W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Mar 10, 2022 – 02:12 am GMT

PDB ID	:	7R1A
EMDB ID	:	EMD-14236
Title	:	Furin Cleaved Alpha Variant SARS-CoV-2 Spike in complex with 3 ACE2
Authors	:	Benton, D.J.; Wrobel, A.G.; Gamblin, S.J.
Deposited on	:	2022-02-02
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.90 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		0.1%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
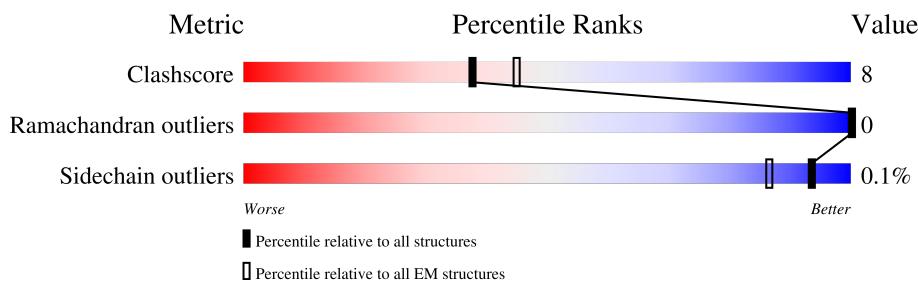
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	1284	58% 19% 22%
1	B	1284	58% 19% 22%
1	C	1284	58% 19% 22%
2	D	654	14% 79% 11% 10%
2	E	654	15% 79% 11% 10%
2	F	654	14% 79% 11% 10%
3	G	2	100%
3	H	2	100%
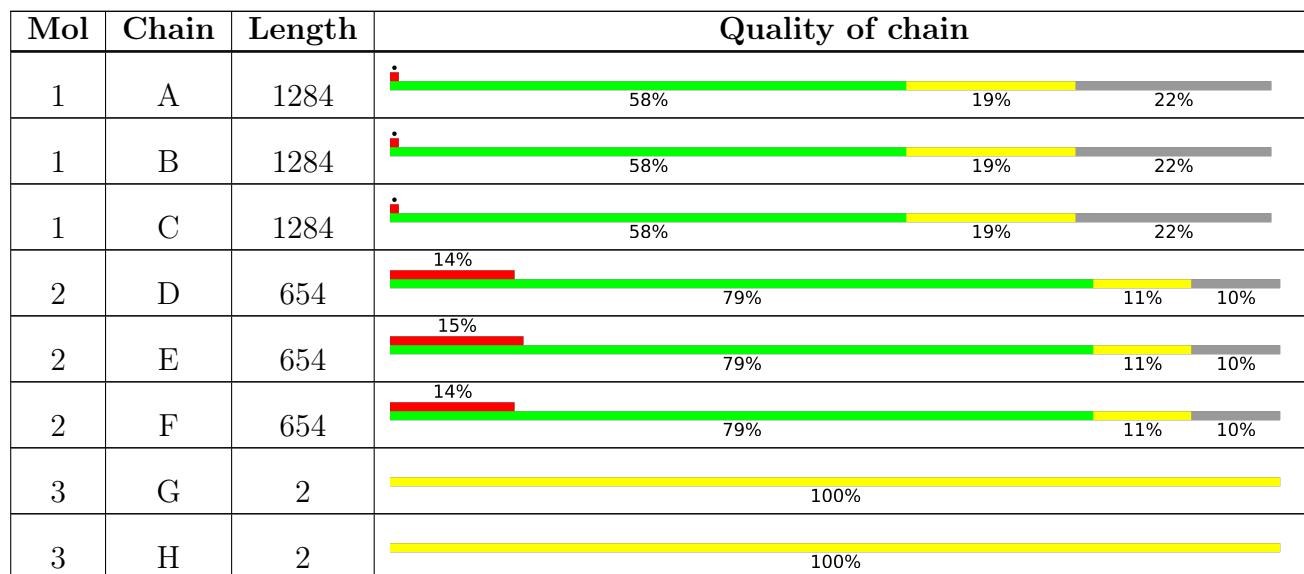
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Mol	Chain	Length	Quality of chain
3	I	2	100%

2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 38616 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	998	Total 7818	C 5002	N 1300	O 1481	S 35	0	0
1	B	998	Total 7818	C 5002	N 1300	O 1481	S 35	0	0
1	C	998	Total 7818	C 5002	N 1300	O 1481	S 35	0	0

There are 273 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP P0DTC2
A	-29	GLY	-	expression tag	UNP P0DTC2
A	-28	ILE	-	expression tag	UNP P0DTC2
A	-27	LEU	-	expression tag	UNP P0DTC2
A	-26	PRO	-	expression tag	UNP P0DTC2
A	-25	SER	-	expression tag	UNP P0DTC2
A	-24	PRO	-	expression tag	UNP P0DTC2
A	-23	GLY	-	expression tag	UNP P0DTC2
A	-22	MET	-	expression tag	UNP P0DTC2
A	-21	PRO	-	expression tag	UNP P0DTC2
A	-20	ALA	-	expression tag	UNP P0DTC2
A	-19	LEU	-	expression tag	UNP P0DTC2
A	-18	LEU	-	expression tag	UNP P0DTC2
A	-17	SER	-	expression tag	UNP P0DTC2
A	-16	LEU	-	expression tag	UNP P0DTC2
A	-15	VAL	-	expression tag	UNP P0DTC2
A	-14	SER	-	expression tag	UNP P0DTC2
A	-13	LEU	-	expression tag	UNP P0DTC2
A	-12	LEU	-	expression tag	UNP P0DTC2
A	-11	SER	-	expression tag	UNP P0DTC2
A	-10	VAL	-	expression tag	UNP P0DTC2
A	-9	LEU	-	expression tag	UNP P0DTC2
A	-8	LEU	-	expression tag	UNP P0DTC2
A	-7	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P0DTC2
A	-5	CYS	-	expression tag	UNP P0DTC2
A	-4	VAL	-	expression tag	UNP P0DTC2
A	-3	ALA	-	expression tag	UNP P0DTC2
A	-2	GLU	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	GLY	-	expression tag	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	570	ASP	ALA	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	716	ILE	THR	variant	UNP P0DTC2
A	982	ALA	SER	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1118	HIS	ASP	variant	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ASN	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	PHE	-	expression tag	UNP P0DTC2
A	1217	GLN	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
B	-30	MET	-	initiating methionine	UNP P0DTC2
B	-29	GLY	-	expression tag	UNP P0DTC2
B	-28	ILE	-	expression tag	UNP P0DTC2
B	-27	LEU	-	expression tag	UNP P0DTC2
B	-26	PRO	-	expression tag	UNP P0DTC2
B	-25	SER	-	expression tag	UNP P0DTC2
B	-24	PRO	-	expression tag	UNP P0DTC2
B	-23	GLY	-	expression tag	UNP P0DTC2
B	-22	MET	-	expression tag	UNP P0DTC2
B	-21	PRO	-	expression tag	UNP P0DTC2
B	-20	ALA	-	expression tag	UNP P0DTC2
B	-19	LEU	-	expression tag	UNP P0DTC2
B	-18	LEU	-	expression tag	UNP P0DTC2
B	-17	SER	-	expression tag	UNP P0DTC2
B	-16	LEU	-	expression tag	UNP P0DTC2
B	-15	VAL	-	expression tag	UNP P0DTC2
B	-14	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	LEU	-	expression tag	UNP P0DTC2
B	-12	LEU	-	expression tag	UNP P0DTC2
B	-11	SER	-	expression tag	UNP P0DTC2
B	-10	VAL	-	expression tag	UNP P0DTC2
B	-9	LEU	-	expression tag	UNP P0DTC2
B	-8	LEU	-	expression tag	UNP P0DTC2
B	-7	MET	-	expression tag	UNP P0DTC2
B	-6	GLY	-	expression tag	UNP P0DTC2
B	-5	CYS	-	expression tag	UNP P0DTC2
B	-4	VAL	-	expression tag	UNP P0DTC2
B	-3	ALA	-	expression tag	UNP P0DTC2
B	-2	GLU	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	GLY	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	570	ASP	ALA	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	716	ILE	THR	variant	UNP P0DTC2
B	982	ALA	SER	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1118	HIS	ASP	variant	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	ARG	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ASN	-	expression tag	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	PHE	-	expression tag	UNP P0DTC2
B	1217	GLN	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	ILE	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	ARG	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLN	-	expression tag	UNP P0DTC2
B	1234	ALA	-	expression tag	UNP P0DTC2
B	1235	TYR	-	expression tag	UNP P0DTC2
B	1236	VAL	-	expression tag	UNP P0DTC2
B	1237	ARG	-	expression tag	UNP P0DTC2
B	1238	LYS	-	expression tag	UNP P0DTC2
B	1239	ASP	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	TRP	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	LEU	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	THR	-	expression tag	UNP P0DTC2
B	1248	PHE	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
C	-30	MET	-	initiating methionine	UNP P0DTC2
C	-29	GLY	-	expression tag	UNP P0DTC2
C	-28	ILE	-	expression tag	UNP P0DTC2
C	-27	LEU	-	expression tag	UNP P0DTC2
C	-26	PRO	-	expression tag	UNP P0DTC2
C	-25	SER	-	expression tag	UNP P0DTC2
C	-24	PRO	-	expression tag	UNP P0DTC2
C	-23	GLY	-	expression tag	UNP P0DTC2
C	-22	MET	-	expression tag	UNP P0DTC2
C	-21	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	ALA	-	expression tag	UNP P0DTC2
C	-19	LEU	-	expression tag	UNP P0DTC2
C	-18	LEU	-	expression tag	UNP P0DTC2
C	-17	SER	-	expression tag	UNP P0DTC2
C	-16	LEU	-	expression tag	UNP P0DTC2
C	-15	VAL	-	expression tag	UNP P0DTC2
C	-14	SER	-	expression tag	UNP P0DTC2
C	-13	LEU	-	expression tag	UNP P0DTC2
C	-12	LEU	-	expression tag	UNP P0DTC2
C	-11	SER	-	expression tag	UNP P0DTC2
C	-10	VAL	-	expression tag	UNP P0DTC2
C	-9	LEU	-	expression tag	UNP P0DTC2
C	-8	LEU	-	expression tag	UNP P0DTC2
C	-7	MET	-	expression tag	UNP P0DTC2
C	-6	GLY	-	expression tag	UNP P0DTC2
C	-5	CYS	-	expression tag	UNP P0DTC2
C	-4	VAL	-	expression tag	UNP P0DTC2
C	-3	ALA	-	expression tag	UNP P0DTC2
C	-2	GLU	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	0	GLY	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	570	ASP	ALA	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	716	ILE	THR	variant	UNP P0DTC2
C	982	ALA	SER	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1118	HIS	ASP	variant	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	expression tag	UNP P0DTC2
C	1211	ARG	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ASN	-	expression tag	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	PHE	-	expression tag	UNP P0DTC2
C	1217	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLY	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	ILE	-	expression tag	UNP P0DTC2
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	ARG	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLN	-	expression tag	UNP P0DTC2
C	1234	ALA	-	expression tag	UNP P0DTC2
C	1235	TYR	-	expression tag	UNP P0DTC2
C	1236	VAL	-	expression tag	UNP P0DTC2
C	1237	ARG	-	expression tag	UNP P0DTC2
C	1238	LYS	-	expression tag	UNP P0DTC2
C	1239	ASP	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	TRP	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	LEU	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	THR	-	expression tag	UNP P0DTC2
C	1248	PHE	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	588	Total	C	N	O	S	0	0
			4801	3076	794	902	29		
2	E	588	Total	C	N	O	S	0	0
			4801	3076	794	902	29		
2	F	588	Total	C	N	O	S	0	0
			4801	3076	794	902	29		

There are 177 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	initiating methionine	UNP Q9BYF1
D	0	GLU	-	expression tag	UNP Q9BYF1
D	1	THR	-	expression tag	UNP Q9BYF1
D	2	ASP	-	expression tag	UNP Q9BYF1
D	3	THR	-	expression tag	UNP Q9BYF1
D	4	LEU	-	expression tag	UNP Q9BYF1
D	5	LEU	-	expression tag	UNP Q9BYF1
D	6	LEU	-	expression tag	UNP Q9BYF1
D	7	TRP	-	expression tag	UNP Q9BYF1
D	8	VAL	-	expression tag	UNP Q9BYF1
D	9	LEU	-	expression tag	UNP Q9BYF1
D	10	LEU	-	expression tag	UNP Q9BYF1
D	11	LEU	-	expression tag	UNP Q9BYF1
D	12	TRP	-	expression tag	UNP Q9BYF1
D	13	VAL	-	expression tag	UNP Q9BYF1
D	14	PRO	-	expression tag	UNP Q9BYF1
D	15	GLY	-	expression tag	UNP Q9BYF1
D	16	SER	-	expression tag	UNP Q9BYF1
D	17	THR	-	expression tag	UNP Q9BYF1
D	18	GLY	-	expression tag	UNP Q9BYF1
D	614	ALA	-	expression tag	UNP Q9BYF1
D	615	ASP	-	expression tag	UNP Q9BYF1
D	616	ASP	-	expression tag	UNP Q9BYF1
D	617	TYR	-	expression tag	UNP Q9BYF1
D	618	LYS	-	expression tag	UNP Q9BYF1
D	619	ASP	-	expression tag	UNP Q9BYF1
D	620	ASP	-	expression tag	UNP Q9BYF1
D	621	ASP	-	expression tag	UNP Q9BYF1
D	622	ASP	-	expression tag	UNP Q9BYF1
D	623	LYS	-	expression tag	UNP Q9BYF1
D	624	TRP	-	expression tag	UNP Q9BYF1
D	625	SER	-	expression tag	UNP Q9BYF1
D	626	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	627	PRO	-	expression tag	UNP Q9BYF1
D	628	GLN	-	expression tag	UNP Q9BYF1
D	629	PHE	-	expression tag	UNP Q9BYF1
D	630	GLU	-	expression tag	UNP Q9BYF1
D	631	LYS	-	expression tag	UNP Q9BYF1
D	632	GLY	-	expression tag	UNP Q9BYF1
D	633	GLY	-	expression tag	UNP Q9BYF1
D	634	GLY	-	expression tag	UNP Q9BYF1
D	635	SER	-	expression tag	UNP Q9BYF1
D	636	GLY	-	expression tag	UNP Q9BYF1
D	637	GLY	-	expression tag	UNP Q9BYF1
D	638	GLY	-	expression tag	UNP Q9BYF1
D	639	SER	-	expression tag	UNP Q9BYF1
D	640	GLY	-	expression tag	UNP Q9BYF1
D	641	GLY	-	expression tag	UNP Q9BYF1
D	642	SER	-	expression tag	UNP Q9BYF1
D	643	SER	-	expression tag	UNP Q9BYF1
D	644	ALA	-	expression tag	UNP Q9BYF1
D	645	TRP	-	expression tag	UNP Q9BYF1
D	646	SER	-	expression tag	UNP Q9BYF1
D	647	HIS	-	expression tag	UNP Q9BYF1
D	648	PRO	-	expression tag	UNP Q9BYF1
D	649	GLN	-	expression tag	UNP Q9BYF1
D	650	PHE	-	expression tag	UNP Q9BYF1
D	651	GLU	-	expression tag	UNP Q9BYF1
D	652	LYS	-	expression tag	UNP Q9BYF1
E	-1	MET	-	initiating methionine	UNP Q9BYF1
E	0	GLU	-	expression tag	UNP Q9BYF1
E	1	THR	-	expression tag	UNP Q9BYF1
E	2	ASP	-	expression tag	UNP Q9BYF1
E	3	THR	-	expression tag	UNP Q9BYF1
E	4	LEU	-	expression tag	UNP Q9BYF1
E	5	LEU	-	expression tag	UNP Q9BYF1
E	6	LEU	-	expression tag	UNP Q9BYF1
E	7	TRP	-	expression tag	UNP Q9BYF1
E	8	VAL	-	expression tag	UNP Q9BYF1
E	9	LEU	-	expression tag	UNP Q9BYF1
E	10	LEU	-	expression tag	UNP Q9BYF1
E	11	LEU	-	expression tag	UNP Q9BYF1
E	12	TRP	-	expression tag	UNP Q9BYF1
E	13	VAL	-	expression tag	UNP Q9BYF1
E	14	PRO	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	15	GLY	-	expression tag	UNP Q9BYF1
E	16	SER	-	expression tag	UNP Q9BYF1
E	17	THR	-	expression tag	UNP Q9BYF1
E	18	GLY	-	expression tag	UNP Q9BYF1
E	614	ALA	-	expression tag	UNP Q9BYF1
E	615	ASP	-	expression tag	UNP Q9BYF1
E	616	ASP	-	expression tag	UNP Q9BYF1
E	617	TYR	-	expression tag	UNP Q9BYF1
E	618	LYS	-	expression tag	UNP Q9BYF1
E	619	ASP	-	expression tag	UNP Q9BYF1
E	620	ASP	-	expression tag	UNP Q9BYF1
E	621	ASP	-	expression tag	UNP Q9BYF1
E	622	ASP	-	expression tag	UNP Q9BYF1
E	623	LYS	-	expression tag	UNP Q9BYF1
E	624	TRP	-	expression tag	UNP Q9BYF1
E	625	SER	-	expression tag	UNP Q9BYF1
E	626	HIS	-	expression tag	UNP Q9BYF1
E	627	PRO	-	expression tag	UNP Q9BYF1
E	628	GLN	-	expression tag	UNP Q9BYF1
E	629	PHE	-	expression tag	UNP Q9BYF1
E	630	GLU	-	expression tag	UNP Q9BYF1
E	631	LYS	-	expression tag	UNP Q9BYF1
E	632	GLY	-	expression tag	UNP Q9BYF1
E	633	GLY	-	expression tag	UNP Q9BYF1
E	634	GLY	-	expression tag	UNP Q9BYF1
E	635	SER	-	expression tag	UNP Q9BYF1
E	636	GLY	-	expression tag	UNP Q9BYF1
E	637	GLY	-	expression tag	UNP Q9BYF1
E	638	GLY	-	expression tag	UNP Q9BYF1
E	639	SER	-	expression tag	UNP Q9BYF1
E	640	GLY	-	expression tag	UNP Q9BYF1
E	641	GLY	-	expression tag	UNP Q9BYF1
E	642	SER	-	expression tag	UNP Q9BYF1
E	643	SER	-	expression tag	UNP Q9BYF1
E	644	ALA	-	expression tag	UNP Q9BYF1
E	645	TRP	-	expression tag	UNP Q9BYF1
E	646	SER	-	expression tag	UNP Q9BYF1
E	647	HIS	-	expression tag	UNP Q9BYF1
E	648	PRO	-	expression tag	UNP Q9BYF1
E	649	GLN	-	expression tag	UNP Q9BYF1
E	650	PHE	-	expression tag	UNP Q9BYF1
E	651	GLU	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	652	LYS	-	expression tag	UNP Q9BYF1
F	-1	MET	-	initiating methionine	UNP Q9BYF1
F	0	GLU	-	expression tag	UNP Q9BYF1
F	1	THR	-	expression tag	UNP Q9BYF1
F	2	ASP	-	expression tag	UNP Q9BYF1
F	3	THR	-	expression tag	UNP Q9BYF1
F	4	LEU	-	expression tag	UNP Q9BYF1
F	5	LEU	-	expression tag	UNP Q9BYF1
F	6	LEU	-	expression tag	UNP Q9BYF1
F	7	TRP	-	expression tag	UNP Q9BYF1
F	8	VAL	-	expression tag	UNP Q9BYF1
F	9	LEU	-	expression tag	UNP Q9BYF1
F	10	LEU	-	expression tag	UNP Q9BYF1
F	11	LEU	-	expression tag	UNP Q9BYF1
F	12	TRP	-	expression tag	UNP Q9BYF1
F	13	VAL	-	expression tag	UNP Q9BYF1
F	14	PRO	-	expression tag	UNP Q9BYF1
F	15	GLY	-	expression tag	UNP Q9BYF1
F	16	SER	-	expression tag	UNP Q9BYF1
F	17	THR	-	expression tag	UNP Q9BYF1
F	18	GLY	-	expression tag	UNP Q9BYF1
F	614	ALA	-	expression tag	UNP Q9BYF1
F	615	ASP	-	expression tag	UNP Q9BYF1
F	616	ASP	-	expression tag	UNP Q9BYF1
F	617	TYR	-	expression tag	UNP Q9BYF1
F	618	LYS	-	expression tag	UNP Q9BYF1
F	619	ASP	-	expression tag	UNP Q9BYF1
F	620	ASP	-	expression tag	UNP Q9BYF1
F	621	ASP	-	expression tag	UNP Q9BYF1
F	622	ASP	-	expression tag	UNP Q9BYF1
F	623	LYS	-	expression tag	UNP Q9BYF1
F	624	TRP	-	expression tag	UNP Q9BYF1
F	625	SER	-	expression tag	UNP Q9BYF1
F	626	HIS	-	expression tag	UNP Q9BYF1
F	627	PRO	-	expression tag	UNP Q9BYF1
F	628	GLN	-	expression tag	UNP Q9BYF1
F	629	PHE	-	expression tag	UNP Q9BYF1
F	630	GLU	-	expression tag	UNP Q9BYF1
F	631	LYS	-	expression tag	UNP Q9BYF1
F	632	GLY	-	expression tag	UNP Q9BYF1
F	633	GLY	-	expression tag	UNP Q9BYF1
F	634	GLY	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	635	SER	-	expression tag	UNP Q9BYF1
F	636	GLY	-	expression tag	UNP Q9BYF1
F	637	GLY	-	expression tag	UNP Q9BYF1
F	638	GLY	-	expression tag	UNP Q9BYF1
F	639	SER	-	expression tag	UNP Q9BYF1
F	640	GLY	-	expression tag	UNP Q9BYF1
F	641	GLY	-	expression tag	UNP Q9BYF1
F	642	SER	-	expression tag	UNP Q9BYF1
F	643	SER	-	expression tag	UNP Q9BYF1
F	644	ALA	-	expression tag	UNP Q9BYF1
F	645	TRP	-	expression tag	UNP Q9BYF1
F	646	SER	-	expression tag	UNP Q9BYF1
F	647	HIS	-	expression tag	UNP Q9BYF1
F	648	PRO	-	expression tag	UNP Q9BYF1
F	649	GLN	-	expression tag	UNP Q9BYF1
F	650	PHE	-	expression tag	UNP Q9BYF1
F	651	GLU	-	expression tag	UNP Q9BYF1
F	652	LYS	-	expression tag	UNP Q9BYF1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
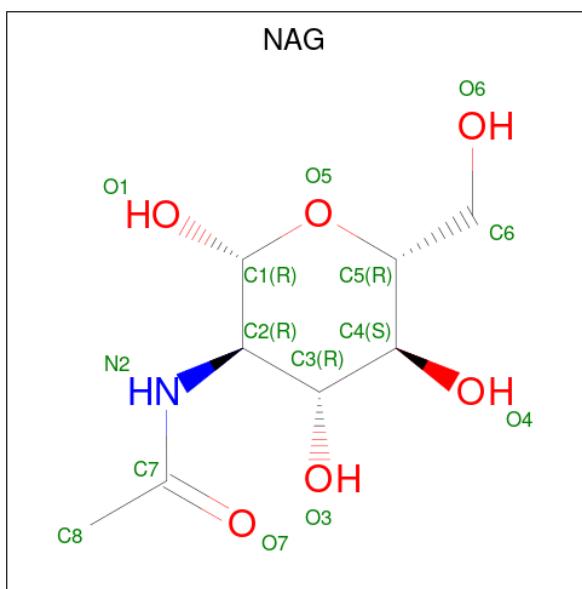
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	D	1	Total	C	N	O	0
			84	48	6	30	
4	D	1	Total	C	N	O	0
			84	48	6	30	
4	D	1	Total	C	N	O	0
			84	48	6	30	
4	D	1	Total	C	N	O	0
			84	48	6	30	

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Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			84	48	6	30	
4	D	1	Total	C	N	O	0
			84	48	6	30	
4	E	1	Total	C	N	O	0
			84	48	6	30	
4	E	1	Total	C	N	O	0
			84	48	6	30	
4	E	1	Total	C	N	O	0
			84	48	6	30	
4	E	1	Total	C	N	O	0
			84	48	6	30	
4	E	1	Total	C	N	O	0
			84	48	6	30	
4	E	1	Total	C	N	O	0
			84	48	6	30	
4	F	1	Total	C	N	O	0
			84	48	6	30	
4	F	1	Total	C	N	O	0
			84	48	6	30	
4	F	1	Total	C	N	O	0
			84	48	6	30	
4	F	1	Total	C	N	O	0
			84	48	6	30	
4	F	1	Total	C	N	O	0
			84	48	6	30	
4	F	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	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: Spike glycoprotein

• Molecule 1: Spike glycoprotein

Chain B:

HIS HIS HIS HIS

• Molecule 1: Spike glycoprotein

Chain C:

HIS HIS HIS HIS HIS

• Molecule 2: Angiotensin-converting enzyme 2

Chain D:

• Molecule 2: Angiotensin-converting enzyme 2

Chain E:

• Molecule 2: Angiotensin-converting enzyme 2

Chain F:

MET GLU THR ASP THR LEU LEU TRP VAL LEU LEU TRP VAL PRO GLY SER THR GLY S19 T20 I21 E22 K26 K31 H34 E35 D38 S44 S77 Q81 Q86 E87 I88 Q89 L97 Q101 Q102 N103 G104 S105 S106 E110 D111 V132 C133 ASN

PRO ASP ASN PRO GLN GLU C141 L142 L143 L144 E145 P146 G147 L148 S167 W168 E171 E182 V185 L186 H195 G211 V212 D213 G214 Y215 T229 F230 E231 E232 I233 R245 M249 N250 A251 Y252 P253 S254 P258 I259 P263 L266 L267 D268 D269 M270 W271 G272

N277 S280 L281 G286 Q287 K288 P289 N290 I291 D292 D295 D299 Q300 A301 I307 M332 W349 D350 L351 G352 K353 L359 D368 F369 L370 T371 H374 E375 H378 Y381 N394 V404 G405 E406 S409 H417 L418 I421 G422 L423 L424 S425

P426 D427 F428 Q429 E430 D431 T453 M462 K465 G466 E467 I468 P469 K470 D471 Q472 P490 V491 P492 H493 D494 D499 P500 A501 S502 F512 Y516 Q524 E527 A532 A533 K534 H535 E536 G537 K541 E549 A550 K562 S563 E564 A569 N572 V573 V574

G575 A576 K577 N578 M579 N580 V581 R582 P583 E589 P590 L591 K596 D597 Q598 N599 K600 N601 S602 F603 V604 G605 T608 D609 P612 Y613 ALA ASP ASP TYR LYS ASP ASP ASP LYS TRP SER HIS PRO GLN PHE GLU LYS GLY GLY SER GLY GLY SER GLY GLY SER SER

ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

NAG1 NAG2

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	45000	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 $(e^-/\text{Å}^2)$	35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.652	Depositor
Minimum map value	-1.968	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	556.544, 556.544, 556.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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, ZN

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	0.29	0/7997	0.48	0/10880
1	B	0.29	0/7997	0.48	0/10880
1	C	0.29	0/7997	0.48	0/10880
2	D	0.25	0/4935	0.44	0/6701
2	E	0.25	0/4935	0.44	0/6701
2	F	0.25	0/4935	0.44	0/6701
All	All	0.27	0/38796	0.46	0/52743

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	7818	0	7615	165	0
1	B	7818	0	7615	170	0
1	C	7818	0	7615	172	0
2	D	4801	0	4583	46	0
2	E	4801	0	4583	44	0
2	F	4801	0	4583	50	0
3	G	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	1	0
3	I	28	0	25	1	0
4	A	140	0	130	1	0
4	B	140	0	130	1	0
4	C	140	0	130	1	0
4	D	84	0	78	0	0
4	E	84	0	78	0	0
4	F	84	0	78	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	38616	0	37293	614	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.

The worst 5 of 614 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:F:31:LYS:HG2	1:C:489:TYR:CD2	2.16	0.81
1:A:599:THR:HG22	1:A:601:GLY:H	1.46	0.79
1:B:599:THR:HG22	1:B:601:GLY:H	1.46	0.79
1:C:599:THR:HG22	1:C:601:GLY:H	1.45	0.79
1:A:323:THR:OG1	1:A:537:LYS:NZ	2.18	0.77

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	978/1284 (76%)	922 (94%)	56 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	978/1284 (76%)	923 (94%)	55 (6%)	0	100	100
1	C	978/1284 (76%)	923 (94%)	55 (6%)	0	100	100
2	D	584/654 (89%)	569 (97%)	15 (3%)	0	100	100
2	E	584/654 (89%)	569 (97%)	15 (3%)	0	100	100
2	F	584/654 (89%)	569 (97%)	15 (3%)	0	100	100
All	All	4686/5814 (81%)	4475 (96%)	211 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	874/1112 (79%)	873 (100%)	1 (0%)	93	97
1	B	874/1112 (79%)	873 (100%)	1 (0%)	93	97
1	C	874/1112 (79%)	873 (100%)	1 (0%)	93	97
2	D	519/573 (91%)	519 (100%)	0	100	100
2	E	519/573 (91%)	519 (100%)	0	100	100
2	F	519/573 (91%)	519 (100%)	0	100	100
All	All	4179/5055 (83%)	4176 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	ARG
1	B	408	ARG
1	C	408	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	544	ASN
1	C	188	ASN
1	C	544	ASN
1	C	343	ASN
1	A	544	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	G	1	3,1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	G	2	3	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	H	1	3,1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	I	1	3,1	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	I	2	3	14,14,15	0.32	0	17,19,21	0.54	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	G	1	3,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0
3	I	2	NAG	1	0
3	H	2	NAG	1	0
3	H	1	NAG	1	0
3	G	2	NAG	1	0
3	G	1	NAG	1	0

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

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
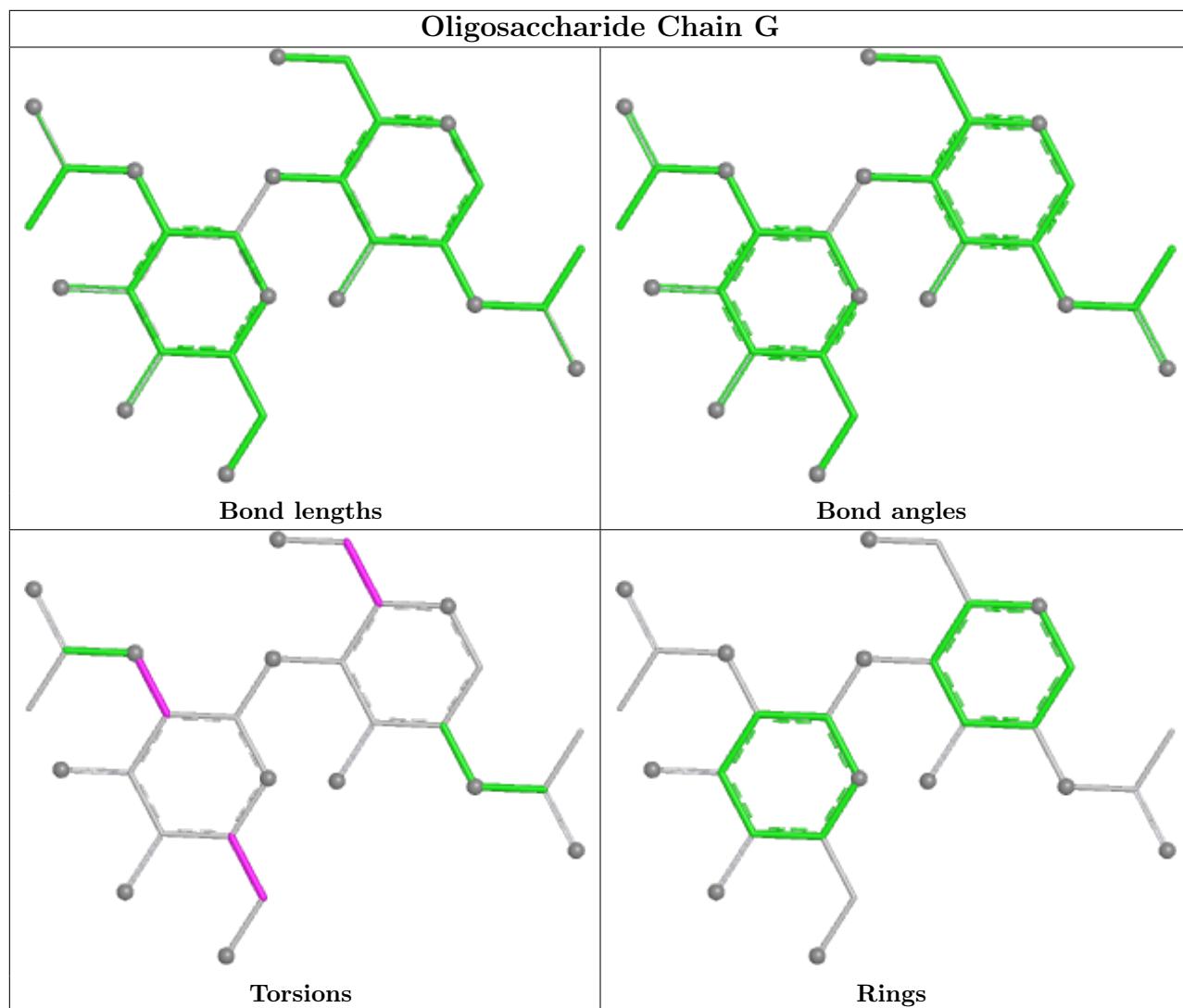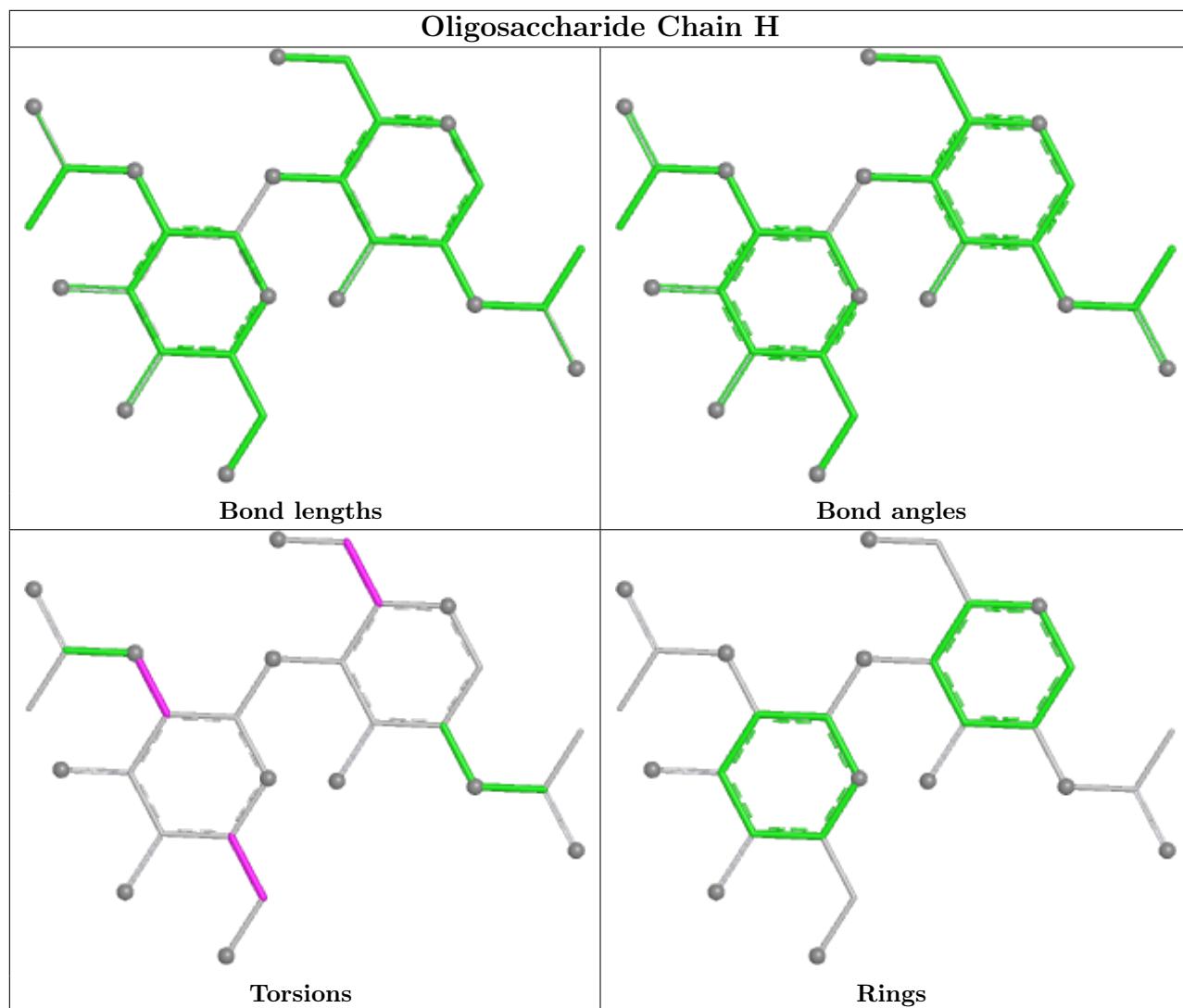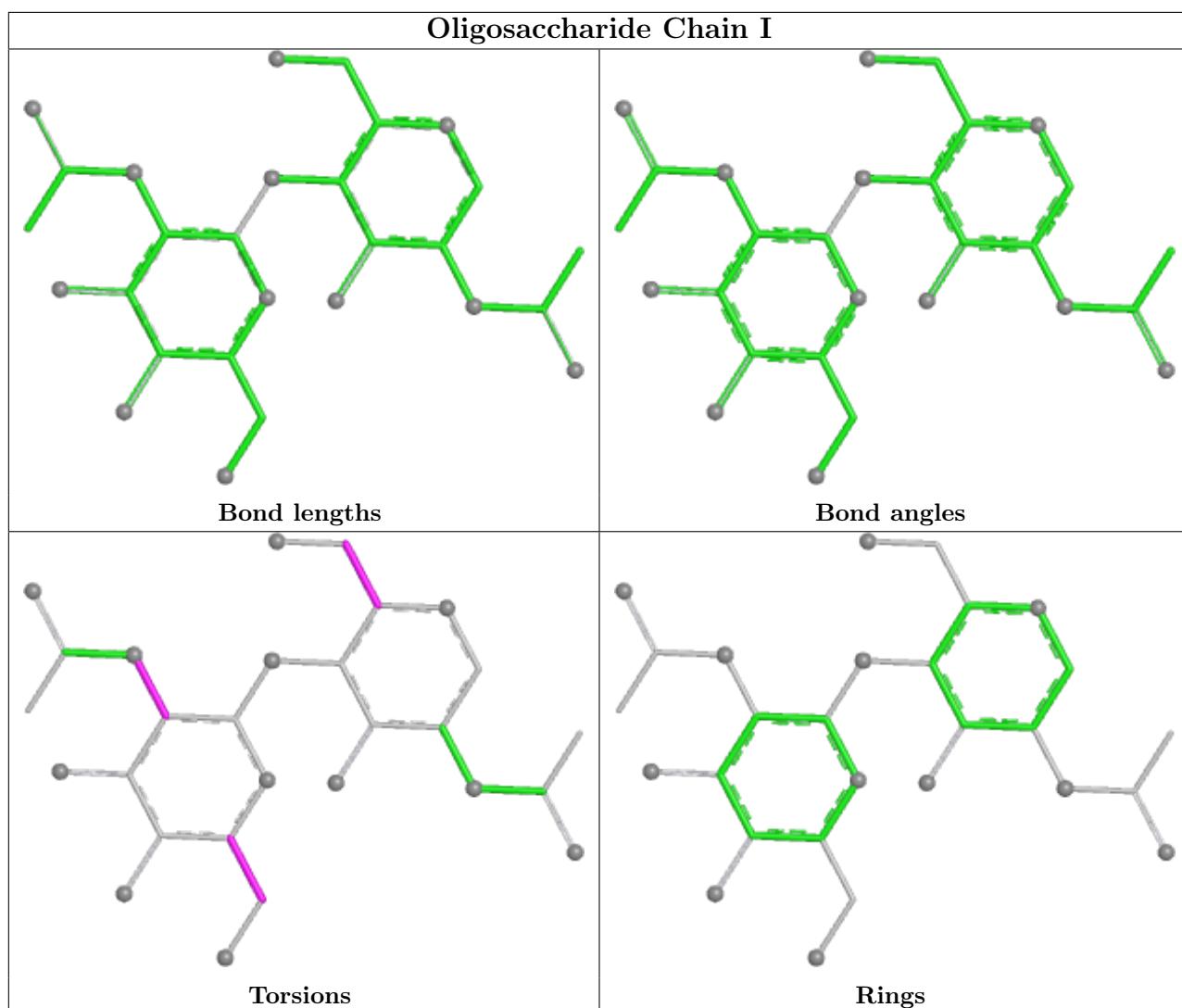
5.6 Ligand geometry ⓘ

Of 51 ligands modelled in this entry, 3 are monoatomic - leaving 48 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	E	906	2	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	C	1306	1	14,14,15	0.17	0	17,19,21	0.39	0
4	NAG	C	1309	1	14,14,15	0.20	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	E	904	2	14,14,15	0.21	0	17,19,21	0.37	0
4	NAG	D	906	2	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	E	903	2	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	B	1308	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	B	1306	1	14,14,15	0.17	0	17,19,21	0.39	0
4	NAG	E	905	2	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	E	902	2	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	B	1307	1	14,14,15	0.18	0	17,19,21	0.51	0
4	NAG	A	1307	1	14,14,15	0.18	0	17,19,21	0.51	0
4	NAG	A	1309	1	14,14,15	0.19	0	17,19,21	0.35	0
4	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.53	0
4	NAG	C	1304	1	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	F	902	2	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	A	1304	1	14,14,15	0.30	0	17,19,21	0.43	0
4	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	A	1302	1	14,14,15	0.26	0	17,19,21	0.35	0
4	NAG	D	903	2	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	D	904	2	14,14,15	0.21	0	17,19,21	0.36	0
4	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	C	1307	1	14,14,15	0.18	0	17,19,21	0.52	0
4	NAG	C	1310	1	14,14,15	0.37	0	17,19,21	0.55	0
4	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.53	0
4	NAG	F	906	2	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	F	904	2	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	A	1308	1	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	D	905	2	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	F	903	2	14,14,15	0.20	0	17,19,21	0.38	0
4	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	C	1302	1	14,14,15	0.27	0	17,19,21	0.34	0
4	NAG	C	1308	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	D	902	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	F	905	2	14,14,15	0.25	0	17,19,21	0.50	0
4	NAG	B	1302	1	14,14,15	0.26	0	17,19,21	0.35	0
4	NAG	E	907	2	14,14,15	0.68	1 (7%)	17,19,21	0.66	1 (5%)
4	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.43	0
4	NAG	B	1310	1	14,14,15	0.37	0	17,19,21	0.54	0
4	NAG	D	907	2	14,14,15	0.68	1 (7%)	17,19,21	0.66	1 (5%)
4	NAG	F	907	2	14,14,15	0.69	1 (7%)	17,19,21	0.66	1 (5%)
4	NAG	A	1306	1	14,14,15	0.17	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	B	1309	1	14,14,15	0.19	0	17,19,21	0.36	0
4	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	A	1310	1	14,14,15	0.37	0	17,19,21	0.54	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	E	906	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	E	904	2	-	2/6/23/26	0/1/1/1
4	NAG	D	906	2	-	2/6/23/26	0/1/1/1
4	NAG	E	903	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	E	905	2	-	2/6/23/26	0/1/1/1
4	NAG	E	902	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	F	902	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	D	903	2	-	0/6/23/26	0/1/1/1
4	NAG	D	904	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	F	906	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	F	904	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	D	905	2	-	2/6/23/26	0/1/1/1
4	NAG	F	903	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	D	902	2	-	4/6/23/26	0/1/1/1
4	NAG	F	905	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	E	907	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	D	907	2	-	4/6/23/26	0/1/1/1
4	NAG	F	907	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	907	NAG	C1-C2	2.27	1.55	1.52
4	D	907	NAG	C1-C2	2.26	1.55	1.52
4	E	907	NAG	C1-C2	2.24	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	907	NAG	C1-O5-C5	2.15	115.10	112.19
4	D	907	NAG	C1-O5-C5	2.14	115.10	112.19
4	F	907	NAG	C1-O5-C5	2.14	115.09	112.19

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1310	NAG	C4-C5-C6-O6
4	D	904	NAG	C4-C5-C6-O6
4	E	904	NAG	C4-C5-C6-O6
4	F	904	NAG	C4-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1310	NAG	1	0
4	B	1310	NAG	1	0
4	A	1310	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14236. 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
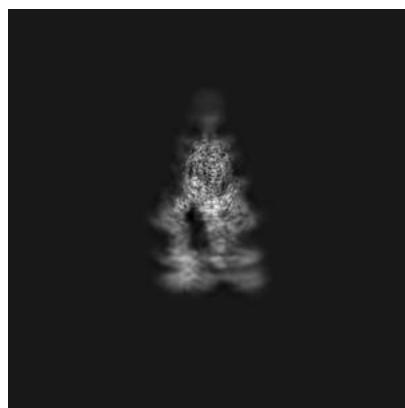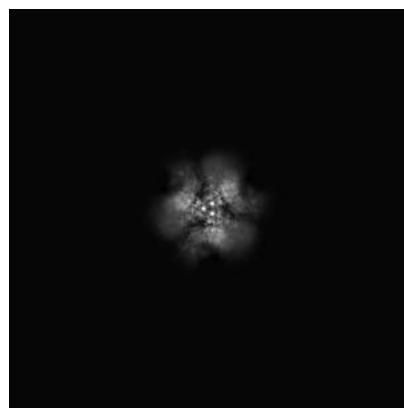
X   Y   Z

6.1.2 Raw map

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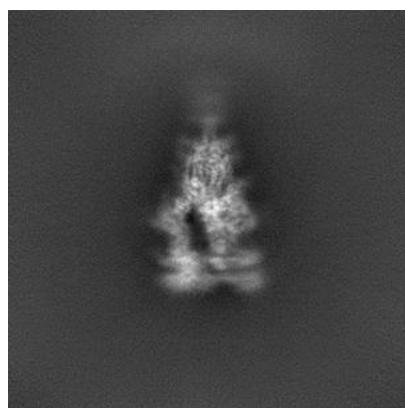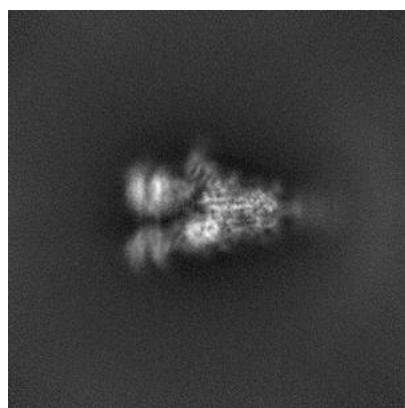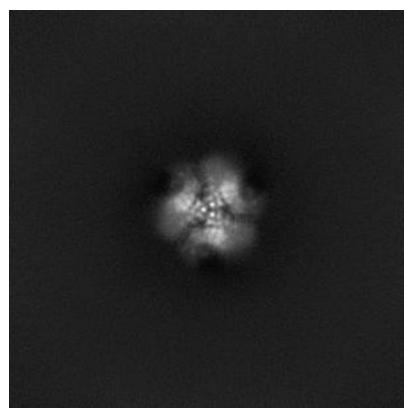
The images above show the map projected in three orthogonal directions.

6.2   Central slices (i)

6.2.1   Primary map
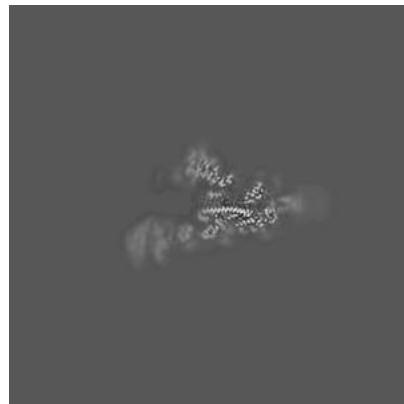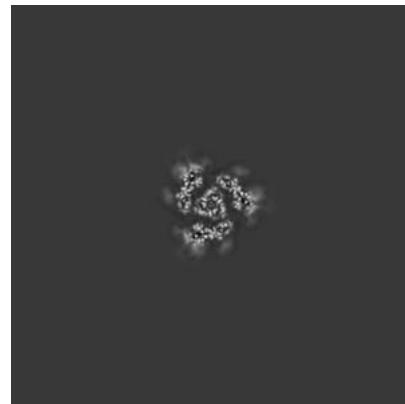
X Index: 256   Y Index: 256   Z Index: 256

6.2.2   Raw map
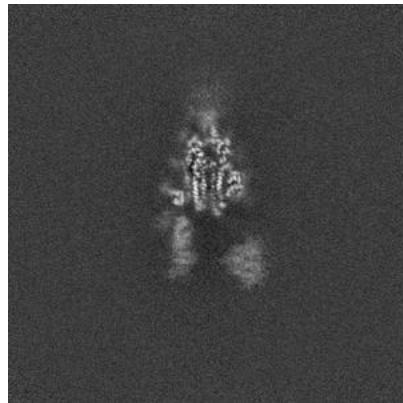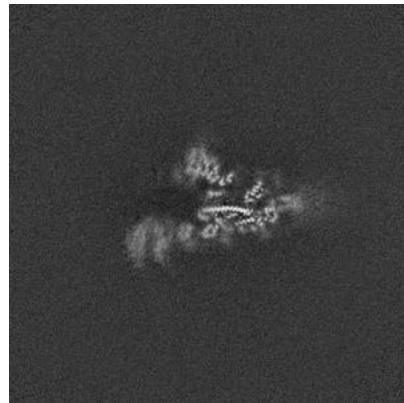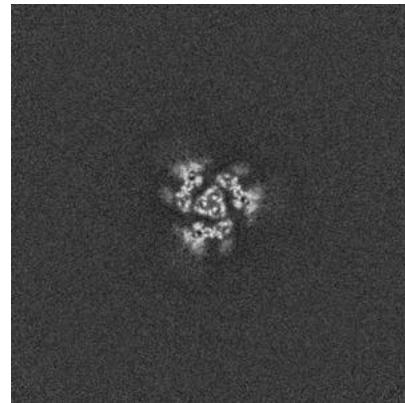
X Index: 256   Y Index: 256   Z Index: 256

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: 260 | Y Index: 263 | Z Index: 265 |
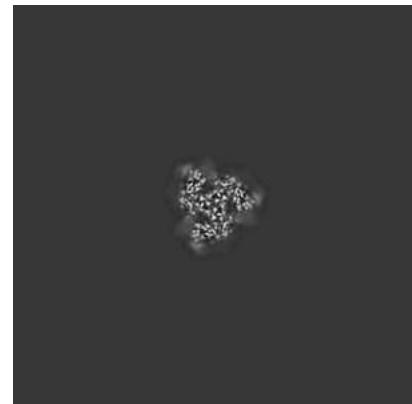
6.3.2 Raw map
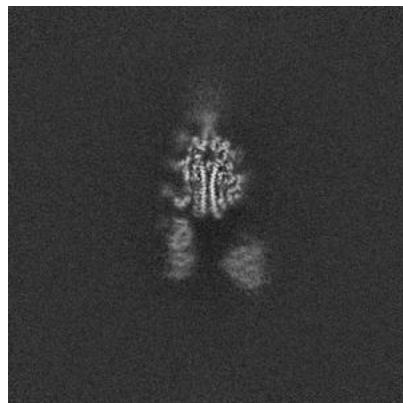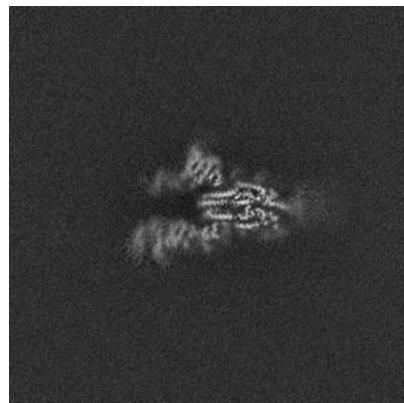
| X Index: 260 | Y Index: 264 | Z Index: 257 |
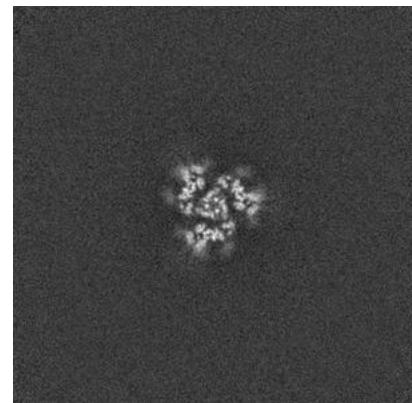
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X	Y	Z
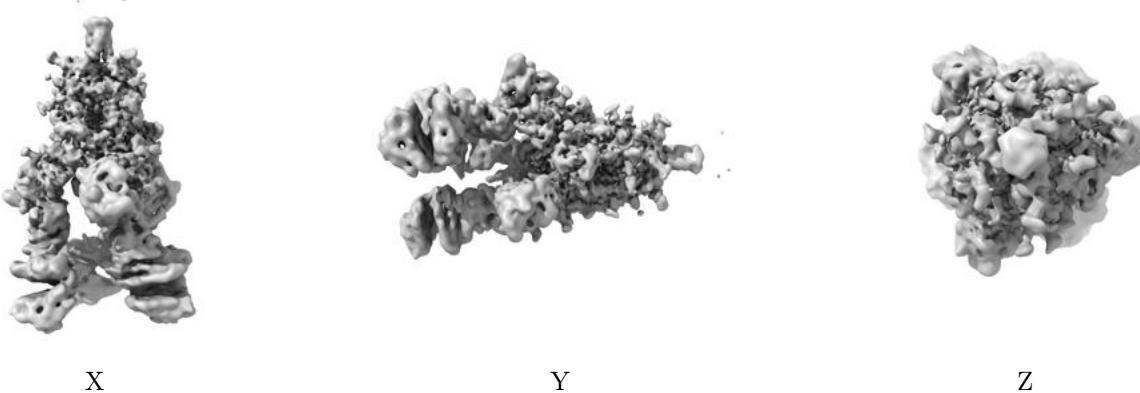
The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X	Y	Z
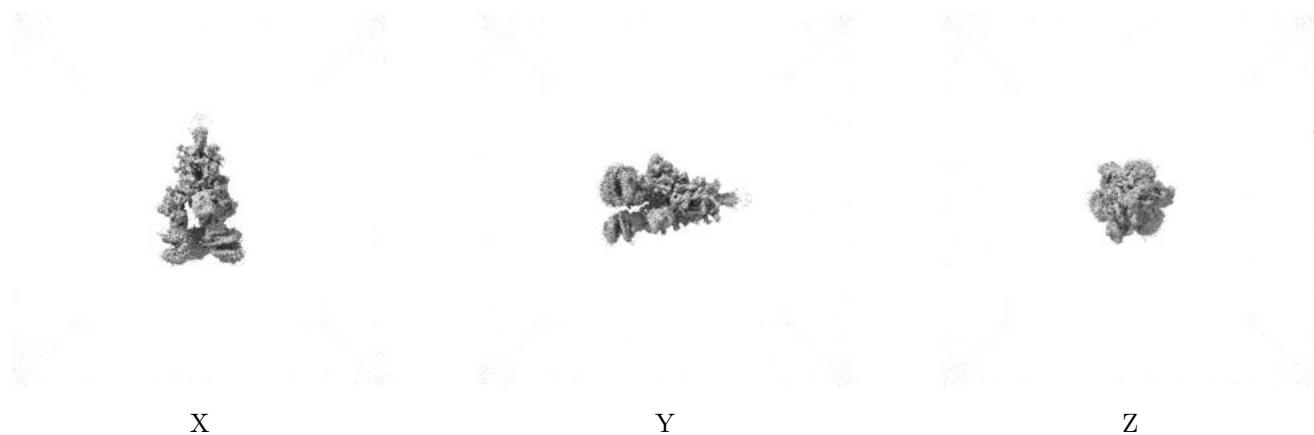
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 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

6.5.1 emd_14236_msk_1.map (i)


X   Y   Z
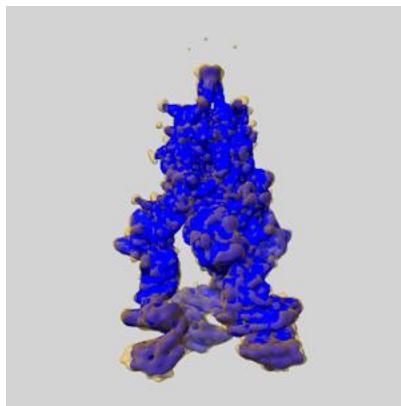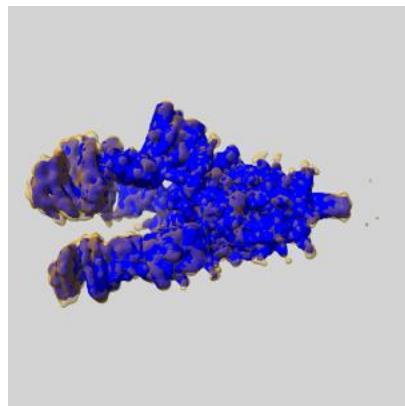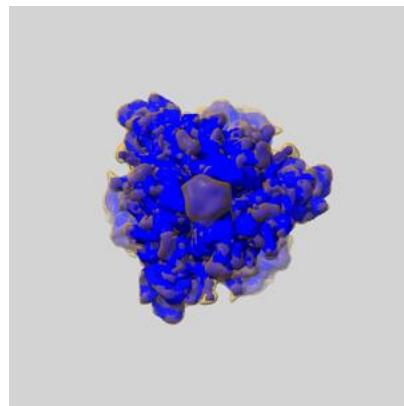
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
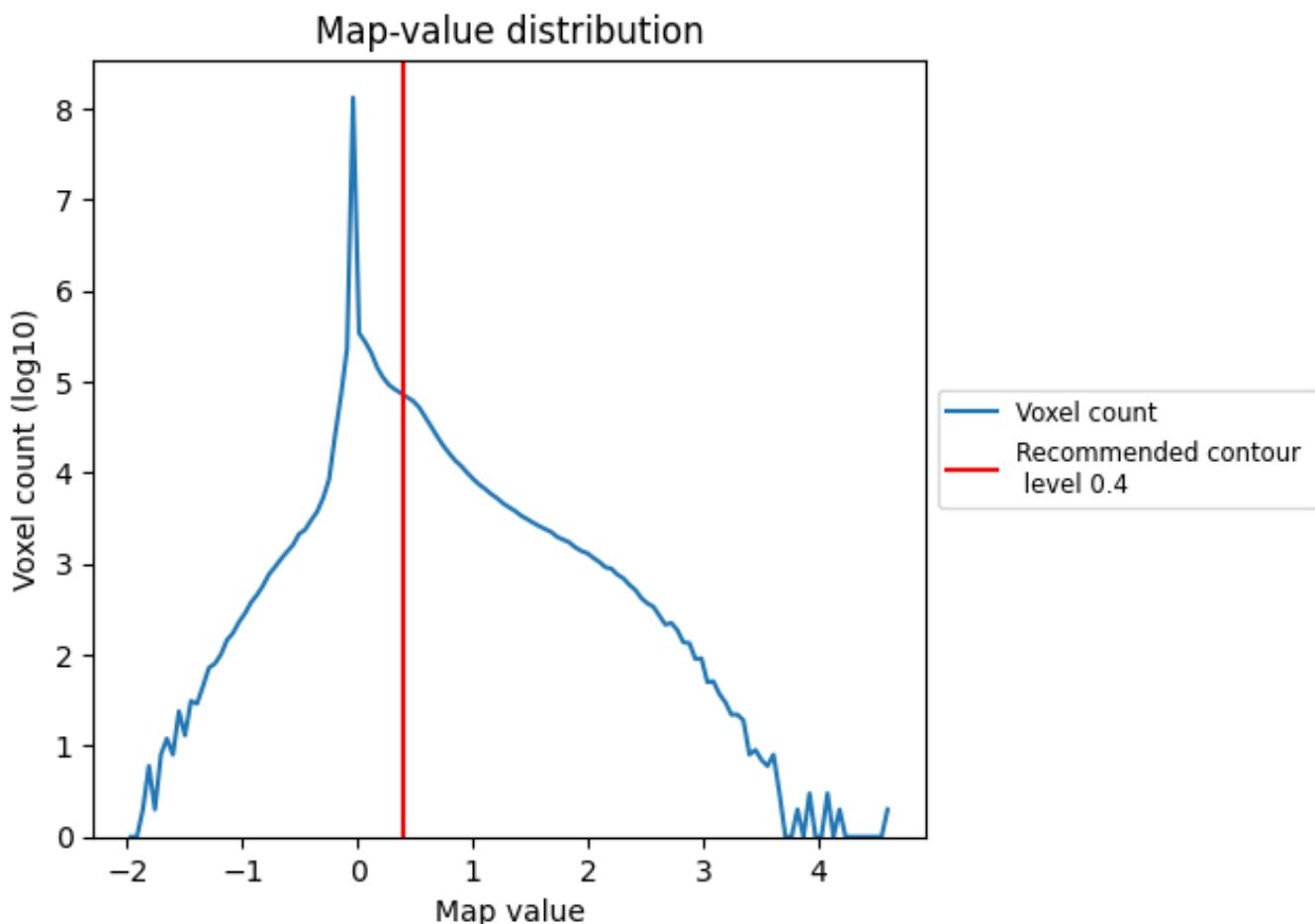
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
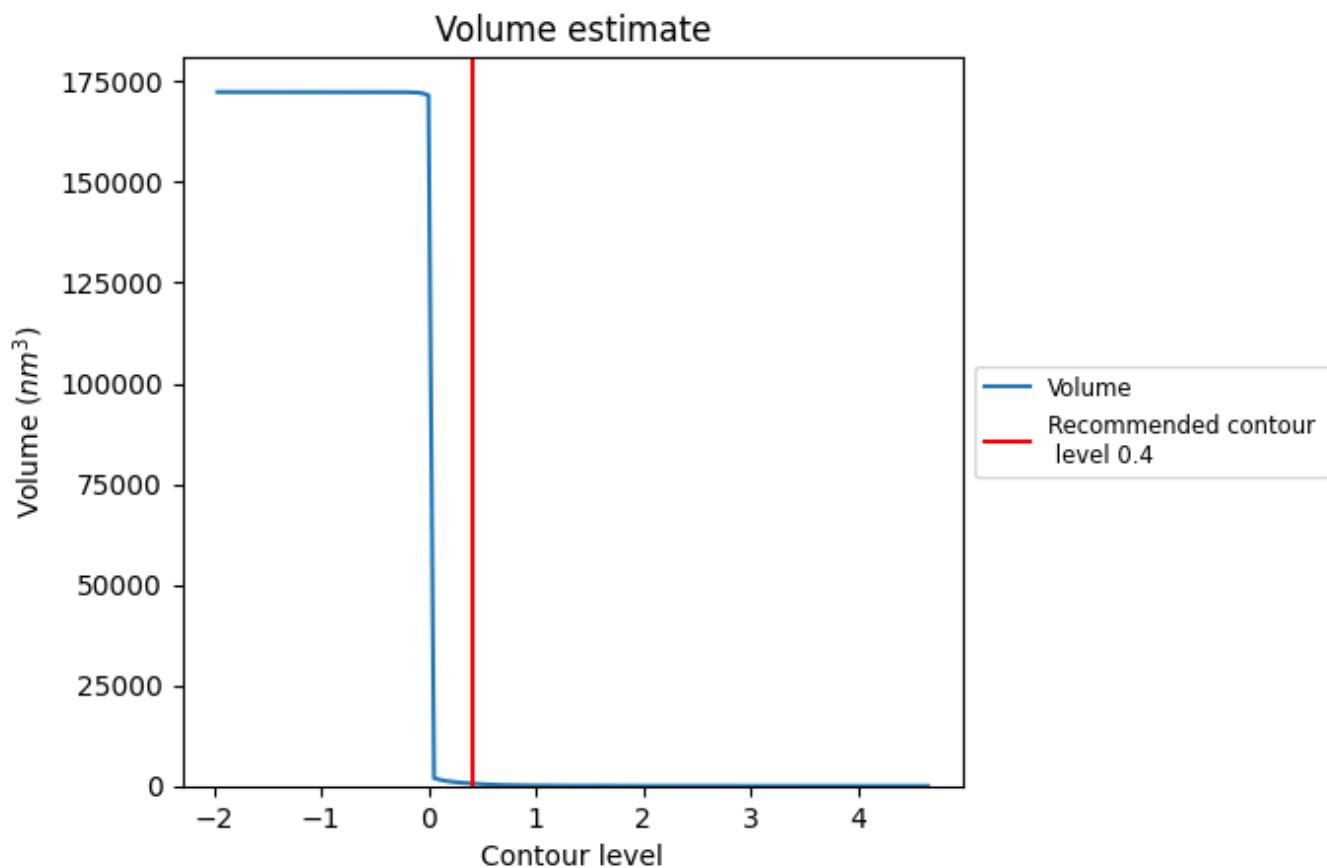
The volume at the recommended contour level is 610 nm^3; this corresponds to an approximate mass of 551 kDa.

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 ⓘ
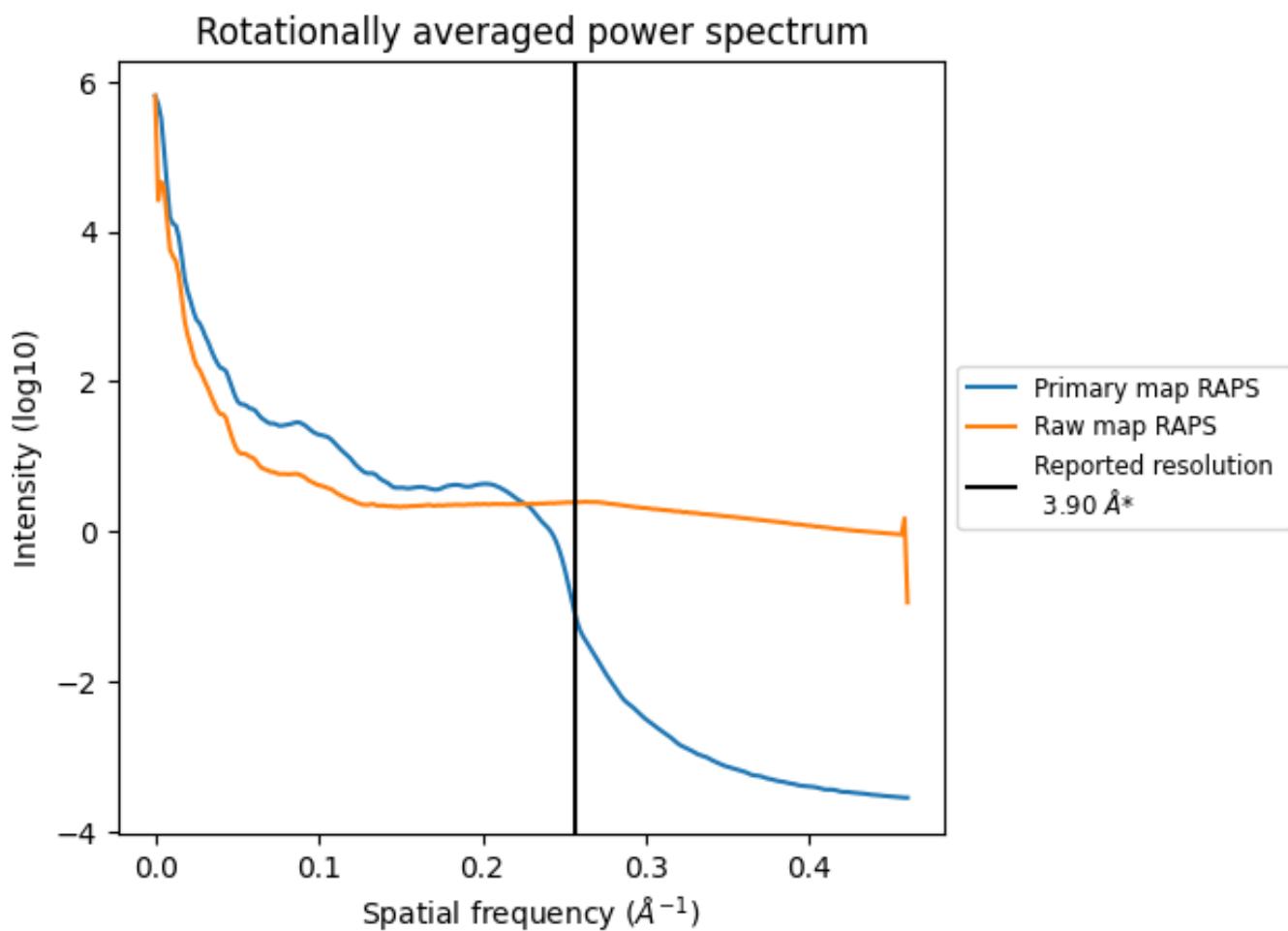
*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
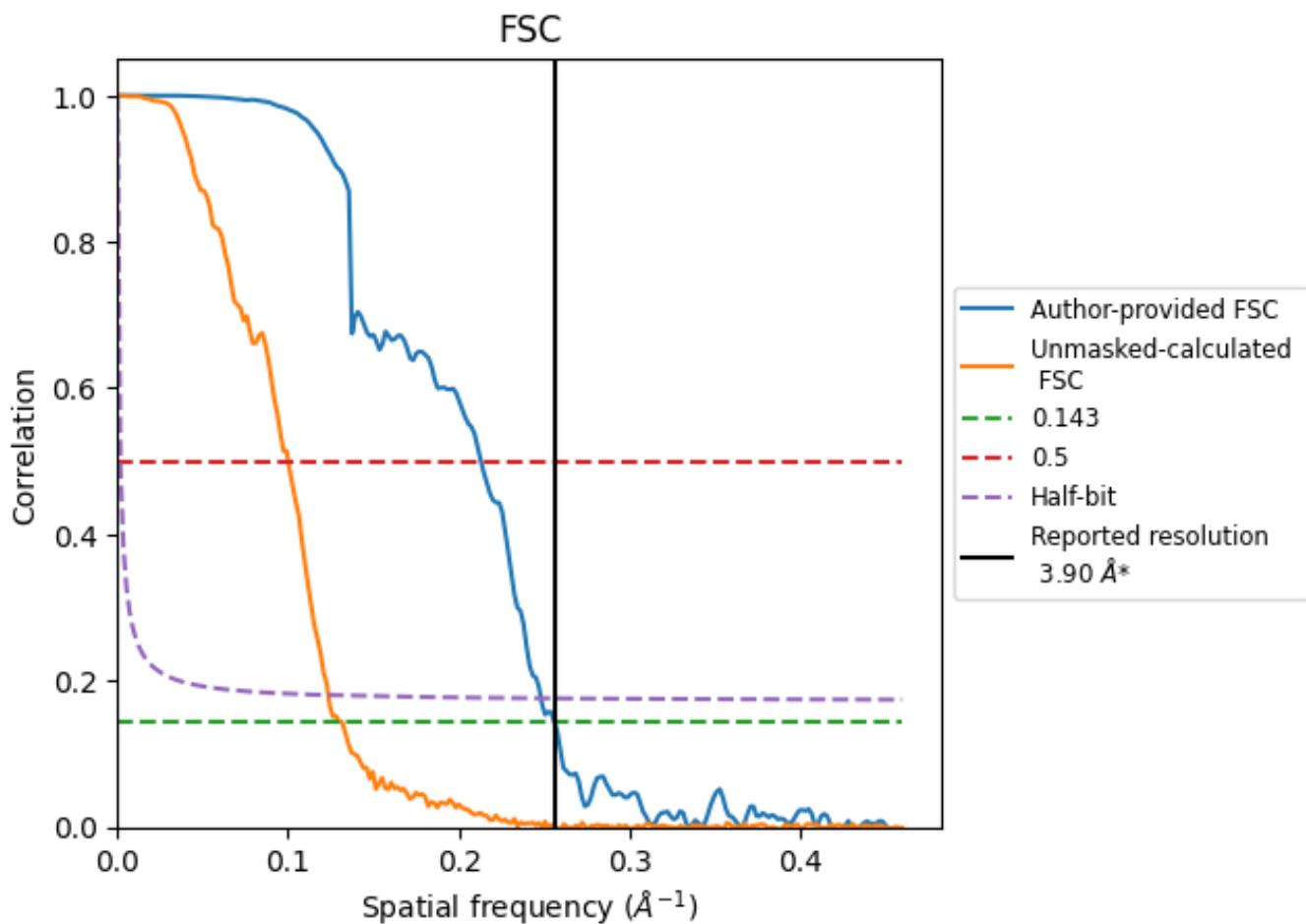
*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	4.69	4.03
Unmasked-calculated*	7.59	9.98	8.09

*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 7.59 differs from the reported value 3.9 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-14236 and PDB model 7R1A. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay ⓘ

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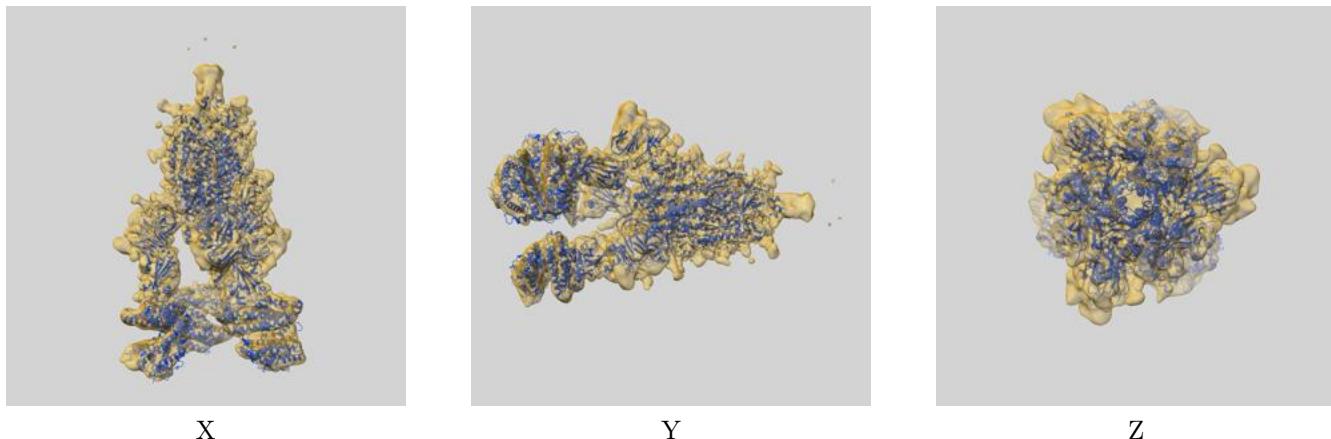
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Atom inclusion　ⓘ
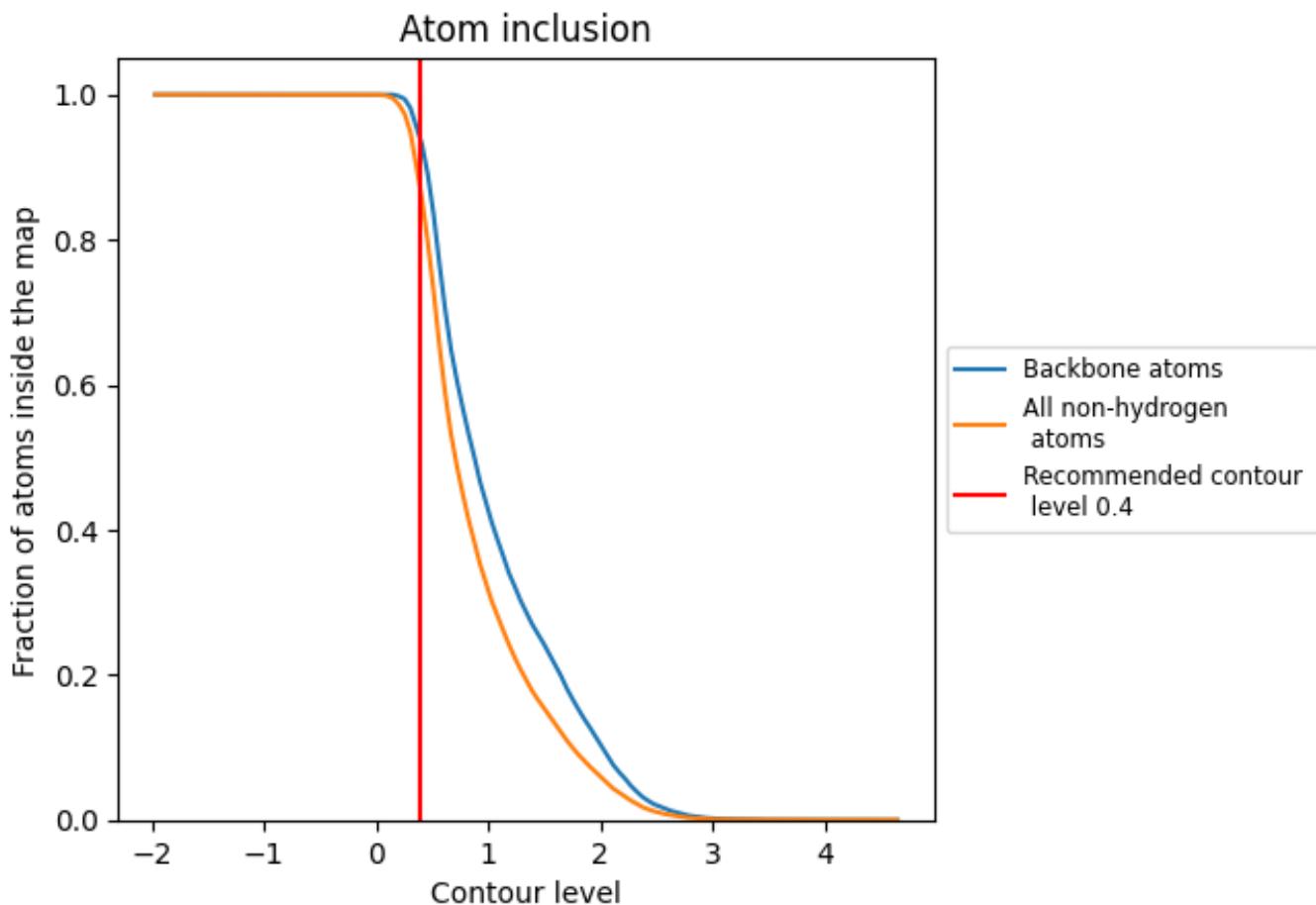
At the recommended contour level, 94% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.