Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID	:	3JCL / pdb_00003jcl
EMDB ID	:	EMD-6526
Title	:	Cryo-electron microscopy structure of a coronavirus spike glycoprotein trimer
Authors	:	Walls, A.C.; Tortorici, M.A.; Bosch, B.J.; Frenz, B.; Rottier, P.J.M.; DiMaio, F.; Rey, F.A.; Veesler, D.
Deposited on	:	2015-12-21
Resolution	:	4.00 Å(reported)
Based on initial models	:	4KQZ, 3R4D, 4H14

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

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

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

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

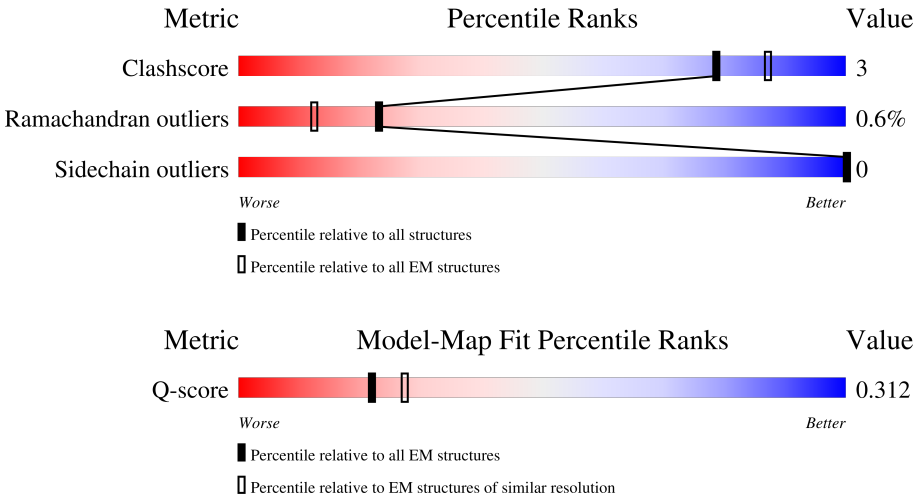
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	1265	32% 75% 8% • 16%
1	B	1265	32% 75% 9% • 16%
1	C	1265	32% 75% 8% • 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 24822 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	1067	Total	C	N	O	S	0	0
			8274	5234	1406	1586	48		
1	B	1067	Total	C	N	O	S	0	0
			8274	5234	1406	1586	48		
1	C	1067	Total	C	N	O	S	0	0
			8274	5234	1406	1586	48		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	717	SER	ARG	conflict	UNP P11224
A	1232	ILE	-	expression tag	UNP P11224
A	1233	LYS	-	expression tag	UNP P11224
A	1234	ARG	-	expression tag	UNP P11224
A	1235	MET	-	expression tag	UNP P11224
A	1236	LYS	-	expression tag	UNP P11224
A	1237	GLN	-	expression tag	UNP P11224
A	1238	ILE	-	expression tag	UNP P11224
A	1239	GLU	-	expression tag	UNP P11224
A	1240	ASP	-	expression tag	UNP P11224
A	1241	LYS	-	expression tag	UNP P11224
A	1242	ILE	-	expression tag	UNP P11224
A	1243	GLU	-	expression tag	UNP P11224
A	1244	GLU	-	expression tag	UNP P11224
A	1245	ILE	-	expression tag	UNP P11224
A	1246	GLU	-	expression tag	UNP P11224
A	1247	SER	-	expression tag	UNP P11224
A	1248	LYS	-	expression tag	UNP P11224
A	1249	GLN	-	expression tag	UNP P11224
A	1250	LYS	-	expression tag	UNP P11224
A	1251	LYS	-	expression tag	UNP P11224
A	1252	ILE	-	expression tag	UNP P11224
A	1253	GLU	-	expression tag	UNP P11224
A	1254	ASN	-	expression tag	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	GLU	-	expression tag	UNP P11224
A	1256	ILE	-	expression tag	UNP P11224
A	1257	ALA	-	expression tag	UNP P11224
A	1258	ARG	-	expression tag	UNP P11224
A	1259	ILE	-	expression tag	UNP P11224
A	1260	LYS	-	expression tag	UNP P11224
A	1261	LYS	-	expression tag	UNP P11224
A	1262	ILE	-	expression tag	UNP P11224
A	1263	LYS	-	expression tag	UNP P11224
A	1264	LEU	-	expression tag	UNP P11224
A	1265	VAL	-	expression tag	UNP P11224
A	1266	PRO	-	expression tag	UNP P11224
A	1267	ARG	-	expression tag	UNP P11224
A	1268	GLY	-	expression tag	UNP P11224
A	1269	SER	-	expression tag	UNP P11224
A	1270	LEU	-	expression tag	UNP P11224
A	1271	GLU	-	expression tag	UNP P11224
A	1272	TRP	-	expression tag	UNP P11224
A	1273	SER	-	expression tag	UNP P11224
A	1274	HIS	-	expression tag	UNP P11224
A	1275	PRO	-	expression tag	UNP P11224
A	1276	GLN	-	expression tag	UNP P11224
A	1277	PHE	-	expression tag	UNP P11224
A	1278	GLU	-	expression tag	UNP P11224
A	1279	LYS	-	expression tag	UNP P11224
B	717	SER	ARG	conflict	UNP P11224
B	1232	ILE	-	expression tag	UNP P11224
B	1233	LYS	-	expression tag	UNP P11224
B	1234	ARG	-	expression tag	UNP P11224
B	1235	MET	-	expression tag	UNP P11224
B	1236	LYS	-	expression tag	UNP P11224
B	1237	GLN	-	expression tag	UNP P11224
B	1238	ILE	-	expression tag	UNP P11224
B	1239	GLU	-	expression tag	UNP P11224
B	1240	ASP	-	expression tag	UNP P11224
B	1241	LYS	-	expression tag	UNP P11224
B	1242	ILE	-	expression tag	UNP P11224
B	1243	GLU	-	expression tag	UNP P11224
B	1244	GLU	-	expression tag	UNP P11224
B	1245	ILE	-	expression tag	UNP P11224
B	1246	GLU	-	expression tag	UNP P11224
B	1247	SER	-	expression tag	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1248	LYS	-	expression tag	UNP P11224
B	1249	GLN	-	expression tag	UNP P11224
B	1250	LYS	-	expression tag	UNP P11224
B	1251	LYS	-	expression tag	UNP P11224
B	1252	ILE	-	expression tag	UNP P11224
B	1253	GLU	-	expression tag	UNP P11224
B	1254	ASN	-	expression tag	UNP P11224
B	1255	GLU	-	expression tag	UNP P11224
B	1256	ILE	-	expression tag	UNP P11224
B	1257	ALA	-	expression tag	UNP P11224
B	1258	ARG	-	expression tag	UNP P11224
B	1259	ILE	-	expression tag	UNP P11224
B	1260	LYS	-	expression tag	UNP P11224
B	1261	LYS	-	expression tag	UNP P11224
B	1262	ILE	-	expression tag	UNP P11224
B	1263	LYS	-	expression tag	UNP P11224
B	1264	LEU	-	expression tag	UNP P11224
B	1265	VAL	-	expression tag	UNP P11224
B	1266	PRO	-	expression tag	UNP P11224
B	1267	ARG	-	expression tag	UNP P11224
B	1268	GLY	-	expression tag	UNP P11224
B	1269	SER	-	expression tag	UNP P11224
B	1270	LEU	-	expression tag	UNP P11224
B	1271	GLU	-	expression tag	UNP P11224
B	1272	TRP	-	expression tag	UNP P11224
B	1273	SER	-	expression tag	UNP P11224
B	1274	HIS	-	expression tag	UNP P11224
B	1275	PRO	-	expression tag	UNP P11224
B	1276	GLN	-	expression tag	UNP P11224
B	1277	PHE	-	expression tag	UNP P11224
B	1278	GLU	-	expression tag	UNP P11224
B	1279	LYS	-	expression tag	UNP P11224
C	717	SER	ARG	conflict	UNP P11224
C	1232	ILE	-	expression tag	UNP P11224
C	1233	LYS	-	expression tag	UNP P11224
C	1234	ARG	-	expression tag	UNP P11224
C	1235	MET	-	expression tag	UNP P11224
C	1236	LYS	-	expression tag	UNP P11224
C	1237	GLN	-	expression tag	UNP P11224
C	1238	ILE	-	expression tag	UNP P11224
C	1239	GLU	-	expression tag	UNP P11224
C	1240	ASP	-	expression tag	UNP P11224

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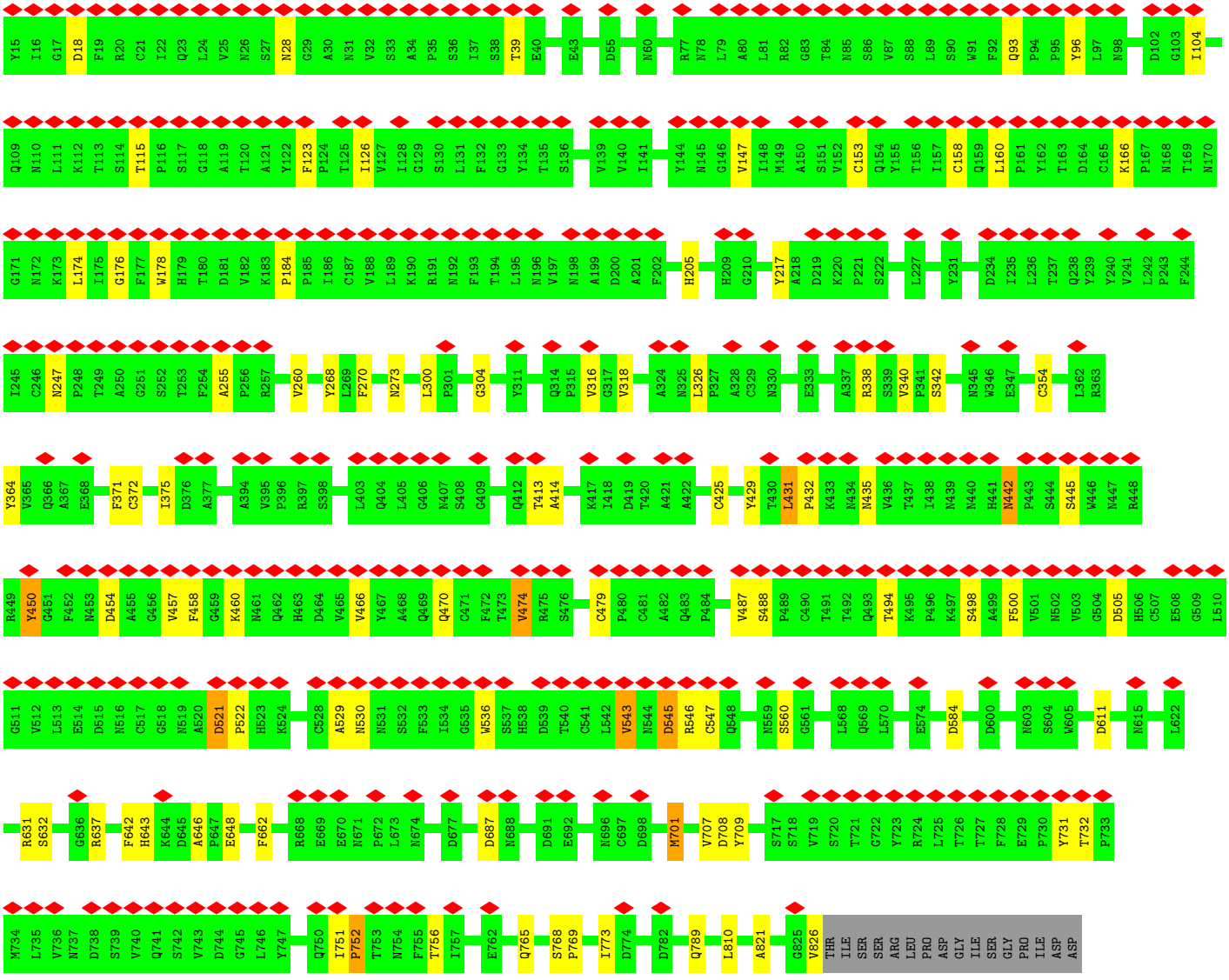
Chain	Residue	Modelled	Actual	Comment	Reference
C	1241	LYS	-	expression tag	UNP P11224
C	1242	ILE	-	expression tag	UNP P11224
C	1243	GLU	-	expression tag	UNP P11224
C	1244	GLU	-	expression tag	UNP P11224
C	1245	ILE	-	expression tag	UNP P11224
C	1246	GLU	-	expression tag	UNP P11224
C	1247	SER	-	expression tag	UNP P11224
C	1248	LYS	-	expression tag	UNP P11224
C	1249	GLN	-	expression tag	UNP P11224
C	1250	LYS	-	expression tag	UNP P11224
C	1251	LYS	-	expression tag	UNP P11224
C	1252	ILE	-	expression tag	UNP P11224
C	1253	GLU	-	expression tag	UNP P11224
C	1254	ASN	-	expression tag	UNP P11224
C	1255	GLU	-	expression tag	UNP P11224
C	1256	ILE	-	expression tag	UNP P11224
C	1257	ALA	-	expression tag	UNP P11224
C	1258	ARG	-	expression tag	UNP P11224
C	1259	ILE	-	expression tag	UNP P11224
C	1260	LYS	-	expression tag	UNP P11224
C	1261	LYS	-	expression tag	UNP P11224
C	1262	ILE	-	expression tag	UNP P11224
C	1263	LYS	-	expression tag	UNP P11224
C	1264	LEU	-	expression tag	UNP P11224
C	1265	VAL	-	expression tag	UNP P11224
C	1266	PRO	-	expression tag	UNP P11224
C	1267	ARG	-	expression tag	UNP P11224
C	1268	GLY	-	expression tag	UNP P11224
C	1269	SER	-	expression tag	UNP P11224
C	1270	LEU	-	expression tag	UNP P11224
C	1271	GLU	-	expression tag	UNP P11224
C	1272	TRP	-	expression tag	UNP P11224
C	1273	SER	-	expression tag	UNP P11224
C	1274	HIS	-	expression tag	UNP P11224
C	1275	PRO	-	expression tag	UNP P11224
C	1276	GLN	-	expression tag	UNP P11224
C	1277	PHE	-	expression tag	UNP P11224
C	1278	GLU	-	expression tag	UNP P11224
C	1279	LYS	-	expression tag	UNP P11224

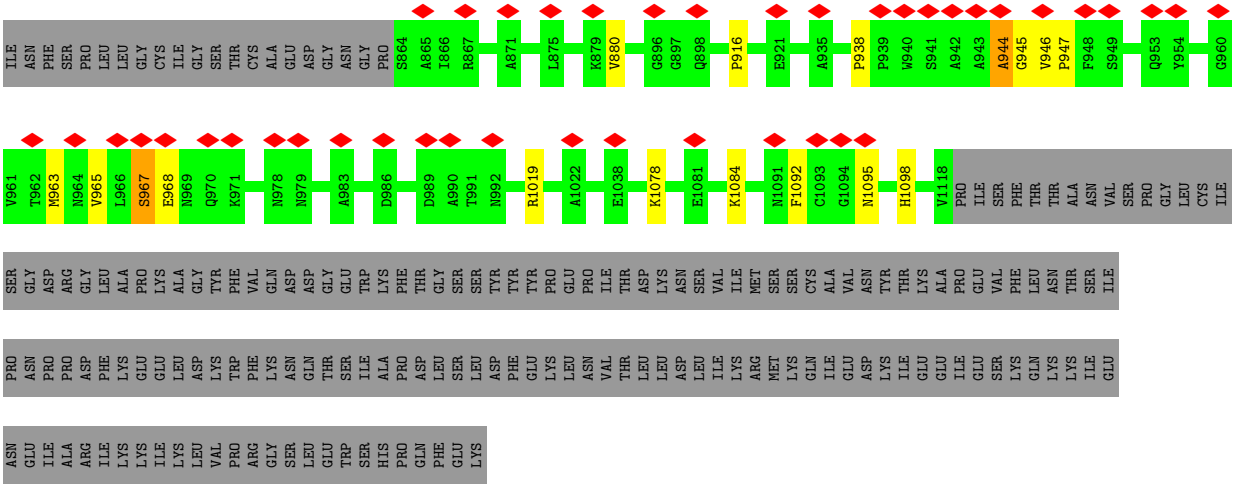
3 Residue-property plots (i)

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: 

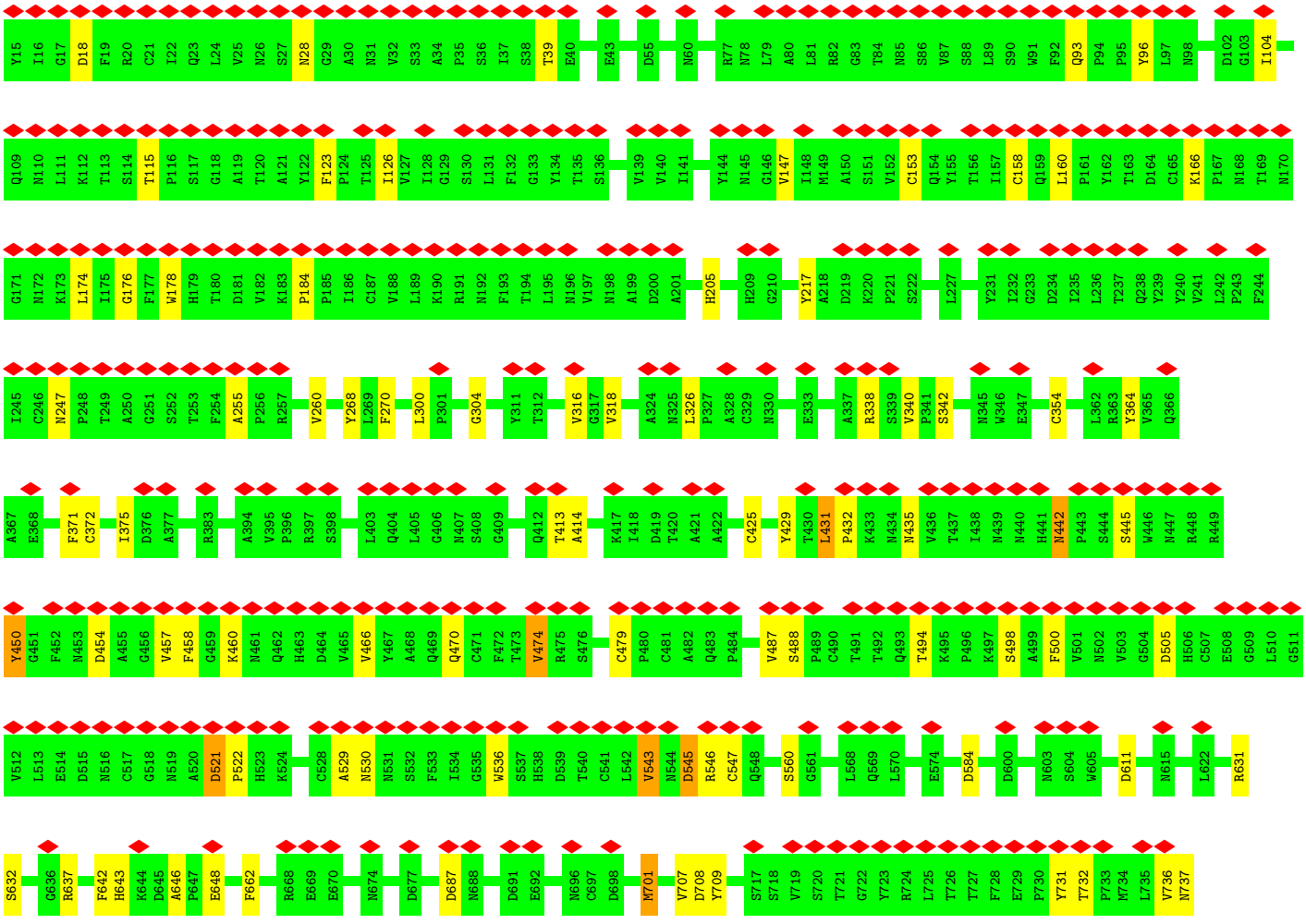


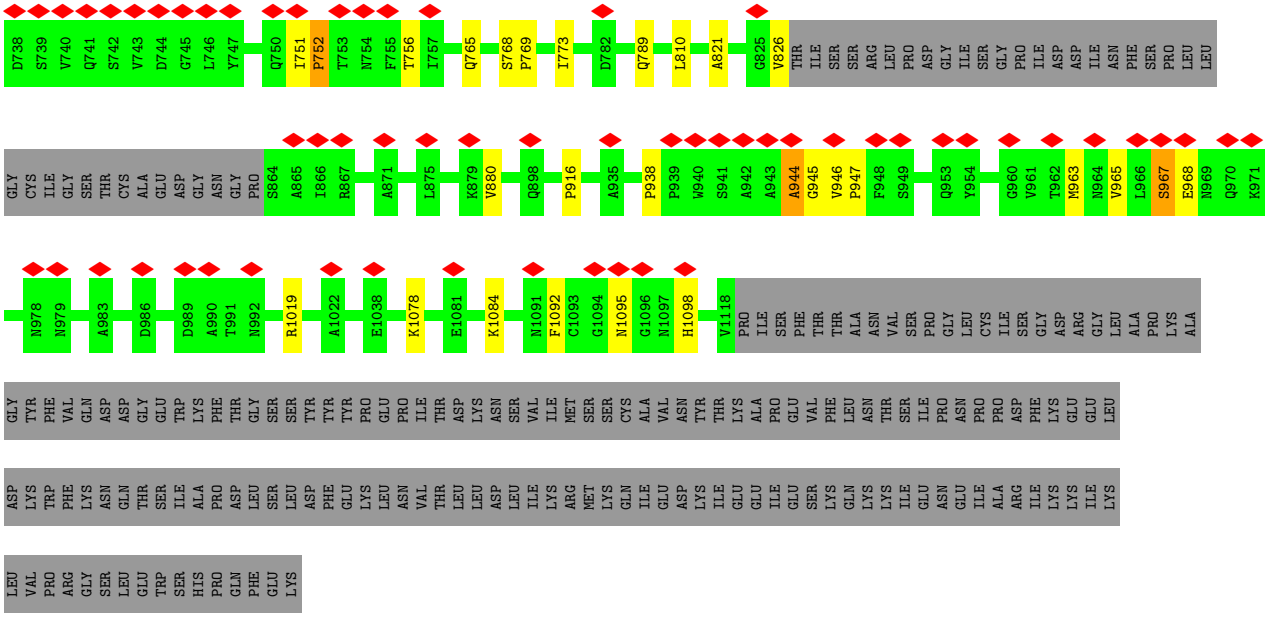


• Molecule 1: Spike glycoprotein

Chain B:



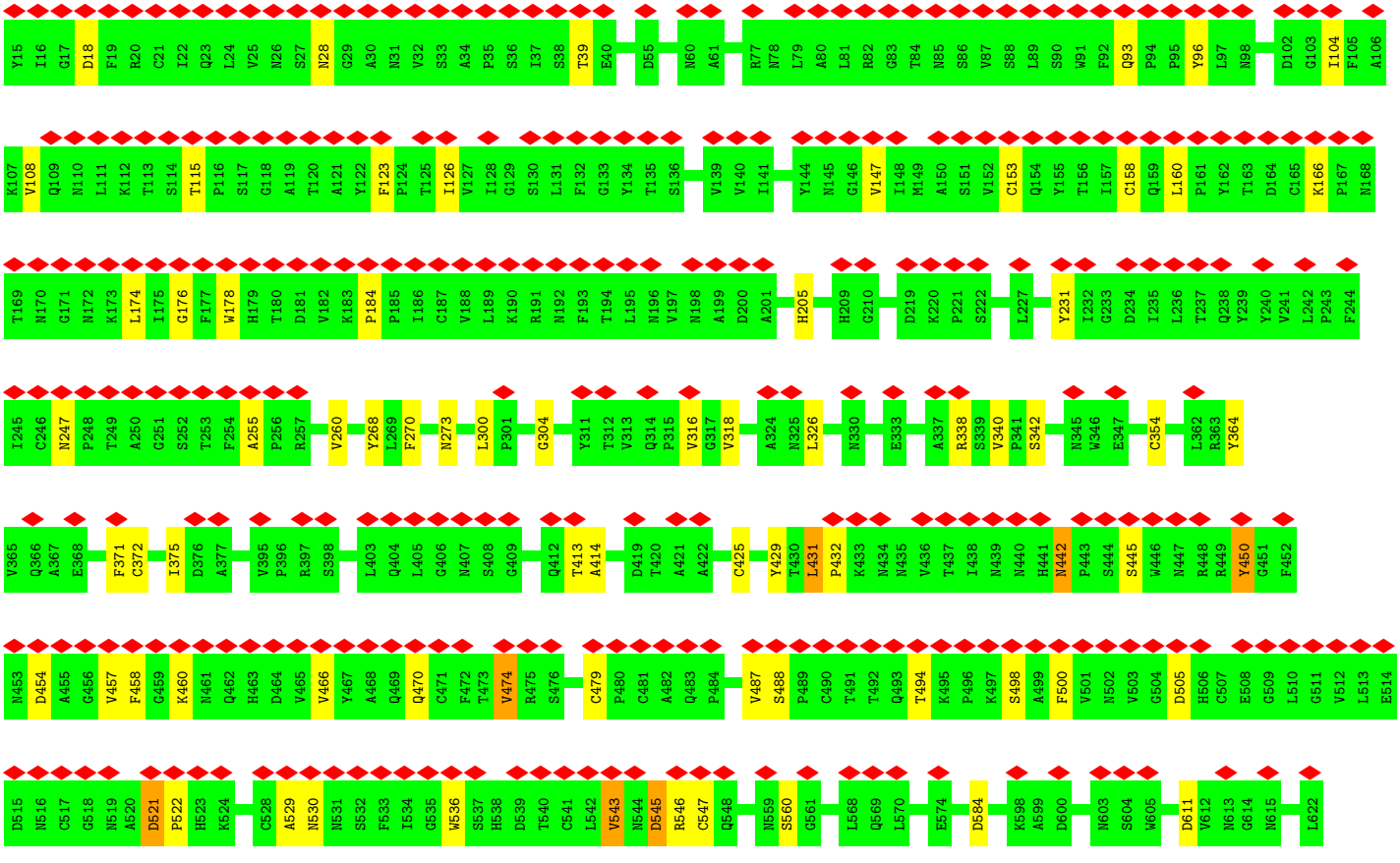


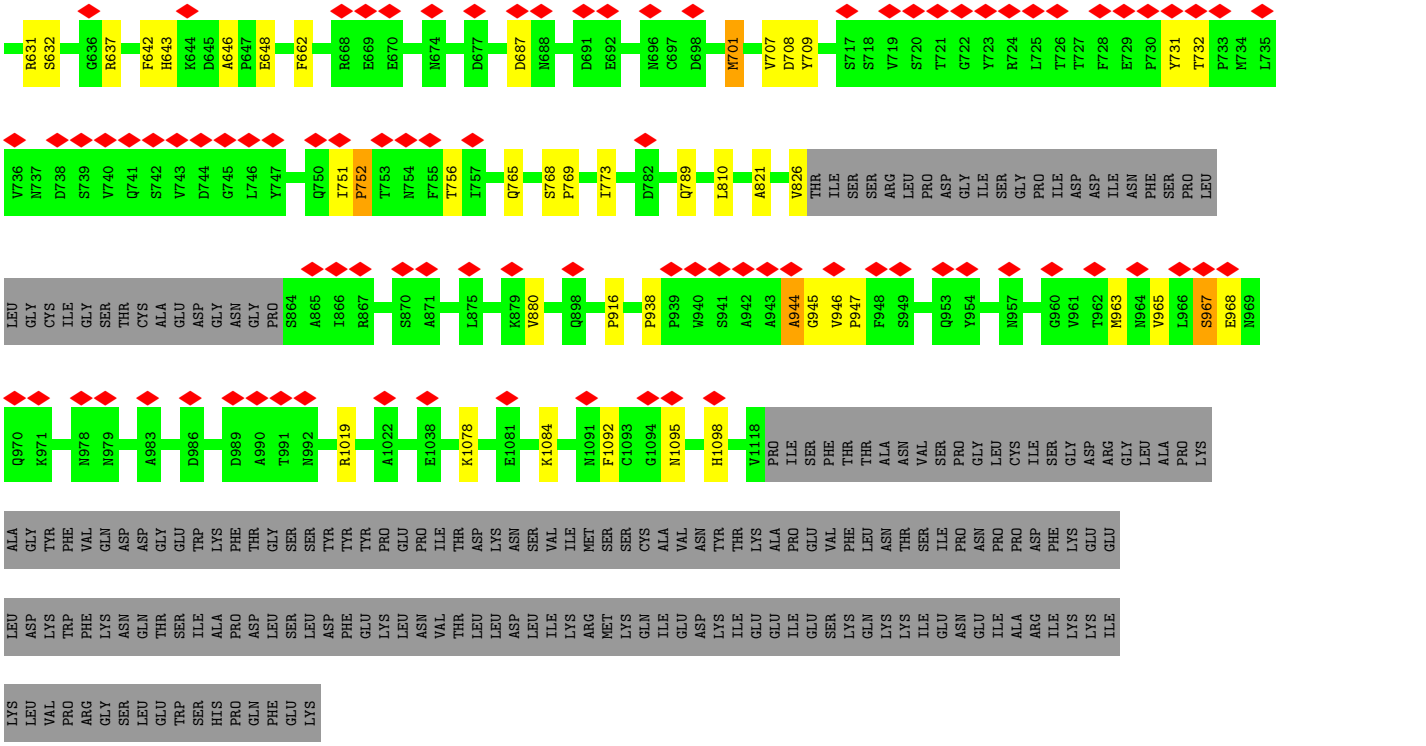


- Molecule 1: Spike glycoprotein

Chain C:






R631 S632 G636 R637 F642 H643 K644 D645 A646 P647 E648 F662 R668 E669 E670 N674 D677 D687 N688 D691 E692 N696 C697 D698 M701 V707 D708 Y709 S717 S718 V719 S720 T721 G722 Y723 R724 L725 T726 T727 F728 E729 P730 Y731 T732 P733 M734 L735
V736 N737 D738 S739 V740 Q741 S742 V743 D744 G745 L746 Y747 Q750 I751 P752 T753 N754 F755 T756 I757 Q765 S768 P769 I773 D782 Q789 L810 A821 V826 THR ILE SER SER ARG LEU PRO ASP GLY ILE SER GLY PRO ILE ASP ASP ILE ASN PHE SER PRO LEU
LEU GLY CYS ILE GLY SER THR CYS ALA GLU ASP GLY ASN GLY PRO S864 A865 I866 R867 S870 A871 L875 K879 V880 Q898 P916 P938 P939 W940 S941 A942 A943 A944 G945 V946 P947 F948 S949 Q953 Y954 N957 G960 V961 T962 M963 N964 V965 L966 S967 E968 N969
Q970 K971 N978 N979 A983 D986 D989 A990 T991 N992 R1019 A1022 E1038 K1078 E1081 K1084 N1091 F1092 C1093 G1094 N1095 H1098 V1118 PRO ILE SER PHE THR THR ALA ASN VAL SER PRO GLY LEU CYS ILE SER GLY ASP ARG GLY LEU ALA PRO LYS
ALA GLY TYR PHE VAL GLN ASP ASP GLY GLU TRP LYS PHE THR GLY SER SER TYR TYR PRO GLU PRO ILE THR ASP LYS ASN SER VAL ILE MET SER SER CYS ALA VAL ASN TYR THR LYS ALA PRO GLU VAL PHE LEU ASN THR SER ILE PRO ASN PRO PRO ASP PHE LYS GLU GLU
LEU ASP LYS TRP PHE LYS ASN GLN THR SER ILE ALA PRO ASP LEU SER LEU ASP PHE GLU LYS LEU ASN VAL THR LEU LEU ASP LEU ILE LYS ARG MET LYS GLN ILE GLU ASP LYS ILE GLU GLU ILE GLU SER LYS GLN LYS LYS ILE GLU ASN GLU ILE ALA ARG ILE LYS LYS ILE
LYS LEU VAL PRO ARG GLY SER LEU GLU TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	82000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	38022	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.456	Depositor
Minimum map value	-0.313	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	420.48, 420.48, 420.48	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.46, 1.46, 1.46	Depositor

5 Model quality

5.1 Standard geometry

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	0.95	3/8458 (0.0%)	1.31	96/11523 (0.8%)
1	B	0.95	3/8458 (0.0%)	1.31	96/11523 (0.8%)
1	C	0.95	3/8458 (0.0%)	1.31	97/11523 (0.8%)
All	All	0.95	9/25374 (0.0%)	1.31	289/34569 (0.8%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	PHE	CB-CG	-5.97	1.36	1.50
1	C	270	PHE	CB-CG	-5.96	1.36	1.50
1	B	270	PHE	CB-CG	-5.91	1.37	1.50
1	A	300	LEU	CB-CG	-5.19	1.43	1.53
1	B	300	LEU	CB-CG	-5.16	1.43	1.53
1	C	300	LEU	CB-CG	-5.16	1.43	1.53
1	A	268	TYR	CB-CG	-5.07	1.40	1.51
1	C	268	TYR	CB-CG	-5.07	1.40	1.51
1	B	268	TYR	CB-CG	-5.06	1.40	1.51

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	946	VAL	N-CA-CB	-10.34	98.69	110.17
1	A	944	ALA	CB-CA-C	-10.34	93.63	110.79
1	B	946	VAL	N-CA-CB	-10.32	98.72	110.17
1	C	946	VAL	N-CA-CB	-10.32	98.72	110.17
1	C	944	ALA	CB-CA-C	-10.30	93.69	110.79
1	B	944	ALA	CB-CA-C	-10.30	93.70	110.79
1	C	708	ASP	CA-CB-CG	8.20	120.80	112.60
1	A	708	ASP	CA-CB-CG	8.17	120.77	112.60
1	B	708	ASP	CA-CB-CG	8.16	120.76	112.60
1	B	916	PRO	CA-C-N	8.10	129.65	120.98
1	B	916	PRO	C-N-CA	8.10	129.65	120.98
1	C	916	PRO	CA-C-N	8.04	129.58	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	916	PRO	C-N-CA	8.04	129.58	120.98
1	A	916	PRO	CA-C-N	8.01	129.55	120.98
1	A	916	PRO	C-N-CA	8.01	129.55	120.98
1	C	709	TYR	N-CA-C	-7.95	102.86	114.39
1	B	709	TYR	N-CA-C	-7.94	102.88	114.39
1	A	709	TYR	N-CA-C	-7.94	102.88	114.39
1	B	643	HIS	N-CA-C	-7.80	97.55	109.95
1	A	643	HIS	N-CA-C	-7.79	97.57	109.95
1	C	643	HIS	N-CA-C	-7.78	97.58	109.95
1	C	247	ASN	CA-C-N	7.73	127.66	119.85
1	C	247	ASN	C-N-CA	7.73	127.66	119.85
1	A	247	ASN	CA-C-N	7.69	127.62	119.85
1	A	247	ASN	C-N-CA	7.69	127.62	119.85
1	B	247	ASN	CA-C-N	7.69	127.62	119.85
1	B	247	ASN	C-N-CA	7.69	127.62	119.85
1	A	642	PHE	N-CA-C	7.54	120.92	109.23
1	C	642	PHE	N-CA-C	7.53	120.89	109.23
1	B	642	PHE	N-CA-C	7.50	120.86	109.23
1	A	560	SER	N-CA-C	7.31	119.04	111.14
1	B	560	SER	N-CA-C	7.31	119.04	111.14
1	C	560	SER	N-CA-C	7.30	119.02	111.14
1	A	123	PHE	CA-CB-CG	7.12	120.92	113.80
1	C	123	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	342	SER	CA-C-N	7.12	126.79	119.82
1	A	342	SER	C-N-CA	7.12	126.79	119.82
1	B	342	SER	CA-C-N	7.11	126.78	119.82
1	B	342	SER	C-N-CA	7.11	126.78	119.82
1	B	123	PHE	CA-CB-CG	7.10	120.90	113.80
1	C	342	SER	CA-C-N	7.05	126.73	119.82
1	C	342	SER	C-N-CA	7.05	126.73	119.82
1	A	536	TRP	CA-CB-CG	6.96	126.82	113.60
1	C	536	TRP	CA-CB-CG	6.96	126.82	113.60
1	B	536	TRP	CA-CB-CG	6.95	126.80	113.60
1	A	498	SER	N-CA-C	6.88	117.12	108.45
1	B	184	PRO	CA-C-N	6.85	127.30	120.52
1	B	184	PRO	C-N-CA	6.85	127.30	120.52
1	B	442	ASN	CA-C-N	6.84	126.54	119.56
1	B	442	ASN	C-N-CA	6.84	126.54	119.56
1	A	184	PRO	CA-C-N	6.84	127.29	120.52
1	A	184	PRO	C-N-CA	6.84	127.29	120.52
1	C	498	SER	N-CA-C	6.83	117.05	108.45
1	A	442	ASN	CA-C-N	6.83	126.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	442	ASN	C-N-CA	6.83	126.52	119.56
1	B	498	SER	N-CA-C	6.83	117.05	108.45
1	C	442	ASN	CA-C-N	6.81	126.51	119.56
1	C	442	ASN	C-N-CA	6.81	126.51	119.56
1	C	184	PRO	CA-C-N	6.78	127.23	120.52
1	C	184	PRO	C-N-CA	6.78	127.23	120.52
1	B	316	VAL	N-CA-C	6.50	118.09	111.00
1	B	789	GLN	N-CA-C	-6.50	105.00	113.12
1	C	316	VAL	N-CA-C	6.49	118.08	111.00
1	A	789	GLN	N-CA-C	-6.49	105.01	113.12
1	B	545	ASP	N-CA-C	-6.49	101.53	110.35
1	A	545	ASP	N-CA-C	-6.47	101.55	110.35
1	C	789	GLN	N-CA-C	-6.47	105.03	113.12
1	A	316	VAL	N-CA-C	6.47	118.05	111.00
1	C	545	ASP	N-CA-C	-6.46	101.57	110.35
1	B	500	PHE	CA-CB-CG	6.43	120.23	113.80
1	C	500	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	500	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	429	TYR	N-CA-C	6.39	118.48	108.96
1	B	429	TYR	N-CA-C	6.38	118.47	108.96
1	C	429	TYR	N-CA-C	6.38	118.47	108.96
1	A	338	ARG	N-CA-C	6.35	118.20	111.28
1	C	338	ARG	N-CA-C	6.35	118.20	111.28
1	B	338	ARG	N-CA-C	6.35	118.20	111.28
1	C	732	THR	CA-C-N	6.29	127.70	119.84
1	C	732	THR	C-N-CA	6.29	127.70	119.84
1	A	304	GLY	N-CA-C	6.28	119.10	110.56
1	B	304	GLY	N-CA-C	6.26	119.07	110.56
1	C	304	GLY	N-CA-C	6.26	119.07	110.56
1	B	160	LEU	CA-C-N	6.25	126.17	119.85
1	B	160	LEU	C-N-CA	6.25	126.17	119.85
1	A	732	THR	CA-C-N	6.25	127.65	119.84
1	A	732	THR	C-N-CA	6.25	127.65	119.84
1	C	160	LEU	CA-C-N	6.25	126.16	119.85
1	C	160	LEU	C-N-CA	6.25	126.16	119.85
1	B	732	THR	CA-C-N	6.24	127.64	119.84
1	B	732	THR	C-N-CA	6.24	127.64	119.84
1	A	160	LEU	CA-C-N	6.23	126.15	119.85
1	A	160	LEU	C-N-CA	6.23	126.15	119.85
1	A	340	VAL	CA-C-N	6.17	127.52	120.85
1	A	340	VAL	C-N-CA	6.17	127.52	120.85
1	B	340	VAL	CA-C-N	6.16	127.50	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	340	VAL	C-N-CA	6.16	127.50	120.85
1	B	255	ALA	CA-C-N	6.16	126.18	119.90
1	B	255	ALA	C-N-CA	6.16	126.18	119.90
1	C	340	VAL	CA-C-N	6.14	127.48	120.85
1	C	340	VAL	C-N-CA	6.14	127.48	120.85
1	A	255	ALA	CA-C-N	6.13	126.15	119.90
1	A	255	ALA	C-N-CA	6.13	126.15	119.90
1	C	255	ALA	CA-C-N	6.11	126.13	119.90
1	C	255	ALA	C-N-CA	6.11	126.13	119.90
1	B	488	SER	CA-C-N	6.10	126.56	120.52
1	B	488	SER	C-N-CA	6.10	126.56	120.52
1	C	494	THR	CB-CA-C	-6.10	102.29	109.80
1	A	880	VAL	N-CA-C	6.08	116.62	107.75
1	B	494	THR	CB-CA-C	-6.08	102.33	109.80
1	B	880	VAL	N-CA-C	6.07	116.61	107.75
1	C	880	VAL	N-CA-C	6.06	116.60	107.75
1	A	488	SER	CA-C-N	6.06	126.52	120.52
1	A	488	SER	C-N-CA	6.06	126.52	120.52
1	C	687	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	494	THR	CB-CA-C	-6.05	102.36	109.80
1	B	687	ASP	CA-CB-CG	6.05	118.65	112.60
1	C	488	SER	CA-C-N	6.05	126.51	120.52
1	C	488	SER	C-N-CA	6.05	126.51	120.52
1	A	153	CYS	N-CA-C	6.05	117.71	108.52
1	C	153	CYS	N-CA-C	6.03	117.69	108.52
1	A	648	GLU	CA-C-N	6.03	126.53	120.14
1	A	648	GLU	C-N-CA	6.03	126.53	120.14
1	A	687	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	104	ILE	N-CA-C	6.02	116.54	108.11
1	C	648	GLU	CA-C-N	6.02	126.52	120.14
1	C	648	GLU	C-N-CA	6.02	126.52	120.14
1	B	153	CYS	N-CA-C	6.01	117.66	108.52
1	B	104	ILE	N-CA-C	6.01	116.52	108.11
1	C	104	ILE	N-CA-C	5.99	116.50	108.11
1	B	648	GLU	CA-C-N	5.99	126.49	120.14
1	B	648	GLU	C-N-CA	5.99	126.49	120.14
1	C	454	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	454	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	454	ASP	CA-CB-CG	5.88	118.47	112.60
1	B	457	VAL	CA-C-N	5.83	128.09	120.28
1	B	457	VAL	C-N-CA	5.83	128.09	120.28
1	C	457	VAL	CA-C-N	5.83	128.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	457	VAL	C-N-CA	5.83	128.09	120.28
1	A	457	VAL	CA-C-N	5.82	128.08	120.28
1	A	457	VAL	C-N-CA	5.82	128.08	120.28
1	A	946	VAL	CA-C-N	5.82	125.79	120.03
1	A	946	VAL	C-N-CA	5.82	125.79	120.03
1	B	521	ASP	CA-C-N	5.81	125.52	119.82
1	B	521	ASP	C-N-CA	5.81	125.52	119.82
1	A	39	THR	N-CA-C	-5.81	106.36	113.50
1	B	946	VAL	CA-C-N	5.81	125.78	120.03
1	B	946	VAL	C-N-CA	5.81	125.78	120.03
1	C	39	THR	N-CA-C	-5.77	106.41	113.50
1	C	521	ASP	CA-C-N	5.77	125.47	119.82
1	C	521	ASP	C-N-CA	5.77	125.47	119.82
1	C	946	VAL	CA-C-N	5.76	125.73	120.03
1	C	946	VAL	C-N-CA	5.76	125.73	120.03
1	A	521	ASP	CA-C-N	5.75	125.46	119.82
1	A	521	ASP	C-N-CA	5.75	125.46	119.82
1	B	39	THR	N-CA-C	-5.75	106.42	113.50
1	B	364	TYR	N-CA-C	-5.75	106.39	113.41
1	C	364	TYR	N-CA-C	-5.72	106.44	113.41
1	A	326	LEU	CA-C-N	5.71	125.68	120.03
1	A	326	LEU	C-N-CA	5.71	125.68	120.03
1	C	326	LEU	CA-C-N	5.70	125.68	120.03
1	C	326	LEU	C-N-CA	5.70	125.68	120.03
1	C	160	LEU	CB-CA-C	-5.66	103.80	111.21
1	B	326	LEU	CA-C-N	5.65	125.63	120.03
1	B	326	LEU	C-N-CA	5.65	125.63	120.03
1	C	662	PHE	CA-CB-CG	-5.65	108.15	113.80
1	B	160	LEU	CB-CA-C	-5.63	103.83	111.21
1	A	160	LEU	CB-CA-C	-5.62	103.86	111.21
1	B	662	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	662	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	450	TYR	N-CA-C	5.57	122.66	110.80
1	C	18	ASP	N-CA-C	5.56	119.37	112.59
1	C	450	TYR	N-CA-C	5.56	122.64	110.80
1	B	18	ASP	N-CA-C	5.56	119.37	112.59
1	A	18	ASP	N-CA-C	5.55	119.36	112.59
1	A	318	VAL	N-CA-C	5.55	116.12	108.12
1	B	318	VAL	N-CA-C	5.55	116.12	108.12
1	B	450	TYR	N-CA-C	5.55	122.62	110.80
1	C	318	VAL	N-CA-C	5.55	116.11	108.12
1	A	967	SER	N-CA-C	-5.46	103.69	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	126	ILE	N-CA-C	5.46	116.53	108.45
1	B	938	PRO	CA-C-N	5.45	125.28	119.28
1	B	938	PRO	C-N-CA	5.45	125.28	119.28
1	B	967	SER	N-CA-C	-5.45	103.70	110.41
1	C	126	ILE	N-CA-C	5.45	116.52	108.45
1	C	938	PRO	CA-C-N	5.44	125.27	119.28
1	C	938	PRO	C-N-CA	5.44	125.27	119.28
1	C	965	VAL	N-CA-C	-5.44	107.55	112.12
1	C	115	THR	CA-C-N	5.43	125.41	120.03
1	C	115	THR	C-N-CA	5.43	125.41	120.03
1	A	938	PRO	CA-C-N	5.43	125.26	119.28
1	A	938	PRO	C-N-CA	5.43	125.26	119.28
1	B	646	ALA	CA-C-N	5.43	125.13	119.64
1	B	646	ALA	C-N-CA	5.43	125.13	119.64
1	A	126	ILE	N-CA-C	5.43	116.48	108.45
1	C	967	SER	N-CA-C	-5.42	103.74	110.41
1	A	965	VAL	N-CA-C	-5.42	107.57	112.12
1	B	965	VAL	N-CA-C	-5.41	107.57	112.12
1	B	115	THR	CA-C-N	5.41	125.39	120.03
1	B	115	THR	C-N-CA	5.41	125.39	120.03
1	C	773	ILE	N-CA-C	5.41	115.77	107.77
1	C	646	ALA	CA-C-N	5.40	125.09	119.64
1	C	646	ALA	C-N-CA	5.40	125.09	119.64
1	B	773	ILE	N-CA-C	5.39	115.75	107.77
1	A	773	ILE	N-CA-C	5.39	115.74	107.77
1	A	364	TYR	N-CA-C	-5.39	106.39	113.12
1	A	115	THR	CA-C-N	5.38	125.35	120.03
1	A	115	THR	C-N-CA	5.38	125.35	120.03
1	B	470	GLN	CA-C-N	5.38	127.75	120.38
1	B	470	GLN	C-N-CA	5.38	127.75	120.38
1	A	646	ALA	CA-C-N	5.38	125.07	119.64
1	A	646	ALA	C-N-CA	5.38	125.07	119.64
1	C	707	VAL	N-CA-C	5.36	116.02	108.36
1	B	707	VAL	N-CA-C	5.35	116.01	108.36
1	A	470	GLN	CA-C-N	5.35	127.71	120.38
1	A	470	GLN	C-N-CA	5.35	127.71	120.38
1	C	470	GLN	CA-C-N	5.35	127.70	120.38
1	C	470	GLN	C-N-CA	5.35	127.70	120.38
1	A	707	VAL	N-CA-C	5.34	116.00	108.36
1	A	431	LEU	N-CA-C	-5.33	101.94	110.10
1	B	701	MET	N-CA-C	5.33	116.11	107.32
1	C	701	MET	N-CA-C	5.32	116.10	107.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1098	HIS	N-CA-C	5.32	118.94	110.70
1	C	431	LEU	N-CA-C	-5.31	101.97	110.10
1	C	1098	HIS	N-CA-C	5.31	118.93	110.70
1	B	431	LEU	N-CA-C	-5.30	101.99	110.10
1	A	1098	HIS	N-CA-C	5.30	118.91	110.70
1	B	260	VAL	N-CA-C	5.30	116.35	108.46
1	A	701	MET	N-CA-C	5.29	116.05	107.32
1	B	547	CYS	N-CA-C	-5.28	102.24	110.10
1	A	260	VAL	N-CA-C	5.27	116.31	108.46
1	A	547	CYS	N-CA-C	-5.26	102.26	110.10
1	C	547	CYS	N-CA-C	-5.26	102.26	110.10
1	C	260	VAL	N-CA-C	5.26	116.29	108.46
1	C	28	ASN	N-CA-C	5.25	116.78	108.96
1	A	28	ASN	N-CA-C	5.22	116.73	108.96
1	B	28	ASN	N-CA-C	5.20	116.71	108.96
1	B	205	HIS	CA-CB-CG	5.20	119.00	113.80
1	B	479	CYS	CA-C-N	5.20	126.34	119.84
1	B	479	CYS	C-N-CA	5.20	126.34	119.84
1	A	205	HIS	CA-CB-CG	5.19	118.99	113.80
1	B	938	PRO	N-CA-C	-5.18	104.38	110.70
1	C	938	PRO	N-CA-C	-5.18	104.37	110.70
1	B	543	VAL	CB-CA-C	-5.18	107.42	113.22
1	C	479	CYS	CA-C-N	5.18	126.31	119.84
1	C	479	CYS	C-N-CA	5.18	126.31	119.84
1	C	147	VAL	N-CA-C	5.17	117.48	108.95
1	C	205	HIS	CA-CB-CG	5.17	118.97	113.80
1	A	479	CYS	CA-C-N	5.17	126.30	119.84
1	A	479	CYS	C-N-CA	5.17	126.30	119.84
1	A	158	CYS	N-CA-C	5.16	117.52	110.55
1	A	938	PRO	N-CA-C	-5.16	104.41	110.70
1	A	147	VAL	N-CA-C	5.16	117.46	108.95
1	A	543	VAL	CB-CA-C	-5.16	107.44	113.22
1	C	174	LEU	CA-C-N	-5.15	116.81	121.65
1	C	174	LEU	C-N-CA	-5.15	116.81	121.65
1	B	147	VAL	N-CA-C	5.15	117.45	108.95
1	C	158	CYS	N-CA-C	5.14	117.50	110.55
1	B	158	CYS	N-CA-C	5.14	117.49	110.55
1	C	543	VAL	CB-CA-C	-5.13	107.47	113.22
1	C	487	VAL	N-CA-C	5.13	115.75	110.36
1	B	487	VAL	N-CA-C	5.12	115.74	110.36
1	A	487	VAL	N-CA-C	5.11	115.73	110.36
1	A	1095	ASN	CA-CB-CG	-5.11	107.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1095	ASN	CA-CB-CG	-5.11	107.49	112.60
1	A	166	LYS	CA-C-N	5.10	126.22	119.84
1	A	166	LYS	C-N-CA	5.10	126.22	119.84
1	A	174	LEU	CA-C-N	-5.10	116.86	121.65
1	A	174	LEU	C-N-CA	-5.10	116.86	121.65
1	B	166	LYS	CA-C-N	5.09	126.20	119.84
1	B	166	LYS	C-N-CA	5.09	126.20	119.84
1	B	174	LEU	CA-C-N	-5.08	116.87	121.65
1	B	174	LEU	C-N-CA	-5.08	116.87	121.65
1	A	765	GLN	N-CA-C	5.08	116.67	111.03
1	C	1095	ASN	CA-CB-CG	-5.08	107.52	112.60
1	C	166	LYS	CA-C-N	5.07	126.18	119.84
1	C	166	LYS	C-N-CA	5.07	126.18	119.84
1	C	93	GLN	CA-C-N	5.07	123.36	119.66
1	C	93	GLN	C-N-CA	5.07	123.36	119.66
1	B	93	GLN	CA-C-N	5.06	123.35	119.66
1	B	93	GLN	C-N-CA	5.06	123.35	119.66
1	A	93	GLN	CA-C-N	5.05	123.34	119.66
1	A	93	GLN	C-N-CA	5.05	123.34	119.66
1	B	765	GLN	N-CA-C	5.04	116.63	111.03
1	A	354	CYS	N-CA-C	5.04	117.64	109.06
1	B	354	CYS	N-CA-C	5.04	117.63	109.06
1	C	354	CYS	N-CA-C	5.02	117.59	109.06
1	C	765	GLN	N-CA-C	5.02	116.60	111.03
1	C	108	VAL	N-CA-C	5.00	115.05	107.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8274	0	8018	45	0
1	B	8274	0	8018	46	0
1	C	8274	0	8018	45	0
All	All	24822	0	24054	133	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 3.

All (133) 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:C:826:VAL:HG12	1:C:826:VAL:O	1.78	0.83
1:A:826:VAL:O	1:A:826:VAL:HG12	1.78	0.83
1:B:826:VAL:O	1:B:826:VAL:HG12	1.78	0.82
1:A:371:PHE:O	1:A:372:CYS:SG	2.38	0.81
1:B:371:PHE:O	1:B:372:CYS:SG	2.38	0.81
1:C:371:PHE:O	1:C:372:CYS:SG	2.38	0.81
1:C:458:PHE:HD1	1:C:458:PHE:H	1.31	0.79
1:B:458:PHE:H	1:B:458:PHE:HD1	1.31	0.76
1:A:458:PHE:H	1:A:458:PHE:HD1	1.31	0.76
1:A:637:ARG:HD2	1:A:637:ARG:H	1.51	0.76
1:B:637:ARG:HD2	1:B:637:ARG:H	1.51	0.75
1:C:637:ARG:HD2	1:C:637:ARG:H	1.51	0.75
1:C:637:ARG:HD2	1:C:637:ARG:N	2.07	0.70
1:B:637:ARG:HD2	1:B:637:ARG:N	2.07	0.70
1:A:637:ARG:HD2	1:A:637:ARG:N	2.07	0.69
1:A:637:ARG:O	1:A:637:ARG:HG2	1.92	0.69
1:B:458:PHE:CD1	1:B:458:PHE:N	2.60	0.68
1:C:458:PHE:CD1	1:C:458:PHE:N	2.60	0.68
1:B:637:ARG:O	1:B:637:ARG:HG2	1.92	0.68
1:C:637:ARG:HG2	1:C:637:ARG:O	1.92	0.67
1:A:458:PHE:HD1	1:A:458:PHE:N	1.93	0.67
1:B:458:PHE:HD1	1:B:458:PHE:N	1.93	0.66
1:A:458:PHE:N	1:A:458:PHE:CD1	2.60	0.65
1:C:1078:LYS:NZ	1:C:1092:PHE:CE1	2.65	0.64
1:B:1078:LYS:NZ	1:B:1092:PHE:CE1	2.65	0.64
1:A:1078:LYS:NZ	1:A:1092:PHE:CE1	2.65	0.64
1:C:458:PHE:HD1	1:C:458:PHE:N	1.93	0.63
1:B:944:ALA:HA	1:C:731:TYR:CG	2.37	0.60
1:A:944:ALA:HA	1:B:731:TYR:CG	2.37	0.60
1:A:731:TYR:CG	1:C:944:ALA:HA	2.37	0.59
1:B:967:SER:O	1:B:968:GLU:C	2.46	0.58
1:A:637:ARG:N	1:A:637:ARG:CD	2.67	0.57
1:A:967:SER:O	1:A:968:GLU:C	2.46	0.57
1:B:637:ARG:N	1:B:637:ARG:CD	2.67	0.57
1:C:637:ARG:N	1:C:637:ARG:CD	2.67	0.57
1:A:751:ILE:O	1:A:752:PRO:C	2.49	0.56
1:A:945:GLY:O	1:A:947:PRO:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:945:GLY:O	1:C:947:PRO:HD3	2.06	0.55
1:B:751:ILE:O	1:B:752:PRO:C	2.49	0.55
1:A:96:TYR:C	1:A:96:TYR:CD2	2.85	0.55
1:C:751:ILE:O	1:C:752:PRO:C	2.49	0.55
1:C:967:SER:O	1:C:968:GLU:C	2.46	0.55
1:B:945:GLY:O	1:B:947:PRO:HD3	2.06	0.55
1:A:637:ARG:O	1:A:637:ARG:CG	2.55	0.55
1:B:96:TYR:CD2	1:B:96:TYR:C	2.85	0.54
1:C:637:ARG:O	1:C:637:ARG:CG	2.55	0.54
1:B:637:ARG:O	1:B:637:ARG:CG	2.55	0.54
1:C:96:TYR:CD2	1:C:96:TYR:C	2.85	0.54
1:C:521:ASP:N	1:C:522:PRO:CD	2.71	0.53
1:A:521:ASP:N	1:A:522:PRO:CD	2.71	0.53
1:B:375:ILE:O	1:B:375:ILE:HG23	2.08	0.53
1:B:521:ASP:N	1:B:522:PRO:CD	2.71	0.53
1:A:375:ILE:O	1:A:375:ILE:HG23	2.08	0.53
1:C:375:ILE:HG23	1:C:375:ILE:O	2.08	0.53
1:C:826:VAL:O	1:C:826:VAL:CG1	2.49	0.53
1:A:545:ASP:O	1:A:546:ARG:C	2.53	0.52
1:C:545:ASP:O	1:C:546:ARG:C	2.53	0.51
1:B:545:ASP:O	1:B:546:ARG:C	2.53	0.50
1:A:372:CYS:SG	1:A:425:CYS:CB	3.01	0.49
1:C:372:CYS:SG	1:C:425:CYS:CB	3.00	0.49
1:B:372:CYS:SG	1:B:425:CYS:CB	3.00	0.49
1:A:371:PHE:C	1:A:372:CYS:SG	2.97	0.48
1:B:466:VAL:HG12	1:B:466:VAL:O	2.14	0.48
1:B:826:VAL:O	1:B:826:VAL:CG1	2.49	0.47
1:A:460:LYS:NZ	1:A:505:ASP:OD2	2.48	0.47
1:C:460:LYS:NZ	1:C:505:ASP:OD2	2.48	0.47
1:A:466:VAL:HG12	1:A:466:VAL:O	2.14	0.47
1:B:371:PHE:C	1:B:372:CYS:SG	2.97	0.47
1:C:371:PHE:C	1:C:372:CYS:SG	2.97	0.47
1:B:460:LYS:NZ	1:B:505:ASP:OD2	2.48	0.47
1:C:466:VAL:O	1:C:466:VAL:HG12	2.14	0.46
1:C:810:LEU:C	1:C:810:LEU:HD23	2.41	0.46
1:B:756:THR:O	1:B:756:THR:HG23	2.16	0.46
1:B:474:VAL:HG23	1:B:474:VAL:O	2.16	0.46
1:A:756:THR:O	1:A:756:THR:HG23	2.16	0.46
1:C:1019:ARG:O	1:C:1019:ARG:HG2	2.16	0.46
1:B:810:LEU:C	1:B:810:LEU:HD23	2.41	0.45
1:A:413:THR:OG1	1:A:414:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:LEU:C	1:A:810:LEU:HD23	2.41	0.45
1:C:701:MET:O	1:C:701:MET:HG2	2.16	0.45
1:B:1019:ARG:HG2	1:B:1019:ARG:O	2.16	0.45
1:B:413:THR:OG1	1:B:414:ALA:N	2.49	0.45
1:B:701:MET:O	1:B:701:MET:HG2	2.16	0.45
1:C:756:THR:HG23	1:C:756:THR:O	2.16	0.45
1:A:1019:ARG:O	1:A:1019:ARG:HG2	2.16	0.45
1:B:611:ASP:C	1:B:611:ASP:OD1	2.60	0.45
1:A:474:VAL:O	1:A:474:VAL:HG23	2.16	0.45
1:A:701:MET:O	1:A:701:MET:HG2	2.16	0.45
1:C:474:VAL:O	1:C:474:VAL:HG23	2.16	0.44
1:C:611:ASP:OD1	1:C:611:ASP:C	2.60	0.44
1:C:413:THR:OG1	1:C:414:ALA:N	2.50	0.44
1:A:611:ASP:OD1	1:A:611:ASP:C	2.60	0.44
1:C:631:ARG:HG2	1:C:632:SER:N	2.34	0.43
1:A:529:ALA:O	1:A:530:ASN:C	2.62	0.43
1:C:963:MET:SD	1:C:963:MET:N	2.92	0.42
1:A:631:ARG:HG2	1:A:632:SER:N	2.34	0.42
1:B:631:ARG:HG2	1:B:632:SER:N	2.34	0.42
1:A:821:ALA:O	1:A:1084:LYS:NZ	2.52	0.42
1:B:529:ALA:O	1:B:530:ASN:C	2.62	0.42
1:A:768:SER:HB2	1:A:769:PRO:HD2	2.02	0.42
1:A:431:LEU:H	1:A:546:ARG:HD3	1.85	0.42
1:B:431:LEU:O	1:B:432:PRO:C	2.63	0.42
1:C:529:ALA:O	1:C:530:ASN:C	2.62	0.42
1:B:584:ASP:C	1:B:584:ASP:OD1	2.63	0.42
1:C:431:LEU:H	1:C:546:ARG:HD3	1.85	0.42
1:B:768:SER:HB2	1:B:769:PRO:HD2	2.02	0.42
1:B:963:MET:SD	1:B:963:MET:N	2.92	0.42
1:C:768:SER:HB2	1:C:769:PRO:HD2	2.02	0.42
1:C:273:ASN:OD1	1:C:273:ASN:C	2.63	0.41
1:A:584:ASP:OD1	1:A:584:ASP:C	2.63	0.41
1:A:963:MET:SD	1:A:963:MET:N	2.92	0.41
1:B:821:ALA:O	1:B:1084:LYS:NZ	2.52	0.41
1:A:442:ASN:H	1:A:543:VAL:HB	1.86	0.41
1:B:431:LEU:H	1:B:546:ARG:HD3	1.85	0.41
1:C:231:TYR:CD2	1:C:231:TYR:C	2.97	0.41
1:A:375:ILE:O	1:A:375:ILE:CG2	2.69	0.41
1:B:435:ASN:OD1	1:B:435:ASN:C	2.63	0.41
1:B:217:TYR:CD2	1:B:217:TYR:N	2.89	0.41
1:B:442:ASN:H	1:B:543:VAL:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:VAL:O	1:B:737:ASN:C	2.64	0.41
1:C:1078:LYS:NZ	1:C:1092:PHE:CD1	2.89	0.41
1:A:431:LEU:O	1:A:432:PRO:C	2.63	0.40
1:C:821:ALA:O	1:C:1084:LYS:NZ	2.53	0.40
1:A:217:TYR:CD2	1:A:217:TYR:N	2.89	0.40
1:A:273:ASN:OD1	1:A:273:ASN:C	2.63	0.40
1:B:375:ILE:O	1:B:375:ILE:CG2	2.69	0.40
1:C:431:LEU:O	1:C:432:PRO:C	2.63	0.40
1:C:442:ASN:H	1:C:543:VAL:HB	1.85	0.40
1:C:584:ASP:OD1	1:C:584:ASP:C	2.63	0.40
1:A:435:ASN:OD1	1:A:435:ASN:C	2.63	0.40
1:A:1078:LYS:NZ	1:A:1092:PHE:CD1	2.89	0.40
1:B:1078:LYS:NZ	1:B:1092:PHE:CD1	2.89	0.40
1:C:375:ILE:O	1:C:375:ILE:CG2	2.69	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	1063/1265 (84%)	1002 (94%)	55 (5%)	6 (1%)	21	57
1	B	1063/1265 (84%)	1002 (94%)	55 (5%)	6 (1%)	21	57
1	C	1063/1265 (84%)	1002 (94%)	55 (5%)	6 (1%)	21	57
All	All	3189/3795 (84%)	3006 (94%)	165 (5%)	18 (1%)	23	57

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	PRO
1	B	752	PRO
1	C	752	PRO

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Mol	Chain	Res	Type
1	A	445	SER
1	B	445	SER
1	C	445	SER
1	A	178	TRP
1	A	450	TYR
1	B	178	TRP
1	B	450	TYR
1	C	178	TRP
1	C	450	TYR
1	A	474	VAL
1	B	474	VAL
1	A	176	GLY
1	B	176	GLY
1	C	176	GLY
1	C	474	VAL

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	918/1095 (84%)	918 (100%)	0	100	100
1	B	918/1095 (84%)	918 (100%)	0	100	100
1	C	918/1095 (84%)	918 (100%)	0	100	100
All	All	2754/3285 (84%)	2754 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	99	GLN
1	A	154	GLN
1	A	192	ASN
1	A	238	GLN

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Mol	Chain	Res	Type
1	A	345	ASN
1	A	523	HIS
1	A	538	HIS
1	A	754	ASN
1	A	824	GLN
1	A	1018	ASN
1	A	1048	ASN
1	A	1104	GLN
1	B	46	GLN
1	B	99	GLN
1	B	154	GLN
1	B	192	ASN
1	B	238	GLN
1	B	345	ASN
1	B	407	ASN
1	B	523	HIS
1	B	538	HIS
1	B	824	GLN
1	B	1048	ASN
1	B	1104	GLN
1	C	46	GLN
1	C	99	GLN
1	C	154	GLN
1	C	192	ASN
1	C	238	GLN
1	C	345	ASN
1	C	357	ASN
1	C	523	HIS
1	C	538	HIS
1	C	754	ASN
1	C	1048	ASN
1	C	1105	ASN

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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

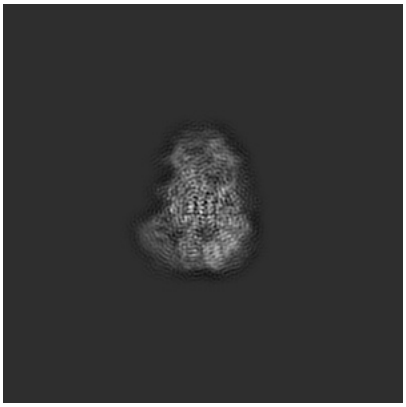
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6526. These allow visual inspection of the internal detail of the map and identification of artifacts.

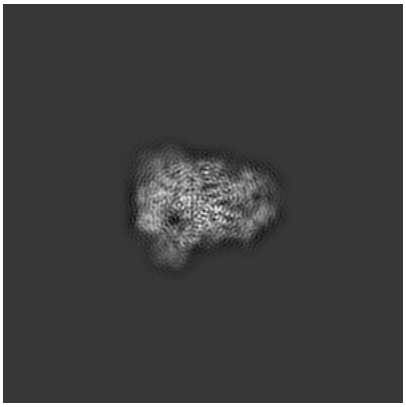
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

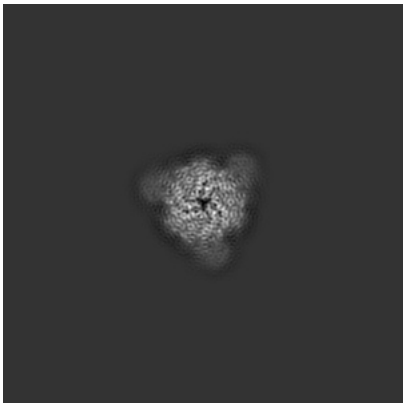
6.1.1 Primary map



X



Y

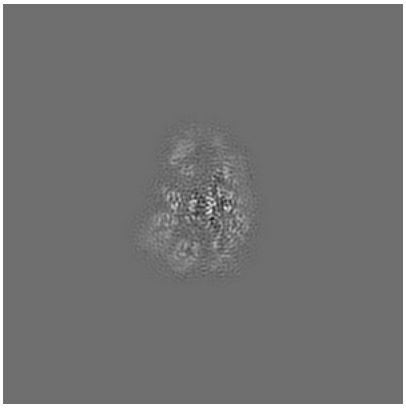


Z

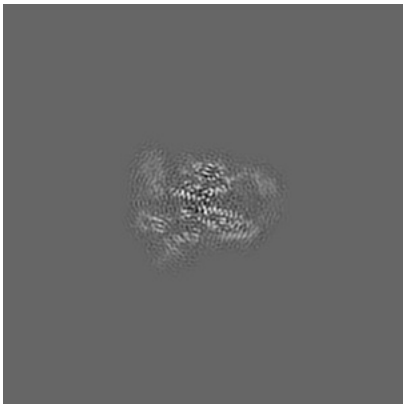
The images above show the map projected in three orthogonal directions.

6.2 Central slices

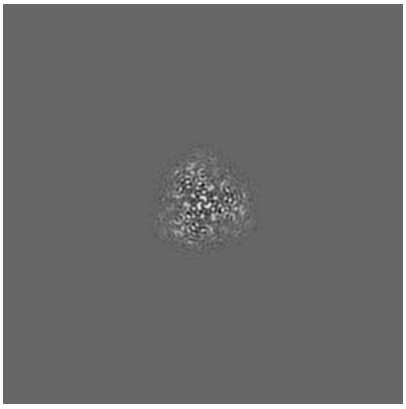
6.2.1 Primary map



X Index: 144



Y Index: 144

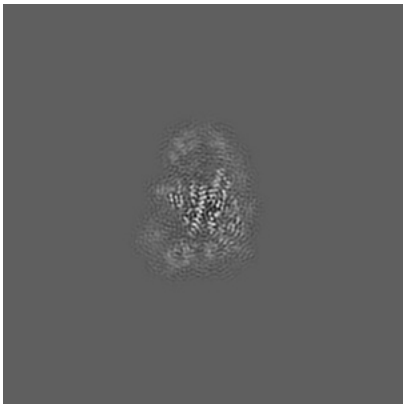


Z Index: 144

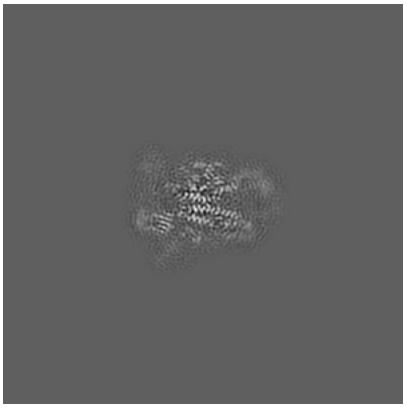
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

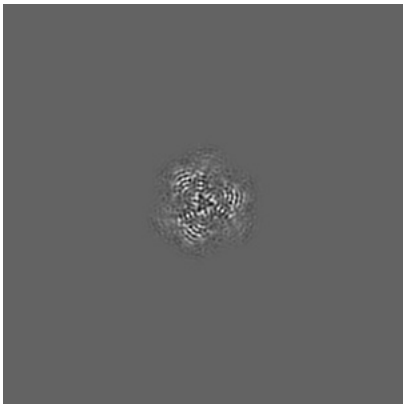
6.3.1 Primary map



X Index: 140



Y Index: 142

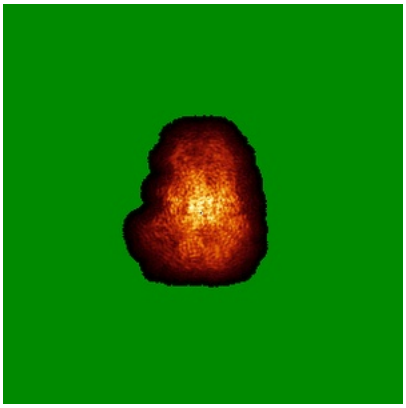


Z Index: 146

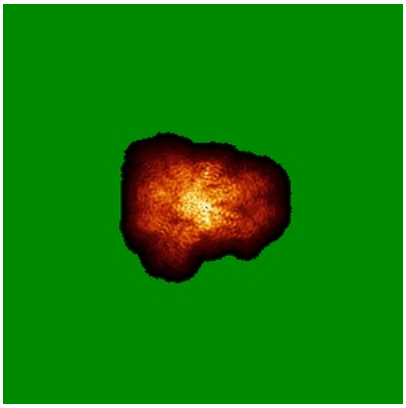
The images above show the largest variance slices of the map in three orthogonal directions.

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

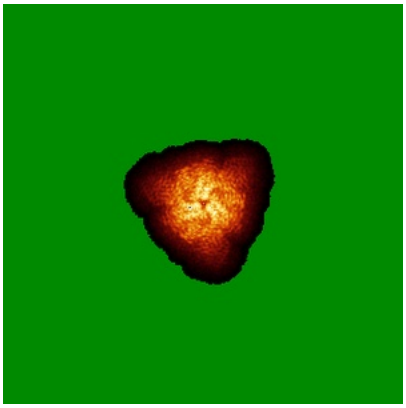
6.4.1 Primary map



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

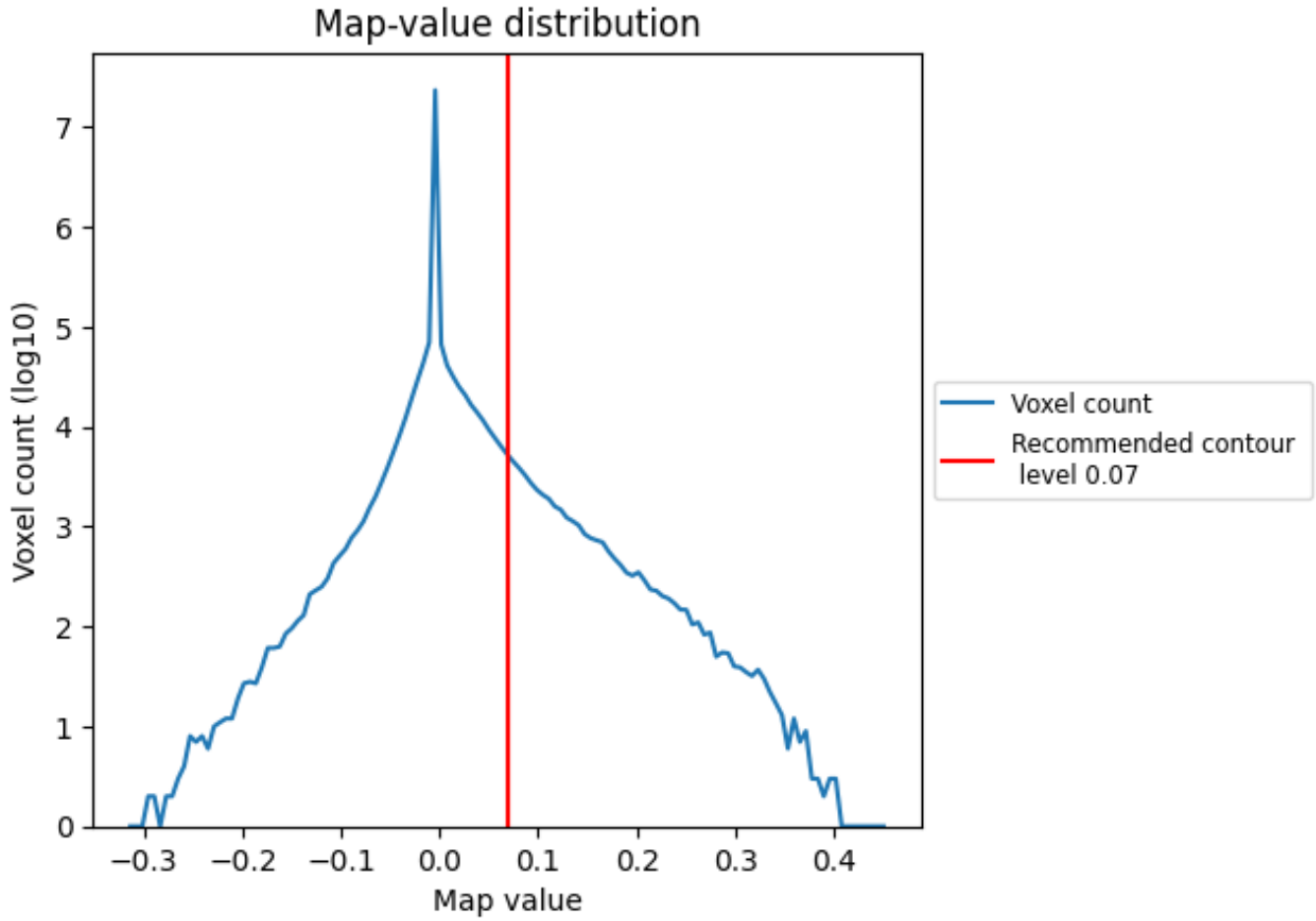
6.6 Mask visualisation (i)

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

7 Map analysis

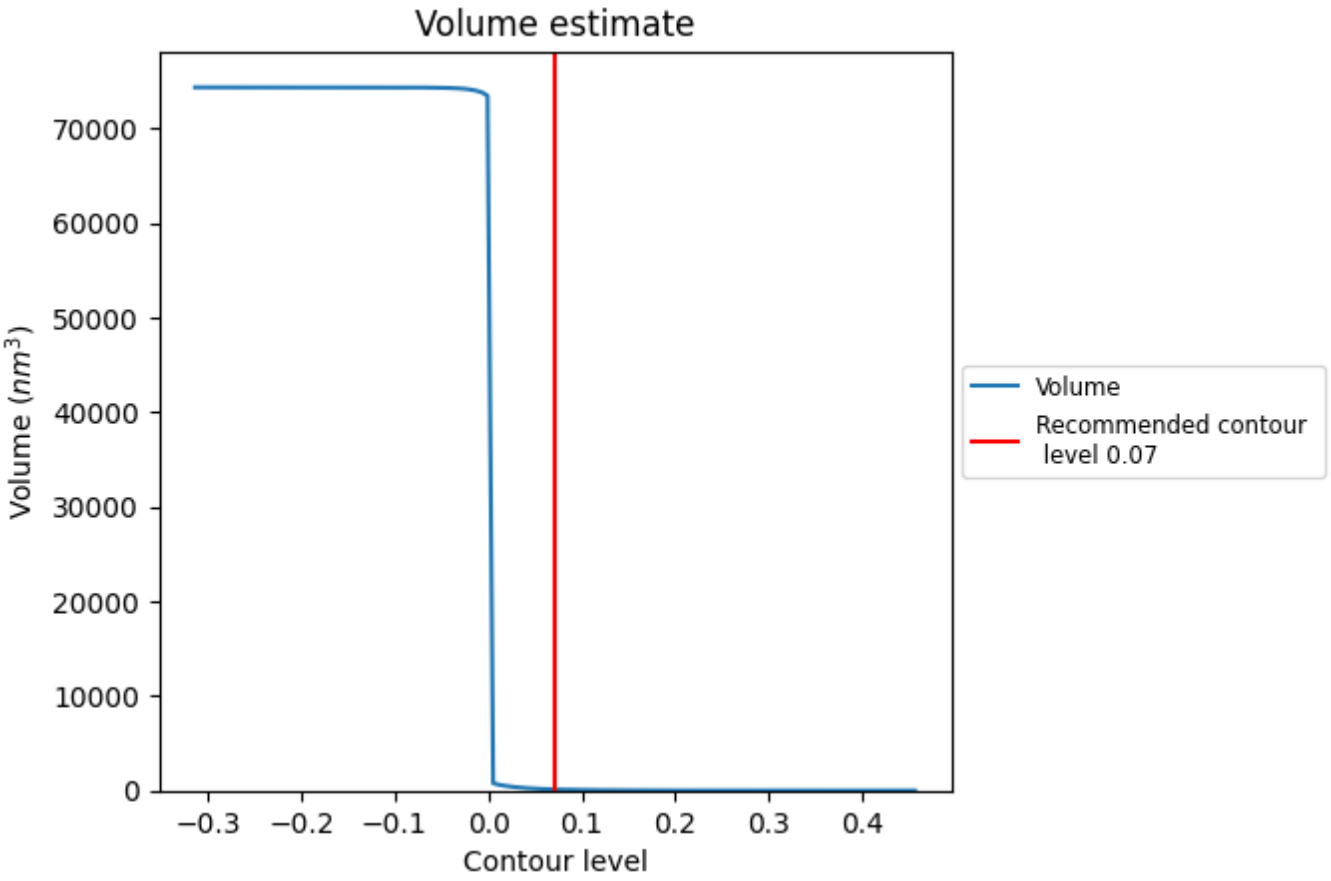
This section contains the results of statistical analysis of the map.

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.

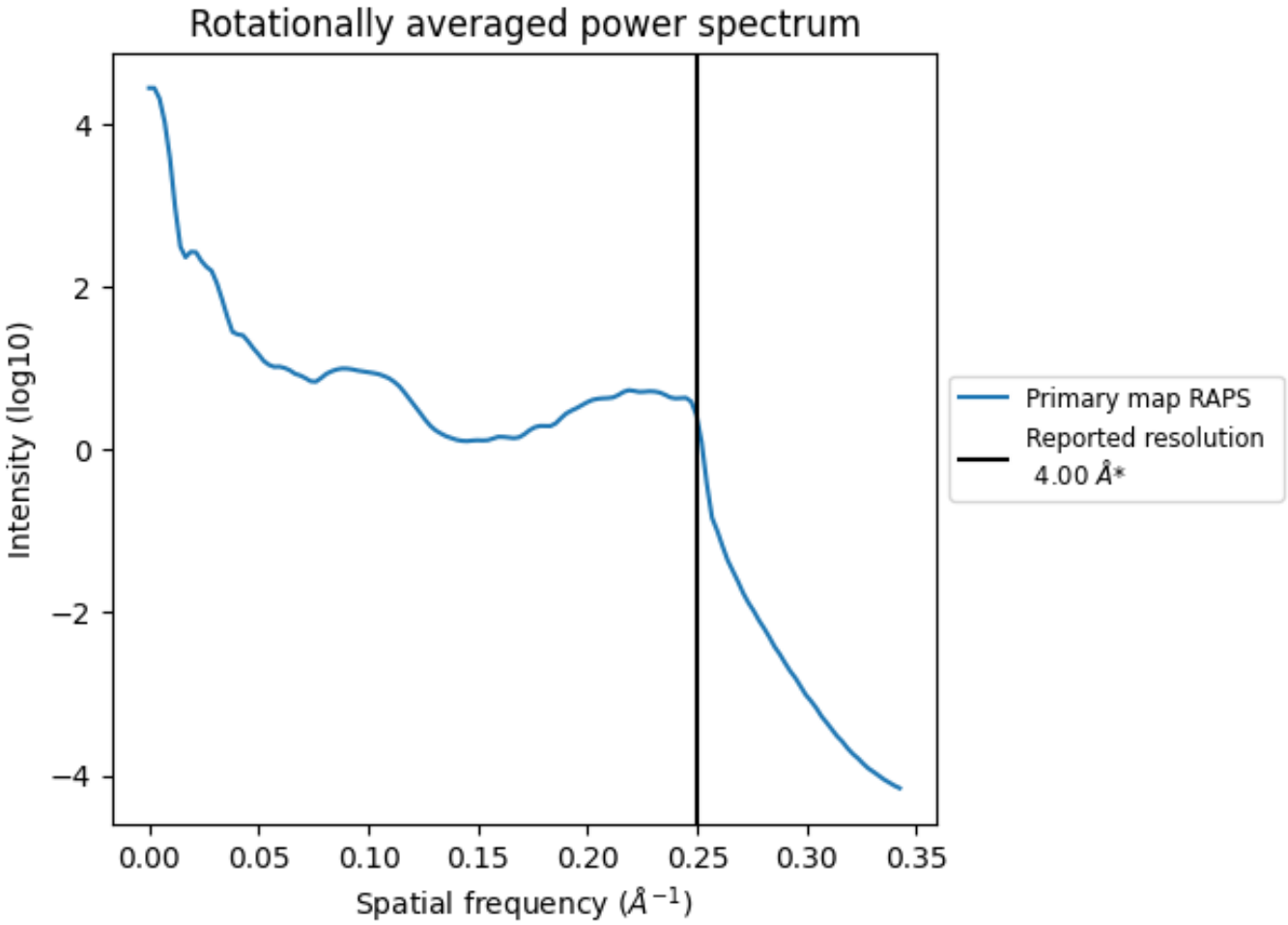
7.2 Volume estimate (i)



The volume at the recommended contour level is 122 nm^3; this corresponds to an approximate mass of 110 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}

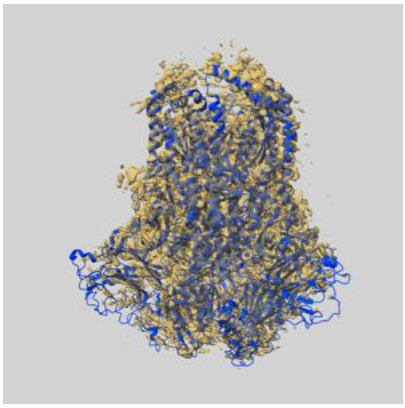
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

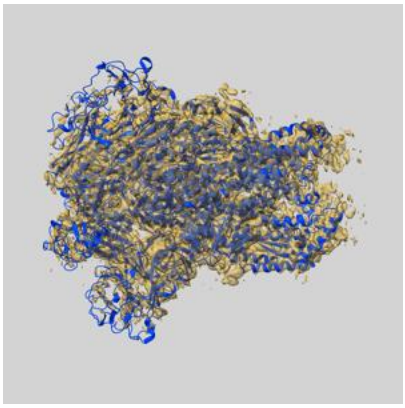
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6526 and PDB model 3JCL. Per-residue inclusion information can be found in section 3 on page 7.

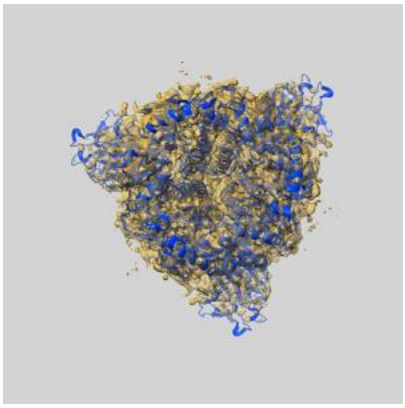
9.1 Map-model overlay



X



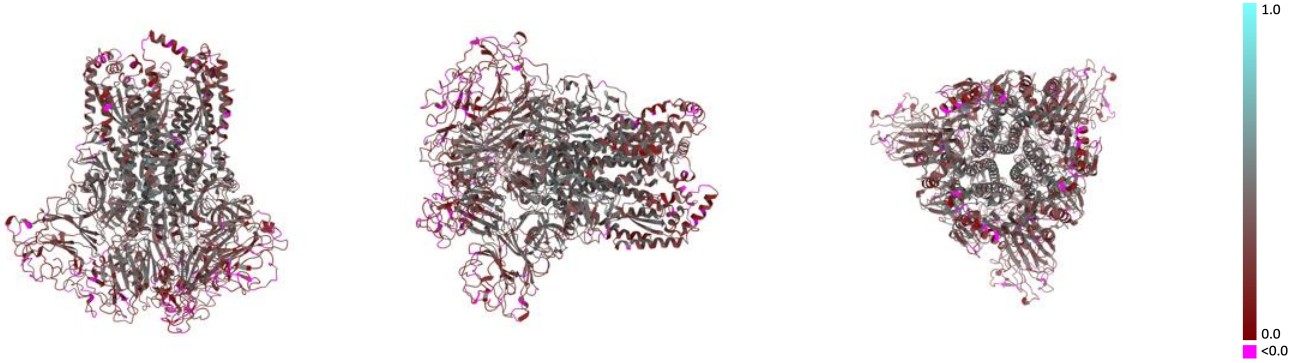
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

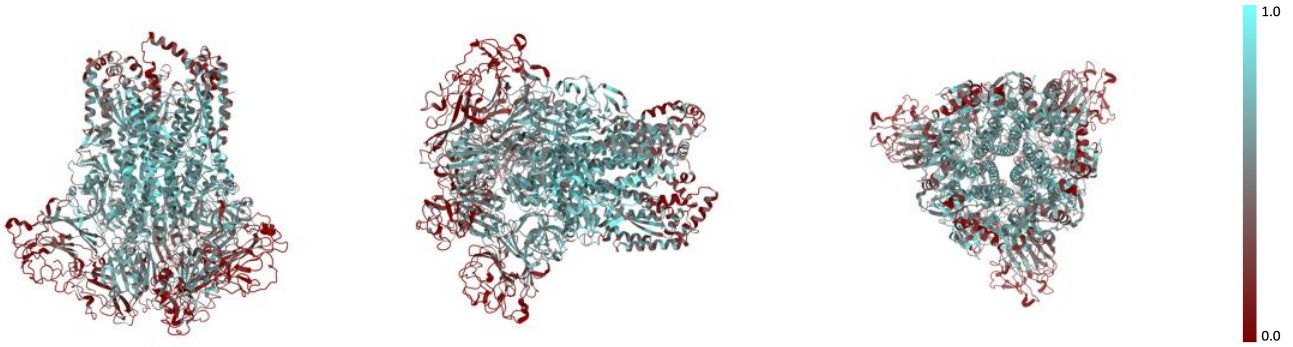
9.2 Q-score mapped to coordinate model (i)



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.

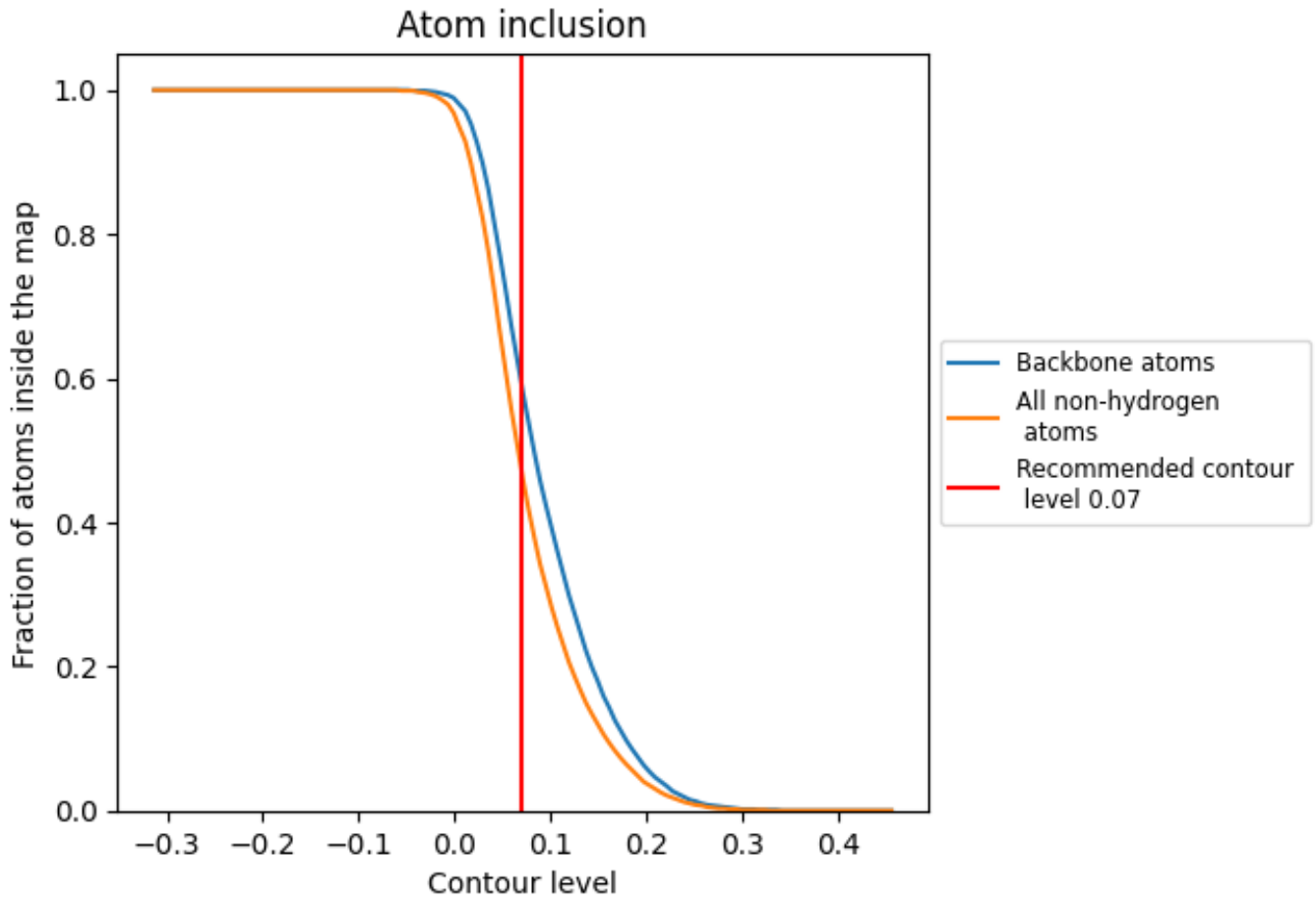
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 47% 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 (0.07) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.4710	0.3120
A	0.4720	0.3120
B	0.4700	0.3120
C	0.4700	0.3120