



Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 11:08 AM JST

PDB ID : 7FCD
EMDB ID : EMD-31524
Title : Structure of the SARS-CoV-2 A372T spike glycoprotein (open)
Authors : Wang, X.; Zhang, S.
Deposited on : 2021-07-14
Resolution : 3.90 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

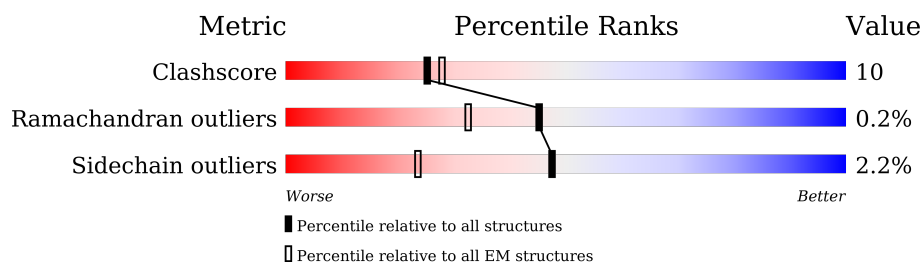
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	1298	
1	B	1298	
1	C	1298	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24444 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	1007	Total	C	N	O	S	0	0
			7901	5050	1319	1496	36		
1	B	1021	Total	C	N	O	S	0	0
			8009	5119	1337	1516	37		
1	C	1027	Total	C	N	O	S	0	0
			8044	5136	1345	1526	37		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	THR	ALA	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	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	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	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	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
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	SER	-	expression tag	UNP P0DTC2
A	1291	ASP	-	expression tag	UNP P0DTC2
A	1292	TYR	-	expression tag	UNP P0DTC2
A	1293	LYS	-	expression tag	UNP P0DTC2
A	1294	ASP	-	expression tag	UNP P0DTC2
A	1295	ASP	-	expression tag	UNP P0DTC2
A	1296	ASP	-	expression tag	UNP P0DTC2
A	1297	ASP	-	expression tag	UNP P0DTC2
A	1298	LYS	-	expression tag	UNP P0DTC2
B	372	THR	ALA	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	SER	-	expression tag	UNP P0DTC2
B	1291	ASP	-	expression tag	UNP P0DTC2
B	1292	TYR	-	expression tag	UNP P0DTC2
B	1293	LYS	-	expression tag	UNP P0DTC2
B	1294	ASP	-	expression tag	UNP P0DTC2
B	1295	ASP	-	expression tag	UNP P0DTC2
B	1296	ASP	-	expression tag	UNP P0DTC2
B	1297	ASP	-	expression tag	UNP P0DTC2
B	1298	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	372	THR	ALA	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	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
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	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2

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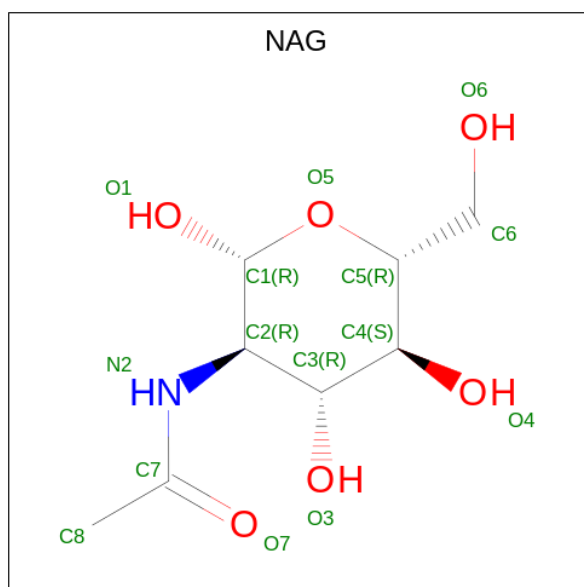
Chain	Residue	Modelled	Actual	Comment	Reference
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	SER	-	expression tag	UNP P0DTC2
C	1291	ASP	-	expression tag	UNP P0DTC2
C	1292	TYR	-	expression tag	UNP P0DTC2
C	1293	LYS	-	expression tag	UNP P0DTC2
C	1294	ASP	-	expression tag	UNP P0DTC2
C	1295	ASP	-	expression tag	UNP P0DTC2
C	1296	ASP	-	expression tag	UNP P0DTC2
C	1297	ASP	-	expression tag	UNP P0DTC2
C	1298	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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	

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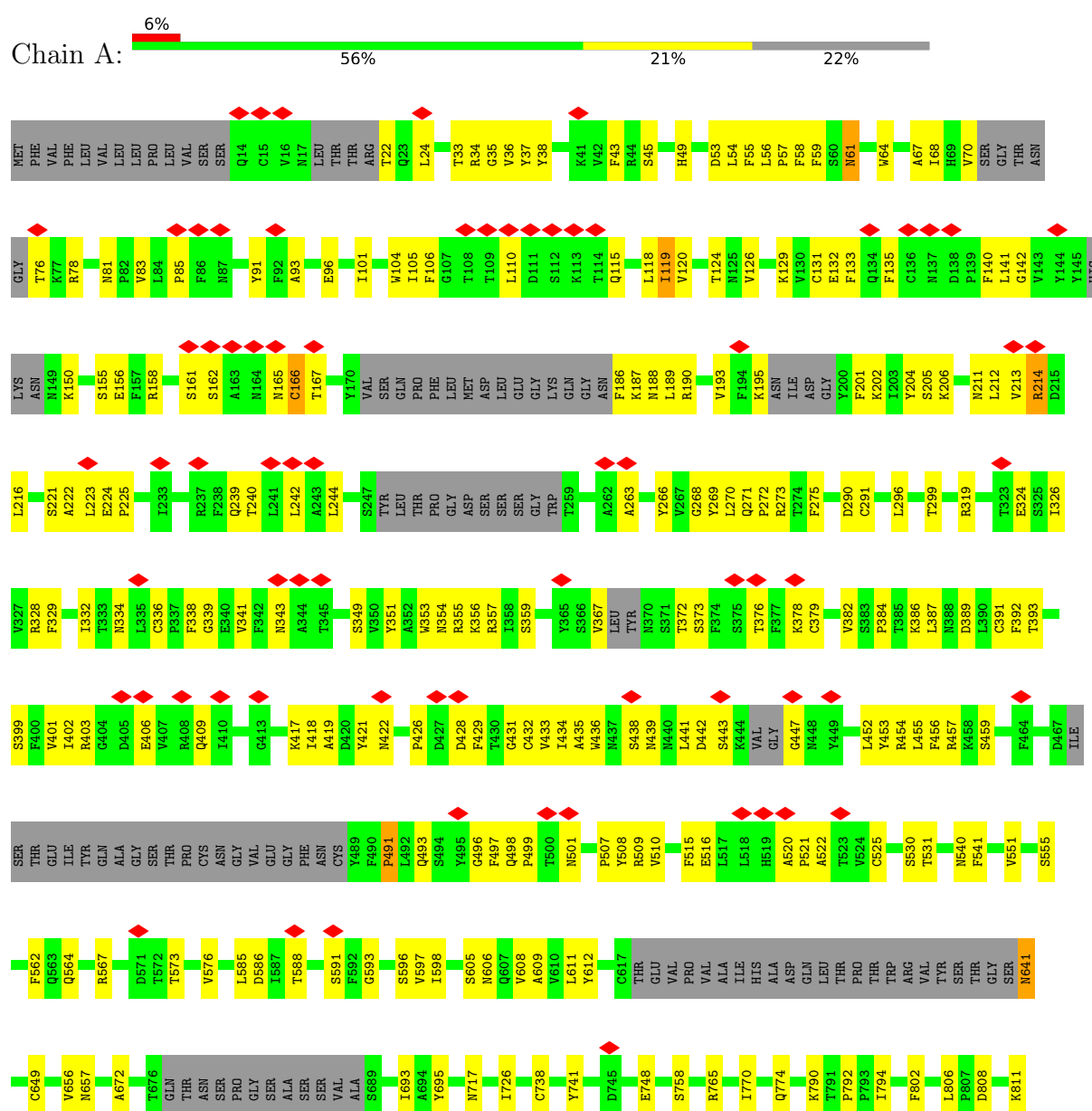
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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C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

3 Residue-property plots

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





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.075	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0104	Depositor
Map size (\AA)	307.41202, 307.41202, 307.41202	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0979, 1.0979, 1.0979	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	0.36	0/8076	0.51	0/10977
1	B	0.57	0/8188	0.61	0/11130
1	C	0.36	0/8224	0.52	0/11183
All	All	0.44	0/24488	0.55	0/33290

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
1	C	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Peptide
1	B	1096	VAL	Peptide
1	B	328	ARG	Peptide
1	B	329	PHE	Peptide
1	B	521	PRO	Peptide
1	B	756	TYR	Peptide
1	C	1074	ASN	Peptide

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	7901	0	7711	192	0
1	B	8009	0	7811	118	0
1	C	8044	0	7846	202	0
2	A	140	0	130	3	0
2	B	154	0	143	0	0
2	C	196	0	182	0	0
All	All	24444	0	23823	494	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 10.

All (494) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:THR:HB	2:A:1309:NAG:C1	1.74	1.16
1:A:213:VAL:HG12	1:A:214:ARG:HG2	1.61	0.81
1:B:214:ARG:HG2	1:B:215:ASP:H	1.43	0.81
1:B:97:LYS:HD3	1:B:187:LYS:HB2	1.64	0.78
1:A:612:TYR:HB2	1:A:649:CYS:HB3	1.65	0.76
1:A:929:SER:OG	1:A:933:LYS:NZ	2.20	0.75
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.20	0.74
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.70	0.74
1:A:37:TYR:HB3	1:A:223:LEU:HB2	1.71	0.73
1:A:521:PRO:HG3	1:A:564:GLN:HG3	1.70	0.72
1:B:86:PHE:H	1:B:237:ARG:HA	1.56	0.71
1:B:379:CYS:HA	1:B:432:CYS:HA	1.72	0.70
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.73	0.70
1:A:37:TYR:HA	1:A:223:LEU:H	1.56	0.70
1:B:33:THR:OG1	1:B:219:GLY:O	2.10	0.69
1:A:193:VAL:HB	1:A:204:TYR:HB2	1.72	0.69
1:C:821:LEU:HD11	1:C:939:SER:HB3	1.74	0.69
1:C:30:ASN:ND2	1:C:31:SER:O	2.26	0.68
1:C:970:PHE:O	1:C:995:ARG:NH1	2.27	0.68
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.75	0.67
1:C:353:TRP:O	1:C:466:ARG:NH2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:NZ	1:C:221:SER:OG	2.28	0.67
1:C:452:LEU:HD13	1:C:492:LEU:HB3	1.76	0.67
1:A:376:THR:HB	1:A:435:ALA:HB3	1.75	0.67
1:C:86:PHE:H	1:C:237:ARG:HA	1.60	0.66
1:B:970:PHE:HA	1:C:756:TYR:HE1	1.60	0.66
1:A:496:GLY:O	1:A:501:ASN:ND2	2.29	0.66
1:A:187:LYS:NZ	1:A:211:ASN:OD1	2.27	0.66
1:C:106:PHE:HB2	1:C:117:LEU:HD23	1.76	0.66
1:A:57:PRO:HB3	1:A:273:ARG:NH1	2.10	0.65
1:A:1031:GLU:OE1	1:C:1039:ARG:NE	2.28	0.65
1:B:30:ASN:HD21	1:B:59:PHE:HD1	1.43	0.65
1:A:457:ARG:NH1	1:A:459:SER:O	2.29	0.65
1:B:417:LYS:HE3	1:B:455:LEU:HD12	1.78	0.65
1:B:1129:VAL:HG12	1:C:917:TYR:HB3	1.79	0.65
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.62	0.65
1:B:291:CYS:HA	1:B:297:SER:HB3	1.79	0.64
1:C:107:GLY:HA3	1:C:110:LEU:HD21	1.79	0.64
1:C:299:THR:HG22	1:C:597:VAL:HG11	1.78	0.64
1:B:204:TYR:HB3	1:B:223:LEU:HG	1.77	0.64
1:A:443:SER:HB3	1:A:499:PRO:HD3	1.79	0.64
1:A:993:ILE:O	1:A:997:ILE:HD12	1.98	0.64
1:C:822:LEU:HD11	1:C:1061:VAL:HG21	1.80	0.64
1:B:156:GLU:OE1	1:B:158:ARG:NH2	2.31	0.63
1:B:201:PHE:HD2	1:B:203:ILE:HD11	1.63	0.63
1:B:134:GLN:HB3	1:B:161:SER:HB2	1.78	0.63
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.81	0.63
1:A:328:ARG:NH1	1:A:531:THR:O	2.31	0.63
1:A:438:SER:HB2	1:A:441:LEU:HD12	1.81	0.63
1:A:239:GLN:NE2	1:A:240:THR:O	2.32	0.62
1:C:612:TYR:HB2	1:C:649:CYS:HB3	1.81	0.62
1:A:329:PHE:O	1:A:530:SER:OG	2.17	0.62
1:C:139:PRO:HB2	1:C:241:LEU:HD21	1.82	0.62
1:C:244:LEU:HD22	1:C:260:ALA:HA	1.82	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HG2	1.81	0.61
1:B:102:ARG:HH22	1:B:154:GLU:HB2	1.65	0.61
1:A:1100:THR:HG22	1:A:1101:HIS:CE1	2.36	0.61
1:A:202:LYS:HE2	1:A:225:PRO:HB2	1.82	0.61
1:C:389:ASP:OD1	1:C:528:LYS:NZ	2.28	0.61
1:B:189:LEU:HD22	1:B:210:ILE:HD13	1.83	0.60
1:C:726:ILE:HG22	1:C:1061:VAL:HG22	1.82	0.60
1:B:132:GLU:HB2	1:B:164:ASN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:CYS:HA	1:C:525:CYS:HA	1.83	0.60
1:A:962:LEU:HD11	1:A:1007:TYR:CD2	2.37	0.60
1:A:212:LEU:HG	1:A:213:VAL:H	1.66	0.59
1:C:290:ASP:OD1	1:C:291:CYS:N	2.34	0.59
1:A:748:GLU:OE2	1:A:748:GLU:N	2.31	0.59
1:C:403:ARG:NH2	1:C:405:ASP:OD2	2.36	0.59
1:A:206:LYS:NZ	1:A:221:SER:OG	2.32	0.59
1:C:409:GLN:NE2	1:C:415:THR:O	2.35	0.59
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.84	0.59
1:A:567:ARG:HD2	1:B:42:VAL:HG11	1.85	0.59
1:A:453:TYR:CZ	1:A:455:LEU:HD11	2.39	0.58
1:C:991:VAL:O	1:C:995:ARG:HG3	2.03	0.58
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.31	0.58
1:A:68:ILE:HG13	1:A:70:VAL:H	1.69	0.58
1:B:712:ILE:HG13	1:B:1077:THR:HG21	1.85	0.58
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.84	0.58
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.86	0.57
1:B:52:GLN:OE1	1:B:274:THR:OG1	2.14	0.57
1:C:409:GLN:HG2	1:C:418:ILE:HB	1.86	0.57
1:A:93:ALA:HB1	1:A:189:LEU:HD11	1.85	0.57
1:C:21:ARG:NH2	1:C:138:ASP:OD2	2.38	0.57
1:A:204:TYR:HA	1:A:225:PRO:HA	1.85	0.57
1:B:193:VAL:HG13	1:B:270:LEU:HD11	1.86	0.57
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.86	0.57
1:A:822:LEU:HD21	1:A:938:LEU:HD13	1.85	0.57
1:C:103:GLY:HA3	1:C:241:LEU:HB2	1.86	0.57
1:A:605:SER:OG	1:A:606:ASN:N	2.37	0.57
1:A:353:TRP:CZ3	1:A:355:ARG:HB2	2.39	0.57
1:B:898:PHE:HZ	1:B:1050:MET:HE1	1.70	0.57
1:C:555:SER:HB3	1:C:584:ILE:HG23	1.85	0.57
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.70	0.57
1:A:85:PRO:O	1:A:269:TYR:OH	2.17	0.56
1:A:391:CYS:SG	1:A:525:CYS:N	2.78	0.56
1:A:403:ARG:HG2	1:A:497:PHE:HE1	1.69	0.56
1:A:765:ARG:NH1	1:C:957:GLN:OE1	2.37	0.56
1:C:121:ASN:CG	1:C:174:PRO:HB3	2.25	0.56
1:C:327:VAL:HA	1:C:542:ASN:OD1	2.05	0.56
1:C:885:GLY:O	1:C:905:ARG:NH2	2.38	0.56
1:C:559:PHE:HB3	1:C:577:ARG:NH2	2.20	0.56
1:C:295:PRO:O	1:C:299:THR:HG23	2.06	0.56
1:C:391:CYS:SG	1:C:525:CYS:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.41	0.56
1:C:563:GLN:O	1:C:577:ARG:NH1	2.38	0.56
1:A:58:PHE:HE1	1:A:275:PHE:HE1	1.54	0.55
1:C:719:THR:N	1:C:1068:VAL:O	2.36	0.55
1:B:330:PRO:HD2	1:B:530:SER:HB2	1.87	0.55
1:C:439:ASN:HD21	1:C:499:PRO:HB3	1.71	0.55
1:C:962:LEU:HD11	1:C:1007:TYR:CG	2.41	0.55
1:A:387:LEU:HD12	1:A:392:PHE:HZ	1.72	0.55
1:B:57:PRO:HG2	1:B:60:SER:HB2	1.89	0.55
1:B:110:LEU:HG	1:B:237:ARG:HH22	1.72	0.55
1:C:141:LEU:HD12	1:C:154:GLU:OE2	2.06	0.55
1:A:439:ASN:O	1:A:443:SER:OG	2.18	0.55
1:C:353:TRP:HH2	1:C:355:ARG:HH11	1.54	0.55
1:A:922:LEU:O	1:A:926:GLN:HG3	2.07	0.55
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.89	0.55
1:B:29:THR:HG23	1:B:62:VAL:HG23	1.90	0.54
1:C:354:ASN:HB3	1:C:399:SER:HB2	1.90	0.54
1:A:22:THR:OG1	1:A:76:THR:O	2.25	0.54
1:A:551:VAL:HB	1:A:588:THR:HB	1.89	0.54
1:A:1045:LYS:H	1:A:1066:THR:HG21	1.72	0.54
1:A:37:TYR:OH	1:A:54:LEU:O	2.14	0.54
1:A:738:CYS:O	1:A:741:TYR:N	2.39	0.54
1:C:457:ARG:NH1	1:C:460:ASN:O	2.40	0.54
1:A:379:CYS:HA	1:A:432:CYS:HA	1.90	0.54
1:B:83:VAL:HG12	1:B:239:GLN:HG3	1.89	0.54
1:A:115:GLN:HA	1:A:132:GLU:HB2	1.90	0.54
1:B:245:HIS:O	1:B:259:THR:HG22	2.08	0.54
1:C:18:LEU:HB2	1:C:21:ARG:HD2	1.90	0.54
1:B:133:PHE:HB3	1:B:160:TYR:HB2	1.90	0.54
1:A:976:VAL:HG12	1:A:979:ASP:H	1.73	0.54
1:C:290:ASP:HB3	1:C:293:LEU:HD23	1.90	0.54
1:C:922:LEU:HD11	1:C:926:GLN:HE21	1.72	0.54
1:A:319:ARG:NH2	1:A:593:GLY:O	2.41	0.54
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.90	0.54
1:C:108:THR:O	1:C:237:ARG:NH1	2.41	0.54
1:A:188:ASN:HB3	1:A:190:ARG:NH1	2.23	0.53
1:A:195:LYS:HD3	1:A:204:TYR:HE1	1.72	0.53
1:C:312:ILE:HD11	1:C:666:ILE:HD13	1.90	0.53
1:C:347:PHE:HB2	1:C:401:VAL:HG13	1.90	0.53
1:A:319:ARG:HD3	1:A:591:SER:HB3	1.90	0.53
1:A:984:LEU:O	1:C:386:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HB2	1:A:78:ARG:HH11	1.74	0.53
1:C:327:VAL:HG12	1:C:530:SER:HA	1.91	0.53
1:A:81:ASN:ND2	1:A:242:LEU:HG	2.23	0.53
1:A:349:SER:OG	1:A:452:LEU:O	2.26	0.53
1:A:1092:GLU:OE2	1:A:1092:GLU:N	2.41	0.53
1:C:851:CYS:HA	1:C:854:LYS:HD2	1.90	0.53
1:A:765:ARG:HH22	1:C:1014:ARG:HH22	1.56	0.53
1:C:349:SER:OG	1:C:350:VAL:N	2.41	0.53
1:A:1100:THR:CB	2:A:1309:NAG:C1	2.66	0.53
1:A:1144:GLU:N	1:A:1144:GLU:OE1	2.42	0.53
1:A:105:ILE:HG22	1:A:118:LEU:HG	1.91	0.52
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.91	0.52
1:C:205:SER:HB3	1:C:226:LEU:HD11	1.91	0.52
1:B:53:ASP:HB3	1:B:55:PHE:CE1	2.44	0.52
1:B:200:TYR:CE1	1:B:230:PRO:HB3	2.45	0.52
1:C:31:SER:HG	1:C:60:SER:H	1.56	0.52
1:A:341:VAL:HG22	1:A:356:LYS:HE2	1.90	0.52
1:A:596:SER:HB2	1:A:611:LEU:HB3	1.91	0.52
1:C:559:PHE:HB3	1:C:577:ARG:HH21	1.74	0.52
1:B:699:LEU:HB2	1:C:788:ILE:HD11	1.90	0.52
1:C:404:GLY:N	1:C:506:GLN:O	2.41	0.52
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.91	0.52
1:C:121:ASN:ND2	1:C:174:PRO:HB3	2.25	0.52
1:C:990:GLU:OE1	1:C:990:GLU:N	2.42	0.52
1:A:447:GLY:HA2	1:A:498:GLN:NE2	2.24	0.52
1:B:53:ASP:OD1	1:B:54:LEU:N	2.31	0.52
1:C:18:LEU:HD13	1:C:258:TRP:CD1	2.45	0.52
1:C:320:VAL:HB	1:C:590:CYS:SG	2.50	0.51
1:B:699:LEU:HB3	1:C:873:TYR:HE1	1.75	0.51
1:A:299:THR:OG1	1:A:597:VAL:HG11	2.09	0.51
1:A:770:ILE:O	1:A:774:GLN:HG2	2.10	0.51
1:B:229:LEU:HD12	1:B:230:PRO:HD2	1.93	0.51
1:B:117:LEU:HD12	1:B:231:ILE:HG21	1.92	0.51
1:B:227:VAL:HG22	1:B:228:ASP:H	1.75	0.51
1:C:112:SER:C	1:C:132:GLU:HG2	2.30	0.51
1:A:129:LYS:HE2	1:A:133:PHE:HZ	1.74	0.51
1:C:457:ARG:NH1	1:C:459:SER:OG	2.44	0.51
1:A:33:THR:HA	1:A:58:PHE:CE2	2.45	0.51
1:A:53:ASP:OD1	1:A:54:LEU:N	2.37	0.51
1:A:290:ASP:OD1	1:A:291:CYS:N	2.44	0.51
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.44	0.50
1:C:346:ARG:HA	1:C:509:ARG:HH22	1.76	0.50
1:C:780:GLU:OE2	1:C:1019:ARG:NH1	2.44	0.50
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.47	0.50
1:A:38:TYR:CE1	1:A:222:ALA:HB3	2.46	0.50
1:A:351:TYR:HB2	1:A:454:ARG:HH21	1.77	0.50
1:A:1100:THR:HG22	1:A:1101:HIS:ND1	2.27	0.50
1:C:516:GLU:HB3	1:C:519:HIS:ND1	2.26	0.50
1:A:567:ARG:HA	1:A:573:THR:HA	1.92	0.50
1:C:329:PHE:N	1:C:530:SER:OG	2.45	0.50
1:A:421:TYR:CE1	1:A:457:ARG:HB3	2.46	0.50
1:A:950:ASP:OD1	1:A:951:VAL:N	2.45	0.50
1:C:92:PHE:CE1	1:C:94:SER:HB2	2.47	0.50
1:C:716:THR:N	1:C:1071:GLN:O	2.43	0.50
1:A:1100:THR:CG2	1:A:1101:HIS:CE1	2.95	0.50
1:A:656:VAL:HG23	1:A:695:TYR:HB3	1.94	0.49
1:A:296:LEU:HB2	1:A:608:VAL:HG11	1.94	0.49
1:C:395:VAL:HG21	1:C:524:VAL:HG11	1.94	0.49
1:C:868:GLU:O	1:C:872:GLN:HG3	2.12	0.49
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.48	0.49
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.47	0.49
1:C:913:GLN:HB3	1:C:917:TYR:CE2	2.48	0.49
1:A:58:PHE:CE1	1:A:275:PHE:HE1	2.30	0.49
1:A:985:ASP:N	1:C:383:SER:OG	2.46	0.49
1:B:102:ARG:HG3	1:B:141:LEU:HG	1.95	0.49
1:B:79:PHE:HE1	1:B:244:LEU:HD21	1.78	0.49
1:C:95:THR:HA	1:C:188:ASN:O	2.12	0.49
1:C:109:THR:HA	1:C:237:ARG:HH12	1.76	0.49
1:C:116:SER:HB2	1:C:133:PHE:HD2	1.77	0.49
1:A:339:GLY:O	1:A:343:ASN:HB3	2.13	0.49
1:B:22:THR:N	1:B:77:LYS:O	2.46	0.49
1:B:201:PHE:N	1:B:229:LEU:O	2.42	0.49
1:C:112:SER:N	1:C:133:PHE:O	2.46	0.49
1:C:807:PRO:HB3	1:C:814:LYS:O	2.13	0.49
1:A:91:TYR:HB3	1:A:268:GLY:O	2.12	0.49
1:C:318:PHE:HE2	1:C:320:VAL:HG22	1.78	0.49
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.94	0.48
1:C:312:ILE:HG12	1:C:598:ILE:HG12	1.94	0.48
1:A:431:GLY:HA2	1:A:515:PHE:CE1	2.48	0.48
1:A:980:ILE:HA	1:A:983:ARG:HG2	1.95	0.48
1:A:67:ALA:HB3	1:A:263:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1307:NAG:O6	2:A:1307:NAG:O4	2.25	0.48
1:C:118:LEU:O	1:C:128:ILE:HA	2.13	0.48
1:C:142:GLY:HA2	1:C:244:LEU:H	1.78	0.48
1:A:91:TYR:HB2	1:A:270:LEU:HD21	1.96	0.48
1:C:215:ASP:OD1	1:C:216:LEU:N	2.45	0.48
1:B:541:PHE:HZ	1:B:587:ILE:HD12	1.77	0.48
1:B:574:ASP:HA	1:B:587:ILE:HG12	1.94	0.48
1:C:79:PHE:CZ	1:C:244:LEU:HD21	2.48	0.48
1:A:960:ASN:O	1:A:964:LYS:HG2	2.13	0.48
1:A:81:ASN:ND2	1:A:240:THR:O	2.47	0.48
1:A:324:GLU:OE2	1:A:326:ILE:HG23	2.14	0.48
1:A:354:ASN:HB3	1:A:399:SER:HB2	1.95	0.48
1:A:355:ARG:NH1	1:A:357:ARG:HB2	2.28	0.48
1:B:331:ASN:HD22	1:B:331:ASN:HA	1.41	0.48
1:A:417:LYS:HZ2	1:A:455:LEU:HA	1.78	0.48
1:C:86:PHE:N	1:C:237:ARG:HA	2.28	0.48
1:C:103:GLY:N	1:C:241:LEU:O	2.41	0.48
1:A:402:ILE:HD11	1:A:510:VAL:HG21	1.96	0.47
1:C:962:LEU:HD11	1:C:1007:TYR:CD2	2.49	0.47
1:A:357:ARG:NH1	1:A:359:SER:OG	2.32	0.47
1:B:44:ARG:NH1	1:B:44:ARG:HB2	2.29	0.47
1:B:676:THR:HA	1:B:690:GLN:HA	1.96	0.47
1:C:143:VAL:HG12	1:C:154:GLU:HB2	1.96	0.47
1:C:756:TYR:O	1:C:758:SER:N	2.47	0.47
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.96	0.47
1:A:83:VAL:HG22	1:A:239:GLN:HG3	1.96	0.47
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.77	0.47
1:A:55:PHE:O	1:A:271:GLN:N	2.29	0.47
1:C:559:PHE:HD2	1:C:577:ARG:HH21	1.63	0.47
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.96	0.47
1:B:358:ILE:HB	1:B:395:VAL:HB	1.97	0.47
1:B:379:CYS:HB3	1:B:382:VAL:HG13	1.96	0.47
1:B:729:VAL:HG11	1:B:781:VAL:HG11	1.97	0.47
1:C:392:PHE:O	1:C:522:ALA:HB1	2.15	0.47
1:C:546:LEU:HD22	1:C:565:PHE:CE2	2.49	0.47
1:C:596:SER:HB2	1:C:611:LEU:HB3	1.96	0.47
1:C:642:VAL:HG22	1:C:651:ILE:HG22	1.97	0.47
1:A:409:GLN:HG2	1:A:419:ALA:HB2	1.96	0.47
1:A:962:LEU:HD11	1:A:1007:TYR:CG	2.50	0.47
1:C:347:PHE:N	1:C:509:ARG:HH12	2.12	0.47
1:B:108:THR:HG23	1:B:114:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:HG2	1:B:215:ASP:N	2.22	0.47
1:C:273:ARG:HD3	1:C:275:PHE:HE1	1.80	0.47
1:C:316:SER:OG	1:C:317:ASN:N	2.48	0.47
1:A:790:LYS:HE3	1:C:702:GLU:HB3	1.97	0.47
1:C:107:GLY:O	1:C:237:ARG:N	2.42	0.47
1:C:962:LEU:HD21	1:C:1007:TYR:HB2	1.97	0.47
1:A:402:ILE:HB	1:A:406:GLU:HB2	1.97	0.46
1:A:641:ASN:HD22	1:A:641:ASN:HA	1.53	0.46
1:B:319:ARG:NH2	1:B:592:PHE:H	2.13	0.46
1:A:496:GLY:O	1:A:498:GLN:N	2.47	0.46
1:A:1100:THR:HG22	1:A:1101:HIS:CG	2.50	0.46
1:C:499:PRO:HA	1:C:506:GLN:NE2	2.30	0.46
1:B:124:THR:O	1:B:174:PRO:HB3	2.16	0.46
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.96	0.46
1:A:726:ILE:HD11	1:A:948:LEU:HD11	1.97	0.46
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.97	0.46
1:C:515:PHE:CE2	1:C:517:LEU:HG	2.51	0.46
1:A:378:LYS:O	1:A:433:VAL:N	2.40	0.46
1:B:102:ARG:O	1:B:121:ASN:HB3	2.15	0.46
1:C:770:ILE:O	1:C:774:GLN:HG2	2.16	0.46
1:C:924:ALA:O	1:C:928:ASN:ND2	2.49	0.46
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.98	0.46
1:B:210:ILE:HD12	1:B:212:LEU:HD12	1.97	0.46
1:C:394:ASN:HB3	1:C:396:TYR:HE1	1.79	0.46
1:C:424:LYS:NZ	1:C:463:PRO:HG3	2.30	0.46
1:A:36:VAL:O	1:A:223:LEU:HG	2.16	0.46
1:A:54:LEU:HD13	1:A:272:PRO:N	2.30	0.46
1:A:991:VAL:O	1:A:995:ARG:HG3	2.15	0.46
1:B:705:VAL:HG12	1:C:895:GLN:HG3	1.98	0.46
1:B:66:HIS:HB2	1:B:78:ARG:NH1	2.31	0.46
1:C:69:HIS:HA	1:C:77:LYS:H	1.81	0.46
1:C:86:PHE:HB2	1:C:238:PHE:HD1	1.81	0.46
1:A:455:LEU:HD13	1:A:493:GLN:HB2	1.98	0.46
1:A:855:PHE:CD2	1:C:589:PRO:HD2	2.51	0.46
1:B:18:LEU:HD13	1:B:258:TRP:CE2	2.51	0.46
1:C:393:THR:HG22	1:C:394:ASN:ND2	2.31	0.46
1:A:96:GLU:OE2	1:A:101:ILE:N	2.45	0.45
1:A:131:CYS:CB	1:A:166:CYS:HA	2.46	0.45
1:B:570:ALA:HB1	1:C:963:VAL:HG11	1.98	0.45
1:C:29:THR:HG23	1:C:62:VAL:HG23	1.99	0.45
1:A:402:ILE:HG13	1:A:508:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:HB2	1:C:466:ARG:HH22	1.82	0.45
1:A:1055:SER:OG	1:A:1056:ALA:N	2.49	0.45
1:C:62:VAL:HG12	1:C:268:GLY:HA3	1.98	0.45
1:C:114:THR:O	1:C:132:GLU:HG3	2.16	0.45
1:C:515:PHE:HE2	1:C:517:LEU:HG	1.80	0.45
1:C:662:CYS:HB2	1:C:697:MET:HE2	1.98	0.45
1:A:58:PHE:HB3	1:A:59:PHE:HD1	1.82	0.45
1:A:351:TYR:CD1	1:A:453:TYR:HA	2.51	0.45
1:A:717:ASN:HB3	1:A:1070:ALA:HB3	1.99	0.45
1:B:188:ASN:HA	1:B:209:PRO:HA	1.98	0.45
1:B:388:ASN:HA	1:B:527:PRO:HD2	1.99	0.45
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.52	0.45
1:C:900:MET:HG2	1:C:917:TYR:OH	2.17	0.45
1:A:61:ASN:HD22	1:A:61:ASN:HA	1.62	0.45
1:B:246:ARG:NH1	1:B:257:GLY:O	2.49	0.45
1:A:393:THR:HB	1:A:516:GLU:HB2	1.99	0.45
1:B:105:ILE:HG22	1:B:118:LEU:HD13	1.98	0.45
1:B:712:ILE:HG22	1:B:714:ILE:HG12	1.99	0.45
1:C:392:PHE:HD2	1:C:515:PHE:CD2	2.35	0.45
1:A:984:LEU:HD21	1:A:988:GLU:OE1	2.17	0.45
1:C:564:GLN:HG3	1:C:565:PHE:CE1	2.51	0.45
1:B:143:VAL:HG11	1:B:152:TRP:HB3	1.99	0.45
1:C:112:SER:HB3	1:C:134:GLN:HB2	1.99	0.45
1:C:453:TYR:HB3	1:C:495:TYR:OH	2.17	0.45
1:A:34:ARG:HG3	1:A:216:LEU:HD21	1.98	0.44
1:B:767:LEU:HD13	1:B:767:LEU:HA	1.82	0.44
1:C:101:ILE:HA	1:C:242:LEU:HD22	1.99	0.44
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.99	0.44
1:C:586:ASP:OD1	1:C:587:ILE:N	2.50	0.44
1:A:64:TRP:HZ2	1:A:214:ARG:HE	1.66	0.44
1:A:332:ILE:HG22	1:A:334:ASN:H	1.82	0.44
1:A:540:ASN:OD1	1:A:541:PHE:N	2.49	0.44
1:B:48:LEU:HD23	1:B:278:LYS:HA	1.99	0.44
1:C:357:ARG:NH1	1:C:396:TYR:OH	2.45	0.44
1:C:437:ASN:HB2	1:C:508:TYR:CZ	2.53	0.44
1:C:538:CYS:HA	1:C:551:VAL:HG22	2.00	0.44
1:C:1055:SER:OG	1:C:1056:ALA:N	2.50	0.44
1:B:78:ARG:NE	1:B:80:ASP:OD2	2.50	0.44
1:B:239:GLN:NE2	1:B:240:THR:O	2.51	0.44
1:B:132:GLU:HG3	1:B:165:ASN:HB2	1.98	0.44
1:B:335:LEU:HD11	1:B:364:ASP:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ILE:HB	1:A:609:ALA:HB3	2.00	0.44
1:B:528:LYS:HA	1:B:528:LYS:HD2	1.82	0.44
1:C:24:LEU:HG	1:C:78:ARG:HD3	1.99	0.44
1:C:189:LEU:HB3	1:C:208:THR:HB	2.00	0.44
1:C:311:GLY:HA2	1:C:664:ILE:HD12	2.00	0.44
1:C:607:GLN:HE21	1:C:674:TYR:HE1	1.66	0.44
1:C:612:TYR:O	1:C:649:CYS:N	2.51	0.44
1:B:55:PHE:HD2	1:B:275:PHE:CD1	2.36	0.44
1:C:172:SER:HB3	1:C:173:GLN:H	1.57	0.44
1:C:600:PRO:HB3	1:C:674:TYR:HB2	2.00	0.44
1:A:379:CYS:SG	1:A:384:PRO:HB3	2.58	0.44
1:A:434:ILE:O	1:A:510:VAL:HG13	2.18	0.44
1:B:66:HIS:O	1:B:78:ARG:NH2	2.50	0.44
1:B:139:PRO:HB2	1:B:241:LEU:HD21	2.00	0.44
1:A:37:TYR:H	1:A:55:PHE:HE1	1.66	0.43
1:A:142:GLY:HA2	1:A:244:LEU:H	1.82	0.43
1:C:100:ILE:O	1:C:102:ARG:HG2	2.18	0.43
1:C:281:GLU:H	1:C:281:GLU:HG3	1.54	0.43
1:B:175:PHE:O	1:B:177:MET:HE2	2.18	0.43
1:B:319:ARG:CZ	1:B:319:ARG:HA	2.48	0.43
1:B:319:ARG:HH22	1:B:592:PHE:H	1.65	0.43
1:C:472:ILE:H	1:C:472:ILE:HG12	1.47	0.43
1:A:271:GLN:O	1:A:273:ARG:N	2.51	0.43
1:A:454:ARG:HA	1:A:491:PRO:O	2.18	0.43
1:A:562:PHE:CE2	1:B:224:GLU:HB3	2.52	0.43
1:A:1145:LEU:HD23	1:A:1146:ASP:OD1	2.18	0.43
1:B:65:PHE:HE2	1:B:84:LEU:HD11	1.82	0.43
1:A:555:SER:HA	1:A:586:ASP:OD2	2.19	0.43
1:A:758:SER:HB3	1:C:965:GLN:OE1	2.19	0.43
1:C:308:VAL:HG12	1:C:599:THR:HG21	2.00	0.43
1:C:351:TYR:CE1	1:C:452:LEU:HB2	2.54	0.43
1:A:336:CYS:HB2	1:A:338:PHE:CZ	2.54	0.43
1:C:569:ILE:H	1:C:569:ILE:HD12	1.83	0.43
1:C:969:ASN:OD1	1:C:975:SER:OG	2.33	0.43
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.52	0.43
1:A:401:VAL:HG12	1:A:509:ARG:HA	1.99	0.43
1:A:576:VAL:HG12	1:A:585:LEU:HB2	2.00	0.43
1:B:347:PHE:HE2	1:B:509:ARG:HD3	1.84	0.43
1:B:433:VAL:HG22	1:B:512:VAL:HG13	2.01	0.43
1:A:43:PHE:CZ	1:A:45:SER:HB3	2.54	0.43
1:A:205:SER:N	1:A:224:GLU:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LYS:HB2	1:B:306:PHE:CE2	2.54	0.43
1:B:878:LEU:HD13	1:B:878:LEU:HA	1.92	0.43
1:C:293:LEU:HD12	1:C:294:ASP:HB2	2.00	0.43
1:C:805:ILE:HG23	1:C:1054:GLN:OE1	2.19	0.43
1:B:85:PRO:HA	1:B:237:ARG:HG2	1.99	0.43
1:B:319:ARG:HA	1:B:319:ARG:NE	2.34	0.43
1:A:418:ILE:HD12	1:A:418:ILE:H	1.84	0.43
1:B:567:ARG:HG3	1:B:573:THR:HA	2.01	0.43
1:B:585:LEU:HD13	1:B:585:LEU:HA	1.89	0.43
1:B:753:LEU:HD13	1:B:997:ILE:HD11	2.00	0.43
1:B:1062:PHE:HB3	1:B:1064:HIS:CD2	2.54	0.43
1:A:355:ARG:CZ	1:A:357:ARG:HB2	2.49	0.42
1:A:890:ALA:HB1	1:C:1046:GLY:HA2	2.01	0.42
1:C:328:ARG:NH1	1:C:531:THR:O	2.52	0.42
1:C:676:THR:HA	1:C:690:GLN:HG2	2.00	0.42
1:C:702:GLU:N	1:C:702:GLU:OE1	2.52	0.42
1:A:81:ASN:HD21	1:A:242:LEU:H	1.68	0.42
1:A:851:CYS:O	1:A:855:PHE:HD1	2.02	0.42
1:C:37:TYR:CB	1:C:223:LEU:HB2	2.49	0.42
1:C:398:ASP:O	1:C:511:VAL:HA	2.19	0.42
1:A:36:VAL:O	1:A:222:ALA:HA	2.19	0.42
1:A:855:PHE:CE2	1:C:589:PRO:HD2	2.53	0.42
1:B:30:ASN:ND2	1:B:31:SER:O	2.52	0.42
1:B:43:PHE:CZ	1:B:45:SER:HB3	2.55	0.42
1:A:386:LYS:HE2	1:A:386:LYS:HB3	1.91	0.42
1:A:794:ILE:HD13	1:A:794:ILE:HA	1.88	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.02	0.42
1:C:45:SER:O	1:C:47:VAL:HG13	2.19	0.42
1:A:186:PHE:CE1	1:A:263:ALA:HA	2.55	0.42
1:C:104:TRP:HZ3	1:C:121:ASN:H	1.66	0.42
1:C:327:VAL:O	1:C:328:ARG:HD2	2.19	0.42
1:A:221:SER:OG	1:A:222:ALA:N	2.53	0.42
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.35	0.42
1:A:418:ILE:HG23	1:A:422:ASN:HB2	2.01	0.42
1:A:802:PHE:HB3	1:A:806:LEU:HD23	2.02	0.42
1:A:977:LEU:O	1:A:981:LEU:HG	2.20	0.42
1:A:985:ASP:HB2	1:A:987:PRO:HD2	2.02	0.42
1:B:443:SER:HB2	1:B:497:PHE:HB3	2.01	0.42
1:C:110:LEU:HB3	1:C:135:PHE:CE2	2.55	0.42
1:B:172:SER:OG	1:B:173:GLN:N	2.53	0.42
1:B:934:ILE:HD12	1:B:934:ILE:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:VAL:H	1:C:531:THR:HG1	1.63	0.42
1:C:401:VAL:HG12	1:C:509:ARG:HG2	2.01	0.42
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.54	0.42
1:B:966:LEU:HD13	1:B:966:LEU:HA	1.85	0.42
1:C:109:THR:O	1:C:237:ARG:NH2	2.43	0.42
1:C:117:LEU:HD11	1:C:119:ILE:HG13	2.00	0.42
1:C:214:ARG:HE	1:C:215:ASP:H	1.67	0.42
1:A:104:TRP:HB3	1:A:119:ILE:HB	2.01	0.41
1:A:386:LYS:HB2	1:A:389:ASP:OD1	2.19	0.41
1:A:885:GLY:HA2	1:A:901:GLN:CD	2.41	0.41
1:A:1080:ALA:HB2	1:A:1089:PHE:HE1	1.85	0.41
1:B:116:SER:O	1:B:130:VAL:HA	2.19	0.41
1:B:294:ASP:HB3	1:B:297:SER:H	1.84	0.41
1:A:393:THR:HG23	1:A:522:ALA:HB2	2.01	0.41
1:A:428:ASP:OD1	1:A:428:ASP:N	2.52	0.41
1:B:68:ILE:HG12	1:B:70:VAL:H	1.86	0.41
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.78	0.41
1:C:88:ASP:OD1	1:C:88:ASP:N	2.52	0.41
1:C:127:VAL:HA	1:C:170:TYR:O	2.20	0.41
1:B:106:PHE:CD2	1:B:238:PHE:HB2	2.55	0.41
1:C:444:LYS:NZ	1:C:448:ASN:OD1	2.44	0.41
1:A:382:VAL:HG11	1:A:515:PHE:HZ	1.85	0.41
1:A:551:VAL:N	1:A:588:THR:O	2.44	0.41
1:C:411:ALA:HB3	1:C:414:GLN:HG2	2.02	0.41
1:C:767:LEU:HD21	1:C:1008:VAL:HG22	2.01	0.41
1:A:455:LEU:O	1:A:456:PHE:HD1	2.04	0.41
1:B:102:ARG:HG2	1:B:243:ALA:HB2	2.02	0.41
1:B:1098:ASN:HD22	1:B:1099:GLY:N	2.17	0.41
1:C:91:TYR:OH	1:C:93:ALA:HB2	2.21	0.41
1:A:896:ILE:HD11	1:A:904:TYR:HE2	1.85	0.41
1:C:299:THR:CG2	1:C:597:VAL:HG11	2.49	0.41
1:C:560:LEU:O	1:C:577:ARG:NH2	2.37	0.41
1:A:456:PHE:HB2	1:A:491:PRO:HA	2.02	0.41
1:B:977:LEU:HD21	1:B:996:LEU:HD22	2.02	0.41
1:C:334:ASN:O	1:C:362:VAL:HG12	2.21	0.41
1:C:347:PHE:CE2	1:C:509:ARG:HB3	2.56	0.41
1:C:452:LEU:O	1:C:495:TYR:OH	2.22	0.41
1:C:550:GLY:HA2	1:C:589:PRO:HA	2.01	0.41
1:C:970:PHE:CD2	1:C:999:GLY:HA3	2.56	0.41
1:A:351:TYR:HD1	1:A:453:TYR:HA	1.86	0.41
1:A:436:TRP:NE1	1:A:509:ARG:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HG	1:B:237:ARG:NH2	2.34	0.41
1:B:281:GLU:H	1:B:281:GLU:HG2	1.53	0.41
1:C:135:PHE:HA	1:C:160:TYR:HA	2.02	0.41
1:C:364:ASP:HA	1:C:388:ASN:HD21	1.86	0.41
1:C:403:ARG:NH2	1:C:505:TYR:HA	2.36	0.41
1:C:466:ARG:HG2	1:C:468:ILE:HG23	2.03	0.41
1:C:887:THR:HG21	1:C:894:LEU:HD12	2.02	0.41
1:A:672:ALA:HA	1:A:693:ILE:O	2.20	0.41
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.54	0.40
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.56	0.40
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.85	0.40
1:C:239:GLN:HG2	1:C:240:THR:H	1.86	0.40
1:C:273:ARG:NE	1:C:290:ASP:OD2	2.43	0.40
1:C:401:VAL:HG21	1:C:451:TYR:CE2	2.55	0.40
1:C:336:CYS:HB2	1:C:338:PHE:CE2	2.56	0.40
1:B:1098:ASN:HD22	1:B:1099:GLY:H	1.68	0.40
1:C:274:THR:HG22	1:C:291:CYS:SG	2.62	0.40
1:A:106:PHE:O	1:A:110:LEU:HD21	2.22	0.40
1:A:118:LEU:HD11	1:A:135:PHE:CZ	2.56	0.40
1:B:18:LEU:HD12	1:B:79:PHE:CZ	2.57	0.40
1:C:133:PHE:HB2	1:C:135:PHE:CE2	2.57	0.40
1:C:672:ALA:HA	1:C:693:ILE:O	2.22	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	979/1298 (75%)	902 (92%)	76 (8%)	1 (0%)	48 80
1	B	993/1298 (76%)	914 (92%)	76 (8%)	3 (0%)	37 70
1	C	1001/1298 (77%)	915 (91%)	83 (8%)	3 (0%)	37 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2973/3894 (76%)	2731 (92%)	235 (8%)	7 (0%)	45 75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	PHE
1	C	172	SER
1	C	491	PRO
1	C	1075	PHE
1	B	1099	GLY
1	A	491	PRO
1	B	412	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	884/1123 (79%)	860 (97%)	24 (3%)	40 60
1	B	896/1123 (80%)	872 (97%)	24 (3%)	40 60
1	C	900/1123 (80%)	888 (99%)	12 (1%)	65 76
All	All	2680/3369 (80%)	2620 (98%)	60 (2%)	47 65

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	61	ASN
1	A	119	ILE
1	A	120	VAL
1	A	124	THR
1	A	126	VAL
1	A	140	PHE
1	A	141	LEU
1	A	150	LYS

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Mol	Chain	Res	Type
1	A	155	SER
1	A	156	GLU
1	A	158	ARG
1	A	161	SER
1	A	162	SER
1	A	165	ASN
1	A	166	CYS
1	A	167	THR
1	A	201	PHE
1	A	367	VAL
1	A	372	THR
1	A	373	SER
1	A	641	ASN
1	A	657	ASN
1	A	1107	ARG
1	B	62	VAL
1	B	281	GLU
1	B	331	ASN
1	B	332	ILE
1	B	366	SER
1	B	370	ASN
1	B	372	THR
1	B	376	THR
1	B	393	THR
1	B	567	ARG
1	B	585	LEU
1	B	587	ILE
1	B	616	ASN
1	B	646	ARG
1	B	657	ASN
1	B	658	ASN
1	B	738	CYS
1	B	758	SER
1	B	767	LEU
1	B	822	LEU
1	B	849	LEU
1	B	878	LEU
1	B	966	LEU
1	B	1098	ASN
1	C	171	VAL
1	C	172	SER
1	C	281	GLU

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Mol	Chain	Res	Type
1	C	345	THR
1	C	370	ASN
1	C	469	SER
1	C	470	THR
1	C	472	ILE
1	C	658	ASN
1	C	1075	PHE
1	C	1098	ASN
1	C	1109	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	69	HIS
1	A	165	ASN
1	A	409	GLN
1	A	641	ASN
1	A	655	HIS
1	B	30	ASN
1	B	196	ASN
1	B	234	ASN
1	B	501	ASN
1	B	658	ASN
1	B	957	GLN
1	B	1098	ASN
1	C	1106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

35 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	A	1304	1	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
2	NAG	C	1306	1	14,14,15	0.44	0	17,19,21	1.09	1 (5%)
2	NAG	C	1307	1	14,14,15	0.54	0	17,19,21	1.41	3 (17%)
2	NAG	B	1302	1	14,14,15	0.35	0	17,19,21	0.76	0
2	NAG	C	1302	1	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
2	NAG	A	1303	1	14,14,15	0.31	0	17,19,21	0.58	0
2	NAG	C	1303	1	14,14,15	0.51	0	17,19,21	2.01	4 (23%)
2	NAG	A	1307	1	14,14,15	0.40	0	17,19,21	0.81	0
2	NAG	B	1308	1	14,14,15	0.41	0	17,19,21	0.81	0
2	NAG	C	1305	1	14,14,15	0.39	0	17,19,21	1.11	1 (5%)
2	NAG	C	1310	1	14,14,15	0.32	0	17,19,21	0.91	0
2	NAG	B	1307	1	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
2	NAG	C	1308	1	14,14,15	0.30	0	17,19,21	1.20	2 (11%)
2	NAG	B	1310	1	14,14,15	0.31	0	17,19,21	0.59	0
2	NAG	A	1309	1	14,14,15	1.33	1 (7%)	17,19,21	3.09	7 (41%)
2	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.66	0
2	NAG	B	1311	1	14,14,15	0.29	0	17,19,21	0.64	0
2	NAG	A	1308	1	14,14,15	0.33	0	17,19,21	0.90	0
2	NAG	C	1304	1	14,14,15	0.53	0	17,19,21	1.55	3 (17%)
2	NAG	C	1313	1	14,14,15	0.26	0	17,19,21	1.26	1 (5%)
2	NAG	A	1305	1	14,14,15	0.30	0	17,19,21	0.63	0
2	NAG	B	1306	1	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	C	1311	1	14,14,15	0.27	0	17,19,21	0.78	0
2	NAG	A	1310	1	14,14,15	0.31	0	17,19,21	0.60	0
2	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.69	0
2	NAG	C	1301	1	14,14,15	0.40	0	17,19,21	0.88	0
2	NAG	B	1301	1	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	1.15	2 (11%)
2	NAG	A	1306	1	14,14,15	0.30	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1304	1	14,14,15	0.29	0	17,19,21	0.60	0
2	NAG	B	1309	1	14,14,15	0.34	0	17,19,21	1.03	1 (5%)
2	NAG	C	1309	1	14,14,15	0.32	0	17,19,21	0.77	1 (5%)
2	NAG	B	1305	1	14,14,15	0.26	0	17,19,21	0.89	1 (5%)
2	NAG	C	1314	1	14,14,15	0.31	0	17,19,21	0.71	0
2	NAG	C	1312	1	14,14,15	0.31	0	17,19,21	0.65	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	5/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1309	NAG	C1-C2	4.58	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1309	NAG	O5-C1-C2	-9.95	95.58	111.29
2	C	1303	NAG	C1-C2-N2	-4.23	103.27	110.49
2	C	1304	NAG	C2-N2-C7	4.12	128.77	122.90
2	A	1309	NAG	C1-O5-C5	3.98	117.58	112.19
2	A	1309	NAG	C4-C3-C2	-3.92	105.27	111.02
2	C	1313	NAG	C2-N2-C7	3.88	128.43	122.90
2	C	1303	NAG	C2-N2-C7	3.85	128.38	122.90
2	C	1307	NAG	C1-O5-C5	3.76	117.29	112.19
2	C	1305	NAG	C1-O5-C5	3.73	117.25	112.19
2	C	1303	NAG	C1-O5-C5	3.67	117.16	112.19
2	C	1304	NAG	C1-O5-C5	3.52	116.97	112.19
2	A	1301	NAG	C2-N2-C7	3.45	127.82	122.90
2	C	1303	NAG	O5-C5-C6	3.28	112.35	107.20
2	C	1308	NAG	C2-N2-C7	2.92	127.06	122.90
2	C	1306	NAG	C1-O5-C5	2.88	116.10	112.19
2	C	1307	NAG	C2-N2-C7	2.86	126.97	122.90
2	B	1307	NAG	C1-O5-C5	2.82	116.01	112.19
2	A	1309	NAG	C2-N2-C7	2.81	126.90	122.90
2	A	1309	NAG	C3-C4-C5	-2.80	105.25	110.24
2	C	1304	NAG	C1-C2-N2	2.60	114.92	110.49
2	B	1309	NAG	C2-N2-C7	-2.46	119.40	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1309	NAG	O3-C3-C2	2.43	114.50	109.47
2	C	1302	NAG	O5-C1-C2	2.25	114.85	111.29
2	B	1305	NAG	C1-O5-C5	2.25	115.24	112.19
2	A	1304	NAG	O5-C5-C6	2.25	110.73	107.20
2	A	1301	NAG	C1-C2-N2	2.18	114.22	110.49
2	C	1307	NAG	C1-C2-N2	2.12	114.11	110.49
2	A	1309	NAG	C6-C5-C4	-2.08	108.12	113.00
2	C	1309	NAG	O5-C1-C2	2.06	114.54	111.29
2	C	1308	NAG	C1-C2-N2	2.05	113.98	110.49

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	NAG	C8-C7-N2-C2
2	A	1301	NAG	O7-C7-N2-C2
2	A	1308	NAG	C8-C7-N2-C2
2	A	1308	NAG	O7-C7-N2-C2
2	A	1309	NAG	C8-C7-N2-C2
2	A	1309	NAG	O7-C7-N2-C2
2	B	1309	NAG	C8-C7-N2-C2
2	B	1309	NAG	O7-C7-N2-C2
2	C	1302	NAG	C8-C7-N2-C2
2	C	1302	NAG	O7-C7-N2-C2
2	C	1304	NAG	C8-C7-N2-C2
2	C	1304	NAG	O7-C7-N2-C2
2	C	1306	NAG	C8-C7-N2-C2
2	C	1306	NAG	O7-C7-N2-C2
2	C	1307	NAG	C8-C7-N2-C2
2	C	1307	NAG	O7-C7-N2-C2
2	C	1311	NAG	O7-C7-N2-C2
2	C	1313	NAG	C8-C7-N2-C2
2	C	1313	NAG	O7-C7-N2-C2
2	C	1308	NAG	C8-C7-N2-C2
2	C	1308	NAG	O7-C7-N2-C2
2	C	1311	NAG	C8-C7-N2-C2
2	C	1304	NAG	C1-C2-N2-C7
2	A	1307	NAG	C4-C5-C6-O6
2	C	1303	NAG	O5-C5-C6-O6
2	A	1302	NAG	C8-C7-N2-C2
2	A	1302	NAG	O7-C7-N2-C2
2	A	1303	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1301	NAG	C8-C7-N2-C2
2	B	1304	NAG	C8-C7-N2-C2
2	B	1304	NAG	O7-C7-N2-C2
2	A	1307	NAG	O5-C5-C6-O6
2	C	1303	NAG	C4-C5-C6-O6
2	A	1303	NAG	O7-C7-N2-C2
2	A	1304	NAG	C8-C7-N2-C2
2	A	1305	NAG	C8-C7-N2-C2
2	B	1301	NAG	O7-C7-N2-C2
2	B	1303	NAG	C8-C7-N2-C2
2	C	1309	NAG	C8-C7-N2-C2
2	C	1310	NAG	C8-C7-N2-C2
2	C	1307	NAG	C1-C2-N2-C7
2	C	1308	NAG	C1-C2-N2-C7
2	B	1303	NAG	O5-C5-C6-O6
2	C	1310	NAG	O5-C5-C6-O6
2	A	1304	NAG	O7-C7-N2-C2
2	C	1309	NAG	O7-C7-N2-C2
2	B	1311	NAG	C8-C7-N2-C2
2	A	1305	NAG	O7-C7-N2-C2
2	B	1303	NAG	O7-C7-N2-C2
2	C	1310	NAG	O7-C7-N2-C2
2	B	1306	NAG	C8-C7-N2-C2
2	B	1311	NAG	O7-C7-N2-C2
2	B	1307	NAG	C8-C7-N2-C2
2	B	1301	NAG	O5-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	B	1307	NAG	O5-C5-C6-O6
2	A	1301	NAG	O5-C5-C6-O6
2	A	1306	NAG	O5-C5-C6-O6
2	B	1306	NAG	O7-C7-N2-C2
2	C	1307	NAG	O5-C5-C6-O6
2	C	1304	NAG	O5-C5-C6-O6
2	B	1307	NAG	O7-C7-N2-C2
2	B	1303	NAG	C4-C5-C6-O6
2	A	1301	NAG	C1-C2-N2-C7
2	C	1313	NAG	C3-C2-N2-C7
2	C	1310	NAG	C4-C5-C6-O6
2	B	1310	NAG	C8-C7-N2-C2
2	B	1310	NAG	O7-C7-N2-C2
2	A	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1307	NAG	1	0
2	A	1309	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

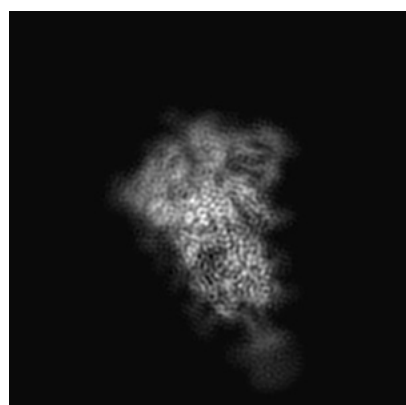
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31524. These allow visual inspection of the internal detail of the map and identification of artifacts.

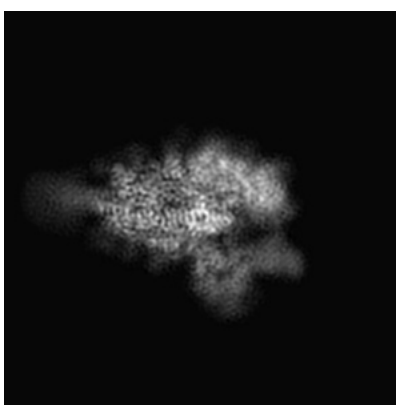
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

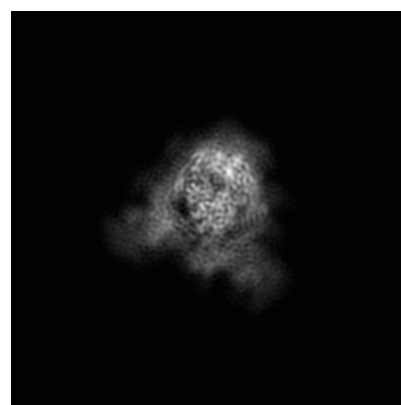
6.1.1 Primary map



X



Y

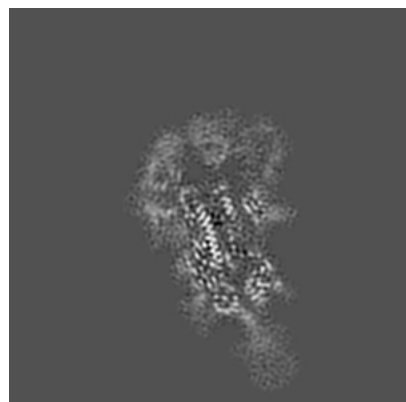


Z

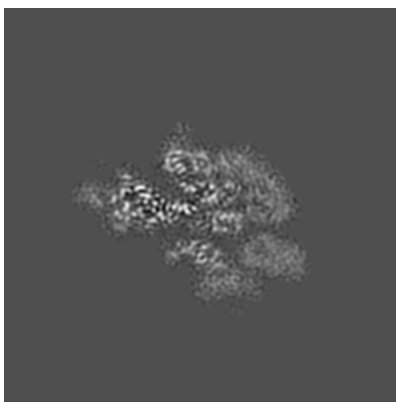
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

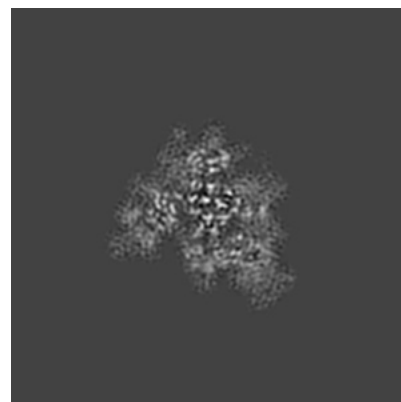
6.2.1 Primary map



X Index: 140



Y Index: 140

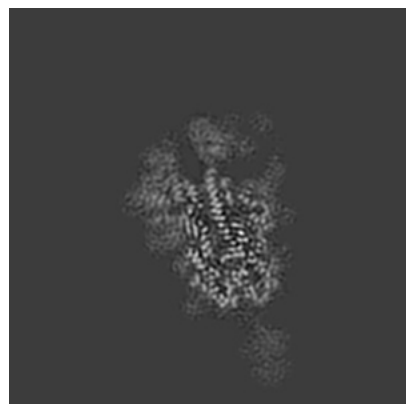


Z Index: 140

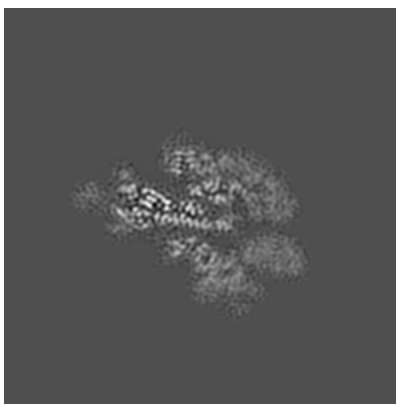
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

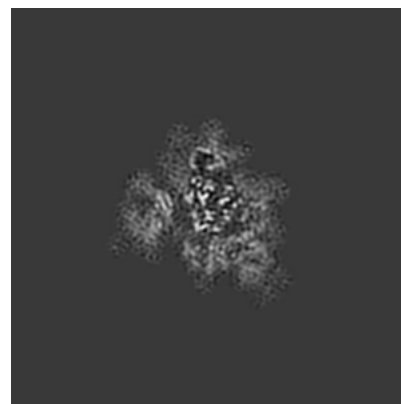
6.3.1 Primary map



X Index: 134



Y Index: 137

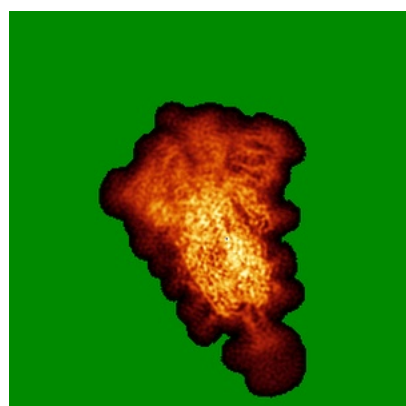


Z Index: 137

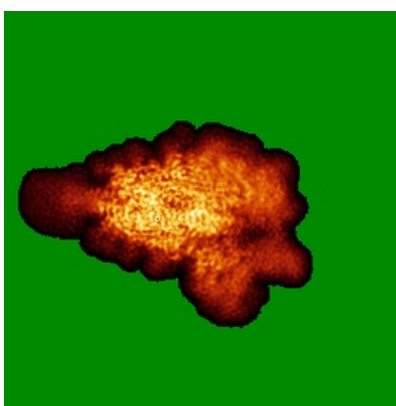
The images above show the largest variance slices of the map in three orthogonal directions.

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

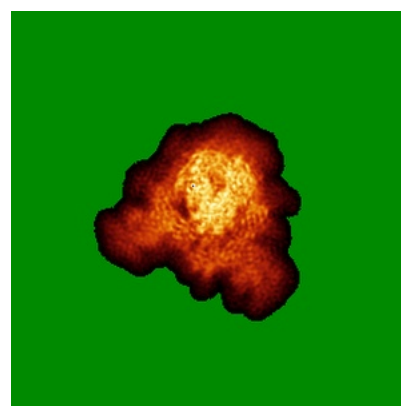
6.4.1 Primary map



X



Y

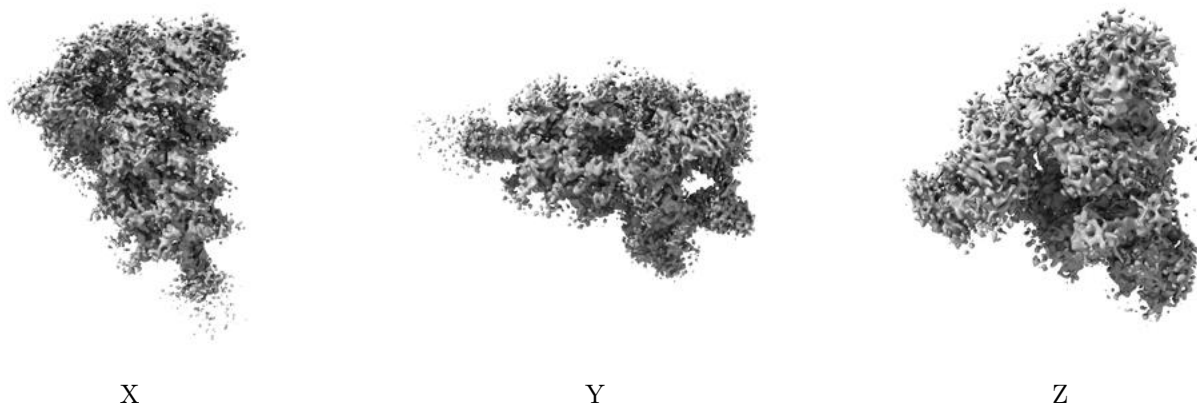


Z

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 0.0104. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

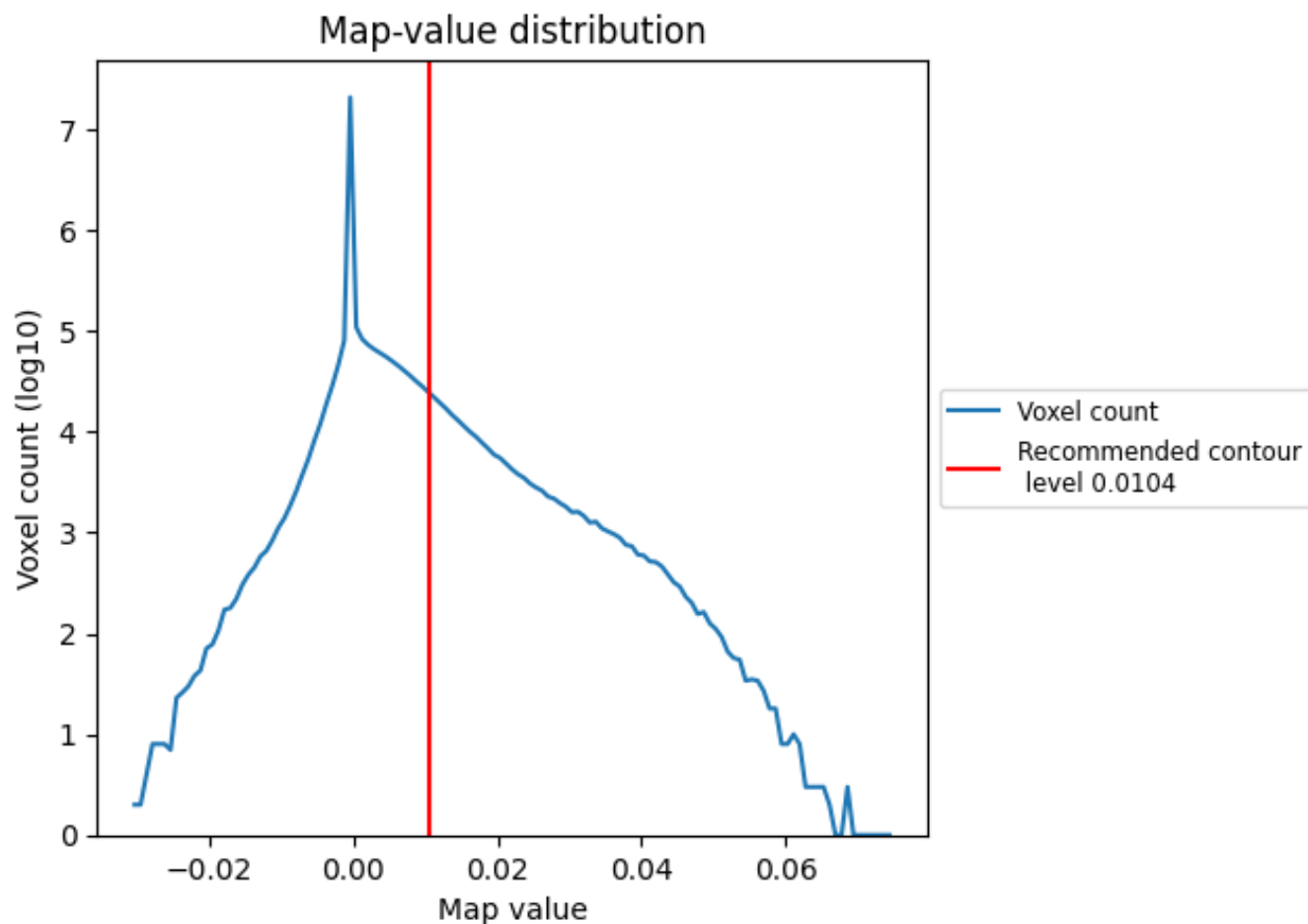
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

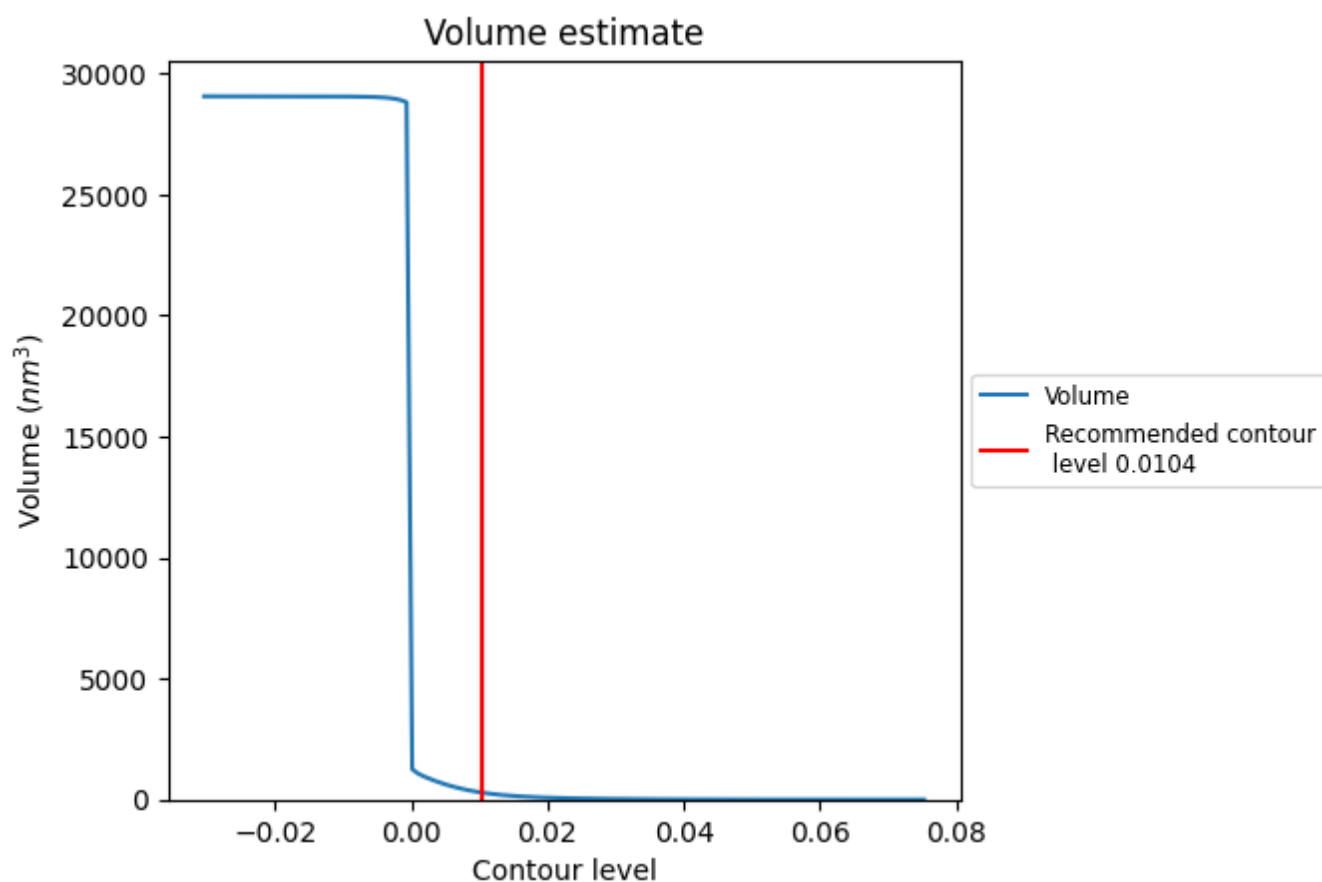
This section contains the results of statistical analysis of the map.

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.

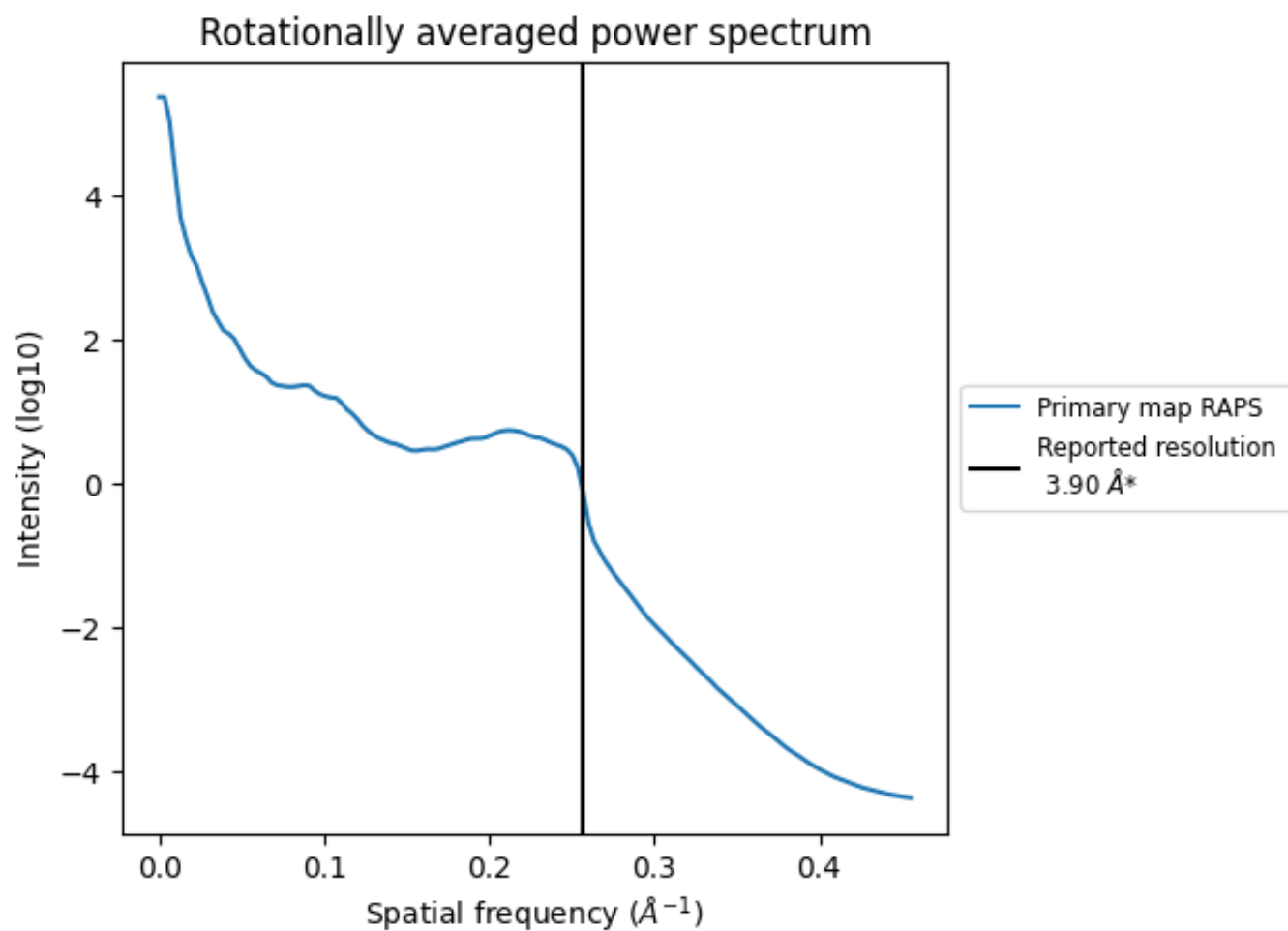
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 289 nm³; this corresponds to an approximate mass of 261 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 0.256 Å⁻¹

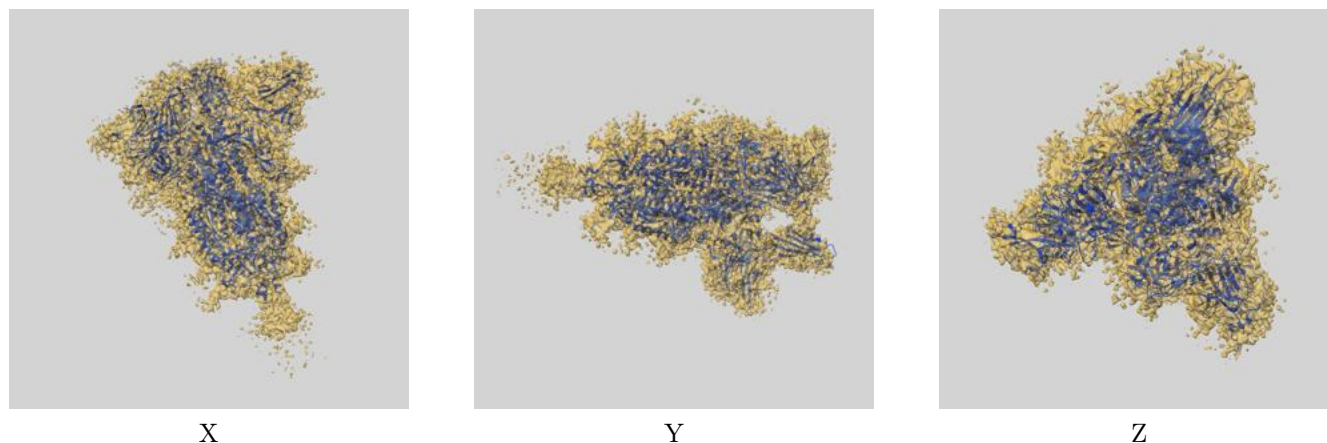
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

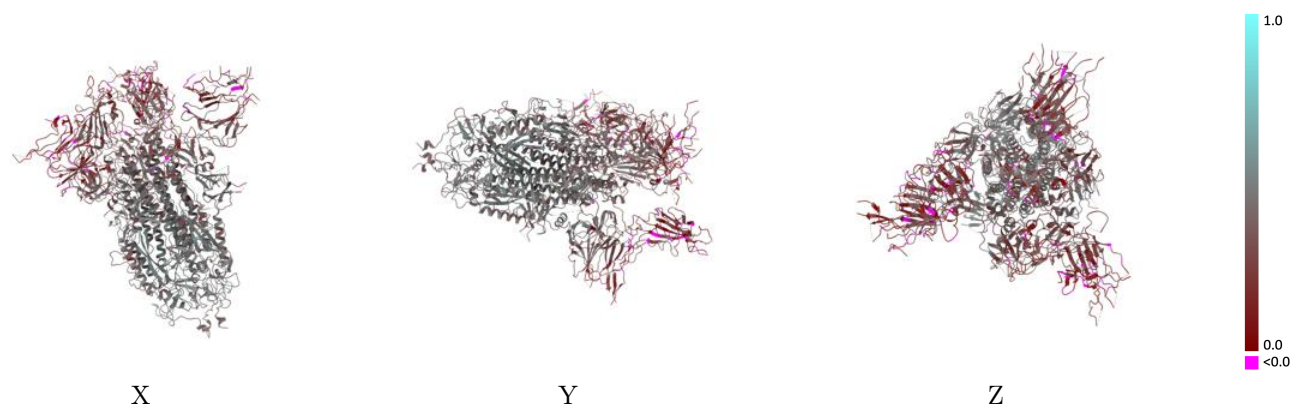
This section contains information regarding the fit between EMDB map EMD-31524 and PDB model 7FCD. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



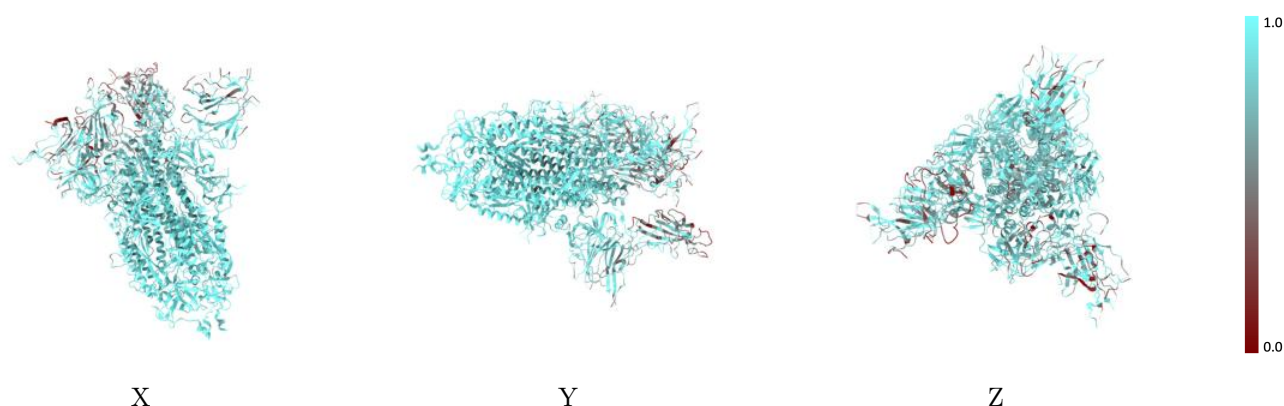
The images above show the 3D surface view of the map at the recommended contour level 0.0104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



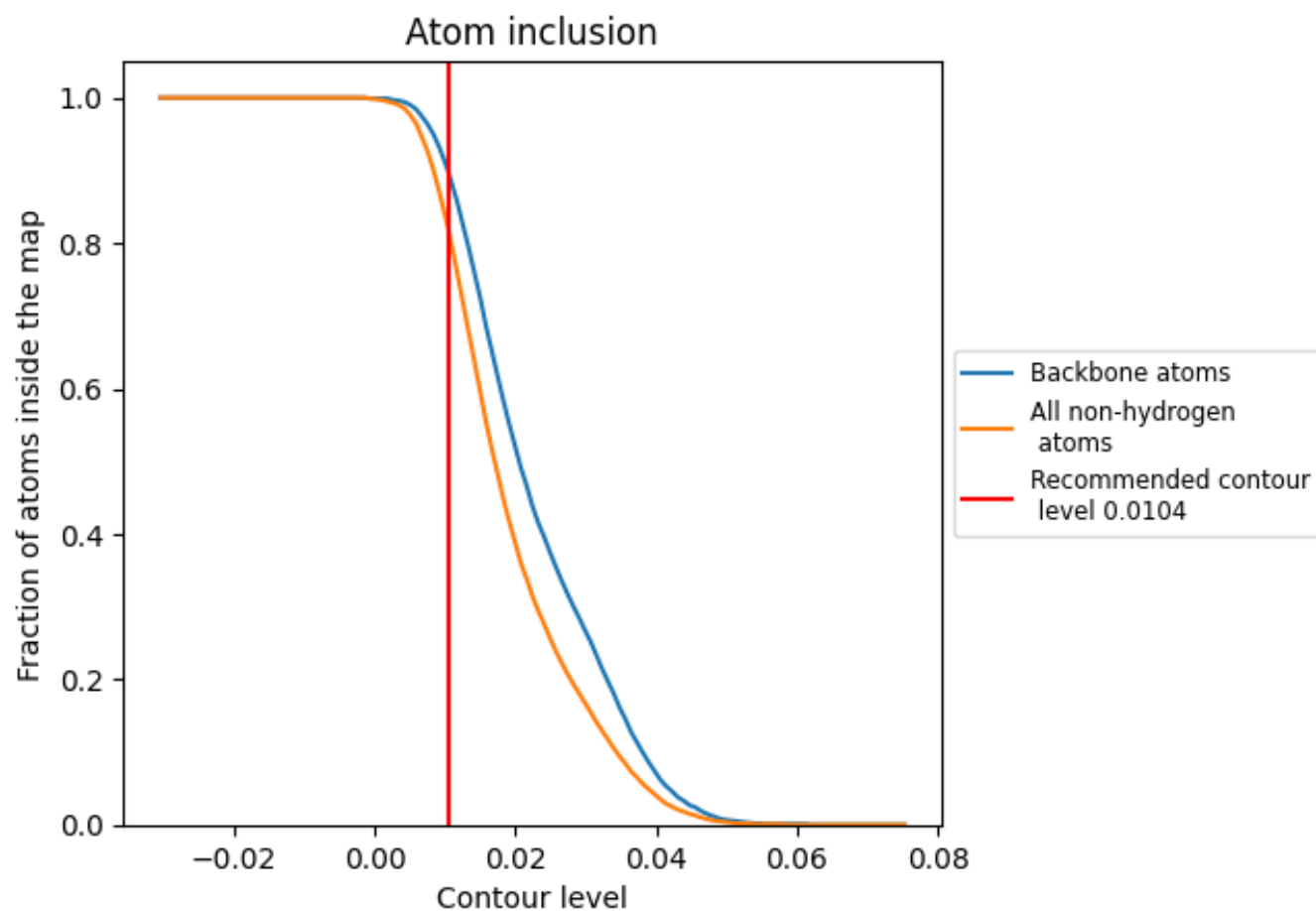
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0104).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.0104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8230	<div></div> 0.3600
A	<div></div> 0.8190	<div></div> 0.3580
B	<div></div> 0.8060	<div></div> 0.3530
C	<div></div> 0.8440	<div></div> 0.3690

