



Full wwPDB EM Validation Report ⓘ

Jun 26, 2025 – 04:57 PM JST

PDB ID : 7WZ2 / pdb_00007wz2
EMDB ID : EMD-32902
Title : SARS-CoV-2 (D614G) Spike trimer
Authors : Zhan, W.Q.; Zhang, X.; Chen, Z.G.; Sun, L.
Deposited on : 2022-02-16
Resolution : 2.70 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

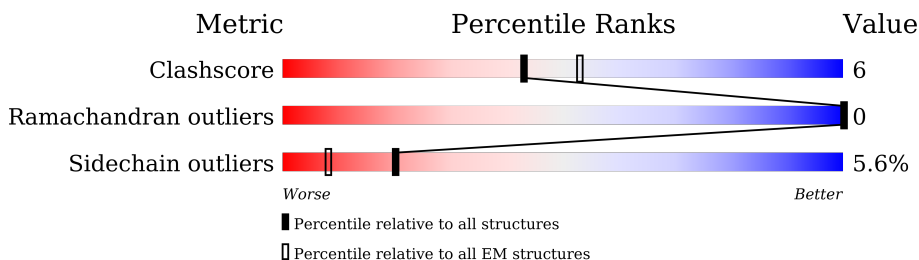
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1288	 65% 17% • 16%
1	C	1288	 65% 18% • 16%
1	E	1288	 69% 14% • 16%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25490 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	1076	Total	C	N	O	S	0	0
			8338	5318	1396	1586	38		
1	C	1076	Total	C	N	O	S	0	0
			8338	5318	1396	1586	38		
1	E	1076	Total	C	N	O	S	0	0
			8338	5318	1396	1586	38		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	PHE	-	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	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2
E	614	GLY	ASP	variant	UNP P0DTC2
E	682	GLY	ARG	conflict	UNP P0DTC2
E	683	SER	ARG	conflict	UNP P0DTC2
E	685	SER	ARG	conflict	UNP P0DTC2
E	986	PRO	LYS	conflict	UNP P0DTC2
E	987	PRO	VAL	conflict	UNP P0DTC2
E	1209	GLY	-	expression tag	UNP P0DTC2
E	1210	SER	-	expression tag	UNP P0DTC2
E	1211	GLY	-	expression tag	UNP P0DTC2
E	1212	TYR	-	expression tag	UNP P0DTC2
E	1213	ILE	-	expression tag	UNP P0DTC2
E	1214	PRO	-	expression tag	UNP P0DTC2
E	1215	GLU	-	expression tag	UNP P0DTC2
E	1216	ALA	-	expression tag	UNP P0DTC2
E	1217	PRO	-	expression tag	UNP P0DTC2
E	1218	ARG	-	expression tag	UNP P0DTC2
E	1219	ASP	-	expression tag	UNP P0DTC2
E	1220	GLY	-	expression tag	UNP P0DTC2
E	1221	GLN	-	expression tag	UNP P0DTC2
E	1222	ALA	-	expression tag	UNP P0DTC2

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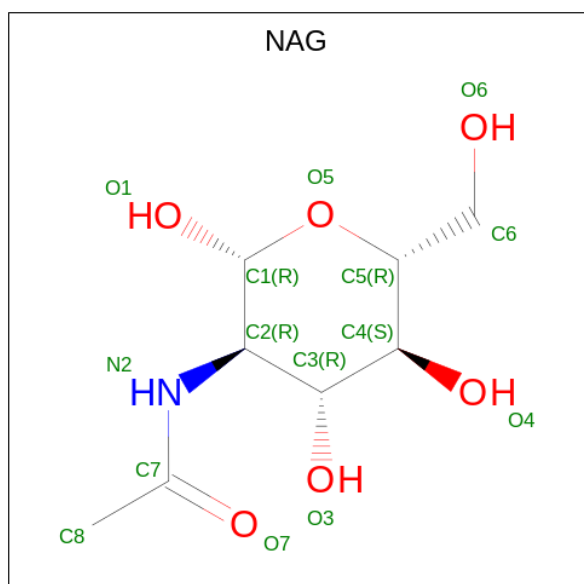
Chain	Residue	Modelled	Actual	Comment	Reference
E	1223	TYR	-	expression tag	UNP P0DTC2
E	1224	VAL	-	expression tag	UNP P0DTC2
E	1225	ARG	-	expression tag	UNP P0DTC2
E	1226	LYS	-	expression tag	UNP P0DTC2
E	1227	ASP	-	expression tag	UNP P0DTC2
E	1228	GLY	-	expression tag	UNP P0DTC2
E	1229	GLU	-	expression tag	UNP P0DTC2
E	1230	TRP	-	expression tag	UNP P0DTC2
E	1231	VAL	-	expression tag	UNP P0DTC2
E	1232	PHE	-	expression tag	UNP P0DTC2
E	1233	LEU	-	expression tag	UNP P0DTC2
E	1234	SER	-	expression tag	UNP P0DTC2
E	1235	THR	-	expression tag	UNP P0DTC2
E	1236	PHE	-	expression tag	UNP P0DTC2
E	1237	LEU	-	expression tag	UNP P0DTC2
E	1238	SER	-	expression tag	UNP P0DTC2
E	1239	GLY	-	expression tag	UNP P0DTC2
E	1240	LEU	-	expression tag	UNP P0DTC2
E	1241	GLU	-	expression tag	UNP P0DTC2
E	1242	VAL	-	expression tag	UNP P0DTC2
E	1243	LEU	-	expression tag	UNP P0DTC2
E	1244	PHE	-	expression tag	UNP P0DTC2
E	1245	GLN	-	expression tag	UNP P0DTC2
E	1246	GLY	-	expression tag	UNP P0DTC2
E	1247	PRO	-	expression tag	UNP P0DTC2
E	1248	GLY	-	expression tag	UNP P0DTC2
E	1249	GLY	-	expression tag	UNP P0DTC2
E	1250	TRP	-	expression tag	UNP P0DTC2
E	1251	SER	-	expression tag	UNP P0DTC2
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	PRO	-	expression tag	UNP P0DTC2
E	1254	GLN	-	expression tag	UNP P0DTC2
E	1255	PHE	-	expression tag	UNP P0DTC2
E	1256	GLU	-	expression tag	UNP P0DTC2
E	1257	LYS	-	expression tag	UNP P0DTC2
E	1258	GLY	-	expression tag	UNP P0DTC2
E	1259	GLY	-	expression tag	UNP P0DTC2
E	1260	GLY	-	expression tag	UNP P0DTC2
E	1261	SER	-	expression tag	UNP P0DTC2
E	1262	GLY	-	expression tag	UNP P0DTC2
E	1263	GLY	-	expression tag	UNP P0DTC2
E	1264	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1265	SER	-	expression tag	UNP P0DTC2
E	1266	GLY	-	expression tag	UNP P0DTC2
E	1267	GLY	-	expression tag	UNP P0DTC2
E	1268	SER	-	expression tag	UNP P0DTC2
E	1269	ALA	-	expression tag	UNP P0DTC2
E	1270	TRP	-	expression tag	UNP P0DTC2
E	1271	SER	-	expression tag	UNP P0DTC2
E	1272	HIS	-	expression tag	UNP P0DTC2
E	1273	PRO	-	expression tag	UNP P0DTC2
E	1274	GLN	-	expression tag	UNP P0DTC2
E	1275	PHE	-	expression tag	UNP P0DTC2
E	1276	GLU	-	expression tag	UNP P0DTC2
E	1277	LYS	-	expression tag	UNP P0DTC2
E	1278	GLY	-	expression tag	UNP P0DTC2
E	1279	GLY	-	expression tag	UNP P0DTC2
E	1280	SER	-	expression tag	UNP P0DTC2
E	1281	HIS	-	expression tag	UNP P0DTC2
E	1282	HIS	-	expression tag	UNP P0DTC2
E	1283	HIS	-	expression tag	UNP P0DTC2
E	1284	HIS	-	expression tag	UNP P0DTC2
E	1285	HIS	-	expression tag	UNP P0DTC2
E	1286	HIS	-	expression tag	UNP P0DTC2
E	1287	HIS	-	expression tag	UNP P0DTC2
E	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



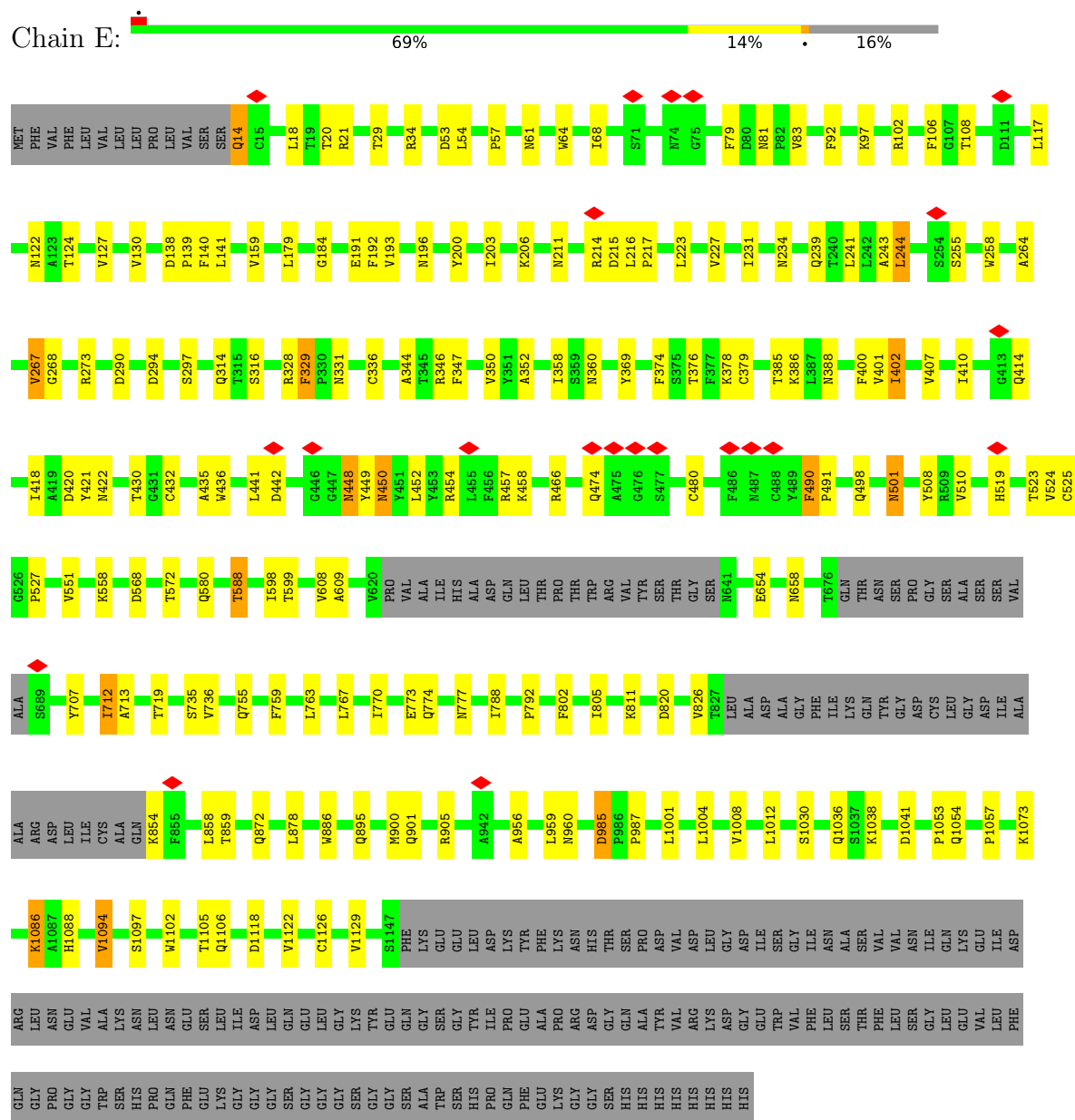
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2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

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 1: Spike glycoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2001157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.834	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	408.576, 408.576, 408.576	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/8534	0.45	5/11626 (0.0%)
1	C	0.18	0/8534	0.44	1/11626 (0.0%)
1	E	0.22	2/8534 (0.0%)	0.43	0/11626
All	All	0.19	2/25602 (0.0%)	0.44	6/34878 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	331	ASN	CA-C	-6.60	1.44	1.52
1	E	61	ASN	CA-C	-6.31	1.46	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASN	CA-C-N	8.59	132.01	120.50
1	A	331	ASN	C-N-CA	8.59	132.01	120.50
1	A	331	ASN	N-CA-C	7.11	121.65	113.19
1	A	368	LEU	N-CA-C	-5.15	108.26	114.75
1	C	805	ILE	N-CA-C	-5.14	108.82	113.71
1	A	330	PRO	O-C-N	-5.11	115.75	122.64

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	8338	0	8068	117	0
1	C	8338	0	8071	119	0
1	E	8338	0	8069	101	0
2	A	168	0	156	3	0
2	C	154	0	143	1	0
2	E	154	0	143	0	0
All	All	25490	0	24650	321	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 6.

All (321) 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:129:LYS:NZ	1:C:131:CYS:SG	2.59	0.75
1:A:97:LYS:HB3	1:A:186:PHE:HA	1.68	0.75
1:A:615:VAL:HG12	1:A:617:CYS:H	1.52	0.75
1:E:18:LEU:HD23	1:E:21:ARG:HH21	1.54	0.73
1:C:532:ASN:HD22	1:C:533:LEU:H	1.35	0.73
1:E:407:VAL:HG21	1:E:508:TYR:HB2	1.71	0.72
1:A:580:GLN:O	2:A:1311:NAG:H83	1.90	0.71
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.71	0.71
1:E:140:PHE:HB3	1:E:244:LEU:HD21	1.70	0.70
1:C:396:TYR:HB2	1:C:514:SER:HB2	1.72	0.70
1:C:339:GLY:HA2	2:C:1302:NAG:H82	1.73	0.70
1:A:92:PHE:HB3	1:A:192:PHE:HB2	1.75	0.68
1:C:706:ALA:O	1:E:895:GLN:NE2	2.28	0.67
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.77	0.67
1:A:132:GLU:O	1:A:164:ASN:ND2	2.28	0.66
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.78	0.66
1:E:130:VAL:HG21	1:E:231:ILE:HG21	1.78	0.66
1:A:547:THR:HG23	1:C:978:ASN:HB3	1.78	0.65
1:A:1037:SER:H	1:A:1048:HIS:HD2	1.45	0.65
1:A:139:PRO:HB3	1:A:159:VAL:HG13	1.79	0.65
1:E:736:VAL:HG11	1:E:1004:LEU:HD11	1.79	0.65
1:C:121:ASN:HD22	1:C:126:VAL:HG22	1.62	0.65
1:C:246:ARG:HH22	1:C:254:SER:HA	1.62	0.64
1:A:580:GLN:O	2:A:1311:NAG:C8	2.46	0.64
1:A:1041:ASP:HB2	1:C:1030:SER:HB3	1.79	0.64
1:C:825:LYS:NZ	1:C:938:LEU:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:448:ASN:ND2	1:E:450:ASN:OD1	2.31	0.64
1:A:149:ASN:ND2	1:A:151:SER:OG	2.31	0.64
1:A:931:ILE:HG22	1:A:935:GLN:HE21	1.63	0.64
1:A:134:GLN:NE2	1:A:136:CYS:SG	2.72	0.63
1:C:407:VAL:HB	1:C:408:ARG:HH11	1.63	0.63
1:A:69:HIS:HD2	1:A:259:THR:HG23	1.65	0.62
1:A:519:HIS:HE1	1:C:41:LYS:H	1.46	0.62
1:A:726:ILE:HD13	1:A:945:LEU:HD23	1.82	0.62
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.82	0.61
1:C:115:GLN:HA	1:C:132:GLU:HG2	1.81	0.61
1:A:580:GLN:HA	2:A:1311:NAG:H82	1.82	0.60
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.34	0.60
1:A:105:ILE:HD11	1:A:241:LEU:HD12	1.84	0.59
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.85	0.59
1:E:454:ARG:HD3	1:E:457:ARG:HB2	1.83	0.59
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.84	0.59
1:C:78:ARG:NH1	1:C:80:ASP:OD1	2.33	0.59
1:E:854:LYS:N	1:E:858:LEU:O	2.36	0.59
1:C:897:PRO:HD2	1:C:900:MET:HE2	1.83	0.58
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.86	0.58
1:E:599:THR:HG22	1:E:608:VAL:HG12	1.85	0.58
1:A:289:VAL:HG21	1:A:300:LYS:HE2	1.85	0.57
1:C:1126:CYS:HB2	1:C:1132:ILE:HG12	1.85	0.57
1:E:196:ASN:ND2	1:E:200:TYR:O	2.37	0.57
1:A:409:GLN:HB3	1:A:419:ALA:HB2	1.85	0.57
1:C:484:GLU:HA	1:C:488:CYS:HB3	1.85	0.57
1:C:328:ARG:HH21	1:C:580:GLN:HB2	1.70	0.57
1:C:404:GLY:O	1:C:408:ARG:NH1	2.38	0.57
1:E:106:PHE:HB2	1:E:117:LEU:HB3	1.87	0.57
1:E:568:ASP:OD1	1:E:572:THR:N	2.38	0.56
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.54	0.56
1:E:378:LYS:NZ	1:E:410:ILE:O	2.38	0.56
1:E:598:ILE:HB	1:E:609:ALA:HB3	1.88	0.56
1:A:102:ARG:NH1	1:A:121:ASN:O	2.38	0.56
1:C:350:VAL:HG11	1:C:418:ILE:HD12	1.86	0.56
1:E:18:LEU:HD12	1:E:255:SER:HB2	1.88	0.56
1:A:18:LEU:HD23	1:A:21:ARG:HH21	1.70	0.56
1:A:319:ARG:HH11	1:A:592:PHE:HB3	1.71	0.55
1:A:328:ARG:NH1	1:A:531:THR:O	2.40	0.55
1:C:144:TYR:HD1	1:C:246:ARG:HG3	1.71	0.55
1:E:102:ARG:HG3	1:E:141:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ASP:OD1	1:A:428:ASP:N	2.39	0.55
1:A:1090:PRO:O	1:C:913:GLN:NE2	2.39	0.55
1:E:81:ASN:ND2	1:E:138:ASP:OD1	2.39	0.55
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.72	0.55
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.89	0.55
1:E:773:GLU:OE2	1:E:777:ASN:ND2	2.40	0.55
1:A:956:ALA:O	1:A:960:ASN:ND2	2.32	0.54
1:A:1076:THR:HG23	1:A:1097:SER:HB3	1.89	0.54
1:A:273:ARG:HH21	1:A:290:ASP:HB3	1.71	0.54
1:E:34:ARG:NH1	1:E:191:GLU:OE2	2.41	0.54
1:E:328:ARG:NH2	1:E:580:GLN:OE1	2.40	0.54
1:C:97:LYS:HB3	1:C:186:PHE:HA	1.90	0.54
1:C:1106:GLN:NE2	1:C:1111:GLU:OE1	2.41	0.54
1:C:115:GLN:NE2	1:C:132:GLU:OE2	2.41	0.54
1:C:966:LEU:O	1:C:975:SER:OG	2.26	0.54
1:A:713:ALA:HB3	1:C:894:LEU:HB2	1.89	0.53
1:A:825:LYS:NZ	1:A:938:LEU:O	2.35	0.53
1:C:244:LEU:HD22	1:C:258:TRP:HB2	1.90	0.53
1:C:1094:VAL:HG23	1:E:900:MET:HE1	1.90	0.53
1:E:369:TYR:OH	1:E:388:ASN:ND2	2.41	0.53
1:A:302:THR:HG21	1:A:315:THR:HA	1.90	0.53
1:C:299:THR:HG22	1:C:308:VAL:HG11	1.91	0.53
1:A:1030:SER:HB3	1:E:1041:ASP:HB2	1.91	0.53
1:A:760:CYS:O	1:A:764:ASN:ND2	2.33	0.53
1:C:110:LEU:HG	1:C:237:ARG:HH12	1.73	0.53
1:A:123:ALA:HB2	1:A:154:GLU:HG3	1.90	0.53
1:C:101:ILE:HD13	1:C:265:TYR:HB3	1.90	0.53
1:C:203:ILE:HB	1:C:227:VAL:HG12	1.90	0.53
1:C:477:SER:OG	1:C:487:ASN:ND2	2.42	0.53
1:C:127:VAL:HG12	1:C:129:LYS:HG3	1.90	0.53
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.91	0.53
1:C:1041:ASP:HB2	1:E:1030:SER:HB3	1.91	0.53
1:A:659:SER:HB3	1:A:698:SER:HB3	1.91	0.52
1:E:350:VAL:HG22	1:E:400:PHE:HB2	1.90	0.52
1:A:516:GLU:HG2	1:A:518:LEU:HG	1.91	0.52
1:C:424:LYS:HB2	1:C:461:LEU:HB3	1.91	0.52
1:C:346:ARG:HH12	1:C:450:ASN:HD22	1.56	0.52
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	1.92	0.52
1:C:490:PHE:HD1	1:C:491:PRO:HD2	1.75	0.52
1:A:125:ASN:HB2	1:A:174:PRO:HA	1.92	0.52
1:A:900:MET:HE1	1:E:1094:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:ARG:NH2	1:E:442:ASP:OD1	2.43	0.52
1:E:376:THR:HB	1:E:435:ALA:HB3	1.92	0.52
1:C:1028:LYS:O	1:C:1032:CYS:HB3	2.09	0.51
1:E:735:SER:HA	1:E:767:LEU:HD13	1.92	0.51
1:A:102:ARG:HD2	1:A:177:MET:HG2	1.92	0.51
1:A:642:VAL:HG12	1:A:651:ILE:HD12	1.92	0.51
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.43	0.51
1:E:402:ILE:HG13	1:E:407:VAL:HG22	1.92	0.51
1:C:314:GLN:NE2	1:C:316:SER:O	2.43	0.51
1:C:379:CYS:HA	1:C:432:CYS:HA	1.92	0.51
1:C:442:ASP:OD2	1:C:509:ARG:NE	2.43	0.51
1:E:448:ASN:HD22	1:E:449:TYR:H	1.57	0.51
1:A:253:ASP:N	1:A:256:SER:OG	2.40	0.51
1:A:444:LYS:HG3	1:A:447:GLY:H	1.75	0.51
1:E:956:ALA:O	1:E:960:ASN:ND2	2.32	0.51
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.93	0.51
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.92	0.51
1:C:1141:LEU:O	1:C:1145:LEU:CB	2.58	0.51
1:E:139:PRO:HB3	1:E:159:VAL:HG13	1.93	0.51
1:E:901:GLN:O	1:E:905:ARG:HG2	2.11	0.51
1:C:330:PRO:HD3	1:C:544:ASN:HD21	1.75	0.51
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.93	0.51
1:A:737:ASP:OD2	1:A:739:THR:OG1	2.24	0.50
1:E:215:ASP:OD1	1:E:216:LEU:N	2.42	0.50
1:E:379:CYS:HA	1:E:432:CYS:HA	1.92	0.50
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.93	0.50
1:E:206:LYS:HB2	1:E:223:LEU:HA	1.93	0.50
1:C:402:ILE:HD11	1:C:510:VAL:HG21	1.94	0.50
1:E:79:PHE:HB2	1:E:258:TRP:HZ3	1.75	0.50
1:E:448:ASN:HD22	1:E:449:TYR:N	2.09	0.50
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	1.93	0.50
1:A:964:LYS:HB2	1:A:964:LYS:HZ2	1.76	0.50
1:C:24:LEU:HD13	1:C:78:ARG:HE	1.76	0.50
1:C:806:LEU:HD23	1:C:878:LEU:HD23	1.93	0.50
1:C:889:GLY:HA3	1:C:1034:LEU:HD23	1.93	0.50
1:A:437:ASN:HD21	1:A:506:GLN:HE21	1.59	0.50
1:C:707:TYR:HB3	1:E:792:PRO:HG3	1.94	0.50
1:A:826:VAL:HG23	1:A:945:LEU:HD13	1.93	0.50
1:A:551:VAL:HB	1:A:588:THR:HG23	1.93	0.49
1:A:825:LYS:NZ	1:A:941:THR:O	2.45	0.49
1:E:122:ASN:OD1	1:E:124:THR:OG1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.41	0.49
1:E:18:LEU:HD11	1:E:258:TRP:CG	2.46	0.49
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.94	0.49
1:C:350:VAL:HA	1:C:400:PHE:HB2	1.94	0.49
1:E:802:PHE:HD1	1:E:805:ILE:HD11	1.77	0.49
1:A:334:ASN:ND2	1:A:335:LEU:O	2.45	0.49
1:E:402:ILE:HD12	1:E:407:VAL:HA	1.94	0.49
1:A:392:PHE:N	1:A:524:VAL:O	2.46	0.49
1:C:968:SER:OG	1:E:755:GLN:O	2.31	0.49
1:C:353:TRP:CD1	1:C:353:TRP:H	2.31	0.49
1:E:57:PRO:HG3	1:E:273:ARG:HD2	1.94	0.49
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.95	0.49
1:C:337:PRO:HG2	1:C:356:LYS:HZ3	1.76	0.49
1:E:139:PRO:HB2	1:E:241:LEU:HD22	1.95	0.49
1:A:103:GLY:HA3	1:A:241:LEU:HB3	1.95	0.48
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.95	0.48
1:E:273:ARG:NH2	1:E:290:ASP:OD2	2.39	0.48
1:A:138:ASP:OD2	1:A:158:ARG:NH2	2.46	0.48
1:C:426:PRO:HB3	1:C:463:PRO:HB3	1.95	0.48
1:E:858:LEU:HD13	1:E:959:LEU:HD22	1.94	0.48
1:A:41:LYS:HE2	1:A:225:PRO:HG2	1.96	0.48
1:E:763:LEU:HD22	1:E:1008:VAL:HG21	1.95	0.48
1:C:788:ILE:HG23	1:C:876:ALA:HB2	1.96	0.48
1:E:551:VAL:HB	1:E:588:THR:HG23	1.96	0.48
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.47	0.48
1:C:102:ARG:NH2	1:C:154:GLU:OE2	2.47	0.48
1:A:92:PHE:HE1	1:A:94:SER:HB3	1.78	0.48
1:C:421:TYR:O	1:C:454:ARG:NH1	2.47	0.48
1:E:108:THR:OG1	1:E:234:ASN:O	2.30	0.48
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.95	0.48
1:E:314:GLN:NE2	1:E:316:SER:O	2.47	0.48
1:A:40:ASP:HB3	1:E:519:HIS:CE1	2.49	0.47
1:A:973:ILE:HD12	1:A:983:ARG:HH11	1.79	0.47
1:E:788:ILE:HG21	1:E:872:GLN:HE21	1.79	0.47
1:C:14:GLN:NE2	1:C:156:GLU:OE1	2.46	0.47
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.46	0.47
1:E:64:TRP:HE1	1:E:264:ALA:HB1	1.79	0.47
1:E:905:ARG:HH11	1:E:1036:GLN:HB2	1.79	0.47
1:A:146:HIS:HB3	1:A:148:ASN:HD21	1.79	0.47
1:E:770:ILE:O	1:E:774:GLN:HG2	2.14	0.47
1:A:102:ARG:HH22	1:A:141:LEU:HD13	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:HA	1:A:432:CYS:HA	1.97	0.47
1:E:352:ALA:HB1	1:E:466:ARG:HH11	1.80	0.47
1:A:294:ASP:OD1	1:A:297:SER:OG	2.28	0.47
1:E:360:ASN:H	1:E:523:THR:HB	1.80	0.47
1:A:253:ASP:H	1:A:256:SER:HG	1.64	0.46
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.97	0.46
1:A:886:TRP:HB3	1:A:1035:GLY:HA2	1.97	0.46
1:A:108:THR:OG1	1:A:234:ASN:O	2.34	0.46
1:A:79:PHE:HE1	1:A:242:LEU:HD22	1.81	0.46
1:A:153:MET:HE3	1:A:154:GLU:H	1.81	0.46
1:A:405:ASP:HA	1:A:408:ARG:HH22	1.81	0.46
1:C:770:ILE:O	1:C:774:GLN:HG2	2.16	0.46
1:A:115:GLN:HA	1:A:132:GLU:HG2	1.97	0.46
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.98	0.46
1:A:166:CYS:HB3	1:A:169:GLU:CD	2.41	0.46
1:C:210:ILE:HG12	1:C:217:PRO:HG3	1.98	0.46
1:C:287:ASP:OD1	1:C:288:ALA:N	2.44	0.46
1:C:729:VAL:HG23	1:C:1059:GLY:HA2	1.98	0.46
1:C:128:ILE:HD12	1:C:170:TYR:HB3	1.98	0.45
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.98	0.45
1:E:385:THR:OG1	1:E:386:LYS:N	2.49	0.45
1:C:858:LEU:HD13	1:C:959:LEU:HD22	1.98	0.45
1:E:985:ASP:OD1	1:E:985:ASP:N	2.39	0.45
1:A:107:GLY:H	1:A:235:ILE:HG23	1.81	0.45
1:E:498:GLN:HB2	1:E:501:ASN:HB2	1.98	0.45
1:A:1090:PRO:HA	1:A:1120:THR:HG22	1.99	0.45
1:C:334:ASN:ND2	1:C:360:ASN:O	2.50	0.45
1:C:733:LYS:HE3	1:C:771:ALA:HB1	1.99	0.45
1:C:403:ARG:HH11	1:C:495:TYR:HE1	1.65	0.45
1:E:203:ILE:HB	1:E:227:VAL:HG12	1.99	0.45
1:A:805:ILE:HG22	1:A:818:ILE:HD12	1.98	0.45
1:C:111:ASP:HB2	1:C:134:GLN:HE22	1.82	0.45
1:C:414:GLN:NE2	1:C:415:THR:O	2.49	0.45
1:E:374:PHE:HA	1:E:436:TRP:HB3	1.99	0.45
1:A:770:ILE:O	1:A:774:GLN:HG2	2.16	0.45
1:C:617:CYS:N	1:C:649:CYS:SG	2.90	0.45
1:E:388:ASN:HB3	1:E:527:PRO:HD2	1.98	0.45
1:E:474:GLN:HG2	1:E:480:CYS:HB3	2.00	0.44
1:A:391:CYS:HA	1:A:525:CYS:HA	1.99	0.44
1:A:578:ASP:HB3	1:A:581:THR:O	2.18	0.44
1:C:105:ILE:HD12	1:C:241:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:OE1	1:C:495:TYR:OH	2.36	0.44
1:C:712:ILE:HD13	1:C:1094:VAL:HG21	1.98	0.44
1:C:805:ILE:HG23	1:C:878:LEU:HD21	1.99	0.44
1:E:712:ILE:HD13	1:E:713:ALA:H	1.83	0.44
1:E:193:VAL:HG23	1:E:223:LEU:HD22	2.00	0.44
1:E:490:PHE:HD1	1:E:490:PHE:HA	1.70	0.44
1:E:1097:SER:HB2	1:E:1102:TRP:CD2	2.52	0.44
1:A:792:PRO:HG3	1:E:707:TYR:HB3	2.00	0.44
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.48	0.44
1:E:811:LYS:NZ	1:E:820:ASP:OD2	2.32	0.44
1:A:196:ASN:HD21	1:A:201:PHE:HD1	1.66	0.44
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	2.00	0.44
1:E:759:PHE:HD2	1:E:1001:LEU:HD21	1.83	0.43
1:C:726:ILE:HD13	1:C:945:LEU:HD23	2.00	0.43
1:A:353:TRP:O	1:A:466:ARG:NH2	2.52	0.43
1:C:985:ASP:HB2	1:C:987:PRO:HD2	1.99	0.43
1:A:1040:VAL:HG21	1:C:1035:GLY:HA3	2.00	0.43
1:C:99:ASN:HD21	1:C:179:LEU:HA	1.84	0.43
1:C:127:VAL:HG13	1:C:171:VAL:HG22	2.00	0.43
1:A:41:LYS:H	1:E:519:HIS:HE1	1.67	0.43
1:A:314:GLN:NE2	1:A:596:SER:OG	2.52	0.43
1:C:32:PHE:CG	1:C:218:GLN:HG2	2.53	0.43
1:C:493:GLN:HE21	1:C:493:GLN:HB2	1.63	0.43
1:E:18:LEU:HB2	1:E:140:PHE:CZ	2.53	0.43
1:E:385:THR:HG23	1:E:386:LYS:HG3	2.01	0.43
1:E:81:ASN:HD22	1:E:239:GLN:HE21	1.66	0.43
1:E:454:ARG:HG3	1:E:491:PRO:HB2	2.00	0.43
1:A:326:ILE:HG23	1:A:541:PHE:HA	2.01	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.51	0.43
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.54	0.42
1:C:714:ILE:HG21	1:C:1105:THR:HG21	2.01	0.42
1:A:146:HIS:HB3	1:A:148:ASN:ND2	2.34	0.42
1:E:1053:PRO:O	1:E:1054:GLN:NE2	2.52	0.42
1:E:1105:THR:OG1	1:E:1106:GLN:N	2.52	0.42
1:C:97:LYS:NZ	1:C:182:LYS:O	2.51	0.42
1:C:294:ASP:OD1	1:C:294:ASP:N	2.52	0.42
1:A:84:LEU:HD22	1:A:267:VAL:HG21	2.01	0.42
1:C:121:ASN:ND2	1:C:126:VAL:HG22	2.32	0.42
1:E:1086:LYS:HG3	1:E:1088:HIS:CE1	2.55	0.42
1:C:22:THR:O	1:C:78:ARG:NH2	2.52	0.42
1:C:445:VAL:HA	1:C:499:PRO:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:GLN:HE21	1:E:14:GLN:HB2	1.69	0.42
1:A:142:GLY:HA3	1:A:155:SER:OG	2.20	0.42
1:A:245:HIS:HB2	1:A:259:THR:HB	2.01	0.42
1:A:341:VAL:HG11	1:A:397:ALA:HB1	2.02	0.42
1:C:388:ASN:HB3	1:C:527:PRO:HD2	2.01	0.42
1:E:886:TRP:HZ3	1:E:905:ARG:HD3	1.83	0.42
1:E:92:PHE:O	1:E:192:PHE:N	2.47	0.41
1:E:216:LEU:HD12	1:E:217:PRO:HD2	2.02	0.41
1:E:418:ILE:HA	1:E:422:ASN:HD22	1.85	0.41
1:E:826:VAL:HB	1:E:1057:PRO:HG2	2.02	0.41
1:A:67:ALA:HB3	1:A:263:ALA:HB3	2.01	0.41
1:A:617:CYS:N	1:A:649:CYS:SG	2.93	0.41
1:E:294:ASP:OD1	1:E:297:SER:N	2.49	0.41
1:A:30:ASN:HD21	1:A:59:PHE:HD1	1.68	0.41
1:C:731:MET:HG3	1:C:1018:ILE:HG21	2.03	0.41
1:A:118:LEU:O	1:A:128:ILE:HA	2.21	0.41
1:A:141:LEU:HD21	1:A:157:PHE:HD1	1.86	0.41
1:C:615:VAL:HG12	1:C:617:CYS:H	1.86	0.41
1:C:960:ASN:O	1:C:964:LYS:HD2	2.20	0.41
1:E:267:VAL:HG12	1:E:268:GLY:H	1.85	0.41
1:C:324:GLU:H	1:C:539:VAL:HG12	1.84	0.41
1:C:811:LYS:O	1:C:813:SER:N	2.48	0.41
1:E:97:LYS:HE2	1:E:184:GLY:H	1.84	0.41
1:A:278:LYS:HB2	1:A:306:PHE:CE1	2.56	0.41
1:A:411:ALA:HB3	1:A:414:GLN:HG3	2.02	0.41
1:C:821:LEU:O	1:C:825:LYS:HB2	2.21	0.41
1:A:403:ARG:HD3	1:A:495:TYR:CD1	2.56	0.41
1:C:1093:GLY:HA2	1:C:1106:GLN:O	2.21	0.41
1:E:759:PHE:CD2	1:E:1001:LEU:HD21	2.56	0.41
1:A:83:VAL:HG13	1:A:237:ARG:HG2	2.03	0.41
1:A:403:ARG:NH1	1:A:406:GLU:OE2	2.54	0.41
1:C:1081:ILE:HD11	1:C:1115:ILE:HG21	2.01	0.41
1:E:18:LEU:HD21	1:E:258:TRP:CE3	2.55	0.41
1:E:141:LEU:HB2	1:E:243:ALA:HA	2.02	0.41
1:E:773:GLU:OE1	1:E:774:GLN:NE2	2.54	0.41
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.45	0.41
1:C:112:SER:H	1:C:134:GLN:NE2	2.18	0.41
1:C:299:THR:O	1:C:302:THR:OG1	2.39	0.41
1:C:281:GLU:H	1:C:281:GLU:HG3	1.69	0.40
1:C:356:LYS:HE3	1:C:356:LYS:HB3	1.83	0.40
1:E:329:PHE:HD1	1:E:329:PHE:HA	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:985:ASP:HB2	1:E:987:PRO:HD2	2.02	0.40
1:E:53:ASP:OD1	1:E:54:LEU:N	2.46	0.40
1:E:344:ALA:HB3	1:E:347:PHE:CE1	2.57	0.40
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.04	0.40
1:A:600:PRO:HB3	1:A:674:TYR:HB2	2.04	0.40
1:C:337:PRO:HG2	1:C:356:LYS:NZ	2.37	0.40
1:C:402:ILE:HB	1:C:406:GLU:HB2	2.03	0.40
1:E:770:ILE:HD11	1:E:1012:LEU:HD23	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	1068/1288 (83%)	997 (93%)	71 (7%)	0	100	100
1	C	1068/1288 (83%)	991 (93%)	77 (7%)	0	100	100
1	E	1068/1288 (83%)	1005 (94%)	63 (6%)	0	100	100
All	All	3204/3864 (83%)	2993 (93%)	211 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	922/1111 (83%)	873 (95%)	49 (5%)	19	43
1	C	922/1111 (83%)	864 (94%)	58 (6%)	15	35
1	E	922/1111 (83%)	875 (95%)	47 (5%)	20	45
All	All	2766/3333 (83%)	2612 (94%)	154 (6%)	20	41

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	51	THR
1	A	63	THR
1	A	70	VAL
1	A	76	THR
1	A	95	THR
1	A	97	LYS
1	A	104	TRP
1	A	128	ILE
1	A	130	VAL
1	A	134	GLN
1	A	141	LEU
1	A	143	VAL
1	A	148	ASN
1	A	149	ASN
1	A	170	TYR
1	A	197	ILE
1	A	202	LYS
1	A	214	ARG
1	A	236	THR
1	A	248	TYR
1	A	249	LEU
1	A	267	VAL
1	A	281	GLU
1	A	307	THR
1	A	326	ILE
1	A	336	CYS
1	A	345	THR
1	A	367	VAL
1	A	396	TYR
1	A	408	ARG
1	A	417	LYS
1	A	424	LYS
1	A	430	THR

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Mol	Chain	Res	Type
1	A	455	LEU
1	A	462	LYS
1	A	468	ILE
1	A	525	CYS
1	A	534	VAL
1	A	569	ILE
1	A	779	GLN
1	A	795	LYS
1	A	820	ASP
1	A	855	PHE
1	A	916	LEU
1	A	1001	LEU
1	A	1104	VAL
1	A	1126	CYS
1	A	1129	VAL
1	C	68	ILE
1	C	70	VAL
1	C	83	VAL
1	C	90	VAL
1	C	122	ASN
1	C	127	VAL
1	C	133	PHE
1	C	145	TYR
1	C	160	TYR
1	C	182	LYS
1	C	233	ILE
1	C	249	LEU
1	C	250	THR
1	C	259	THR
1	C	291	CYS
1	C	293	LEU
1	C	303	LEU
1	C	307	THR
1	C	335	LEU
1	C	336	CYS
1	C	341	VAL
1	C	357	ARG
1	C	358	ILE
1	C	376	THR
1	C	387	LEU
1	C	402	ILE
1	C	408	ARG

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Mol	Chain	Res	Type
1	C	414	GLN
1	C	417	LYS
1	C	423	TYR
1	C	424	LYS
1	C	429	PHE
1	C	430	THR
1	C	455	LEU
1	C	458	LYS
1	C	480	CYS
1	C	486	PHE
1	C	488	CYS
1	C	489	TYR
1	C	493	GLN
1	C	517	LEU
1	C	525	CYS
1	C	532	ASN
1	C	581	THR
1	C	616	ASN
1	C	642	VAL
1	C	738	CYS
1	C	740	MET
1	C	826	VAL
1	C	855	PHE
1	C	916	LEU
1	C	947	LYS
1	C	964	LYS
1	C	995	ARG
1	C	1094	VAL
1	C	1104	VAL
1	C	1107	ARG
1	C	1129	VAL
1	E	14	GLN
1	E	20	THR
1	E	29	THR
1	E	68	ILE
1	E	83	VAL
1	E	127	VAL
1	E	179	LEU
1	E	211	ASN
1	E	214	ARG
1	E	244	LEU
1	E	267	VAL

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Mol	Chain	Res	Type
1	E	329	PHE
1	E	336	CYS
1	E	358	ILE
1	E	401	VAL
1	E	402	ILE
1	E	414	GLN
1	E	420	ASP
1	E	421	TYR
1	E	430	THR
1	E	441	LEU
1	E	448	ASN
1	E	450	ASN
1	E	452	LEU
1	E	458	LYS
1	E	490	PHE
1	E	501	ASN
1	E	510	VAL
1	E	524	VAL
1	E	525	CYS
1	E	558	LYS
1	E	588	THR
1	E	654	GLU
1	E	658	ASN
1	E	712	ILE
1	E	719	THR
1	E	859	THR
1	E	878	LEU
1	E	985	ASP
1	E	1038	LYS
1	E	1073	LYS
1	E	1086	LYS
1	E	1094	VAL
1	E	1118	ASP
1	E	1122	VAL
1	E	1126	CYS
1	E	1129	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	81	ASN

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Mol	Chain	Res	Type
1	A	115	GLN
1	A	121	ASN
1	A	125	ASN
1	A	134	GLN
1	A	137	ASN
1	A	149	ASN
1	A	173	GLN
1	A	218	GLN
1	A	314	GLN
1	A	334	ASN
1	A	439	ASN
1	A	493	GLN
1	A	498	GLN
1	A	501	ASN
1	A	506	GLN
1	A	519	HIS
1	A	556	ASN
1	A	580	GLN
1	A	641	ASN
1	A	658	ASN
1	A	784	GLN
1	A	804	GLN
1	A	872	GLN
1	A	901	GLN
1	A	907	ASN
1	A	926	GLN
1	A	935	GLN
1	A	954	GLN
1	A	1005	GLN
1	A	1048	HIS
1	A	1106	GLN
1	C	23	GLN
1	C	66	HIS
1	C	99	ASN
1	C	115	GLN
1	C	121	ASN
1	C	134	GLN
1	C	218	GLN
1	C	414	GLN
1	C	437	ASN
1	C	460	ASN
1	C	487	ASN

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Mol	Chain	Res	Type
1	C	493	GLN
1	C	498	GLN
1	C	506	GLN
1	C	532	ASN
1	C	544	ASN
1	C	563	GLN
1	C	762	GLN
1	C	804	GLN
1	C	856	ASN
1	C	935	GLN
1	C	954	GLN
1	C	957	GLN
1	C	1064	HIS
1	C	1071	GLN
1	C	1083	HIS
1	C	1106	GLN
1	E	23	GLN
1	E	81	ASN
1	E	121	ASN
1	E	137	ASN
1	E	196	ASN
1	E	218	GLN
1	E	354	ASN
1	E	388	ASN
1	E	414	GLN
1	E	437	ASN
1	E	448	ASN
1	E	450	ASN
1	E	474	GLN
1	E	493	GLN
1	E	501	ASN
1	E	506	GLN
1	E	519	HIS
1	E	540	ASN
1	E	556	ASN
1	E	613	GLN
1	E	644	GLN
1	E	675	GLN
1	E	755	GLN
1	E	784	GLN
1	E	872	GLN
1	E	895	GLN

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Mol	Chain	Res	Type
1	E	901	GLN
1	E	919	ASN
1	E	949	GLN
1	E	954	GLN
1	E	969	ASN
1	E	992	GLN
1	E	1011	GLN
1	E	1058	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1311	1	14,14,15	0.34	0	17,19,21	0.75	0
2	NAG	C	1305	1	14,14,15	0.34	0	17,19,21	0.70	0
2	NAG	E	1304	1	14,14,15	0.37	0	17,19,21	0.99	2 (11%)
2	NAG	C	1306	1	14,14,15	0.36	0	17,19,21	0.65	0
2	NAG	C	1309	1	14,14,15	0.29	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1303	1	14,14,15	0.29	0	17,19,21	1.02	1 (5%)
2	NAG	E	1308	1	14,14,15	0.39	0	17,19,21	0.69	0
2	NAG	C	1302	1	14,14,15	0.27	0	17,19,21	1.08	1 (5%)
2	NAG	E	1305	1	14,14,15	0.33	0	17,19,21	0.77	0
2	NAG	A	1304	1	14,14,15	0.25	0	17,19,21	0.52	0
2	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	A	1310	1	14,14,15	0.32	0	17,19,21	0.71	0
2	NAG	E	1310	1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
2	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	E	1307	1	14,14,15	0.34	0	17,19,21	0.78	0
2	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	0.65	0
2	NAG	C	1304	1	14,14,15	0.30	0	17,19,21	0.63	0
2	NAG	C	1308	1	14,14,15	0.43	0	17,19,21	0.91	1 (5%)
2	NAG	C	1310	1	14,14,15	0.36	0	17,19,21	0.70	0
2	NAG	A	1309	1	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
2	NAG	E	1302	1	14,14,15	0.43	0	17,19,21	0.74	0
2	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	1.06	1 (5%)
2	NAG	C	1307	1	14,14,15	0.34	0	17,19,21	0.77	0
2	NAG	A	1311	1	14,14,15	0.40	0	17,19,21	0.81	0
2	NAG	E	1301	1	14,14,15	0.25	0	17,19,21	1.05	1 (5%)
2	NAG	E	1306	1	14,14,15	0.32	0	17,19,21	0.99	1 (5%)
2	NAG	E	1311	1	14,14,15	0.34	0	17,19,21	0.71	0
2	NAG	E	1309	1	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
2	NAG	A	1308	1	14,14,15	0.33	0	17,19,21	0.75	1 (5%)
2	NAG	A	1307	1	14,14,15	0.33	0	17,19,21	0.80	0
2	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	A	1312	1	14,14,15	0.32	0	17,19,21	0.72	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	E	1304	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
2	NAG	E	1303	1	-	5/6/23/26	0/1/1/1
2	NAG	E	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
2	NAG	E	1305	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1310	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	E	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1302	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	E	1306	1	-	3/6/23/26	0/1/1/1
2	NAG	E	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	E	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1302	NAG	C1-O5-C5	2.96	116.20	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1301	NAG	C2-N2-C7	2.68	126.72	122.90
2	E	1303	NAG	C2-N2-C7	2.65	126.68	122.90
2	C	1308	NAG	C1-O5-C5	2.51	115.60	112.19
2	C	1301	NAG	C2-N2-C7	2.32	126.21	122.90
2	E	1310	NAG	C1-O5-C5	2.20	115.17	112.19
2	E	1304	NAG	C2-N2-C7	-2.13	119.87	122.90
2	A	1308	NAG	C1-O5-C5	2.12	115.06	112.19
2	A	1309	NAG	C1-O5-C5	2.12	115.06	112.19
2	E	1304	NAG	C4-C3-C2	-2.11	107.93	111.02
2	E	1309	NAG	C1-O5-C5	2.10	115.03	112.19
2	E	1306	NAG	C1-O5-C5	2.08	115.01	112.19
2	A	1312	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1302	NAG	C8-C7-N2-C2
2	C	1302	NAG	O7-C7-N2-C2
2	E	1301	NAG	C3-C2-N2-C7
2	E	1301	NAG	C8-C7-N2-C2
2	E	1301	NAG	O7-C7-N2-C2
2	E	1303	NAG	C3-C2-N2-C7
2	E	1303	NAG	C8-C7-N2-C2
2	E	1303	NAG	O7-C7-N2-C2
2	E	1306	NAG	O7-C7-N2-C2
2	E	1310	NAG	C8-C7-N2-C2
2	E	1310	NAG	O7-C7-N2-C2
2	A	1308	NAG	C8-C7-N2-C2
2	A	1308	NAG	O7-C7-N2-C2
2	C	1304	NAG	C8-C7-N2-C2
2	C	1304	NAG	O7-C7-N2-C2
2	E	1302	NAG	C8-C7-N2-C2
2	E	1302	NAG	O7-C7-N2-C2
2	E	1306	NAG	C8-C7-N2-C2
2	E	1310	NAG	O5-C5-C6-O6
2	E	1302	NAG	O5-C5-C6-O6
2	E	1305	NAG	O5-C5-C6-O6
2	A	1305	NAG	C8-C7-N2-C2
2	A	1305	NAG	O7-C7-N2-C2
2	C	1301	NAG	C8-C7-N2-C2
2	C	1309	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	1309	NAG	O7-C7-N2-C2
2	E	1311	NAG	C8-C7-N2-C2
2	A	1301	NAG	O5-C5-C6-O6
2	E	1303	NAG	O5-C5-C6-O6
2	E	1310	NAG	C4-C5-C6-O6
2	A	1301	NAG	C4-C5-C6-O6
2	A	1303	NAG	C4-C5-C6-O6
2	C	1301	NAG	O7-C7-N2-C2
2	E	1308	NAG	C8-C7-N2-C2
2	E	1311	NAG	O7-C7-N2-C2
2	E	1302	NAG	C4-C5-C6-O6
2	E	1305	NAG	C4-C5-C6-O6
2	A	1307	NAG	C8-C7-N2-C2
2	C	1306	NAG	C8-C7-N2-C2
2	C	1308	NAG	C8-C7-N2-C2
2	C	1308	NAG	O7-C7-N2-C2
2	E	1307	NAG	C8-C7-N2-C2
2	E	1308	NAG	O7-C7-N2-C2
2	A	1303	NAG	O5-C5-C6-O6
2	E	1303	NAG	C4-C5-C6-O6
2	E	1306	NAG	C1-C2-N2-C7
2	A	1306	NAG	O5-C5-C6-O6
2	C	1306	NAG	O7-C7-N2-C2
2	E	1307	NAG	O7-C7-N2-C2
2	C	1301	NAG	C1-C2-N2-C7
2	A	1307	NAG	O7-C7-N2-C2
2	C	1303	NAG	C8-C7-N2-C2
2	A	1312	NAG	C8-C7-N2-C2
2	C	1303	NAG	O7-C7-N2-C2
2	C	1305	NAG	C8-C7-N2-C2
2	C	1309	NAG	O5-C5-C6-O6
2	A	1306	NAG	C4-C5-C6-O6
2	A	1312	NAG	O7-C7-N2-C2
2	E	1304	NAG	O5-C5-C6-O6
2	E	1304	NAG	C4-C5-C6-O6
2	C	1308	NAG	O5-C5-C6-O6
2	C	1302	NAG	C1-C2-N2-C7
2	C	1305	NAG	O7-C7-N2-C2
2	A	1304	NAG	C3-C2-N2-C7
2	E	1305	NAG	C8-C7-N2-C2
2	C	1308	NAG	C4-C5-C6-O6
2	E	1305	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	E	1309	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1302	NAG	1	0
2	A	1311	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

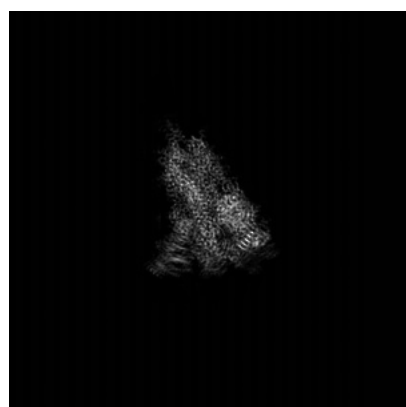
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32902. These allow visual inspection of the internal detail of the map and identification of artifacts.

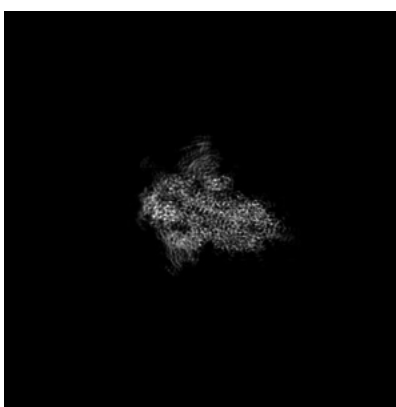
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

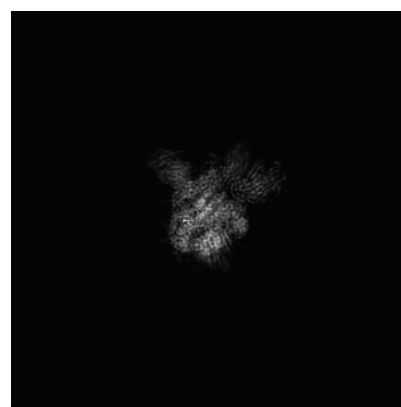
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192

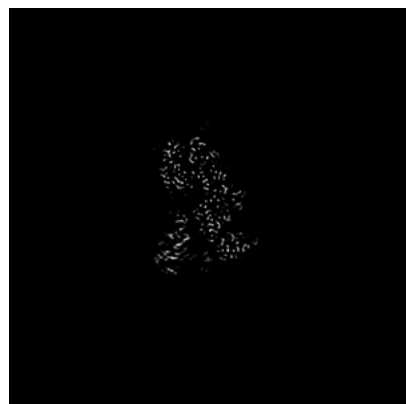


Z Index: 192

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

6.3 Largest variance slices [i](#)

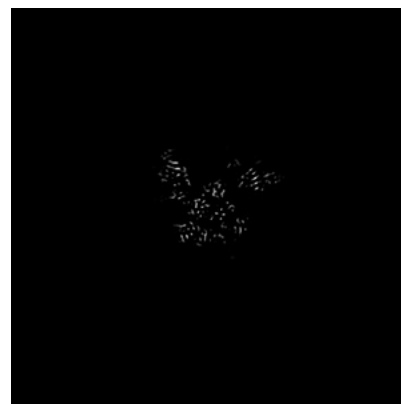
6.3.1 Primary map



X Index: 186



Y Index: 182

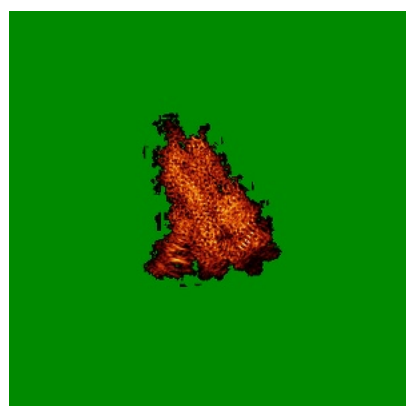


Z Index: 179

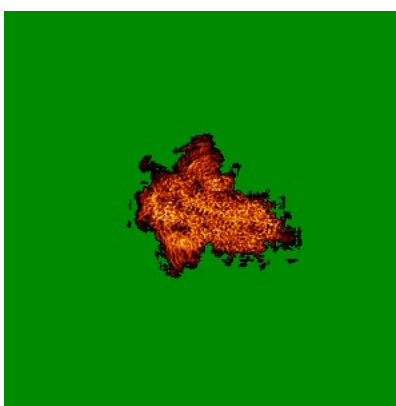
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

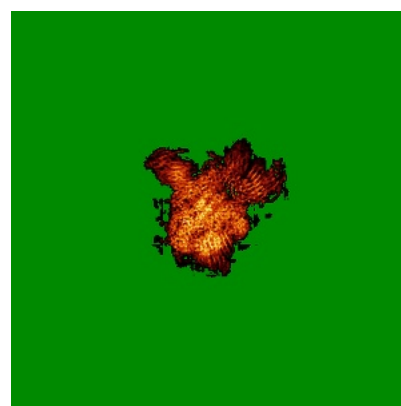
6.4.1 Primary map



X



Y

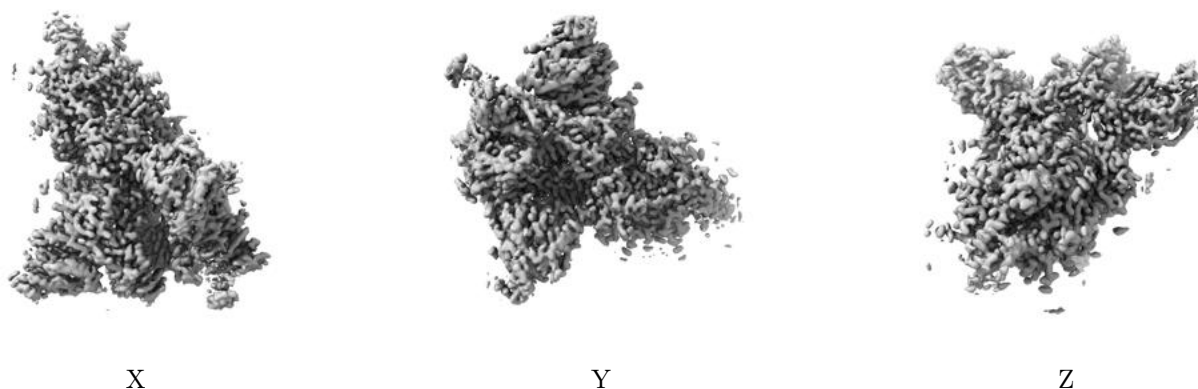


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

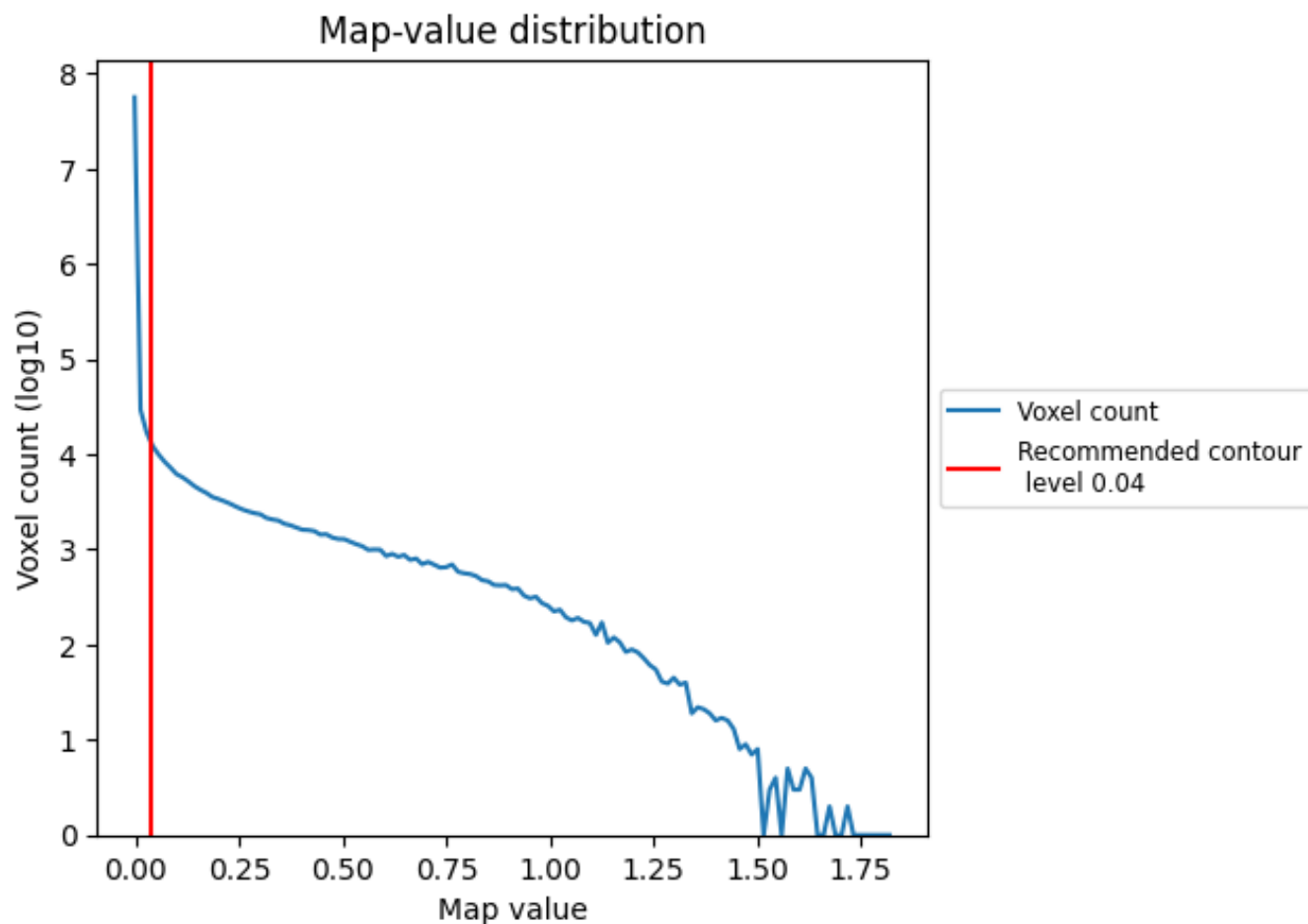
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

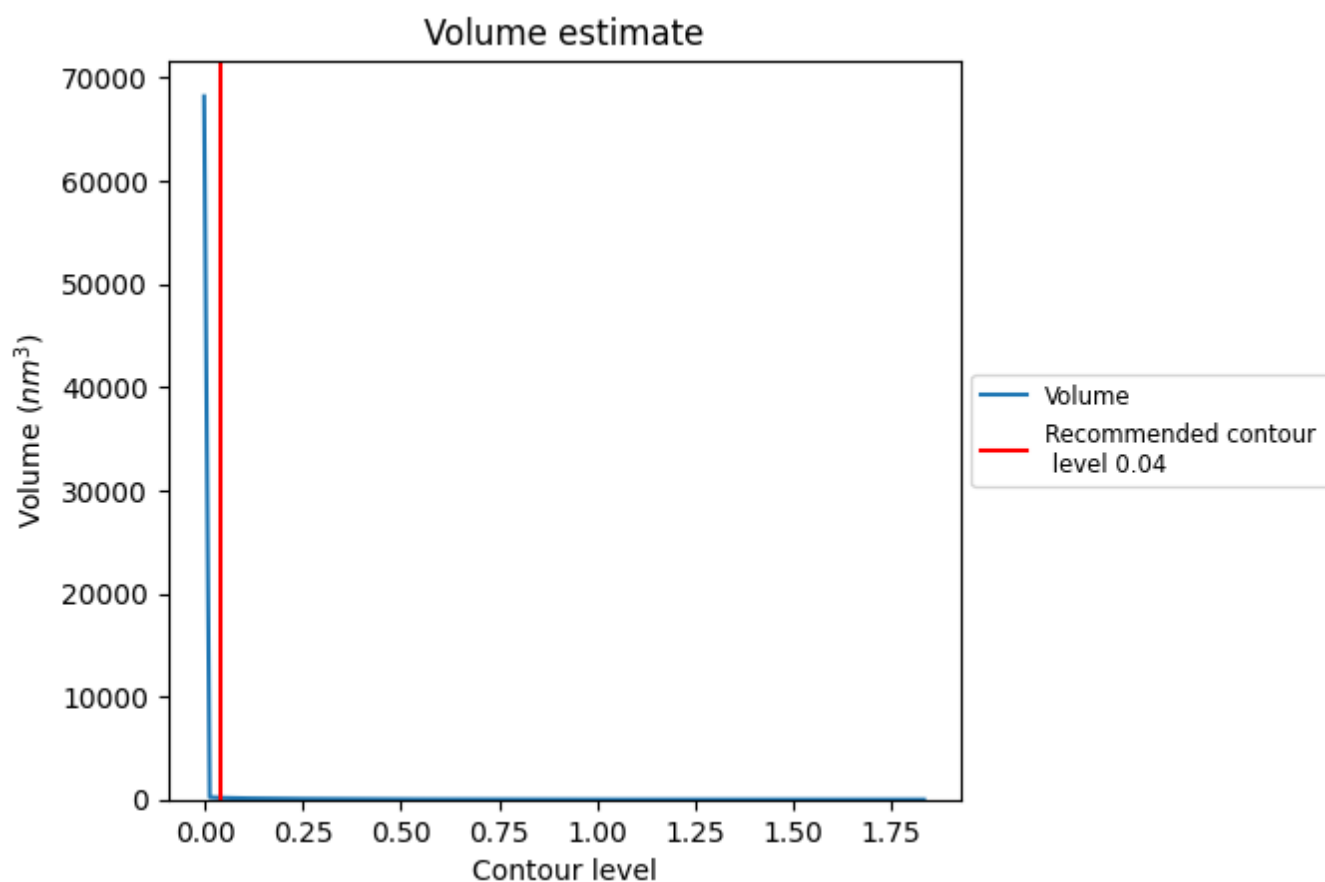
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

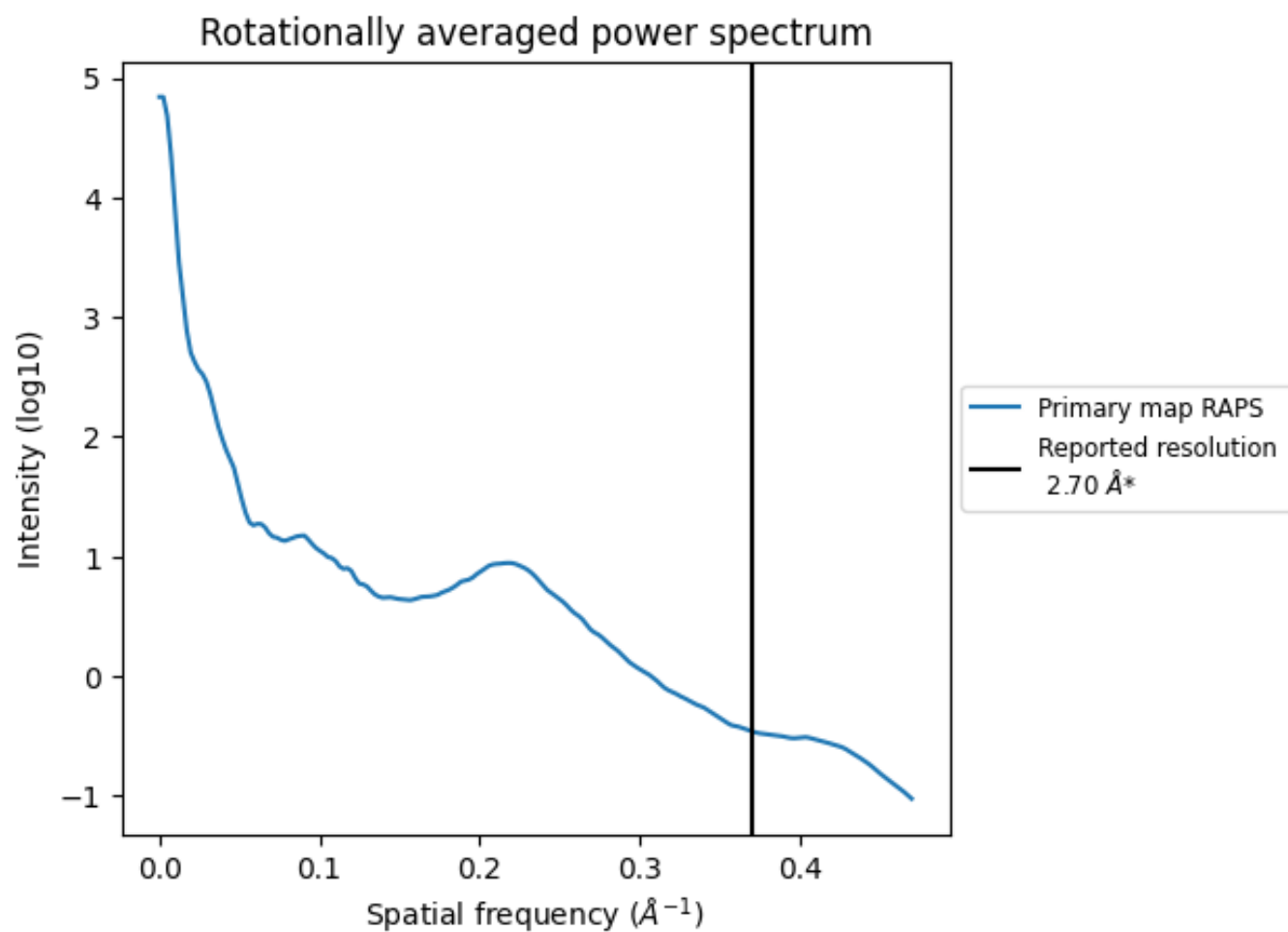
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 156 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

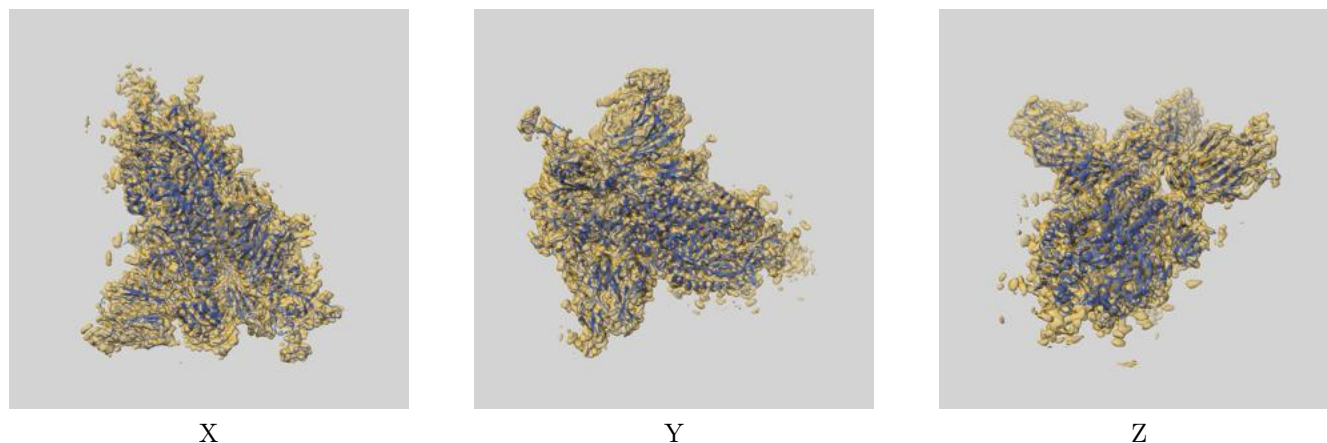
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

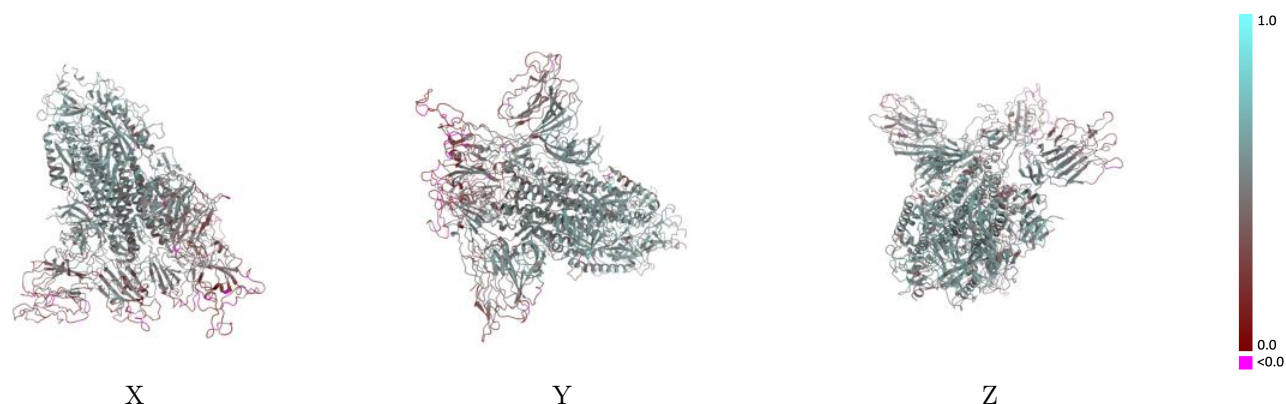
This section contains information regarding the fit between EMDB map EMD-32902 and PDB model 7WZ2. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



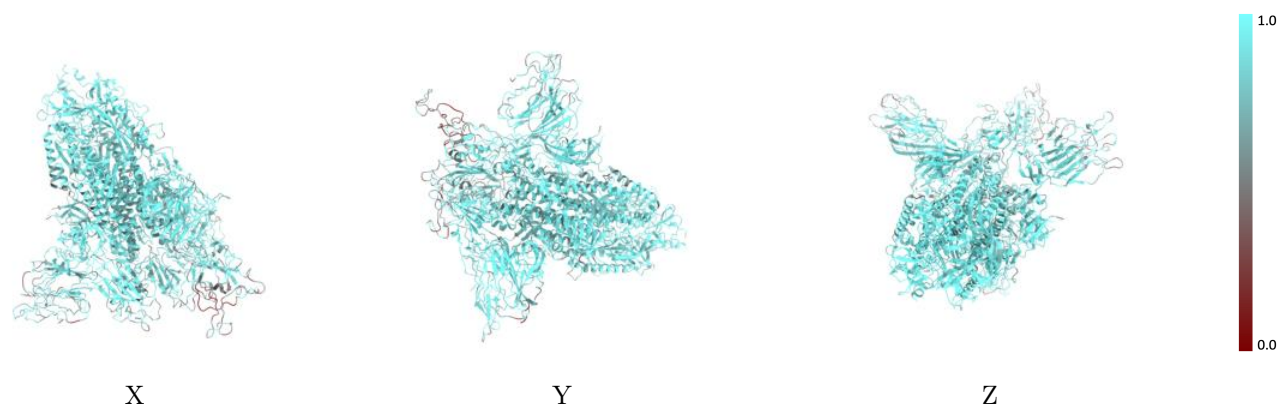
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



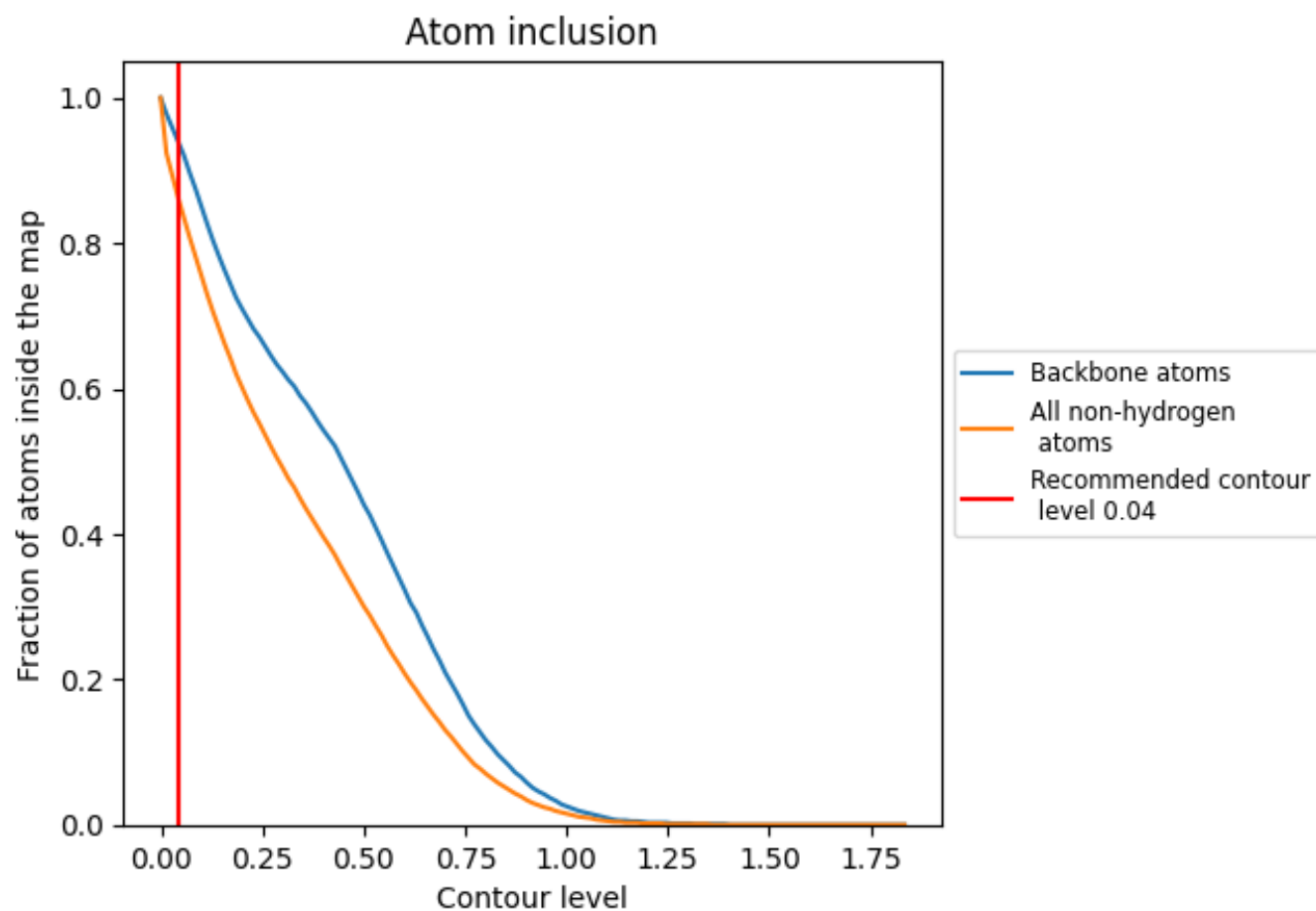
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 86% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8650	<div></div> 0.4560
A	<div></div> 0.8640	<div></div> 0.4500
C	<div></div> 0.8570	<div></div> 0.4550
E	<div></div> 0.8740	<div></div> 0.4620

