Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 06:19 AM EST

PDB ID	:	7M6I
EMDB ID	:	EMD-23697
Title	:	Structure of the SARS-CoV-2 S 2P trimer in complex with the human neutralizing antibody Fab fragment, BG1-24
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2021-03-25
Resolution	:	4.00 Å(reported)
Based on initial model	:	6XKL

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

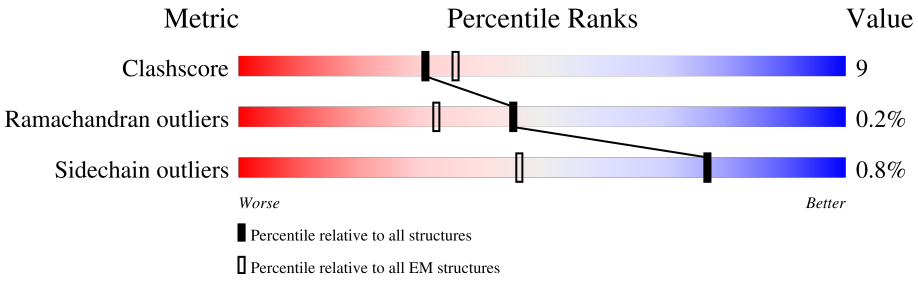
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



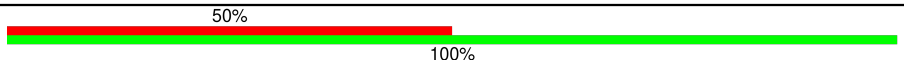
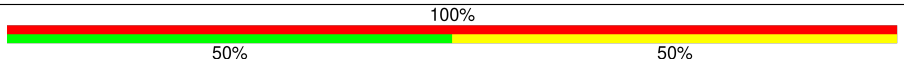
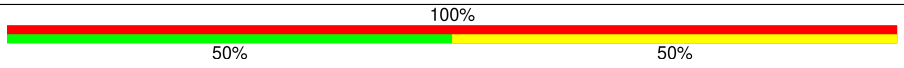
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	1259	10% 63% 16% • 20%
1	B	1259	19% 62% 17% 20%
1	C	1259	10% 61% 18% • 20%
2	H	229	28% 36% 14% • 49%
2	M	229	31% 38% 13% 49%
3	L	215	34% 27% 19% • 51%
3	N	215	40% 30% 18% • 51%
4	D	2	50% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	2	
4	I	2	
5	E	4	
6	G	3	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27359 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	1002	Total	C	N	O	S	0	0
			7814	4989	1299	1491	35		
1	B	1001	Total	C	N	O	S	0	0
			7801	4981	1297	1490	33		
1	C	1001	Total	C	N	O	S	0	0
			7809	4987	1298	1490	34		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	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
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	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
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	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
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called BG1-24 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	117	Total	C	N	O	S	0	0
			897	566	150	176	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	117	Total	C	N	O	S	0	0
			897	566	150	176	5		

- Molecule 3 is a protein called BG1-24 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			802	501	142	157	2		
3	N	106	Total	C	N	O	S	0	0
			802	501	142	157	2		

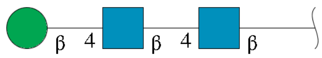
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

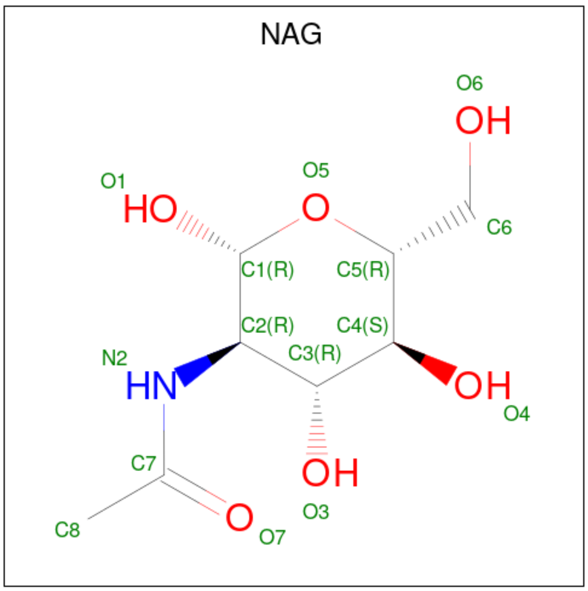
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
6	G	3	Total C N O 39 22 2 15	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

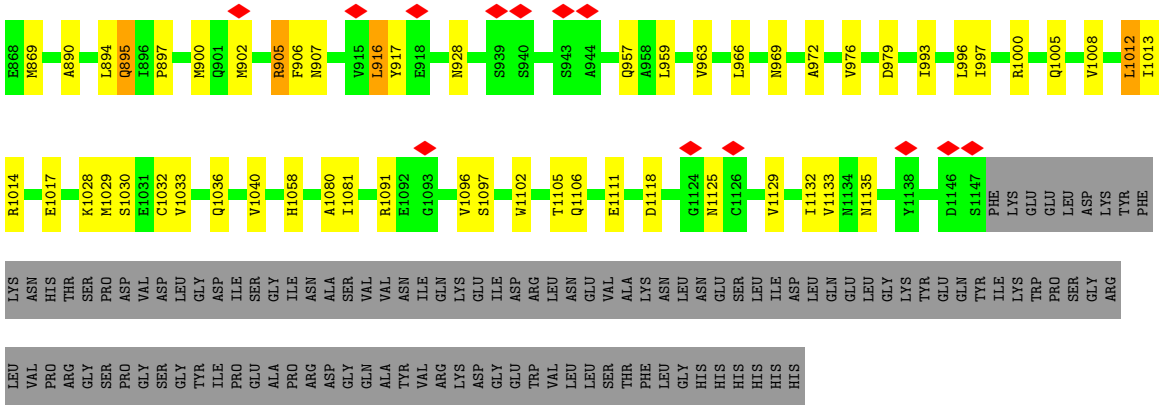
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	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.

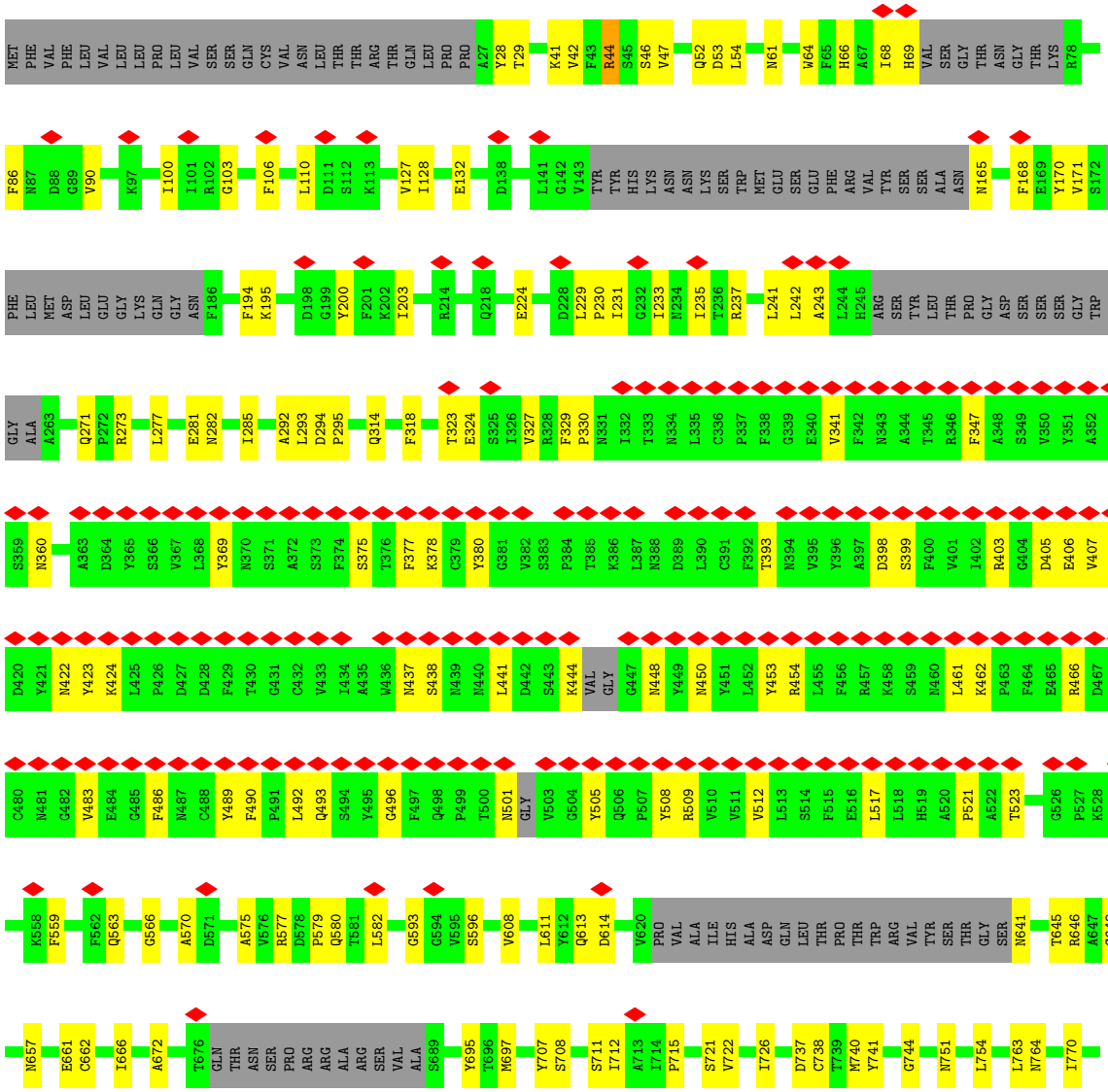
- Molecule 1: Spike glycoprotein

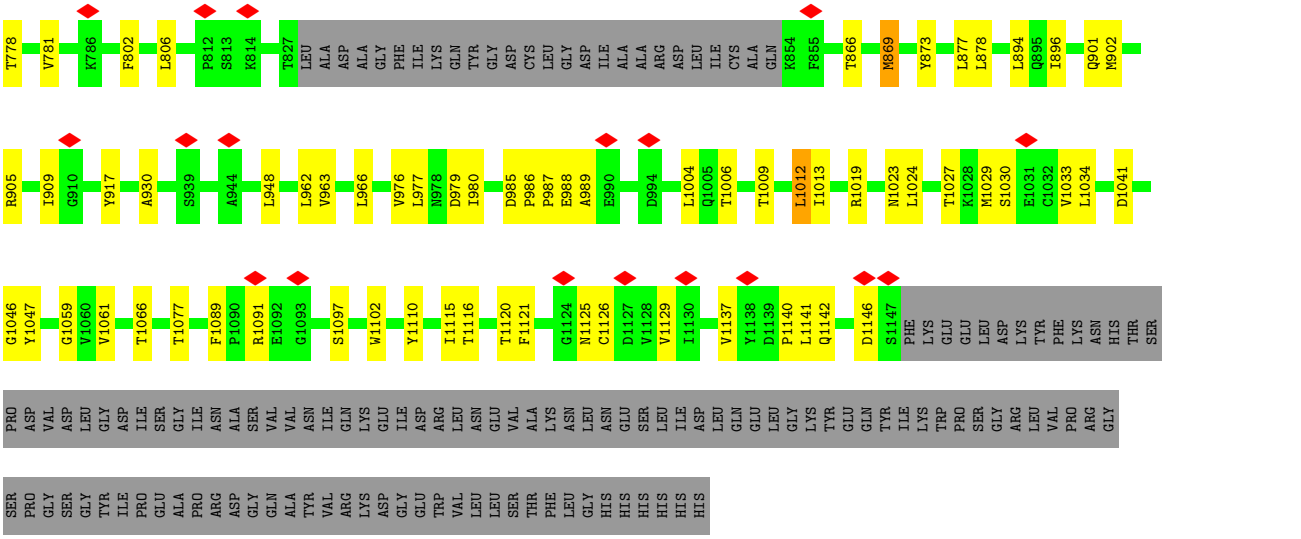
Chain A:



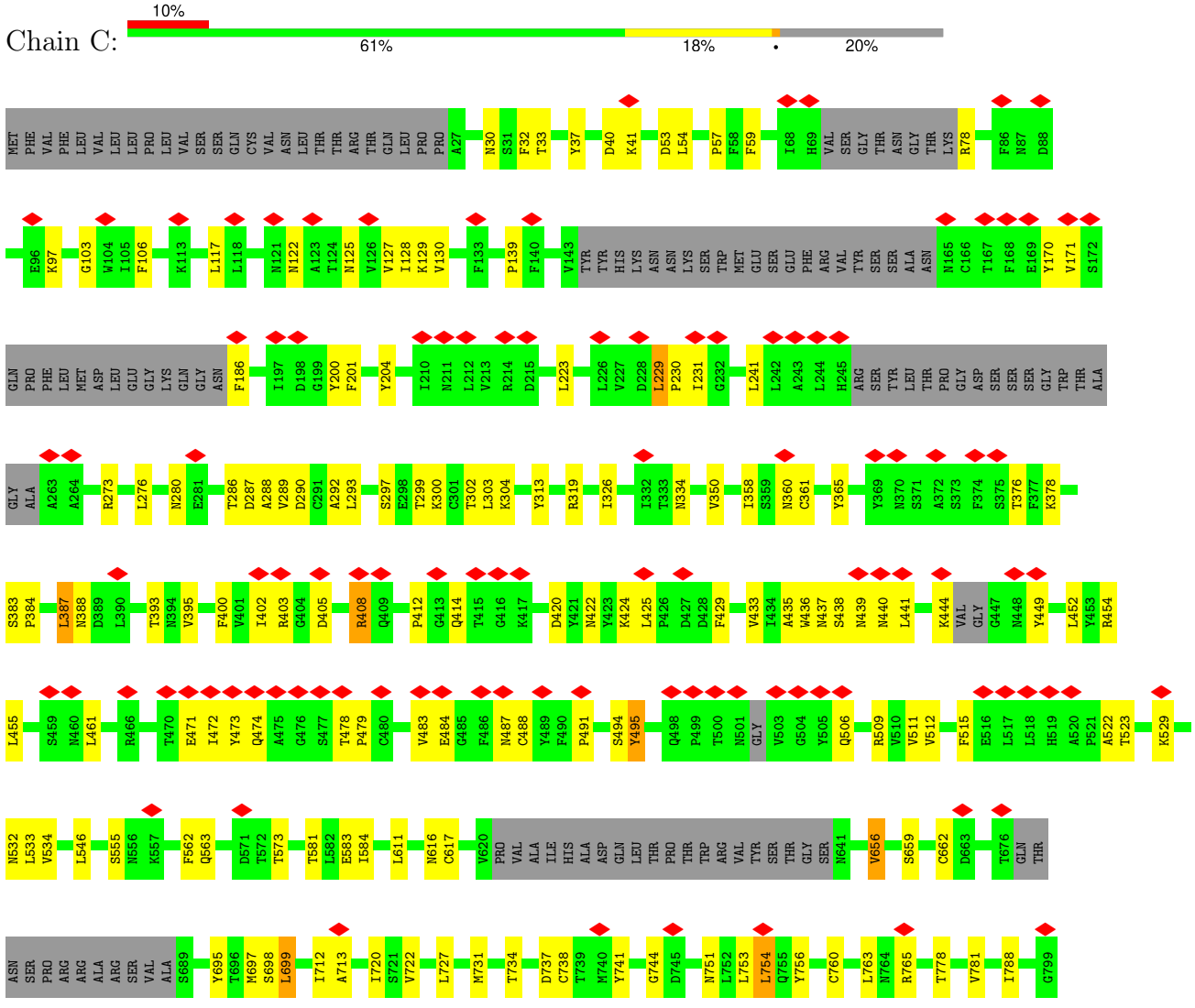
• Molecule 1: Spike glycoprotein

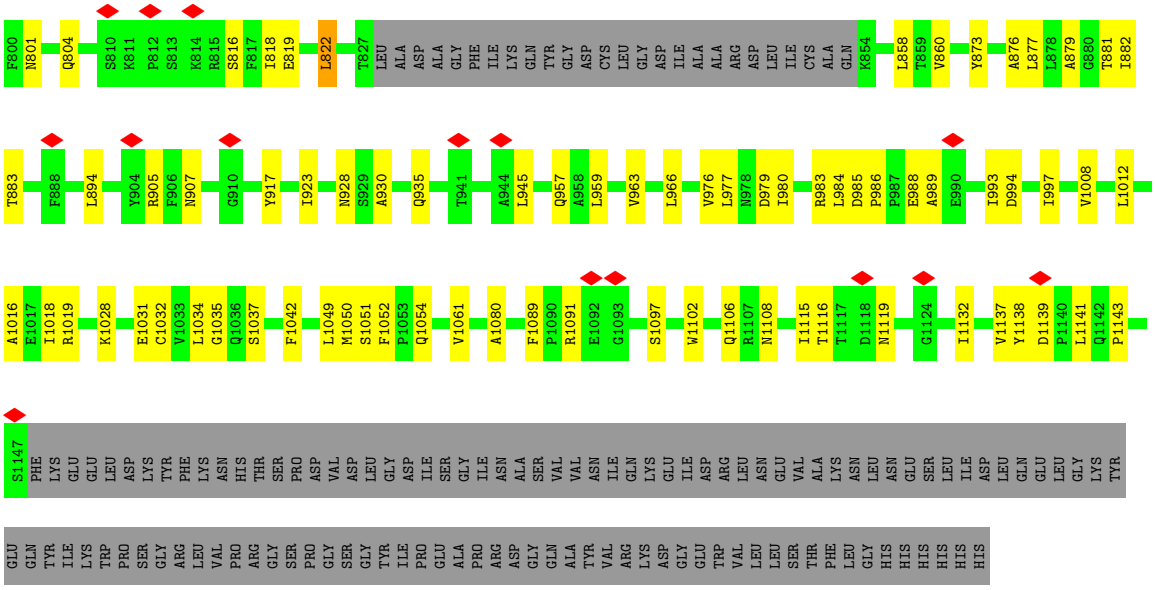
Chain B:





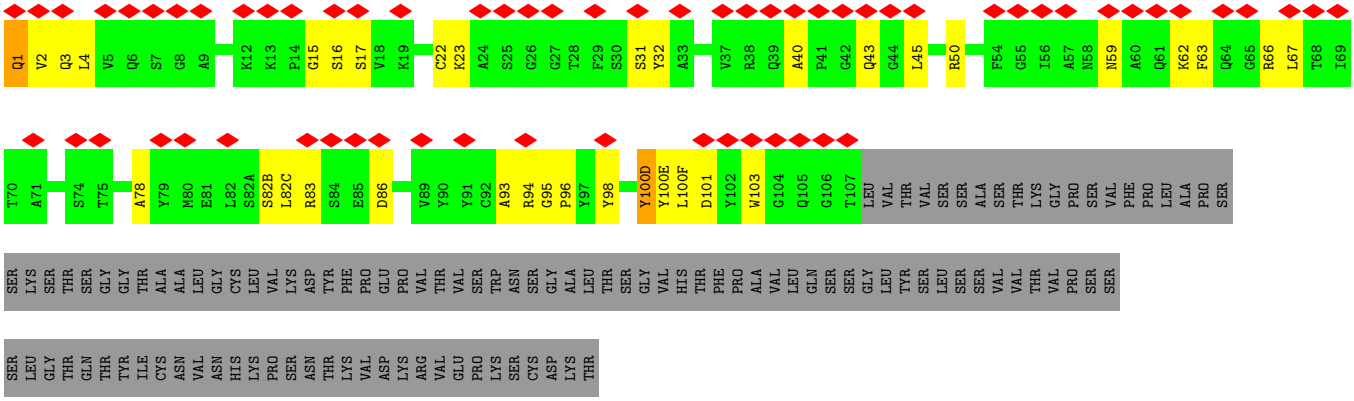
• Molecule 1: Spike glycoprotein





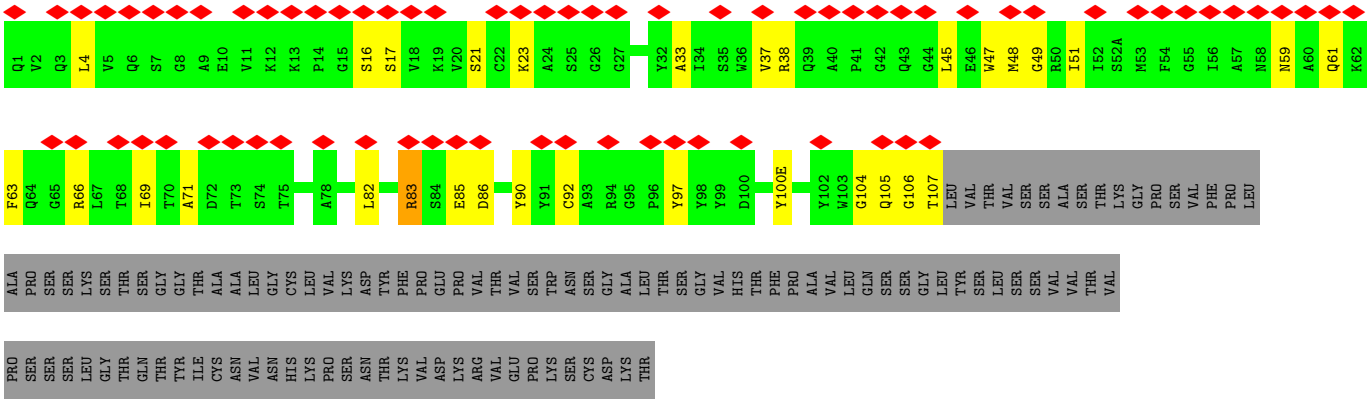
• Molecule 2: BG1-24 Fab Heavy Chain

Chain H:



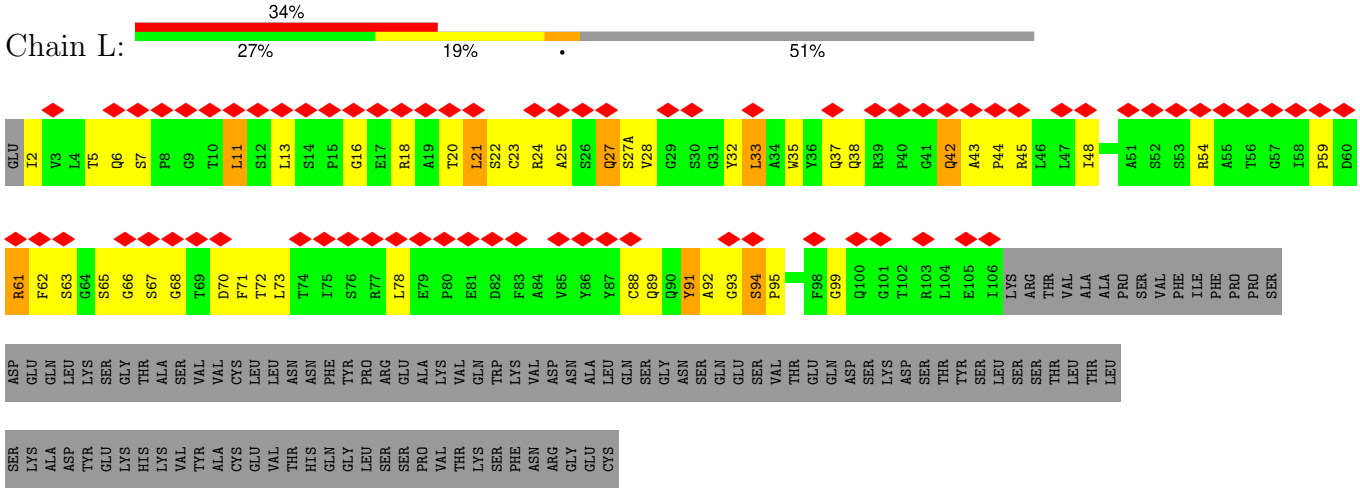
• Molecule 2: BG1-24 Fab Heavy Chain

Chain M:



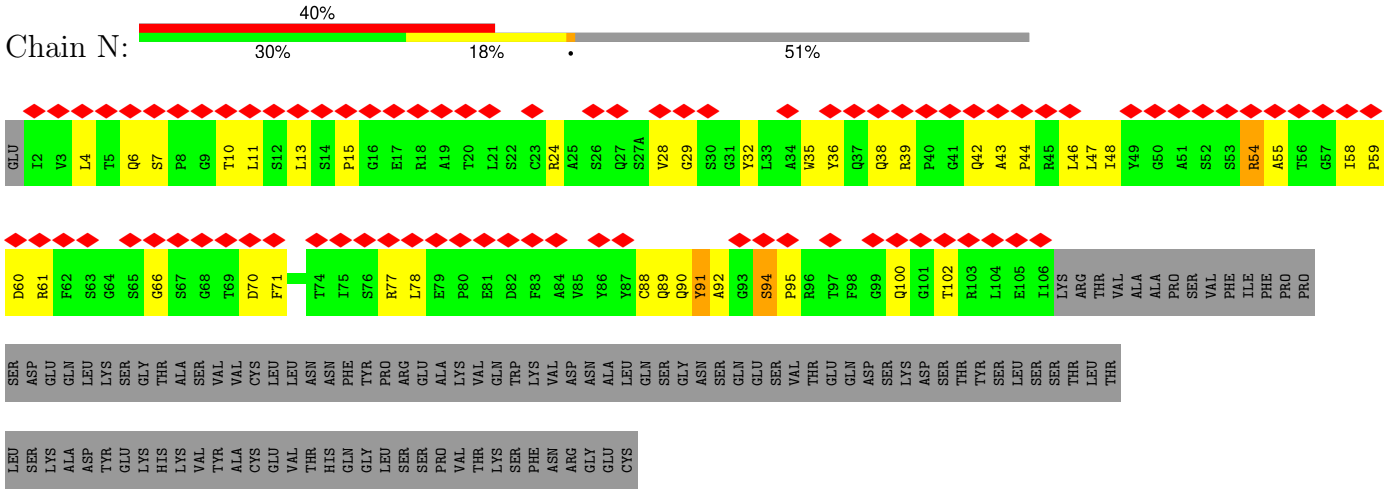
• Molecule 3: BG1-24 Fab Light Chain

Chain L:



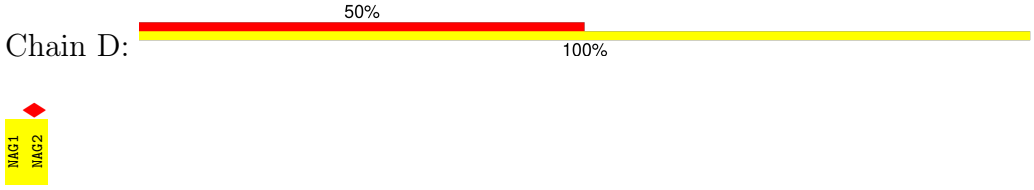
• Molecule 3: BG1-24 Fab Light Chain

Chain N:



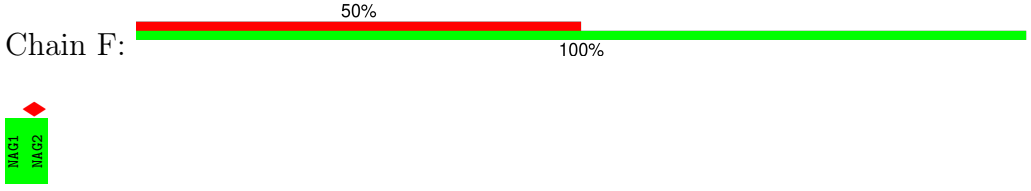
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain F:

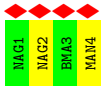


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain G:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84059	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.416	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	375.40802, 375.40802, 375.40802	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/7989	0.74	8/10872 (0.1%)
1	B	0.35	0/7973	0.75	12/10850 (0.1%)
1	C	0.37	0/7983	0.74	10/10863 (0.1%)
2	H	0.38	0/918	0.88	2/1242 (0.2%)
2	M	0.37	0/918	0.86	0/1242
3	L	0.40	0/820	0.92	5/1113 (0.4%)
3	N	0.36	0/820	0.91	2/1113 (0.2%)
All	All	0.36	0/27421	0.76	39/37295 (0.1%)

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	B	0	3
1	C	0	4
2	M	0	1
3	L	0	1
3	N	0	1
All	All	0	10

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	878	LEU	CA-CB-CG	8.54	134.94	115.30
1	A	1012	LEU	CA-CB-CG	7.55	132.66	115.30
3	N	91	TYR	CA-CB-CG	7.21	127.09	113.40
1	B	614	ASP	CB-CG-OD1	7.11	124.70	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	582	LEU	CA-CB-CG	6.96	131.31	115.30
1	C	822	LEU	CA-CB-CG	6.96	131.30	115.30
2	H	45	LEU	CA-CB-CG	6.91	131.19	115.30
1	B	902	MET	CA-CB-CG	6.81	124.87	113.30
1	A	754	LEU	CA-CB-CG	6.71	130.73	115.30
1	C	1141	LEU	CA-CB-CG	6.54	130.33	115.30
1	B	282	ASN	CB-CA-C	6.42	123.23	110.40
1	C	945	LEU	CA-CB-CG	6.21	129.57	115.30
1	A	905	ARG	CA-CB-CG	-6.19	99.79	113.40
1	B	1141	LEU	CA-CB-CG	5.97	129.03	115.30
3	N	4	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	905	ARG	CB-CG-CD	5.89	126.93	111.60
3	L	11	LEU	CA-CB-CG	5.76	128.55	115.30
2	H	1	GLN	CA-CB-CG	5.65	125.84	113.40
1	C	1034	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	616	ASN	CB-CA-C	5.59	121.58	110.40
1	C	387	LEU	CB-CG-CD2	5.59	120.50	111.00
3	L	33	LEU	CB-CG-CD2	5.56	120.45	111.00
1	A	916	LEU	CB-CG-CD1	-5.56	101.56	111.00
1	C	387	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	877	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	806	LEU	CA-CB-CG	5.39	127.69	115.30
3	L	21	LEU	CA-CB-CG	5.38	127.67	115.30
3	L	91	TYR	CA-CB-CG	5.36	123.58	113.40
1	C	229	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	242	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	754	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	1012	LEU	CA-CB-CG	5.20	127.27	115.30
1	B	869	MET	CB-CG-SD	-5.17	96.89	112.40
3	L	42	GLN	C-N-CA	5.15	134.57	121.70
1	B	44	ARG	CA-CB-CG	5.14	124.71	113.40
1	C	611	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	869	MET	CA-CB-CG	5.12	122.00	113.30
1	C	414	GLN	N-CA-CB	5.09	119.77	110.60
1	B	44	ARG	CB-CG-CD	5.03	124.68	111.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	471	GLU	Peptide
1	B	474	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	483	VAL	Peptide
1	C	122	ASN	Peptide
1	C	33	THR	Peptide
1	C	471	GLU	Peptide
1	C	474	GLN	Peptide
3	L	7	SER	Peptide
2	M	106	GLY	Peptide
3	N	7	SER	Peptide

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	7814	0	7600	133	0
1	B	7801	0	7577	142	0
1	C	7809	0	7597	144	0
2	H	897	0	858	22	0
2	M	897	0	858	19	0
3	L	802	0	777	32	0
3	N	802	0	777	24	0
4	D	28	0	25	0	0
4	F	28	0	25	0	0
4	I	28	0	25	0	0
5	E	50	0	43	0	0
6	G	39	0	34	0	0
7	A	140	0	130	3	0
7	B	112	0	104	3	0
7	C	112	0	104	0	0
All	All	27359	0	26534	470	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 9.

All (470) 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:475:ALA:HB3	1:A:488:CYS:HA	1.51	0.89
2:M:33:ALA:HB2	2:M:97:TYR:HB2	1.57	0.84
1:C:106:PHE:HB2	1:C:117:LEU:HD21	1.64	0.78
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.67	0.77
1:B:866:THR:H	1:B:869:MET:HE2	1.51	0.75
2:M:61:GLN:HE22	3:N:95:PRO:HD3	1.51	0.75
3:N:94:SER:HB3	3:N:95:PRO:HD2	1.69	0.74
1:A:394:ASN:ND2	1:C:200:TYR:OH	2.20	0.74
1:B:360:ASN:H	1:B:523:THR:HB	1.51	0.74
3:L:94:SER:HB3	3:L:95:PRO:HD2	1.70	0.73
1:A:780:GLU:O	1:A:784:GLN:NE2	2.21	0.73
1:A:293:LEU:HD23	1:A:294:ASP:HB2	1.69	0.73
3:L:6:GLN:HE22	3:L:99:GLY:HA3	1.55	0.72
1:A:271:GLN:HE21	1:A:273:ARG:HD3	1.55	0.71
1:B:356:LYS:NZ	1:B:399:SER:OG	2.25	0.70
1:B:132:GLU:OE1	1:B:165:ASN:N	2.25	0.70
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.75	0.69
1:C:360:ASN:H	1:C:523:THR:HB	1.57	0.69
1:B:438:SER:HB2	1:B:509:ARG:HB2	1.73	0.69
1:A:1013:ILE:HD13	1:C:1012:LEU:HG	1.72	0.69
1:A:310:LYS:HG2	1:A:664:ILE:HD11	1.75	0.68
2:M:105:GLN:HG3	3:N:42:GLN:HE22	1.59	0.68
1:A:905:ARG:HE	1:A:1036:GLN:HB2	1.59	0.68
1:C:376:THR:HB	1:C:435:ALA:HB3	1.77	0.67
1:C:455:LEU:H	1:C:491:PRO:HB2	1.58	0.67
1:B:738:CYS:H	1:B:764:ASN:HD21	1.42	0.66
1:A:417:LYS:O	1:A:421:TYR:HB2	1.94	0.66
3:L:21:LEU:HD23	3:L:73:LEU:HD23	1.78	0.66
2:M:21:SER:OG	2:M:23:LYS:NZ	2.28	0.66
1:C:484:GLU:HA	3:L:93:GLY:HA2	1.77	0.66
1:B:1091:ARG:HE	1:B:1121:PHE:HB3	1.62	0.65
3:L:6:GLN:NE2	3:L:88:CYS:SG	2.70	0.64
1:B:380:TYR:H	7:B:1304:NAG:H3	1.61	0.64
1:B:466:ARG:HH21	1:B:468:ILE:HG13	1.61	0.64
1:A:378:LYS:NZ	1:A:380:TYR:OH	2.29	0.63
1:B:988:GLU:OE2	1:C:383:SER:OG	2.16	0.63
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.79	0.63
1:A:360:ASN:H	1:A:523:THR:HB	1.63	0.63
1:B:369:TYR:OH	1:C:487:ASN:ND2	2.32	0.62
2:M:100(E):TYR:HB2	3:N:91:TYR:CE2	2.34	0.62
1:B:424:LYS:HD2	1:B:461:LEU:HB3	1.81	0.62
1:A:406:GLU:HA	1:A:409:GLN:HB3	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:HD13	3:L:27:GLN:HG3	1.82	0.62
2:M:4:LEU:HG	2:M:104:GLY:HA3	1.80	0.62
1:A:280:ASN:ND2	1:A:281:GLU:OE1	2.32	0.61
1:B:200:TYR:HA	1:B:230:PRO:HA	1.82	0.61
1:B:403:ARG:HB2	1:B:406:GLU:HG2	1.81	0.61
1:C:393:THR:HA	1:C:522:ALA:HA	1.82	0.61
3:N:89:GLN:NE2	3:N:90:GLN:O	2.34	0.61
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.82	0.61
1:C:656:VAL:HG23	1:C:695:TYR:HB3	1.81	0.61
1:C:905:ARG:NH1	1:C:1050:MET:SD	2.73	0.61
1:A:393:THR:HA	1:A:522:ALA:HA	1.82	0.61
1:B:559:PHE:HB2	1:B:577:ARG:HH21	1.63	0.61
1:C:289:VAL:HG21	1:C:300:LYS:HD2	1.82	0.61
1:A:712:ILE:HG21	1:A:1096:VAL:HG12	1.81	0.61
1:C:405:ASP:O	1:C:408:ARG:NH1	2.33	0.61
1:A:395:VAL:HB	1:A:513:LEU:HD21	1.83	0.60
1:C:1115:ILE:HG22	1:C:1137:VAL:HG23	1.82	0.60
3:L:22:SER:HA	3:L:72:THR:HA	1.83	0.60
1:A:92:PHE:HE1	1:A:94:SER:HB2	1.66	0.60
3:L:42:GLN:HG3	3:L:43:ALA:H	1.67	0.60
3:N:59:PRO:HB2	3:N:61:ARG:HG2	1.82	0.60
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.84	0.60
3:L:38:GLN:HA	3:L:44:PRO:HA	1.83	0.60
1:C:326:ILE:HD11	1:C:534:VAL:HG12	1.83	0.60
1:C:376:THR:HG23	1:C:378:LYS:HE3	1.83	0.60
3:L:16:GLY:H	3:L:78:LEU:HB3	1.65	0.60
1:C:280:ASN:ND2	1:C:286:THR:OG1	2.33	0.59
1:C:350:VAL:HG12	1:C:400:PHE:HB2	1.84	0.59
1:B:408:ARG:HH22	3:L:63:SER:HB3	1.67	0.59
1:C:734:THR:HG21	1:C:959:LEU:HD21	1.83	0.59
1:B:405:ASP:HA	1:B:408:ARG:HD3	1.84	0.59
1:B:596:SER:HB2	1:B:611:LEU:HB3	1.84	0.59
3:N:10:THR:HA	3:N:102:THR:HG23	1.85	0.59
1:A:897:PRO:HB2	1:A:900:MET:HG2	1.85	0.59
1:C:1054:GLN:HB2	1:C:1061:VAL:HG13	1.85	0.59
1:C:662:CYS:HB2	1:C:697:MET:HG3	1.83	0.59
1:A:300:LYS:NZ	1:A:306:PHE:O	2.32	0.58
1:A:342:PHE:HZ	1:A:513:LEU:HD12	1.67	0.58
2:H:32:TYR:CD1	2:H:96:PRO:HB3	2.38	0.58
1:C:473:TYR:HB3	1:C:488:CYS:HB3	1.84	0.58
1:C:1028:LYS:O	1:C:1032:CYS:HB3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:HE2	1:B:521:PRO:HD3	1.68	0.58
1:B:611:LEU:HD11	1:B:666:ILE:HG23	1.84	0.58
1:C:424:LYS:HZ3	1:C:461:LEU:HB3	1.68	0.58
1:C:276:LEU:HD11	1:C:304:LYS:HA	1.86	0.58
1:A:134:GLN:NE2	1:A:135:PHE:O	2.37	0.58
1:C:139:PRO:HG2	1:C:241:LEU:HD21	1.86	0.58
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.69	0.57
1:B:103:GLY:HA3	1:B:241:LEU:HD12	1.87	0.57
1:B:454:ARG:HB2	1:B:492:LEU:HD13	1.85	0.57
1:C:659:SER:HB2	1:C:698:SER:HB2	1.86	0.57
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.22	0.57
1:C:438:SER:HB2	1:C:509:ARG:HG3	1.87	0.57
1:A:187:LYS:NZ	1:A:211:ASN:OD1	2.38	0.57
1:B:341:VAL:HG11	1:B:356:LYS:HE3	1.86	0.57
1:B:110:LEU:HD13	1:B:237:ARG:HB2	1.87	0.57
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.37	0.56
2:M:83:ARG:NE	2:M:85:GLU:OE2	2.33	0.56
3:L:35:TRP:HB2	3:L:48:ILE:HG22	1.86	0.56
2:M:51:ILE:HD11	2:M:69:ILE:HG22	1.88	0.56
3:N:61:ARG:NH2	3:N:77:ARG:O	2.38	0.56
1:C:273:ARG:HE	1:C:292:ALA:HB3	1.71	0.56
1:C:788:ILE:HG13	1:C:876:ALA:HB2	1.88	0.56
1:A:917:TYR:HB3	1:B:1129:VAL:HG23	1.88	0.56
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.86	0.56
1:A:295:PRO:HA	1:A:298:GLU:HG2	1.87	0.56
2:H:40:ALA:HB3	2:H:43:GLN:HB3	1.88	0.55
1:B:469:SER:OG	1:B:471:GLU:OE1	2.23	0.55
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.88	0.55
1:A:618:THR:HG21	7:A:1306:NAG:H62	1.88	0.55
1:B:271:GLN:OE1	1:B:273:ARG:NH2	2.39	0.55
1:A:801:ASN:OD1	1:A:928:ASN:ND2	2.40	0.55
1:A:439:ASN:OD1	1:A:506:GLN:NE2	2.40	0.55
1:B:408:ARG:HH21	3:L:54:ARG:HH12	1.54	0.55
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.88	0.55
1:A:108:THR:O	1:A:237:ARG:NH2	2.40	0.55
1:B:437:ASN:HA	1:B:508:TYR:HD2	1.72	0.55
1:C:201:PHE:HB2	1:C:231:ILE:HG12	1.89	0.55
1:C:858:LEU:HD11	1:C:959:LEU:HD23	1.88	0.55
1:C:882:ILE:HG23	1:C:883:THR:HG23	1.88	0.55
2:H:82(B):SER:O	2:H:83:ARG:NH1	2.40	0.54
1:B:405:ASP:OD1	1:B:408:ARG:NH1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1019:ARG:NH1	1:B:1023:ASN:OD1	2.40	0.54
1:A:403:ARG:NH1	1:A:505:TYR:HB3	2.22	0.54
3:L:11:LEU:HB2	3:L:13:LEU:HD13	1.88	0.54
1:A:1028:LYS:O	1:A:1032:CYS:HB3	2.06	0.54
1:C:737:ASP:O	1:C:741:TYR:HB3	2.06	0.54
1:C:440:ASN:OD1	1:C:441:LEU:N	2.41	0.54
3:N:39:ARG:NH2	3:N:43:ALA:O	2.41	0.54
1:B:873:TYR:CE1	1:C:699:LEU:HB3	2.42	0.53
1:A:858:LEU:HD23	1:A:959:LEU:HD12	1.89	0.53
3:N:6:GLN:HB3	3:N:100:GLN:HE22	1.73	0.53
1:C:472:ILE:HG22	1:C:473:TYR:HD1	1.72	0.53
1:A:389:ASP:HA	1:A:528:LYS:HZ2	1.73	0.53
1:A:403:ARG:HH11	1:A:505:TYR:HB3	1.73	0.53
1:B:393:THR:HG23	1:B:517:LEU:HB2	1.91	0.53
1:C:412:PRO:HG3	1:C:429:PHE:HE1	1.74	0.53
1:C:905:ARG:HD3	1:C:1049:LEU:HB3	1.90	0.53
1:C:984:LEU:HD12	1:C:988:GLU:HG3	1.91	0.53
1:C:979:ASP:O	1:C:983:ARG:HG2	2.09	0.53
3:N:66:GLY:HA3	3:N:71:PHE:HA	1.91	0.53
1:B:66:HIS:HB3	1:B:68:ILE:HG22	1.90	0.52
2:M:4:LEU:HD22	2:M:92:CYS:HB3	1.92	0.52
2:M:90:TYR:H	2:M:107:THR:HG22	1.75	0.52
1:B:330:PRO:HA	1:B:579:PRO:HB2	1.90	0.52
1:B:722:VAL:HG12	1:B:930:ALA:HB1	1.90	0.52
1:C:402:ILE:HA	1:C:495:TYR:HE1	1.74	0.52
1:A:644:GLN:NE2	1:A:645:THR:O	2.43	0.52
1:B:273:ARG:HD2	1:B:292:ALA:HB3	1.91	0.52
1:C:1032:CYS:SG	1:C:1051:SER:OG	2.68	0.52
1:C:801:ASN:ND2	1:C:928:ASN:OD1	2.42	0.52
3:L:21:LEU:N	3:L:73:LEU:O	2.41	0.52
1:A:319:ARG:NH1	1:A:590:CYS:SG	2.83	0.52
1:C:879:ALA:HA	1:C:882:ILE:HG22	1.91	0.52
1:B:444:LYS:HZ2	1:B:448:ASN:HA	1.75	0.52
1:B:770:ILE:HD11	1:B:1012:LEU:HG	1.92	0.52
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.75	0.51
2:M:37:VAL:HB	2:M:45:LEU:HD21	1.93	0.51
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.92	0.51
1:B:501:ASN:HB3	1:B:505:TYR:HB2	1.91	0.51
1:A:751:ASN:HA	1:A:754:LEU:HG	1.92	0.51
1:B:917:TYR:HD2	1:C:1089:PHE:HE2	1.59	0.51
1:C:744:GLY:H	1:C:977:LEU:HD23	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47:TRP:NE1	2:M:49:GLY:O	2.43	0.51
1:A:302:THR:HG21	1:A:315:THR:HA	1.92	0.51
1:B:90:VAL:H	1:B:195:LYS:NZ	2.07	0.51
1:B:329:PHE:O	1:B:580:GLN:NE2	2.44	0.51
3:N:47:LEU:HA	3:N:58:ILE:HG12	1.93	0.51
3:L:2:ILE:HD11	3:L:25:ALA:HB1	1.93	0.51
1:B:314:GLN:OE1	1:B:613:GLN:NE2	2.42	0.51
1:A:736:VAL:O	1:A:764:ASN:ND2	2.44	0.50
1:C:816:SER:HB2	1:C:819:GLU:OE1	2.10	0.50
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.44	0.50
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.30	0.50
1:B:490:PHE:O	1:B:493:GLN:NE2	2.44	0.50
1:B:194:PHE:HD2	1:B:203:ILE:HD12	1.77	0.50
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.93	0.50
3:N:11:LEU:HG	3:N:13:LEU:HG	1.93	0.50
3:N:38:GLN:HA	3:N:44:PRO:HA	1.94	0.50
1:A:402:ILE:HB	1:A:406:GLU:HB2	1.92	0.50
1:A:791:THR:HG21	1:A:806:LEU:HD21	1.94	0.50
1:A:763:LEU:HD22	1:A:1008:VAL:HG11	1.92	0.49
1:B:741:TYR:OH	1:B:962:LEU:O	2.30	0.49
1:C:422:ASN:HD21	1:C:454:ARG:N	2.09	0.49
1:C:422:ASN:HD21	1:C:454:ARG:H	1.60	0.49
3:N:29:GLY:HA3	3:N:32:TYR:HD1	1.75	0.49
1:C:763:LEU:HD12	1:C:1008:VAL:HG11	1.94	0.49
1:A:1105:THR:HG23	1:A:1111:GLU:H	1.77	0.49
1:B:909:ILE:HG21	1:B:1047:TYR:HB3	1.94	0.49
1:A:659:SER:HB2	1:A:698:SER:HB2	1.94	0.49
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.94	0.49
1:A:769:GLY:O	1:A:773:GLU:HB2	2.11	0.49
1:A:778:THR:HA	1:A:781:VAL:HG12	1.94	0.49
1:A:917:TYR:HD2	1:B:1089:PHE:HE2	1.60	0.49
1:C:616:ASN:OD1	1:C:617:CYS:N	2.45	0.49
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.47	0.49
1:B:68:ILE:HG13	1:B:69:HIS:H	1.78	0.49
1:B:403:ARG:HH22	1:B:496:GLY:H	1.58	0.49
1:C:986:PRO:HA	1:C:989:ALA:HB3	1.94	0.49
3:N:54:ARG:NH1	3:N:60:ASP:OD1	2.46	0.49
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.94	0.49
1:C:818:ILE:O	1:C:822:LEU:HD12	2.12	0.49
1:C:1139:ASP:O	1:C:1143:PRO:HD2	2.13	0.48
1:A:1091:ARG:NH2	1:A:1118:ASP:O	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLY:C	1:A:487:ASN:H	2.16	0.48
1:C:1031:GLU:HG3	1:C:1037:SER:HB2	1.96	0.48
3:L:61:ARG:NH1	3:L:62:PHE:HD2	2.12	0.48
2:M:59:ASN:ND2	2:M:63:PHE:O	2.46	0.48
1:B:407:VAL:HG21	1:B:508:TYR:HB2	1.95	0.48
1:B:42:VAL:O	1:C:563:GLN:NE2	2.46	0.48
1:B:662:CYS:HB2	1:B:697:MET:SD	2.53	0.48
1:B:744:GLY:H	1:B:977:LEU:HD23	1.79	0.48
2:H:100(D):TYR:HB3	2:H:100(E):TYR:HD1	1.78	0.48
1:C:424:LYS:NZ	1:C:461:LEU:HB3	2.27	0.48
1:A:902:MET:HB3	1:A:916:LEU:HD11	1.96	0.48
1:B:41:LYS:HE2	1:C:562:PHE:HB2	1.95	0.48
1:A:731:MET:HG2	1:A:774:GLN:HE21	1.79	0.48
1:A:666:ILE:HD13	1:A:670:ILE:HG22	1.96	0.47
3:N:42:GLN:HG3	3:N:43:ALA:H	1.78	0.47
1:A:513:LEU:HD22	1:A:515:PHE:CE2	2.50	0.47
1:B:52:GLN:NE2	1:B:273:ARG:O	2.47	0.47
1:C:437:ASN:OD1	1:C:438:SER:N	2.48	0.47
1:A:328:ARG:HA	1:A:530:SER:HB2	1.95	0.47
1:B:44:ARG:HB3	1:B:47:VAL:HB	1.96	0.47
1:B:46:SER:HB3	1:B:281:GLU:HG3	1.95	0.47
2:H:1:GLN:OE1	2:H:2:VAL:N	2.47	0.47
1:C:494:SER:HB2	2:H:98:TYR:OH	2.15	0.47
1:C:532:ASN:OD1	1:C:533:LEU:N	2.47	0.47
1:A:566:GLY:HA3	1:A:575:ALA:HB3	1.95	0.47
1:C:402:ILE:HA	1:C:495:TYR:CE1	2.49	0.47
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.40	0.47
1:A:993:ILE:O	1:A:997:ILE:HG12	2.15	0.47
1:C:976:VAL:O	1:C:980:ILE:HD12	2.15	0.47
1:B:1125:ASN:OD1	1:B:1126:CYS:N	2.47	0.47
1:C:130:VAL:HG21	1:C:231:ILE:HG22	1.96	0.47
1:C:963:VAL:HA	1:C:966:LEU:HD23	1.95	0.47
1:B:763:LEU:HD11	1:B:1004:LEU:HB3	1.96	0.47
1:B:873:TYR:HE1	1:C:699:LEU:HB3	1.79	0.47
1:C:993:ILE:O	1:C:997:ILE:HG12	2.15	0.47
2:H:93:ALA:HA	2:H:103:TRP:CD1	2.50	0.47
2:M:38:ARG:HB3	2:M:48:MET:HE3	1.96	0.47
1:B:1009:THR:O	1:B:1013:ILE:HG12	2.15	0.47
1:B:168:PHE:HE2	1:B:229:LEU:HD22	1.80	0.46
1:B:347:PHE:HE2	1:B:509:ARG:HD3	1.80	0.46
1:B:751:ASN:HA	1:B:754:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLY:HA3	1:C:241:LEU:HD12	1.97	0.46
1:C:200:TYR:CE1	1:C:230:PRO:HG3	2.50	0.46
1:A:1081:ILE:HG23	1:A:1135:ASN:HB3	1.97	0.46
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.51	0.46
3:N:35:TRP:CZ2	3:N:88:CYS:HB3	2.50	0.46
1:C:403:ARG:NH1	1:C:405:ASP:HB2	2.30	0.46
2:M:83:ARG:HD3	2:M:86:ASP:HB2	1.97	0.46
1:A:555:SER:HB2	1:A:557:LYS:HG2	1.97	0.46
1:A:715:PRO:HD3	1:C:894:LEU:HD13	1.98	0.46
1:C:449:TYR:CE1	2:H:31:SER:HB2	2.50	0.46
3:L:35:TRP:CE2	3:L:88:CYS:HB3	2.50	0.46
1:A:444:LYS:HG3	1:A:448:ASN:HB2	1.97	0.46
1:C:37:TYR:OH	1:C:54:LEU:O	2.25	0.46
1:C:1050:MET:HE3	1:C:1052:PHE:HE1	1.80	0.46
2:M:51:ILE:HD13	2:M:71:ALA:HB2	1.97	0.46
1:A:969:ASN:OD1	1:A:972:ALA:N	2.36	0.46
1:B:327:VAL:HA	1:B:542:ASN:HB3	1.98	0.46
1:B:721:SER:O	1:B:1066:THR:OG1	2.32	0.46
1:C:358:ILE:HB	1:C:395:VAL:HB	1.98	0.46
1:C:125:ASN:HD21	1:C:171:VAL:HG13	1.81	0.46
3:L:5:THR:O	3:L:24:ARG:N	2.46	0.46
1:A:230:PRO:HB3	1:B:521:PRO:HD2	1.98	0.46
1:B:1142:GLN:NE2	1:B:1146:ASP:OD1	2.49	0.46
1:C:59:PHE:HD2	1:C:293:LEU:HD21	1.81	0.46
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	1.97	0.46
3:N:15:PRO:HA	3:N:78:LEU:HB3	1.97	0.46
1:C:303:LEU:HD21	1:C:313:TYR:CD1	2.51	0.45
1:A:42:VAL:O	1:B:563:GLN:NE2	2.50	0.45
1:A:966:LEU:HD12	1:A:966:LEU:HA	1.85	0.45
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.30	0.45
1:B:29:THR:HG22	1:B:64:TRP:HB2	1.98	0.45
1:C:738:CYS:SG	1:C:753:LEU:HD21	2.57	0.45
1:A:1029:MET:HE2	1:A:1033:VAL:HG21	1.99	0.45
1:C:478:THR:OG1	1:C:479:PRO:HD3	2.17	0.45
1:A:421:TYR:CE1	1:A:459:SER:HA	2.51	0.45
1:A:737:ASP:OD1	1:A:738:CYS:N	2.49	0.45
2:H:66:ARG:HD2	2:H:83:ARG:HH12	1.81	0.45
3:N:36:TYR:HE1	3:N:46:LEU:HD13	1.82	0.45
1:A:452:LEU:HA	1:A:494:SER:HA	1.97	0.45
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.98	0.45
1:A:963:VAL:HG11	1:B:570:ALA:HB1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:VAL:HG22	1:C:515:PHE:HD1	1.82	0.45
1:C:756:TYR:OH	1:C:994:ASP:OD2	2.28	0.45
3:L:24:ARG:HG2	3:L:70:ASP:HA	1.98	0.45
1:A:894:LEU:HD13	1:B:715:PRO:HD3	1.98	0.45
1:B:277:LEU:HD23	1:B:285:ILE:HD13	1.98	0.45
1:C:731:MET:HB3	1:C:1018:ILE:HD13	1.98	0.45
1:C:1016:ALA:HA	1:C:1019:ARG:HG2	1.98	0.45
1:A:83:VAL:HB	1:A:237:ARG:HD2	1.99	0.45
1:A:406:GLU:O	1:A:410:ILE:HG22	2.17	0.45
1:B:53:ASP:OD1	1:B:54:LEU:N	2.48	0.45
1:C:424:LYS:HB3	1:C:424:LYS:HE3	1.71	0.45
1:B:486:PHE:HA	1:B:489:TYR:HE2	1.82	0.45
1:C:751:ASN:HA	1:C:754:LEU:HG	1.99	0.45
3:L:23:CYS:HB2	3:L:35:TRP:CZ2	2.52	0.44
1:B:737:ASP:HB3	1:B:740:MET:HB2	1.98	0.44
3:L:33:LEU:HD12	3:L:89:GLN:O	2.18	0.44
1:A:611:LEU:HD22	1:A:666:ILE:HG23	2.00	0.44
1:A:813:SER:O	1:A:815:ARG:N	2.50	0.44
1:C:365:TYR:HB2	1:C:388:ASN:HB3	1.99	0.44
1:C:425:LEU:HD23	1:C:429:PHE:CE1	2.52	0.44
2:H:62:LYS:HE2	2:H:63:PHE:CE2	2.53	0.44
3:N:28:VAL:HG13	3:N:92:ALA:HB2	2.00	0.44
1:A:906:PHE:CD2	1:A:916:LEU:HD12	2.53	0.44
1:B:708:SER:HB3	1:B:711:SER:HB3	1.99	0.44
1:B:1030:SER:HA	1:B:1034:LEU:HD12	2.00	0.44
1:A:900:MET:SD	1:A:917:TYR:OH	2.72	0.44
1:B:778:THR:HA	1:B:781:VAL:HG12	1.98	0.44
3:L:32:TYR:C	3:L:91:TYR:HB3	2.38	0.44
1:A:976:VAL:HG12	1:A:979:ASP:H	1.83	0.44
1:B:715:PRO:O	1:B:1110:TYR:N	2.51	0.44
1:A:357:ARG:HE	1:C:230:PRO:HB3	1.82	0.44
1:A:526:GLY:HA3	1:A:528:LYS:HZ3	1.82	0.44
1:B:375:SER:HB2	3:L:67:SER:HB2	1.99	0.44
1:A:409:GLN:NE2	1:A:419:ALA:H	2.15	0.44
1:A:662:CYS:HB2	1:A:697:MET:HG3	2.00	0.44
1:B:28:TYR:CD1	1:B:61:ASN:HB3	2.53	0.43
1:B:726:ILE:HG23	1:B:1061:VAL:HG22	2.00	0.43
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.99	0.43
1:C:420:ASP:O	1:C:424:LYS:NZ	2.39	0.43
1:A:401:VAL:HB	1:A:451:TYR:CE2	2.52	0.43
1:B:127:VAL:HG12	1:B:171:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ARG:HD2	1:B:582:LEU:HG	1.99	0.43
1:A:1040:VAL:HG11	1:C:1035:GLY:HA3	2.00	0.43
1:B:441:LEU:HD13	1:B:509:ARG:HH22	1.81	0.43
1:B:1116:THR:HB	1:B:1140:PRO:HG3	2.00	0.43
1:C:334:ASN:HB3	1:C:361:CYS:HA	2.00	0.43
2:H:22:CYS:HB3	2:H:78:ALA:HB3	2.00	0.43
3:L:27(A):SER:HA	3:L:68:GLY:O	2.19	0.43
3:L:28:VAL:O	3:L:32:TYR:HB2	2.18	0.43
1:A:869:MET:HE3	1:B:697:MET:HG2	2.00	0.43
1:C:1116:THR:HA	1:C:1138:TYR:O	2.18	0.43
1:B:566:GLY:HA3	1:B:575:ALA:HB3	2.00	0.43
1:C:877:LEU:O	1:C:881:THR:HG23	2.18	0.43
2:H:4:LEU:HA	2:H:23:LYS:HB3	2.00	0.43
3:N:55:ALA:HB3	3:N:58:ILE:HD13	2.01	0.43
1:A:43:PHE:HB3	1:B:566:GLY:HA2	2.01	0.43
1:B:231:ILE:HG22	1:B:233:ILE:HG13	2.00	0.43
1:A:200:TYR:CE2	1:B:521:PRO:HD3	2.52	0.43
1:A:792:PRO:HG3	1:B:707:TYR:HB3	1.99	0.43
1:A:890:ALA:HA	1:B:1046:GLY:HA2	2.01	0.43
1:B:657:ASN:HB3	7:B:1307:NAG:HN2	1.83	0.43
1:B:976:VAL:HG12	1:B:979:ASP:H	1.83	0.43
1:A:287:ASP:OD1	1:A:288:ALA:N	2.52	0.43
2:M:66:ARG:NH2	2:M:82:LEU:HD11	2.34	0.43
1:A:996:LEU:HG	1:A:1000:ARG:HD2	2.00	0.43
1:B:661:GLU:O	1:B:695:TYR:OH	2.33	0.43
1:B:985:ASP:HB3	1:B:987:PRO:HD2	2.01	0.43
1:C:734:THR:HG22	1:C:860:VAL:HG22	2.00	0.43
1:A:167:THR:OG1	1:A:168:PHE:N	2.50	0.43
1:B:802:PHE:HB3	1:B:806:LEU:HD23	1.99	0.43
1:C:778:THR:HA	1:C:781:VAL:HG12	2.00	0.43
1:A:383:SER:HB2	1:A:386:LYS:HB2	2.01	0.42
1:B:422:ASN:ND2	1:B:453:TYR:O	2.52	0.42
1:B:645:THR:HG23	1:B:648:GLY:H	1.84	0.42
1:B:963:VAL:HA	1:B:966:LEU:HD23	2.01	0.42
1:B:224:GLU:HB3	1:C:562:PHE:CE1	2.54	0.42
1:C:1106:GLN:NE2	1:C:1108:ASN:H	2.17	0.42
2:H:94:ARG:HG2	2:H:95:GLY:H	1.82	0.42
2:M:48:MET:HG3	2:M:63:PHE:CD2	2.54	0.42
1:B:369:TYR:HD1	1:B:377:PHE:CD2	2.37	0.42
1:B:645:THR:OG1	1:B:646:ARG:N	2.52	0.42
1:A:1080:ALA:O	1:A:1132:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:ARG:NH1	3:L:65:SER:HB3	2.34	0.42
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.55	0.42
3:L:93:GLY:O	3:L:94:SER:HB2	2.19	0.42
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.33	0.42
1:A:1106:GLN:H	1:A:1106:GLN:HG3	1.56	0.42
1:B:712:ILE:HG22	1:B:1077:THR:HB	2.00	0.42
1:B:896:ILE:HG22	1:C:712:ILE:HD12	2.01	0.42
1:C:53:ASP:OD1	1:C:54:LEU:N	2.50	0.42
1:C:127:VAL:HG13	1:C:171:VAL:HG22	2.00	0.42
1:A:418:ILE:O	1:A:422:ASN:HB2	2.19	0.42
1:A:1133:VAL:HA	7:A:1310:NAG:H82	2.01	0.42
1:B:86:PHE:HE1	1:B:90:VAL:HG22	1.85	0.42
1:B:293:LEU:HD23	1:B:294:ASP:HB3	2.01	0.42
2:H:15:GLY:N	2:H:82(C):LEU:O	2.52	0.42
1:A:1030:SER:HB2	1:B:1041:ASP:HB3	2.00	0.42
1:B:347:PHE:CE2	1:B:509:ARG:HD3	2.53	0.42
1:B:378:LYS:HZ2	1:B:412:PRO:HG3	1.84	0.42
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	2.02	0.42
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	2.02	0.42
1:B:1116:THR:O	1:B:1120:THR:HG22	2.20	0.42
1:C:483:VAL:HG22	2:H:50:ARG:HD3	2.02	0.42
1:C:1080:ALA:O	1:C:1132:ILE:HG13	2.19	0.42
2:H:16:SER:OG	2:H:17:SER:N	2.52	0.42
1:A:349:SER:HA	1:A:451:TYR:CE2	2.54	0.42
1:A:422:ASN:ND2	1:A:454:ARG:O	2.38	0.42
1:C:384:PRO:O	1:C:387:LEU:HD22	2.20	0.42
1:C:412:PRO:HG3	1:C:429:PHE:CE1	2.55	0.42
1:C:129:LYS:HE2	1:C:129:LYS:HB2	1.80	0.42
1:C:441:LEU:O	1:C:444:LYS:NZ	2.53	0.42
1:A:37:TYR:OH	1:A:53:ASP:OD2	2.38	0.42
1:A:770:ILE:HD11	1:A:1012:LEU:HD12	2.02	0.42
1:B:976:VAL:O	1:B:980:ILE:HG12	2.20	0.42
1:C:546:LEU:HD11	1:C:573:THR:HG21	2.00	0.42
3:N:48:ILE:HD12	3:N:54:ARG:HA	2.02	0.42
1:A:730:SER:O	1:A:1058:HIS:HB3	2.19	0.41
1:B:398:ASP:HB2	1:B:512:VAL:HB	2.02	0.41
2:M:16:SER:OG	2:M:17:SER:N	2.53	0.41
1:A:1014:ARG:O	1:A:1017:GLU:HG2	2.20	0.41
1:B:128:ILE:HD13	1:B:170:TYR:HD2	1.84	0.41
1:B:378:LYS:NZ	7:B:1304:NAG:O6	2.53	0.41
1:A:389:ASP:OD1	1:A:390:LEU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:GLN:OE1	1:C:765:ARG:NH1	2.53	0.41
1:B:369:TYR:HD1	1:B:377:PHE:HD2	1.69	0.41
1:C:30:ASN:HB2	1:C:32:PHE:CE1	2.56	0.41
1:C:57:PRO:HB3	1:C:273:ARG:HH12	1.84	0.41
1:A:341:VAL:HG13	1:A:342:PHE:CD1	2.55	0.41
1:A:895:GLN:HE21	1:A:895:GLN:HB2	1.60	0.41
1:B:462:LYS:HE2	1:B:462:LYS:HB2	1.69	0.41
1:C:97:LYS:HE3	1:C:186:PHE:HD1	1.84	0.41
1:C:433:VAL:HG13	1:C:512:VAL:HG12	2.01	0.41
1:C:473:TYR:HD2	1:C:488:CYS:HB2	1.85	0.41
3:N:24:ARG:HG3	3:N:70:ASP:HA	2.02	0.41
1:A:52:GLN:OE1	1:A:274:THR:OG1	2.37	0.41
1:A:435:ALA:HA	1:A:510:VAL:HA	2.03	0.41
1:B:295:PRO:HB2	1:B:608:VAL:HG21	2.01	0.41
1:B:1029:MET:HA	1:B:1033:VAL:HG13	2.02	0.41
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.61	0.41
1:A:386:LYS:HE2	1:C:985:ASP:HB3	2.03	0.41
1:C:128:ILE:HG21	1:C:229:LEU:HD21	2.03	0.41
1:C:287:ASP:OD1	1:C:288:ALA:N	2.54	0.41
1:C:299:THR:HA	1:C:302:THR:HG22	2.01	0.41
2:H:59:ASN:HD21	2:H:67:LEU:HB2	1.86	0.41
1:A:133:PHE:HE2	1:A:135:PHE:HD1	1.69	0.41
1:B:712:ILE:CG2	1:B:1077:THR:HB	2.50	0.41
1:B:901:GLN:O	1:B:905:ARG:HG2	2.21	0.41
1:C:40:ASP:OD1	1:C:41:LYS:N	2.52	0.41
1:C:581:THR:O	1:C:583:GLU:N	2.54	0.41
1:C:720:ILE:HD12	1:C:923:ILE:HB	2.03	0.41
2:H:1:GLN:CD	2:H:2:VAL:H	2.25	0.41
2:H:59:ASN:HD21	2:H:67:LEU:H	1.69	0.41
3:L:18:ARG:HH22	3:L:20:THR:HG22	1.86	0.41
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG21	2.56	0.41
1:A:1125:ASN:OD1	1:A:1125:ASN:N	2.54	0.41
1:A:1129:VAL:HG23	1:C:917:TYR:HB3	2.03	0.41
1:B:418:ILE:CD1	1:B:453:TYR:HB2	2.51	0.41
1:C:455:LEU:N	1:C:491:PRO:HB2	2.31	0.41
1:C:763:LEU:HD11	1:C:1008:VAL:HG21	2.04	0.41
1:A:396:TYR:O	1:A:514:SER:N	2.36	0.40
1:A:503:VAL:HA	1:A:506:GLN:HB2	2.03	0.40
1:A:895:GLN:HE22	1:B:711:SER:HB3	1.86	0.40
1:B:100:ILE:HG23	1:B:243:ALA:HB3	2.03	0.40
1:B:318:PHE:N	1:B:593:GLY:O	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:LEU:HA	1:B:1027:THR:HG22	2.03	0.40
1:A:439:ASN:HD21	1:A:506:GLN:HG3	1.86	0.40
1:A:560:LEU:N	1:A:563:GLN:OE1	2.50	0.40
1:C:555:SER:OG	1:C:584:ILE:O	2.37	0.40
1:C:1091:ARG:N	1:C:1119:ASN:O	2.50	0.40
1:A:216:LEU:HA	1:A:217:PRO:HD3	1.92	0.40
1:C:290:ASP:O	1:C:297:SER:HB3	2.22	0.40
1:C:319:ARG:HE	1:C:319:ARG:HB2	1.55	0.40
1:A:699:LEU:HD12	1:C:873:TYR:CE1	2.56	0.40
1:A:1005:GLN:HE22	1:B:1006:THR:HG23	1.86	0.40
3:L:59:PRO:HB2	3:L:61:ARG:CD	2.52	0.40
1:A:616:ASN:OD1	7:A:1306:NAG:N2	2.55	0.40
1:B:894:LEU:HD12	1:C:713:ALA:O	2.22	0.40
1:C:436:TRP:HZ3	1:C:511:VAL:HG12	1.87	0.40
1:C:441:LEU:HB3	1:C:509:ARG:HH21	1.86	0.40
1:C:483:VAL:HG13	2:H:100(D):TYR:OH	2.20	0.40
1:C:738:CYS:HB2	1:C:760:CYS:HB2	1.83	0.40
3:L:37:GLN:O	3:L:45:ARG:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	984/1259 (78%)	929 (94%)	51 (5%)	4 (0%)	30 66
1	B	981/1259 (78%)	915 (93%)	66 (7%)	0	100 100
1	C	981/1259 (78%)	926 (94%)	55 (6%)	0	100 100
2	H	115/229 (50%)	107 (93%)	7 (6%)	1 (1%)	14 49
2	M	115/229 (50%)	111 (96%)	4 (4%)	0	100 100
3	L	104/215 (48%)	94 (90%)	8 (8%)	2 (2%)	6 35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	N	104/215 (48%)	94 (90%)	9 (9%)	1 (1%)	13 47
All	All	3384/4665 (72%)	3176 (94%)	200 (6%)	8 (0%)	45 76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	471	GLU
1	A	477	SER
1	A	605	SER
2	H	101	ASP
3	L	92	ALA
1	A	454	ARG
3	L	94	SER
3	N	94	SER

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	872/1096 (80%)	865 (99%)	7 (1%)	79 84
1	B	867/1096 (79%)	865 (100%)	2 (0%)	92 93
1	C	871/1096 (80%)	862 (99%)	9 (1%)	73 81
2	H	93/191 (49%)	90 (97%)	3 (3%)	34 55
2	M	93/191 (49%)	92 (99%)	1 (1%)	70 80
3	L	85/183 (46%)	83 (98%)	2 (2%)	44 63
3	N	85/183 (46%)	84 (99%)	1 (1%)	67 78
All	All	2966/4036 (74%)	2941 (99%)	25 (1%)	77 84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	120	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	444	LYS
1	A	602	THR
1	A	604	THR
1	A	895	GLN
1	A	907	ASN
1	B	450	ASN
1	B	641	ASN
1	C	78	ARG
1	C	408	ARG
1	C	452	LEU
1	C	495	TYR
1	C	529	LYS
1	C	656	VAL
1	C	699	LEU
1	C	907	ASN
1	C	957	GLN
2	H	3	GLN
2	H	100(D)	TYR
2	H	100(F)	LEU
3	L	27	GLN
3	L	61	ARG
2	M	83	ARG
3	N	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
1	A	394	ASN
1	A	409	GLN
1	A	439	ASN
1	A	460	ASN
1	A	474	GLN
1	A	487	ASN
1	A	506	GLN
1	A	774	GLN
1	A	801	ASN
1	A	895	GLN
1	A	928	ASN
1	B	764	ASN
1	C	487	ASN
1	C	498	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	6	GLN
3	L	27	GLN
3	N	42	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.74	1 (5%)
5	NAG	E	1	5,1	14,14,15	0.63	0	17,19,21	0.52	0
5	NAG	E	2	5	14,14,15	0.99	2 (14%)	17,19,21	1.16	1 (5%)
5	BMA	E	3	5	11,11,12	0.65	0	15,15,17	0.76	0
5	MAN	E	4	5	11,11,12	1.29	2 (18%)	15,15,17	1.28	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	F	2	4	14,14,15	0.26	0	17,19,21	0.64	0
6	NAG	G	1	6,1	14,14,15	0.52	0	17,19,21	0.71	0
6	NAG	G	2	6	14,14,15	0.72	1 (7%)	17,19,21	0.65	0
6	BMA	G	3	6	11,11,12	0.71	0	15,15,17	0.78	0
4	NAG	I	1	4,1	14,14,15	0.60	0	17,19,21	1.48	3 (17%)
4	NAG	I	2	4	14,14,15	0.53	0	17,19,21	0.44	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	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
6	NAG	G	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	4	MAN	C2-C3	2.85	1.56	1.52
5	E	2	NAG	C1-C2	2.70	1.56	1.52
5	E	4	MAN	C1-C2	2.60	1.58	1.52
6	G	2	NAG	O5-C1	2.31	1.47	1.43
5	E	2	NAG	O5-C1	2.26	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C1-O5-C5	3.78	117.25	112.19
4	I	1	NAG	C1-O5-C5	3.63	117.05	112.19
5	E	4	MAN	C1-C2-C3	3.12	114.19	109.64
4	I	1	NAG	O4-C4-C3	-2.79	103.79	110.38
4	I	1	NAG	C2-N2-C7	2.51	126.27	122.90
4	D	2	NAG	C1-O5-C5	2.34	115.32	112.19
5	E	4	MAN	O2-C2-C3	-2.23	105.53	110.15
4	D	1	NAG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (19) torsion outliers are listed below:

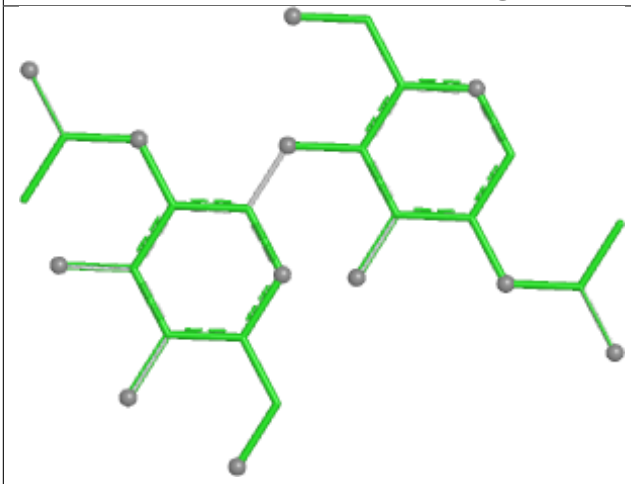
Mol	Chain	Res	Type	Atoms
5	E	4	MAN	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	I	1	NAG	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O7-C7-N2-C2
6	G	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7
6	G	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
4	I	1	NAG	C1-C2-N2-C7
4	F	2	NAG	C8-C7-N2-C2

There are no ring outliers.

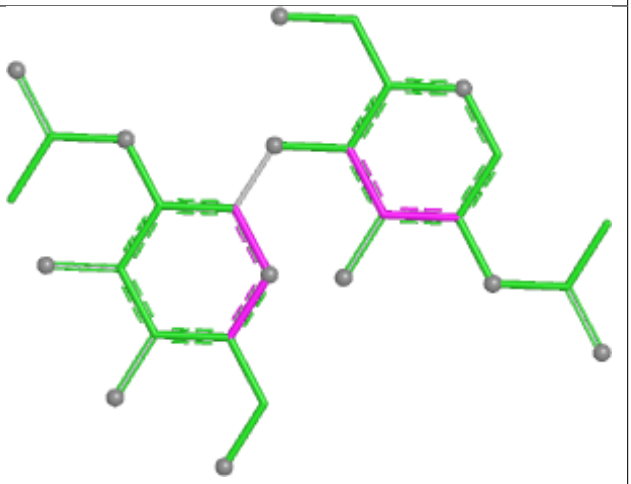
No monomer is involved in short contacts.

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

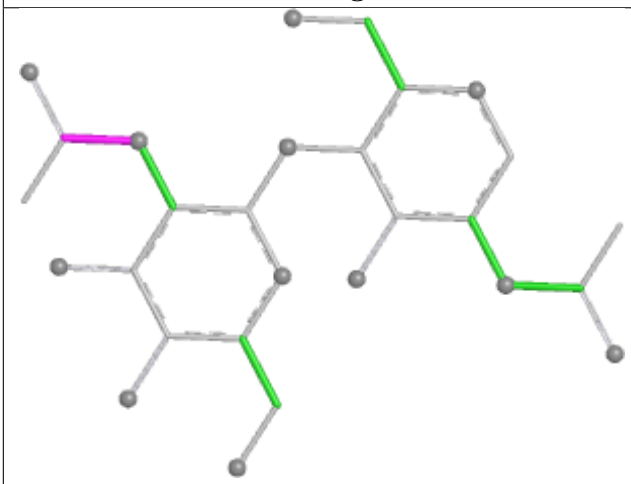
Oligosaccharide Chain D



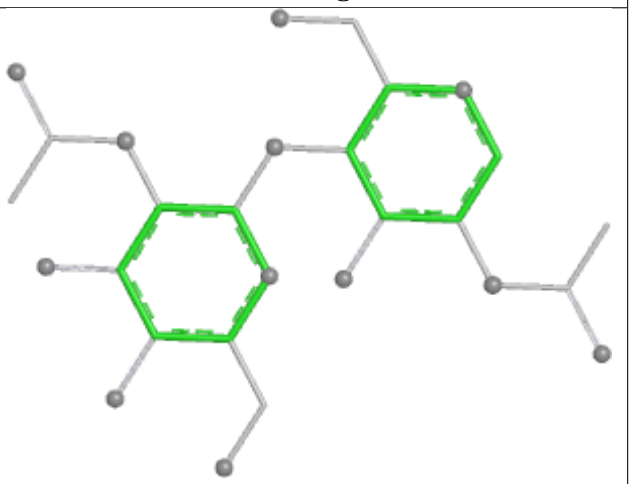
Bond lengths



Bond angles

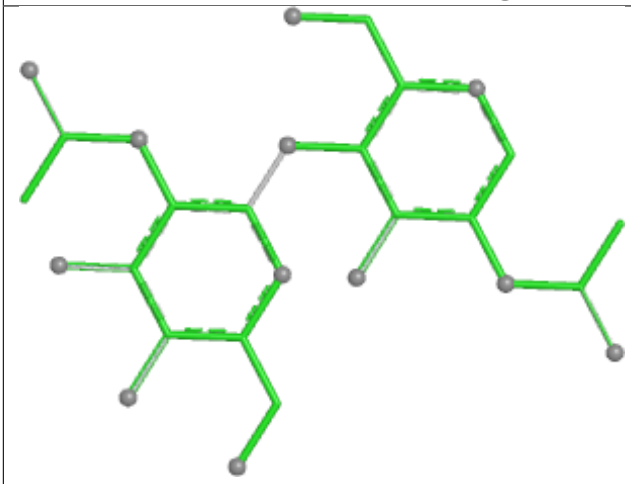


Torsions

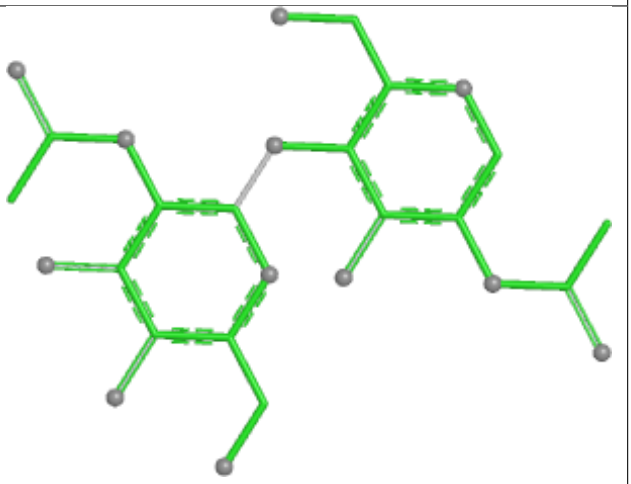


Rings

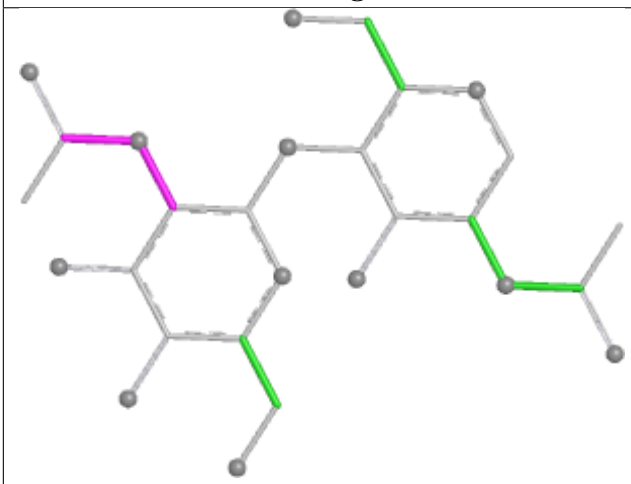
Oligosaccharide Chain F



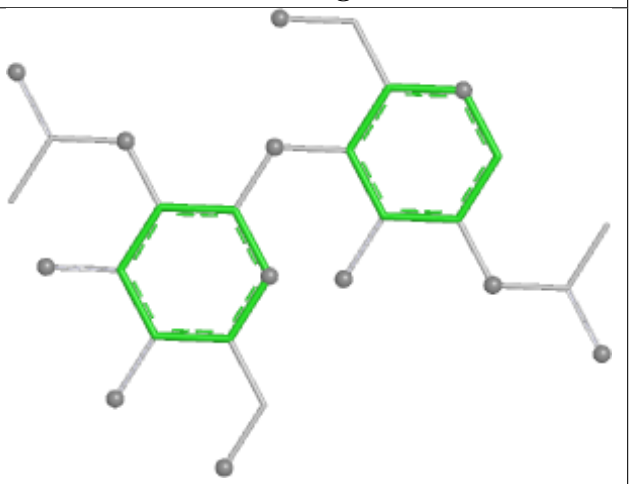
Bond lengths



Bond angles

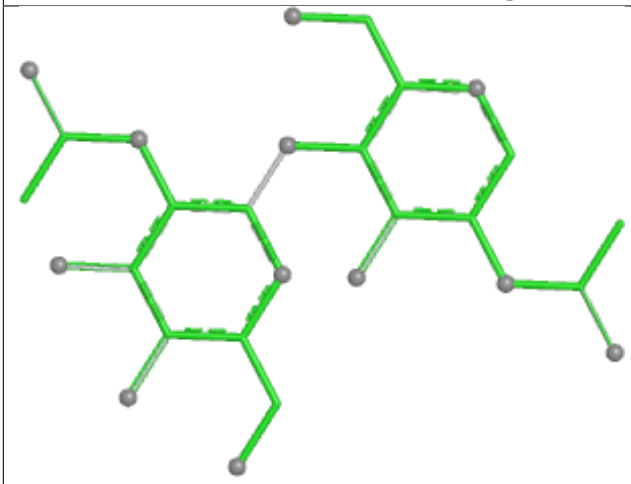


Torsions

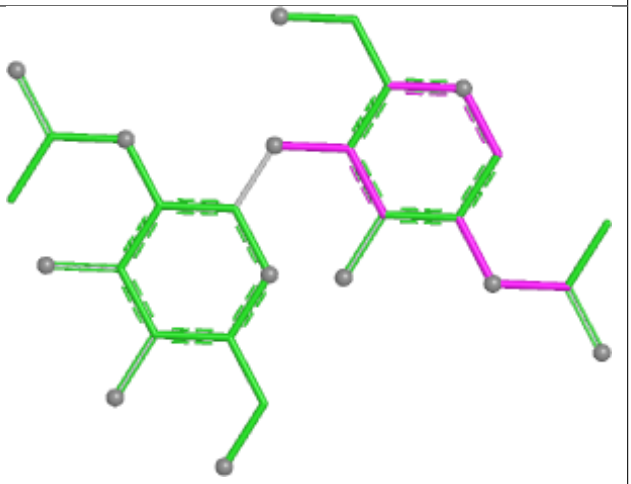


Rings

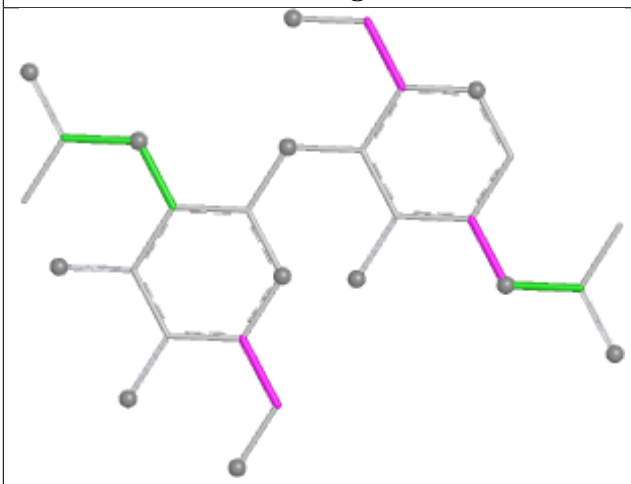
Oligosaccharide Chain I



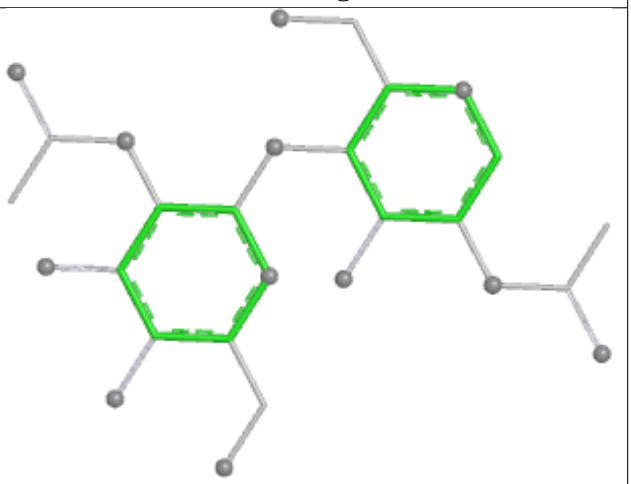
Bond lengths



Bond angles

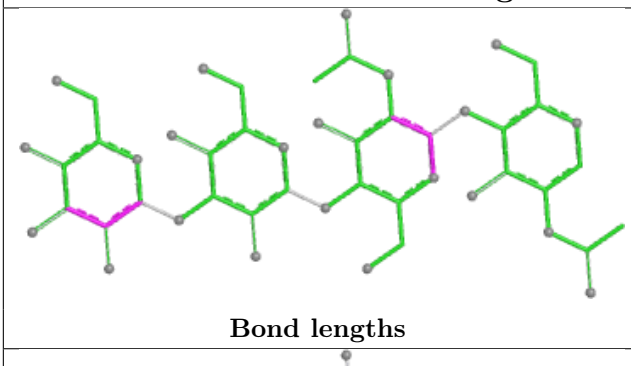


Torsions

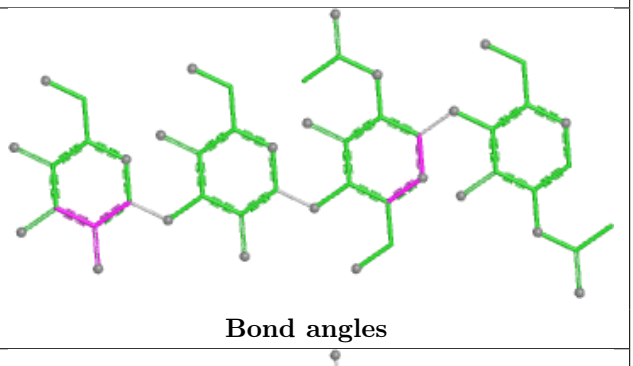


Rings

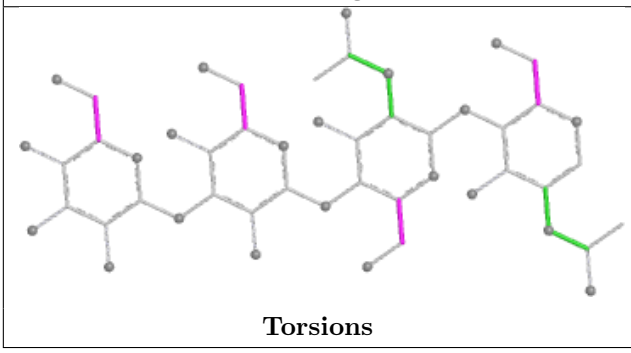
Oligosaccharide Chain E



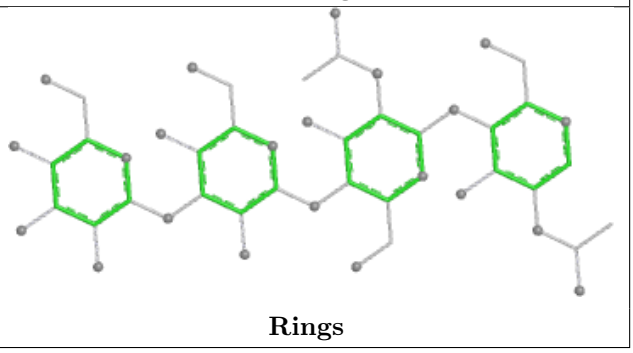
Bond lengths



Bond angles

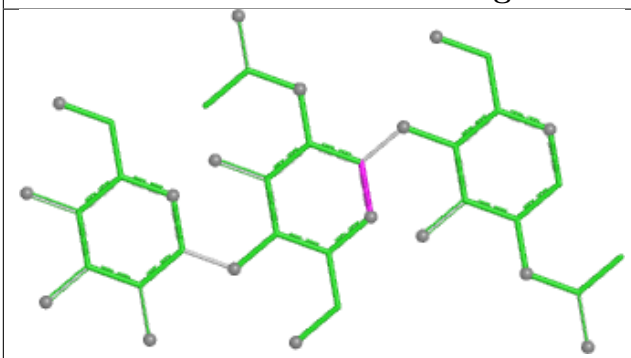


Torsions

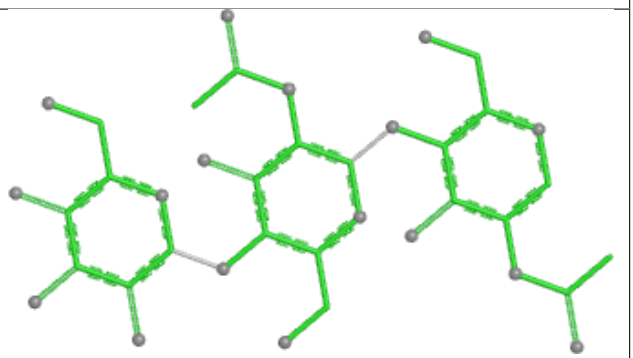


Rings

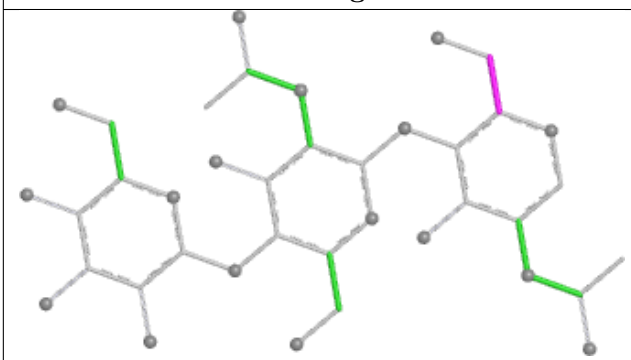
Oligosaccharide Chain G



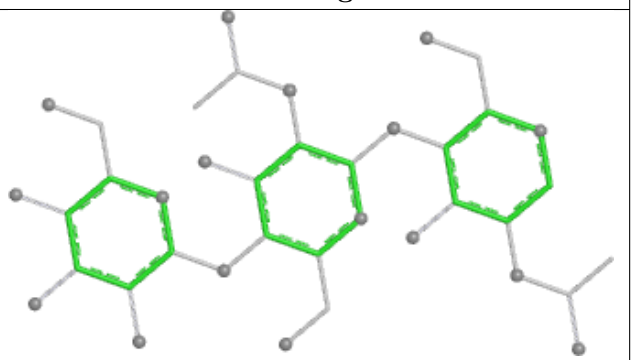
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

26 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	$\#\|Z\| > 2$
7	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.63	0
7	NAG	B	1302	1	14,14,15	0.68	0	17,19,21	2.33	3 (17%)
7	NAG	B	1301	1	14,14,15	0.45	0	17,19,21	0.51	0
7	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.58	0
7	NAG	A	1305	1	14,14,15	0.35	0	17,19,21	0.49	0
7	NAG	A	1301	1	14,14,15	0.42	0	17,19,21	0.68	0
7	NAG	C	1305	1	14,14,15	0.40	0	17,19,21	0.66	1 (5%)
7	NAG	A	1302	1	14,14,15	0.40	0	17,19,21	0.91	1 (5%)
7	NAG	C	1308	1	14,14,15	0.41	0	17,19,21	0.75	0
7	NAG	A	1303	1	14,14,15	0.27	0	17,19,21	0.41	0
7	NAG	A	1307	1	14,14,15	0.70	1 (7%)	17,19,21	0.61	0
7	NAG	C	1306	1	14,14,15	0.40	0	17,19,21	0.45	0
7	NAG	B	1308	1	14,14,15	0.78	1 (7%)	17,19,21	0.78	1 (5%)
7	NAG	A	1309	1	14,14,15	0.48	0	17,19,21	1.08	1 (5%)
7	NAG	B	1303	1	14,14,15	0.43	0	17,19,21	0.60	0
7	NAG	C	1301	1	14,14,15	0.23	0	17,19,21	0.45	0
7	NAG	B	1304	-	14,14,15	0.24	0	17,19,21	0.53	0
7	NAG	B	1307	1	14,14,15	0.54	0	17,19,21	0.47	0
7	NAG	B	1306	1	14,14,15	0.32	0	17,19,21	0.70	0
7	NAG	A	1310	1	14,14,15	1.56	2 (14%)	17,19,21	1.12	1 (5%)
7	NAG	C	1303	1	14,14,15	0.46	0	17,19,21	0.33	0
7	NAG	A	1304	1	14,14,15	0.40	0	17,19,21	0.46	0
7	NAG	A	1306	1	14,14,15	0.75	1 (7%)	17,19,21	0.66	0
7	NAG	C	1302	1	14,14,15	0.54	0	17,19,21	1.13	2 (11%)
7	NAG	C	1304	-	14,14,15	0.26	0	17,19,21	0.50	0
7	NAG	B	1305	1	14,14,15	0.71	0	17,19,21	0.71	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
7	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	6/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
7	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1310	NAG	C1-C2	4.86	1.59	1.52
7	A	1310	NAG	O5-C1	3.05	1.48	1.43
7	B	1308	NAG	C1-C2	2.68	1.56	1.52
7	A	1306	NAG	C1-C2	2.34	1.55	1.52
7	A	1307	NAG	C1-C2	2.24	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1302	NAG	C2-N2-C7	7.91	133.51	122.90
7	B	1302	NAG	C1-C2-N2	3.84	116.49	110.43
7	A	1310	NAG	C1-O5-C5	3.79	117.26	112.19
7	A	1309	NAG	C1-O5-C5	3.68	117.12	112.19
7	C	1302	NAG	C2-N2-C7	2.83	126.70	122.90
7	C	1302	NAG	C1-O5-C5	2.82	115.97	112.19
7	A	1302	NAG	C2-N2-C7	2.55	126.32	122.90
7	B	1308	NAG	C2-N2-C7	2.33	126.03	122.90
7	B	1302	NAG	C4-C3-C2	-2.11	107.92	111.02
7	C	1305	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1307	NAG	C4-C5-C6-O6
7	B	1305	NAG	O5-C5-C6-O6
7	B	1306	NAG	O5-C5-C6-O6
7	C	1302	NAG	O5-C5-C6-O6
7	C	1301	NAG	O5-C5-C6-O6
7	C	1304	NAG	O5-C5-C6-O6
7	C	1302	NAG	C4-C5-C6-O6
7	A	1307	NAG	O5-C5-C6-O6
7	A	1302	NAG	C4-C5-C6-O6
7	A	1309	NAG	C4-C5-C6-O6
7	B	1303	NAG	O5-C5-C6-O6
7	C	1307	NAG	O5-C5-C6-O6
7	B	1301	NAG	O5-C5-C6-O6
7	B	1305	NAG	C4-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6
7	A	1302	NAG	O5-C5-C6-O6
7	B	1306	NAG	C4-C5-C6-O6
7	A	1309	NAG	O5-C5-C6-O6
7	B	1301	NAG	C4-C5-C6-O6
7	C	1301	NAG	C4-C5-C6-O6
7	B	1302	NAG	C4-C5-C6-O6
7	B	1302	NAG	O5-C5-C6-O6
7	A	1307	NAG	C4-C5-C6-O6
7	B	1308	NAG	O5-C5-C6-O6
7	B	1302	NAG	C8-C7-N2-C2
7	B	1302	NAG	O7-C7-N2-C2
7	A	1304	NAG	O5-C5-C6-O6
7	A	1303	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	1304	NAG	C4-C5-C6-O6
7	B	1303	NAG	C4-C5-C6-O6
7	C	1306	NAG	O5-C5-C6-O6
7	A	1305	NAG	O5-C5-C6-O6
7	A	1308	NAG	O5-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6
7	B	1308	NAG	C4-C5-C6-O6
7	B	1307	NAG	O5-C5-C6-O6
7	C	1303	NAG	O5-C5-C6-O6
7	A	1306	NAG	C4-C5-C6-O6
7	B	1308	NAG	C1-C2-N2-C7
7	A	1304	NAG	C4-C5-C6-O6
7	A	1303	NAG	C4-C5-C6-O6
7	A	1306	NAG	O5-C5-C6-O6
7	C	1306	NAG	C4-C5-C6-O6
7	B	1308	NAG	C3-C2-N2-C7
7	C	1302	NAG	C3-C2-N2-C7
7	A	1305	NAG	C4-C5-C6-O6
7	A	1308	NAG	C4-C5-C6-O6
7	A	1302	NAG	C1-C2-N2-C7
7	B	1302	NAG	C1-C2-N2-C7
7	C	1302	NAG	C1-C2-N2-C7
7	C	1308	NAG	C1-C2-N2-C7
7	A	1302	NAG	C3-C2-N2-C7
7	A	1309	NAG	C3-C2-N2-C7
7	B	1302	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1304	NAG	2	0
7	B	1307	NAG	1	0
7	A	1310	NAG	1	0
7	A	1306	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

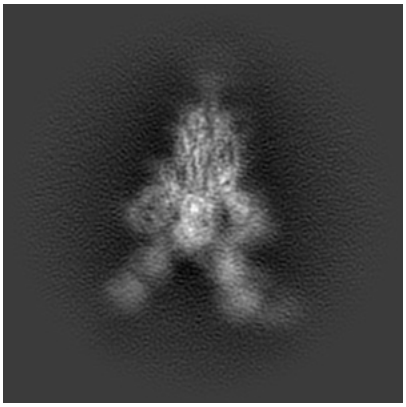
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23697. These allow visual inspection of the internal detail of the map and identification of artifacts.

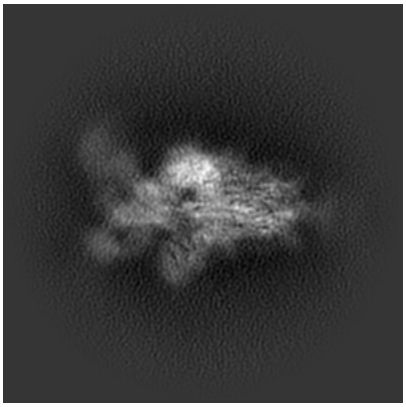
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

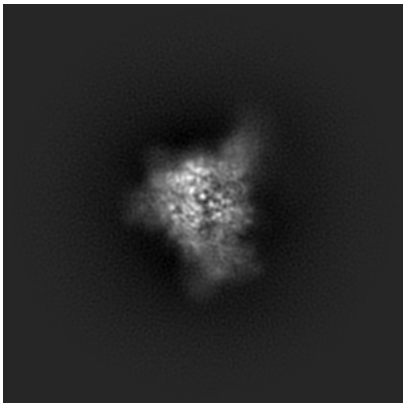
6.1.1 Primary map



X



Y

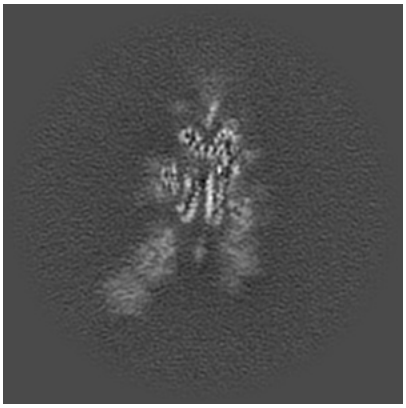


Z

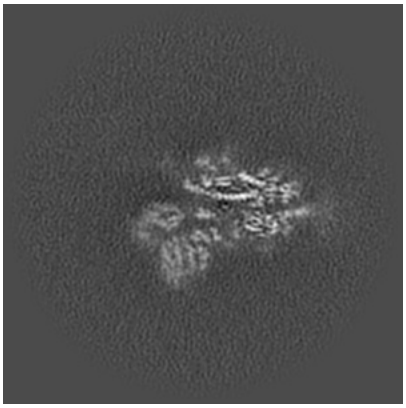
The images above show the map projected in three orthogonal directions.

6.2 Central slices

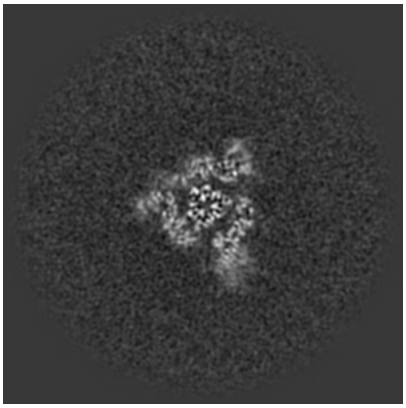
6.2.1 Primary map



X Index: 216



Y Index: 216

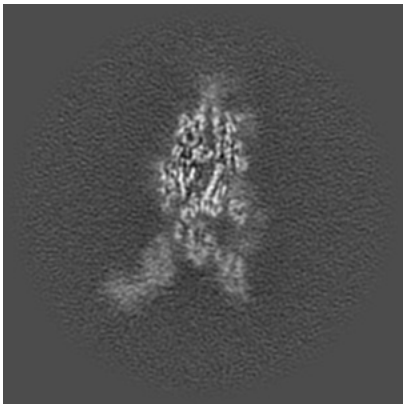


Z Index: 216

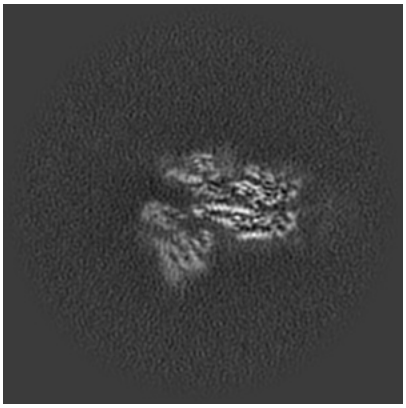
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

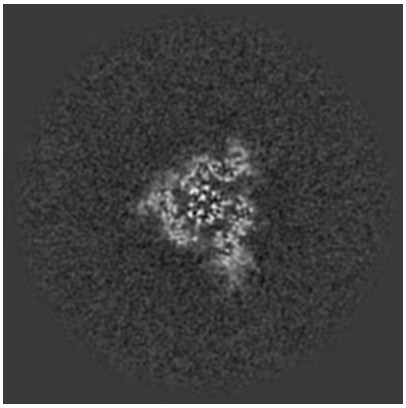
6.3.1 Primary map



X Index: 204



Y Index: 210

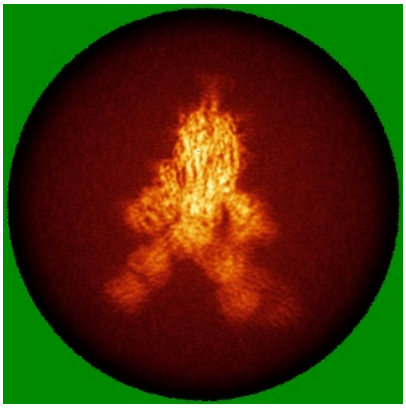


Z Index: 218

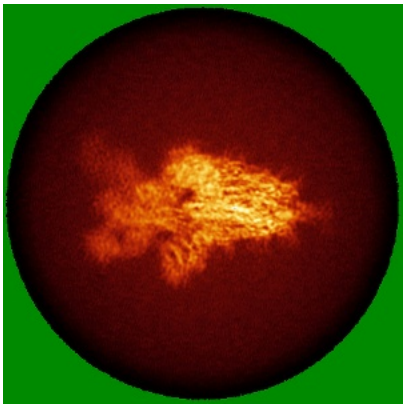
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

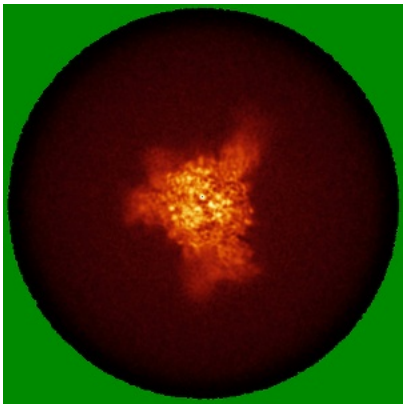
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

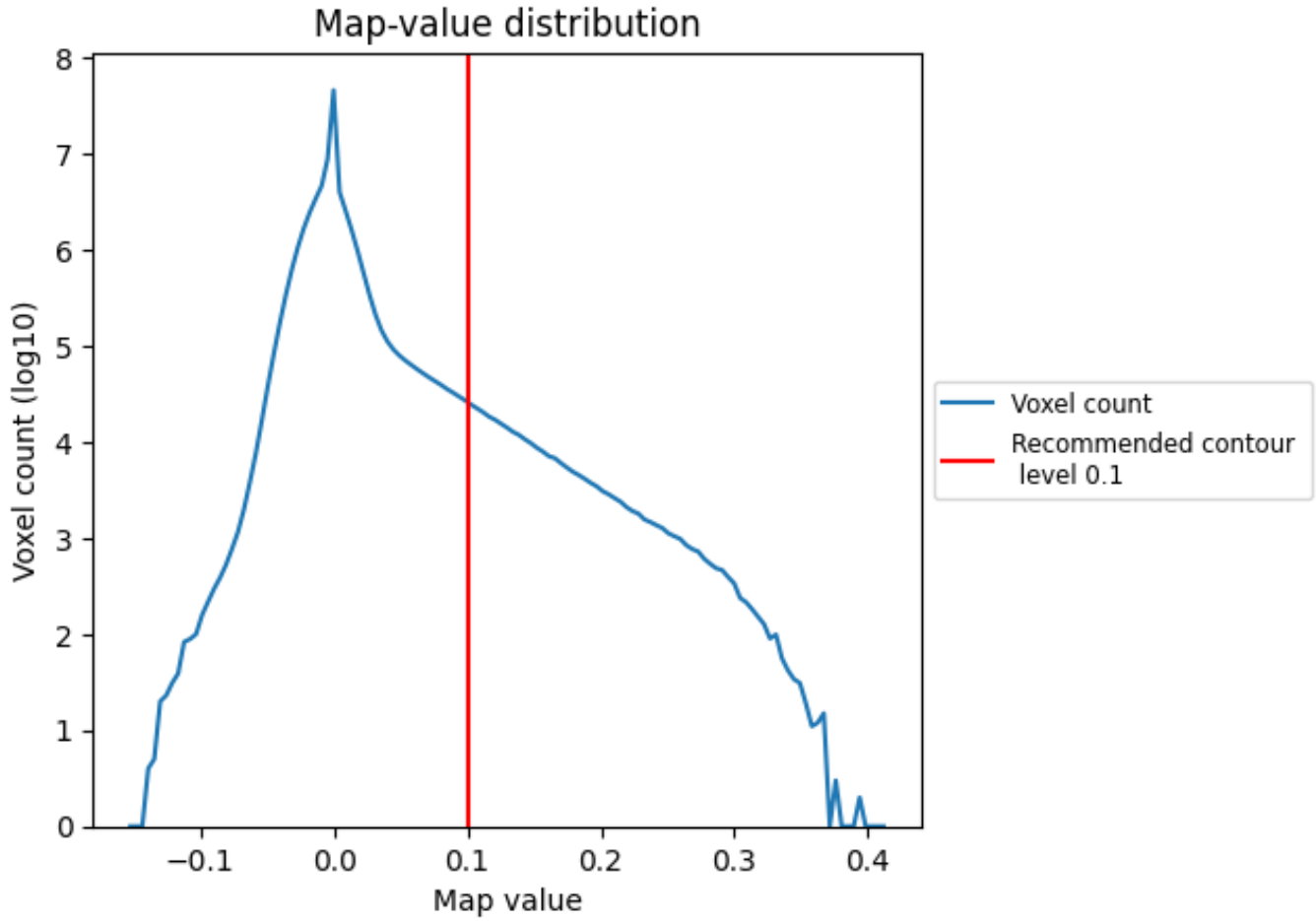
6.6 Mask visualisation (i)

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

7 Map analysis

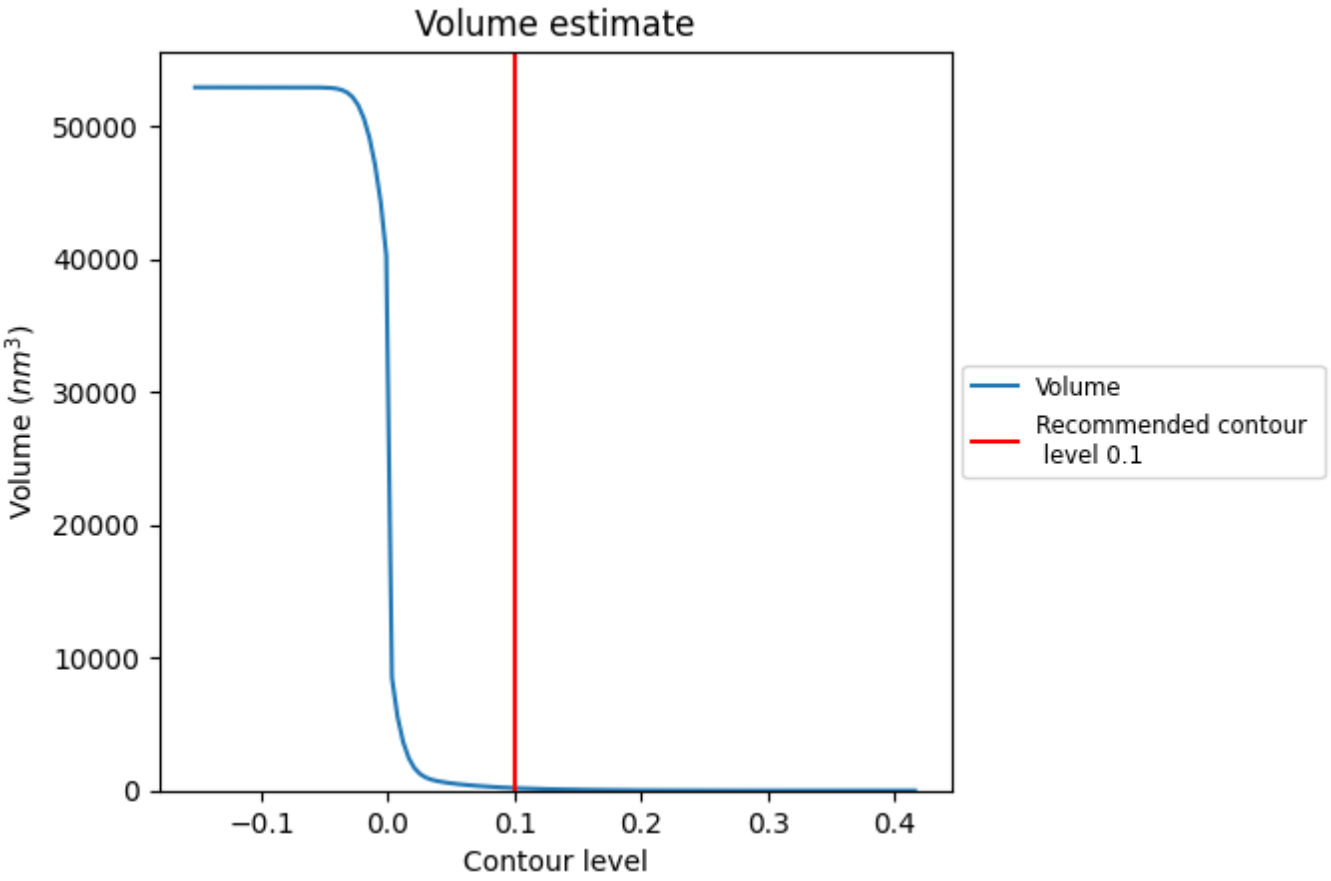
This section contains the results of statistical analysis of the map.

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.

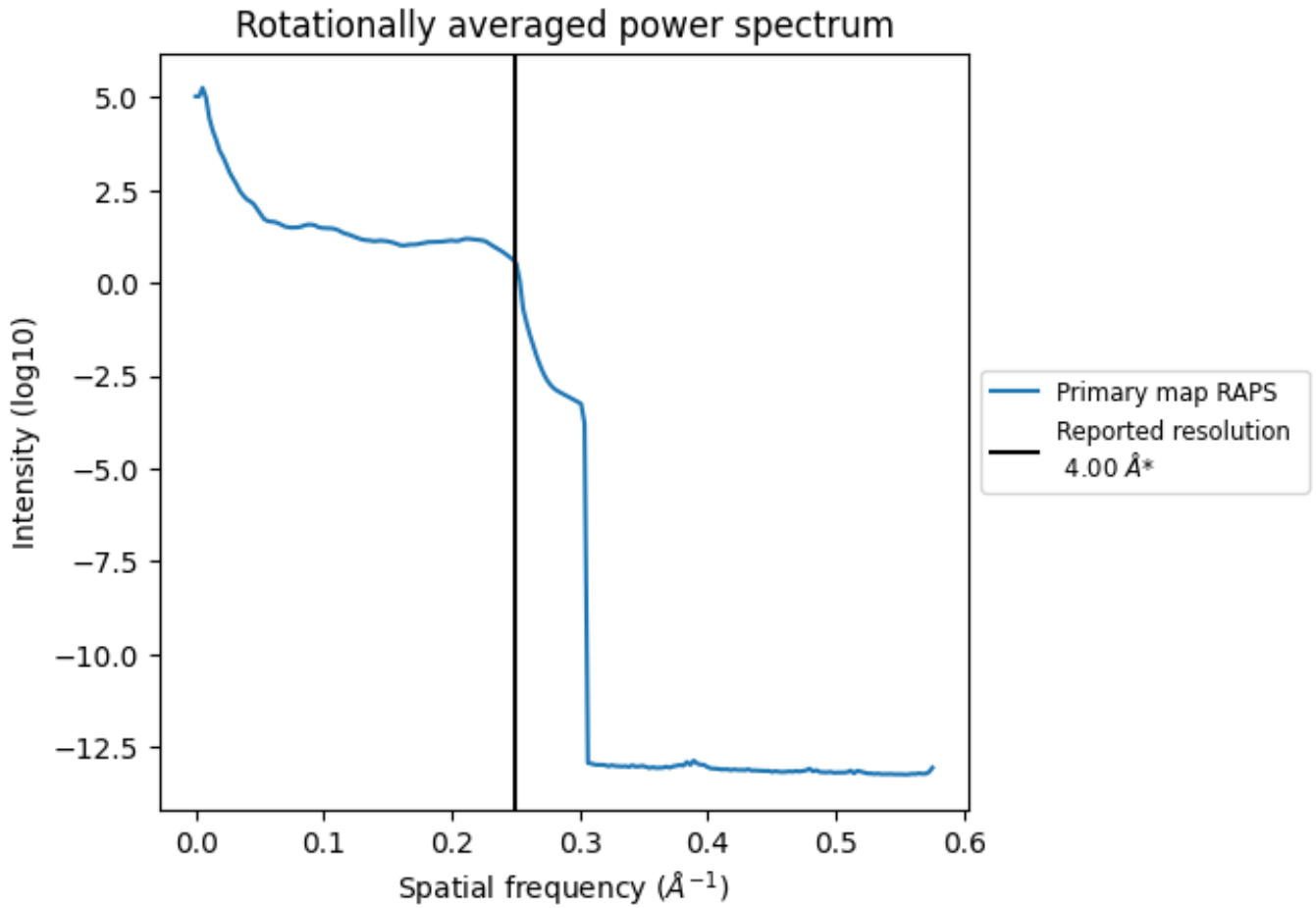
7.2 Volume estimate



The volume at the recommended contour level is 190 nm^3; this corresponds to an approximate mass of 172 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)

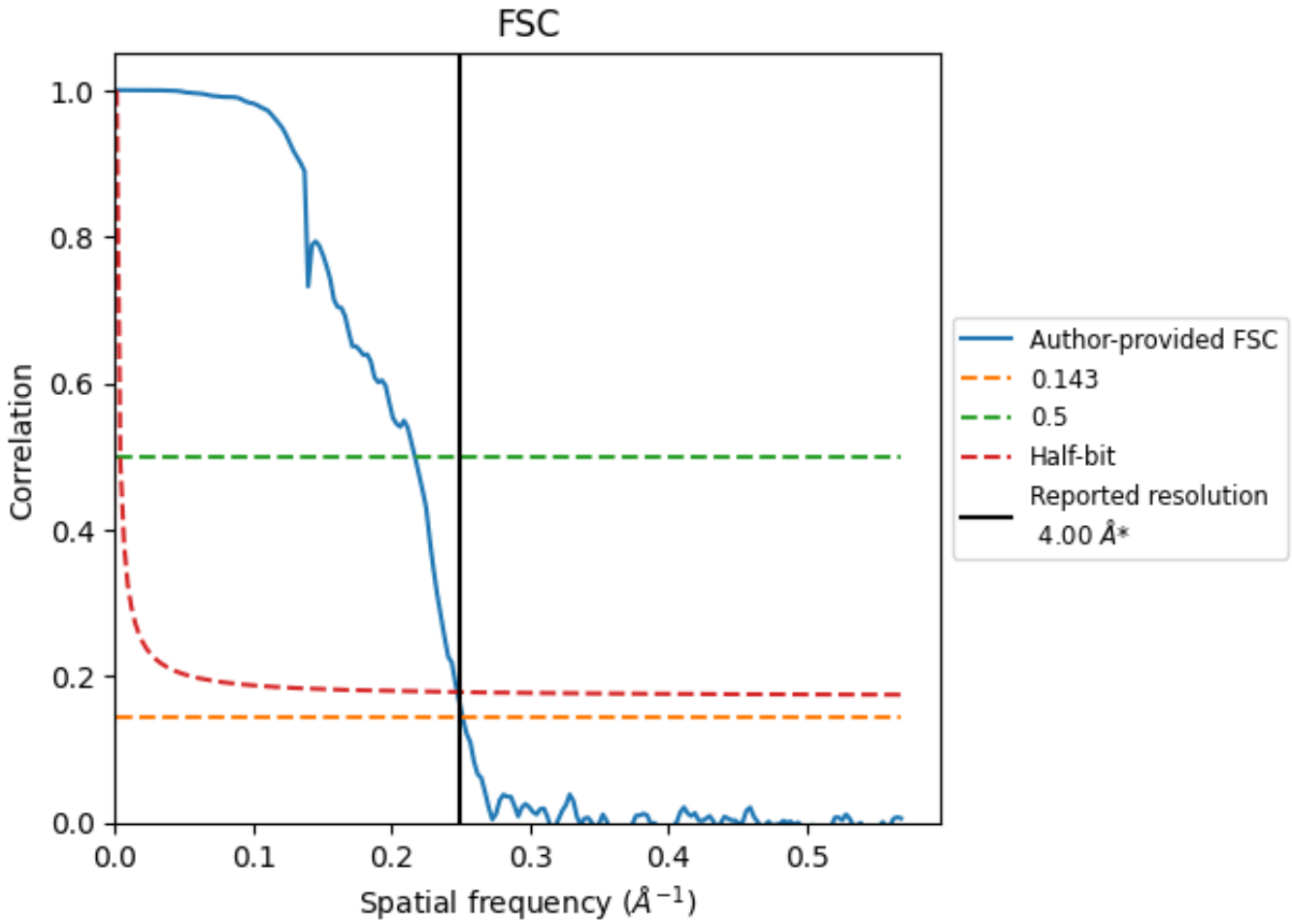


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

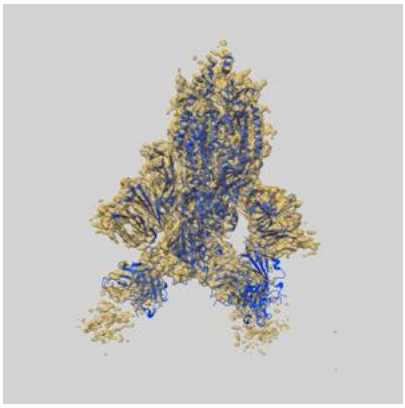
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	4.61	4.04
Unmasked-calculated*	-	-	-

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

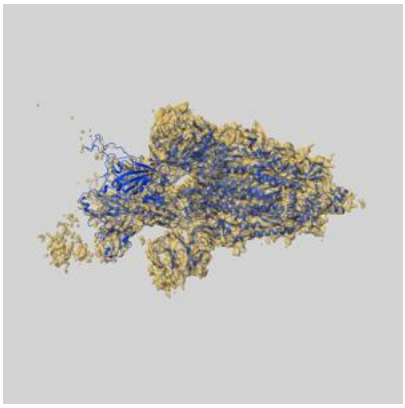
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23697 and PDB model 7M6I. Per-residue inclusion information can be found in section 3 on page 11.

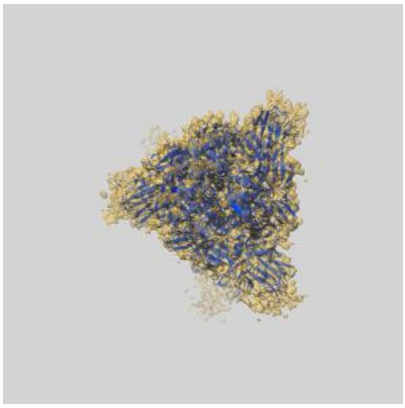
9.1 Map-model overlay



X



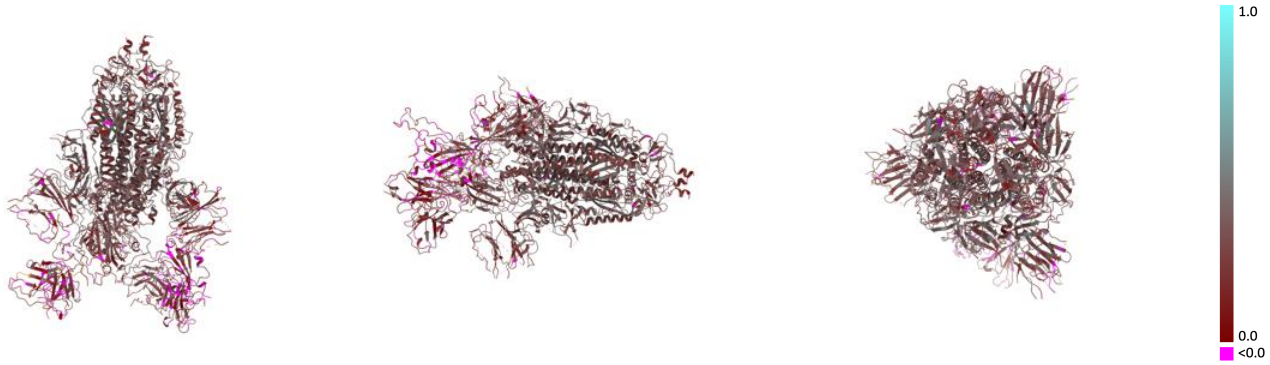
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

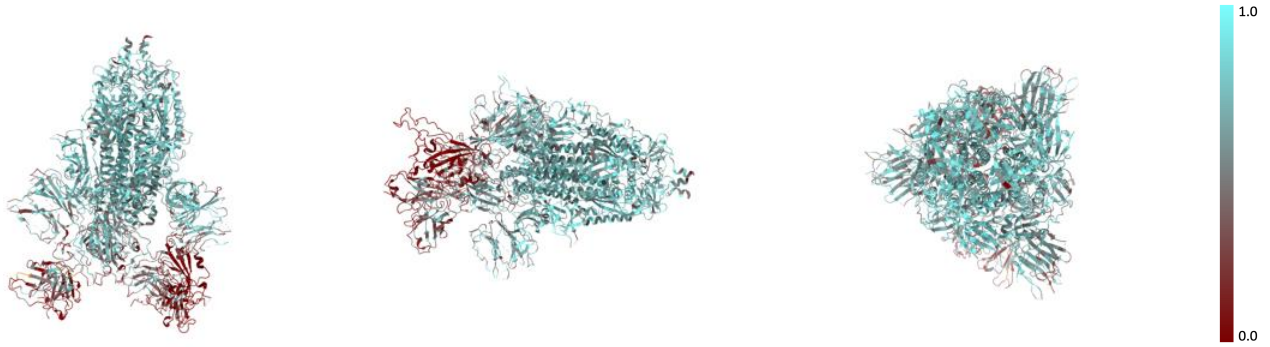
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

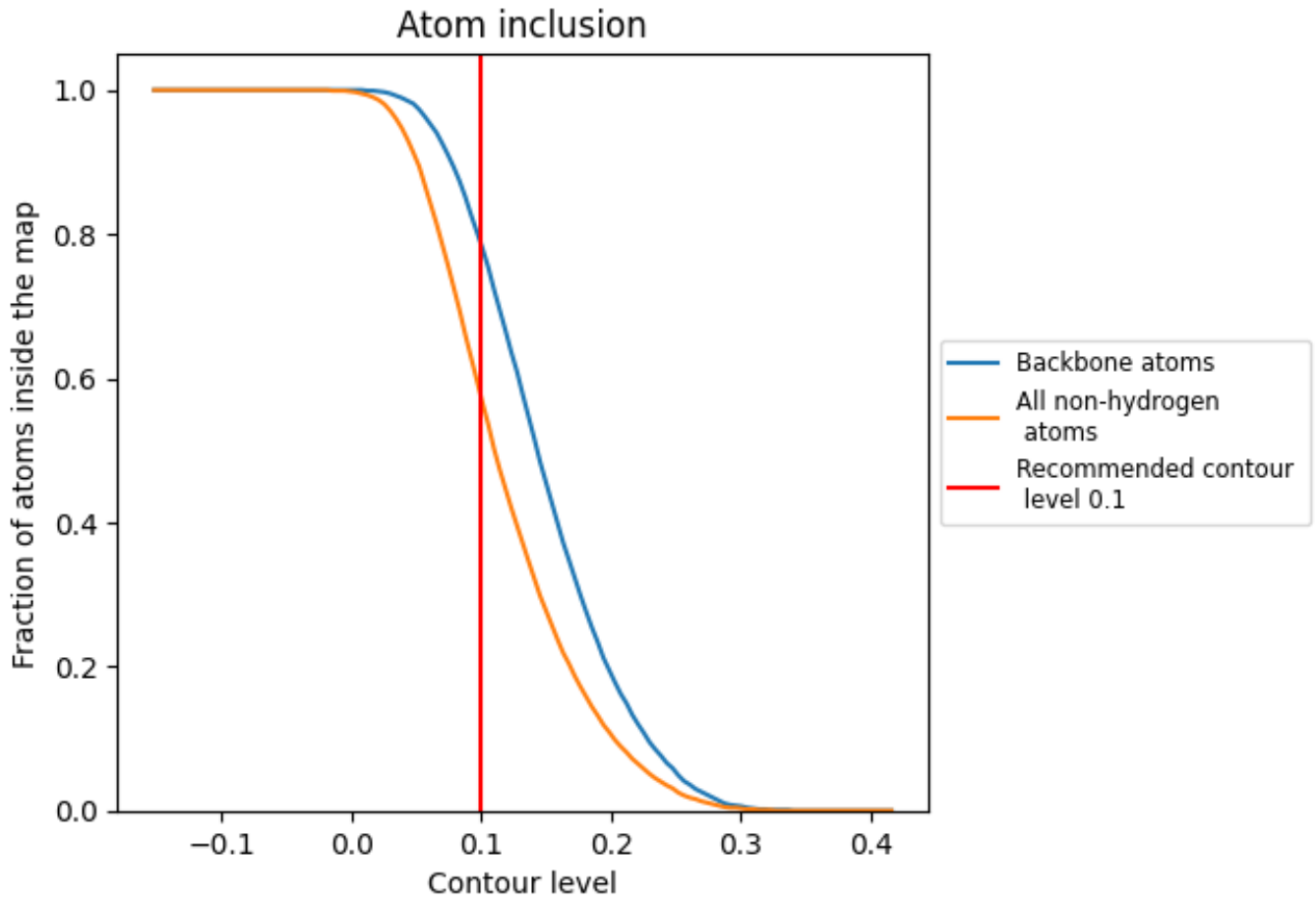
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5720	0.2770
A	0.6390	0.2960
B	0.5620	0.2760
C	0.6420	0.3030
D	0.2860	0.2740
E	0.0800	0.2560
F	0.3210	0.2430
G	0.3330	0.3270
H	0.3590	0.2130
I	0.1430	0.1080
L	0.2730	0.1930
M	0.3190	0.1510
N	0.2060	0.1300