



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 04:38 PM JST

PDB ID : 7WOB  
EMDB ID : EMD-32647  
Title : SARS-CoV-2 Spike in complex with IgG 553-60 (2-up trimer)  
Authors : Zhan, W.Q.; Zhang, X.; Chen, Z.G.; Sun, L.  
Deposited on : 2022-01-21  
Resolution : 3.25 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](mailto: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>.

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

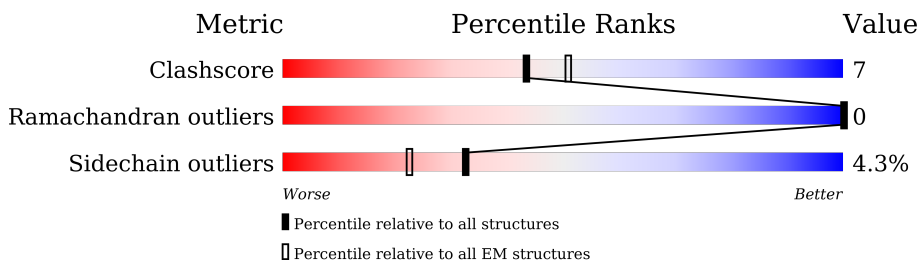
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.25 Å.

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



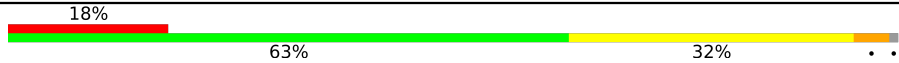
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	C	1288	
1	E	1288	
2	D	226	
2	F	226	
2	H	226	
3	B	215	
3	G	215	

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Mol	Chain	Length	Quality of chain
3	I	215	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '18%', a green segment in the middle labeled '63%', and a yellow segment on the right labeled '32%'. There are two small black dots at the far right end of the bar.</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 35134 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
			Total	C	N	O	S		
1	A	1076	8338	5318	1396	1586	38	0	0
1	C	1076	8338	5318	1396	1586	38	0	0
1	E	1076	8338	5318	1396	1586	38	0	0

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 a protein called mAb60 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	204	Total	C	N	O	S	0	0
			1560	997	262	295	6		
2	F	204	Total	C	N	O	S	0	0
			1560	997	262	295	6		
2	H	204	Total	C	N	O	S	0	0
			1560	997	262	295	6		

- Molecule 3 is a protein called mAb60 VL.

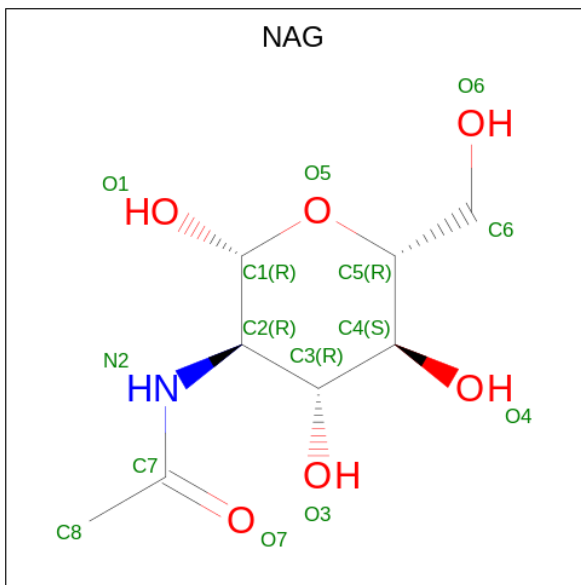
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	212	Total	C	N	O	S	0	0
			1636	1022	285	325	4		
3	G	212	Total	C	N	O	S	0	0
			1636	1022	285	325	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	212	1636	1022	285	325	4	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	A	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	C	1	182	104	13	65	0
4	E	1	168	96	12	60	0
4	E	1	168	96	12	60	0
4	E	1	168	96	12	60	0
4	E	1	168	96	12	60	0
4	E	1	168	96	12	60	0

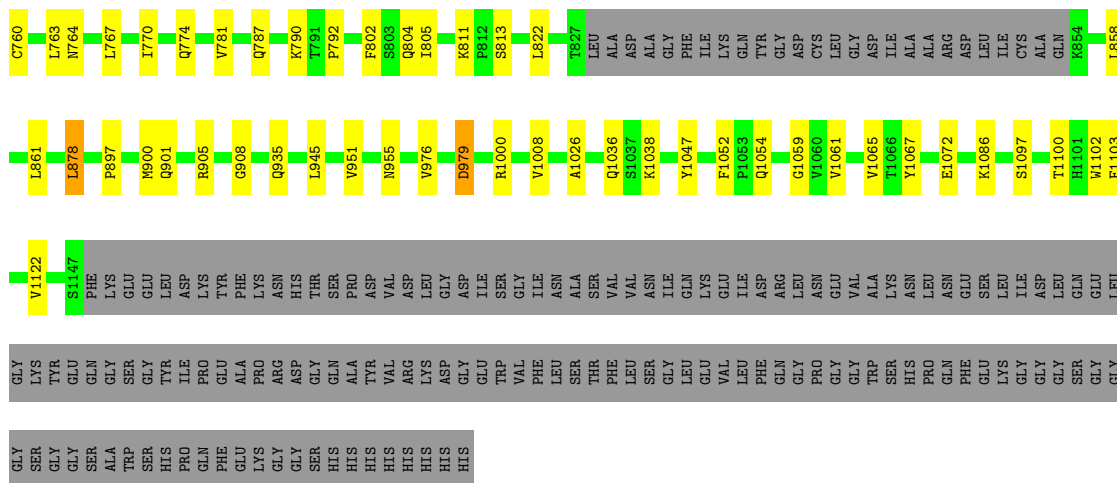
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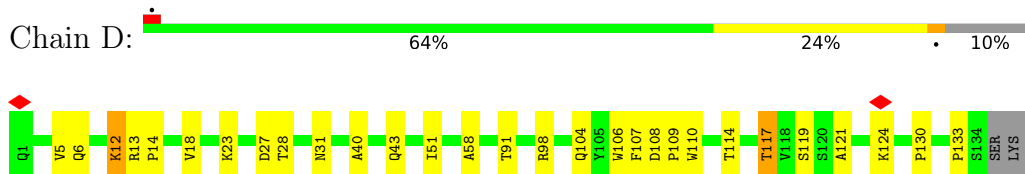
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>
4	E	1	Total	C	N	O	0
			168	96	12	60	
4	E	1	Total	C	N	O	0
			168	96	12	60	
4	E	1	Total	C	N	O	0
			168	96	12	60	
4	E	1	Total	C	N	O	0
			168	96	12	60	
4	E	1	Total	C	N	O	0
			168	96	12	60	
4	E	1	Total	C	N	O	0
			168	96	12	60	



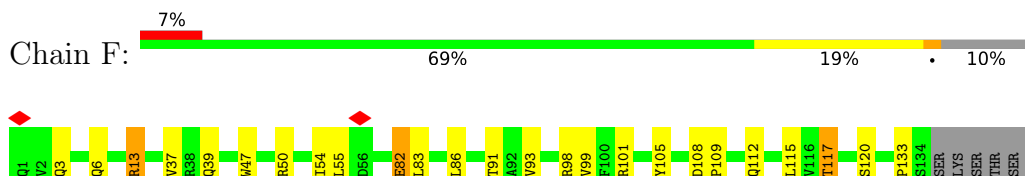




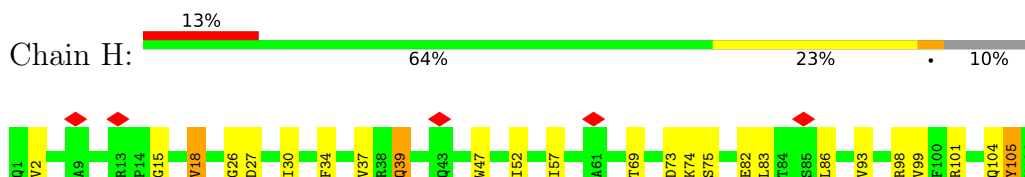
• Molecule 2: mAb60 VH



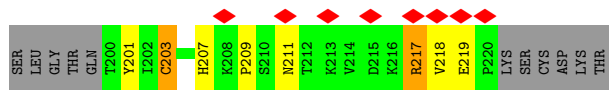
• Molecule 2: mAb60 VH



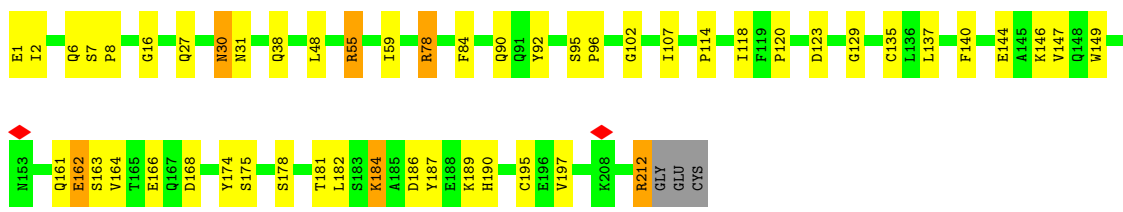
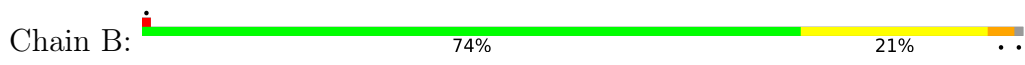
• Molecule 2: mAb60 VH



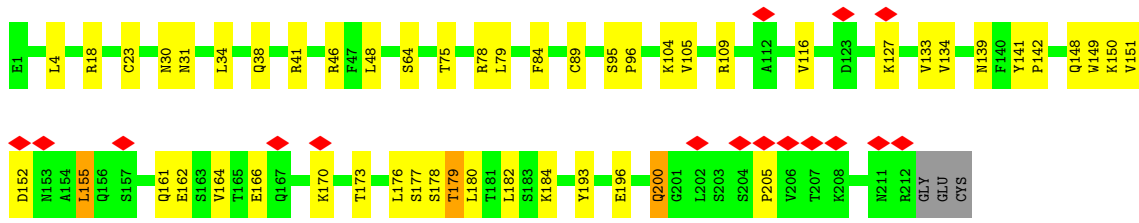
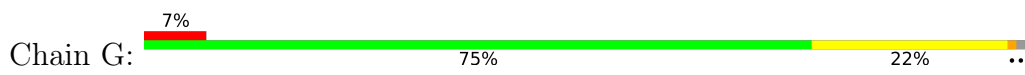




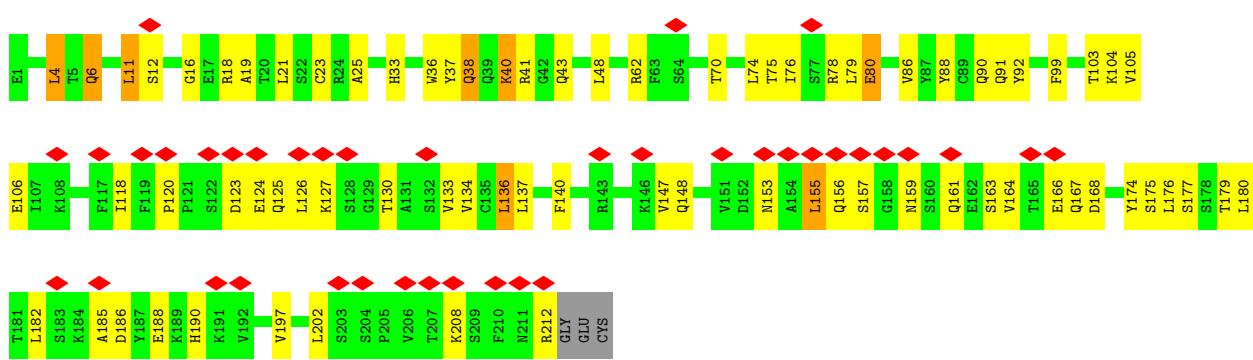
• Molecule 3: mAb60 VL



• Molecule 3: mAb60 VL



• Molecule 3: mAb60 VL



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99762	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 ( $e^-/\text{\AA}^2$ )	61	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	0.074	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.24	0/8534	0.42	0/11626
1	C	0.24	0/8534	0.42	0/11626
1	E	0.24	0/8534	0.42	0/11626
2	D	0.25	0/1599	0.45	0/2178
2	F	0.24	0/1599	0.45	0/2178
2	H	0.24	0/1599	0.46	0/2178
3	B	0.25	0/1672	0.43	0/2269
3	G	0.25	0/1672	0.46	0/2269
3	I	0.25	0/1672	0.45	0/2269
All	All	0.24	0/35415	0.43	0/48219

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8338	0	8067	109	0
1	C	8338	0	8067	96	0
1	E	8338	0	8068	102	0
2	D	1560	0	1538	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1560	0	1538	25	0
2	H	1560	0	1538	35	0
3	B	1636	0	1591	31	0
3	G	1636	0	1591	26	0
3	I	1636	0	1591	51	0
4	A	182	0	169	2	0
4	C	182	0	169	0	0
4	E	168	0	156	4	0
All	All	35134	0	34083	485	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (485) 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)
3:B:6:GLN:HG3	3:B:102:GLY:H	1.53	0.73
1:C:132:GLU:HB3	1:C:164:ASN:HB2	1.70	0.71
1:E:103:GLY:HA3	1:E:120:VAL:HA	1.74	0.70
3:B:55:ARG:H	3:B:55:ARG:HE	1.37	0.70
2:D:133:PRO:HA	3:B:120:PRO:HD2	1.74	0.70
1:E:498:GLN:O	1:E:501:ASN:ND2	2.26	0.69
1:E:439:ASN:HA	1:E:507:PRO:HD2	1.76	0.68
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.76	0.67
1:A:102:ARG:HG3	1:A:141:LEU:HB2	1.78	0.66
1:A:977:LEU:HD11	1:A:993:ILE:HG12	1.78	0.65
1:A:617:CYS:N	1:A:649:CYS:SG	2.69	0.65
2:F:98:ARG:HB3	2:F:109:PRO:HG2	1.77	0.65
3:B:1:GLU:HB2	3:B:27:GLN:HB2	1.79	0.65
2:D:98:ARG:HB3	2:D:109:PRO:HG2	1.79	0.65
2:H:39:GLN:HB3	2:H:93:VAL:HB	1.79	0.65
3:G:116:VAL:HG23	3:G:205:PRO:HB2	1.80	0.64
2:H:130:PRO:O	3:I:125:GLN:NE2	2.30	0.64
2:H:173:PHE:HB3	3:I:164:VAL:HG11	1.79	0.64
1:C:562:PHE:O	1:E:41:LYS:NZ	2.31	0.63
1:C:115:GLN:NE2	1:C:130:VAL:O	2.30	0.63
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.31	0.63
1:E:897:PRO:HD2	1:E:900:MET:HE2	1.79	0.63
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.80	0.63
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.81	0.62
1:E:108:THR:HB	1:E:114:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:135:CYS:HB3	3:B:178:SER:HB2	1.80	0.62
1:A:981:LEU:HD21	1:A:993:ILE:HD11	1.81	0.62
3:G:200:GLN:H	3:G:200:GLN:HE21	1.46	0.62
1:C:212:LEU:HD22	1:C:217:PRO:HD3	1.81	0.62
3:I:21:LEU:HB2	3:I:74:LEU:HB3	1.82	0.62
1:C:365:TYR:HB2	1:C:387:LEU:HD13	1.81	0.62
2:D:27:ASP:OD2	2:D:98:ARG:NH2	2.32	0.62
3:G:139:ASN:HA	3:G:173:THR:HB	1.82	0.62
3:G:164:VAL:HG12	3:G:177:SER:H	1.65	0.62
1:C:726:ILE:HB	1:C:947:LYS:HD3	1.81	0.61
1:E:1086:LYS:HD3	1:E:1122:VAL:HG21	1.81	0.61
3:I:6:GLN:NE2	3:I:23:CYS:SG	2.73	0.61
3:I:40:LYS:O	3:I:43:GLN:NE2	2.32	0.61
1:E:94:SER:HB2	1:E:190:ARG:HB2	1.79	0.61
1:E:715:PRO:HA	1:E:1072:GLU:HA	1.83	0.61
1:E:1047:TYR:HB2	1:E:1067:TYR:HB3	1.83	0.61
2:D:155:GLU:HG3	2:D:156:PRO:HD3	1.82	0.61
2:H:98:ARG:HB3	2:H:109:PRO:HG2	1.82	0.61
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.82	0.61
1:E:491:PRO:HB2	1:E:492:LEU:HD22	1.83	0.61
3:G:34:LEU:HD11	3:G:89:CYS:HB3	1.82	0.61
1:C:210:ILE:HG12	1:C:217:PRO:HG2	1.83	0.61
3:B:30:ASN:HD22	3:B:31:ASN:HD22	1.46	0.61
2:F:13:ARG:HB3	2:F:120:SER:HB2	1.82	0.61
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.82	0.61
2:F:151:ASP:HA	2:F:182:LEU:HD22	1.82	0.61
1:A:99:ASN:O	1:A:102:ARG:NH1	2.28	0.60
2:D:158:THR:OG1	2:D:206:ASN:ND2	2.34	0.60
1:E:149:ASN:ND2	1:E:151:SER:OG	2.35	0.60
1:A:61:ASN:N	1:A:61:ASN:OD1	2.35	0.60
1:E:763:LEU:HD22	1:E:1008:VAL:HG21	1.83	0.59
3:I:166:GLU:HB3	3:I:174:TYR:HB3	1.83	0.59
3:I:125:GLN:HB3	3:I:130:THR:HB	1.84	0.59
3:G:38:GLN:HB2	3:G:48:LEU:HD11	1.83	0.59
1:A:246:ARG:NH2	1:A:253:ASP:O	2.36	0.59
1:C:905:ARG:HH11	1:C:1036:GLN:HB2	1.68	0.58
1:C:212:LEU:HD13	1:C:217:PRO:HG3	1.84	0.58
1:C:276:LEU:HD22	1:C:301:CYS:HA	1.85	0.58
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.84	0.58
1:C:1086:LYS:HD2	1:C:1122:VAL:HG21	1.85	0.58
1:A:206:LYS:HB2	1:A:223:LEU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:18:ARG:HH11	3:G:75:THR:HG23	1.69	0.57
1:E:568:ASP:OD1	1:E:572:THR:N	2.34	0.57
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.87	0.57
1:A:365:TYR:HB2	1:A:387:LEU:HD13	1.85	0.57
1:E:760:CYS:O	1:E:764:ASN:ND2	2.31	0.57
1:E:607:GLN:HE22	1:E:691:SER:HA	1.70	0.57
3:G:30:ASN:OD1	3:G:31:ASN:ND2	2.38	0.57
3:G:38:GLN:OE1	3:G:46:ARG:NH2	2.38	0.57
1:E:392:PHE:N	1:E:524:VAL:O	2.35	0.56
2:H:175:ALA:HB1	2:H:183:TYR:HB3	1.85	0.56
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.85	0.56
1:C:131:CYS:HA	1:C:166:CYS:HA	1.87	0.56
4:E:1312:NAG:H83	4:E:1312:NAG:H3	1.87	0.56
1:A:97:LYS:HB3	1:A:186:PHE:HA	1.86	0.56
1:A:122:ASN:ND2	1:A:125:ASN:O	2.39	0.56
3:I:161:GLN:NE2	3:I:163:SER:OG	2.39	0.56
3:I:182:LEU:HD13	3:I:186:ASP:HB2	1.88	0.56
1:C:117:LEU:HD23	1:C:130:VAL:HG13	1.87	0.56
2:D:159:VAL:HG13	2:D:205:VAL:HG22	1.88	0.56
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.87	0.56
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.39	0.56
3:I:12:SER:HA	3:I:106:GLU:HB3	1.88	0.56
2:D:200:THR:OG1	2:D:201:TYR:N	2.38	0.55
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.88	0.55
3:G:79:LEU:HD11	3:G:105:VAL:HG11	1.87	0.55
1:E:132:GLU:O	1:E:164:ASN:ND2	2.39	0.55
3:I:37:TYR:OH	3:I:90:GLN:NE2	2.39	0.55
2:D:133:PRO:HD2	2:D:220:PRO:HA	1.88	0.55
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.39	0.55
3:G:4:LEU:HD11	3:G:23:CYS:HB3	1.88	0.55
3:G:162:GLU:HB3	3:G:178:SER:HA	1.88	0.55
1:A:458:LYS:NZ	1:A:474:GLN:O	2.39	0.55
1:C:555:SER:HB2	1:C:586:ASP:HB2	1.88	0.55
1:E:115:GLN:NE2	1:E:132:GLU:OE2	2.39	0.55
1:A:431:GLY:HA2	1:A:515:PHE:HD2	1.71	0.55
1:A:903:ALA:O	1:A:907:ASN:ND2	2.40	0.55
1:E:104:TRP:HB3	1:E:238:PHE:HE1	1.72	0.55
1:C:615:VAL:HG12	1:C:617:CYS:H	1.71	0.55
1:A:329:PHE:O	1:A:580:GLN:NE2	2.40	0.54
1:E:1100:THR:OG1	4:E:1311:NAG:O7	2.24	0.54
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:VAL:HG12	2:H:47:TRP:HA	1.89	0.54
1:E:193:VAL:HG23	1:E:223:LEU:HD22	1.88	0.54
3:I:62:ARG:HH22	3:I:80:GLU:HB2	1.71	0.54
2:F:93:VAL:HG22	2:F:115:LEU:HD23	1.88	0.54
1:E:439:ASN:HB3	1:E:506:GLN:HE21	1.72	0.54
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.90	0.54
1:E:102:ARG:NH1	1:E:121:ASN:O	2.40	0.54
1:E:280:ASN:ND2	4:E:1304:NAG:O7	2.41	0.54
3:G:148:GLN:HG3	3:G:196:GLU:HG3	1.89	0.54
2:H:108:ASP:HB3	2:H:109:PRO:HD3	1.90	0.54
1:E:118:LEU:HB2	1:E:133:PHE:HZ	1.73	0.54
1:C:81:ASN:O	1:C:239:GLN:NE2	2.39	0.53
2:H:145:LEU:H	2:H:189:VAL:HG13	1.73	0.53
1:A:395:VAL:HG12	1:A:515:PHE:HA	1.90	0.53
1:A:1076:THR:HG23	1:A:1097:SER:HB3	1.89	0.53
1:C:186:PHE:HD2	1:C:213:VAL:HA	1.74	0.53
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.91	0.53
1:A:895:GLN:NE2	1:E:711:SER:OG	2.41	0.53
1:E:722:VAL:HG22	1:E:1065:VAL:HG22	1.90	0.53
3:G:133:VAL:HB	3:G:180:LEU:HD13	1.89	0.53
1:A:855:PHE:HB2	1:A:858:LEU:HB2	1.91	0.53
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.90	0.53
3:I:148:GLN:HE21	3:I:155:LEU:HD11	1.74	0.53
1:A:424:LYS:NZ	1:A:425:LEU:O	2.36	0.53
1:E:555:SER:HB2	1:E:586:ASP:HB2	1.91	0.52
3:I:6:GLN:NE2	3:I:103:THR:OG1	2.43	0.52
1:A:327:VAL:HG11	1:A:528:LYS:HD2	1.92	0.52
1:E:15:CYS:HA	1:E:158:ARG:HD3	1.91	0.52
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.90	0.52
2:H:207:HIS:HB3	2:H:211:ASN:HA	1.90	0.52
3:I:25:ALA:HB3	3:I:70:THR:HG23	1.91	0.52
1:E:131:CYS:HA	1:E:166:CYS:HA	1.90	0.52
3:B:187:TYR:O	3:B:212:ARG:NH2	2.43	0.52
1:E:494:SER:HB3	2:H:30:ILE:HD11	1.90	0.52
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.92	0.52
1:C:738:CYS:SG	1:C:739:THR:N	2.82	0.52
1:A:406:GLU:HB3	1:A:418:ILE:HG21	1.92	0.52
1:A:798:GLY:O	1:A:920:GLN:NE2	2.43	0.52
1:C:735:SER:HB3	1:C:859:THR:HG23	1.92	0.52
2:D:14:PRO:HG3	2:D:119:SER:HA	1.92	0.52
3:I:188:GLU:O	3:I:212:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:147:VAL:HG22	3:B:197:VAL:HG13	1.91	0.51
1:A:128:ILE:O	1:A:170:TYR:N	2.43	0.51
2:F:164:GLY:N	2:F:167:THR:OG1	2.42	0.51
1:E:388:ASN:HB2	1:E:527:PRO:HD2	1.92	0.51
1:E:133:PHE:HB3	1:E:163:ALA:HA	1.91	0.51
3:B:162:GLU:OE1	3:B:163:SER:N	2.44	0.51
1:A:1086:LYS:HD3	1:A:1122:VAL:HG21	1.93	0.51
1:E:822:LEU:HD22	1:E:945:LEU:HD11	1.92	0.51
1:E:802:PHE:HD1	1:E:805:ILE:HD11	1.76	0.50
3:I:86:VAL:HG22	3:I:104:LYS:HD3	1.93	0.50
3:I:120:PRO:HA	3:I:133:VAL:HG23	1.93	0.50
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.44	0.50
1:E:951:VAL:O	1:E:955:ASN:ND2	2.37	0.50
3:I:180:LEU:HD22	3:I:182:LEU:HG	1.93	0.50
1:E:143:VAL:HG12	1:E:154:GLU:HG2	1.94	0.50
2:H:39:GLN:O	2:H:39:GLN:NE2	2.44	0.50
1:A:326:ILE:HD11	1:A:328:ARG:HD3	1.93	0.50
3:B:114:PRO:HB3	3:B:140:PHE:HB3	1.92	0.50
1:E:908:GLY:O	1:E:1038:LYS:NZ	2.44	0.50
1:E:97:LYS:HD3	1:E:262:ALA:HB3	1.93	0.50
2:F:91:THR:HG23	2:F:117:THR:HA	1.93	0.50
3:I:18:ARG:HH12	3:I:75:THR:HB	1.77	0.50
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.94	0.50
2:H:107:PHE:O	2:H:110:TRP:NE1	2.44	0.50
1:E:314:GLN:NE2	1:E:316:SER:O	2.45	0.49
2:D:162:ASN:H	2:D:203:CYS:HA	1.76	0.49
1:A:328:ARG:HE	1:A:533:LEU:HB2	1.77	0.49
1:A:1114:ILE:HD13	1:A:1114:ILE:H	1.77	0.49
1:C:317:ASN:HB2	1:C:319:ARG:HH11	1.76	0.49
1:E:276:LEU:HD22	1:E:301:CYS:HA	1.93	0.49
1:A:707:TYR:HB3	1:C:792:PRO:HG3	1.94	0.49
1:C:303:LEU:HD12	1:C:308:VAL:HG12	1.93	0.49
1:C:428:ASP:OD1	1:C:428:ASP:N	2.45	0.49
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.94	0.49
1:E:146:HIS:HA	1:E:248:TYR:HE2	1.78	0.49
1:E:328:ARG:NH2	1:E:531:THR:O	2.45	0.49
2:H:104:GLN:HB2	3:I:92:TYR:HD2	1.77	0.49
1:A:79:PHE:HE2	1:A:244:LEU:HB3	1.76	0.49
1:A:90:VAL:HG23	1:A:267:VAL:HG13	1.94	0.49
2:D:152:TYR:CE1	2:D:184:SER:HA	2.48	0.49
2:F:208:LYS:HB3	2:F:209:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ILE:HD13	1:C:921:LYS:HE2	1.94	0.49
3:I:126:LEU:HB3	3:I:185:ALA:HB2	1.94	0.49
1:C:567:ARG:HG2	1:E:42:VAL:HG11	1.93	0.49
1:E:742:ILE:O	1:E:1000:ARG:NH1	2.45	0.49
2:D:108:ASP:HB3	2:D:109:PRO:HD3	1.95	0.49
2:H:177:LEU:HG	2:H:183:TYR:HE1	1.77	0.49
1:C:1141:LEU:HD23	1:C:1141:LEU:H	1.78	0.49
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.95	0.49
2:F:145:LEU:HD22	2:F:166:LEU:HD21	1.93	0.49
1:A:77:LYS:NZ	1:A:258:TRP:O	2.46	0.49
1:E:339:GLY:HA2	1:E:343:ASN:HD21	1.77	0.49
2:F:158:THR:HB	2:F:206:ASN:HB2	1.94	0.48
1:A:521:PRO:HG3	1:A:564:GLN:HG3	1.93	0.48
1:A:1072:GLU:HG2	4:A:1311:NAG:H81	1.95	0.48
2:H:27:ASP:OD1	2:H:27:ASP:N	2.44	0.48
1:A:904:TYR:HA	1:A:907:ASN:HD21	1.79	0.48
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	1.95	0.48
3:B:16:GLY:O	3:B:78:ARG:NH1	2.46	0.48
3:I:33:HIS:HB3	3:I:92:TYR:HB2	1.94	0.48
1:A:788:ILE:HG23	1:A:876:ALA:HB2	1.95	0.48
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.60	0.48
1:E:905:ARG:HH11	1:E:1036:GLN:HB2	1.78	0.48
1:A:895:GLN:HG2	1:E:713:ALA:HB2	1.95	0.48
2:F:108:ASP:HB3	2:F:109:PRO:HD3	1.96	0.48
1:A:745:ASP:OD1	1:E:319:ARG:NH1	2.47	0.48
1:C:752:LEU:HD21	1:C:990:GLU:HG3	1.96	0.48
2:D:148:LEU:HD23	2:D:186:SER:HB3	1.96	0.48
3:G:41:ARG:HH11	3:G:104:LYS:HE2	1.79	0.48
1:A:367:VAL:O	1:A:371:SER:OG	2.32	0.48
3:B:48:LEU:HA	3:B:59:ILE:HG13	1.96	0.48
1:E:125:ASN:HB3	1:E:174:PRO:HA	1.94	0.48
1:E:644:GLN:NE2	1:E:645:THR:O	2.39	0.48
1:C:115:GLN:NE2	1:C:167:THR:OG1	2.47	0.47
1:C:126:VAL:H	1:C:172:SER:HB2	1.78	0.47
1:E:244:LEU:HD13	1:E:246:ARG:HG3	1.96	0.47
1:E:318:PHE:N	1:E:593:GLY:O	2.46	0.47
1:E:676:THR:HB	1:E:690:GLN:HG2	1.96	0.47
1:E:901:GLN:O	1:E:905:ARG:HG2	2.14	0.47
3:I:148:GLN:HB3	3:I:155:LEU:HD11	1.96	0.47
1:E:770:ILE:O	1:E:774:GLN:HG2	2.14	0.47
2:H:83:LEU:HD22	2:H:86:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:NH1	1:C:531:THR:O	2.45	0.47
1:E:24:LEU:HD23	1:E:78:ARG:HH11	1.79	0.47
1:A:388:ASN:HB3	1:A:527:PRO:HD2	1.96	0.47
1:C:149:ASN:ND2	1:C:151:SER:OG	2.48	0.47
1:C:393:THR:O	1:C:523:THR:OG1	2.31	0.47
1:E:374:PHE:HA	1:E:436:TRP:HB3	1.95	0.47
1:E:666:ILE:HD11	1:E:672:ALA:HB2	1.95	0.47
3:I:41:ARG:NH1	3:I:168:ASP:OD2	2.47	0.47
1:A:738:CYS:SG	1:A:739:THR:N	2.87	0.47
1:A:792:PRO:HG3	1:E:707:TYR:HB3	1.95	0.47
1:C:452:LEU:HD13	1:C:492:LEU:HD22	1.97	0.47
1:E:379:CYS:HA	1:E:432:CYS:HA	1.97	0.47
1:A:886:TRP:HB3	1:A:1035:GLY:HA2	1.95	0.47
1:C:1054:GLN:N	1:C:1061:VAL:O	2.48	0.47
1:E:105:ILE:HD11	1:E:239:GLN:HB3	1.95	0.47
2:D:179:SER:HB3	3:B:161:GLN:HE21	1.80	0.47
2:F:6:GLN:H	2:F:112:GLN:NE2	2.13	0.47
2:H:161:TRP:HA	2:H:203:CYS:HA	1.97	0.47
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.97	0.47
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.96	0.47
1:C:81:ASN:HD22	1:C:239:GLN:HE21	1.63	0.47
1:C:379:CYS:HA	1:C:432:CYS:HA	1.95	0.47
1:C:901:GLN:O	1:C:905:ARG:HG2	2.14	0.47
1:E:804:GLN:OE1	1:E:935:GLN:NE2	2.47	0.47
3:I:159:ASN:HD21	3:I:182:LEU:HD23	1.79	0.47
1:C:117:LEU:HG	1:C:233:ILE:HD11	1.97	0.46
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	1.95	0.46
1:E:600:PRO:HD3	1:E:692:ILE:HD11	1.97	0.46
2:H:128:VAL:HG13	2:H:147:CYS:HB2	1.97	0.46
3:I:104:LYS:NZ	3:I:105:VAL:O	2.46	0.46
1:C:130:VAL:HB	1:C:167:THR:HB	1.97	0.46
2:D:154:PRO:HB2	2:D:207:HIS:NE2	2.30	0.46
2:F:83:LEU:HD13	2:F:86:LEU:HD21	1.98	0.46
3:I:118:ILE:HG13	3:I:208:LYS:HE2	1.97	0.46
1:A:498:GLN:HG3	1:A:500:THR:H	1.80	0.46
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.97	0.46
1:C:403:ARG:NH2	1:C:406:GLU:OE2	2.49	0.46
2:H:130:PRO:HB2	2:H:218:VAL:HG12	1.97	0.46
1:C:457:ARG:HG2	1:C:458:LYS:H	1.81	0.46
2:F:37:VAL:HG12	2:F:47:TRP:HA	1.98	0.46
2:H:153:PHE:HB3	2:H:154:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:137:LEU:O	3:I:175:SER:OG	2.29	0.46
1:C:788:ILE:HG23	1:C:876:ALA:HB2	1.97	0.46
1:A:483:VAL:HG12	2:D:104:GLN:HB2	1.98	0.46
2:F:47:TRP:HE1	2:F:50:ARG:HB2	1.80	0.46
1:C:555:SER:HB3	1:C:584:ILE:HG22	1.98	0.46
1:C:773:GLU:HA	1:C:776:LYS:HG2	1.98	0.46
1:A:404:GLY:O	1:A:408:ARG:NH1	2.49	0.45
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.98	0.45
3:B:162:GLU:HB2	3:B:164:VAL:HG23	1.99	0.45
1:A:276:LEU:HB3	1:A:289:VAL:HG22	1.97	0.45
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.97	0.45
1:E:195:LYS:HD2	1:E:202:LYS:HD2	1.98	0.45
3:G:64:SER:HB3	3:G:75:THR:HB	1.98	0.45
1:A:985:ASP:OD1	1:A:985:ASP:N	2.49	0.45
1:E:112:SER:HB2	1:E:134:GLN:HB2	1.97	0.45
1:E:289:VAL:HG12	1:E:291:CYS:H	1.81	0.45
1:E:729:VAL:HG23	1:E:1059:GLY:HA2	1.98	0.45
2:H:2:VAL:HG12	2:H:26:GLY:HA3	1.98	0.45
2:H:15:GLY:H	2:H:86:LEU:HB2	1.82	0.45
1:A:379:CYS:HA	1:A:432:CYS:HA	1.98	0.45
3:G:155:LEU:HD13	3:G:161:GLN:HE22	1.81	0.45
1:A:106:PHE:O	1:A:117:LEU:N	2.44	0.45
1:C:533:LEU:HD21	1:C:585:LEU:HD21	1.98	0.45
1:E:454:ARG:NH1	1:E:467:ASP:O	2.49	0.45
1:E:709:ASN:OD1	1:E:709:ASN:N	2.40	0.45
1:E:878:LEU:HD21	1:E:1052:PHE:HB3	1.97	0.45
1:A:980:ILE:HG23	1:A:984:LEU:HD13	1.98	0.45
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.99	0.45
1:C:659:SER:HB3	1:C:698:SER:HB3	1.99	0.45
1:A:889:GLY:HA3	1:A:1034:LEU:HD23	1.98	0.45
3:I:156:GLN:HG2	3:I:157:SER:H	1.81	0.45
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.52	0.45
1:C:728:PRO:HD3	1:C:947:LYS:HG3	1.99	0.45
1:E:147:LYS:HD3	1:E:248:TYR:HD2	1.81	0.45
2:D:171:HIS:CE1	3:B:175:SER:HB2	2.52	0.45
1:A:156:GLU:OE1	1:A:158:ARG:NH2	2.48	0.45
1:C:530:SER:OG	1:C:580:GLN:NE2	2.49	0.45
1:E:97:LYS:NZ	1:E:182:LYS:O	2.41	0.45
1:E:14:GLN:O	1:E:14:GLN:NE2	2.50	0.45
2:D:12:LYS:HE2	2:D:18:VAL:HG12	1.99	0.45
1:A:439:ASN:HD22	1:A:507:PRO:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:147:VAL:HG13	3:B:197:VAL:HG22	1.99	0.44
1:A:878:LEU:HD21	1:A:1052:PHE:HB3	1.99	0.44
3:G:151:VAL:HG12	3:G:152:ASP:H	1.82	0.44
3:I:38:GLN:O	3:I:38:GLN:NE2	2.51	0.44
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.81	0.44
1:C:277:LEU:HD22	1:C:285:ILE:HD13	1.99	0.44
1:E:380:TYR:HB2	1:E:429:PHE:HD2	1.83	0.44
2:F:54:ILE:HG21	2:F:101:ARG:HH21	1.82	0.44
2:H:129:PHE:HB2	2:H:148:LEU:HB3	1.98	0.44
1:E:1097:SER:HB2	1:E:1102:TRP:CD2	2.53	0.44
1:C:145:TYR:HB3	1:C:247:SER:HB3	1.99	0.44
1:C:976:VAL:HB	1:C:979:ASP:HB2	1.99	0.44
2:F:82:GLU:OE1	2:F:83:LEU:N	2.50	0.44
3:G:134:VAL:HG22	3:G:179:THR:HB	1.99	0.44
1:A:735:SER:HA	1:A:767:LEU:HD13	2.00	0.44
1:A:986:PRO:N	1:A:987:PRO:HD2	2.33	0.44
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.44
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.93	0.44
1:A:415:THR:OG1	1:A:420:ASP:OD2	2.32	0.44
1:A:736:VAL:HG22	1:A:858:LEU:HD13	2.00	0.44
1:C:355:ARG:HB2	1:C:466:ARG:HH12	1.82	0.44
3:B:95:SER:HB3	3:B:96:PRO:HD3	1.99	0.44
1:A:21:ARG:HD2	1:A:79:PHE:H	1.82	0.44
1:C:770:ILE:O	1:C:774:GLN:HG2	2.18	0.44
2:D:28:THR:OG1	2:D:31:ASN:ND2	2.51	0.44
2:H:207:HIS:CD2	2:H:209:PRO:HD2	2.53	0.44
3:I:134:VAL:HG11	3:I:179:THR:HA	1.99	0.44
1:E:431:GLY:HA2	1:E:515:PHE:HD2	1.82	0.43
2:D:145:LEU:HD22	2:D:191:VAL:HG22	1.98	0.43
3:B:123:ASP:OD1	3:B:123:ASP:N	2.51	0.43
1:A:770:ILE:O	1:A:774:GLN:HG2	2.18	0.43
1:A:825:LYS:HD2	1:A:942:ALA:HA	1.99	0.43
1:E:733:LYS:O	1:E:861:LEU:N	2.49	0.43
2:D:107:PHE:O	2:D:110:TRP:NE1	2.51	0.43
3:G:79:LEU:HG	3:G:84:PHE:HE1	1.83	0.43
1:A:190:ARG:HG2	1:A:207:HIS:HD2	1.83	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.52	0.43
2:D:121:ALA:HB3	2:D:153:PHE:HB2	2.00	0.43
1:C:403:ARG:HG2	1:C:497:PHE:HE1	1.82	0.43
1:E:811:LYS:HG2	1:E:813:SER:H	1.83	0.43
2:D:146:GLY:HA2	2:D:161:TRP:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:38:GLN:HB2	3:B:48:LEU:HD11	1.99	0.43
2:H:18:VAL:HG13	2:H:86:LEU:HD11	2.00	0.43
3:I:4:LEU:HD12	3:I:91:GLN:HB2	2.00	0.43
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.00	0.43
1:C:1054:GLN:HB2	1:C:1061:VAL:HB	2.00	0.43
1:E:805:ILE:HB	1:E:1054:GLN:HE22	1.82	0.43
1:A:106:PHE:HB2	1:A:117:LEU:HD12	2.00	0.43
1:A:122:ASN:HD22	1:A:122:ASN:H	1.66	0.43
1:A:988:GLU:O	1:A:992:GLN:HG2	2.18	0.43
1:C:148:ASN:ND2	1:C:149:ASN:OD1	2.52	0.43
2:F:99:VAL:HB	2:F:105:TYR:HB2	1.99	0.43
3:I:37:TYR:HB2	3:I:88:TYR:HB2	2.00	0.43
1:C:105:ILE:HG13	1:C:241:LEU:HD11	2.01	0.43
2:D:5:VAL:O	2:D:23:LYS:N	2.44	0.43
3:B:55:ARG:HB2	3:B:59:ILE:HB	2.00	0.43
1:A:102:ARG:HB2	1:A:141:LEU:HD13	2.00	0.43
1:E:44:ARG:HD2	1:E:47:VAL:HG11	2.00	0.43
3:B:137:LEU:HD11	3:B:197:VAL:HG21	2.01	0.43
1:A:86:PHE:HB2	1:A:238:PHE:HD1	1.84	0.42
1:C:425:LEU:HD12	1:C:426:PRO:HD2	2.00	0.42
1:C:661:GLU:O	1:C:695:TYR:OH	2.30	0.42
3:B:7:SER:HB2	3:B:8:PRO:HD3	2.00	0.42
1:C:108:THR:HG23	1:C:114:THR:HG21	2.01	0.42
1:E:204:TYR:HB3	1:E:223:LEU:HB3	2.02	0.42
3:B:129:GLY:HA2	3:B:184:LYS:HG3	2.01	0.42
2:H:134:SER:HA	2:H:143:ALA:HB3	2.01	0.42
3:I:11:LEU:HD12	3:I:19:ALA:HB1	2.01	0.42
3:I:153:ASN:HD21	3:I:156:GLN:NE2	2.18	0.42
1:C:24:LEU:HD12	1:C:25:PRO:HD2	2.01	0.42
1:C:131:CYS:HB2	1:C:133:PHE:CZ	2.54	0.42
1:C:671:CYS:SG	1:C:697:MET:HB3	2.59	0.42
2:D:40:ALA:HB3	2:D:43:GLN:HB3	2.00	0.42
2:D:130:PRO:HA	2:D:218:VAL:HG22	2.01	0.42
2:D:175:ALA:HB2	2:D:185:LEU:HD23	2.01	0.42
3:I:147:VAL:HA	3:I:197:VAL:HA	2.00	0.42
1:A:167:THR:HG22	1:A:168:PHE:H	1.84	0.42
3:G:149:TRP:HZ3	3:G:193:TYR:HB3	1.83	0.42
1:E:438:SER:HB3	1:E:441:LEU:HB2	2.01	0.42
2:F:133:PRO:HB2	2:F:220:PRO:HB3	2.02	0.42
1:A:142:GLY:HA2	1:A:243:ALA:HB1	2.02	0.42
1:A:185:ASN:HD22	1:A:211:ASN:HD22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:GLY:HA3	1:C:430:THR:HA	2.01	0.42
1:C:985:ASP:OD1	1:C:985:ASP:N	2.52	0.42
1:E:90:VAL:HG13	1:E:267:VAL:HG13	2.01	0.42
1:E:276:LEU:HB3	1:E:289:VAL:HB	2.01	0.42
1:E:976:VAL:HB	1:E:979:ASP:HB2	2.01	0.42
3:I:36:TRP:CD2	3:I:74:LEU:HD22	2.55	0.42
1:E:126:VAL:HG12	1:E:128:ILE:HG13	2.02	0.42
2:H:69:THR:HB	2:H:82:GLU:HB3	2.01	0.42
2:H:173:PHE:HE2	3:I:177:SER:HB2	1.84	0.42
1:C:275:PHE:HD2	1:C:288:ALA:HB1	1.85	0.42
2:D:173:PHE:HB3	3:B:164:VAL:HG11	2.02	0.42
3:G:109:ARG:HD2	3:G:109:ARG:HA	1.95	0.42
1:A:374:PHE:HA	1:A:436:TRP:HB3	2.01	0.42
1:A:391:CYS:HA	1:A:525:CYS:HA	2.01	0.42
1:C:68:ILE:H	1:C:68:ILE:HG13	1.54	0.42
1:C:1091:ARG:NH1	1:C:1120:THR:O	2.53	0.42
1:E:118:LEU:HG	1:E:120:VAL:HG22	2.02	0.42
3:B:168:ASP:HA	3:B:174:TYR:HE1	1.85	0.42
2:F:54:ILE:HG23	2:F:55:LEU:HD12	2.01	0.42
1:A:444:LYS:HE2	1:A:448:ASN:HA	2.02	0.41
3:B:144:GLU:OE2	3:B:146:LYS:NZ	2.50	0.41
2:H:190:THR:HG22	3:I:136:LEU:HD21	2.02	0.41
1:C:991:VAL:HG12	1:C:995:ARG:NE	2.35	0.41
3:B:84:PHE:CE2	3:B:107:ILE:HG12	2.56	0.41
3:B:118:ILE:HD11	3:B:195:CYS:HB3	2.02	0.41
2:F:175:ALA:HB2	2:F:185:LEU:HB2	2.01	0.41
3:I:62:ARG:NH2	3:I:80:GLU:HB2	2.36	0.41
1:A:245:HIS:HB2	1:A:259:THR:HB	2.03	0.41
1:C:201:PHE:HB2	1:C:231:ILE:HD11	2.02	0.41
1:E:91:TYR:HD1	1:E:193:VAL:HG22	1.84	0.41
1:E:165:ASN:HD22	1:E:165:ASN:H	1.67	0.41
3:B:90:GLN:HE22	3:B:92:TYR:HB3	1.85	0.41
2:F:149:VAL:HG21	2:F:205:VAL:HG11	2.02	0.41
2:F:208:LYS:HB3	2:F:208:LYS:HE3	1.91	0.41
1:A:15:CYS:HA	1:A:158:ARG:HD3	2.03	0.41
1:E:735:SER:HA	1:E:767:LEU:HD13	2.03	0.41
2:D:6:GLN:HE21	2:D:114:THR:HG23	1.86	0.41
3:B:55:ARG:HE	3:B:55:ARG:N	2.12	0.41
3:G:95:SER:HB3	3:G:96:PRO:HD3	2.01	0.41
2:H:52:ILE:HD12	2:H:57:ILE:HD11	2.02	0.41
3:I:38:GLN:HE21	3:I:38:GLN:HB3	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:124:GLU:HB2	3:I:127:LYS:HD3	2.03	0.41
1:A:351:TYR:HE1	1:A:452:LEU:HB2	1.85	0.41
1:A:979:ASP:HB3	1:A:983:ARG:NH1	2.36	0.41
2:F:6:GLN:H	2:F:112:GLN:HE22	1.68	0.41
3:G:141:TYR:HB3	3:G:142:PRO:HD3	2.02	0.41
1:A:615:VAL:HG23	1:A:649:CYS:SG	2.61	0.41
1:E:781:VAL:HG22	1:E:1026:ALA:HB2	2.02	0.41
2:D:106:TRP:CD1	2:D:108:ASP:HB2	2.55	0.41
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.56	0.41
1:C:408:ARG:H	1:C:408:ARG:HD2	1.86	0.41
2:H:99:VAL:HB	2:H:105:TYR:HB2	2.02	0.41
3:I:16:GLY:H	3:I:79:LEU:HD23	1.84	0.41
1:A:77:LYS:HE3	1:A:258:TRP:CE2	2.55	0.41
1:C:81:ASN:HD22	1:C:239:GLN:NE2	2.18	0.41
1:E:1103:PHE:HZ	4:E:1311:NAG:H62	1.86	0.41
2:D:91:THR:HG22	2:D:117:THR:HA	2.01	0.41
3:I:19:ALA:HB3	3:I:76:ILE:HD11	2.02	0.41
1:A:180:GLU:HG3	1:A:182:LYS:HG3	2.03	0.41
1:A:210:ILE:HG12	1:A:217:PRO:HG3	2.02	0.41
1:C:545:GLY:HA3	1:C:565:PHE:CE1	2.56	0.41
1:C:790:LYS:HE2	1:C:790:LYS:HB2	1.95	0.41
1:E:39:PRO:HG3	1:E:55:PHE:HZ	1.85	0.41
1:E:671:CYS:SG	1:E:697:MET:HB3	2.61	0.41
2:F:157:VAL:HG23	2:F:207:HIS:CD2	2.56	0.41
3:G:127:LYS:HA	3:G:184:LYS:HD3	2.03	0.41
2:H:47:TRP:HB2	3:I:99:PHE:HE2	1.86	0.41
3:I:38:GLN:OE1	3:I:40:LYS:NZ	2.54	0.41
1:C:108:THR:O	1:C:237:ARG:NH1	2.51	0.41
1:E:115:GLN:HG3	1:E:130:VAL:HG12	2.03	0.41
3:B:182:LEU:HD22	3:B:186:ASP:HB2	2.03	0.41
1:A:86:PHE:N	1:A:236:THR:O	2.54	0.40
1:A:1131:GLY:HA2	4:A:1308:NAG:H81	2.02	0.40
3:I:134:VAL:HB	3:I:180:LEU:HB2	2.03	0.40
1:A:485:GLY:H	1:A:488:CYS:HB2	1.85	0.40
1:C:947:LYS:HE3	1:C:947:LYS:HB3	1.89	0.40
3:I:140:PHE:CZ	3:I:175:SER:HA	2.56	0.40
1:A:21:ARG:HG3	1:A:78:ARG:HA	2.02	0.40
1:C:472:ILE:HD13	1:C:472:ILE:H	1.85	0.40
1:C:707:TYR:HB3	1:E:792:PRO:HG3	2.02	0.40
1:E:491:PRO:O	2:H:101:ARG:NH2	2.45	0.40
1:E:206:LYS:HB2	1:E:223:LEU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1054:GLN:HB2	1:E:1061:VAL:HB	2.04	0.40
2:H:217:ARG:NH2	3:I:123:ASP:OD2	2.54	0.40
3:I:41:ARG:HB2	3:I:43:GLN:HE22	1.86	0.40
1:C:439:ASN:O	1:C:441:LEU:HD23	2.21	0.40
1:E:654:GLU:O	1:E:694:ALA:N	2.53	0.40
2:D:51:ILE:HG13	2:D:58:ALA:HB2	2.02	0.40
2:F:157:VAL:HG22	2:F:206:ASN:O	2.21	0.40
3:G:196:GLU:HA	3:G:205:PRO:HD2	2.02	0.40
2:H:73:ASP:OD1	2:H:75:SER:OG	2.34	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%)	1030 (96%)	38 (4%)	0	100	100
1	C	1068/1288 (83%)	1028 (96%)	40 (4%)	0	100	100
1	E	1068/1288 (83%)	1030 (96%)	38 (4%)	0	100	100
2	D	198/226 (88%)	186 (94%)	12 (6%)	0	100	100
2	F	198/226 (88%)	188 (95%)	10 (5%)	0	100	100
2	H	198/226 (88%)	186 (94%)	12 (6%)	0	100	100
3	B	210/215 (98%)	195 (93%)	15 (7%)	0	100	100
3	G	210/215 (98%)	182 (87%)	28 (13%)	0	100	100
3	I	210/215 (98%)	182 (87%)	28 (13%)	0	100	100
All	All	4428/5187 (85%)	4207 (95%)	221 (5%)	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%)	891 (97%)	31 (3%)	37	64
1	C	922/1111 (83%)	886 (96%)	36 (4%)	32	61
1	E	922/1111 (83%)	894 (97%)	28 (3%)	41	67
2	D	173/192 (90%)	165 (95%)	8 (5%)	27	57
2	F	173/192 (90%)	160 (92%)	13 (8%)	13	39
2	H	173/192 (90%)	158 (91%)	15 (9%)	10	34
3	B	182/185 (98%)	170 (93%)	12 (7%)	16	45
3	G	182/185 (98%)	173 (95%)	9 (5%)	25	55
3	I	182/185 (98%)	168 (92%)	14 (8%)	13	38
All	All	3831/4464 (86%)	3665 (96%)	166 (4%)	33	59

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	61	ASN
1	A	68	ILE
1	A	70	VAL
1	A	79	PHE
1	A	146	HIS
1	A	157	PHE
1	A	167	THR
1	A	211	ASN
1	A	214	ARG
1	A	259	THR
1	A	326	ILE
1	A	335	LEU
1	A	336	CYS
1	A	345	THR
1	A	362	VAL
1	A	364	ASP
1	A	387	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	408	ARG
1	A	430	THR
1	A	455	LEU
1	A	719	THR
1	A	804	GLN
1	A	855	PHE
1	A	873	TYR
1	A	878	LEU
1	A	1001	LEU
1	A	1076	THR
1	A	1082	CYS
1	A	1086	LYS
1	A	1114	ILE
1	C	68	ILE
1	C	69	HIS
1	C	108	THR
1	C	113	LYS
1	C	144	TYR
1	C	166	CYS
1	C	277	LEU
1	C	291	CYS
1	C	307	THR
1	C	319	ARG
1	C	335	LEU
1	C	336	CYS
1	C	357	ARG
1	C	364	ASP
1	C	378	LYS
1	C	387	LEU
1	C	393	THR
1	C	408	ARG
1	C	429	PHE
1	C	440	ASN
1	C	441	LEU
1	C	458	LYS
1	C	472	ILE
1	C	493	GLN
1	C	495	TYR
1	C	525	CYS
1	C	581	THR
1	C	617	CYS
1	C	740	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	760	CYS
1	C	820	ASP
1	C	855	PHE
1	C	873	TYR
1	C	878	LEU
1	C	947	LYS
1	C	995	ARG
1	E	14	GLN
1	E	61	ASN
1	E	63	THR
1	E	133	PHE
1	E	150	LYS
1	E	165	ASN
1	E	170	TYR
1	E	187	LYS
1	E	244	LEU
1	E	249	LEU
1	E	277	LEU
1	E	307	THR
1	E	335	LEU
1	E	356	LYS
1	E	408	ARG
1	E	422	ASN
1	E	455	LEU
1	E	489	TYR
1	E	517	LEU
1	E	525	CYS
1	E	709	ASN
1	E	712	ILE
1	E	719	THR
1	E	787	GLN
1	E	790	LYS
1	E	858	LEU
1	E	878	LEU
1	E	979	ASP
2	D	12	LYS
2	D	13	ARG
2	D	117	THR
2	D	124	LYS
2	D	155	GLU
2	D	161	TRP
2	D	170	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	177	LEU
3	B	2	ILE
3	B	30	ASN
3	B	55	ARG
3	B	78	ARG
3	B	149	TRP
3	B	162	GLU
3	B	166	GLU
3	B	181	THR
3	B	184	LYS
3	B	189	LYS
3	B	190	HIS
3	B	212	ARG
2	F	3	GLN
2	F	13	ARG
2	F	39	GLN
2	F	82	GLU
2	F	117	THR
2	F	157	VAL
2	F	161	TRP
2	F	167	THR
2	F	170	VAL
2	F	171	HIS
2	F	214	VAL
2	F	217	ARG
2	F	218	VAL
3	G	78	ARG
3	G	150	LYS
3	G	155	LEU
3	G	166	GLU
3	G	170	LYS
3	G	176	LEU
3	G	179	THR
3	G	182	LEU
3	G	200	GLN
2	H	18	VAL
2	H	34	PHE
2	H	39	GLN
2	H	74	LYS
2	H	105	TYR
2	H	115	LEU
2	H	117	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	150	LYS
2	H	159	VAL
2	H	166	LEU
2	H	177	LEU
2	H	201	TYR
2	H	203	CYS
2	H	217	ARG
2	H	219	GLU
3	I	4	LEU
3	I	6	GLN
3	I	11	LEU
3	I	38	GLN
3	I	40	LYS
3	I	48	LEU
3	I	78	ARG
3	I	80	GLU
3	I	136	LEU
3	I	155	LEU
3	I	167	GLN
3	I	176	LEU
3	I	190	HIS
3	I	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	14	GLN
1	A	23	GLN
1	A	49	HIS
1	A	122	ASN
1	A	134	GLN
1	A	173	GLN
1	A	196	ASN
1	A	207	HIS
1	A	211	ASN
1	A	218	GLN
1	A	394	ASN
1	A	439	ASN
1	A	498	GLN
1	A	644	GLN
1	A	784	GLN
1	A	804	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	872	GLN
1	A	895	GLN
1	A	901	GLN
1	A	907	ASN
1	A	926	GLN
1	A	954	GLN
1	A	969	ASN
1	A	1005	GLN
1	A	1048	HIS
1	C	23	GLN
1	C	81	ASN
1	C	115	GLN
1	C	148	ASN
1	C	149	ASN
1	C	207	HIS
1	C	218	GLN
1	C	394	ASN
1	C	409	GLN
1	C	414	GLN
1	C	440	ASN
1	C	493	GLN
1	C	498	GLN
1	C	580	GLN
1	C	641	ASN
1	C	690	GLN
1	C	762	GLN
1	C	787	GLN
1	C	804	GLN
1	C	913	GLN
1	C	954	GLN
1	E	14	GLN
1	E	23	GLN
1	E	49	HIS
1	E	115	GLN
1	E	148	ASN
1	E	149	ASN
1	E	188	ASN
1	E	207	HIS
1	E	218	GLN
1	E	343	ASN
1	E	388	ASN
1	E	439	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	440	ASN
1	E	450	ASN
1	E	493	GLN
1	E	506	GLN
1	E	580	GLN
1	E	675	GLN
1	E	690	GLN
1	E	755	GLN
1	E	762	GLN
1	E	784	GLN
1	E	787	GLN
1	E	913	GLN
1	E	954	GLN
1	E	1002	GLN
1	E	1011	GLN
1	E	1054	GLN
1	E	1101	HIS
1	E	1106	GLN
2	D	31	ASN
2	D	62	GLN
2	D	112	GLN
2	D	204	ASN
2	D	206	ASN
3	B	6	GLN
3	B	31	ASN
3	B	43	GLN
3	B	148	GLN
2	F	3	GLN
2	F	171	HIS
3	G	27	GLN
3	G	30	ASN
3	G	31	ASN
3	G	43	GLN
3	G	91	GLN
3	G	148	GLN
3	G	159	ASN
3	G	161	GLN
3	G	200	GLN
2	H	1	GLN
2	H	3	GLN
2	H	31	ASN
2	H	39	GLN

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Mol	Chain	Res	Type
2	H	65	GLN
2	H	112	GLN
3	I	6	GLN
3	I	90	GLN
3	I	139	ASN
3	I	148	GLN
3	I	156	GLN
3	I	161	GLN
3	I	167	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

38 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	$\# Z  > 2$
4	NAG	E	1306	1	14,14,15	0.27	0	17,19,21	0.53	0
4	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1306	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	1302	1	14,14,15	0.29	0	17,19,21	0.53	0
4	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	A	1311	1	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	E	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1304	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	A	1313	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1312	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	A	1303	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	E	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1313	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	E	1307	1	14,14,15	0.35	0	17,19,21	0.58	0
4	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	E	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	E	1311	1	14,14,15	0.24	0	17,19,21	0.55	0
4	NAG	E	1310	1	14,14,15	0.27	0	17,19,21	0.54	0
4	NAG	A	1301	1	14,14,15	0.35	0	17,19,21	0.40	0
4	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	E	1308	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1311	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	A	1312	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	E	1305	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	E	1312	1	14,14,15	0.45	0	17,19,21	1.26	1 (5%)
4	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	E	1303	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	E	1301	1	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	A	1310	1	14,14,15	0.26	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	3/6/23/26	0/1/1/1
4	NAG	E	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1312	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1312	NAG	C2-N2-C7	4.29	129.01	122.90

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C4-C5-C6-O6
4	C	1310	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	E	1305	NAG	C4-C5-C6-O6
4	E	1306	NAG	C4-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1313	NAG	O5-C5-C6-O6
4	C	1310	NAG	C4-C5-C6-O6
4	E	1304	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	E	1305	NAG	O5-C5-C6-O6
4	E	1306	NAG	O5-C5-C6-O6
4	E	1312	NAG	O5-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	E	1309	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	E	1304	NAG	C8-C7-N2-C2
4	E	1304	NAG	O7-C7-N2-C2
4	E	1312	NAG	C8-C7-N2-C2
4	E	1312	NAG	O7-C7-N2-C2
4	C	1312	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	E	1309	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1312	NAG	C4-C5-C6-O6
4	A	1311	NAG	C4-C5-C6-O6
4	E	1307	NAG	C4-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	E	1304	NAG	O5-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1313	NAG	C4-C5-C6-O6
4	E	1307	NAG	O5-C5-C6-O6
4	E	1308	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	E	1302	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	E	1308	NAG	O5-C5-C6-O6
4	E	1312	NAG	C4-C5-C6-O6
4	A	1310	NAG	C3-C2-N2-C7
4	A	1311	NAG	C3-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7
4	E	1306	NAG	C3-C2-N2-C7
4	E	1307	NAG	C3-C2-N2-C7
4	E	1310	NAG	C3-C2-N2-C7
4	E	1311	NAG	C3-C2-N2-C7
4	C	1304	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	E	1312	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1311	NAG	1	0
4	E	1304	NAG	1	0
4	E	1311	NAG	2	0
4	E	1312	NAG	1	0
4	A	1308	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

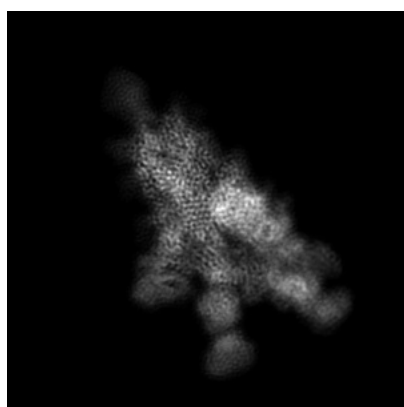
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32647. These allow visual inspection of the internal detail of the map and identification of artifacts.

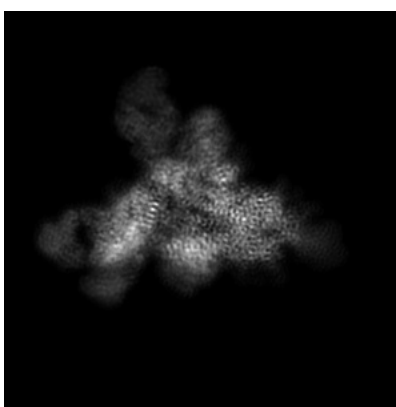
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

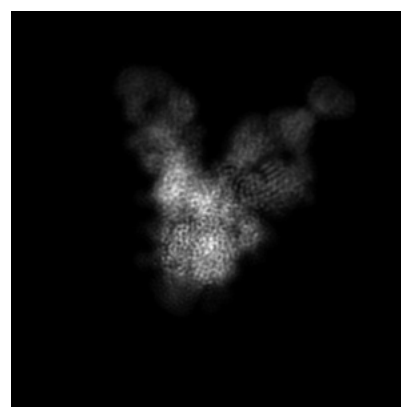
#### 6.1.1 Primary map



X



Y



Z

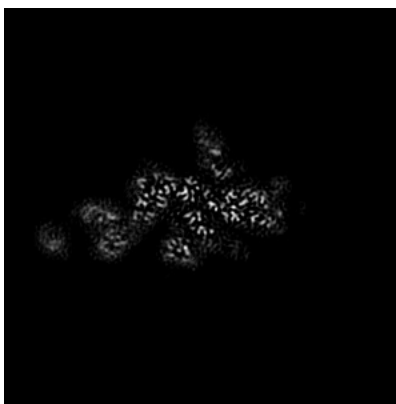
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 192



Y Index: 192

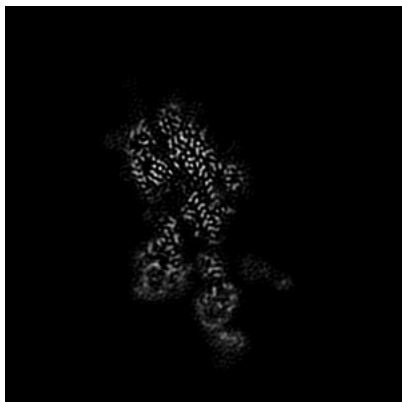


Z Index: 192

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

## 6.3 Largest variance slices [i](#)

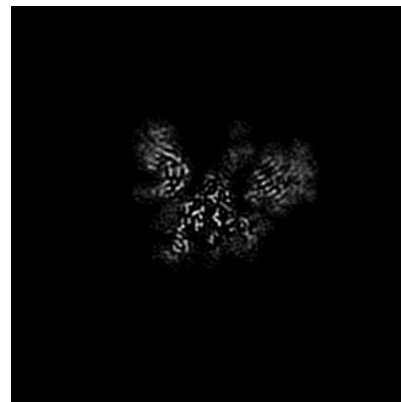
### 6.3.1 Primary map



X Index: 184



Y Index: 164

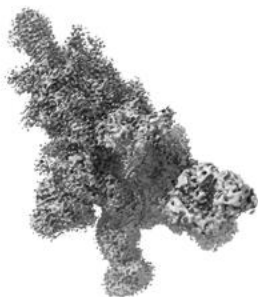


Z Index: 192

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

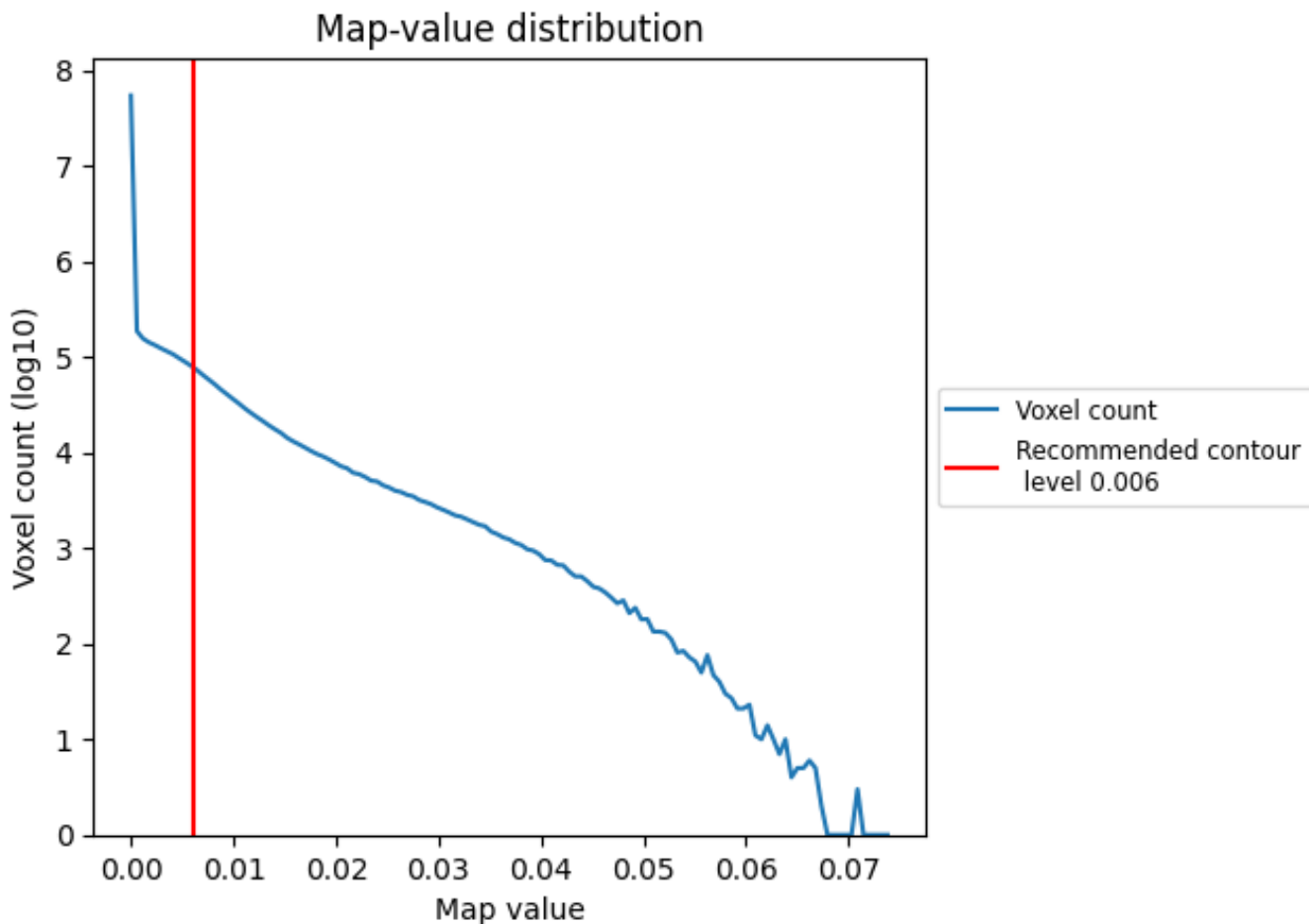
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

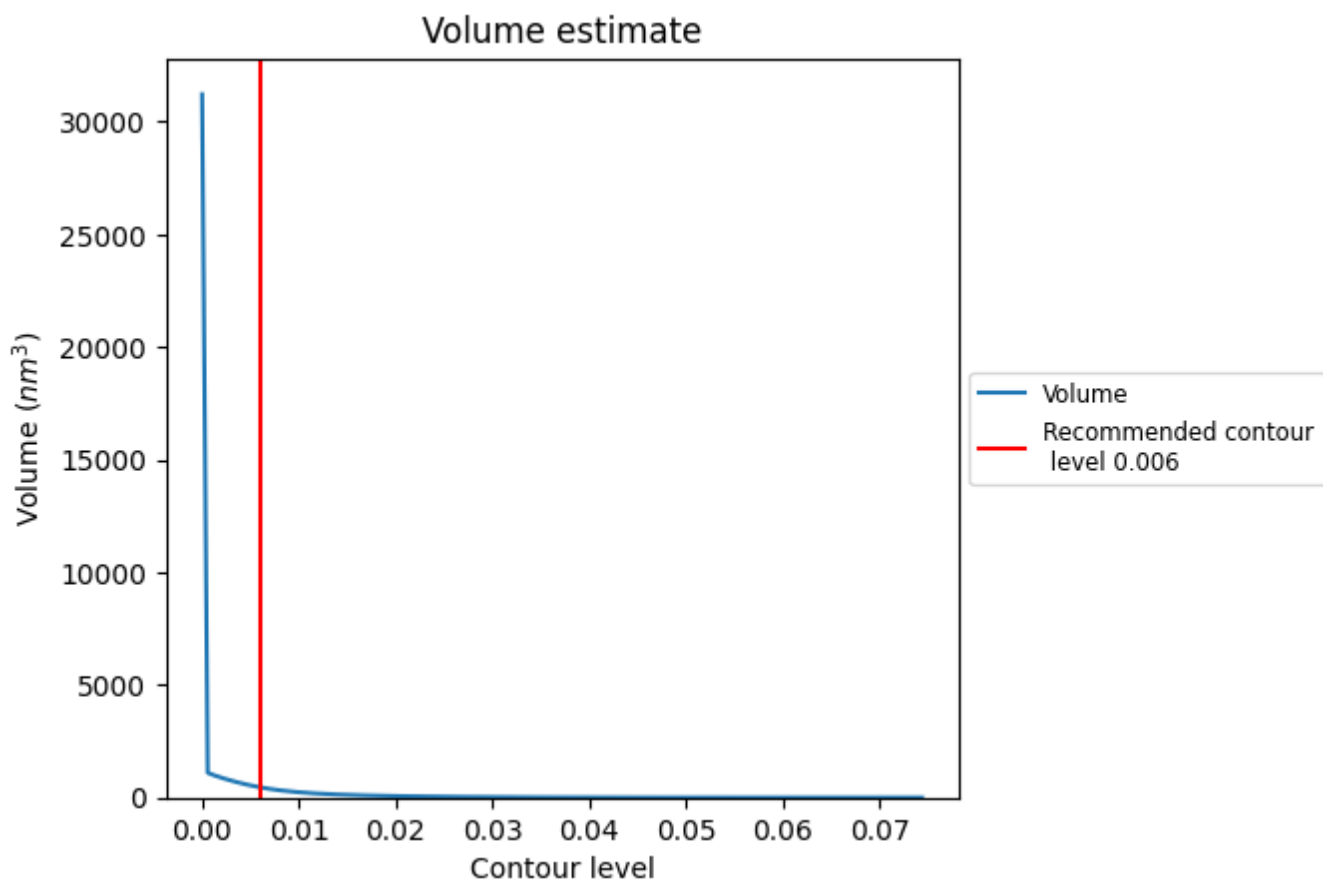
This section contains the results of statistical analysis of the map.

### 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.

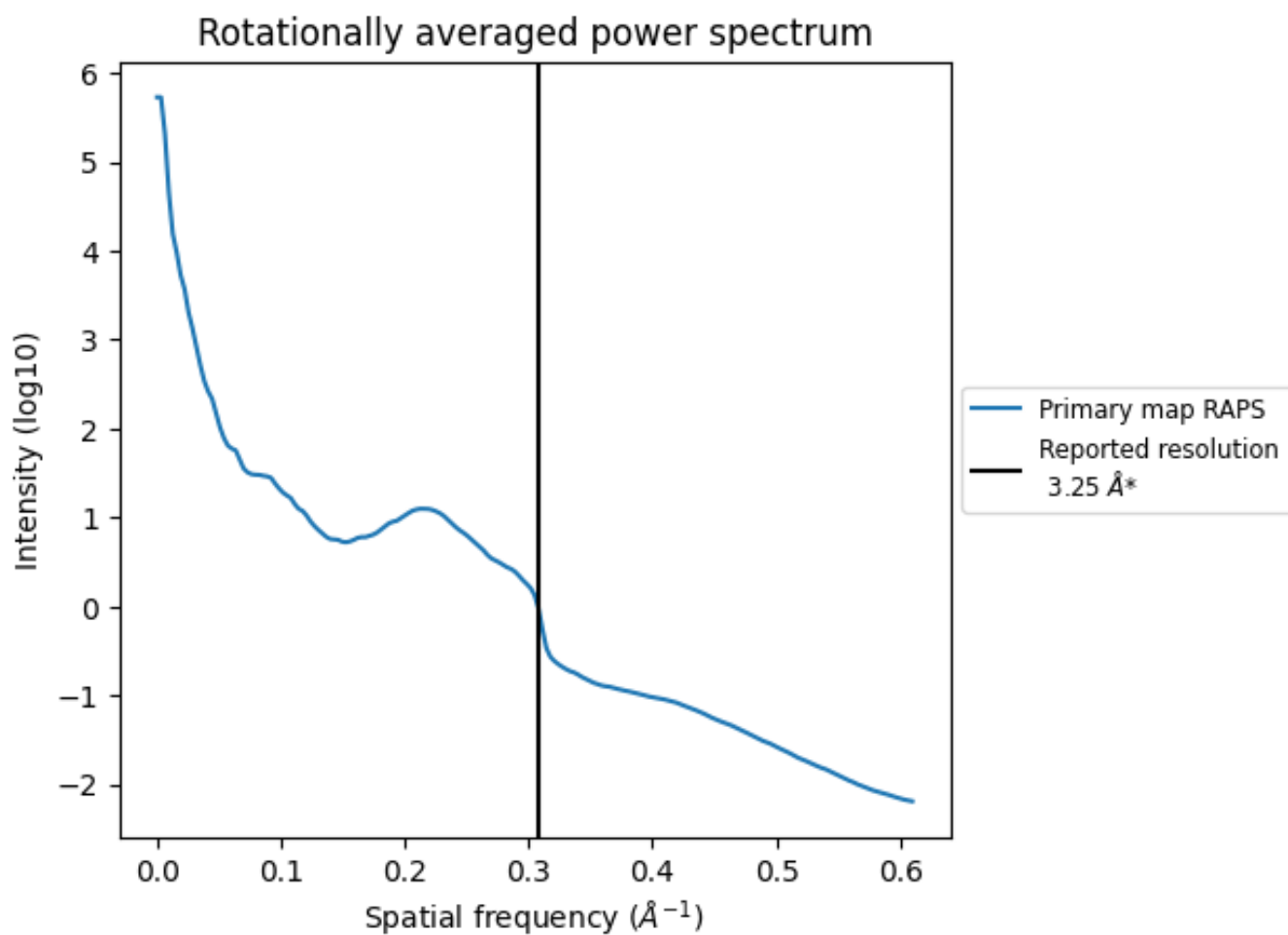
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 456 nm<sup>3</sup>; this corresponds to an approximate mass of 412 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.308 \text{\AA}^{-1}$

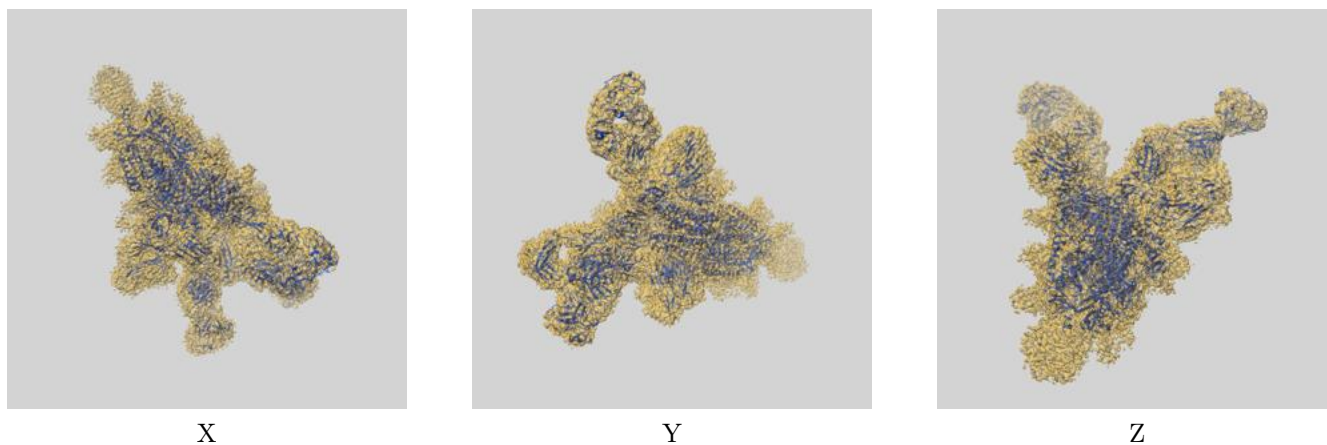
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

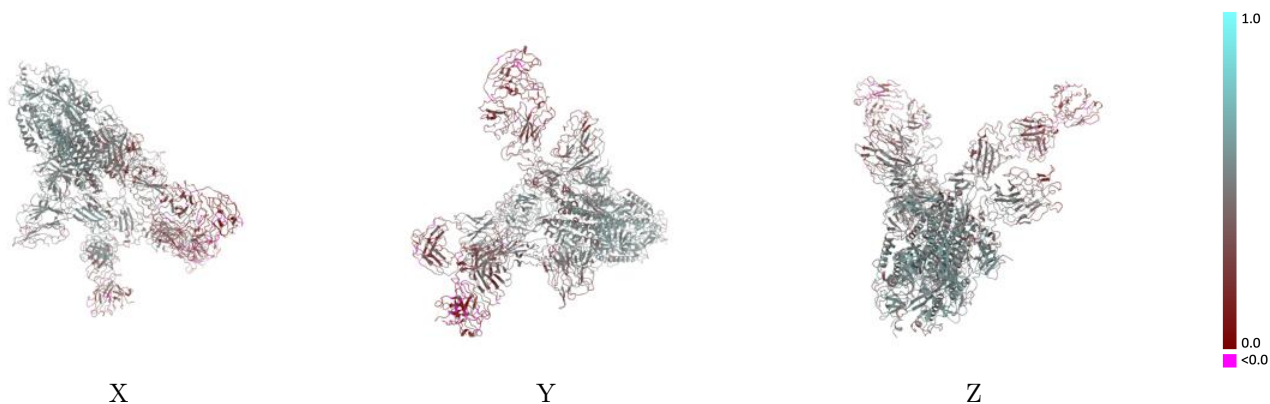
This section contains information regarding the fit between EMDB map EMD-32647 and PDB model 7WOB. Per-residue inclusion information can be found in section [3](#) on page [14](#).

### 9.1 Map-model overlay [i](#)



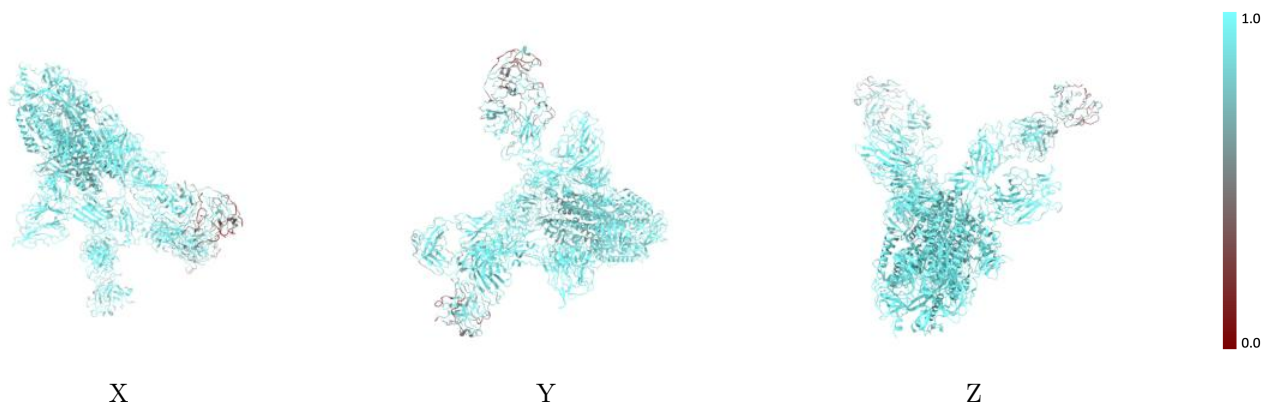
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



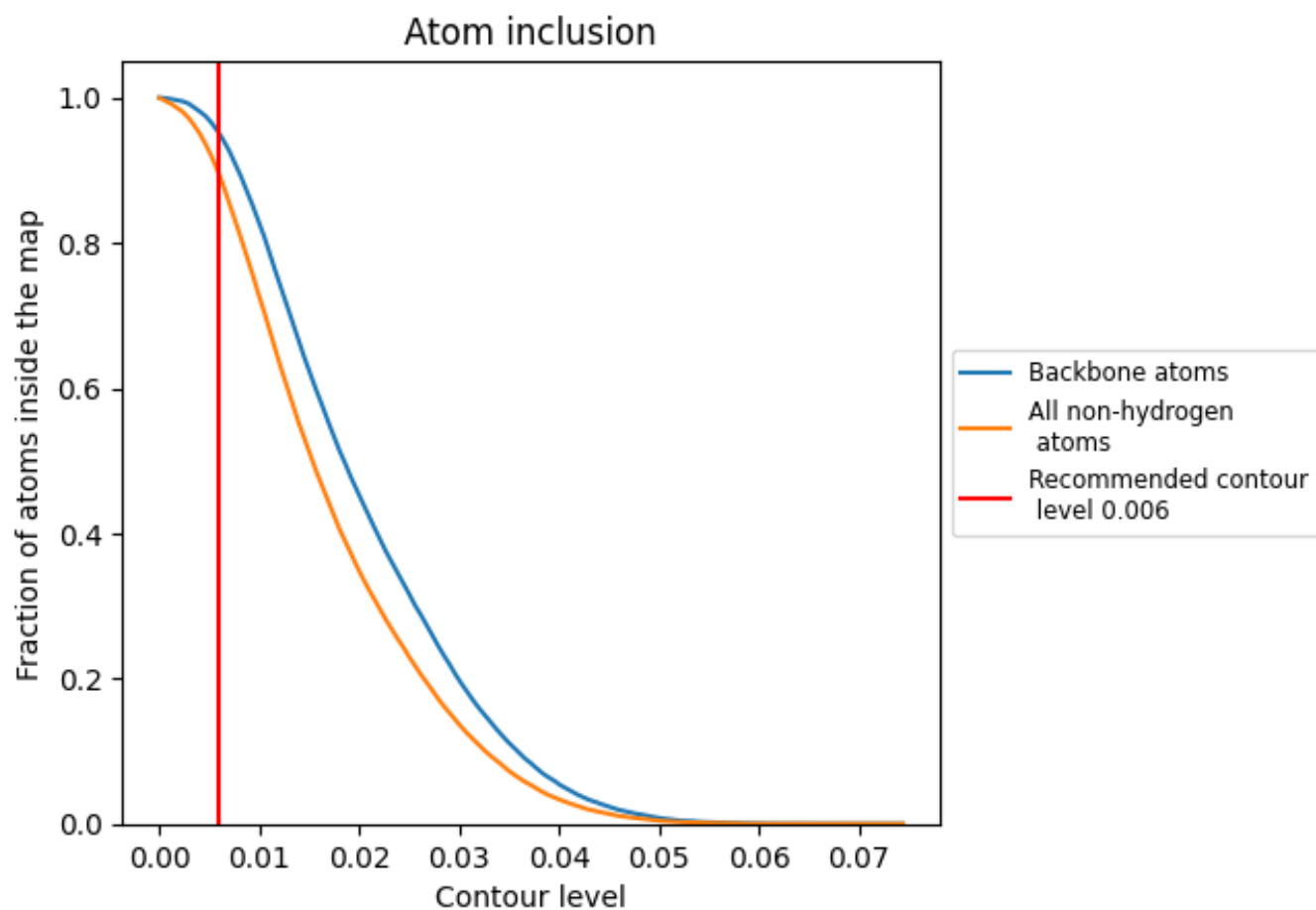
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).





















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8932	 0.4170
A	 0.9322	 0.4680
B	 0.8808	 0.3260
C	 0.9388	 0.4750
D	 0.8891	 0.3610
E	 0.9312	 0.4540
F	 0.8141	 0.3130
G	 0.7555	 0.2480
H	 0.7143	 0.2520
I	 0.6532	 0.2230

