wwPDB EM Validation Summary Report (i)

May 31, 2022 – 07:20 pm BST

PDB ID	:	7R4Q
EMDB ID	:	EMD-14314
Title	:	The SARS-CoV-2 spike in complex with the 1.29 neutralizing nanobody
Authors	:	Casasnovas, J.M.; Melero, R.; Arranz, R.; Fernandez, L.A.
Deposited on	:	2022-02-09
Resolution	:	3.60 Å(reported)
Based on initial models	:	6ZXN, 3TPK

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:

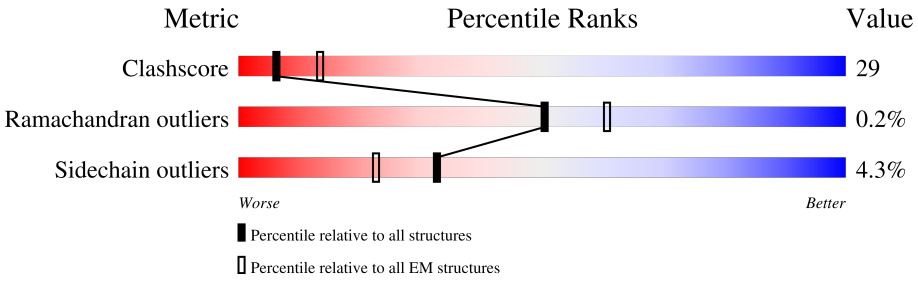
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	1264	28% 51% 25% 5% • 16%
1	B	1264	25% 49% 27% 5% • 17%
1	C	1264	25% 51% 25% 6% • 16%
2	D	126	44% 37% 56% • 5%
2	E	126	25% 36% 56% • 5%
3	F	2	50% 50% 50%
3	G	2	100% 100%
3	H	2	100% 100%

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Mol	Chain	Length	Quality of chain
3	I	2	50% 50%
3	J	2	50% 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1307	-	-	X	-
4	NAG	B	1310	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 51957 atoms, of which 24719 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	1060	Total	C	H	N	O	S	3	0
			16380	5297	8079	1383	1583	38		
1	B	1054	Total	C	H	N	O	S	3	0
			16287	5268	8034	1376	1571	38		
1	C	1060	Total	C	H	N	O	S	1	0
			16361	5292	8069	1382	1580	38		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	TYR	-	expression tag	UNP P0DTC2
A	1215	ILE	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	GLU	-	expression tag	UNP P0DTC2
A	1218	ALA	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	ASP	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLN	-	expression tag	UNP P0DTC2
A	1224	ALA	-	expression tag	UNP P0DTC2
A	1225	TYR	-	expression tag	UNP P0DTC2
A	1226	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	LYS	-	expression tag	UNP P0DTC2
A	1229	ASP	-	expression tag	UNP P0DTC2
A	1230	GLY	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	TRP	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	SER	-	expression tag	UNP P0DTC2
A	1237	THR	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	ASN	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	TYR	-	expression tag	UNP P0DTC2
A	1246	PHE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	TYR	-	expression tag	UNP P0DTC2
A	1251	LYS	-	expression tag	UNP P0DTC2
A	1252	ASP	-	expression tag	UNP P0DTC2
A	1253	ASP	-	expression tag	UNP P0DTC2
A	1254	ASP	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	LYS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	HIS	-	expression tag	UNP P0DTC2
A	1264	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	TYR	-	expression tag	UNP P0DTC2
B	1215	ILE	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	GLU	-	expression tag	UNP P0DTC2
B	1218	ALA	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	ASP	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLN	-	expression tag	UNP P0DTC2
B	1224	ALA	-	expression tag	UNP P0DTC2
B	1225	TYR	-	expression tag	UNP P0DTC2
B	1226	VAL	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	LYS	-	expression tag	UNP P0DTC2
B	1229	ASP	-	expression tag	UNP P0DTC2
B	1230	GLY	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	TRP	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	SER	-	expression tag	UNP P0DTC2
B	1237	THR	-	expression tag	UNP P0DTC2
B	1238	PHE	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	ASN	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	TYR	-	expression tag	UNP P0DTC2
B	1246	PHE	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	TYR	-	expression tag	UNP P0DTC2
B	1251	LYS	-	expression tag	UNP P0DTC2
B	1252	ASP	-	expression tag	UNP P0DTC2
B	1253	ASP	-	expression tag	UNP P0DTC2
B	1254	ASP	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	LYS	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	HIS	-	expression tag	UNP P0DTC2
B	1264	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	TYR	-	expression tag	UNP P0DTC2
C	1215	ILE	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	GLU	-	expression tag	UNP P0DTC2
C	1218	ALA	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	ASP	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLN	-	expression tag	UNP P0DTC2
C	1224	ALA	-	expression tag	UNP P0DTC2
C	1225	TYR	-	expression tag	UNP P0DTC2
C	1226	VAL	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	ASP	-	expression tag	UNP P0DTC2
C	1230	GLY	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	TRP	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	SER	-	expression tag	UNP P0DTC2
C	1237	THR	-	expression tag	UNP P0DTC2
C	1238	PHE	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	ASN	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	TYR	-	expression tag	UNP P0DTC2
C	1246	PHE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	TYR	-	expression tag	UNP P0DTC2
C	1251	LYS	-	expression tag	UNP P0DTC2
C	1252	ASP	-	expression tag	UNP P0DTC2
C	1253	ASP	-	expression tag	UNP P0DTC2
C	1254	ASP	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	LYS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	HIS	-	expression tag	UNP P0DTC2
C	1264	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Camel-derived nanobody 1.29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	120	Total	C	N	O	S	0	0
			895	554	154	184	3		

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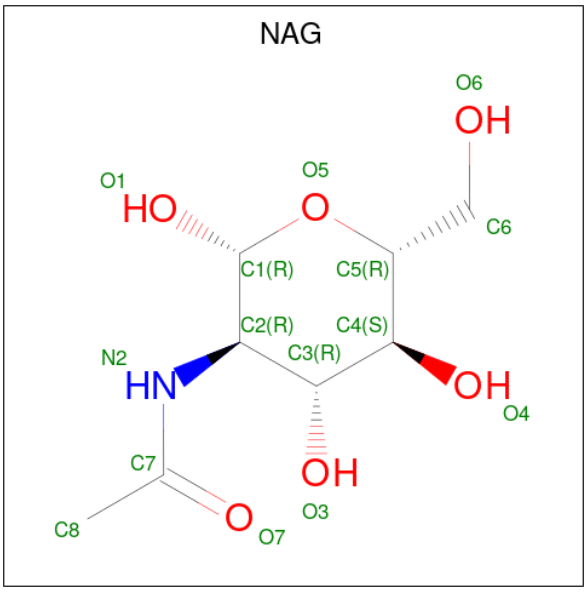
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	120	Total	C	N	O	S	0	0
			895	554	154	184	3		

- Molecule 3 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
3	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	J	2	Total	C	H	N	O	0	0
			53	16	25	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 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0

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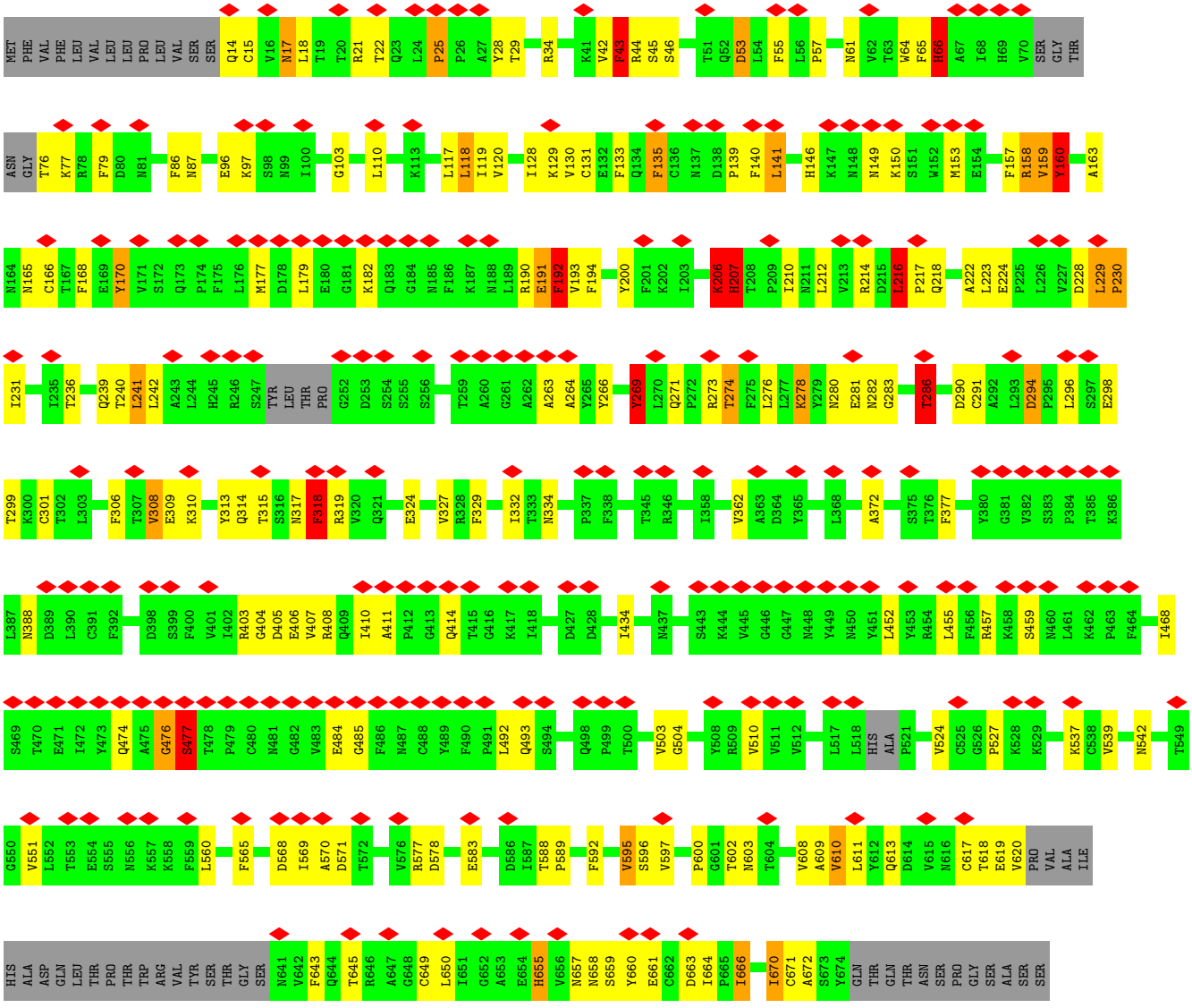
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0

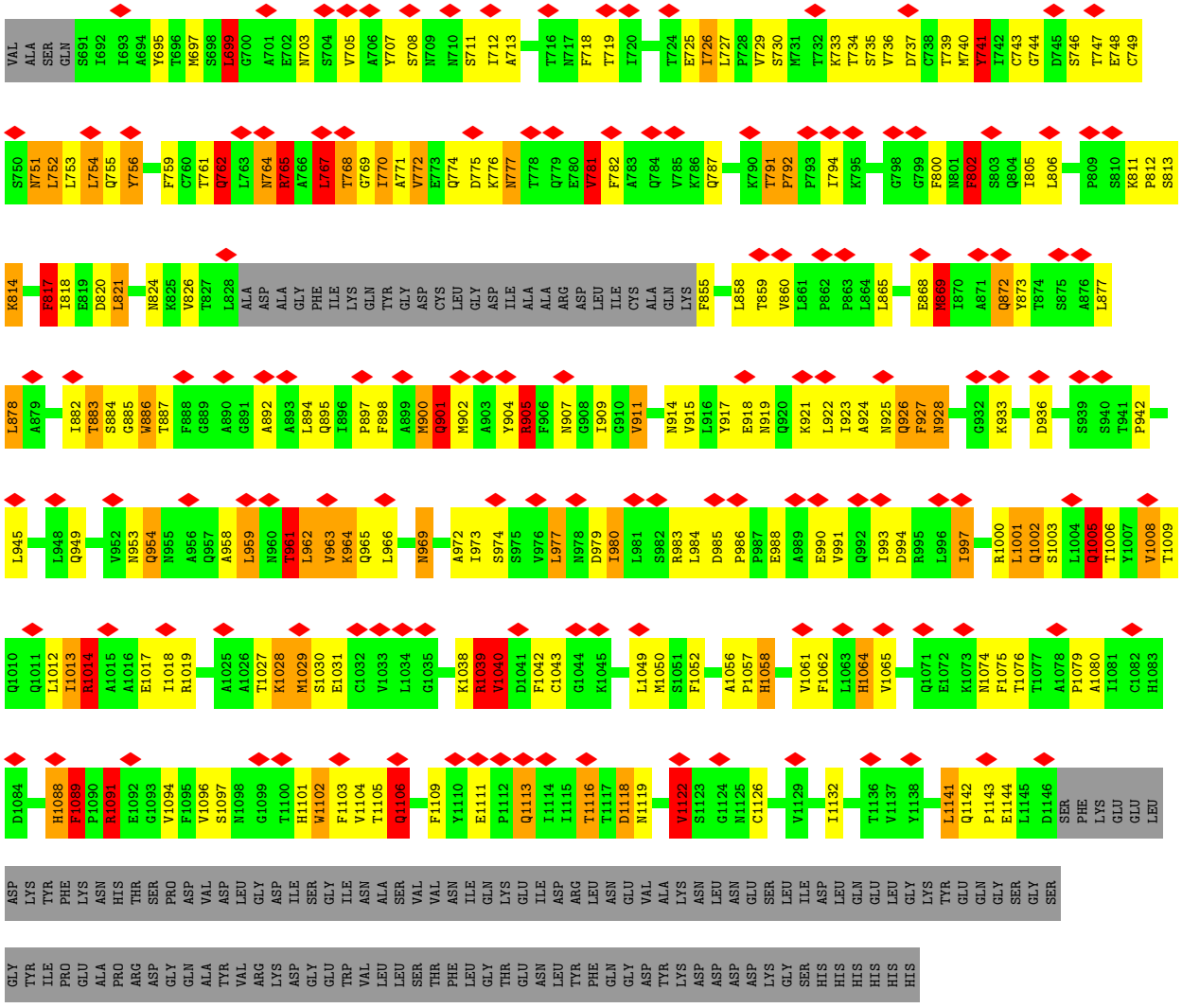
3 Residue-property plots (i)

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

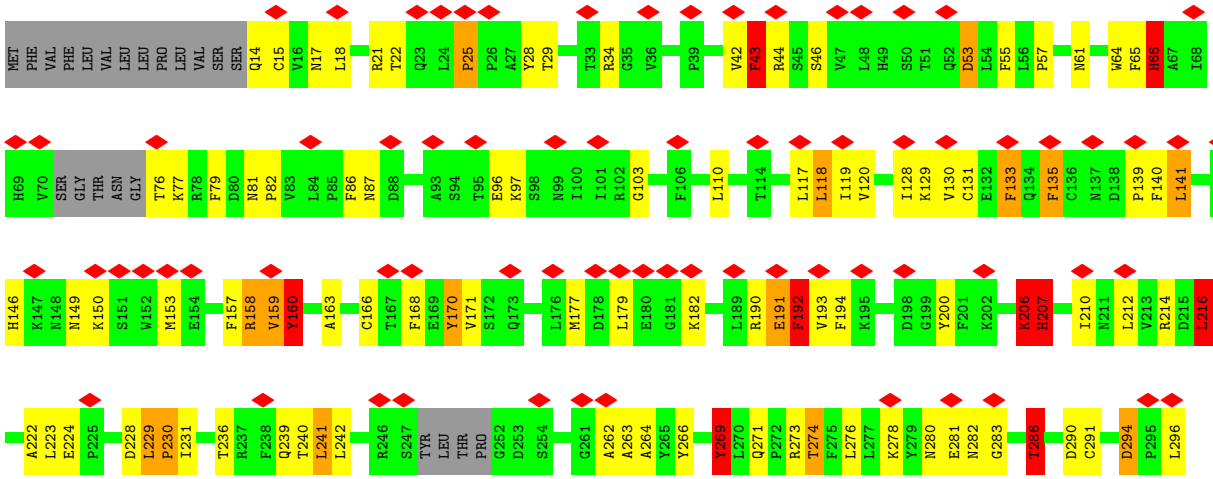
Chain A:

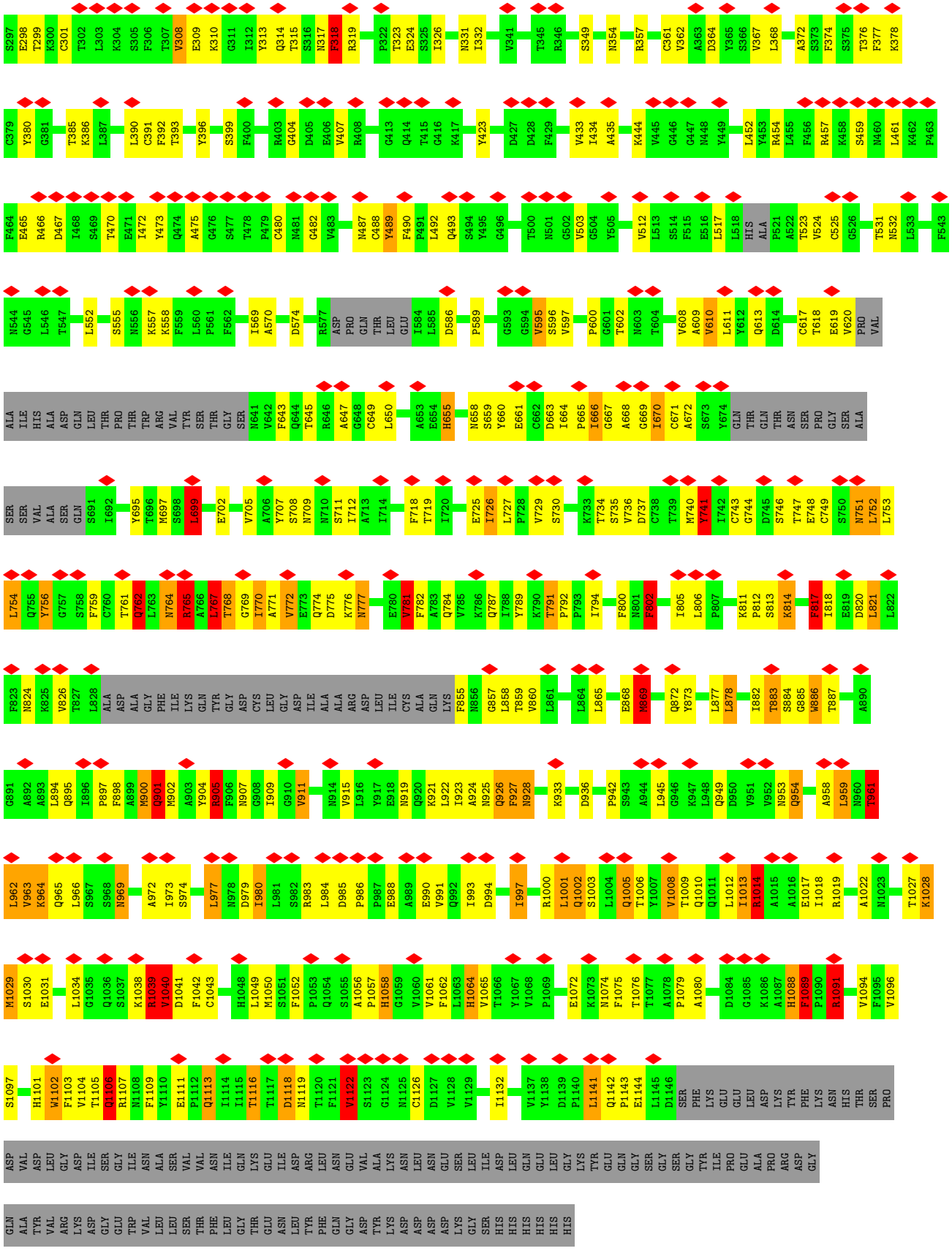




• Molecule 1: Spike glycoprotein

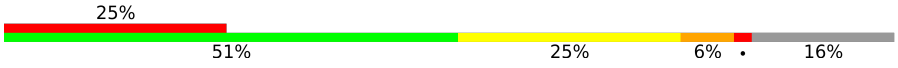
Chain B:

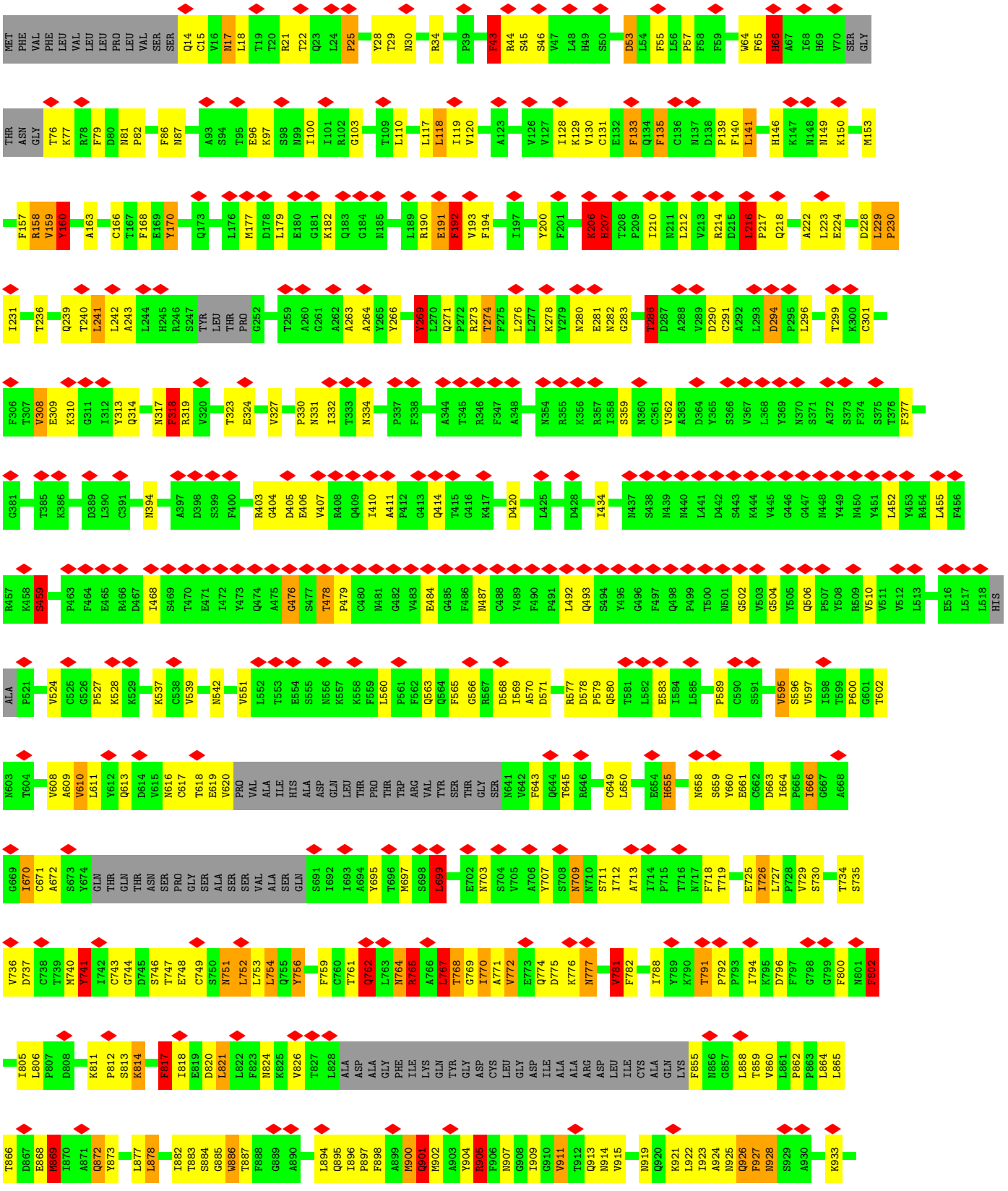


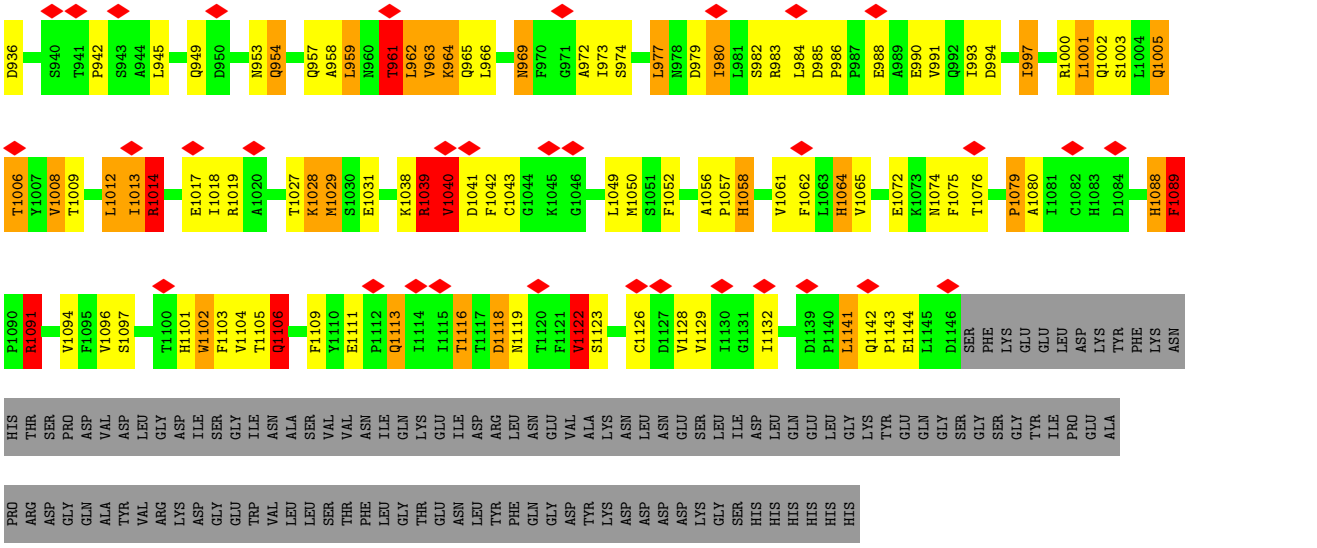


- Molecule 1: Spike glycoprotein

Chain C:

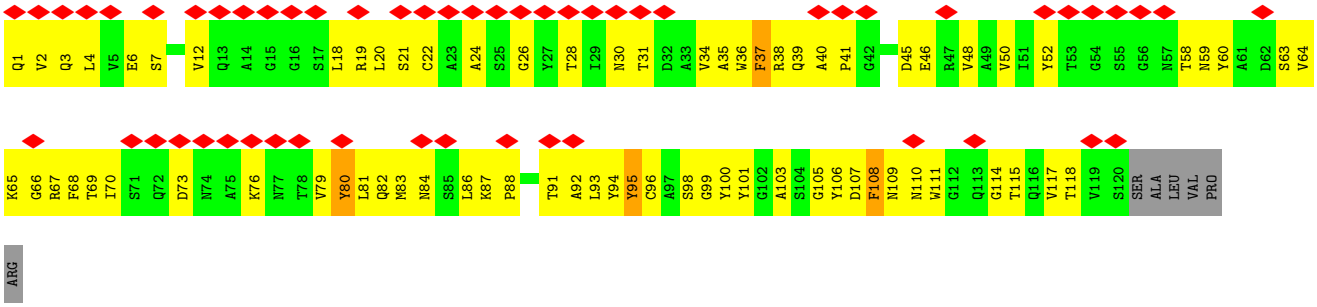






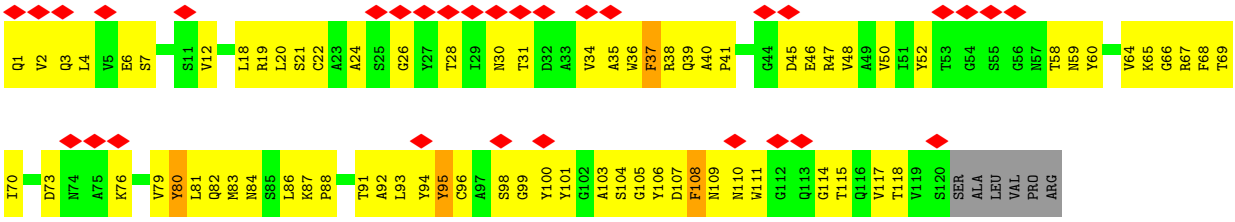
• Molecule 2: Camel-derived nanobody 1.29

Chain D:



• Molecule 2: Camel-derived nanobody 1.29

Chain E:

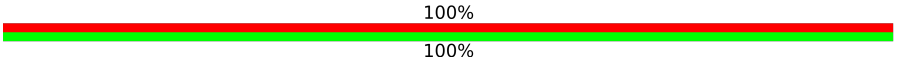


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

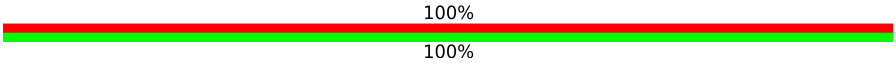
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



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

Chain I:

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

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.963	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	418.2, 418.2, 418.2	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.05	65/8501 (0.8%)	2.07	240/11563 (2.1%)
1	B	1.06	66/8452 (0.8%)	2.08	238/11495 (2.1%)
1	C	1.05	66/8488 (0.8%)	2.07	239/11544 (2.1%)
2	D	0.34	0/912	0.54	0/1238
2	E	0.34	0/912	0.54	0/1238
All	All	1.02	197/27265 (0.7%)	2.01	717/37078 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	11	40
1	B	11	38
1	C	11	38
All	All	33	116

The worst 5 of 197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	PHE	CE1-CZ	-24.11	0.91	1.37
1	A	192	PHE	CE1-CZ	-24.04	0.91	1.37
1	B	192	PHE	CE1-CZ	-24.04	0.91	1.37
1	B	741	TYR	CG-CD1	-17.29	1.16	1.39
1	C	741	TYR	CG-CD1	-17.27	1.16	1.39

The worst 5 of 717 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	PHE	CB-CG-CD1	56.88	160.62	120.80
1	C	192	PHE	CB-CG-CD1	56.85	160.60	120.80
1	A	192	PHE	CB-CG-CD1	56.80	160.56	120.80
1	B	192	PHE	CB-CG-CD2	-51.66	84.64	120.80
1	A	192	PHE	CB-CG-CD2	-51.65	84.65	120.80

5 of 33 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	274	THR	CB
1	A	286	THR	CB
1	A	299	THR	CB
1	A	719	THR	CB
1	A	761	THR	CB

5 of 116 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	159	VAL	Peptide
1	A	25	PRO	Peptide
1	A	43	PHE	Sidechain
1	A	66	HIS	Sidechain

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	8301	8079	8081	468	0
1	B	8253	8034	8043	502	0
1	C	8292	8069	8072	473	0
2	D	895	0	839	124	0
2	E	895	0	839	146	0
3	F	28	25	25	2	0
3	G	28	25	25	0	0
3	H	28	25	25	0	0
3	I	28	25	25	1	0
3	J	28	25	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	196	181	182	15	0
4	B	182	167	169	26	0
4	C	84	64	78	8	0
All	All	27238	24719	26428	1551	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 29.

The worst 5 of 1551 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)
1:A:770:ILE:CB	1:A:770:ILE:CG2	1.76	1.63
1:C:699:LEU:CD2	1:C:699:LEU:CG	1.76	1.63
1:C:959:LEU:CG	1:C:959:LEU:CD2	1.77	1.62
1:B:911:VAL:CG2	1:B:911:VAL:HG13	1.28	1.61
1:C:911:VAL:CG1	1:C:911:VAL:CG2	1.78	1.61

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	1044/1264 (83%)	948 (91%)	94 (9%)	2 (0%)	47 79
1	B	1039/1264 (82%)	938 (90%)	99 (10%)	2 (0%)	47 79
1	C	1042/1264 (82%)	946 (91%)	92 (9%)	4 (0%)	34 71
2	D	118/126 (94%)	114 (97%)	4 (3%)	0	100 100
2	E	118/126 (94%)	114 (97%)	4 (3%)	0	100 100
All	All	3361/4044 (83%)	3060 (91%)	293 (9%)	8 (0%)	50 79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	459	SER
1	A	25	PRO
1	A	699	LEU
1	B	25	PRO
1	B	699	LEU

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	931/1100 (85%)	891 (96%)	40 (4%)	29	63
1	B	925/1100 (84%)	887 (96%)	38 (4%)	30	64
1	C	929/1100 (84%)	892 (96%)	37 (4%)	31	65
2	D	92/97 (95%)	86 (94%)	6 (6%)	17	51
2	E	92/97 (95%)	86 (94%)	6 (6%)	17	51
All	All	2969/3494 (85%)	2842 (96%)	127 (4%)	33	63

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	777	ASN
1	C	1091	ARG
1	B	1014	ARG
1	C	1040	VAL
2	D	80	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	ASN
1	C	957	GLN
1	C	1119	ASN
1	C	616	ASN
1	B	66	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
3	NAG	F	1	3	14,14,15	1.19	1 (7%)	17,19,21	0.87	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.32	0
3	NAG	G	1	3	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	H	1	3	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	I	1	3	14,14,15	0.70	1 (7%)	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.18	0	17,19,21	0.38	0
3	NAG	J	1	1,3	14,14,15	0.44	0	17,19,21	0.70	1 (5%)
3	NAG	J	2	3	14,14,15	0.24	0	17,19,21	0.46	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	F	1	3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C1-C2	4.21	1.58	1.52
3	I	1	NAG	O5-C1	-2.59	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

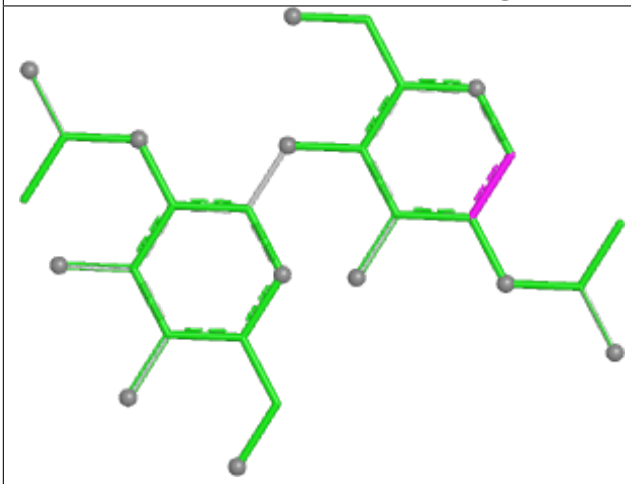
There are no ring outliers.

3 monomers are involved in 5 short contacts:

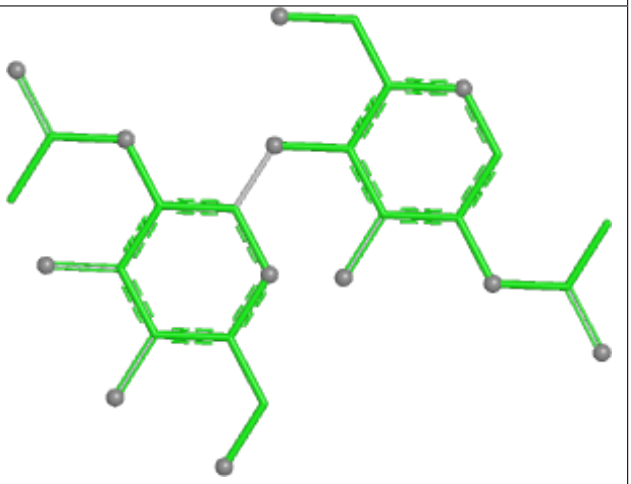
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	2	0
3	F	1	NAG	2	0
3	I	1	NAG	1	0

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

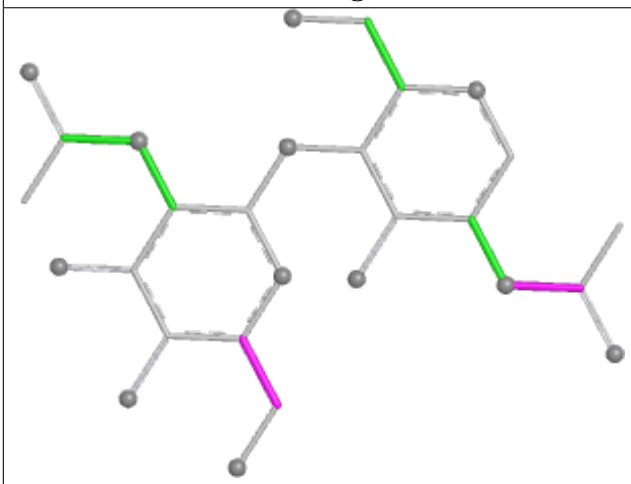
Oligosaccharide Chain F



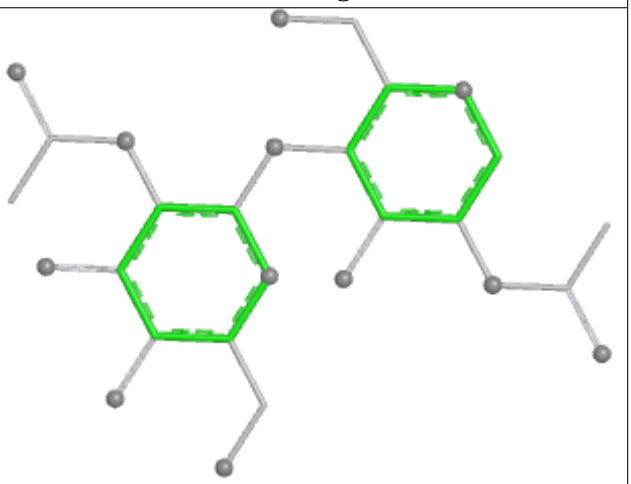
Bond lengths



Bond angles

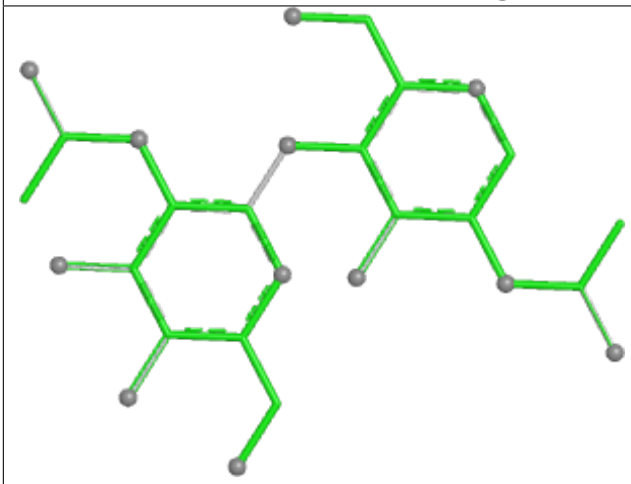


Torsions

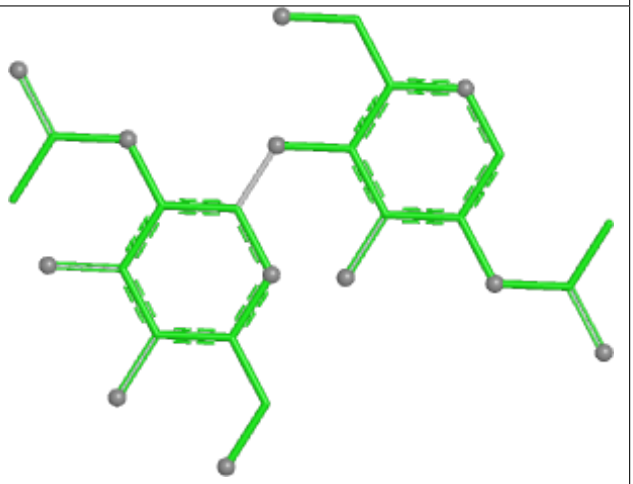


Rings

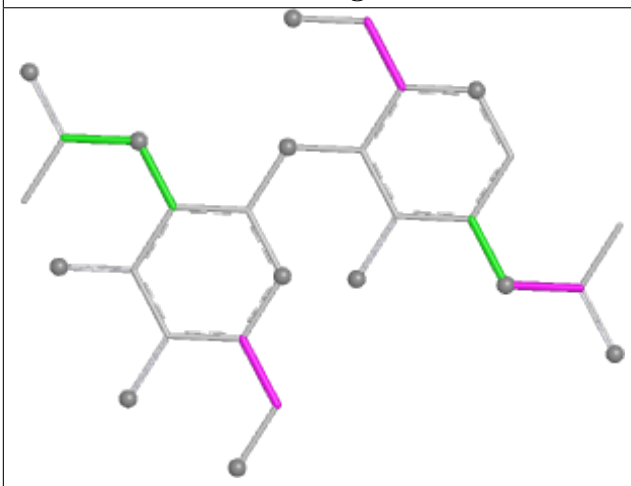
Oligosaccharide Chain G



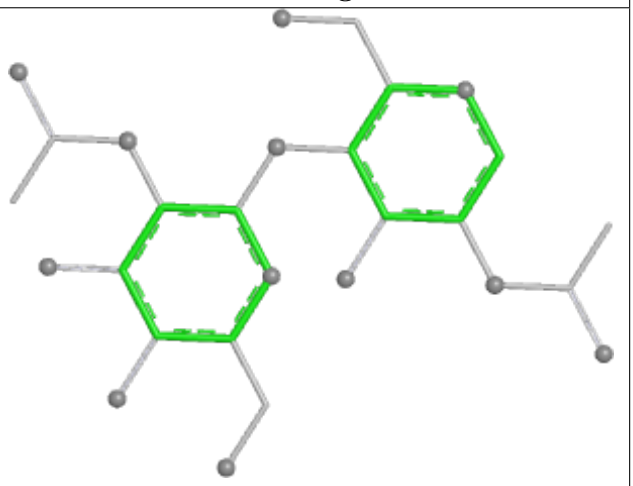
Bond lengths



Bond angles

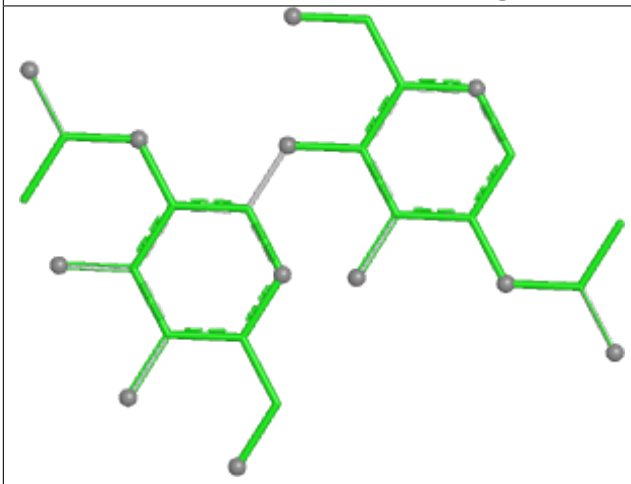


Torsions

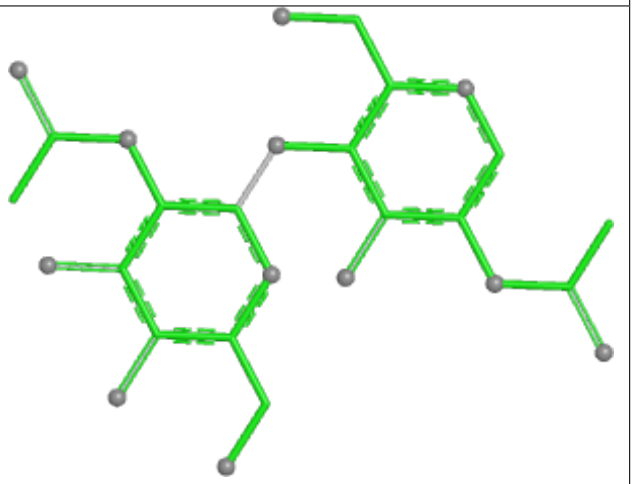


Rings

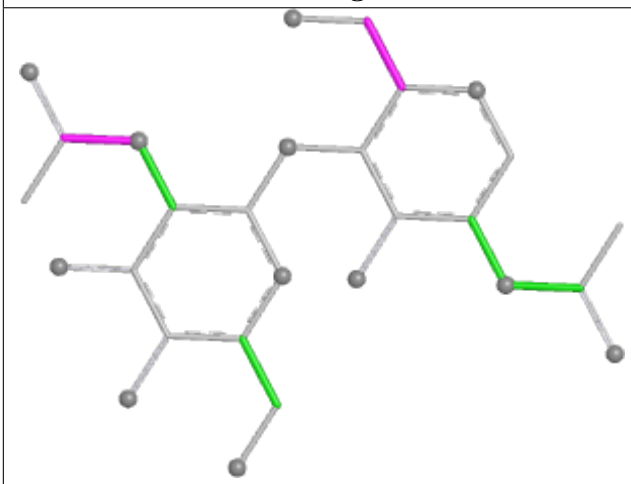
Oligosaccharide Chain H



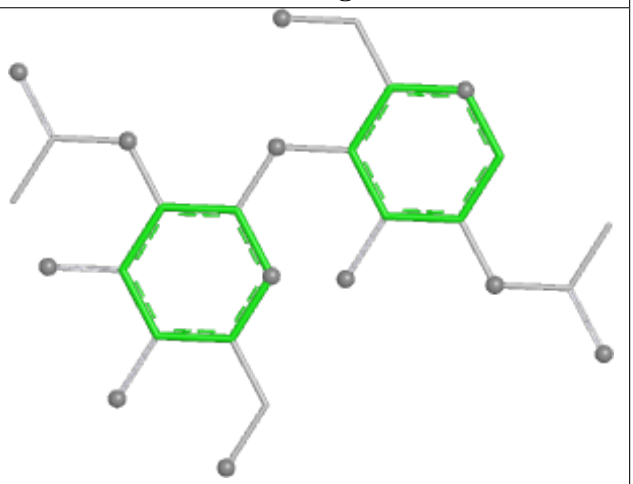
Bond lengths



Bond angles

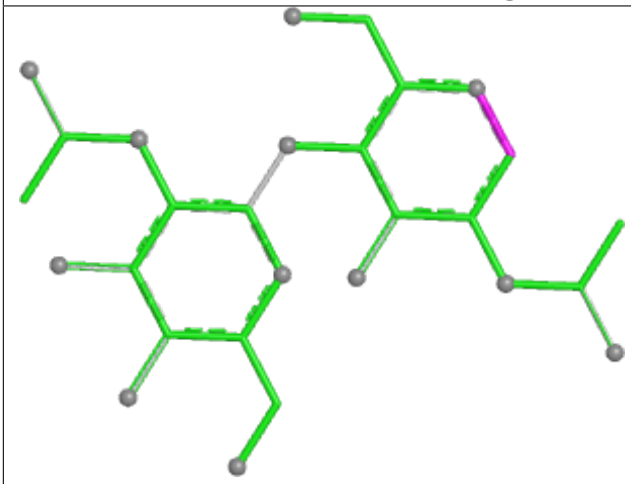


Torsions

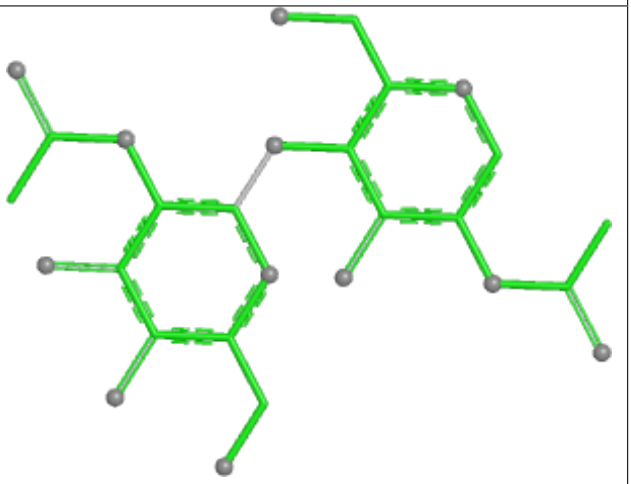


Rings

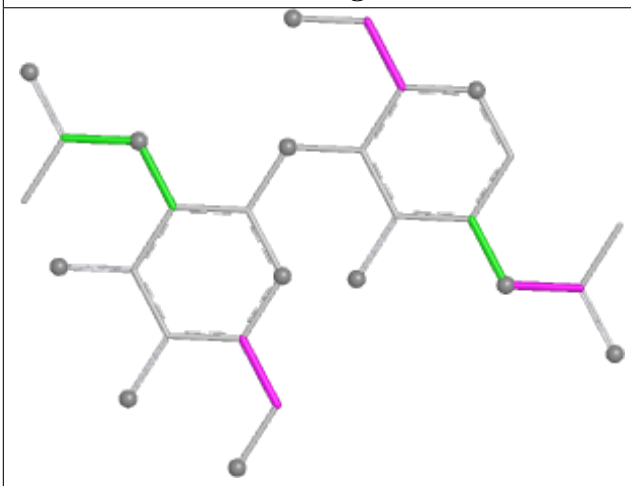
Oligosaccharide Chain I



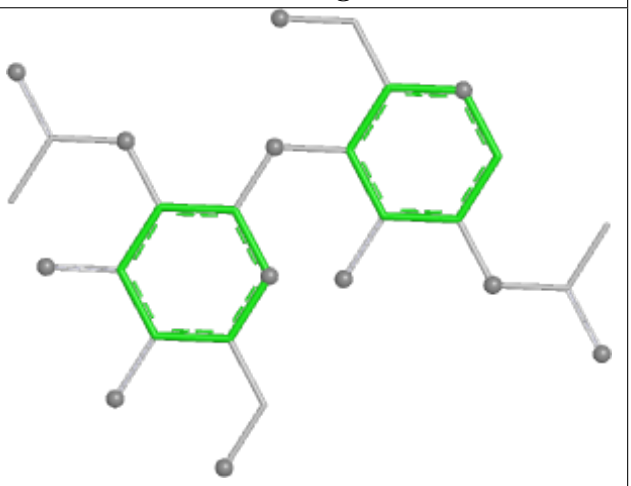
Bond lengths



Bond angles

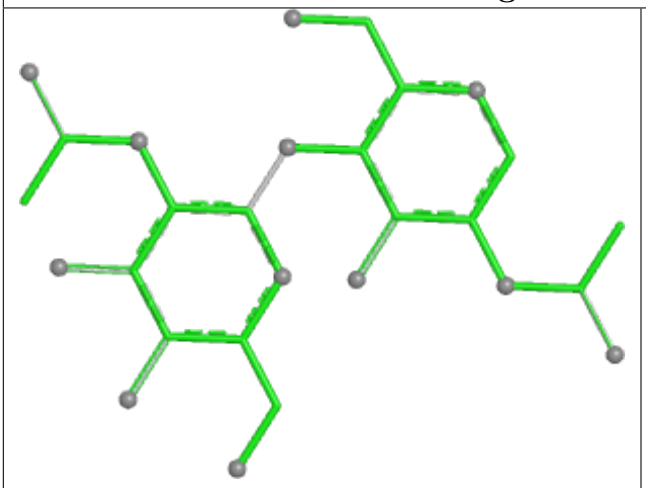


Torsions

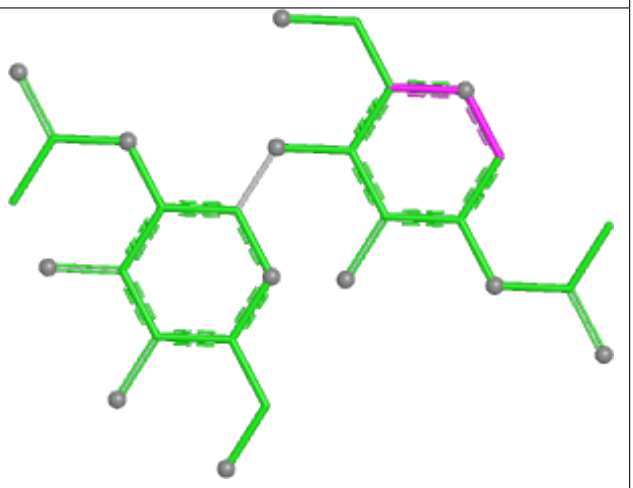


Rings

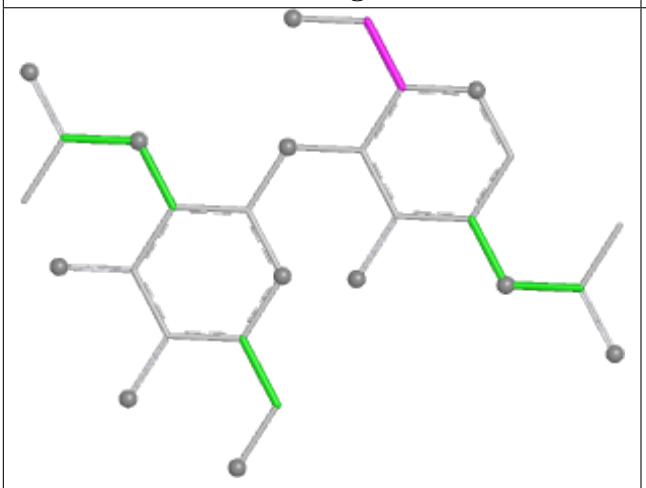
Oligosaccharide Chain J



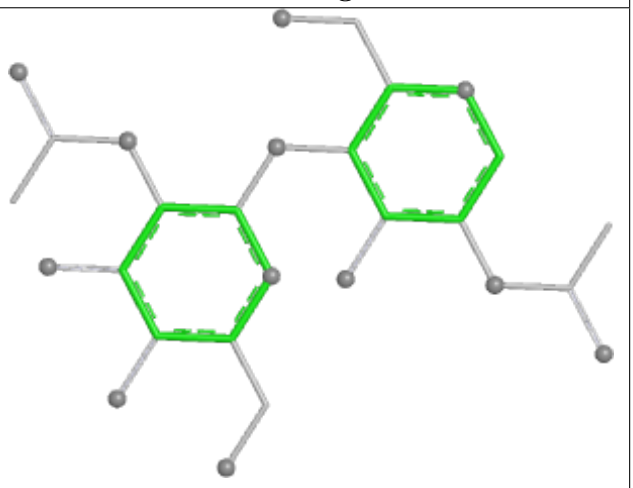
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1310	1	14,14,15	3.30	2 (14%)	17,19,21	2.13	1 (5%)
4	NAG	A	1312	-	14,14,15	0.65	1 (7%)	17,19,21	0.77	1 (5%)
4	NAG	B	1306	-	14,14,15	0.30	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1314	1	14,14,15	0.36	0	17,19,21	0.46	0
4	NAG	C	1303	1	14,14,15	0.87	1 (7%)	17,19,21	0.66	1 (5%)
4	NAG	B	1311	1	14,14,15	1.66	2 (14%)	17,19,21	1.35	2 (11%)
4	NAG	A	1311	1	14,14,15	1.76	2 (14%)	17,19,21	1.44	1 (5%)
4	NAG	B	1312	-	14,14,15	2.78	2 (14%)	17,19,21	1.04	1 (5%)
4	NAG	A	1308	1	14,14,15	0.47	0	17,19,21	1.37	1 (5%)
4	NAG	B	1313	1	14,14,15	0.98	1 (7%)	17,19,21	0.69	1 (5%)
4	NAG	A	1305	1	14,14,15	1.74	2 (14%)	17,19,21	0.66	0
4	NAG	A	1304	1	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	B	1309	1	14,14,15	1.06	1 (7%)	17,19,21	0.69	0
4	NAG	B	1301	-	14,14,15	0.35	0	17,19,21	0.46	0
4	NAG	B	1308	1	14,14,15	1.17	2 (14%)	17,19,21	0.94	1 (5%)
4	NAG	A	1302	-	14,14,15	0.16	0	17,19,21	0.61	0
4	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.35	0
4	NAG	A	1303	-	14,14,15	1.41	2 (14%)	17,19,21	1.02	2 (11%)
4	NAG	A	1301	-	14,14,15	0.89	1 (7%)	17,19,21	0.66	0
4	NAG	C	1301	1	14,14,15	0.92	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	B	1307	-	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
4	NAG	B	1302	-	14,14,15	0.56	0	17,19,21	0.44	0
4	NAG	B	1305	-	14,14,15	0.69	1 (7%)	17,19,21	0.51	0
4	NAG	B	1304	1	14,14,15	1.81	2 (14%)	17,19,21	1.12	2 (11%)
4	NAG	A	1306	-	14,14,15	0.63	0	17,19,21	0.45	0
4	NAG	A	1307	1	14,14,15	1.66	2 (14%)	17,19,21	2.00	1 (5%)
4	NAG	C	1305	1	14,14,15	2.18	1 (7%)	17,19,21	2.18	1 (5%)
4	NAG	C	1302	1	14,14,15	0.51	0	17,19,21	1.10	2 (11%)
4	NAG	A	1313	1	14,14,15	0.74	1 (7%)	17,19,21	0.41	0
4	NAG	B	1303	-	14,14,15	0.20	0	17,19,21	0.52	0
4	NAG	C	1306	1	14,14,15	2.34	2 (14%)	17,19,21	1.28	1 (5%)
4	NAG	C	1304	-	14,14,15	1.00	2 (14%)	17,19,21	1.45	3 (17%)
4	NAG	A	1309	1	14,14,15	1.29	1 (7%)	17,19,21	1.02	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
4	NAG	B	1310	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1312	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1310	NAG	O5-C1	11.92	1.62	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1312	NAG	O5-C1	9.95	1.59	1.43
4	C	1306	NAG	O5-C1	8.02	1.56	1.43
4	C	1305	NAG	O5-C1	7.93	1.56	1.43
4	B	1304	NAG	C1-C2	6.29	1.61	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1305	NAG	C1-O5-C5	8.40	123.57	112.19
4	B	1310	NAG	C1-O5-C5	8.22	123.33	112.19
4	A	1307	NAG	C1-O5-C5	7.87	122.86	112.19
4	A	1311	NAG	C1-O5-C5	5.35	119.44	112.19
4	A	1308	NAG	C1-O5-C5	5.23	119.28	112.19

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1307	NAG	C3-C2-N2-C7
4	C	1306	NAG	C1-C2-N2-C7
4	A	1304	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1310	NAG	9	0
4	C	1303	NAG	1	0
4	B	1301	NAG	2	0
4	A	1302	NAG	2	0
4	A	1303	NAG	4	0
4	A	1301	NAG	4	0
4	C	1301	NAG	1	0
4	B	1307	NAG	7	0
4	B	1302	NAG	2	0
4	B	1305	NAG	2	0
4	B	1304	NAG	4	0
4	A	1306	NAG	2	0
4	A	1313	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1306	NAG	2	0
4	C	1304	NAG	4	0
4	A	1309	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	A	3
1	B	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	332:ILE	C	333:THR	N	6.23
1	C	527:PRO	C	528:LYS	N	4.26
1	B	481:ASN	C	482:GLY	N	3.38
1	C	528:LYS	C	529:LYS	N	3.28
1	A	527:PRO	C	528:LYS	N	3.23

6 Map visualisation

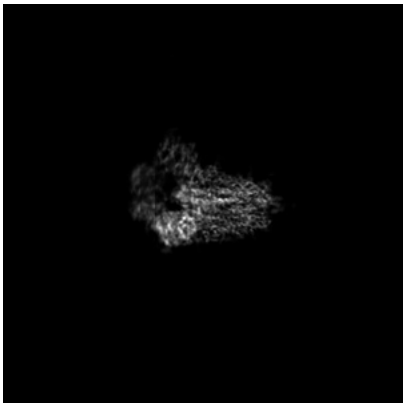
This section contains visualisations of the EMDB entry EMD-14314. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

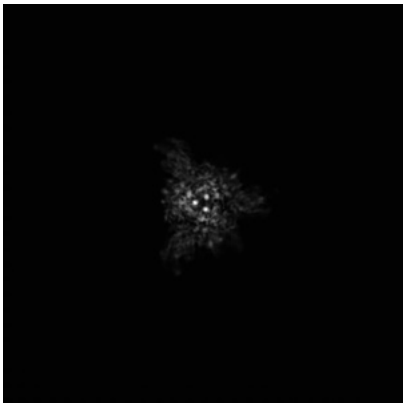
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



Z

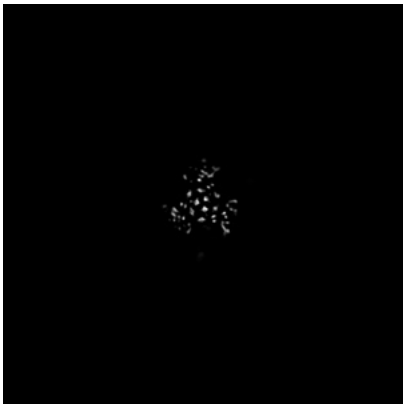
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 246

Y Index: 246



Z Index: 246

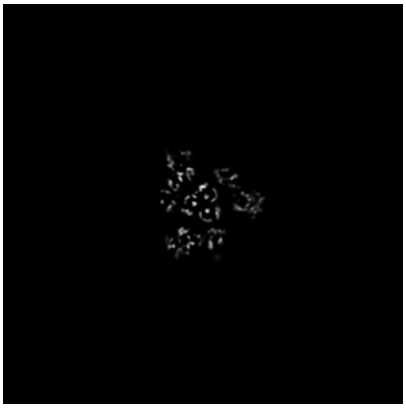
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 249

Y Index: 238



Z Index: 222

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

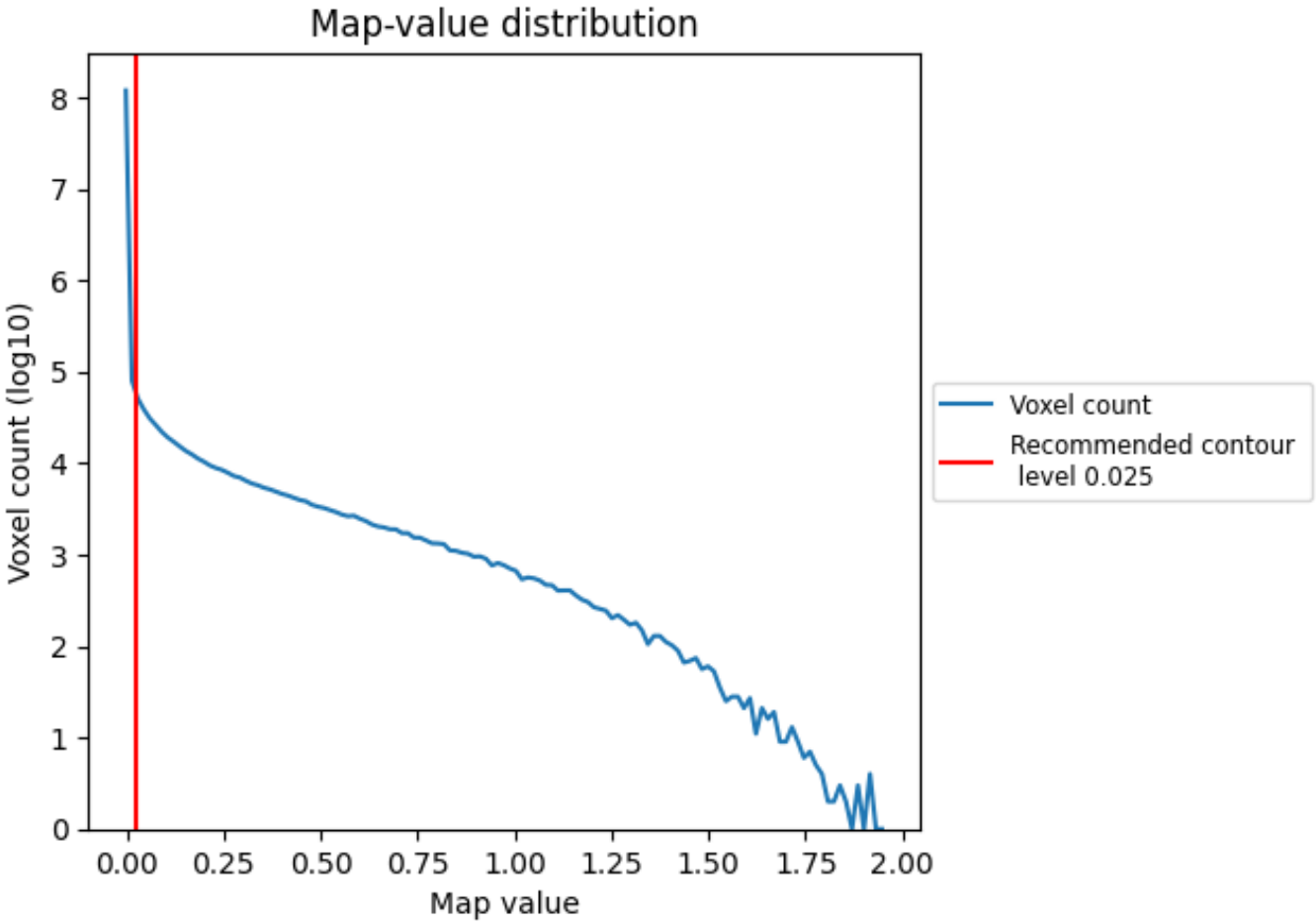
6.5 Mask visualisation (i)

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

7 Map analysis

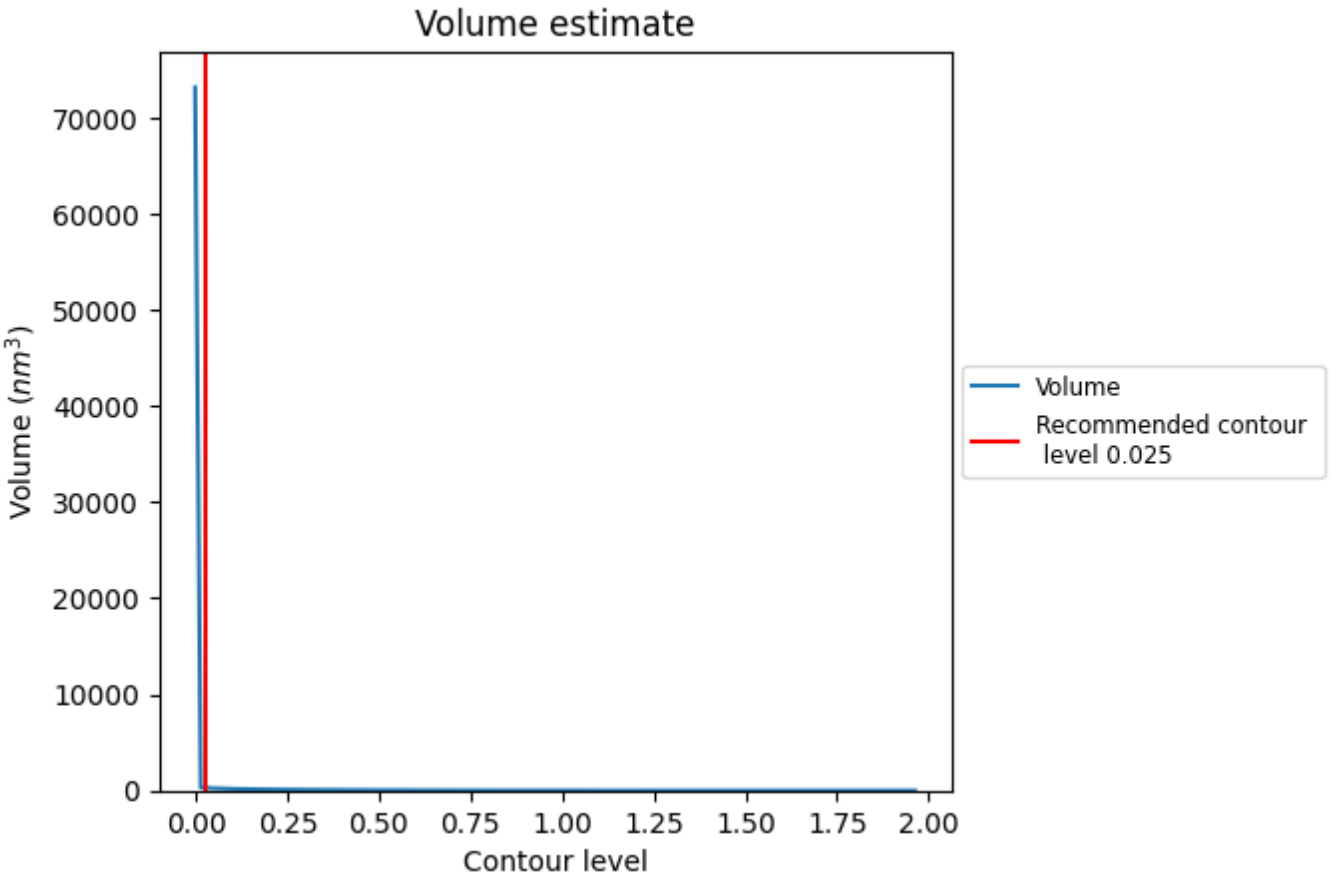
This section contains the results of statistical analysis of the map.

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.

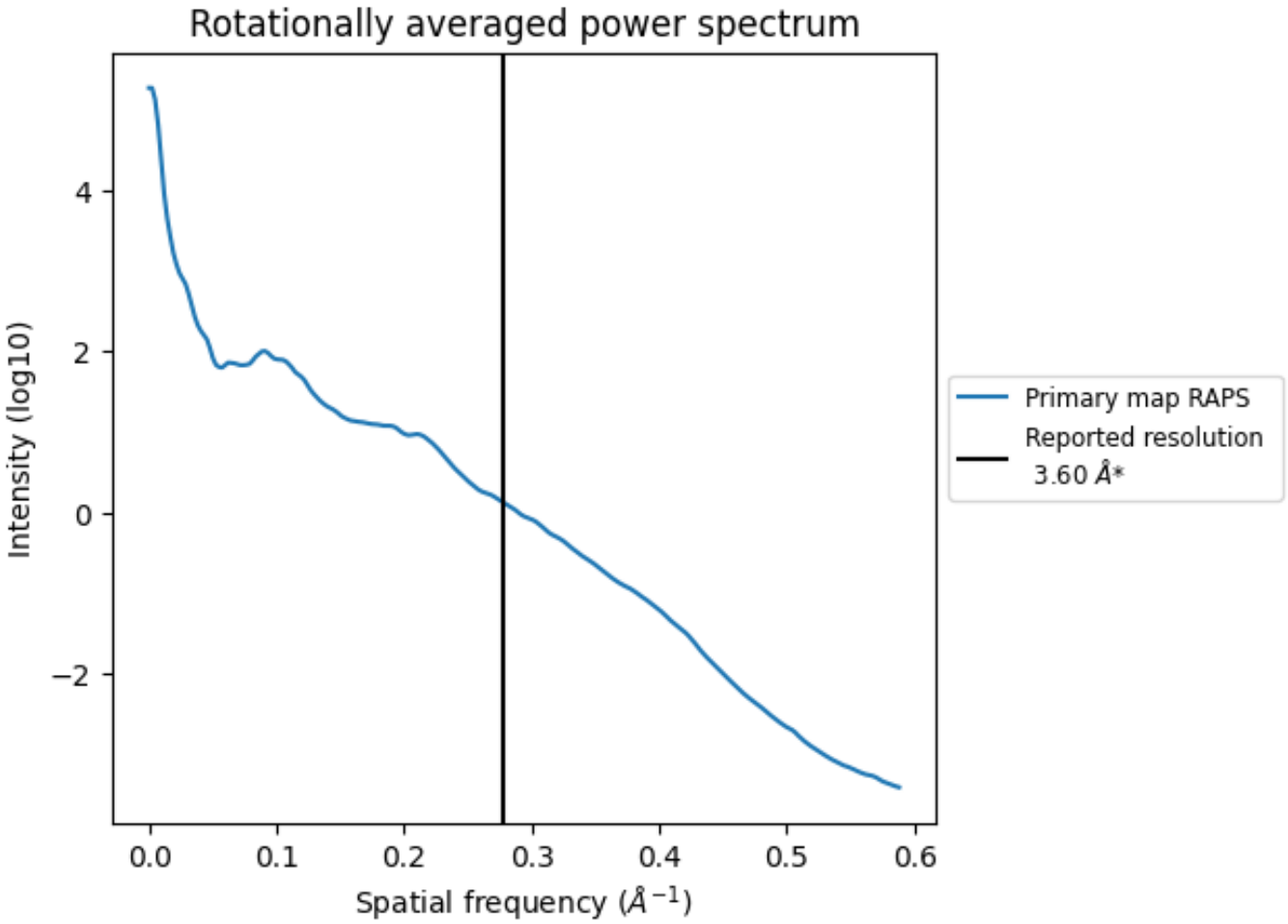
7.2 Volume estimate (i)



The volume at the recommended contour level is 284 nm^3; this corresponds to an approximate mass of 256 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 (i)

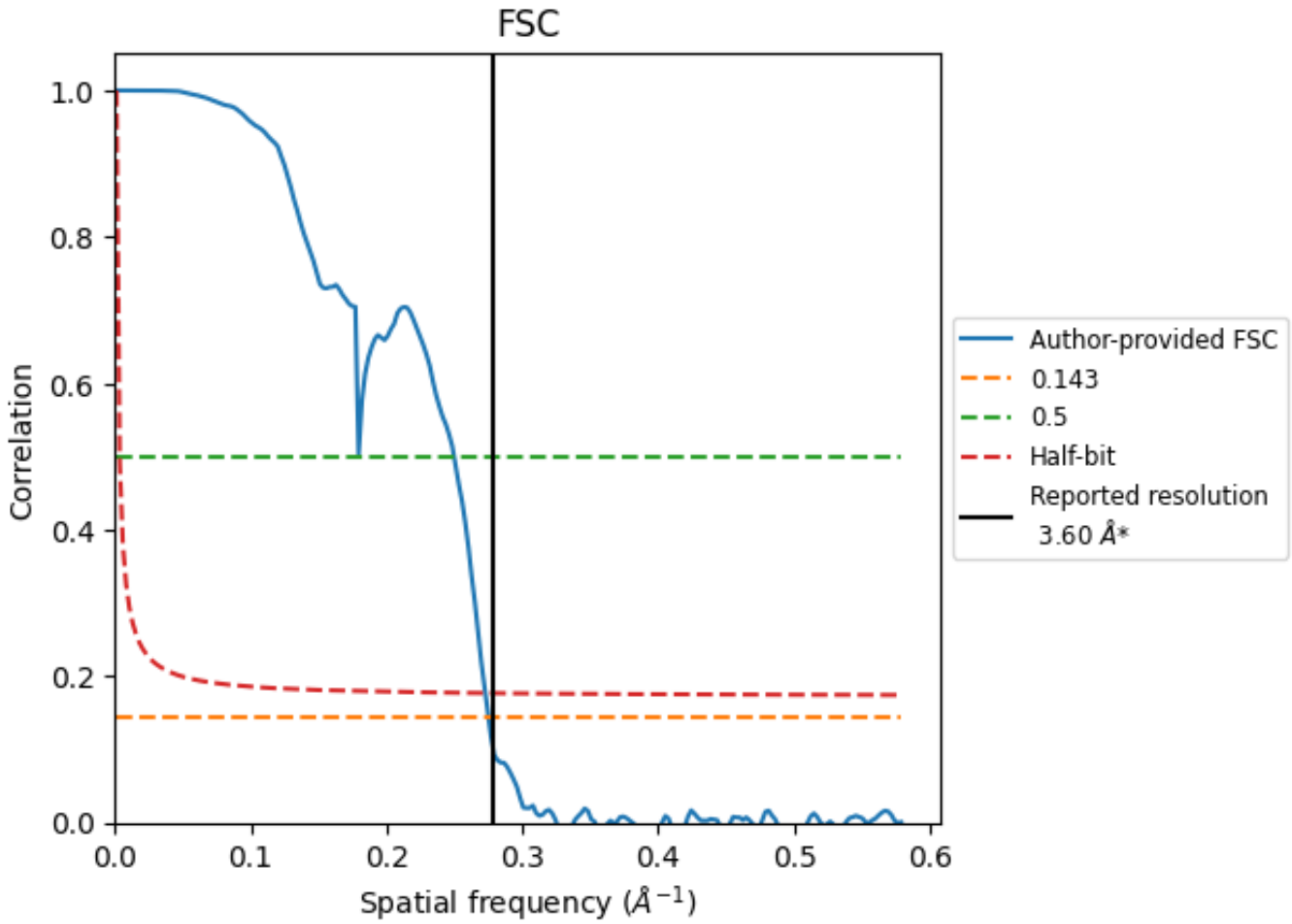


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

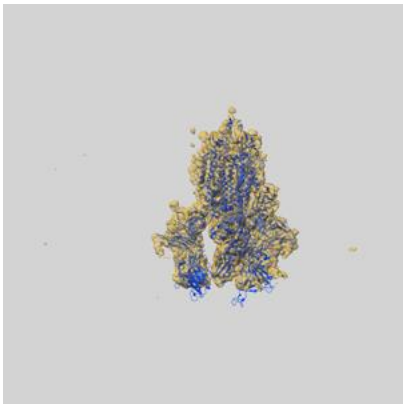
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.64	4.00	3.67
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

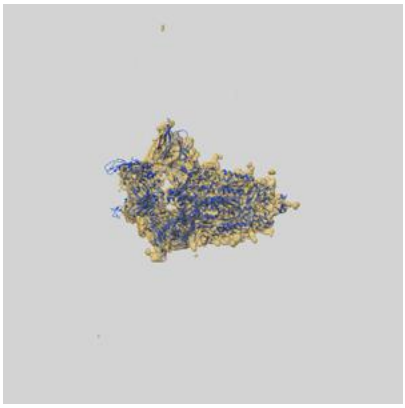
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14314 and PDB model 7R4Q. Per-residue inclusion information can be found in section 3 on page 12.

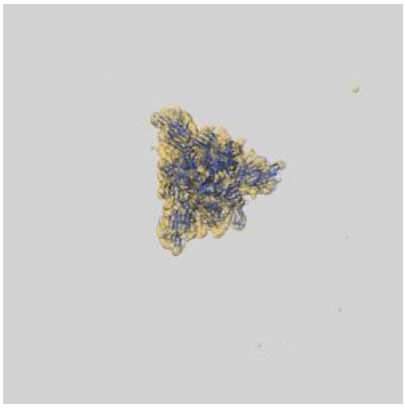
9.1 Map-model overlay



X



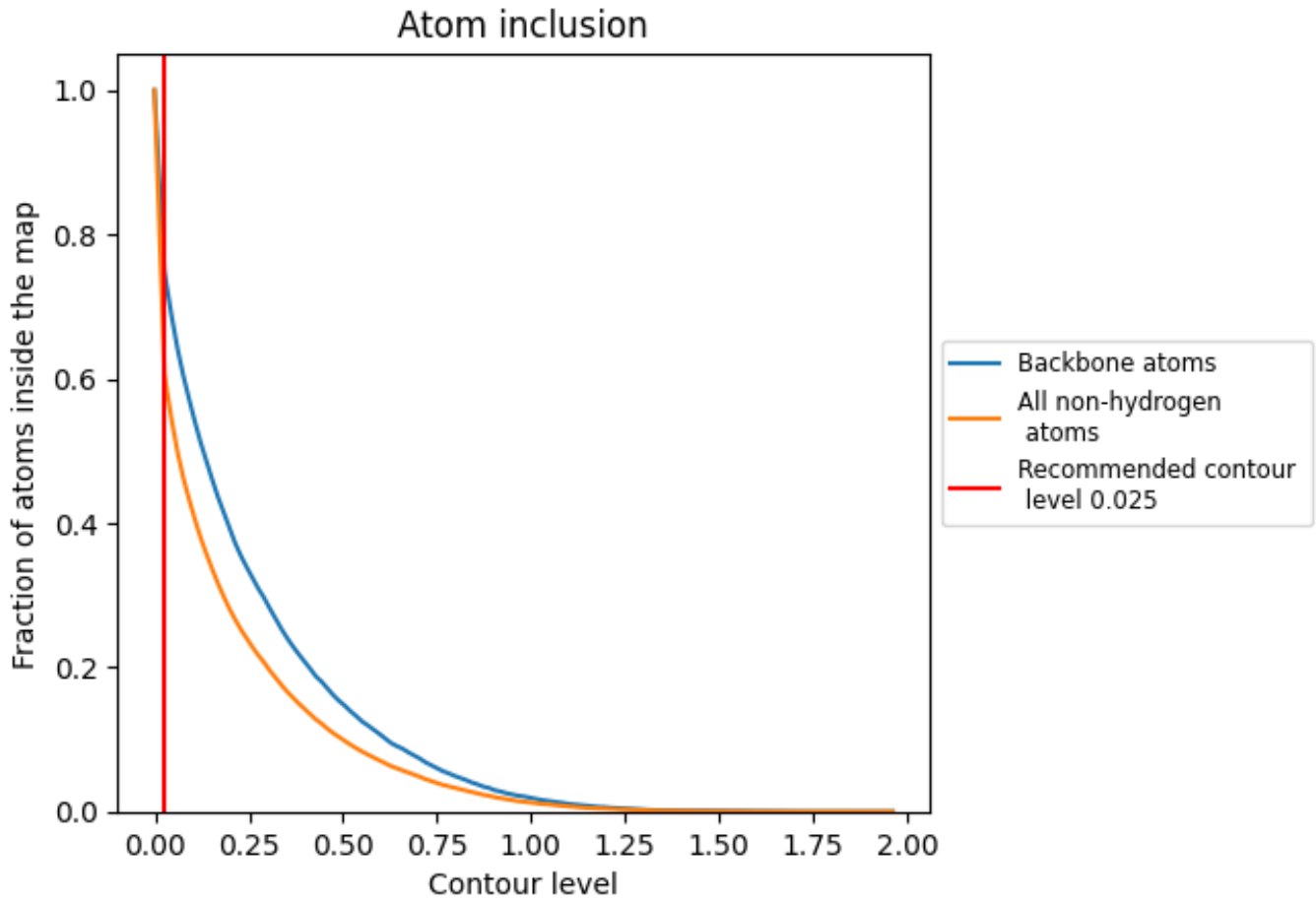
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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 (i)



At the recommended contour level, 75% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.