Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 05:17 AM JST

PDB ID	:	7VXD
EMDB ID	:	EMD-32176
Title	:	SARS-CoV-2 spike protein in complex with ACE2, Beta variant, C1 state
Authors	:	Xu, C.; Cong, Y.
Deposited on	:	2021-11-12
Resolution	:	4.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

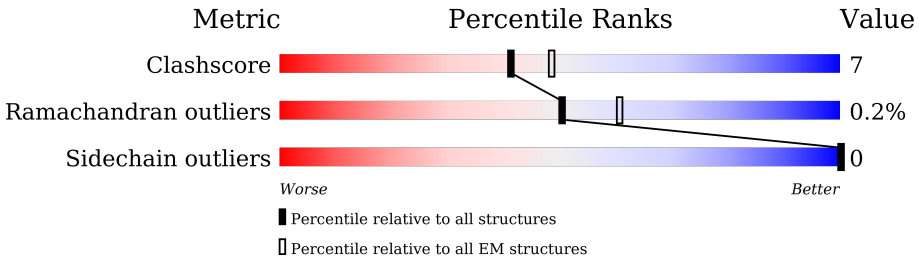
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1258	10% 69% 17% 14%
1	B	1258	8% 68% 18% 14%
1	D	1258	9% 68% 17% 15%
2	C	625	46% 81% 14% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30194 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	1079	Total 8453	C 5398	N 1410	O 1606	S 39	0	0
1	D	1075	Total 8423	C 5382	N 1403	O 1599	S 39	0	0
1	B	1078	Total 8448	C 5396	N 1409	O 1604	S 39	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	243	ILE	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	ASN	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	TYR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	TYR	-	expression tag	UNP P0DTC2
A	1247	LYS	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	ASP	-	expression tag	UNP P0DTC2
A	1251	ASP	-	expression tag	UNP P0DTC2
A	1252	LYS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
D	18	PHE	LEU	variant	UNP P0DTC2
D	80	ALA	ASP	variant	UNP P0DTC2
D	215	GLY	ASP	variant	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	ALA	deletion	UNP P0DTC2
D	243	ILE	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	484	LYS	GLU	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	682	GLY	ARG	variant	UNP P0DTC2
D	683	SER	ARG	variant	UNP P0DTC2
D	685	SER	ARG	variant	UNP P0DTC2
D	701	VAL	ALA	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1207	GLU	-	expression tag	UNP P0DTC2
D	1208	GLN	-	expression tag	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLU	-	expression tag	UNP P0DTC2
D	1239	ASN	-	expression tag	UNP P0DTC2
D	1240	LEU	-	expression tag	UNP P0DTC2
D	1241	TYR	-	expression tag	UNP P0DTC2
D	1242	PHE	-	expression tag	UNP P0DTC2
D	1243	GLN	-	expression tag	UNP P0DTC2
D	1244	GLY	-	expression tag	UNP P0DTC2
D	1245	ASP	-	expression tag	UNP P0DTC2
D	1246	TYR	-	expression tag	UNP P0DTC2
D	1247	LYS	-	expression tag	UNP P0DTC2
D	1248	ASP	-	expression tag	UNP P0DTC2
D	1249	ASP	-	expression tag	UNP P0DTC2
D	1250	ASP	-	expression tag	UNP P0DTC2
D	1251	ASP	-	expression tag	UNP P0DTC2
D	1252	LYS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	HIS	-	expression tag	UNP P0DTC2
D	1259	HIS	-	expression tag	UNP P0DTC2
D	1260	HIS	-	expression tag	UNP P0DTC2
D	1261	HIS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	243	ILE	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	701	VAL	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	ASN	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	TYR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	TYR	-	expression tag	UNP P0DTC2
B	1247	LYS	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	ASP	-	expression tag	UNP P0DTC2
B	1251	ASP	-	expression tag	UNP P0DTC2
B	1252	LYS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q9BYF1
C	1	HIS	-	expression tag	UNP Q9BYF1
C	2	SER	-	expression tag	UNP Q9BYF1
C	3	SER	-	expression tag	UNP Q9BYF1
C	4	ALA	-	expression tag	UNP Q9BYF1
C	5	LEU	-	expression tag	UNP Q9BYF1
C	6	LEU	-	expression tag	UNP Q9BYF1
C	7	CYS	-	expression tag	UNP Q9BYF1

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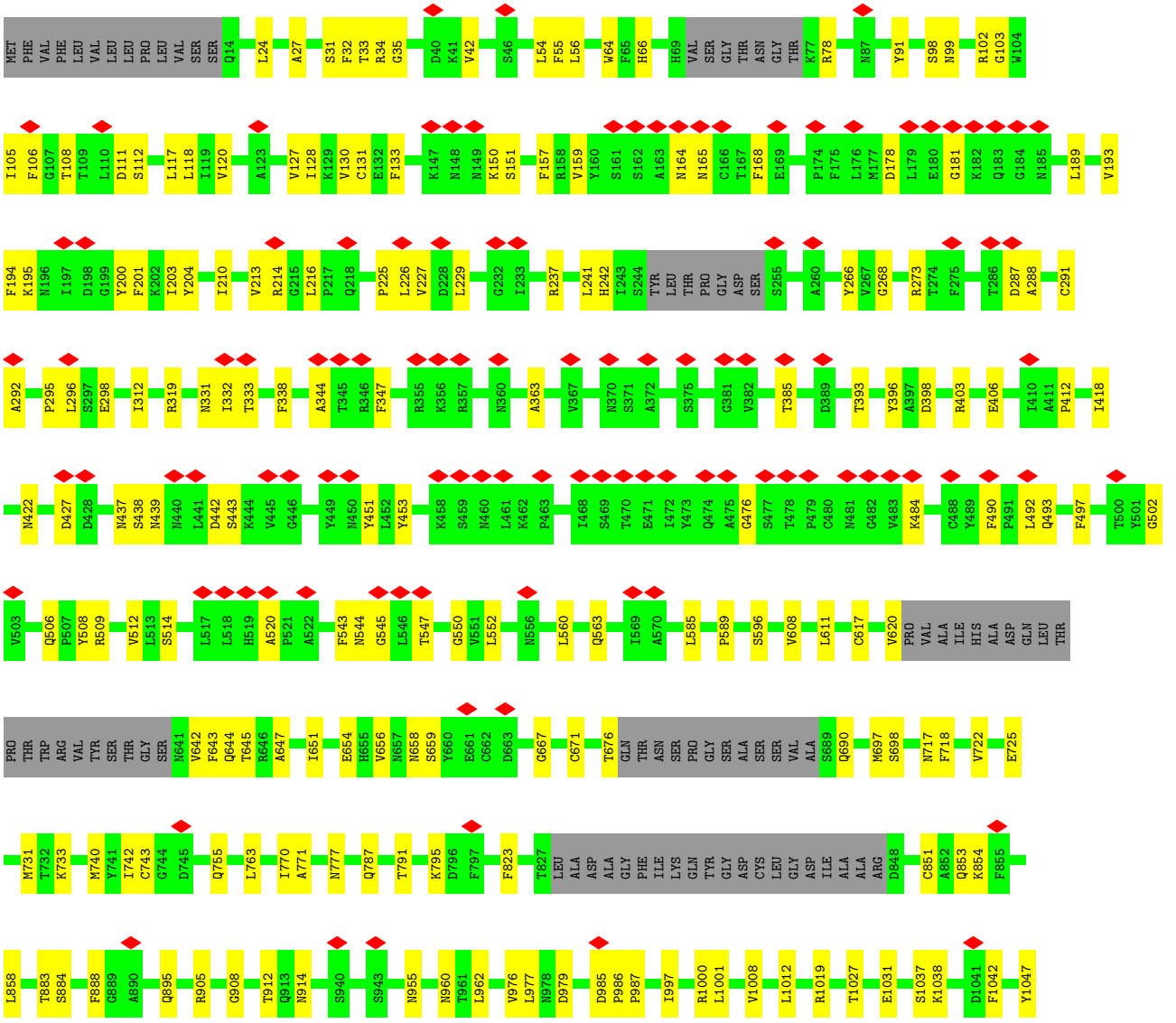
Chain	Residue	Modelled	Actual	Comment	Reference
C	8	CYS	-	expression tag	UNP Q9BYF1
C	9	LEU	-	expression tag	UNP Q9BYF1
C	10	VAL	-	expression tag	UNP Q9BYF1
C	11	LEU	-	expression tag	UNP Q9BYF1
C	12	LEU	-	expression tag	UNP Q9BYF1
C	13	THR	-	expression tag	UNP Q9BYF1
C	14	GLY	-	expression tag	UNP Q9BYF1
C	15	VAL	-	expression tag	UNP Q9BYF1
C	16	ARG	-	expression tag	UNP Q9BYF1
C	616	HIS	-	expression tag	UNP Q9BYF1
C	617	HIS	-	expression tag	UNP Q9BYF1
C	618	HIS	-	expression tag	UNP Q9BYF1
C	619	HIS	-	expression tag	UNP Q9BYF1
C	620	HIS	-	expression tag	UNP Q9BYF1
C	621	HIS	-	expression tag	UNP Q9BYF1
C	622	HIS	-	expression tag	UNP Q9BYF1
C	623	HIS	-	expression tag	UNP Q9BYF1
C	624	HIS	-	expression tag	UNP Q9BYF1

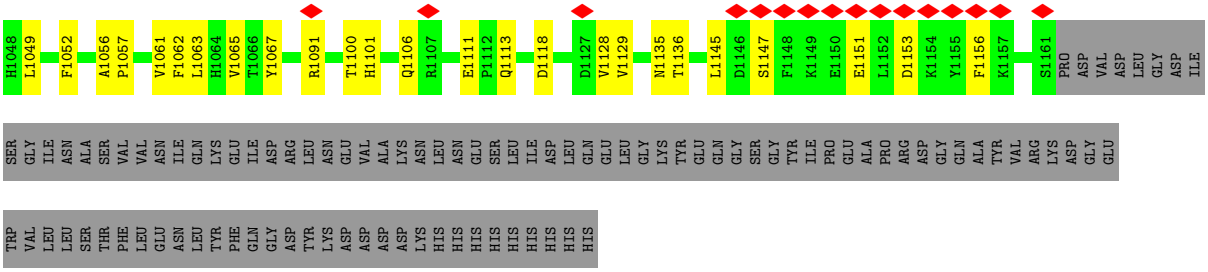
3 Residue-property plots (i)

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

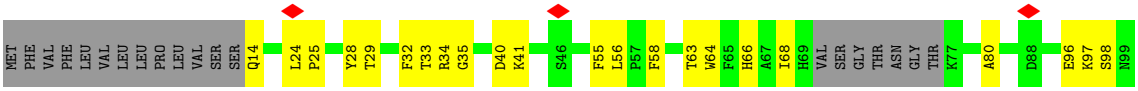
Chain A:

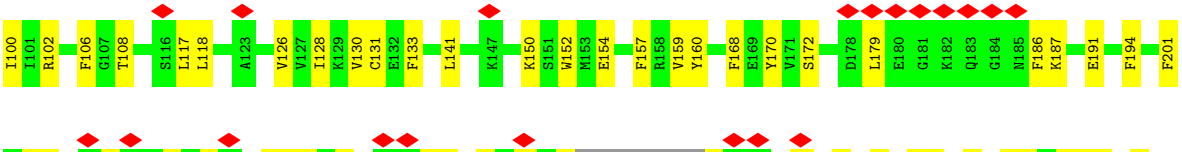


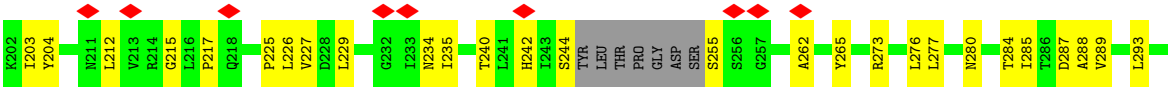


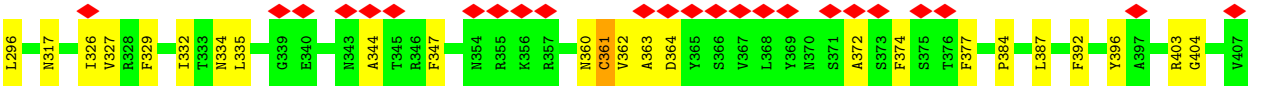
• Molecule 1: Spike glycoprotein

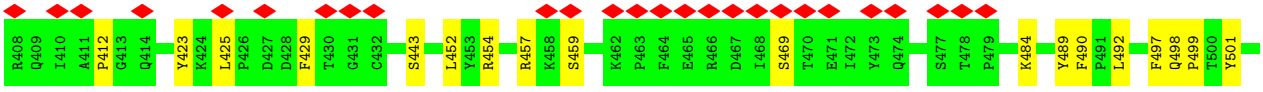
Chain D:

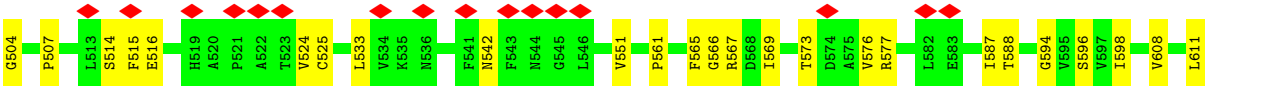


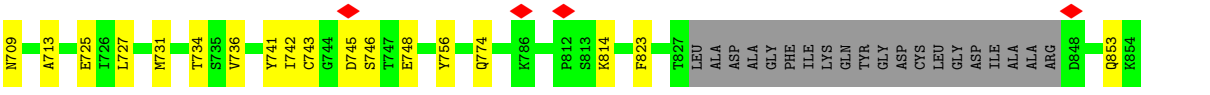


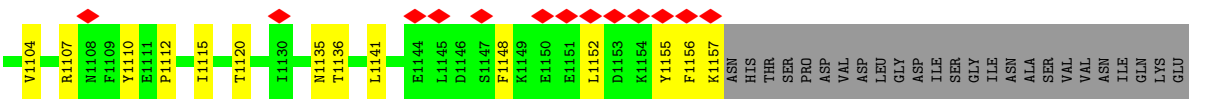


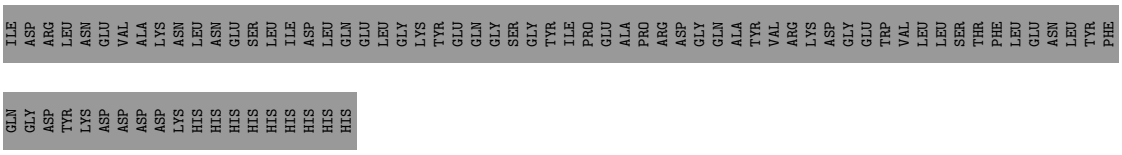






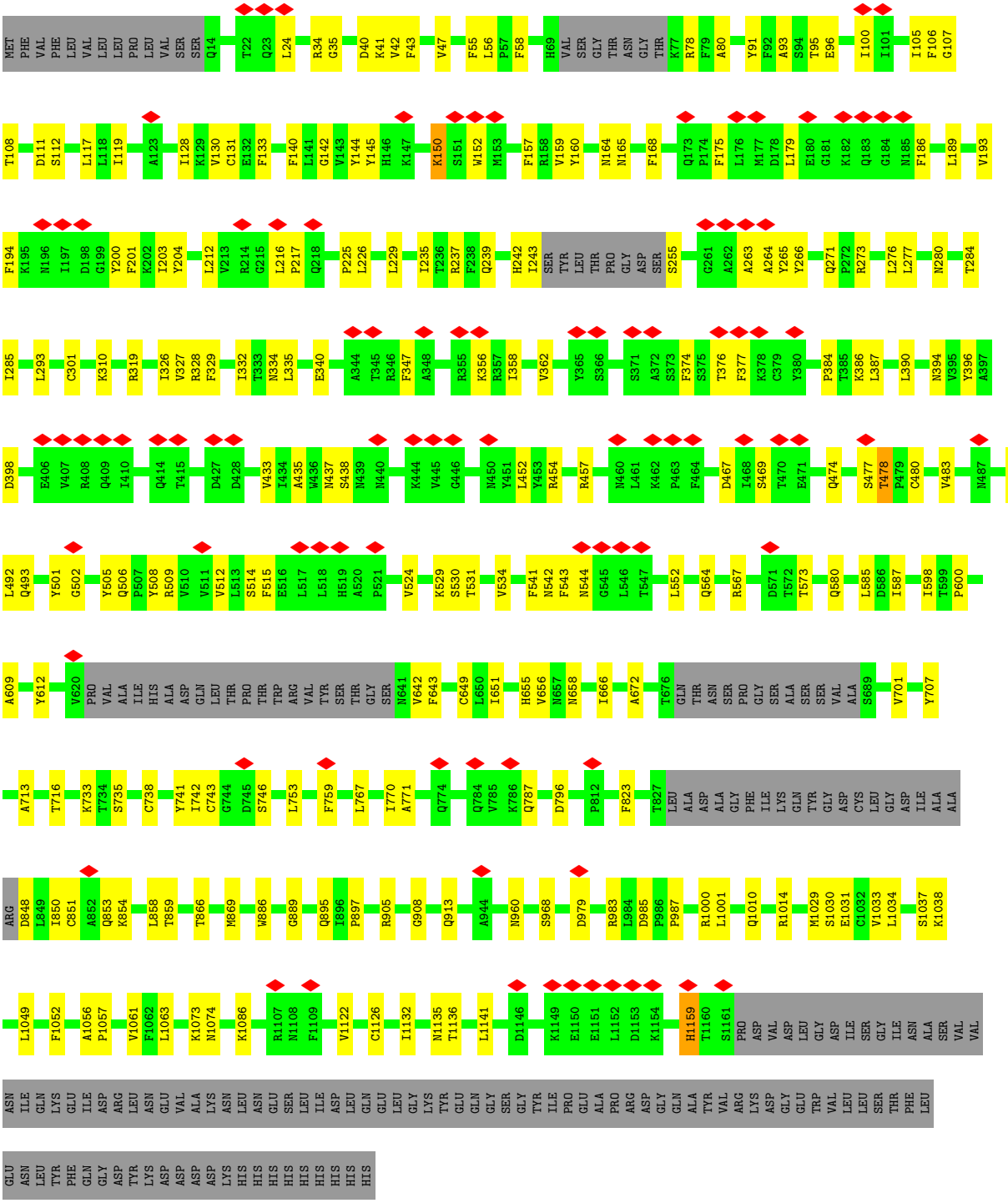






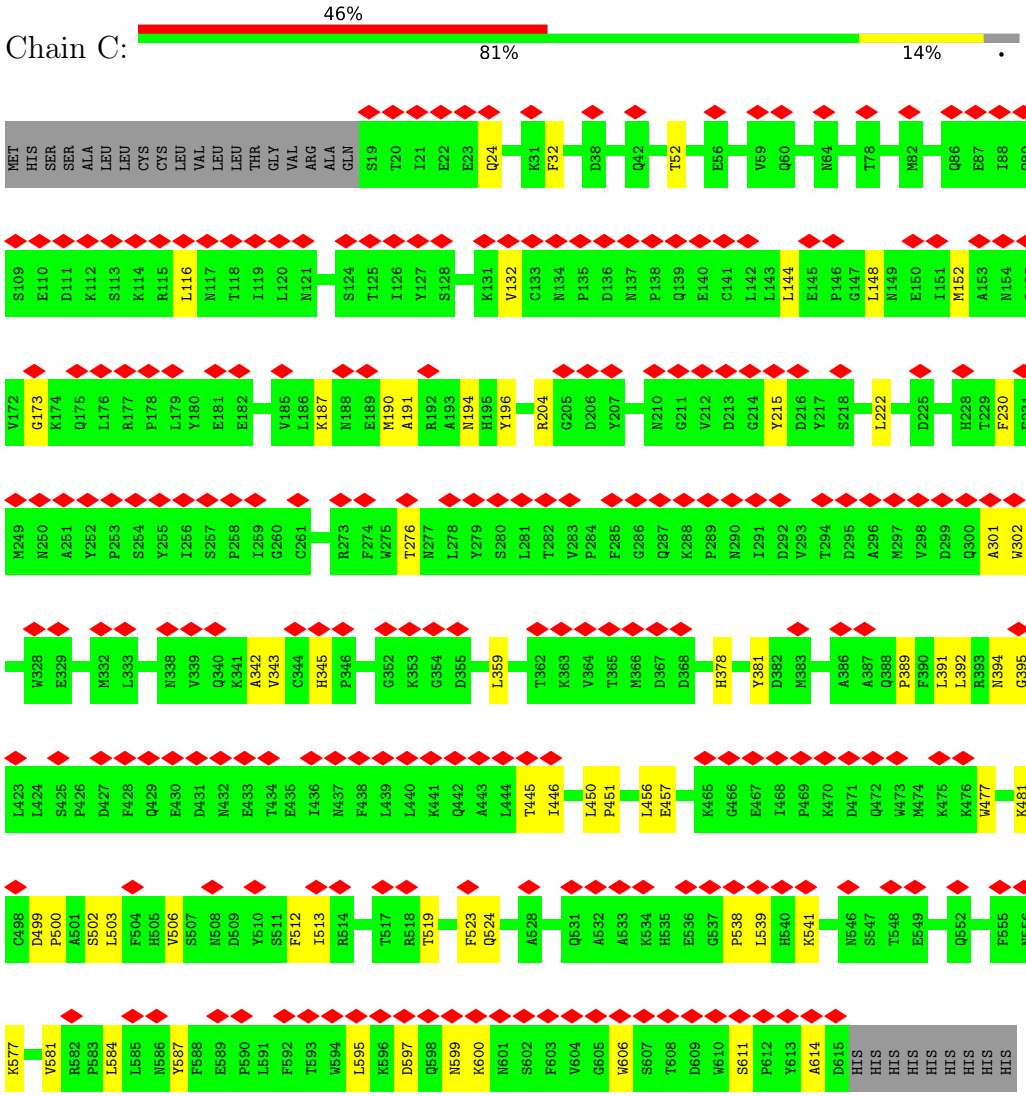
• Molecule 1: Spike glycoprotein

Chain B:



• Molecule 2: Angiotensin-converting enzyme 2

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9689	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.006	Depositor
Minimum map value	-1.514	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.703	Depositor
Map size (Å)	393.48, 393.48, 393.48	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	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	0.25	0/8651	0.42	0/11766
1	B	0.29	2/8646 (0.0%)	0.42	0/11760
1	D	0.26	1/8620 (0.0%)	0.42	0/11724
2	C	0.23	0/5007	0.37	0/6803
All	All	0.26	3/30924 (0.0%)	0.41	0/42053

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	GLN	C-N	12.05	1.57	1.34
1	B	478	THR	C-N	6.48	1.46	1.34
1	D	25	PRO	C-N	5.11	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8453	0	8240	134	0
1	B	8448	0	8243	152	0
1	D	8423	0	8223	143	0
2	C	4870	0	4643	51	0
All	All	30194	0	29349	442	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 7.

All (442) 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:D:332:ILE:HG23	1:D:362:VAL:HG21	1.38	1.04
1:D:332:ILE:CG2	1:D:362:VAL:HG21	1.90	1.01
1:D:362:VAL:HG22	1:D:524:VAL:HG11	1.51	0.90
1:A:273:ARG:NH2	1:A:291:CYS:O	2.09	0.85
1:D:361:CYS:HB3	1:D:392:PHE:H	1.40	0.84
1:A:55:PHE:HB2	1:A:273:ARG:HB2	1.60	0.83
1:D:1157:LYS:C	1:B:1159:HIS:CE1	2.52	0.83
1:D:1089:PHE:HB3	1:B:913:GLN:HE21	1.47	0.79
1:D:361:CYS:HB2	1:D:392:PHE:HB2	1.65	0.79
1:B:142:GLY:HA3	1:B:243:ILE:HG22	1.64	0.77
1:B:398:ASP:HB3	1:B:512:VAL:HB	1.66	0.76
1:D:332:ILE:HG23	1:D:362:VAL:CG2	2.15	0.76
1:B:452:LEU:HB3	1:B:492:LEU:HD11	1.69	0.73
1:A:31:SER:HB2	1:A:34:ARG:HB2	1.70	0.72
1:A:24:LEU:HD21	1:A:78:ARG:HB3	1.73	0.71
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.73	0.69
1:D:102:ARG:HH12	1:D:244:SER:HA	1.57	0.69
1:B:193:VAL:HB	1:B:204:TYR:HD2	1.58	0.68
1:B:362:VAL:HG22	1:B:524:VAL:HG21	1.75	0.68
1:D:361:CYS:CB	1:D:392:PHE:HB2	2.23	0.68
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.76	0.68
1:A:193:VAL:HB	1:A:204:TYR:HD2	1.59	0.67
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.27	0.67
1:B:80:ALA:O	1:B:242:HIS:NE2	2.27	0.67
1:D:713:ALA:HB3	1:B:895:GLN:H	1.60	0.66
1:B:201:PHE:HB2	1:B:229:LEU:HB2	1.78	0.66
1:B:327:VAL:O	1:B:531:THR:OG1	2.14	0.66
2:C:152:MET:O	2:C:161:ARG:NH1	2.29	0.65
1:B:1052:PHE:HB2	1:B:1063:LEU:HB2	1.78	0.65
1:D:326:ILE:HG21	1:D:533:LEU:HD13	1.78	0.65
2:C:538:PRO:HD2	2:C:541:LYS:HD2	1.80	0.64
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.27	0.64
1:D:334:ASN:OD1	1:D:335:LEU:N	2.30	0.64
1:D:1045:LYS:NZ	1:B:889:GLY:O	2.29	0.64
1:D:335:LEU:HD23	1:D:364:ASP:HA	1.80	0.64
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.31	0.63
1:D:126:VAL:HB	1:D:172:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.32	0.63
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.31	0.63
1:B:452:LEU:HD13	1:B:492:LEU:HD21	1.79	0.63
1:A:740:MET:SD	1:B:319:ARG:NH2	2.69	0.63
2:C:457:GLU:HG2	2:C:513:ILE:HD13	1.81	0.63
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.32	0.63
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.81	0.62
1:B:384:PRO:HA	1:B:387:LEU:HB2	1.82	0.62
1:A:201:PHE:HB2	1:A:229:LEU:HB2	1.82	0.62
1:A:99:ASN:ND2	1:A:178:ASP:O	2.30	0.62
1:D:742:ILE:O	1:D:1000:ARG:NH1	2.33	0.61
2:C:524:GLN:HB3	2:C:574:VAL:HG11	1.82	0.61
1:D:1052:PHE:HB2	1:D:1063:LEU:HB2	1.82	0.61
1:B:376:THR:HB	1:B:435:ALA:HB3	1.82	0.61
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.82	0.61
1:B:457:ARG:NH1	1:B:467:ASP:OD2	2.33	0.61
1:B:853:GLN:NE2	1:B:960:ASN:OD1	2.33	0.61
1:D:1135:ASN:OD1	1:D:1136:THR:N	2.30	0.61
1:A:105:ILE:HB	1:A:241:LEU:HD11	1.83	0.60
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.83	0.60
2:C:595:LEU:O	2:C:599:ASN:ND2	2.31	0.60
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.31	0.60
1:D:108:THR:OG1	1:D:234:ASN:O	2.19	0.60
1:A:189:LEU:HD22	1:A:210:ILE:HD13	1.84	0.60
1:D:201:PHE:HB2	1:D:229:LEU:HB2	1.84	0.60
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.31	0.60
1:D:454:ARG:NH1	1:D:469:SER:O	2.34	0.60
1:D:317:ASN:HD22	1:D:594:GLY:HA2	1.67	0.59
1:D:396:TYR:HB2	1:D:514:SER:HB2	1.84	0.59
1:B:552:LEU:HB3	1:B:585:LEU:HD11	1.83	0.59
1:B:387:LEU:HD13	1:B:515:PHE:HE2	1.66	0.59
1:D:1077:THR:HG21	1:B:897:PRO:HG2	1.83	0.59
1:B:55:PHE:HB2	1:B:273:ARG:HB2	1.84	0.59
1:A:164:ASN:OD1	1:A:165:ASN:N	2.36	0.59
1:D:332:ILE:HG21	1:D:362:VAL:HG21	1.80	0.59
2:C:394:ASN:OD1	2:C:395:GLY:N	2.36	0.59
1:A:319:ARG:NH1	1:D:745:ASP:OD1	2.32	0.59
1:A:443:SER:HA	1:A:497:PHE:HB3	1.83	0.59
1:B:454:ARG:NH1	1:B:469:SER:O	2.34	0.59
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.30	0.59
1:A:200:TYR:OH	1:B:394:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:PRO:HD2	2:C:392:LEU:HD12	1.84	0.59
1:A:547:THR:OG1	1:D:978:ASN:ND2	2.35	0.59
2:C:190:MET:O	2:C:194:ASN:ND2	2.34	0.59
1:A:438:SER:HB3	1:A:509:ARG:HG3	1.85	0.59
2:C:451:PRO:HB2	2:C:485:VAL:HG12	1.85	0.58
1:D:883:THR:O	1:D:901:GLN:NE2	2.36	0.58
1:D:14:GLN:N	1:D:255:SER:HG	2.00	0.58
1:B:58:PHE:HB2	1:B:293:LEU:HD22	1.85	0.58
1:B:194:PHE:HE1	1:B:203:ILE:HG23	1.69	0.58
1:D:725:GLU:OE2	1:D:1028:LYS:NZ	2.34	0.58
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.68	0.58
1:D:277:LEU:HD22	1:D:285:ILE:HD13	1.86	0.58
1:A:103:GLY:O	1:A:242:HIS:NE2	2.27	0.58
1:D:746:SER:OG	1:D:748:GLU:OE1	2.20	0.58
2:C:144:LEU:HA	2:C:148:LEU:HB2	1.84	0.58
2:C:204:ARG:HG2	2:C:222:LEU:HD23	1.86	0.58
1:B:216:LEU:HD21	1:B:266:TYR:HE2	1.68	0.57
1:B:329:PHE:HE1	1:B:544:ASN:H	1.50	0.57
1:A:385:THR:HG1	1:B:477:SER:HG	1.48	0.57
1:A:895:GLN:NE2	1:B:1074:ASN:OD1	2.37	0.57
1:B:612:TYR:HB2	1:B:649:CYS:HB3	1.86	0.57
2:C:378:HIS:HE1	2:C:402:GLU:HA	1.70	0.57
1:B:164:ASN:OD1	1:B:165:ASN:N	2.32	0.57
1:A:32:PHE:CD2	1:A:33:THR:HG23	2.39	0.57
1:A:717:ASN:OD1	1:A:718:PHE:N	2.36	0.57
1:A:412:PRO:HB3	1:A:427:ASP:HA	1.87	0.57
2:C:503:LEU:HD23	2:C:506:VAL:HG23	1.87	0.57
1:A:106:PHE:HD2	1:A:117:LEU:HD23	1.70	0.57
1:D:106:PHE:HB3	1:D:235:ILE:HD13	1.87	0.57
2:C:446:ILE:HD13	2:C:523:PHE:HZ	1.69	0.57
1:B:100:ILE:HD12	1:B:263:ALA:HB2	1.87	0.57
1:B:334:ASN:OD1	1:B:335:LEU:N	2.31	0.57
1:B:642:VAL:HG22	1:B:651:ILE:HG12	1.87	0.57
1:D:403:ARG:HG2	1:D:497:PHE:HE1	1.70	0.56
1:A:883:THR:OG1	1:B:707:TYR:OH	2.17	0.56
1:D:55:PHE:HB2	1:D:273:ARG:HB2	1.85	0.56
1:D:1039:ARG:NE	1:B:1031:GLU:OE2	2.32	0.56
1:A:451:TYR:HD2	1:A:497:PHE:HE2	1.52	0.56
1:A:656:VAL:HG12	1:A:658:ASN:H	1.70	0.56
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.36	0.56
1:D:551:VAL:N	1:D:588:THR:O	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD21	1:A:266:TYR:HE2	1.71	0.55
2:C:32:PHE:HE2	2:C:391:LEU:HD21	1.71	0.55
2:C:539:LEU:HD23	2:C:587:TYR:HB2	1.89	0.55
1:B:1010:GLN:HB3	1:B:1014:ARG:HH12	1.72	0.55
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.89	0.55
1:D:1152:LEU:HD23	1:D:1155:TYR:HD2	1.71	0.55
1:A:755:GLN:O	1:B:968:SER:OG	2.24	0.55
1:B:140:PHE:HZ	1:B:255:SER:HB2	1.72	0.55
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.88	0.54
1:A:883:THR:HG23	1:B:707:TYR:HE1	1.72	0.54
1:D:35:GLY:HA3	1:D:56:LEU:HB3	1.89	0.54
1:D:452:LEU:HB3	1:D:492:LEU:HD11	1.90	0.54
1:A:42:VAL:HG13	1:B:567:ARG:H	1.72	0.54
1:B:387:LEU:HD23	1:B:390:LEU:HD12	1.89	0.54
1:D:32:PHE:CD2	1:D:33:THR:HG23	2.42	0.54
1:D:736:VAL:HG22	1:D:858:LEU:HG	1.90	0.54
1:D:457:ARG:NH1	1:D:459:SER:OG	2.41	0.54
1:A:120:VAL:HB	1:A:127:VAL:HB	1.90	0.54
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.41	0.54
1:D:152:TRP:CD2	1:D:179:LEU:HB2	2.43	0.54
1:D:756:TYR:OH	1:D:994:ASP:OD1	2.26	0.54
1:B:128:ILE:HD13	1:B:229:LEU:HD11	1.90	0.54
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.89	0.53
1:B:374:PHE:H	1:B:377:PHE:HZ	1.54	0.53
1:B:474:GLN:NE2	1:B:478:THR:O	2.41	0.53
1:D:212:LEU:HD22	1:D:217:PRO:HD3	1.91	0.53
1:B:853:GLN:HB3	1:B:858:LEU:HD12	1.90	0.53
2:C:611:SER:HB3	2:C:614:ALA:HB3	1.90	0.53
2:C:235:PRO:O	2:C:239:HIS:ND1	2.37	0.53
1:D:360:ASN:N	1:D:360:ASN:HD22	2.07	0.53
1:D:977:LEU:HD22	1:D:993:ILE:HG12	1.91	0.53
1:B:280:ASN:OD1	1:B:284:THR:N	2.37	0.53
1:B:850:ILE:HG22	1:B:854:LYS:HE3	1.91	0.53
1:D:814:LYS:NZ	1:D:872:GLN:OE1	2.41	0.52
1:B:656:VAL:HG12	1:B:658:ASN:H	1.74	0.52
1:A:213:VAL:HG13	1:A:214:ARG:H	1.73	0.52
1:D:194:PHE:HE1	1:D:203:ILE:HG23	1.74	0.52
1:D:361:CYS:HB3	1:D:392:PHE:N	2.17	0.52
1:D:905:ARG:NH1	1:D:1049:LEU:O	2.40	0.52
2:C:96:GLN:HE21	2:C:392:LEU:HG	1.73	0.52
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:GLN:HG2	2:C:104:GLY:H	1.74	0.52
1:D:709:ASN:ND2	1:B:796:ASP:OD2	2.43	0.52
1:B:327:VAL:HG22	1:B:542:ASN:HB3	1.91	0.52
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.73	0.52
1:A:117:LEU:HD11	1:A:128:ILE:HG23	1.91	0.52
1:A:131:CYS:HB2	1:A:133:PHE:CE1	2.44	0.52
2:C:482:ARG:O	2:C:606:TRP:NE1	2.38	0.52
1:B:866:THR:HG22	1:B:869:MET:HG2	1.91	0.52
1:A:439:ASN:O	1:A:443:SER:OG	2.27	0.52
1:D:29:THR:HG23	1:D:64:TRP:HB2	1.91	0.52
1:B:738:CYS:HA	1:B:741:TYR:HB3	1.91	0.52
2:C:557:MET:HG3	2:C:569:ALA:HB1	1.91	0.52
1:B:133:PHE:HB3	1:B:160:TYR:CD1	2.45	0.52
1:A:24:LEU:HD13	1:A:66:HIS:CE1	2.45	0.51
1:A:398:ASP:HB3	1:A:512:VAL:HB	1.91	0.51
2:C:52:THR:HG22	2:C:359:LEU:HD13	1.92	0.51
1:B:131:CYS:HB2	1:B:133:PHE:CE1	2.45	0.51
1:B:152:TRP:CD2	1:B:179:LEU:HB2	2.44	0.51
1:A:150:LYS:HG3	1:A:151:SER:H	1.76	0.51
1:A:643:PHE:HE2	1:A:654:GLU:HA	1.75	0.51
1:D:573:THR:HG22	1:D:587:ILE:HG13	1.92	0.51
1:D:1156:PHE:HA	1:B:1159:HIS:CD2	2.45	0.51
1:A:986:PRO:HD3	1:B:386:LYS:HZ1	1.74	0.51
1:B:152:TRP:HB3	1:B:179:LEU:HD12	1.92	0.51
1:B:716:THR:HG21	1:B:1073:LYS:HD2	1.91	0.51
1:A:853:GLN:NE2	1:A:960:ASN:OD1	2.43	0.51
1:A:858:LEU:HD21	1:A:962:LEU:HD23	1.92	0.51
1:A:102:ARG:H	1:A:242:HIS:CE1	2.28	0.51
1:A:550:GLY:HA2	1:A:589:PRO:HA	1.91	0.51
1:A:194:PHE:HE1	1:A:203:ILE:HG23	1.74	0.51
1:A:1111:GLU:HG2	1:A:1113:GLN:HE21	1.76	0.51
2:C:103:ASN:HB3	2:C:106:SER:HB2	1.92	0.51
2:C:144:LEU:HD12	2:C:148:LEU:HB2	1.93	0.51
2:C:301:ALA:O	2:C:306:ARG:NH2	2.44	0.51
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.93	0.51
1:B:742:ILE:HG13	1:B:753:LEU:HD21	1.93	0.51
1:A:1153:ASP:HA	1:A:1156:PHE:HE2	1.76	0.51
1:B:552:LEU:HD22	1:B:585:LEU:HD21	1.92	0.51
1:D:287:ASP:OD1	1:D:288:ALA:N	2.43	0.50
2:C:276:THR:OG1	2:C:445:THR:OG1	2.29	0.50
1:A:287:ASP:OD1	1:A:288:ALA:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:701:VAL:O	1:B:787:GLN:NE2	2.44	0.50
1:A:543:PHE:O	1:A:545:GLY:N	2.44	0.50
1:D:703:ASN:OD1	1:D:704:SER:N	2.45	0.50
1:B:573:THR:HG22	1:B:587:ILE:HG13	1.93	0.50
1:A:108:THR:O	1:A:237:ARG:NH2	2.36	0.50
1:A:1031:GLU:HB3	1:A:1037:SER:HB2	1.94	0.50
1:A:1153:ASP:HA	1:A:1156:PHE:CE2	2.47	0.50
1:D:452:LEU:HD13	1:D:492:LEU:HD21	1.93	0.50
1:B:24:LEU:HG	1:B:78:ARG:HD2	1.93	0.50
1:B:347:PHE:HE2	1:B:509:ARG:HB3	1.76	0.50
1:B:502:GLY:O	1:B:506:GLN:HG3	2.12	0.50
1:B:332:ILE:HG12	1:B:529:LYS:HD3	1.95	0.49
1:D:396:TYR:O	1:D:514:SER:N	2.38	0.49
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.47	0.49
1:A:667:GLY:HA2	1:D:864:LEU:HA	1.94	0.49
1:B:105:ILE:HB	1:B:239:GLN:HB2	1.94	0.49
1:A:676:THR:HA	1:A:690:GLN:HG2	1.94	0.49
1:A:787:GLN:NE2	1:B:701:VAL:O	2.46	0.49
1:D:80:ALA:O	1:D:265:TYR:OH	2.29	0.49
1:B:150:LYS:C	1:B:152:TRP:H	2.16	0.49
1:A:560:LEU:HB2	1:A:563:GLN:HG2	1.95	0.48
1:D:96:GLU:OE1	1:D:100:ILE:N	2.46	0.48
1:D:204:TYR:HD1	1:D:225:PRO:HA	1.78	0.48
1:B:643:PHE:HE2	1:B:655:HIS:H	1.60	0.48
1:D:497:PHE:CE2	1:D:507:PRO:HB3	2.48	0.48
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.94	0.48
1:A:484:LYS:HE2	1:A:490:PHE:HB2	1.94	0.48
1:A:1147:SER:O	1:A:1151:GLU:N	2.46	0.48
2:C:132:VAL:HG23	2:C:168:TRP:HE3	1.78	0.48
1:B:276:LEU:HD11	1:B:301:CYS:HA	1.96	0.48
1:B:108:THR:O	1:B:237:ARG:NH2	2.39	0.48
1:D:226:LEU:HG	1:D:227:VAL:HG13	1.95	0.48
1:D:360:ASN:N	1:D:360:ASN:ND2	2.60	0.48
1:D:567:ARG:HE	1:B:42:VAL:HG11	1.79	0.48
1:D:1157:LYS:C	1:B:1159:HIS:HE1	2.13	0.48
2:C:168:TRP:HE1	2:C:502:SER:HB2	1.78	0.48
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.95	0.48
1:B:144:TYR:HD1	1:B:145:TYR:HD2	1.61	0.48
1:D:484:LYS:HD2	1:D:490:PHE:HB2	1.95	0.47
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.96	0.47
1:B:356:LYS:HE2	1:B:358:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:CYS:HB3	1:A:298:GLU:OE2	2.14	0.47
1:D:332:ILE:HA	1:D:524:VAL:HG22	1.95	0.47
1:D:344:ALA:HB3	1:D:347:PHE:HE1	1.78	0.47
1:D:404:GLY:HA3	1:D:504:GLY:HA2	1.96	0.47
1:A:596:SER:HB2	1:A:611:LEU:HB3	1.97	0.47
2:C:581:VAL:HG13	2:C:584:LEU:HD23	1.97	0.47
2:C:191:ALA:HB1	2:C:196:TYR:HB2	1.95	0.47
1:B:96:GLU:OE1	1:B:100:ILE:N	2.47	0.47
1:A:403:ARG:HB2	1:A:406:GLU:HG2	1.97	0.47
1:B:107:GLY:H	1:B:235:ILE:HG23	1.78	0.47
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.96	0.47
1:D:240:THR:HG21	1:D:242:HIS:CE1	2.50	0.47
1:D:569:ILE:HG22	1:B:47:VAL:HG23	1.97	0.47
1:D:374:PHE:HB2	1:D:377:PHE:CE1	2.50	0.46
1:D:484:LYS:HE3	1:D:489:TYR:HA	1.97	0.46
1:A:986:PRO:HD3	1:B:386:LYS:NZ	2.30	0.46
1:D:276:LEU:HB3	1:D:289:VAL:HB	1.96	0.46
2:C:230:PHE:HA	2:C:233:ILE:HD12	1.96	0.46
1:D:24:LEU:HD13	1:D:66:HIS:CE1	2.50	0.46
1:D:296:LEU:HB2	1:D:608:VAL:HG21	1.98	0.46
1:D:596:SER:HB2	1:D:611:LEU:HB3	1.97	0.46
1:B:95:THR:HG22	1:B:189:LEU:HD13	1.98	0.46
1:A:642:VAL:HA	1:A:651:ILE:HG22	1.96	0.46
1:A:733:LYS:HE3	1:A:771:ALA:HB1	1.96	0.46
1:D:853:GLN:NE2	1:D:960:ASN:OD1	2.46	0.46
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.97	0.46
1:B:212:LEU:HD13	1:B:217:PRO:HD3	1.96	0.46
1:D:58:PHE:HB2	1:D:293:LEU:HD22	1.98	0.46
1:D:1090:PRO:HA	1:D:1120:THR:HG22	1.97	0.46
1:B:979:ASP:O	1:B:983:ARG:NE	2.48	0.46
1:A:552:LEU:HB3	1:A:585:LEU:HD13	1.97	0.46
1:D:97:LYS:HG2	1:D:187:LYS:H	1.80	0.46
1:A:725:GLU:HB3	1:A:1062:PHE:HB2	1.97	0.46
1:D:130:VAL:HB	1:D:168:PHE:HB3	1.98	0.46
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.98	0.46
1:D:329:PHE:HB2	1:D:525:CYS:HB2	1.98	0.46
1:D:332:ILE:HG12	1:D:524:VAL:HG13	1.98	0.46
1:D:662:CYS:HB2	1:D:697:MET:HG3	1.98	0.46
1:B:437:ASN:HA	1:B:508:TYR:HD1	1.79	0.46
1:A:437:ASN:HA	1:A:508:TYR:HD1	1.80	0.45
1:D:131:CYS:HB2	1:D:133:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:PHE:HD2	1:D:525:CYS:HB2	1.80	0.45
1:B:490:PHE:CE2	1:B:492:LEU:HB3	2.51	0.45
1:A:1056:ALA:HB2	1:A:1061:VAL:HG23	1.98	0.45
1:A:1100:THR:HG23	1:A:1101:HIS:H	1.81	0.45
2:C:302:TRP:HA	2:C:306:ARG:HH21	1.80	0.45
1:B:326:ILE:HD13	1:B:534:VAL:H	1.80	0.45
1:D:128:ILE:HD13	1:D:170:TYR:HD2	1.81	0.45
1:A:1027:THR:HG22	1:A:1042:PHE:HZ	1.81	0.45
1:D:280:ASN:OD1	1:D:284:THR:N	2.49	0.45
1:D:561:PRO:HA	1:D:577:ARG:HH12	1.82	0.45
1:B:733:LYS:HE3	1:B:771:ALA:HB1	1.98	0.45
1:D:1107:ARG:HD3	1:B:886:TRP:HZ2	1.81	0.45
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.81	0.45
1:A:453:TYR:CZ	1:A:493:GLN:HB2	2.52	0.45
2:C:450:LEU:HD21	2:C:519:THR:HB	1.99	0.45
2:C:499:ASP:HB3	2:C:500:PRO:HD3	1.99	0.45
1:B:157:PHE:CZ	1:B:159:VAL:HB	2.52	0.45
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.97	0.45
1:D:40:ASP:OD1	1:D:41:LYS:N	2.44	0.45
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.99	0.44
1:D:98:SER:HB2	1:D:179:LEU:HA	1.99	0.44
1:A:98:SER:HB3	1:A:181:GLY:HA2	2.00	0.44
1:D:141:LEU:HD23	1:D:154:GLU:HG3	1.99	0.44
1:D:374:PHE:HB2	1:D:377:PHE:HE1	1.82	0.44
1:D:598:ILE:HG23	1:D:664:ILE:HG21	1.98	0.44
2:C:450:LEU:HB2	2:C:451:PRO:HD3	1.99	0.44
1:B:242:HIS:HE1	1:B:265:TYR:HE2	1.65	0.44
1:A:851:CYS:HA	1:A:854:LYS:HD3	1.98	0.44
1:D:858:LEU:HD21	1:D:962:LEU:HD23	1.98	0.44
2:C:574:VAL:HG23	2:C:576:ALA:H	1.83	0.44
1:B:106:PHE:HD2	1:B:117:LEU:HD23	1.81	0.44
1:A:91:TYR:HB3	1:A:268:GLY:HA3	2.00	0.44
1:A:157:PHE:CZ	1:A:159:VAL:HB	2.52	0.44
1:A:791:THR:HG21	1:A:795:LYS:HE3	1.99	0.44
1:D:565:PHE:O	1:B:43:PHE:N	2.46	0.44
2:C:456:LEU:HB3	2:C:512:PHE:CE2	2.53	0.44
1:B:1031:GLU:HB3	1:B:1037:SER:HB2	2.00	0.44
1:A:130:VAL:HB	1:A:168:PHE:HB3	2.00	0.44
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.99	0.44
1:D:106:PHE:HD2	1:D:117:LEU:HD23	1.83	0.44
1:D:212:LEU:HD21	1:D:215:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.99	0.44
1:A:617:CYS:H	1:A:644:GLN:HE21	1.66	0.44
1:B:501:TYR:HB3	1:B:505:TYR:HB2	2.00	0.44
1:B:743:CYS:SG	1:B:746:SER:HB2	2.58	0.44
1:D:1141:LEU:HD13	1:B:1141:LEU:HD21	1.99	0.43
1:A:193:VAL:HB	1:A:204:TYR:CD2	2.47	0.43
1:D:823:PHE:CD1	1:D:1057:PRO:HD3	2.52	0.43
1:B:328:ARG:NH2	1:B:580:GLN:OE1	2.51	0.43
1:A:502:GLY:O	1:A:506:GLN:HG3	2.18	0.43
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.00	0.43
1:A:985:ASP:HB3	1:A:987:PRO:HD2	2.00	0.43
1:D:516:GLU:OE2	1:B:200:TYR:OH	2.32	0.43
1:D:1104:VAL:HG23	1:D:1115:ILE:HG12	2.01	0.43
1:B:335:LEU:HD23	1:B:362:VAL:HB	2.00	0.43
1:A:54:LEU:HB2	1:A:195:LYS:HD2	1.99	0.43
1:A:743:CYS:HA	1:A:977:LEU:HD11	2.01	0.43
2:C:157:ASP:HB3	2:C:160:GLU:HB3	2.01	0.43
1:A:671:CYS:SG	1:A:697:MET:HG2	2.59	0.43
1:D:157:PHE:CZ	1:D:159:VAL:HB	2.54	0.43
1:B:186:PHE:HB2	1:B:212:LEU:HB3	2.01	0.43
1:A:1129:VAL:HG22	1:D:917:TYR:HB3	2.00	0.43
1:B:759:PHE:CE2	1:B:1001:LEU:HB3	2.53	0.43
1:D:372:ALA:H	1:D:377:PHE:HE2	1.66	0.43
2:C:116:LEU:HD11	2:C:187:LYS:HD3	2.01	0.43
2:C:597:ASP:HA	2:C:600:LYS:HE3	2.01	0.43
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.52	0.43
1:A:331:ASN:OD1	1:A:333:THR:HG23	2.19	0.43
1:A:1128:VAL:HG13	1:A:1129:VAL:N	2.34	0.43
1:D:327:VAL:HG22	1:D:542:ASN:H	1.84	0.43
1:D:423:TYR:OH	1:D:514:SER:OG	2.36	0.43
2:C:381:TYR:HD1	2:C:558:LEU:HD22	1.84	0.43
1:B:1126:CYS:HB2	1:B:1132:ILE:HG21	2.00	0.43
1:A:884:SER:HB2	1:A:888:PHE:HB3	2.01	0.42
1:B:823:PHE:HD1	1:B:1057:PRO:HD3	1.84	0.42
1:A:895:GLN:NE2	1:B:713:ALA:HB2	2.34	0.42
1:A:997:ILE:O	1:A:1001:LEU:HG	2.19	0.42
1:A:1128:VAL:HG13	1:A:1129:VAL:H	1.82	0.42
1:D:1056:ALA:HB2	1:D:1061:VAL:HG23	2.01	0.42
1:B:175:PHE:HZ	1:B:226:LEU:HD11	1.83	0.42
1:A:347:PHE:CE2	1:A:509:ARG:HD3	2.53	0.42
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:THR:HG23	1:A:647:ALA:H	1.84	0.42
2:C:157:ASP:OD1	2:C:158:TYR:N	2.51	0.42
2:C:343:VAL:HG12	2:C:345:HIS:H	1.84	0.42
2:C:477:TRP:HE1	2:C:481:LYS:HZ1	1.67	0.42
1:B:194:PHE:CE1	1:B:203:ILE:HG23	2.53	0.42
1:A:204:TYR:CE1	1:A:225:PRO:HG3	2.54	0.42
1:D:743:CYS:SG	1:D:746:SER:HB3	2.60	0.42
2:C:396:ALA:HB3	2:C:400:PHE:CD2	2.54	0.42
1:A:111:ASP:OD1	1:A:112:SER:N	2.46	0.42
1:A:213:VAL:HG13	1:A:214:ARG:N	2.35	0.42
1:D:384:PRO:HA	1:D:387:LEU:HG	2.02	0.42
1:B:35:GLY:HA3	1:B:56:LEU:HB3	2.00	0.42
1:B:735:SER:N	1:B:859:THR:O	2.46	0.42
1:D:68:ILE:HA	1:D:262:ALA:HA	2.00	0.42
1:D:150:LYS:C	1:D:152:TRP:H	2.23	0.42
1:D:34:ARG:NE	1:D:191:GLU:OE2	2.53	0.42
1:D:727:LEU:HD11	1:D:1028:LYS:HD2	2.02	0.42
1:B:91:TYR:CE2	1:B:93:ALA:HB2	2.55	0.42
1:B:340:GLU:OE2	1:B:356:LYS:NZ	2.44	0.42
1:A:823:PHE:HD1	1:A:1057:PRO:HD3	1.85	0.41
1:D:97:LYS:HG3	1:D:186:PHE:HA	2.01	0.41
1:D:731:MET:HB2	1:D:774:GLN:NE2	2.35	0.41
2:C:215:TYR:HE1	2:C:577:LYS:HE2	1.85	0.41
1:A:731:MET:HG3	1:A:955:ASN:HD21	1.85	0.41
1:D:1029:MET:O	1:D:1033:VAL:HB	2.20	0.41
2:C:103:ASN:HB2	2:C:107:VAL:HG13	2.03	0.41
1:A:296:LEU:HB2	1:A:608:VAL:HG21	2.02	0.41
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	2.02	0.41
1:D:361:CYS:SG	1:D:361:CYS:O	2.79	0.41
1:B:544:ASN:ND2	1:B:564:GLN:HB3	2.35	0.41
1:D:28:TYR:HD1	1:D:63:THR:HA	1.84	0.41
1:D:498:GLN:HB3	1:D:501:TYR:CD2	2.55	0.41
1:D:676:THR:HA	1:D:690:GLN:HG2	2.02	0.41
1:B:848:ASP:HB3	1:B:851:CYS:HB2	2.01	0.41
1:B:1030:SER:HA	1:B:1034:LEU:HD12	2.01	0.41
1:A:331:ASN:OD1	1:A:332:ILE:N	2.54	0.41
1:B:91:TYR:HD1	1:B:193:VAL:HG22	1.84	0.41
1:B:100:ILE:CG2	1:B:243:ILE:H	2.33	0.41
1:B:111:ASP:OD1	1:B:112:SER:N	2.45	0.41
1:B:277:LEU:HD22	1:B:285:ILE:HD13	2.02	0.41
1:A:976:VAL:HG12	1:A:979:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1156:PHE:C	1:B:1159:HIS:CD2	2.94	0.41
1:B:34:ARG:NH1	1:B:216:LEU:HD13	2.36	0.41
1:A:620:VAL:HG21	1:A:642:VAL:HG22	2.02	0.41
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	2.02	0.41
1:D:429:PHE:HA	1:D:515:PHE:HB2	2.03	0.41
1:D:1090:PRO:HD2	1:B:913:GLN:HE22	1.86	0.41
1:A:338:PHE:HE2	1:A:363:ALA:HA	1.86	0.41
1:A:476:GLY:HA3	2:C:24:GLN:HE21	1.86	0.41
1:A:659:SER:HB3	1:A:698:SER:HB2	2.02	0.41
1:D:443:SER:HB3	1:D:499:PRO:HD3	2.02	0.41
1:D:565:PHE:HB2	1:D:576:VAL:HG12	2.02	0.41
1:D:656:VAL:HG12	1:D:658:ASN:H	1.86	0.41
1:D:1107:ARG:HD3	1:B:886:TRP:CZ2	2.56	0.41
1:B:490:PHE:O	1:B:493:GLN:NE2	2.53	0.41
1:A:312:ILE:HD11	1:A:596:SER:HB3	2.02	0.40
1:A:1100:THR:HG23	1:A:1101:HIS:N	2.36	0.40
1:D:412:PRO:HA	1:D:425:LEU:HB2	2.04	0.40
1:D:566:GLY:HA2	1:B:43:PHE:O	2.21	0.40
1:B:186:PHE:HD2	1:B:212:LEU:HD23	1.85	0.40
1:B:541:PHE:HB2	1:B:543:PHE:CE2	2.55	0.40
1:B:1029:MET:O	1:B:1033:VAL:HB	2.21	0.40
1:B:40:ASP:OD1	1:B:41:LYS:N	2.45	0.40
1:B:96:GLU:HG2	1:B:264:ALA:H	1.84	0.40
1:D:734:THR:HG21	1:D:959:LEU:HD21	2.02	0.40
1:D:741:TYR:CE2	1:D:1000:ARG:HB3	2.56	0.40
1:B:1056:ALA:HB2	1:B:1061:VAL:HG23	2.03	0.40
1:A:912:THR:HG22	1:A:914:ASN:H	1.87	0.40
1:A:1145:LEU:HD23	1:D:1148:PHE:CG	2.56	0.40
1:D:118:LEU:HD22	1:D:160:TYR:HE2	1.86	0.40
2:C:169:ARG:HA	2:C:173:GLY:H	1.86	0.40
1:B:242:HIS:HE1	1:B:265:TYR:CE2	2.38	0.40
1:A:118:LEU:HG	1:A:133:PHE:CE2	2.56	0.40
1:D:1110:TYR:CZ	1:D:1112:PRO:HG3	2.56	0.40
2:C:342:ALA:HB1	2:C:359:LEU:HD11	2.02	0.40
1:B:480:CYS:O	1:B:483:VAL:HG12	2.22	0.40
1:B:985:ASP:HB3	1:B:987:PRO:HD2	2.04	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	1067/1258 (85%)	1020 (96%)	45 (4%)	2 (0%)	47	79
1	B	1066/1258 (85%)	1018 (96%)	45 (4%)	3 (0%)	41	75
1	D	1063/1258 (84%)	1010 (95%)	51 (5%)	2 (0%)	47	79
2	C	595/625 (95%)	586 (98%)	9 (2%)	0	100	100
All	All	3791/4399 (86%)	3634 (96%)	150 (4%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	361	CYS
1	A	292	ALA
1	A	544	ASN
1	B	150	LYS
1	B	1159	HIS
1	D	363	ALA
1	B	530	SER

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	944/1095 (86%)	944 (100%)	0	100	100
1	B	943/1095 (86%)	943 (100%)	0	100	100
1	D	940/1095 (86%)	940 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	527/552 (96%)	527 (100%)	0	100 100
All	All	3354/3837 (87%)	3354 (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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	394	ASN
1	A	422	ASN
1	A	563	GLN
1	A	644	GLN
1	A	787	GLN
1	A	955	ASN
1	A	1088	HIS
1	A	1106	GLN
1	A	1113	GLN
1	D	69	HIS
1	D	317	ASN
1	D	787	GLN
1	D	978	ASN
2	C	24	GLN
2	C	380	GLN
2	C	401	HIS
2	C	417	HIS
2	C	535	HIS
1	B	61	ASN
1	B	81	ASN
1	B	99	ASN
1	B	188	ASN
1	B	394	ASN
1	B	703	ASN
1	B	787	GLN
1	B	913	GLN

5.3.3 RNA

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 monosaccharides 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.

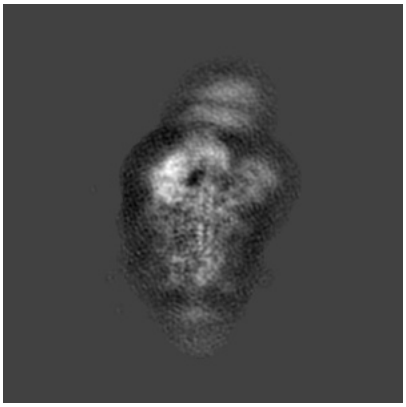
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32176. These allow visual inspection of the internal detail of the map and identification of artifacts.

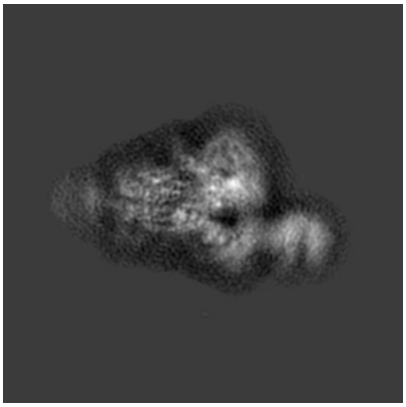
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

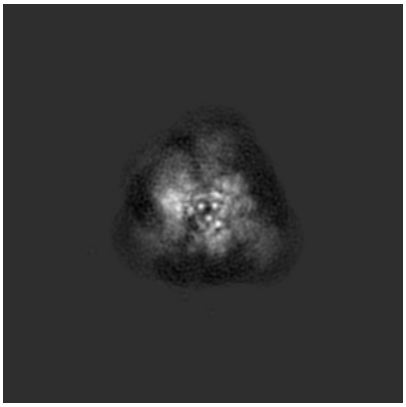
6.1.1 Primary map



X



Y

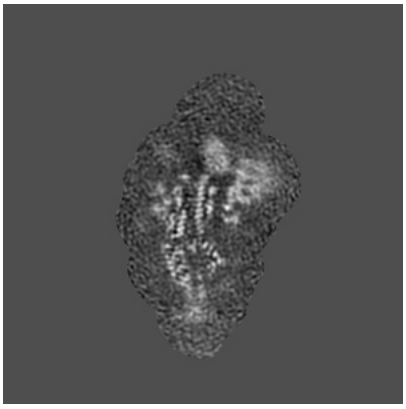


Z

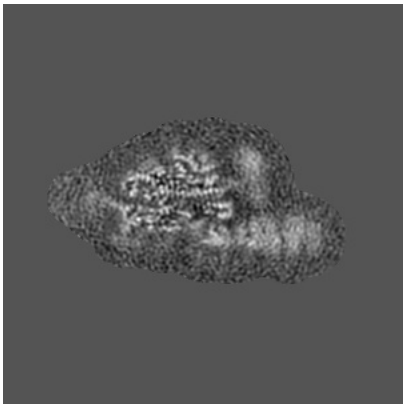
The images above show the map projected in three orthogonal directions.

6.2 Central slices

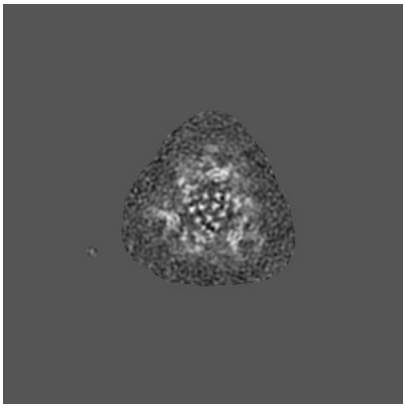
6.2.1 Primary map



X Index: 180



Y Index: 180

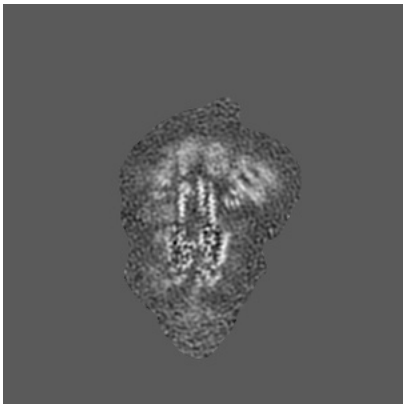


Z Index: 180

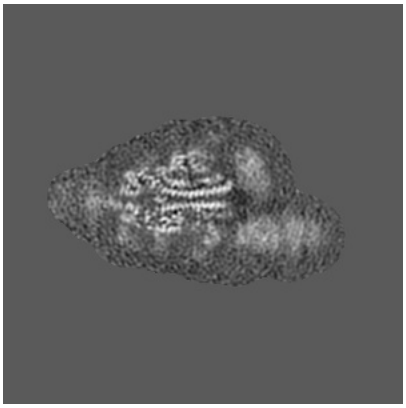
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

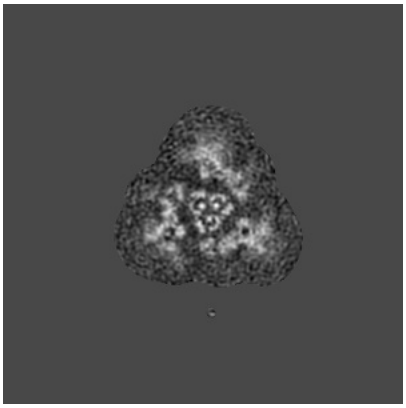
6.3.1 Primary map



X Index: 192



Y Index: 177



Z Index: 193

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.703. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

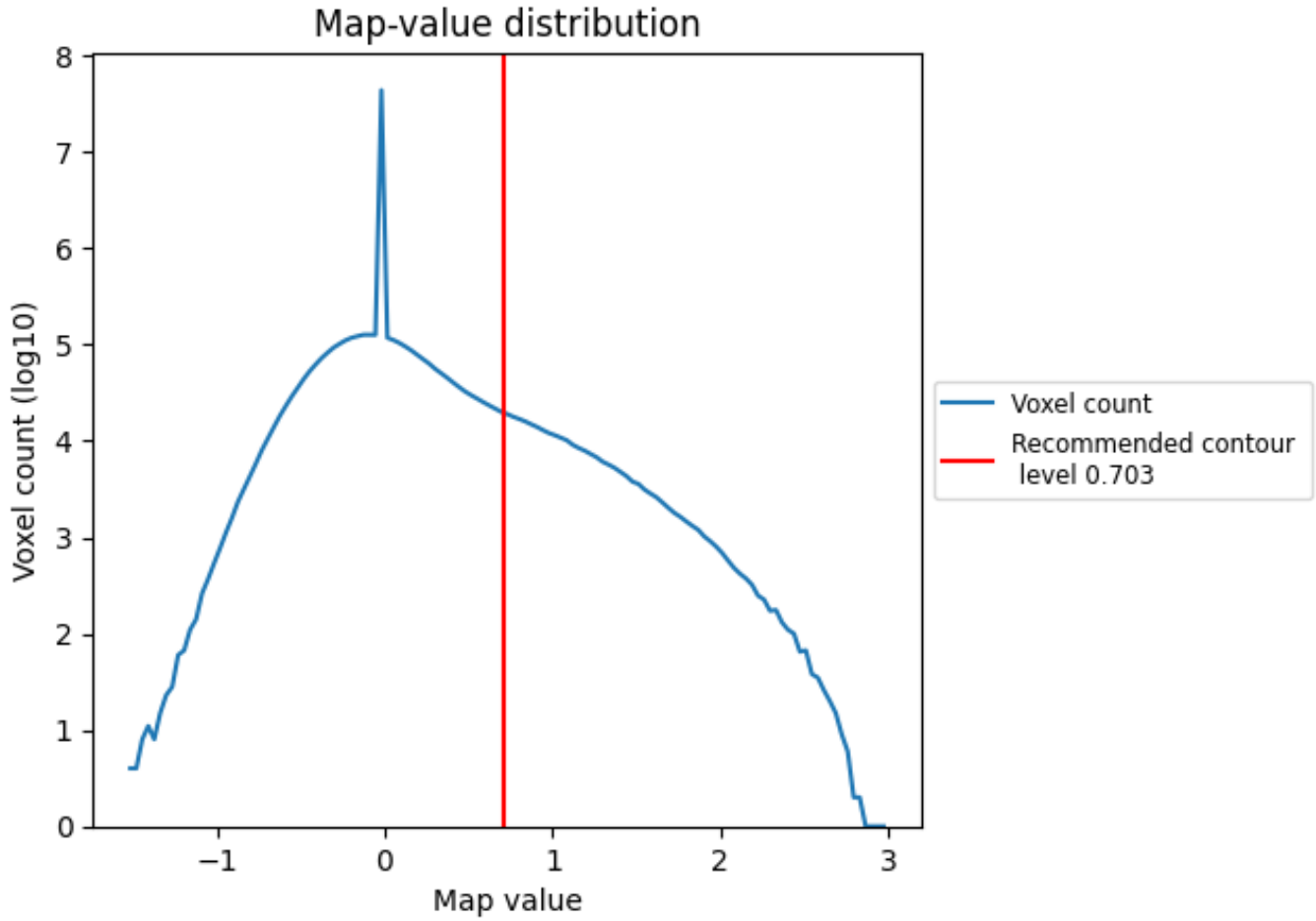
6.5 Mask visualisation (i)

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

7 Map analysis

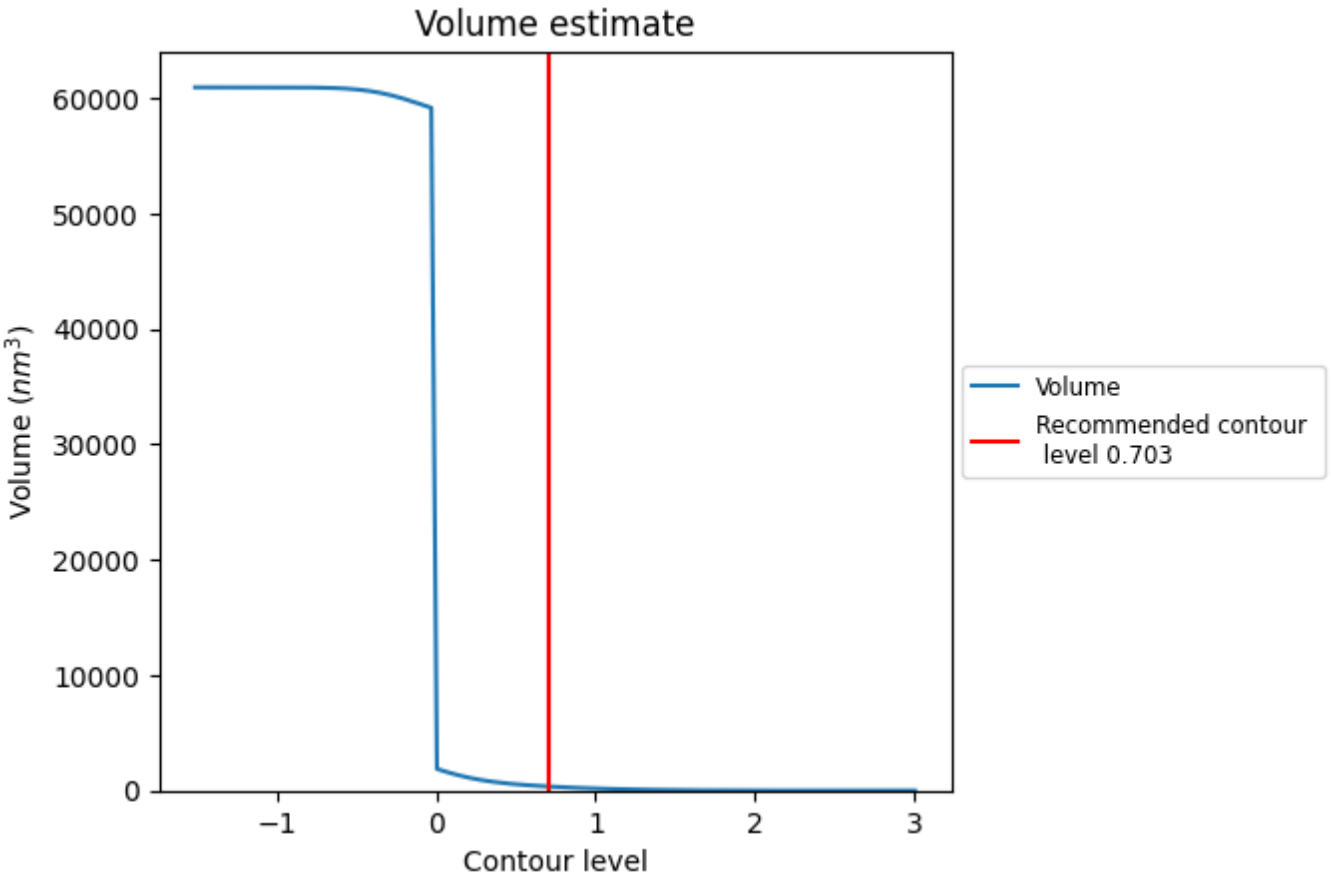
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

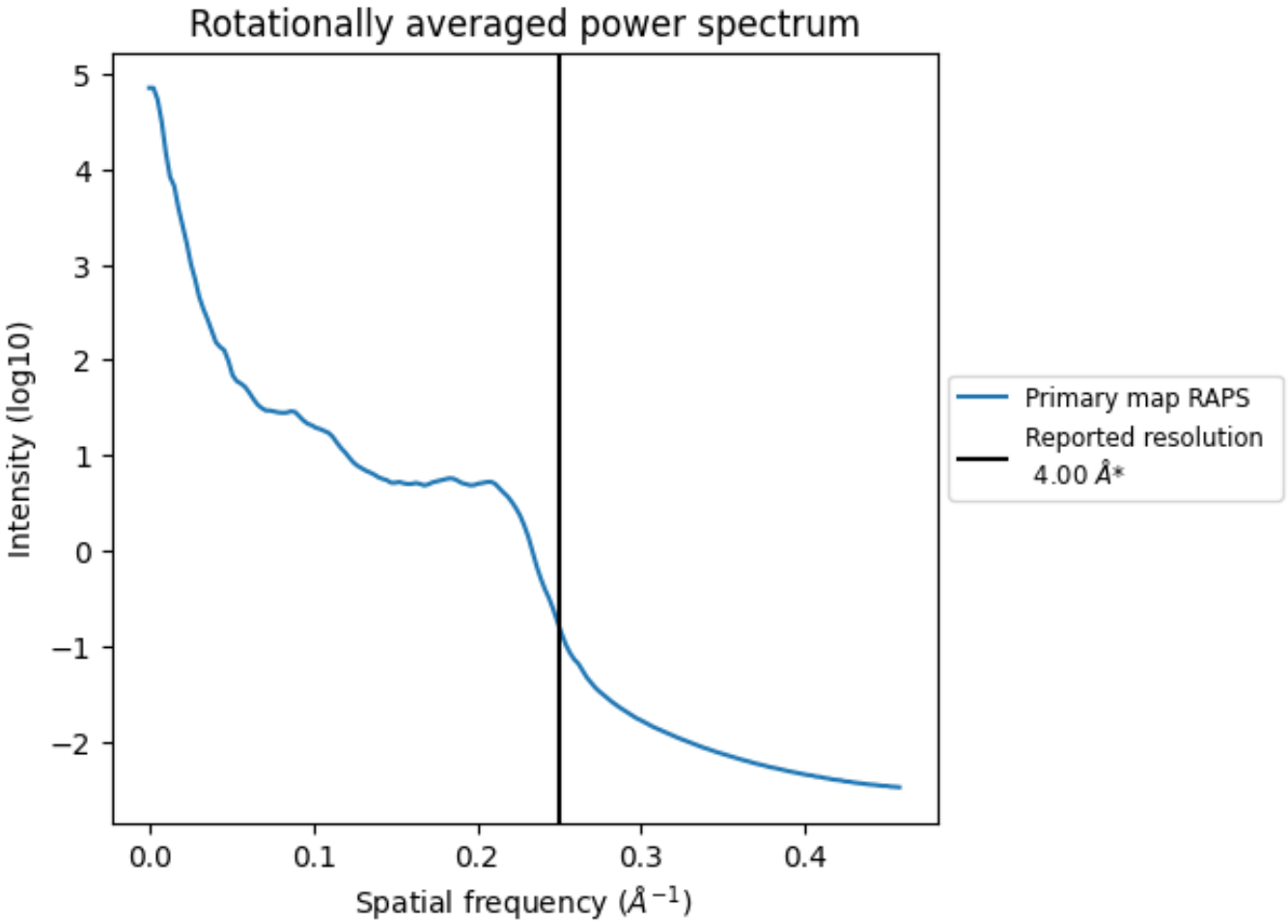
7.2 Volume estimate



The volume at the recommended contour level is 354 nm^3; this corresponds to an approximate mass of 320 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}

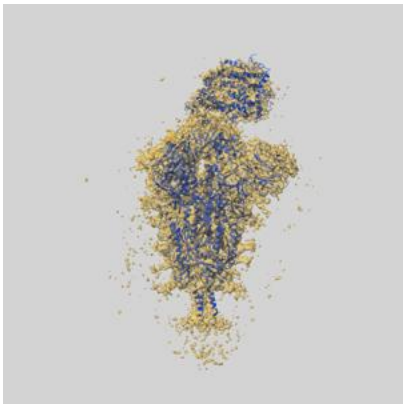
8 Fourier-Shell correlation (i)

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

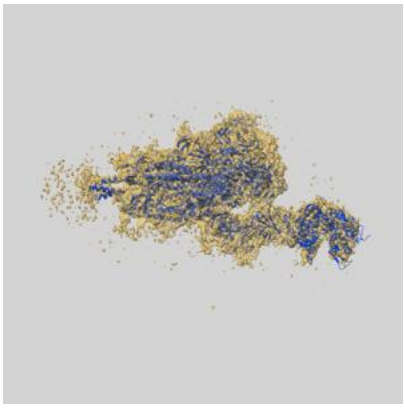
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32176 and PDB model 7VXD. Per-residue inclusion information can be found in section 3 on page 10.

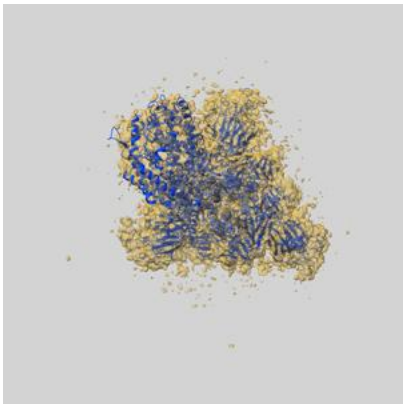
9.1 Map-model overlay



X



Y



Z

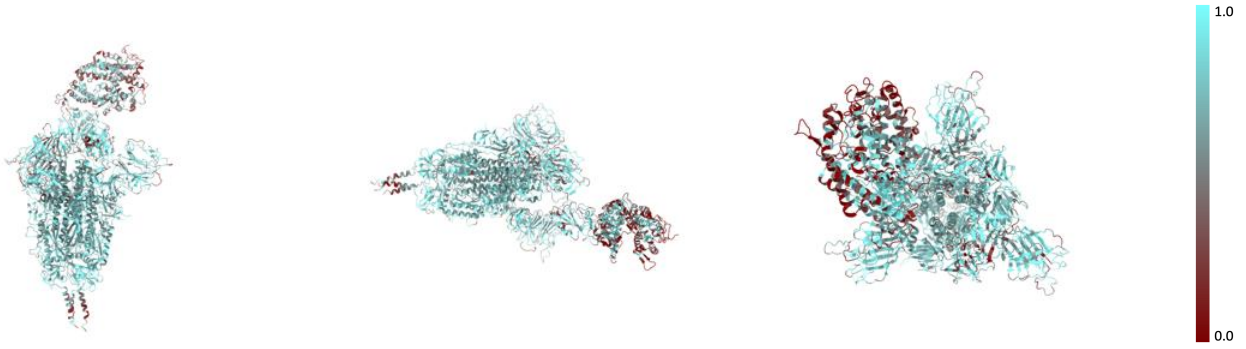
The images above show the 3D surface view of the map at the recommended contour level 0.703 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

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.

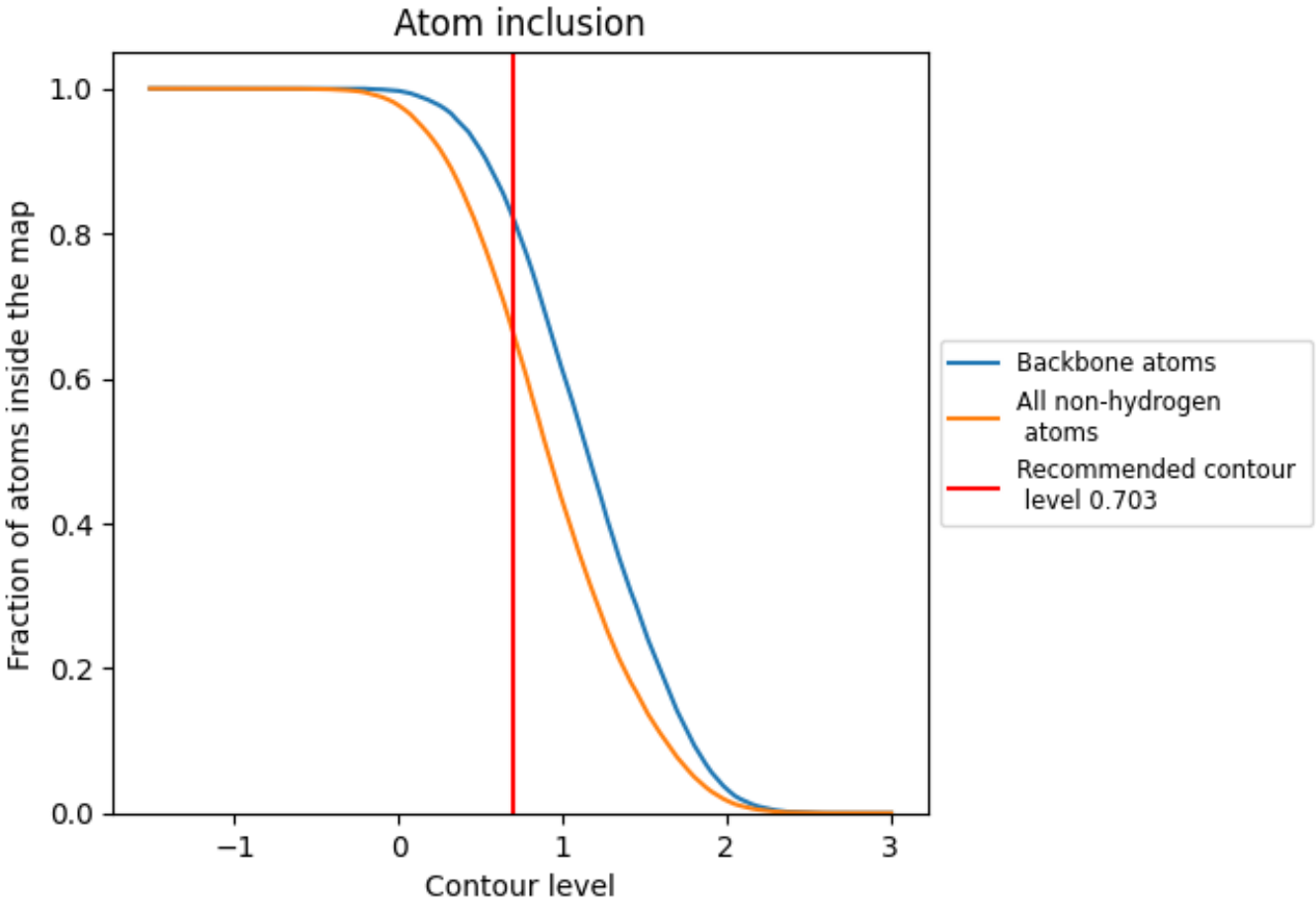
9.3 Atom inclusion mapped to coordinate model



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 (0.703).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.703) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6617	0.1820
A	0.6971	0.2120
B	0.7066	0.2130
C	0.4503	0.0380
D	0.7033	0.2030