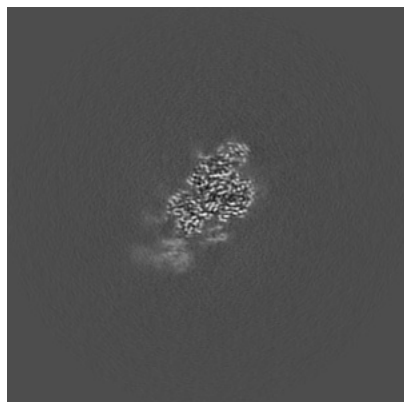


Z Index: 192

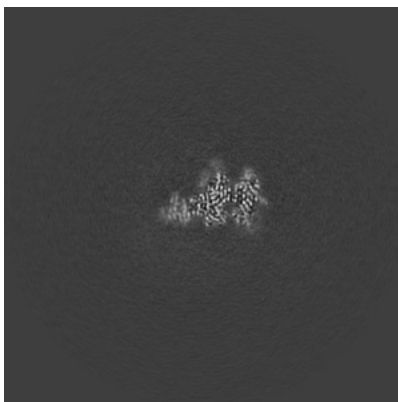
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

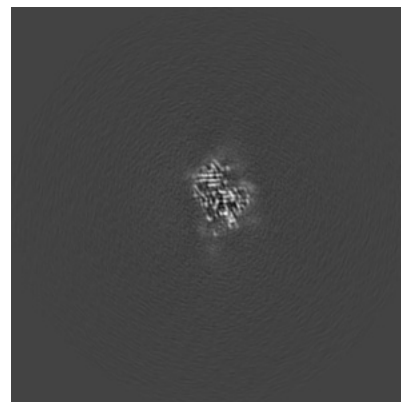
6.3.1 Primary map



X Index: 198

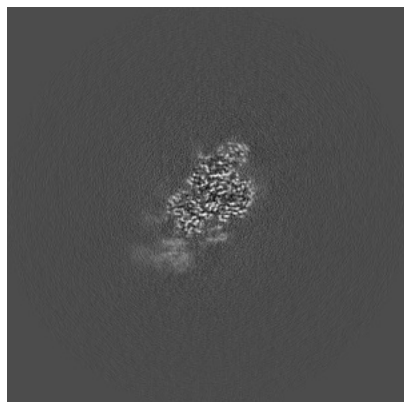


Y Index: 205

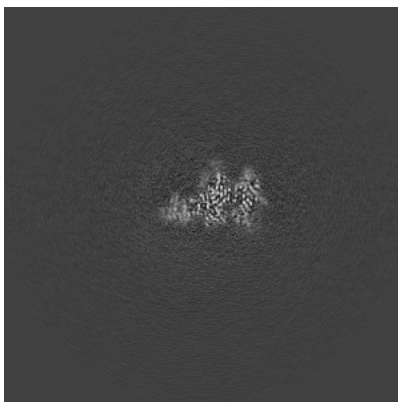


Z Index: 208

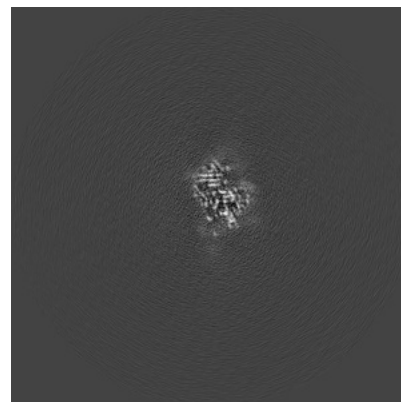
6.3.2 Raw map



X Index: 198



Y Index: 205

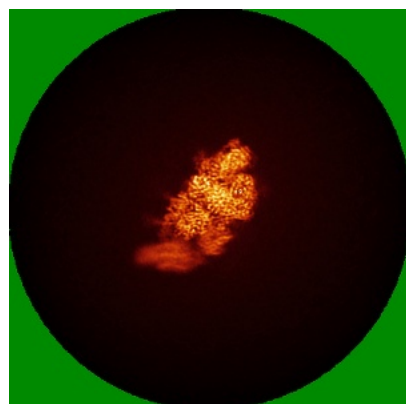


Z Index: 208

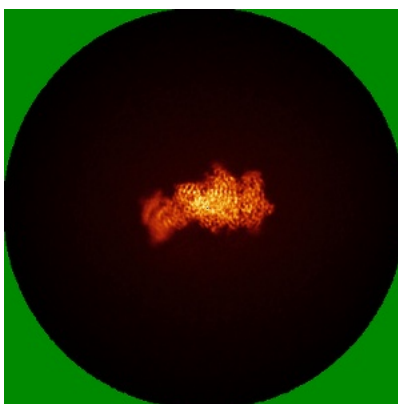
The images above show the largest variance slices of the map in three orthogonal directions.

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

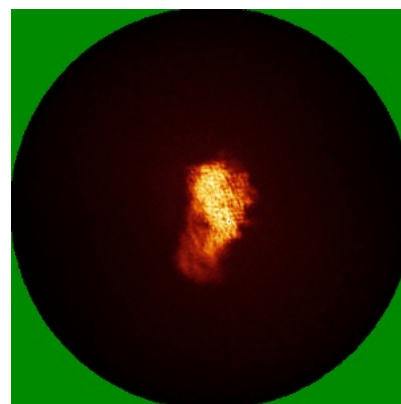
6.4.1 Primary map



X

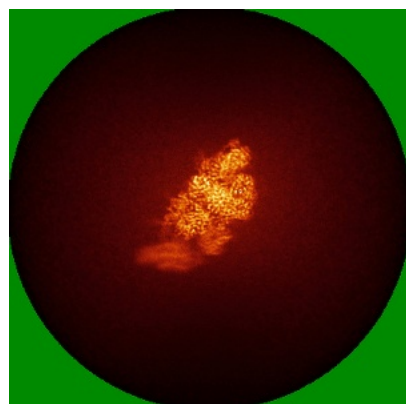


Y

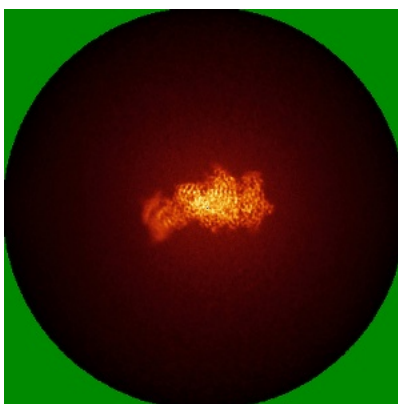


Z

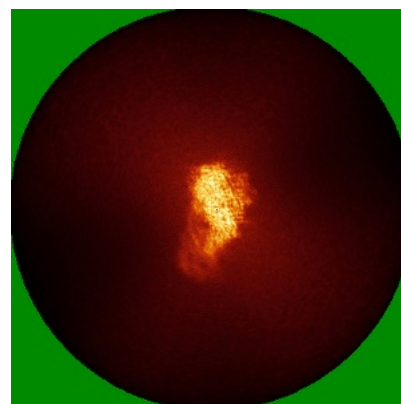
6.4.2 Raw map



X



Y

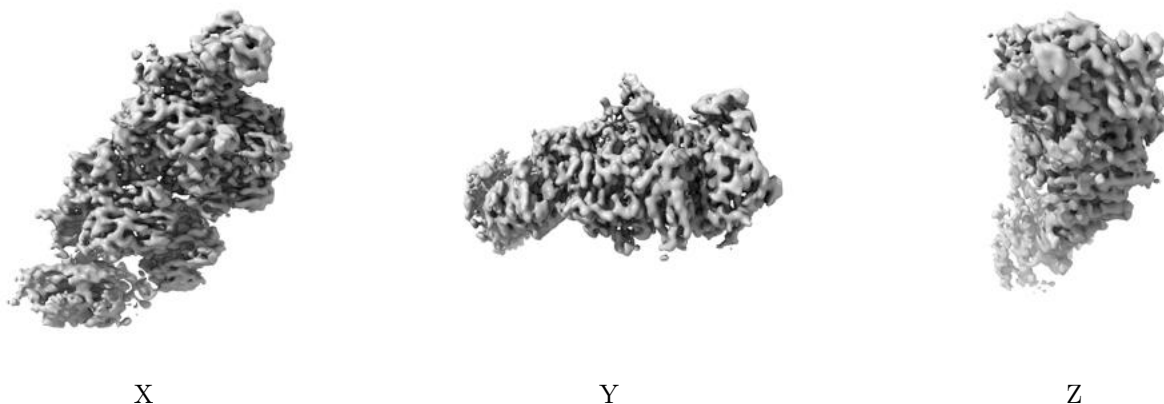


Z

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.

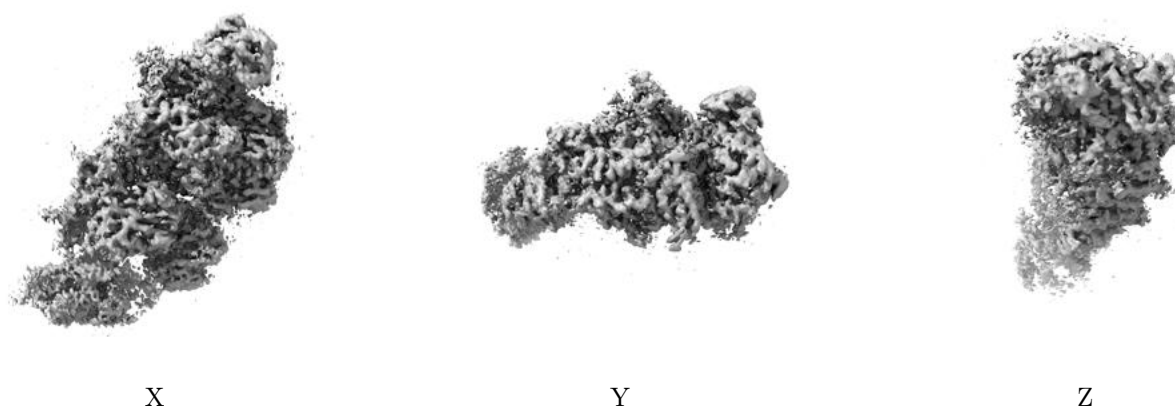
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0145. 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.

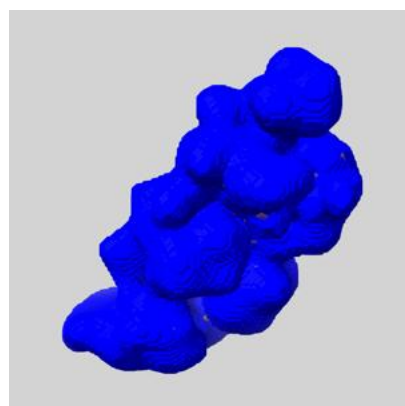
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

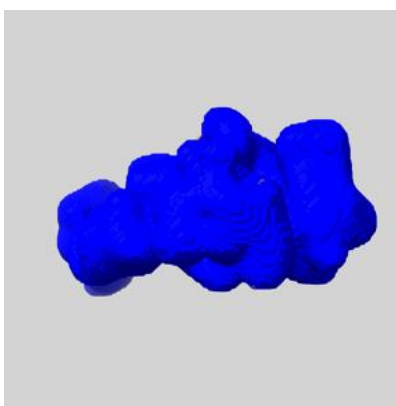
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

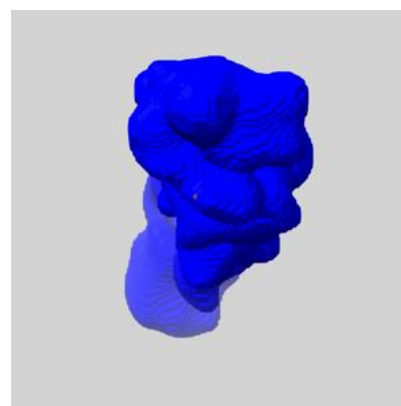
6.6.1 emd_23057_msk_1.map [i](#)



X



Y

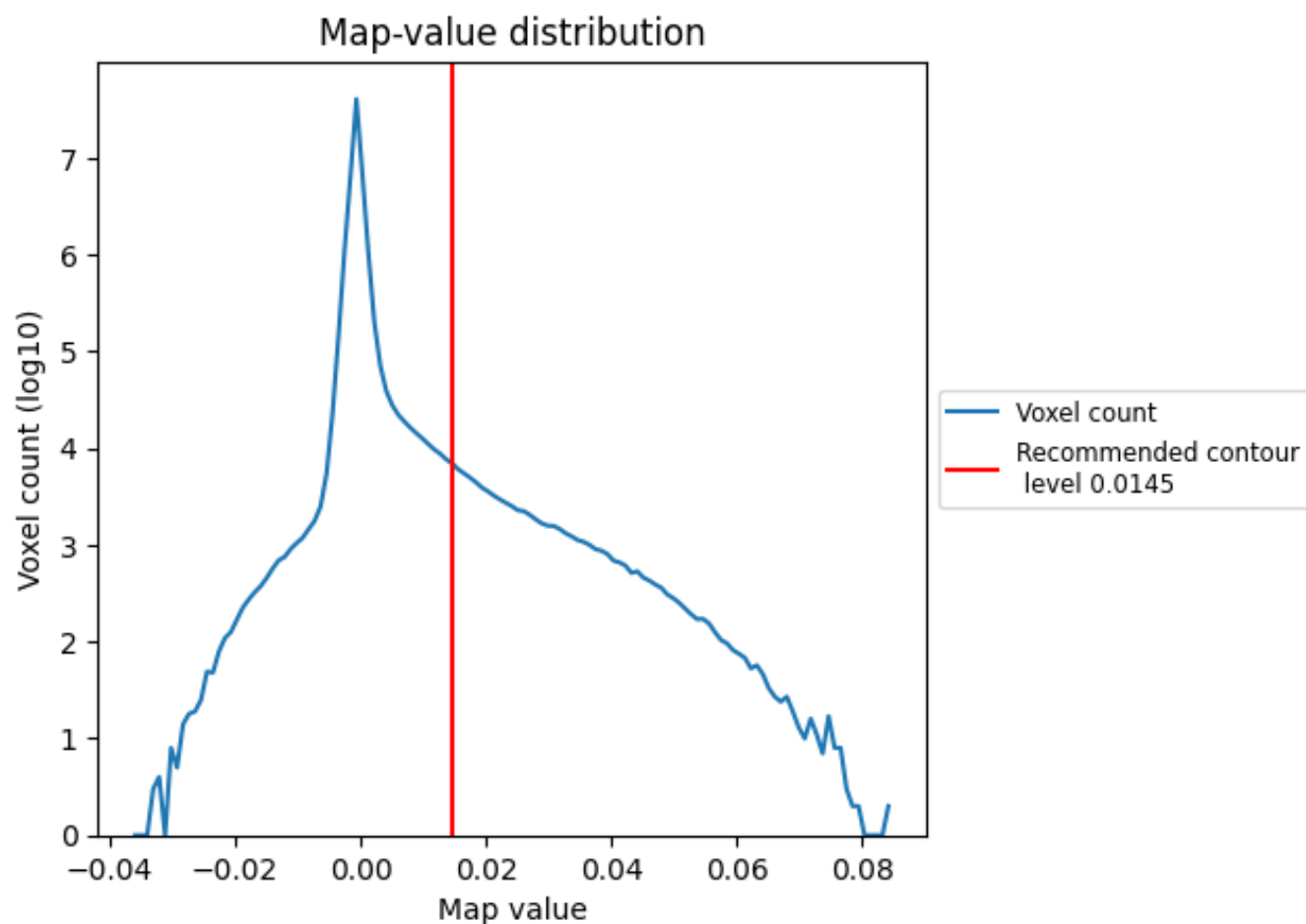


Z

7 Map analysis [i](#)

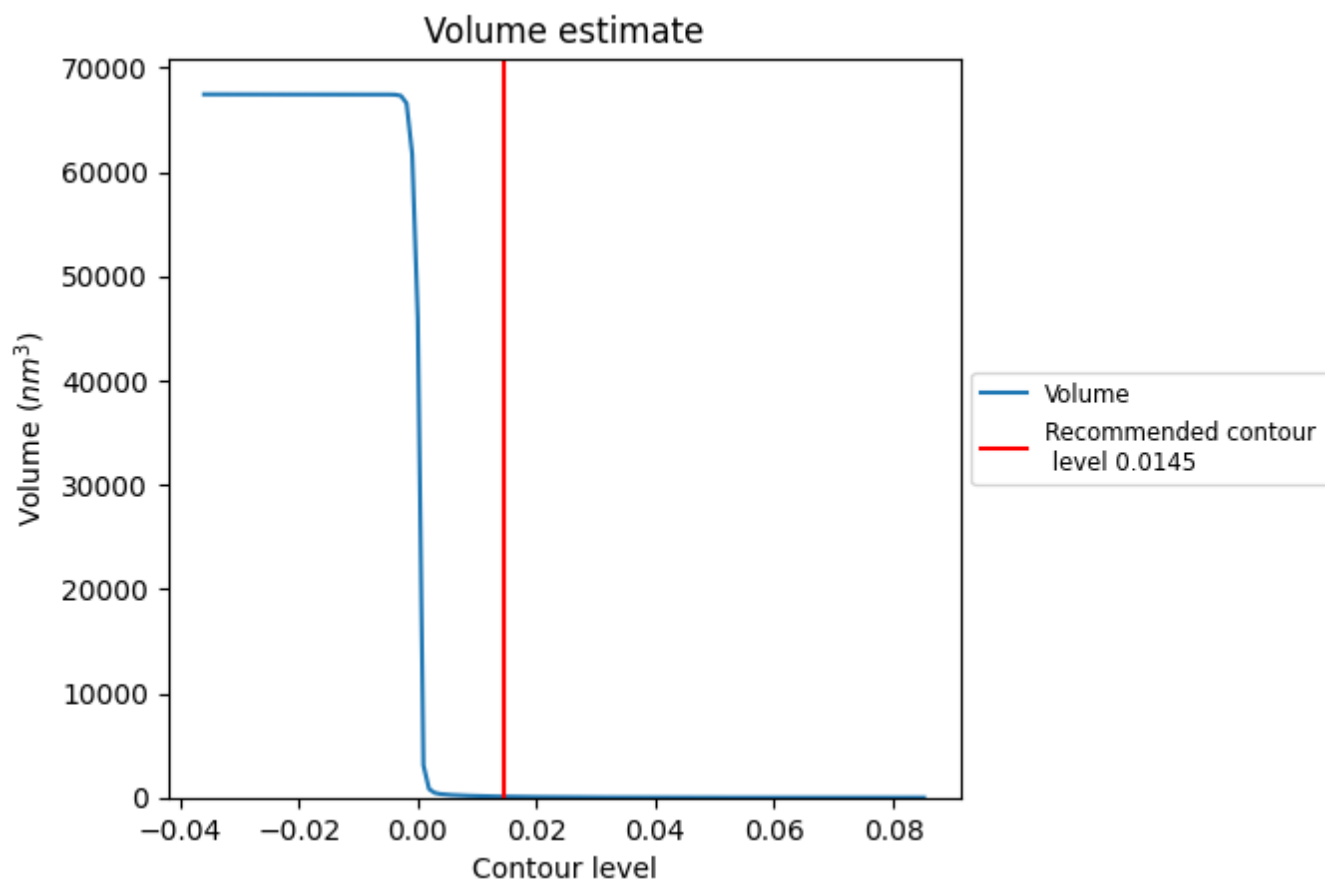
This section contains the results of statistical analysis of the map.

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.

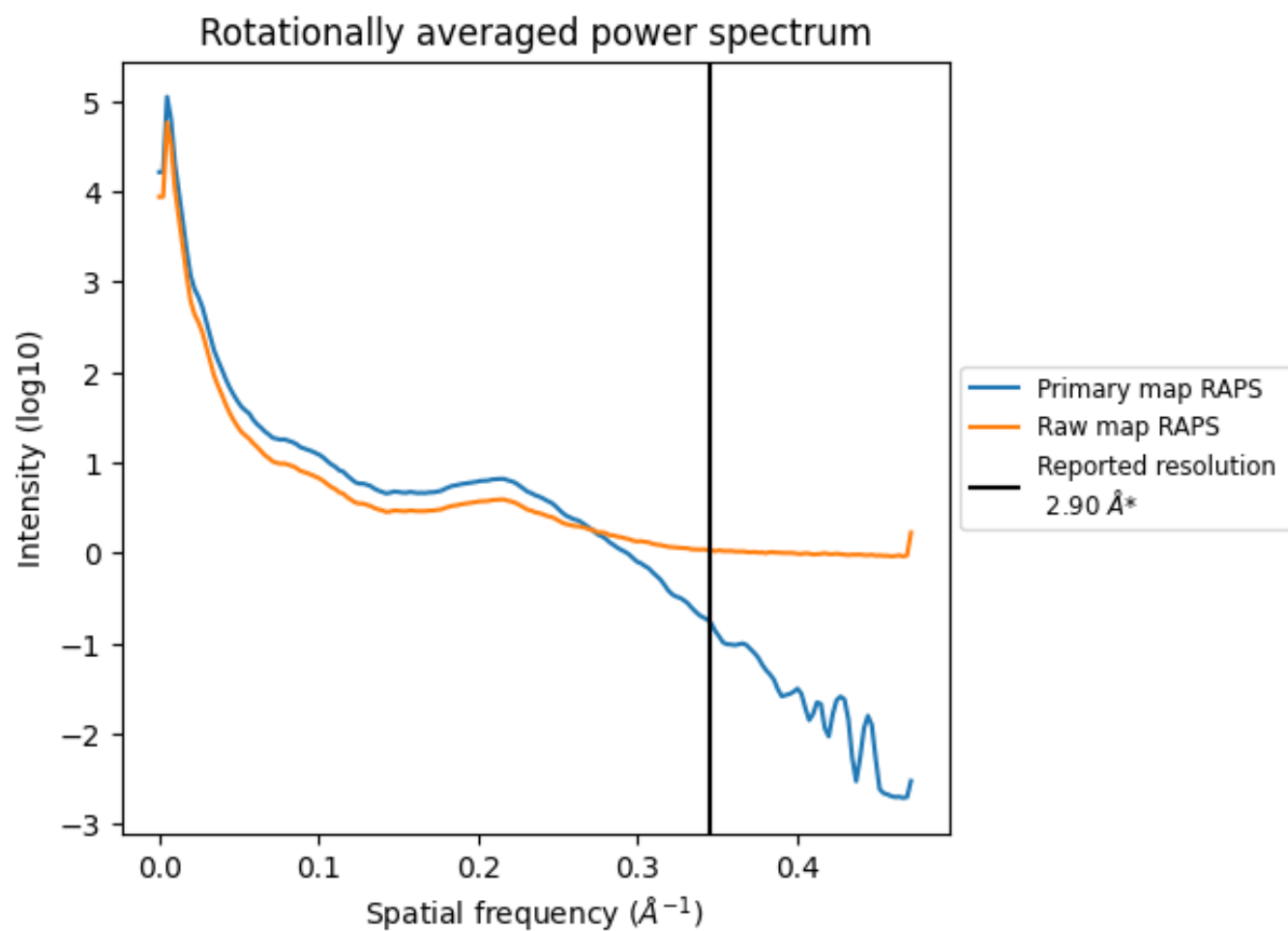
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

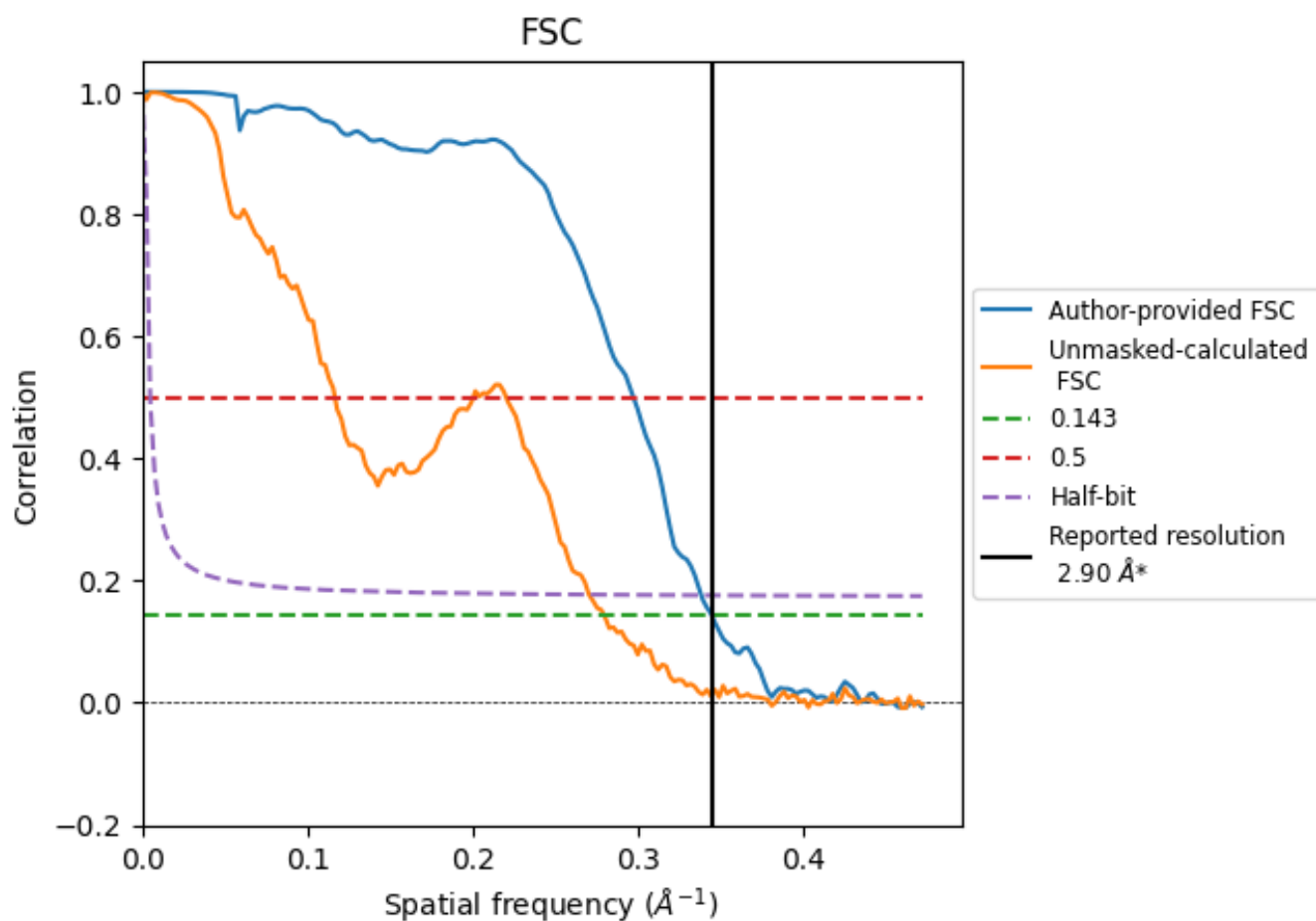


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

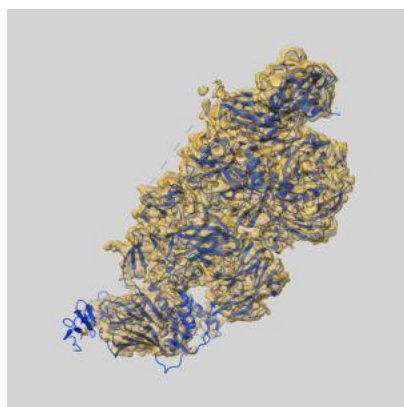
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.37	2.96
Unmasked-calculated*	3.58	8.58	3.70

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

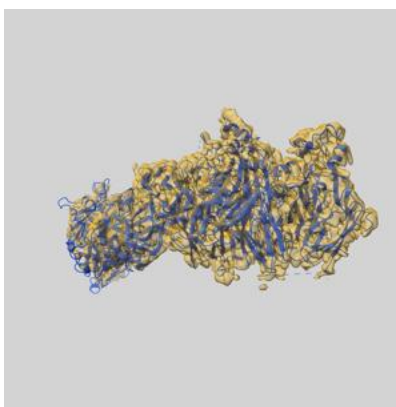
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23057 and PDB model 7KWO. Per-residue inclusion information can be found in section 3 on page 5.

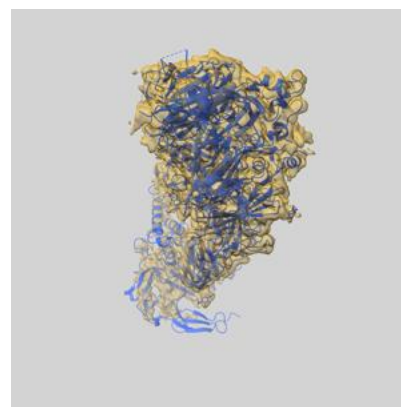
9.1 Map-model overlay [i](#)



X



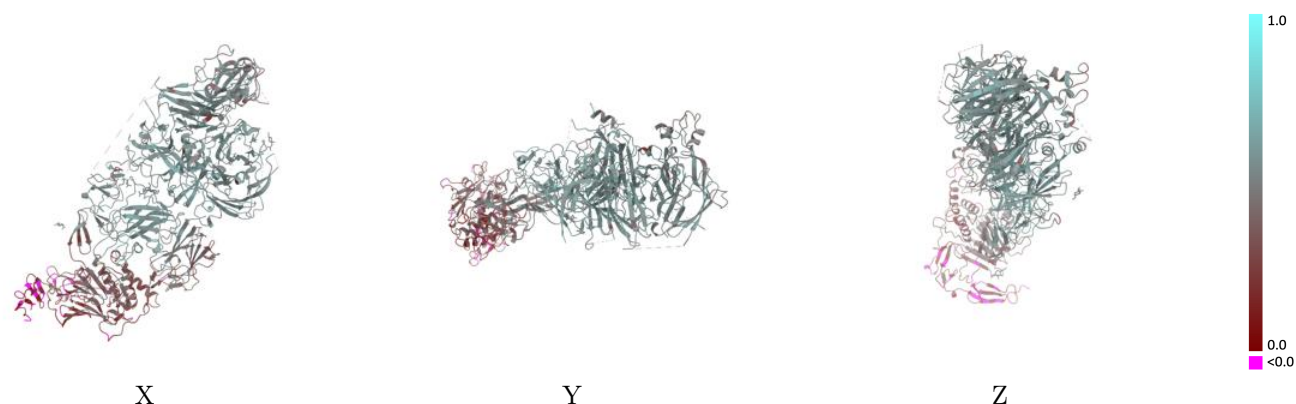
Y



Z

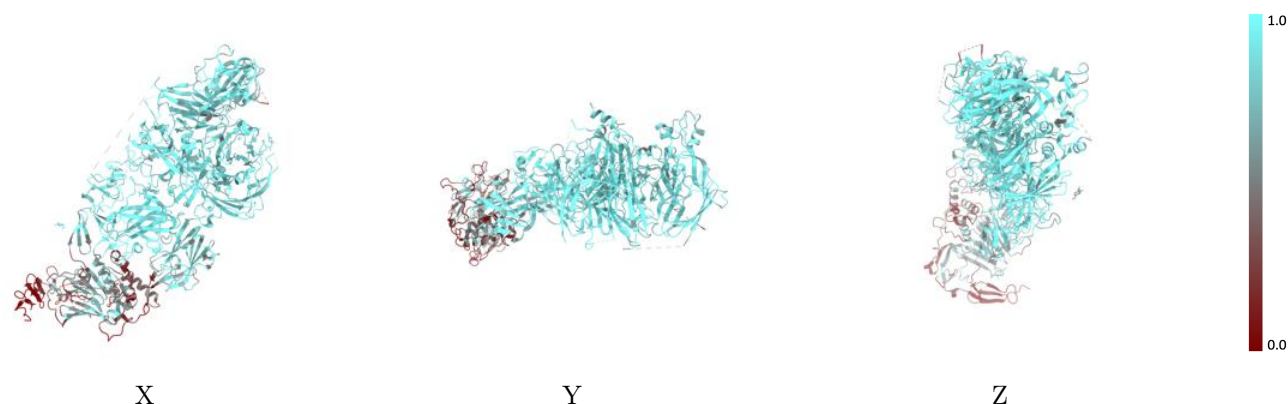
The images above show the 3D surface view of the map at the recommended contour level 0.0145 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



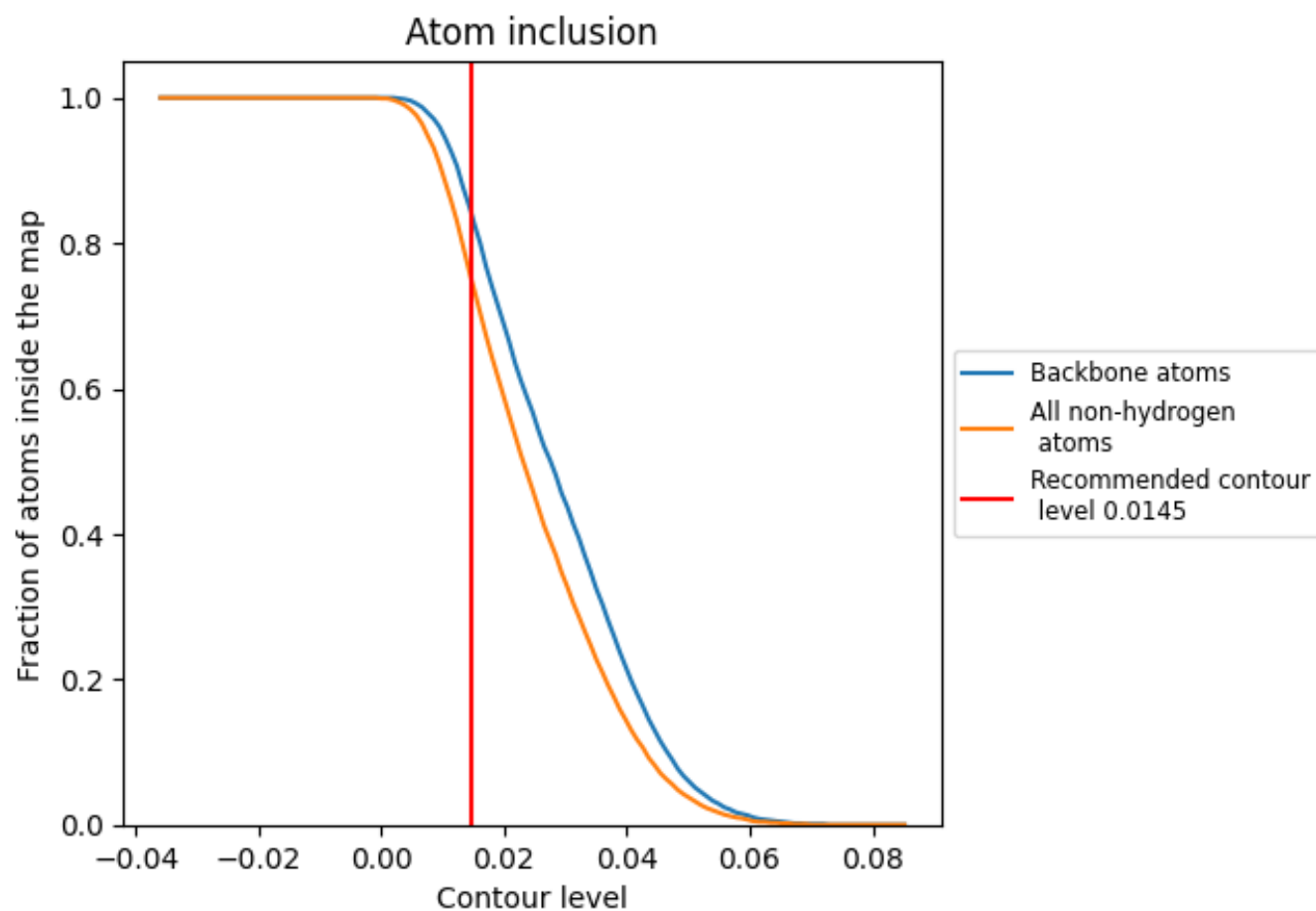
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0145).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 76% 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 (0.0145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.4620
A	0.8730	0.5270
B	0.8970	0.5130
V	0.4400	0.2880

