



## Full wwPDB EM Validation Report ⓘ

Aug 30, 2025 – 07:06 am BST

PDB ID : 9HBK / pdb\_00009hbk  
EMDB ID : EMD-52019  
Title : Structure of A16/G9 in complex with A56/K2 (vaccinia virus)  
Authors : Vernuccio, R.; Meola, A.; Guardado-Calvo, P.  
Deposited on : 2024-11-07  
Resolution : 3.20 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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

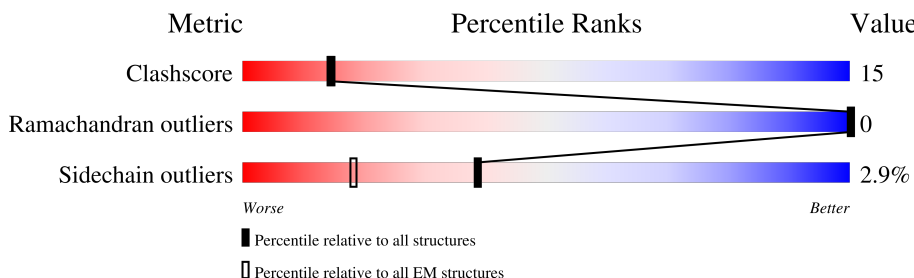
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	340	<div> <div>11%</div> <div>56%</div> <div>28%</div> <div>•</div> <div>16%</div> </div>
2	B	316	<div> <div>27%</div> <div>51%</div> <div>32%</div> <div>17%</div> </div>
3	C	413	<div> <div>6%</div> <div>55%</div> <div>29%</div> <div>•</div> <div>14%</div> </div>
4	D	139	<div> <div>•</div> <div>48%</div> <div>32%</div> <div>•</div> <div>18%</div> </div>
5	E	4	<div> <div>25%</div> <div>100%</div> </div>
6	F	4	<div> <div>50%</div> <div>25%</div> <div>75%</div> </div>
7	G	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8372 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 Virion membrane protein OPG143.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	286	Total	C	N	O	S	0	0
			2351	1489	404	435	23		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ARG	-	expression tag	UNP P16710
A	1	SER	-	expression tag	UNP P16710
A	2	ALA	-	expression tag	UNP P16710
A	296	GLY	-	expression tag	UNP P16710
A	297	SER	-	expression tag	UNP P16710
A	298	GLY	-	expression tag	UNP P16710
A	299	LEU	-	expression tag	UNP P16710
A	300	VAL	-	expression tag	UNP P16710
A	301	PRO	-	expression tag	UNP P16710
A	302	ARG	-	expression tag	UNP P16710
A	303	GLY	-	expression tag	UNP P16710
A	304	SER	-	expression tag	UNP P16710
A	305	GLY	-	expression tag	UNP P16710
A	306	GLY	-	expression tag	UNP P16710
A	307	SER	-	expression tag	UNP P16710
A	308	GLY	-	expression tag	UNP P16710
A	309	GLY	-	expression tag	UNP P16710
A	310	SER	-	expression tag	UNP P16710
A	311	HIS	-	expression tag	UNP P16710
A	312	HIS	-	expression tag	UNP P16710
A	313	HIS	-	expression tag	UNP P16710
A	314	HIS	-	expression tag	UNP P16710
A	315	HIS	-	expression tag	UNP P16710
A	316	HIS	-	expression tag	UNP P16710
A	317	HIS	-	expression tag	UNP P16710
A	318	HIS	-	expression tag	UNP P16710
A	319	GLY	-	expression tag	UNP P16710
A	320	GLY	-	expression tag	UNP P16710

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Chain	Residue	Modelled	Actual	Comment	Reference
A	321	SER	-	expression tag	UNP P16710
A	322	GLY	-	expression tag	UNP P16710
A	323	THR	-	expression tag	UNP P16710
A	324	GLY	-	expression tag	UNP P16710
A	325	GLY	-	expression tag	UNP P16710
A	326	LEU	-	expression tag	UNP P16710
A	327	ASN	-	expression tag	UNP P16710
A	328	ASP	-	expression tag	UNP P16710
A	329	ILE	-	expression tag	UNP P16710
A	330	PHE	-	expression tag	UNP P16710
A	331	GLU	-	expression tag	UNP P16710
A	332	ALA	-	expression tag	UNP P16710
A	333	GLN	-	expression tag	UNP P16710
A	334	LYS	-	expression tag	UNP P16710
A	335	ILE	-	expression tag	UNP P16710
A	336	GLU	-	expression tag	UNP P16710
A	337	TRP	-	expression tag	UNP P16710
A	338	HIS	-	expression tag	UNP P16710
A	339	GLU	-	expression tag	UNP P16710

- Molecule 2 is a protein called Entry-fusion complex protein OPG094.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	261	Total	C	N	O	S	0	0
			2109	1319	372	401	17		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	expression tag	UNP P07611
B	82	ALA	ASN	conflict	UNP P07611
B	93	GLN	ASN	conflict	UNP P07611
B	156	ALA	SER	conflict	UNP P07611
B	157	ASP	ASN	conflict	UNP P07611
B	272	GLY	-	expression tag	UNP P07611
B	273	SER	-	expression tag	UNP P07611
B	274	GLY	-	expression tag	UNP P07611
B	275	LEU	-	expression tag	UNP P07611
B	276	VAL	-	expression tag	UNP P07611
B	277	PRO	-	expression tag	UNP P07611
B	278	ARG	-	expression tag	UNP P07611
B	279	GLY	-	expression tag	UNP P07611

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Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	-	expression tag	UNP P07611
B	281	LEU	-	expression tag	UNP P07611
B	282	GLU	-	expression tag	UNP P07611
B	283	ASP	-	expression tag	UNP P07611
B	284	ASP	-	expression tag	UNP P07611
B	285	ASP	-	expression tag	UNP P07611
B	286	ASP	-	expression tag	UNP P07611
B	287	LYS	-	expression tag	UNP P07611
B	288	ALA	-	expression tag	UNP P07611
B	289	GLY	-	expression tag	UNP P07611
B	290	TRP	-	expression tag	UNP P07611
B	291	SER	-	expression tag	UNP P07611
B	292	HIS	-	expression tag	UNP P07611
B	293	PRO	-	expression tag	UNP P07611
B	294	GLN	-	expression tag	UNP P07611
B	295	PHE	-	expression tag	UNP P07611
B	296	GLU	-	expression tag	UNP P07611
B	297	LYS	-	expression tag	UNP P07611
B	298	GLY	-	expression tag	UNP P07611
B	299	GLY	-	expression tag	UNP P07611
B	300	GLY	-	expression tag	UNP P07611
B	301	SER	-	expression tag	UNP P07611
B	302	GLY	-	expression tag	UNP P07611
B	303	GLY	-	expression tag	UNP P07611
B	304	GLY	-	expression tag	UNP P07611
B	305	SER	-	expression tag	UNP P07611
B	306	GLY	-	expression tag	UNP P07611
B	307	GLY	-	expression tag	UNP P07611
B	308	GLY	-	expression tag	UNP P07611
B	309	SER	-	expression tag	UNP P07611
B	310	TRP	-	expression tag	UNP P07611
B	311	SER	-	expression tag	UNP P07611
B	312	HIS	-	expression tag	UNP P07611
B	313	PRO	-	expression tag	UNP P07611
B	314	GLN	-	expression tag	UNP P07611
B	315	PHE	-	expression tag	UNP P07611
B	316	GLU	-	expression tag	UNP P07611
B	317	LYS	-	expression tag	UNP P07611

- Molecule 3 is a protein called Superinfection exclusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	354	Total	C	N	O	S	0	0
			2866	1841	474	534	17		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	109	SER	CYS	conflict	UNP P18384
C	370	GLY	-	expression tag	UNP P18384
C	371	SER	-	expression tag	UNP P18384
C	372	GLY	-	expression tag	UNP P18384
C	373	LEU	-	expression tag	UNP P18384
C	374	VAL	-	expression tag	UNP P18384
C	375	PRO	-	expression tag	UNP P18384
C	376	ARG	-	expression tag	UNP P18384
C	377	GLY	-	expression tag	UNP P18384
C	378	SER	-	expression tag	UNP P18384
C	379	GLY	-	expression tag	UNP P18384
C	380	SER	-	expression tag	UNP P18384
C	381	ALA	-	expression tag	UNP P18384
C	382	GLY	-	expression tag	UNP P18384
C	383	TRP	-	expression tag	UNP P18384
C	384	SER	-	expression tag	UNP P18384
C	385	HIS	-	expression tag	UNP P18384
C	386	PRO	-	expression tag	UNP P18384
C	387	GLN	-	expression tag	UNP P18384
C	388	PHE	-	expression tag	UNP P18384
C	389	GLU	-	expression tag	UNP P18384
C	390	LYS	-	expression tag	UNP P18384
C	391	GLY	-	expression tag	UNP P18384
C	392	GLY	-	expression tag	UNP P18384
C	393	GLY	-	expression tag	UNP P18384
C	394	SER	-	expression tag	UNP P18384
C	395	GLY	-	expression tag	UNP P18384
C	396	GLY	-	expression tag	UNP P18384
C	397	GLY	-	expression tag	UNP P18384
C	398	SER	-	expression tag	UNP P18384
C	399	GLY	-	expression tag	UNP P18384
C	400	GLY	-	expression tag	UNP P18384
C	401	GLY	-	expression tag	UNP P18384
C	402	SER	-	expression tag	UNP P18384
C	403	TRP	-	expression tag	UNP P18384
C	404	SER	-	expression tag	UNP P18384
C	405	HIS	-	expression tag	UNP P18384

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Chain	Residue	Modelled	Actual	Comment	Reference
C	406	PRO	-	expression tag	UNP P18384
C	407	GLN	-	expression tag	UNP P18384
C	408	PHE	-	expression tag	UNP P18384
C	409	GLU	-	expression tag	UNP P18384
C	410	LYS	-	expression tag	UNP P18384
C	411	GLY	-	expression tag	UNP P18384
C	412	THR	-	expression tag	UNP P18384
C	413	GLY	-	expression tag	UNP P18384
C	414	GLY	-	expression tag	UNP P18384
C	415	LEU	-	expression tag	UNP P18384
C	416	ASN	-	expression tag	UNP P18384
C	417	ASP	-	expression tag	UNP P18384
C	418	ILE	-	expression tag	UNP P18384
C	419	PHE	-	expression tag	UNP P18384
C	420	GLU	-	expression tag	UNP P18384
C	421	ALA	-	expression tag	UNP P18384
C	422	GLN	-	expression tag	UNP P18384
C	423	LYS	-	expression tag	UNP P18384
C	424	ILE	-	expression tag	UNP P18384
C	425	GLU	-	expression tag	UNP P18384
C	426	TRP	-	expression tag	UNP P18384
C	427	HIS	-	expression tag	UNP P18384
C	428	GLU	-	expression tag	UNP P18384

- Molecule 4 is a protein called Protein OPG185.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	114	Total	C	N	O	S	0	0
			905	571	138	192	4		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	15	ARG	-	expression tag	UNP Q01218
D	16	SER	-	expression tag	UNP Q01218
D	134	GLY	-	expression tag	UNP Q01218
D	135	SER	-	expression tag	UNP Q01218
D	136	GLY	-	expression tag	UNP Q01218
D	137	LEU	-	expression tag	UNP Q01218
D	138	VAL	-	expression tag	UNP Q01218
D	139	PRO	-	expression tag	UNP Q01218
D	140	ARG	-	expression tag	UNP Q01218

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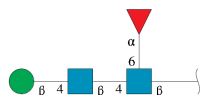
Chain	Residue	Modelled	Actual	Comment	Reference
D	141	GLY	-	expression tag	UNP Q01218
D	142	SER	-	expression tag	UNP Q01218
D	143	GLY	-	expression tag	UNP Q01218
D	144	SER	-	expression tag	UNP Q01218
D	145	GLY	-	expression tag	UNP Q01218
D	146	HIS	-	expression tag	UNP Q01218
D	147	HIS	-	expression tag	UNP Q01218
D	148	HIS	-	expression tag	UNP Q01218
D	149	HIS	-	expression tag	UNP Q01218
D	150	HIS	-	expression tag	UNP Q01218
D	151	HIS	-	expression tag	UNP Q01218
D	152	HIS	-	expression tag	UNP Q01218
D	153	HIS	-	expression tag	UNP Q01218

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
5	E	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			49	28	2	19		

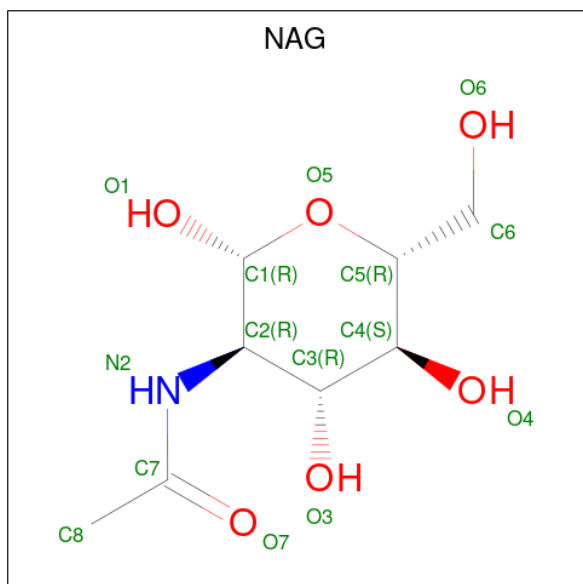
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).

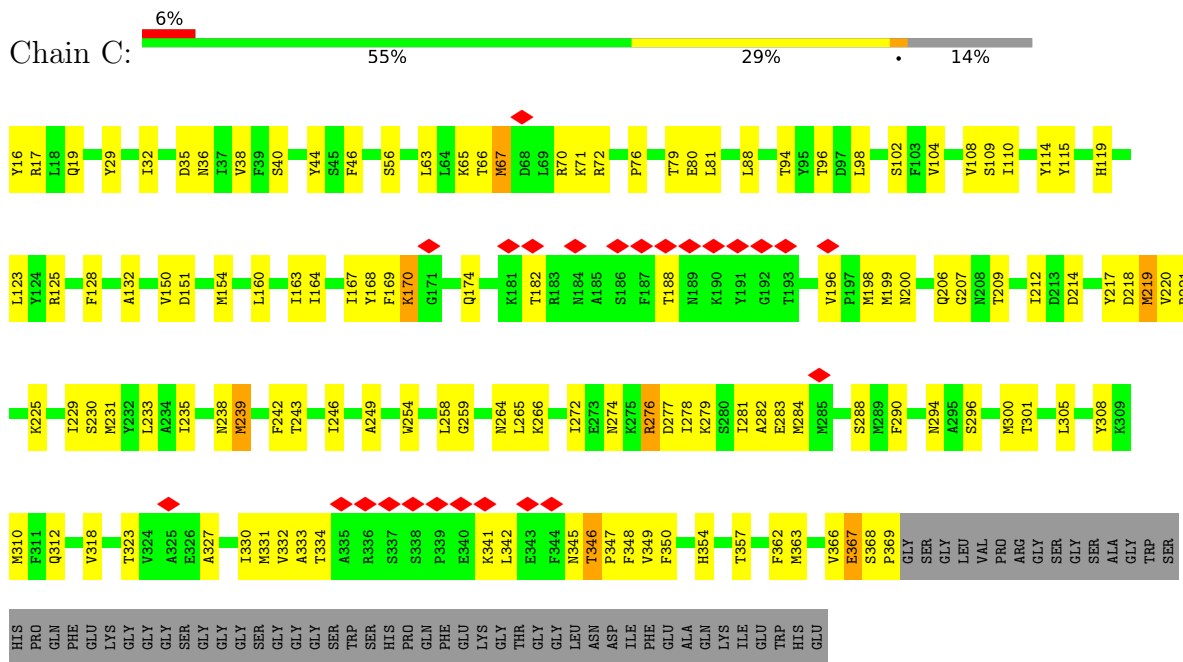


Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			14	8	1	5	

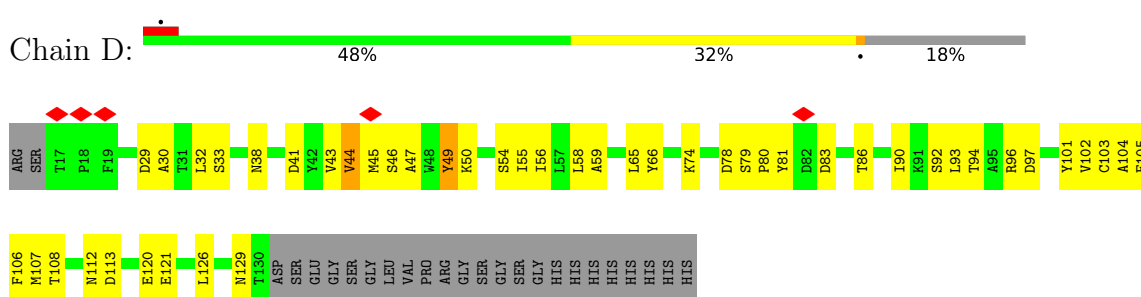


GLY  
SER  
GLY  
GLY  
GLY  
GLY  
GLY  
GLY  
TRP  
SER  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS

• Molecule 3: Superinfection exclusion protein



• Molecule 4: Protein OPG185



• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 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	228433	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.565	Depositor
Minimum map value	-0.283	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	232.2, 232.2, 232.2	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.29, 1.29, 1.29	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: NAG, FUC, BMA, MAN

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	0.14	0/2419	0.35	0/3268
2	B	0.13	0/2160	0.35	0/2923
3	C	0.13	0/2932	0.35	0/3965
4	D	0.13	0/923	0.36	0/1260
All	All	0.13	0/8434	0.35	0/11416

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	2351	0	2217	77	0
2	B	2109	0	2023	69	0
3	C	2866	0	2845	86	0
4	D	905	0	860	32	0
5	E	50	0	43	0	0
6	F	49	0	43	0	0
7	G	28	0	25	0	0
8	D	14	0	13	1	0
All	All	8372	0	8069	248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:ILE:HD11	3:C:312:GLN:HB2	1.49	0.94
3:C:279:LYS:O	3:C:283:GLU:HB2	1.71	0.91
2:B:84:THR:HG22	2:B:86:PRO:HD2	1.64	0.80
4:D:45:MET:HB2	4:D:106:PHE:HB2	1.63	0.79
4:D:45:MET:HE1	4:D:58:LEU:HD11	1.64	0.79
3:C:354:HIS:HD2	3:C:357:THR:H	1.33	0.76
1:A:242:ASN:HB3	1:A:245:CYS:HB3	1.71	0.73
1:A:58:LYS:HA	1:A:127:ARG:HH12	1.55	0.71
4:D:97:ASP:OD1	4:D:101:TYR:OH	2.08	0.70
2:B:217:LYS:HG3	2:B:218:GLN:HG3	1.73	0.70
1:A:105:ASN:OD1	1:A:106:GLU:N	2.23	0.70
2:B:257:LEU:HB2	2:B:260:ASN:HB2	1.73	0.70
3:C:16:TYR:HB3	3:C:76:PRO:HB2	1.75	0.69
4:D:38:ASN:ND2	4:D:41:ASP:OD2	2.26	0.69
4:D:44:VAL:HG11	4:D:108:THR:HG23	1.75	0.68
3:C:163:ILE:HB	3:C:331:MET:HB2	1.76	0.68
2:B:189:PHE:HE2	2:B:204:MET:HE1	1.58	0.68
3:C:40:SER:OG	3:C:312:GLN:NE2	2.27	0.67
3:C:366:VAL:HG12	3:C:367:GLU:H	1.61	0.66
2:B:63:PHE:HB3	2:B:76:LEU:HD22	1.78	0.65
1:A:133:LYS:NZ	2:B:42:TYR:O	2.29	0.65
1:A:264:VAL:HG21	1:A:284:GLN:HG3	1.78	0.65
1:A:193:ARG:HG2	1:A:195:PRO:HD2	1.78	0.64
1:A:74:ILE:HB	1:A:79:ALA:HB2	1.80	0.63
1:A:192:LYS:NZ	1:A:219:ILE:O	2.31	0.62
1:A:169:ASP:OD1	1:A:188:TRP:NE1	2.29	0.61
3:C:94:THR:HA	3:C:170:LYS:O	2.00	0.61
1:A:94:LYS:HG3	1:A:123:ALA:HB2	1.83	0.61
2:B:99:LYS:HG2	2:B:113:VAL:HB	1.81	0.61
3:C:119:HIS:HA	3:C:123:LEU:HD12	1.83	0.61
2:B:178:SER:HB2	2:B:208:ILE:HD12	1.83	0.60
3:C:128:PHE:HD1	3:C:132:ALA:HB1	1.67	0.60
3:C:217:TYR:OH	3:C:238:ASN:O	2.20	0.60
1:A:92:SER:O	1:A:122:ILE:HA	2.02	0.60
4:D:29:ASP:HA	4:D:90:ILE:O	2.02	0.59
2:B:227:THR:O	2:B:231:LEU:N	2.32	0.59
1:A:103:TYR:O	3:C:19:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:ALA:HB3	4:D:104:ALA:HB3	1.85	0.58
1:A:109:PRO:HG2	3:C:17:ARG:NH2	2.19	0.58
2:B:51:ASP:OD1	2:B:52:LYS:N	2.37	0.58
2:B:205:ILE:HD13	2:B:259:ARG:HB2	1.85	0.58
2:B:173:MET:HE1	2:B:189:PHE:CG	2.39	0.57
4:D:30:ALA:HB2	4:D:93:LEU:HD11	1.86	0.57
4:D:112:ASN:HB3	8:D:201:NAG:O5	2.04	0.57
3:C:308:TYR:HB2	3:C:333:ALA:HA	1.87	0.57
1:A:96:ARG:HH21	2:B:10:PRO:HB2	1.69	0.57
1:A:105:ASN:HB3	3:C:249:ALA:HB2	1.87	0.57
4:D:97:ASP:O	4:D:101:TYR:OH	2.18	0.56
2:B:128:ASP:HA	2:B:148:TRP:HZ2	1.71	0.56
4:D:46:SER:HB2	4:D:59:ALA:HB3	1.88	0.56
1:A:216:PHE:O	1:A:220:ILE:HG12	2.05	0.56
1:A:242:ASN:ND2	1:A:244:ASN:OD1	2.39	0.56
3:C:154:MET:HG3	3:C:334:THR:O	2.06	0.56
1:A:160:ASN:C	1:A:160:ASN:HD22	2.12	0.56
1:A:240:LYS:HG3	1:A:251:PRO:HB3	1.87	0.56
4:D:94:THR:HG22	4:D:96:ARG:H	1.68	0.56
2:B:21:ASP:OD1	2:B:21:ASP:N	2.33	0.56
1:A:145:LYS:HD3	1:A:151:ASN:HB3	1.88	0.55
1:A:126:GLN:NE2	2:B:70:PRO:HB3	2.21	0.55
3:C:188:THR:HG21	3:C:345:ASN:HD22	1.70	0.55
3:C:108:VAL:HG13	3:C:301:THR:HG21	1.88	0.55
1:A:42:GLU:HG2	1:A:58:LYS:HB2	1.90	0.54
2:B:116:SER:OG	2:B:117:CYS:N	2.39	0.54
2:B:135:CYS:HB2	2:B:140:PHE:HA	1.88	0.54
3:C:98:LEU:HD13	3:C:167:ILE:HG12	1.90	0.54
1:A:67:ILE:HD11	2:B:23:MET:HB3	1.89	0.53
1:A:217:ILE:HD12	1:A:278:LYS:HB2	1.89	0.53
1:A:257:ASP:N	1:A:257:ASP:OD1	2.39	0.53
3:C:290:PHE:HZ	3:C:310:MET:HE3	1.73	0.53
1:A:254:ASN:HB2	1:A:258:LYS:HE2	1.90	0.53
1:A:197:MET:HE1	1:A:220:ILE:HD12	1.90	0.53
3:C:44:TYR:HE2	3:C:282:ALA:HB2	1.73	0.53
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.74	0.53
3:C:278:ILE:HB	3:C:310:MET:HG3	1.91	0.52
3:C:38:VAL:HG21	3:C:272:ILE:HB	1.92	0.52
3:C:206:GLN:HB3	3:C:258:LEU:HD12	1.92	0.52
1:A:172:MET:HA	1:A:175:PHE:HB3	1.92	0.52
3:C:151:ASP:OD1	3:C:154:MET:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:VAL:H	3:C:274:ASN:HD22	1.58	0.51
3:C:246:ILE:HG21	3:C:363:MET:HE1	1.92	0.51
3:C:220:VAL:HG11	3:C:265:LEU:HD11	1.92	0.51
4:D:105:PHE:HB2	4:D:120:GLU:HB2	1.91	0.51
3:C:196:VAL:HG11	3:C:368:SER:HB2	1.92	0.51
2:B:206:ASP:HA	2:B:210:ARG:HB2	1.93	0.51
1:A:105:ASN:CG	1:A:106:GLU:H	2.18	0.51
1:A:219:ILE:HG22	1:A:220:ILE:HD13	1.93	0.51
2:B:98:TRP:HB3	2:B:112:ALA:HB1	1.93	0.51
3:C:348:PHE:HD2	3:C:369:PRO:HG3	1.75	0.51
2:B:186:CYS:O	2:B:190:LEU:HD12	2.11	0.50
1:A:156:PRO:HG2	1:A:159:PHE:HD2	1.74	0.50
3:C:239:MET:HE3	3:C:349:VAL:HG23	1.94	0.50
2:B:257:LEU:O	2:B:261:TYR:N	2.45	0.50
4:D:50:LYS:HG3	4:D:56:ILE:HD11	1.94	0.50
1:A:59:PHE:HE1	1:A:61:LEU:HD23	1.76	0.50
2:B:150:GLY:O	2:B:154:ASN:ND2	2.33	0.50
3:C:32:ILE:HG12	3:C:276:ARG:HD3	1.93	0.50
3:C:221:ARG:NH1	3:C:230:SER:OG	2.38	0.50
3:C:114:TYR:HE1	3:C:123:LEU:HD11	1.76	0.50
1:A:221:ARG:HH12	1:A:277:ARG:HD3	1.77	0.50
2:B:169:LEU:O	2:B:173:MET:HG2	2.12	0.50
1:A:104:GLN:O	1:A:107:VAL:HG12	2.12	0.49
3:C:114:TYR:CE1	3:C:123:LEU:HD11	2.47	0.49
1:A:259:TYR:HA	1:A:263:ARG:HE	1.76	0.49
1:A:230:THR:HG21	2:B:143:ASN:HA	1.94	0.49
3:C:219:MET:HA	3:C:233:LEU:O	2.13	0.49
1:A:6:THR:OG1	1:A:7:LEU:N	2.41	0.49
3:C:66:THR:HG23	3:C:67:MET:HG2	1.93	0.49
2:B:20:THR:OG1	2:B:23:MET:SD	2.60	0.49
3:C:76:PRO:O	3:C:79:THR:OG1	2.29	0.48
4:D:74:LYS:NZ	4:D:92:SER:O	2.45	0.48
3:C:182:THR:HG22	3:C:198:MET:HB3	1.96	0.48
2:B:37:ALA:O	2:B:78:ARG:NH1	2.46	0.48
1:A:276:ASP:HB3	1:A:278:LYS:HG2	1.96	0.48
2:B:152:ALA:HB1	2:B:196:HIS:CD2	2.49	0.48
3:C:345:ASN:OD1	3:C:346:THR:N	2.39	0.48
1:A:137:LEU:HB2	1:A:156:PRO:HD2	1.96	0.48
1:A:266:TRP:HB3	2:B:268:ASN:C	2.39	0.48
1:A:280:LEU:HB3	1:A:284:GLN:HB2	1.95	0.48
2:B:128:ASP:HB3	2:B:169:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:LEU:HD12	4:D:66:TYR:H	1.79	0.48
2:B:45:ILE:HD12	2:B:48:LEU:HD21	1.96	0.48
3:C:200:ASN:ND2	3:C:264:ASN:OD1	2.41	0.48
2:B:243:CYS:H	2:B:264:LEU:HG	1.80	0.47
3:C:347:PRO:HB3	3:C:366:VAL:O	2.14	0.47
1:A:137:LEU:HD21	1:A:143:VAL:HA	1.96	0.47
3:C:36:ASN:ND2	3:C:367:GLU:OE2	2.48	0.47
3:C:109:SER:O	3:C:301:THR:HG23	2.14	0.47
3:C:199:MET:O	3:C:266:LYS:HA	2.14	0.47
2:B:205:ILE:HG23	2:B:257:LEU:HD13	1.95	0.47
2:B:153:PHE:HD2	2:B:196:HIS:HB2	1.79	0.47
3:C:318:VAL:HG22	3:C:323:THR:HG22	1.96	0.47
1:A:263:ARG:HH12	2:B:244:TRP:HE3	1.61	0.47
2:B:35:ALA:HB3	2:B:36:PRO:HD3	1.97	0.47
3:C:115:TYR:O	3:C:119:HIS:HB3	2.14	0.47
3:C:174:GLN:HA	3:C:225:LYS:HB2	1.95	0.47
3:C:231:MET:SD	3:C:350:PHE:HB2	2.55	0.47
1:A:137:LEU:HD11	1:A:142:SER:HB2	1.96	0.47
2:B:155:ARG:HG3	2:B:166:LEU:HD13	1.96	0.46
2:B:135:CYS:O	2:B:185:ILE:HD11	2.15	0.46
3:C:102:SER:HB3	3:C:123:LEU:HD23	1.97	0.46
3:C:29:TYR:CE2	3:C:243:THR:HG23	2.50	0.46
1:A:9:ARG:HA	1:A:9:ARG:HD3	1.72	0.46
1:A:72:SER:HB2	2:B:18:VAL:H	1.79	0.46
3:C:207:GLY:HA3	3:C:220:VAL:HG22	1.97	0.46
4:D:105:PHE:HB3	4:D:107:MET:SD	2.55	0.46
2:B:97:TYR:CE1	2:B:115:GLU:HB2	2.51	0.46
2:B:239:GLU:HB3	2:B:242:GLU:HB3	1.96	0.46
3:C:150:VAL:HA	3:C:154:MET:CE	2.46	0.46
4:D:102:VAL:HG13	4:D:121:GLU:HG3	1.96	0.46
2:B:59:ARG:NH1	2:B:108:TYR:OH	2.49	0.46
2:B:134:TRP:CE3	2:B:135:CYS:HB3	2.51	0.46
2:B:91:THR:HA	2:B:144:ILE:HD12	1.97	0.45
4:D:105:PHE:HB3	4:D:107:MET:HE1	1.96	0.45
2:B:205:ILE:HD11	2:B:258:THR:OG1	2.17	0.45
3:C:108:VAL:O	3:C:125:ARG:NH2	2.49	0.45
1:A:10:ILE:O	1:A:10:ILE:HG13	2.16	0.45
3:C:278:ILE:HB	3:C:310:MET:CG	2.47	0.45
1:A:57:PRO:O	1:A:127:ARG:NH1	2.49	0.45
3:C:209:THR:HG23	3:C:218:ASP:OD2	2.16	0.45
2:B:49:ALA:O	2:B:53:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:GLN:HE21	2:B:147:GLN:HB2	1.61	0.45
3:C:281:ILE:HA	3:C:284:MET:SD	2.57	0.45
3:C:327:ALA:HB2	3:C:362:PHE:HE1	1.81	0.45
1:A:271:THR:O	1:A:288:ARG:HD2	2.17	0.45
3:C:46:PHE:HE1	3:C:81:LEU:HD21	1.82	0.45
2:B:158:ARG:HD2	4:D:129:ASN:HD21	1.81	0.44
2:B:226:PRO:HB2	2:B:230:LYS:HB3	1.99	0.44
3:C:154:MET:HA	3:C:334:THR:O	2.17	0.44
2:B:40:LEU:HD13	4:D:33:SER:OG	2.17	0.44
3:C:88:LEU:HD22	3:C:96:THR:HG21	2.00	0.44
1:A:55:ILE:HG22	1:A:57:PRO:HD3	1.98	0.44
3:C:239:MET:CE	3:C:349:VAL:HG23	2.48	0.44
1:A:160:ASN:O	1:A:160:ASN:ND2	2.43	0.44
1:A:204:CYS:HB3	1:A:208:MET:HE2	1.98	0.44
2:B:151:SER:O	2:B:155:ARG:HG2	2.18	0.44
3:C:212:ILE:HD12	3:C:254:TRP:CZ2	2.52	0.44
1:A:88:GLU:H	1:A:88:GLU:HG3	1.63	0.43
2:B:8:GLU:O	2:B:9:LEU:HD13	2.17	0.43
3:C:354:HIS:CD2	3:C:357:THR:H	2.24	0.43
2:B:217:LYS:O	2:B:222:ARG:HA	2.18	0.43
1:A:24:MET:HE2	1:A:24:MET:HB3	1.91	0.43
3:C:70:ARG:HH22	3:C:72:ARG:NH2	2.16	0.43
3:C:278:ILE:HG22	3:C:282:ALA:HB2	2.00	0.43
1:A:182:ASN:ND2	1:A:184:ASN:HB2	2.34	0.43
1:A:82:TYR:O	2:B:22:GLU:HG3	2.19	0.43
2:B:173:MET:HE1	2:B:189:PHE:CD1	2.53	0.43
3:C:169:PHE:HE2	3:C:229:ILE:HD13	1.84	0.42
4:D:32:LEU:HD11	4:D:126:LEU:HD22	2.01	0.42
3:C:279:LYS:O	3:C:283:GLU:CB	2.56	0.42
4:D:44:VAL:HG13	4:D:106:PHE:O	2.20	0.42
1:A:97:PRO:HG2	2:B:14:PRO:HD3	2.01	0.42
3:C:56:SER:OG	3:C:296:SER:O	2.25	0.42
2:B:97:TYR:CD1	2:B:97:TYR:C	2.97	0.42
1:A:225:PHE:CE1	1:A:282:TYR:HB2	2.54	0.42
2:B:171:ASN:O	2:B:175:THR:HG23	2.19	0.42
3:C:239:MET:HE1	3:C:348:PHE:HA	2.02	0.42
3:C:277:ASP:OD1	3:C:277:ASP:C	2.63	0.42
1:A:10:ILE:HG12	2:B:8:GLU:O	2.19	0.42
3:C:63:LEU:HA	3:C:66:THR:HG22	2.01	0.42
1:A:161:ASN:OD1	1:A:164:LYS:N	2.51	0.42
3:C:242:PHE:O	3:C:246:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:SER:HA	4:D:86:THR:O	2.20	0.42
1:A:166:GLU:HG2	1:A:193:ARG:HE	1.85	0.42
1:A:92:SER:OG	1:A:93:PHE:N	2.53	0.41
2:B:23:MET:HB3	2:B:23:MET:HE3	1.94	0.41
2:B:202:LYS:HG3	2:B:258:THR:OG1	2.20	0.41
2:B:224:SER:O	2:B:226:PRO:HD3	2.20	0.41
1:A:105:ASN:CG	1:A:106:GLU:N	2.77	0.41
1:A:172:MET:HB3	1:A:172:MET:HE3	1.83	0.41
3:C:330:ILE:HG22	3:C:332:VAL:HG13	2.02	0.41
1:A:216:PHE:CE1	1:A:220:ILE:HG13	2.55	0.41
2:B:68:THR:H	2:B:74:SER:HA	1.86	0.41
2:B:196:HIS:CE1	2:B:197:ASN:HB2	2.55	0.41
2:B:241:ARG:HG3	2:B:246:PRO:HG3	2.02	0.41
3:C:164:ILE:HG12	3:C:330:ILE:HD13	2.01	0.41
1:A:250:TYR:HA	1:A:257:ASP:HB3	2.01	0.41
3:C:35:ASP:HB2	3:C:342:LEU:O	2.18	0.41
1:A:20:ARG:HH21	1:A:58:LYS:HZ3	1.67	0.41
4:D:79:SER:N	4:D:80:PRO:HD3	2.36	0.41
3:C:96:THR:HA	3:C:168:TYR:O	2.21	0.41
3:C:218:ASP:HB2	3:C:235:ILE:CG2	2.51	0.41
1:A:56:LYS:O	1:A:127:ARG:NH2	2.53	0.41
3:C:125:ARG:HA	3:C:125:ARG:HD2	1.89	0.41
1:A:196:ALA:HA	1:A:199:THR:HG22	2.03	0.41
3:C:305:LEU:HD12	3:C:305:LEU:HA	1.86	0.41
4:D:45:MET:CB	4:D:106:PHE:HB2	2.43	0.41
4:D:78:ASP:OD1	4:D:78:ASP:N	2.49	0.41
4:D:83:ASP:OD1	4:D:83:ASP:N	2.47	0.41
1:A:180:PRO:HB2	1:A:212:TYR:CD2	2.56	0.41
3:C:110:ILE:HG22	3:C:300:MET:HG3	2.02	0.41
3:C:288:SER:HB2	3:C:294:ASN:HB3	2.03	0.41
4:D:49:TYR:HB3	4:D:54:SER:O	2.21	0.41
2:B:157:ASP:OD1	2:B:157:ASP:N	2.53	0.40
3:C:65:LYS:HZ2	3:C:65:LYS:C	2.28	0.40
3:C:160:LEU:HB2	3:C:305:LEU:HD11	2.03	0.40
1:A:62:ILE:HD12	1:A:62:ILE:N	2.36	0.40
1:A:193:ARG:O	1:A:197:MET:HG2	2.21	0.40
1:A:220:ILE:HG22	1:A:224:TYR:HB2	2.02	0.40
2:B:243:CYS:O	2:B:244:TRP:HD1	2.04	0.40
4:D:86:THR:HG22	4:D:105:PHE:CZ	2.56	0.40
4:D:106:PHE:C	4:D:107:MET:HE3	2.46	0.40
3:C:341:LYS:C	3:C:342:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:TYR:CD1	4:D:55:ILE:HG12	2.57	0.40
1:A:59:PHE:CE1	1:A:61:LEU:HD23	2.56	0.40
2:B:123:ASP:OD1	2:B:155:ARG:HA	2.21	0.40
3:C:206:GLN:HA	3:C:259:GLY:O	2.22	0.40
1:A:109:PRO:HA	1:A:112:ILE:HB	2.03	0.40
1:A:157:LYS:O	1:A:161:ASN:ND2	2.54	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	284/340 (84%)	275 (97%)	9 (3%)	0	100	100
2	B	259/316 (82%)	232 (90%)	27 (10%)	0	100	100
3	C	352/413 (85%)	336 (96%)	16 (4%)	0	100	100
4	D	112/139 (81%)	108 (96%)	4 (4%)	0	100	100
All	All	1007/1208 (83%)	951 (94%)	56 (6%)	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	259/296 (88%)	254 (98%)	5 (2%)	52	76
2	B	234/272 (86%)	229 (98%)	5 (2%)	48	74
3	C	318/358 (89%)	307 (96%)	11 (4%)	31	63
4	D	105/125 (84%)	99 (94%)	6 (6%)	17	50
All	All	916/1051 (87%)	889 (97%)	27 (3%)	39	67

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	90	CYS
1	A	107	VAL
1	A	160	ASN
1	A	245	CYS
2	B	31	HIS
2	B	81	TYR
2	B	139	THR
2	B	213	SER
2	B	248	CYS
3	C	67	MET
3	C	71	LYS
3	C	80	GLU
3	C	104	VAL
3	C	170	LYS
3	C	214	ASP
3	C	219	MET
3	C	239	MET
3	C	276	ARG
3	C	346	THR
3	C	367	GLU
4	D	43	VAL
4	D	44	VAL
4	D	49	TYR
4	D	81	TYR
4	D	103	CYS
4	D	113	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN

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Mol	Chain	Res	Type
2	B	44	HIS
3	C	19	GLN
3	C	119	HIS
3	C	241	HIS
3	C	312	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

10 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	$\# Z  > 2$
5	NAG	E	1	3,5	14,14,15	0.83	1 (7%)	17,19,21	1.52	3 (17%)
5	NAG	E	2	5	14,14,15	0.76	0	17,19,21	1.46	4 (23%)
5	BMA	E	3	5	11,11,12	0.86	0	15,15,17	2.45	5 (33%)
5	MAN	E	4	5	11,11,12	0.78	0	15,15,17	1.00	1 (6%)
6	NAG	F	1	3,6	14,14,15	0.74	0	17,19,21	0.96	0
6	NAG	F	2	6	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
6	BMA	F	3	6	11,11,12	0.86	0	15,15,17	2.11	3 (20%)
6	FUC	F	4	6	10,10,11	0.72	0	14,14,16	1.56	3 (21%)
7	NAG	G	1	4,7	14,14,15	0.72	0	17,19,21	1.15	1 (5%)
7	NAG	G	2	7	14,14,15	0.72	0	17,19,21	0.80	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	E	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	FUC	F	4	6	-	-	0/1/1/1
7	NAG	G	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	O5-C1	-2.04	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	BMA	C1-O5-C5	7.46	122.30	112.19
6	F	3	BMA	C1-O5-C5	6.39	120.85	112.19
5	E	1	NAG	O5-C1-C2	-4.18	104.69	111.29
6	F	4	FUC	C1-C2-C3	3.44	113.89	109.67
7	G	1	NAG	C2-N2-C7	3.02	127.21	122.90
5	E	2	NAG	C4-C3-C2	-2.98	106.65	111.02
6	F	4	FUC	C1-O5-C5	2.96	119.48	112.78
5	E	4	MAN	C1-O5-C5	2.42	115.47	112.19
5	E	2	NAG	O4-C4-C5	2.35	115.14	109.30
5	E	3	BMA	C2-C3-C4	2.35	114.96	110.89
5	E	2	NAG	C1-O5-C5	2.29	115.29	112.19
6	F	3	BMA	C3-C4-C5	2.26	114.27	110.24
6	F	3	BMA	C2-C3-C4	2.23	114.76	110.89
5	E	3	BMA	C3-C4-C5	2.21	114.19	110.24
5	E	2	NAG	O5-C5-C4	-2.21	105.44	110.83
6	F	4	FUC	C3-C4-C5	-2.20	106.35	109.77
5	E	3	BMA	O3-C3-C2	-2.18	105.83	109.99
6	F	2	NAG	O5-C1-C2	-2.15	107.89	111.29
5	E	1	NAG	C3-C4-C5	2.10	113.99	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	BMA	O4-C4-C3	-2.07	105.56	110.35
5	E	1	NAG	O4-C4-C3	-2.02	105.68	110.35

There are no chirality outliers.

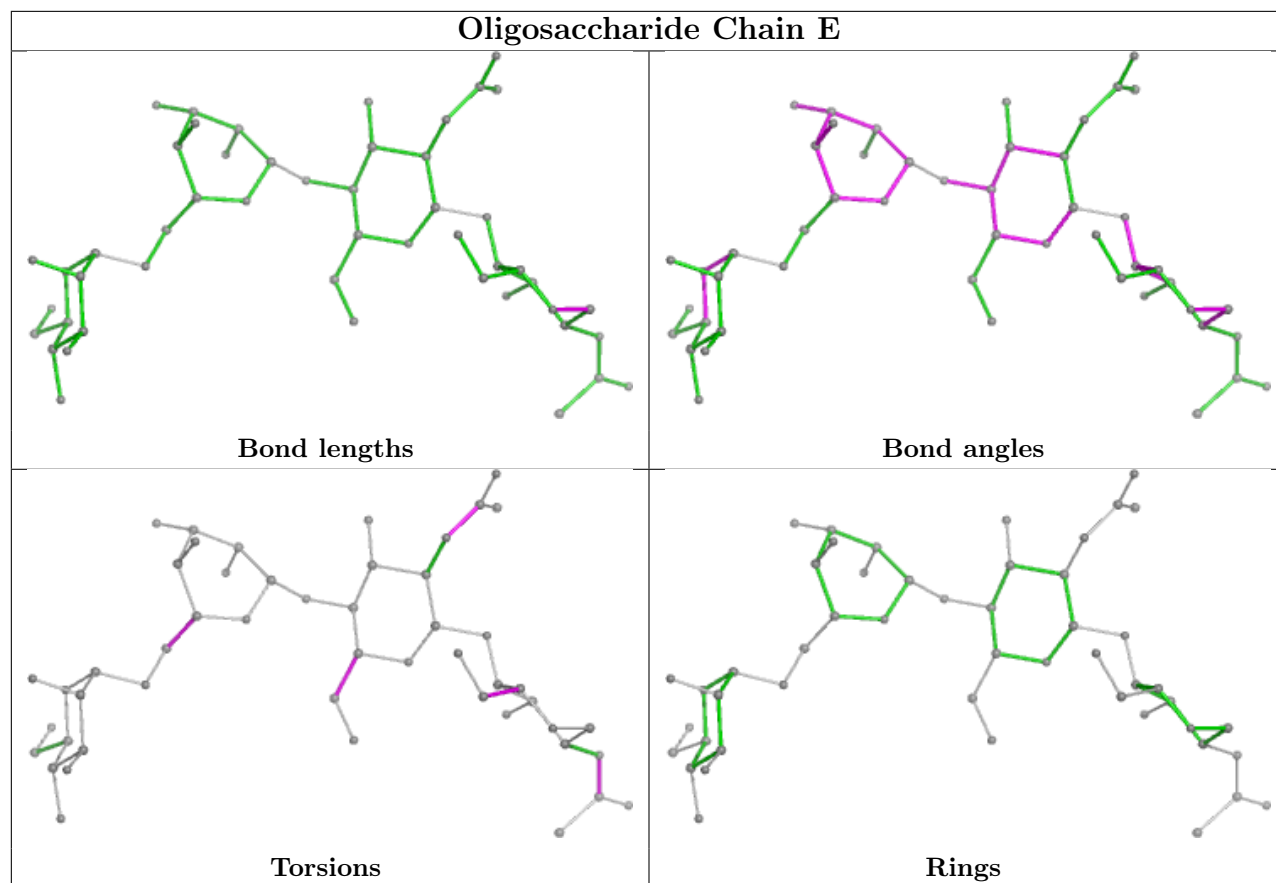
All (15) torsion outliers are listed below:

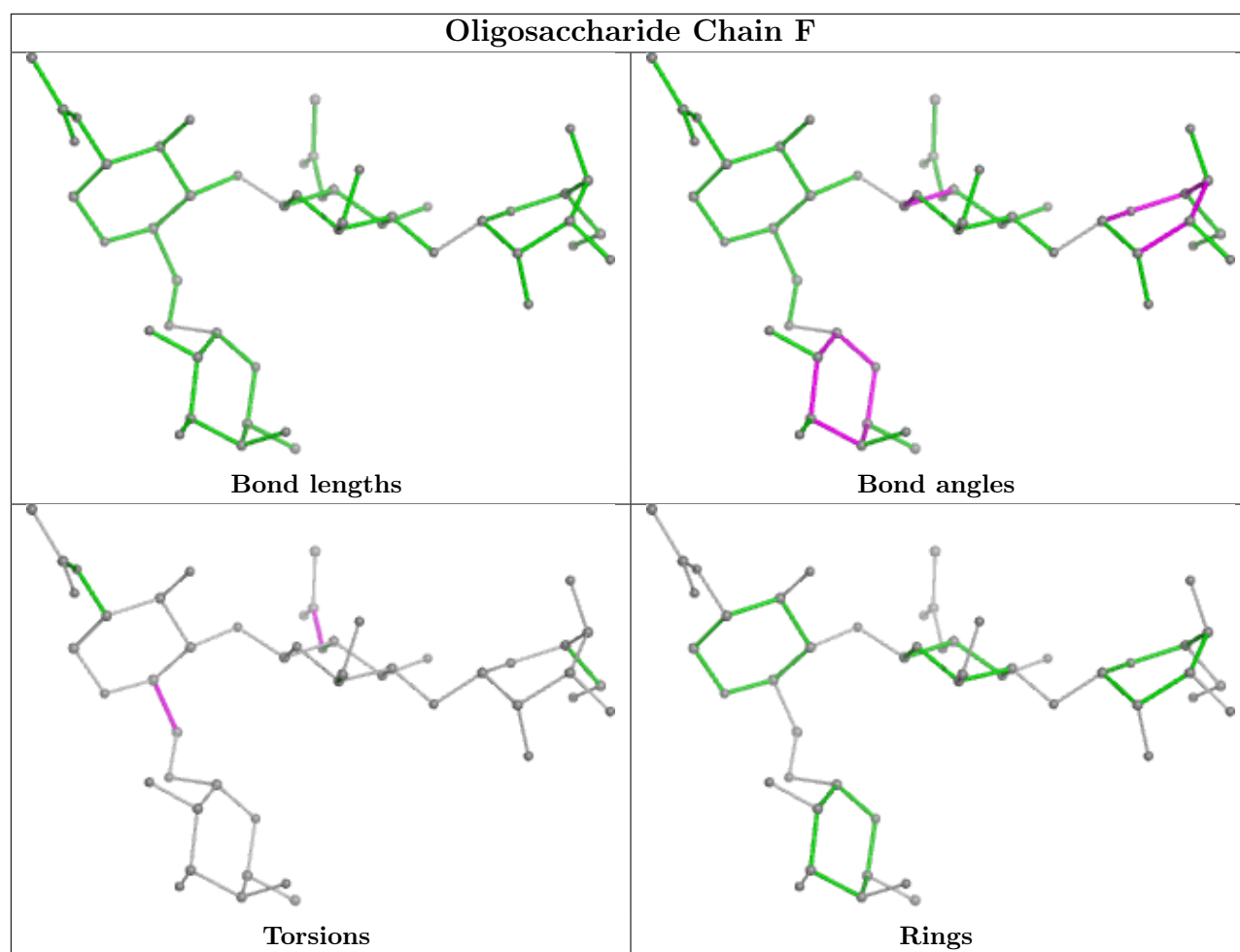
Mol	Chain	Res	Type	Atoms
5	E	3	BMA	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
5	E	1	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	G	1	NAG	C3-C2-N2-C7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

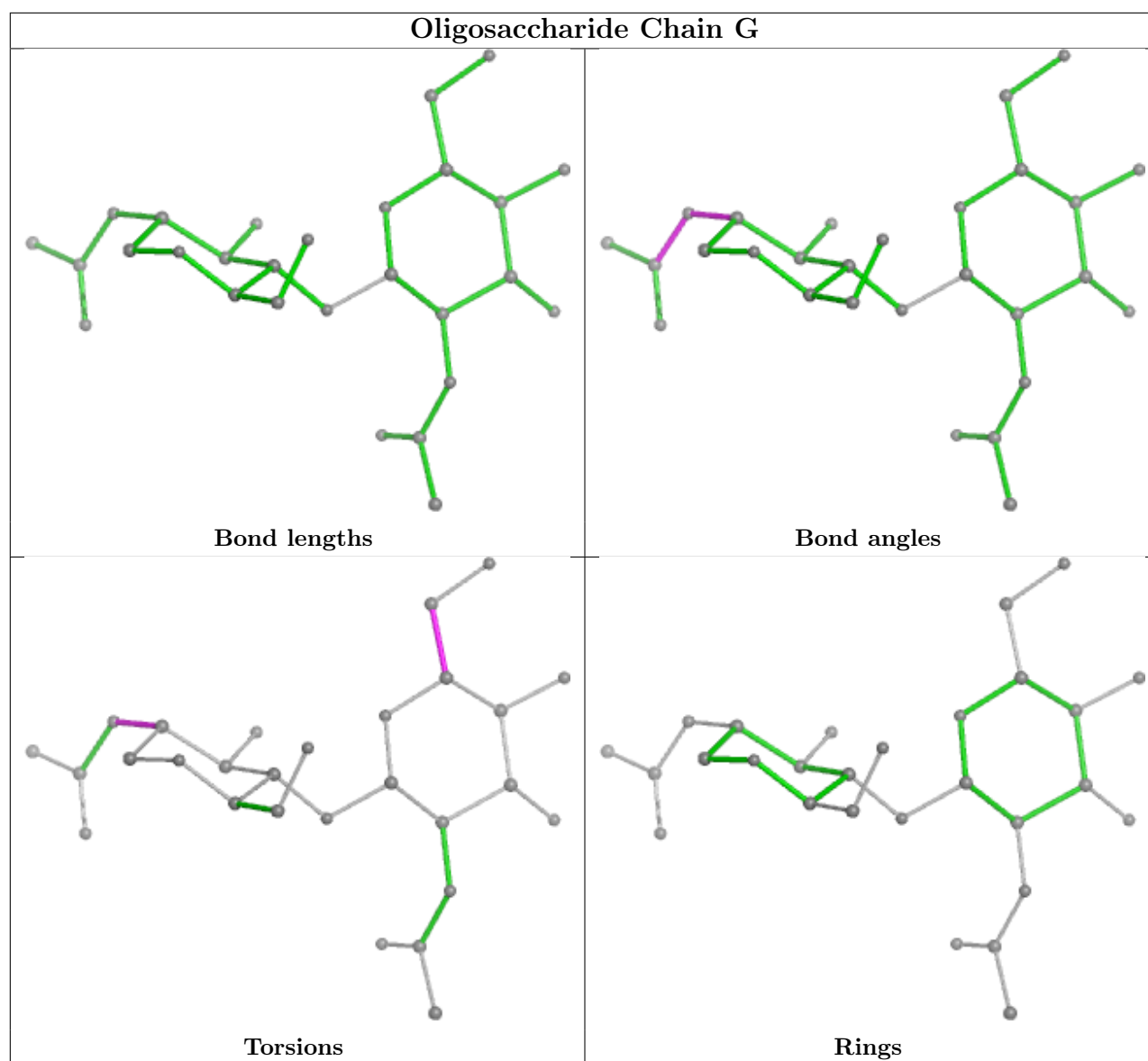
There are no ring outliers.

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 oligosaccharide.







## 5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z  > 2$
8	NAG	D	201	4	14,14,15	0.72	0	17,19,21	0.98	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	201	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	201	NAG	O5-C1-C2	-2.85	106.79	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

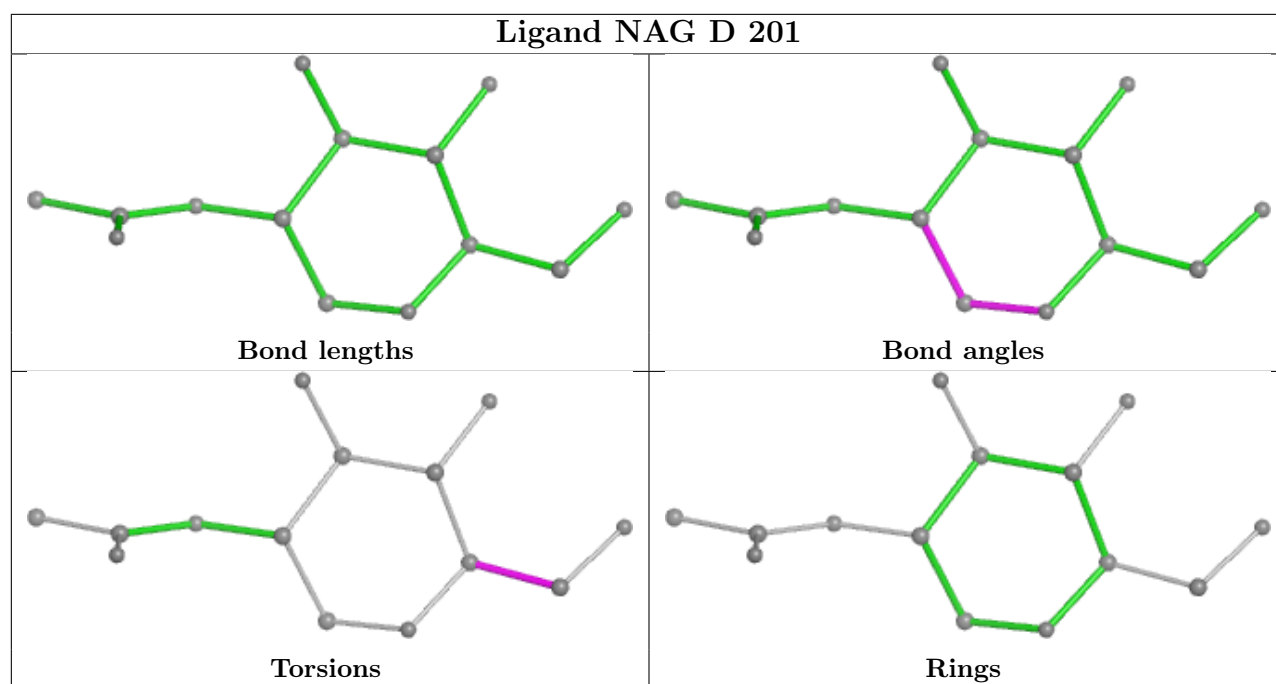
Mol	Chain	Res	Type	Atoms
8	D	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	201	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 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.

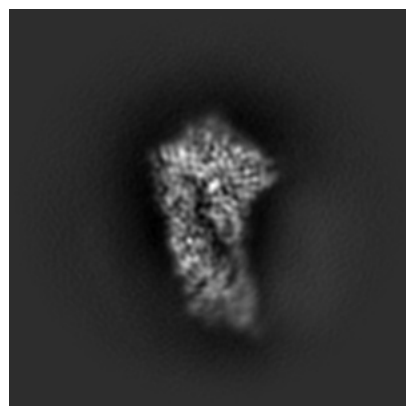
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52019. These allow visual inspection of the internal detail of the map and identification of artifacts.

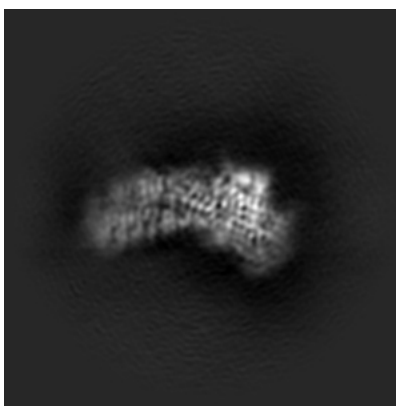
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

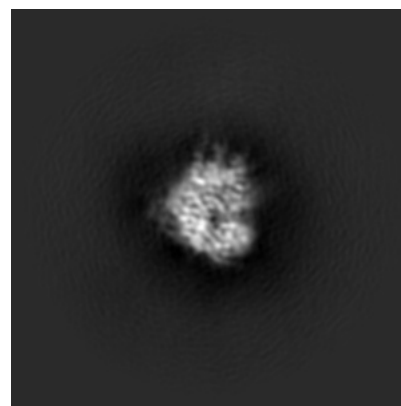
#### 6.1.1 Primary map



X

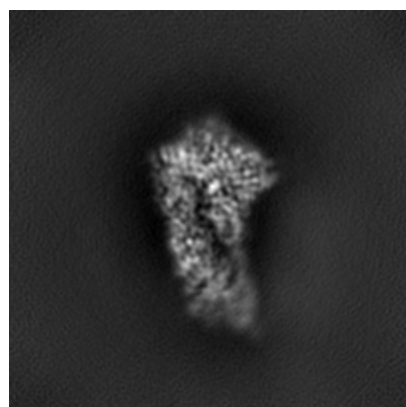


Y

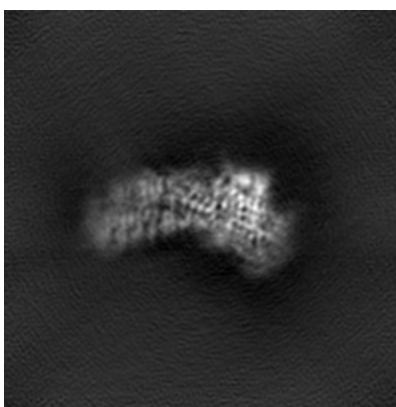


Z

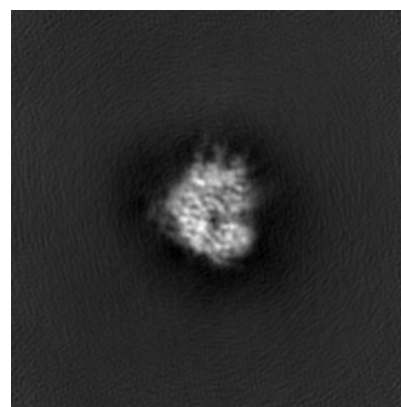
#### 6.1.2 Raw map



X



Y

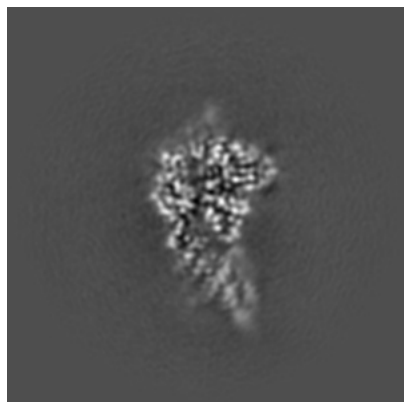


Z

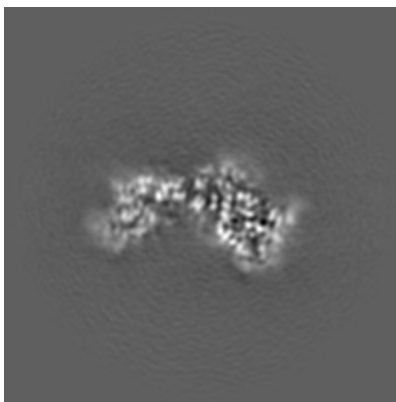
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

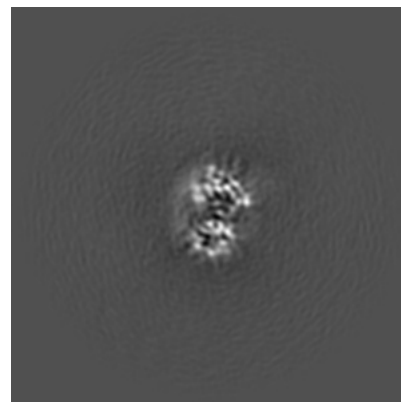
### 6.2.1 Primary map



X Index: 90

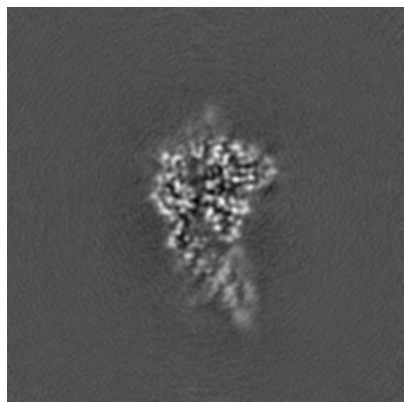


Y Index: 90

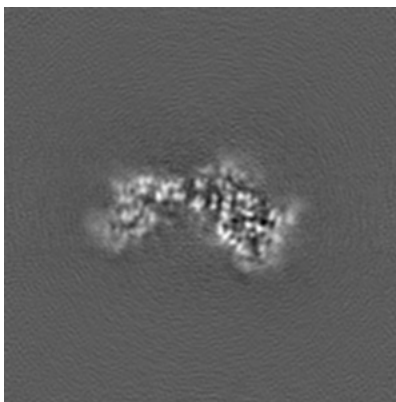


Z Index: 90

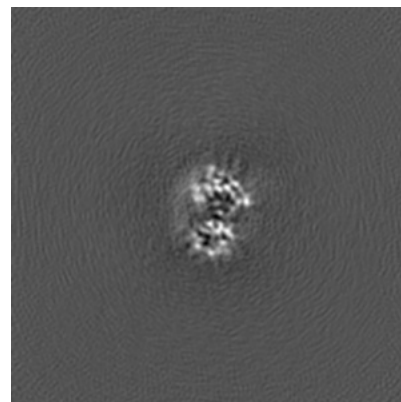
### 6.2.2 Raw map



X Index: 90



Y Index: 90



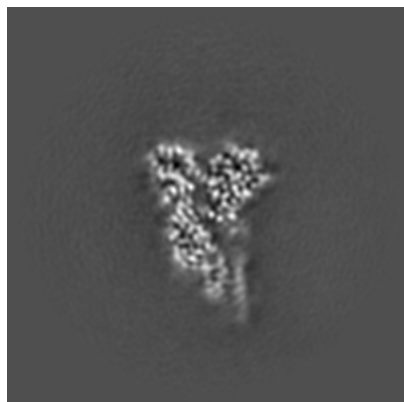
Z Index: 90

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

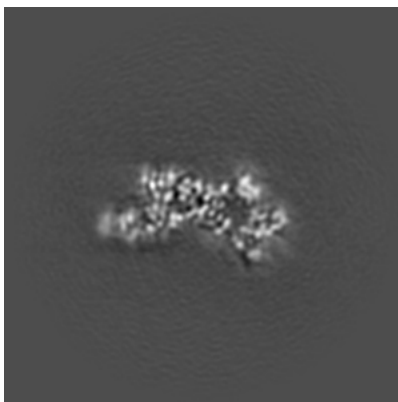


## 6.3 Largest variance slices [i](#)

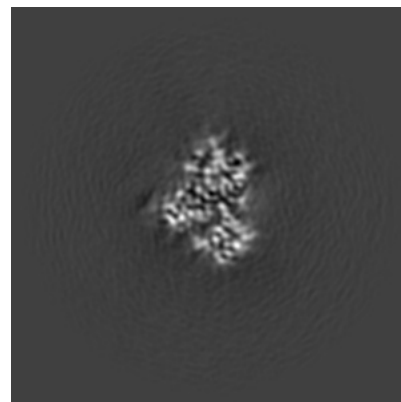
### 6.3.1 Primary map



X Index: 98

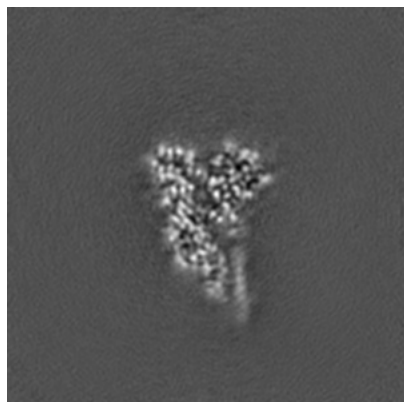


Y Index: 82

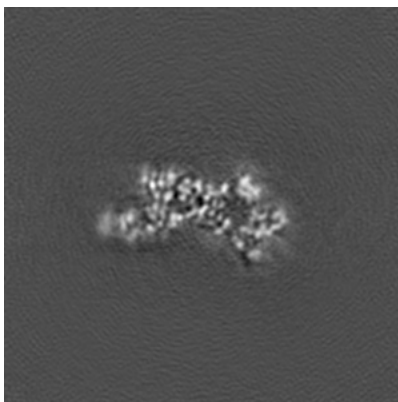


Z Index: 106

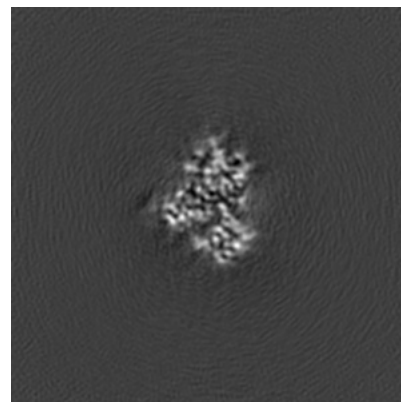
### 6.3.2 Raw map



X Index: 97



Y Index: 82

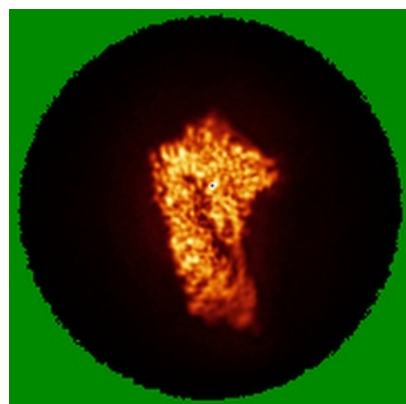


Z Index: 106

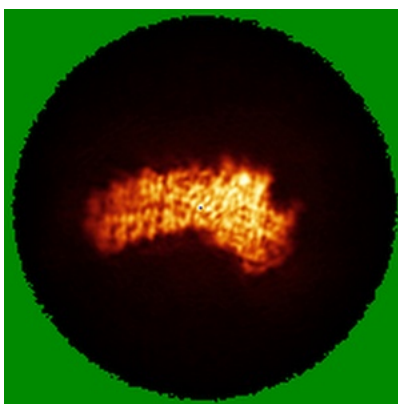
The images above show the largest variance slices of the map in three orthogonal directions.

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

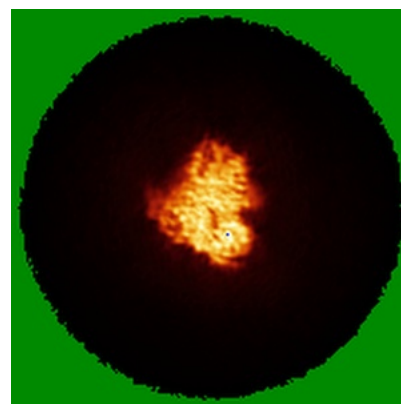
### 6.4.1 Primary map



X

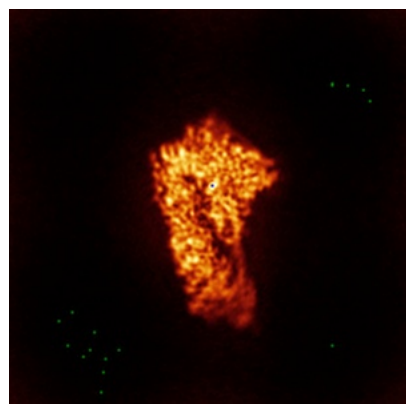


Y

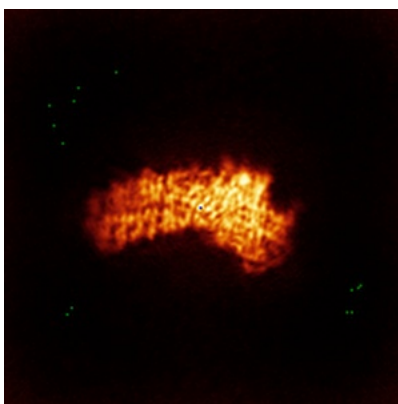


Z

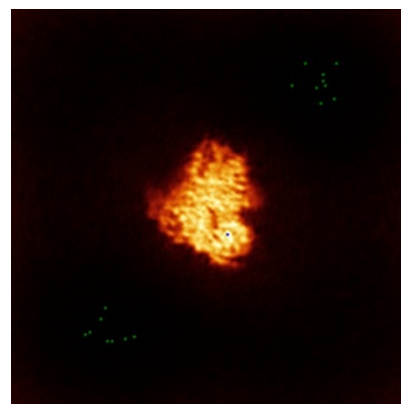
### 6.4.2 Raw map



X



Y

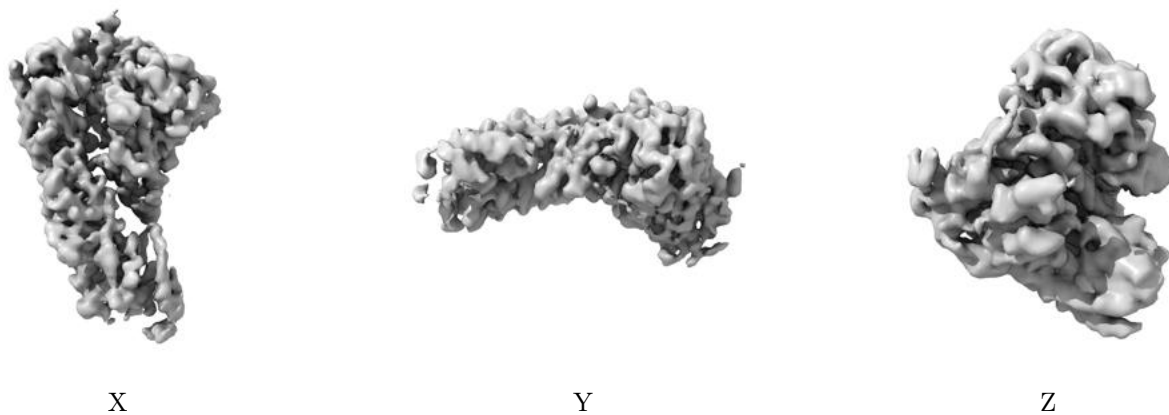


Z

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 0.12. 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.

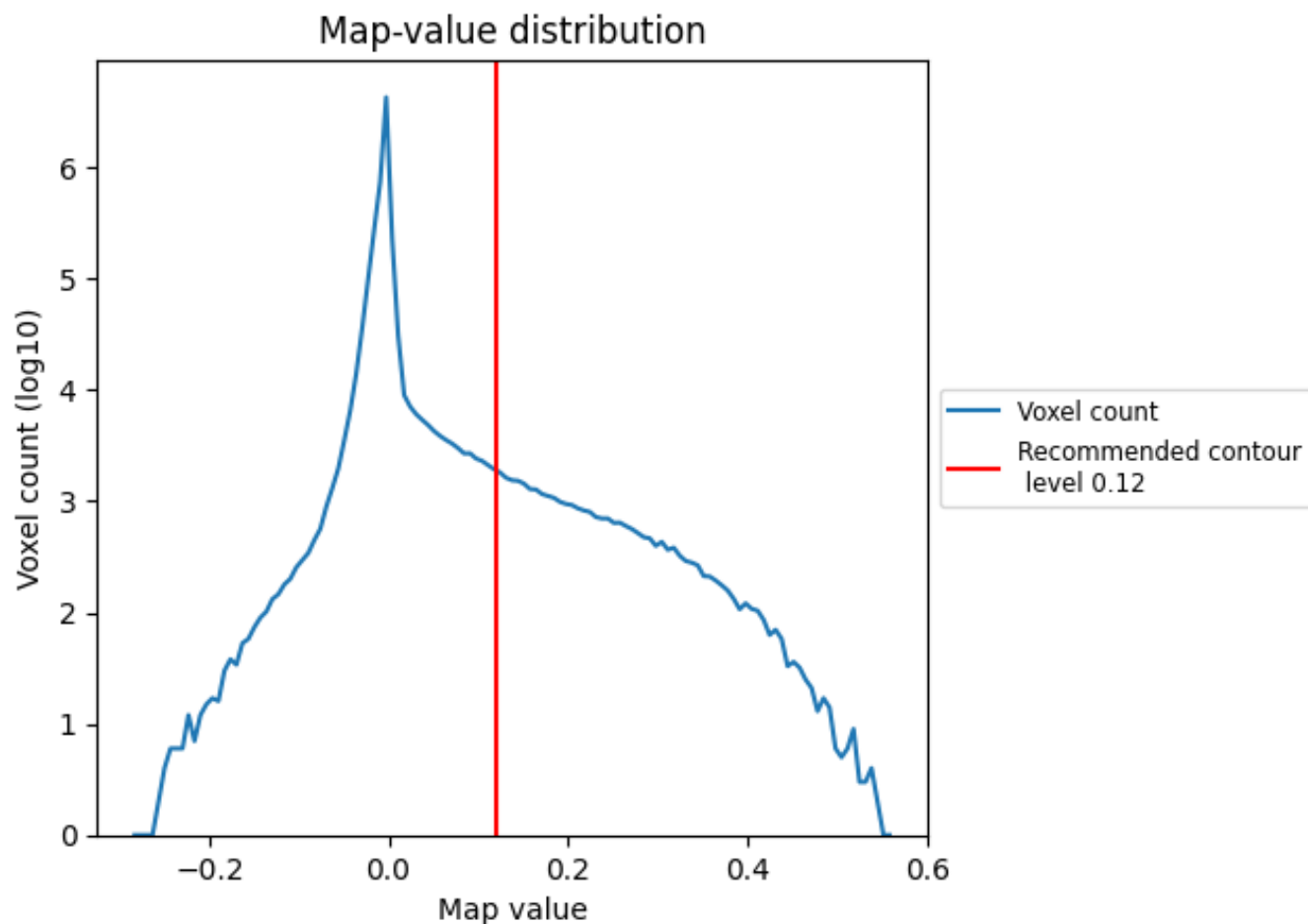
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

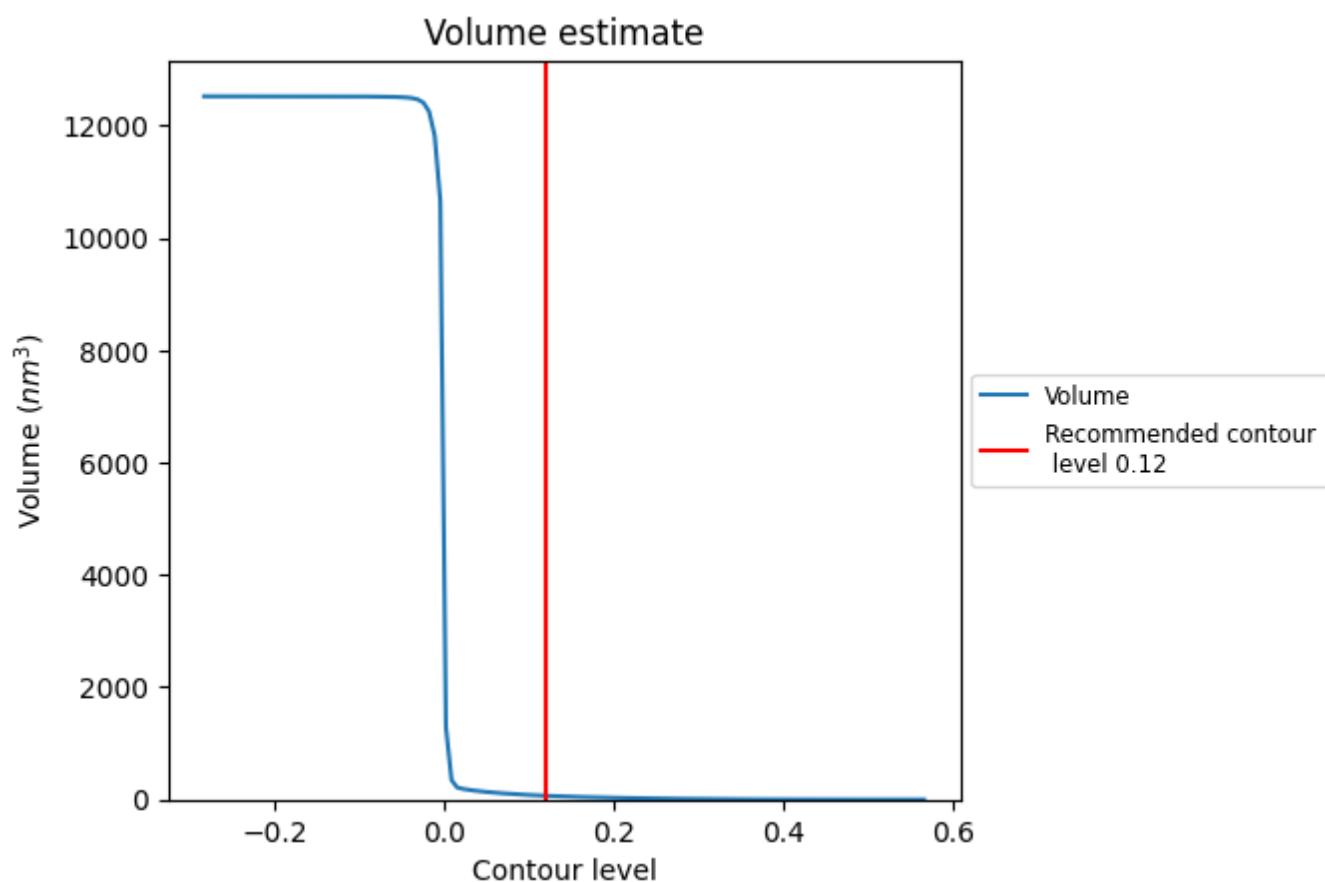
This section contains the results of statistical analysis of the map.

### 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.

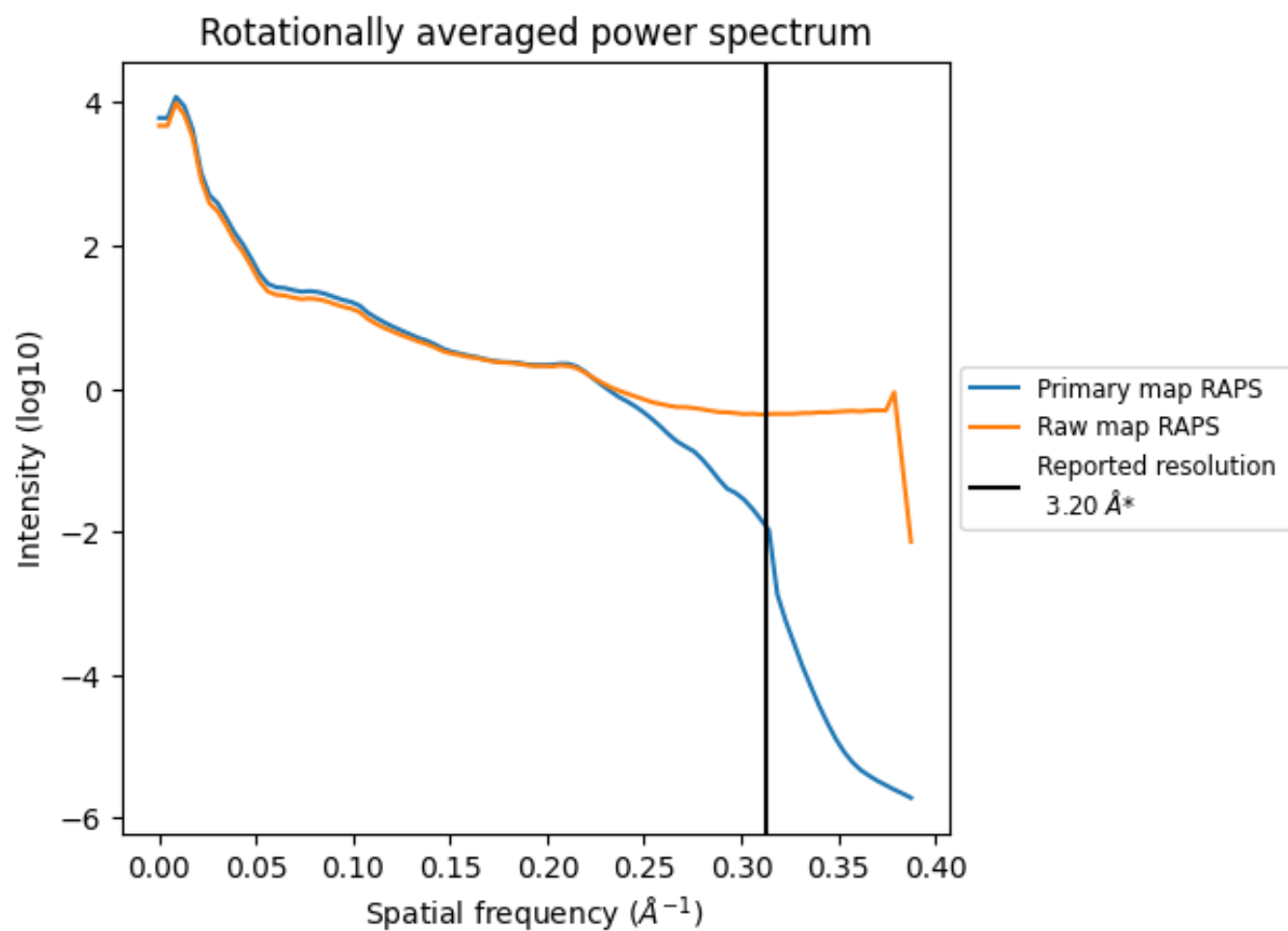
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm<sup>3</sup>; this corresponds to an approximate mass of 61 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 ⓘ

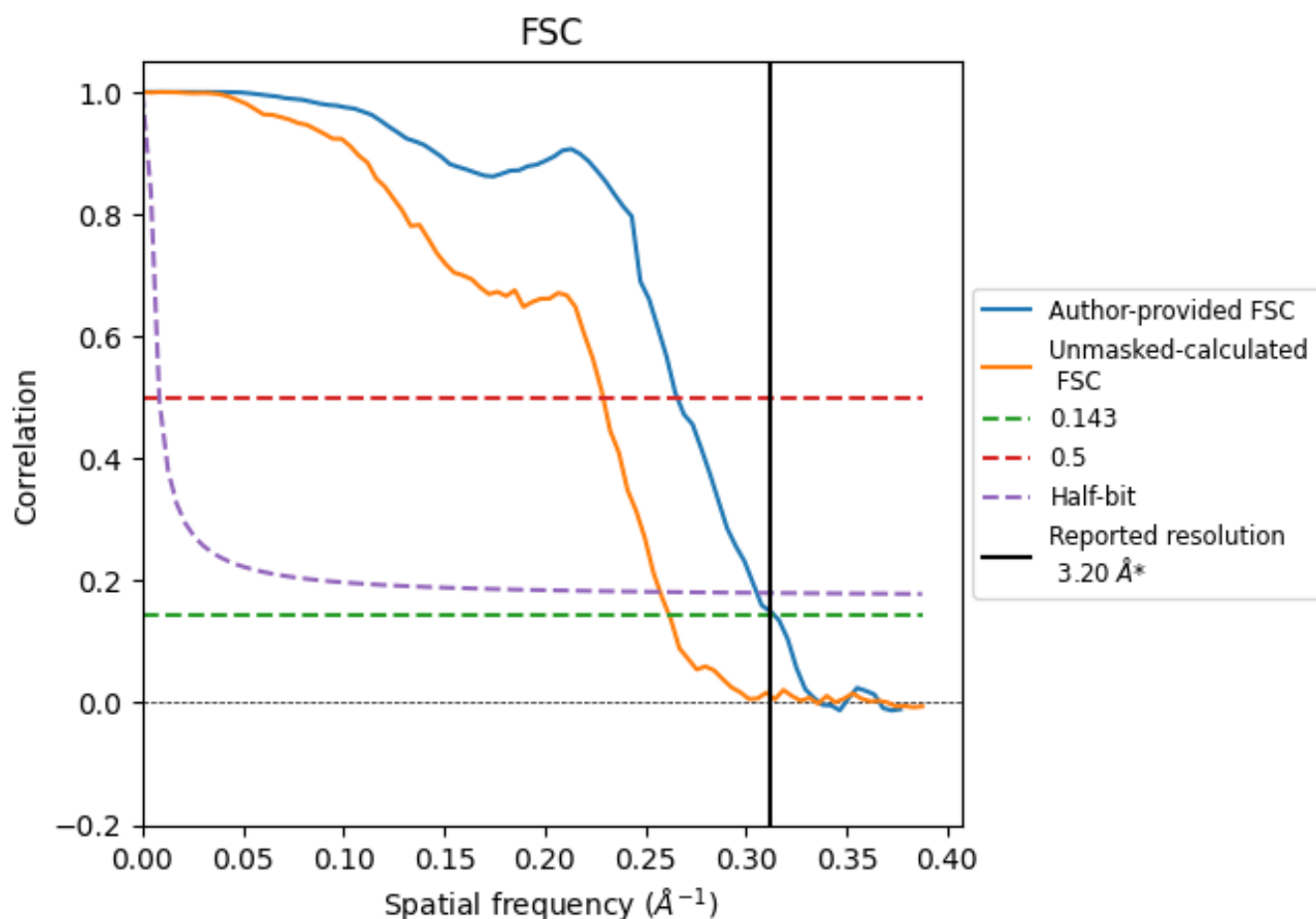


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.76	3.27
Unmasked-calculated*	3.82	4.37	3.89

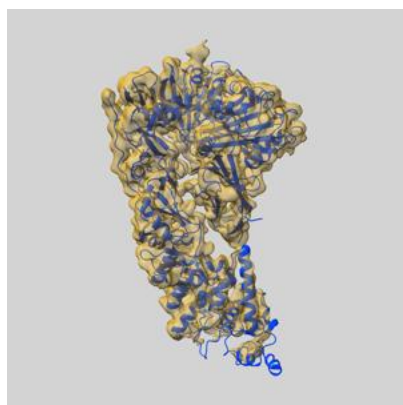
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.2 by more than 10 %



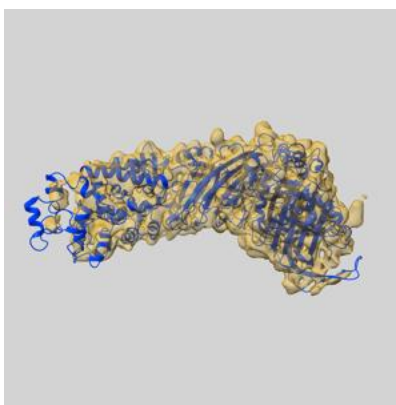
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52019 and PDB model 9HBK. Per-residue inclusion information can be found in section [3](#) on page [10](#).

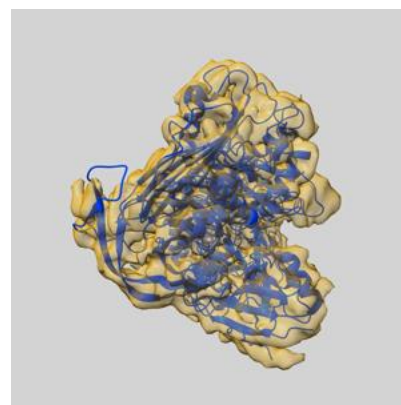
### 9.1 Map-model overlay [i](#)



X



Y



Z

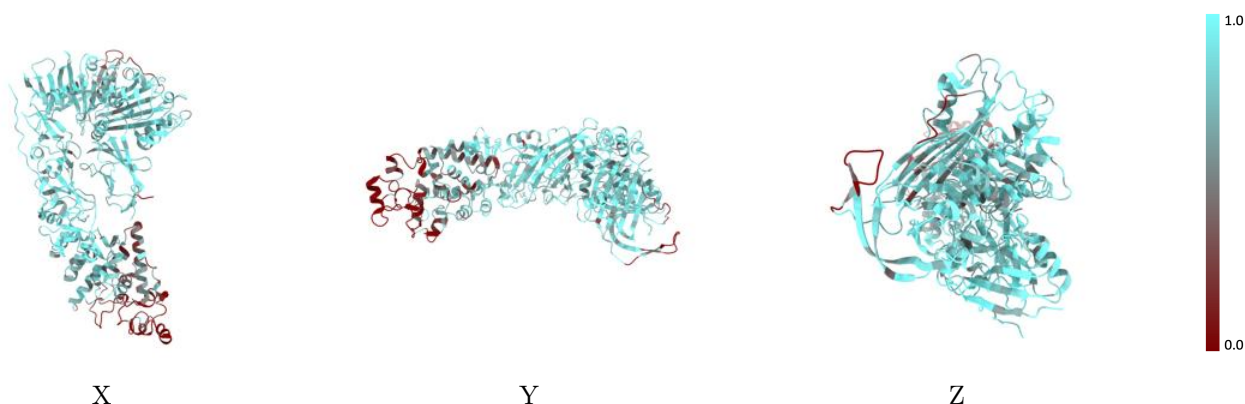
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



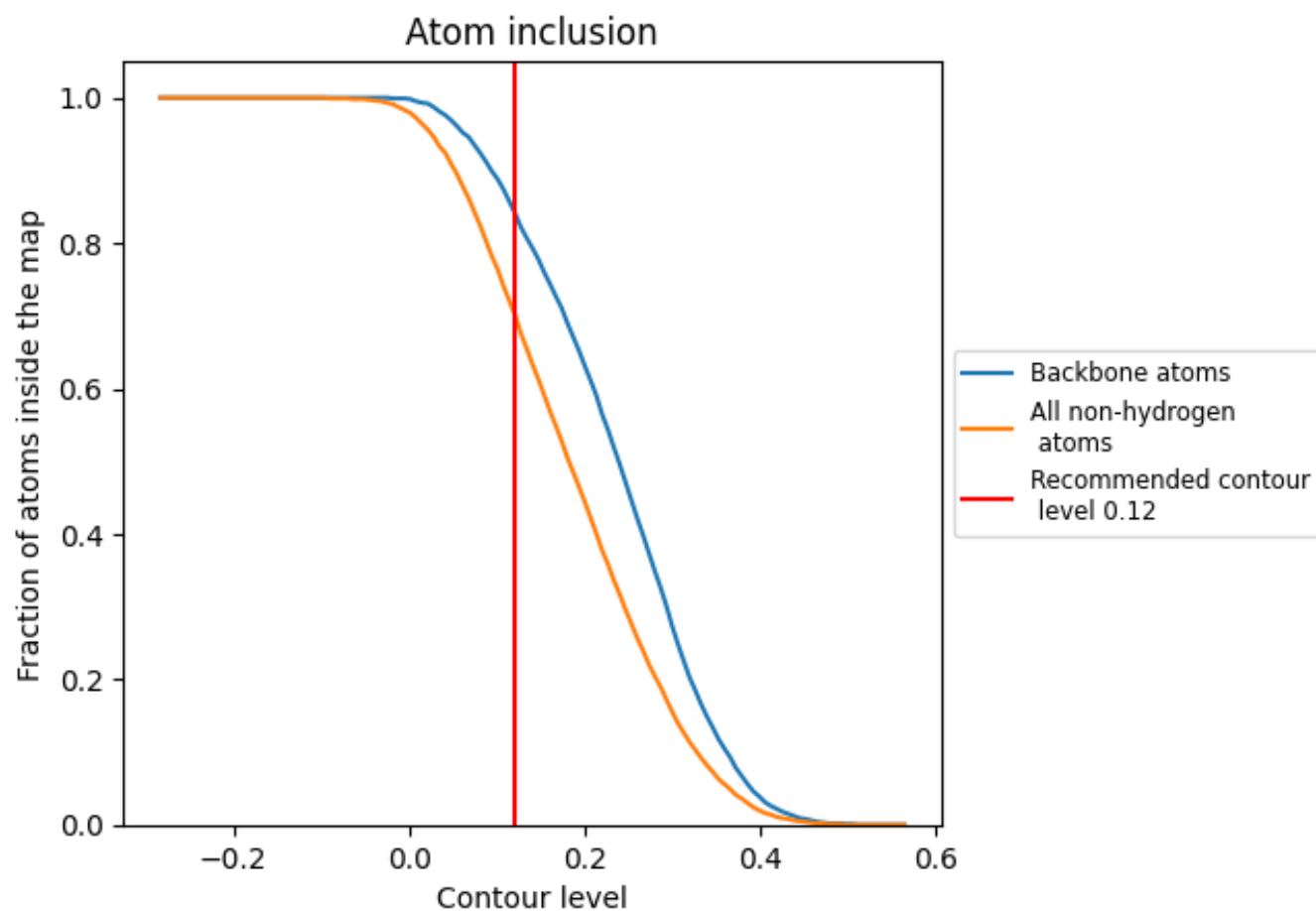
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 70% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7040	<div></div> 0.3560
A	<div></div> 0.7280	<div></div> 0.3510
B	<div></div> 0.5580	<div></div> 0.2920
C	<div></div> 0.7740	<div></div> 0.3860
D	<div></div> 0.7770	<div></div> 0.4150
E	<div></div> 0.7600	<div></div> 0.4020
F	<div></div> 0.4490	<div></div> 0.3810
G	<div></div> 0.3570	<div></div> 0.3130

1.0

0.0

<0.0