



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 01:37 PM JST

PDB ID : 7WHK  
EMDB ID : EMD-32503  
Title : The state 3 complex structure of Omicron spike with Bn03 (2-up RBD, 5 nanobodies)  
Authors : Zhan, W.Q.; Zhang, X.; Chen, Z.G.; Sun, L.  
Deposited on : 2021-12-30  
Resolution : 3.01 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:

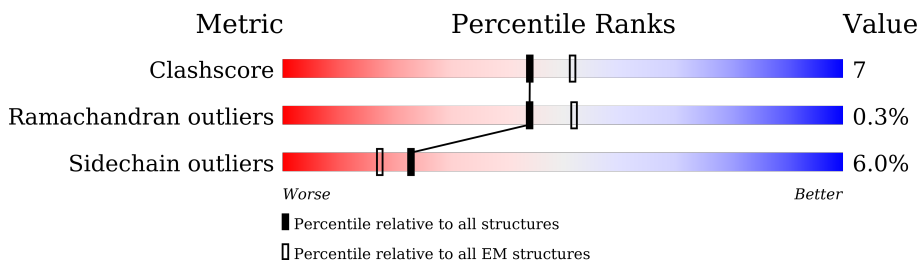
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 3.01 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	1285	
1	B	1285	
1	C	1285	
2	D	120	
2	H	120	
3	E	138	
3	F	138	
3	G	138	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 29150 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	1040	8101	5193	1348	1522	38	0	0
1	B	1027	7999	5131	1329	1502	37	0	0
1	C	1043	8129	5208	1357	1526	38	0	0

There are 384 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	209	ILE	LEU	variant	UNP P0DTC2
A	212	GLU	-	insertion	UNP P0DTC2
A	213	PRO	-	insertion	UNP P0DTC2
A	214	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	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	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	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	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
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	variant	UNP P0DTC2
B	212	GLU	-	insertion	UNP P0DTC2
B	213	PRO	-	insertion	UNP P0DTC2
B	214	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	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	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	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
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	145	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	209	ILE	LEU	variant	UNP P0DTC2
C	212	GLU	-	insertion	UNP P0DTC2
C	213	PRO	-	insertion	UNP P0DTC2
C	214	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	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	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
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

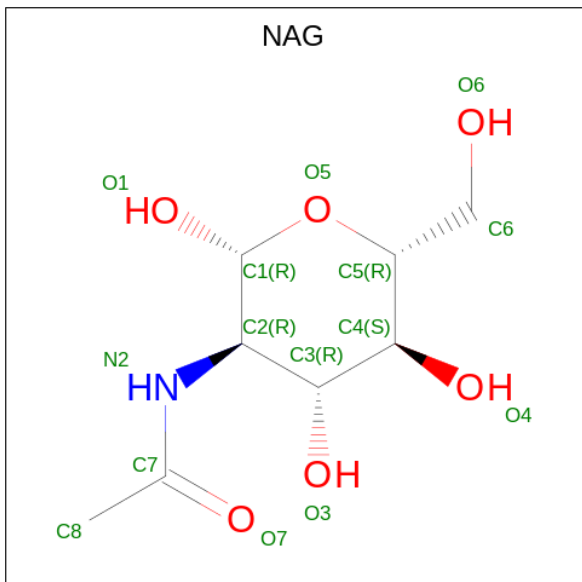
- Molecule 2 is a protein called Bn03\_nano2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	119	Total	C	N	O	S	0	0
			922	585	151	182	4		
2	H	119	Total	C	N	O	S	0	0
			922	585	151	182	4		

- Molecule 3 is a protein called Bn03\_nano1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	117	Total	C	N	O	S	0	0
			899	562	148	182	7		
3	F	116	Total	C	N	O	S	0	0
			893	559	147	180	7		
3	G	116	Total	C	N	O	S	0	0
			893	559	147	180	7		

- 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	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			112	64	8	40	
4	B	1	Total	C	N	O	0
			112	64	8	40	

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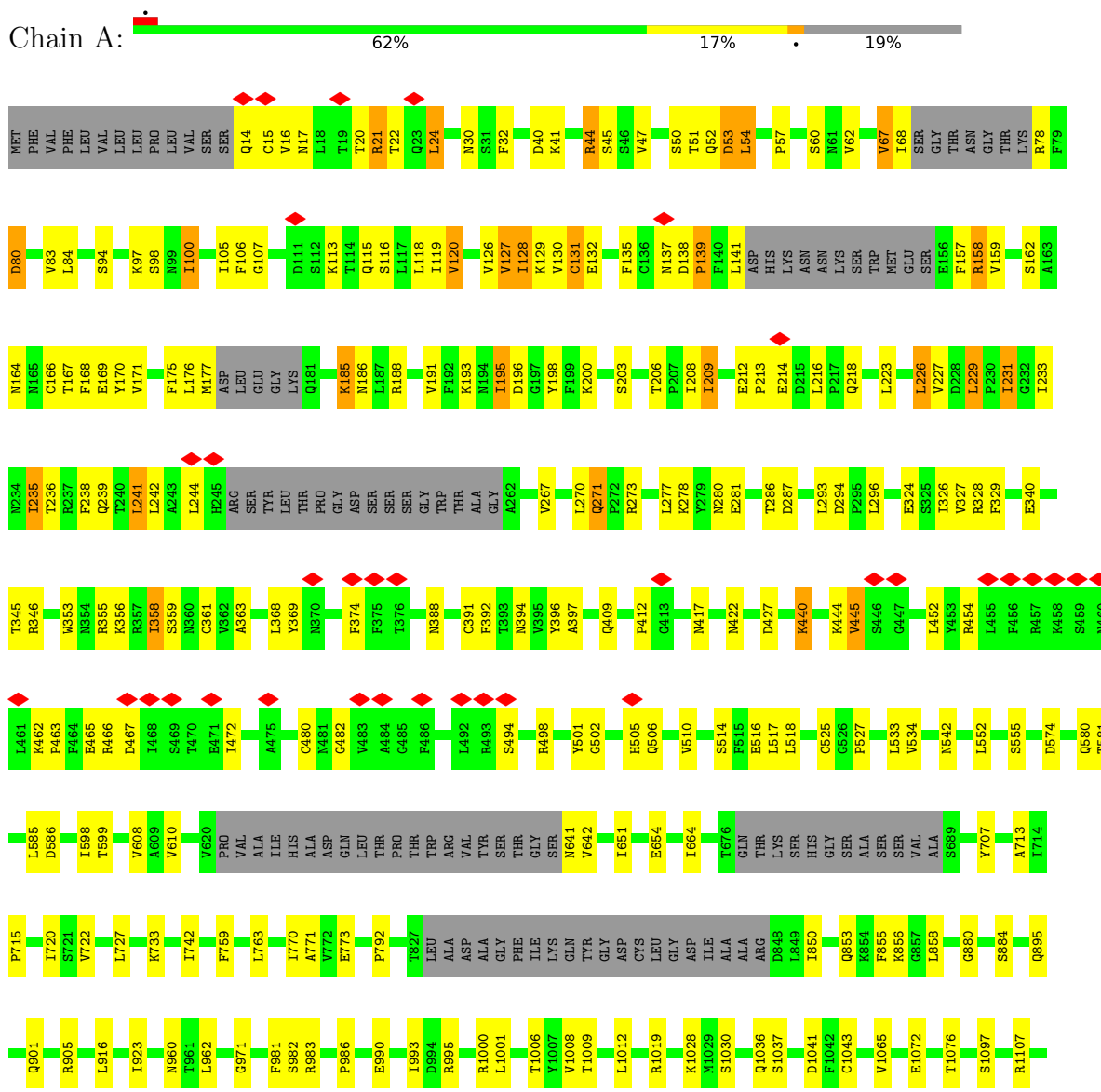
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0
4	C	1	140	80	10	50	0

### 3 Residue-property plots [i](#)

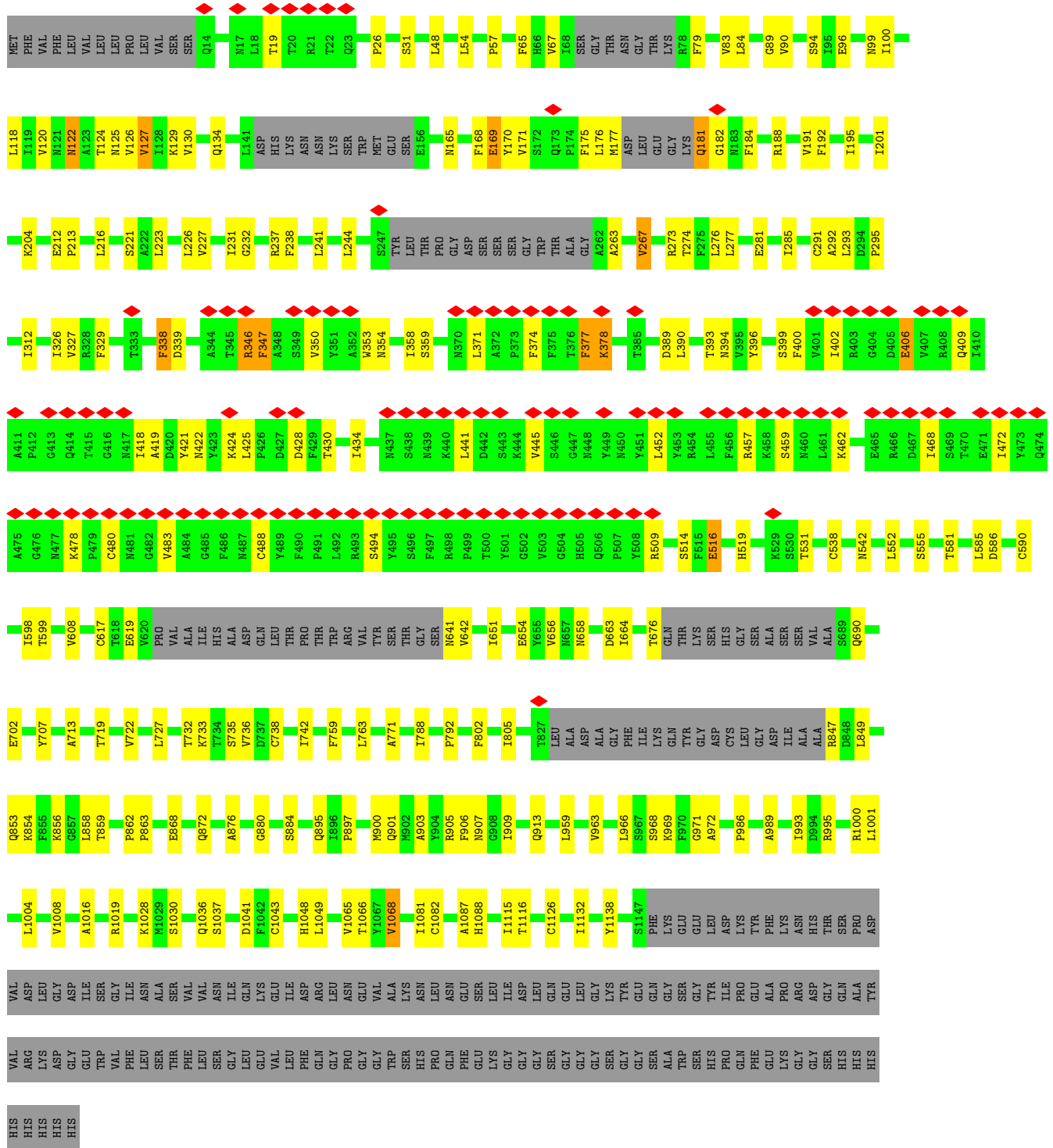
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Spike glycoprotein

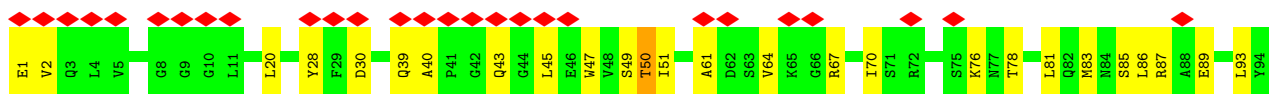








• Molecule 2: Bn03\_nano2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.477	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	340.48, 340.48, 340.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.064, 1.064, 1.064	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	0.30	0/8293	0.46	0/11295
1	B	0.27	0/8189	0.44	0/11150
1	C	0.27	0/8321	0.44	0/11331
2	D	0.24	0/945	0.42	0/1283
2	H	0.24	0/945	0.42	0/1283
3	E	0.24	0/920	0.46	0/1251
3	F	0.24	0/914	0.46	0/1243
3	G	0.24	0/914	0.46	0/1243
All	All	0.27	0/29441	0.45	0/40079

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	8101	0	7882	102	0
1	B	7999	0	7786	99	0
1	C	8129	0	7913	126	0
2	D	922	0	866	22	0
2	H	922	0	866	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	899	0	852	17	0
3	F	893	0	847	16	0
3	G	893	0	847	21	0
4	A	140	0	130	1	0
4	B	112	0	104	1	0
4	C	140	0	130	1	0
All	All	29150	0	28223	395	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 (395) 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:E:90:THR:HA	3:E:114:VAL:O	1.71	0.91
3:E:34:MET:HB2	3:E:51:MET:HB3	1.71	0.71
1:B:555:SER:HB2	1:B:586:ASP:HB2	1.74	0.70
1:C:327:VAL:HA	1:C:542:ASN:HB3	1.73	0.69
2:D:47:TRP:HE1	2:D:50:THR:HG23	1.58	0.68
1:C:374:PHE:HB3	1:C:434:ILE:HD11	1.76	0.67
1:C:126:VAL:HG23	1:C:175:PHE:HA	1.77	0.67
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.76	0.66
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.78	0.66
2:H:47:TRP:HE1	2:H:50:THR:HG23	1.62	0.65
1:A:327:VAL:HA	1:A:542:ASN:HB3	1.77	0.64
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.79	0.64
3:E:39:GLN:HE22	3:E:45:PRO:HG3	1.63	0.64
1:A:130:VAL:HG11	1:A:231:ILE:HG21	1.81	0.63
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.32	0.63
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.28	0.63
1:C:452:LEU:HA	1:C:494:SER:HA	1.81	0.63
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.29	0.62
1:B:271:GLN:OE1	1:B:273:ARG:NH1	2.33	0.62
1:A:107:GLY:H	1:A:235:ILE:HG23	1.63	0.62
1:A:853:GLN:NE2	1:A:960:ASN:OD1	2.33	0.62
1:C:897:PRO:HD2	1:C:900:MET:HE2	1.82	0.61
1:B:34:ARG:HH21	1:B:217:PRO:HB2	1.64	0.61
2:H:45:LEU:HD22	2:H:110:TRP:HH2	1.66	0.61
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.82	0.61
1:A:353:TRP:O	1:A:466:ARG:NH1	2.34	0.61
1:C:312:ILE:HG12	1:C:598:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.83	0.61
1:B:108:THR:O	1:B:237:ARG:NH2	2.33	0.61
1:C:480:CYS:HB2	1:C:483:VAL:HG22	1.83	0.61
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.33	0.60
1:A:356:LYS:HD2	1:A:358:ILE:HG12	1.81	0.60
1:B:790:LYS:NZ	1:C:702:GLU:OE2	2.33	0.60
1:B:858:LEU:HD13	1:B:959:LEU:HD22	1.84	0.60
1:C:96:GLU:OE2	1:C:188:ARG:NH1	2.34	0.59
1:A:599:THR:HG22	1:A:608:VAL:HG12	1.84	0.59
1:B:476:GLY:HA3	1:B:487:ASN:HD21	1.68	0.59
2:D:107:PHE:HB2	2:D:110:TRP:HE1	1.68	0.59
2:D:1:GLU:HG3	2:D:2:VAL:HG23	1.85	0.59
1:A:57:PRO:HG3	1:A:271:GLN:HG2	1.83	0.59
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.85	0.59
1:A:412:PRO:HB3	1:A:427:ASP:HA	1.85	0.59
2:D:99:ARG:NH1	2:D:104:ASP:O	2.36	0.58
2:D:51:ILE:HG12	2:D:70:ILE:HG21	1.86	0.58
1:A:326:ILE:HD11	1:A:534:VAL:HG22	1.86	0.58
3:F:47:TRP:HE1	3:F:50:SER:HB3	1.69	0.58
1:B:792:PRO:HG3	1:C:707:TYR:HB3	1.86	0.57
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.85	0.57
1:B:642:VAL:HA	1:B:651:ILE:HG22	1.86	0.57
1:B:1030:SER:HB3	1:C:1041:ASP:HB2	1.87	0.57
3:G:22:CYS:HB3	3:G:78:LEU:HB2	1.87	0.57
2:H:1:GLU:HG3	2:H:2:VAL:HG23	1.85	0.57
3:E:73:ASN:HD21	3:E:77:MET:H	1.51	0.57
3:E:90:THR:HG22	3:E:116:VAL:H	1.69	0.57
1:B:389:ASP:OD2	1:B:547:LYS:NZ	2.38	0.56
1:C:719:THR:HG23	1:C:1068:VAL:HG13	1.86	0.56
3:F:68:THR:HG23	3:F:81:GLN:HB3	1.88	0.56
1:C:735:SER:OG	1:C:859:THR:OG1	2.23	0.56
1:A:296:LEU:HB2	1:A:608:VAL:HG11	1.86	0.56
1:A:880:GLY:O	1:A:884:SER:OG	2.21	0.56
1:B:455:LEU:HD11	1:B:493:ARG:HB2	1.88	0.56
1:B:552:LEU:HD23	1:B:585:LEU:HD13	1.87	0.56
1:C:231:ILE:HG13	1:C:232:GLY:H	1.68	0.56
1:C:274:THR:HG23	1:C:291:CYS:HB2	1.88	0.55
3:G:38:ARG:HE	3:G:46:GLU:HB3	1.70	0.55
1:A:982:SER:HB3	1:B:390:LEU:HD21	1.88	0.55
1:B:478:LYS:HD3	1:B:487:ASN:HB3	1.88	0.55
1:B:905:ARG:HH11	1:B:1036:GLN:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:54:SER:OG	3:E:56:ARG:NH2	2.40	0.55
1:A:905:ARG:HH11	1:A:1036:GLN:HB2	1.72	0.55
1:C:641:ASN:HD21	1:C:654:GLU:HA	1.72	0.55
1:B:357:ARG:NH2	1:B:396:TYR:OH	2.40	0.55
1:A:363:ALA:N	1:A:525:CYS:O	2.35	0.55
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.89	0.54
1:A:345:THR:HG22	1:A:346:ARG:HG2	1.89	0.54
1:C:1126:CYS:HB2	1:C:1132:ILE:HG12	1.88	0.54
3:F:90:THR:HG23	3:F:115:THR:HA	1.89	0.54
1:C:204:LYS:NZ	1:C:221:SER:O	2.38	0.54
1:C:359:SER:OG	1:C:394:ASN:ND2	2.40	0.54
1:B:735:SER:HA	1:B:767:LEU:HD13	1.89	0.54
1:A:105:ILE:HG22	1:A:118:LEU:HD13	1.89	0.54
1:A:707:TYR:HB3	1:C:792:PRO:HG3	1.90	0.54
1:C:99:ASN:ND2	1:C:177:MET:SD	2.80	0.54
1:C:759:PHE:HD2	1:C:1001:LEU:HD21	1.73	0.54
1:C:378:LYS:H	1:C:378:LYS:HD3	1.72	0.53
1:B:231:ILE:HG22	1:B:232:GLY:H	1.72	0.53
1:A:392:PHE:HD2	1:A:517:LEU:HB2	1.74	0.53
1:B:96:GLU:OE2	1:B:101:ILE:N	2.41	0.53
1:B:610:VAL:HG23	1:B:651:ILE:HG13	1.90	0.53
1:C:100:ILE:HD13	1:C:263:ALA:HB2	1.91	0.53
1:A:128:ILE:HG23	1:A:170:TYR:HB3	1.90	0.53
1:A:552:LEU:HD23	1:A:585:LEU:HD13	1.91	0.53
1:C:346:ARG:HG2	1:C:347:PHE:H	1.72	0.53
1:C:868:GLU:OE2	1:C:872:GLN:NE2	2.42	0.53
1:C:354:ASN:ND2	1:C:399:SER:OG	2.42	0.53
1:C:424:LYS:NZ	1:C:425:LEU:O	2.42	0.53
1:A:452:LEU:HA	1:A:494:SER:HA	1.91	0.52
1:C:1016:ALA:O	1:C:1019:ARG:NH1	2.42	0.52
1:B:895:GLN:HG2	1:C:713:ALA:HB2	1.91	0.52
1:C:338:PHE:HB2	1:C:358:ILE:HG21	1.92	0.52
1:A:462:LYS:HD2	1:A:463:PRO:HD2	1.91	0.52
1:A:642:VAL:HG12	1:A:651:ILE:HG12	1.90	0.52
2:H:99:ARG:NH1	2:H:104:ASP:O	2.39	0.52
1:C:191:VAL:HG23	1:C:223:LEU:HD22	1.91	0.52
3:F:19:ARG:HH11	3:F:79:TYR:HB3	1.74	0.52
1:A:359:SER:HB2	1:A:394:ASN:HD22	1.73	0.52
1:B:1125:ASN:OD1	1:B:1126:CYS:N	2.43	0.52
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	1.92	0.52
1:C:909:ILE:HD13	1:C:1049:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:VAL:HA	1:A:498:ARG:HH12	1.75	0.52
1:B:1037:SER:OG	1:B:1043:CYS:SG	2.67	0.52
1:A:97:LYS:HD3	1:A:185:LYS:HA	1.92	0.52
2:D:40:ALA:HB3	2:D:43:GLN:HE21	1.75	0.52
3:E:96:VAL:HG12	3:E:108:TRP:HA	1.91	0.51
3:F:73:ASN:HD21	3:F:75:GLU:HB3	1.73	0.51
3:G:103:SER:N	3:G:106:ASP:OD2	2.42	0.51
1:B:34:ARG:NH1	1:B:189:GLU:OE2	2.42	0.51
1:B:409:GLN:HE22	1:B:418:ILE:H	1.56	0.51
1:B:1066:THR:OG1	1:B:1067:TYR:N	2.43	0.51
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.92	0.51
1:B:212:GLU:HB3	1:B:213:PRO:HD3	1.93	0.51
1:A:454:ARG:NH2	1:A:467:ASP:O	2.43	0.51
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.44	0.51
1:B:326:ILE:HD12	1:B:539:VAL:HG21	1.91	0.51
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.75	0.51
1:A:355:ARG:HA	1:A:397:ALA:O	2.11	0.51
1:C:901:GLN:O	1:C:905:ARG:HG2	2.11	0.51
1:A:1037:SER:OG	1:A:1043:CYS:SG	2.68	0.50
1:C:89:GLY:HA2	1:C:192:PHE:O	2.11	0.50
1:C:122:ASN:HB3	1:C:124:THR:H	1.75	0.50
2:D:45:LEU:HD22	2:D:110:TRP:HH2	1.76	0.50
3:G:69:ILE:HB	3:G:80:LEU:HD12	1.92	0.50
1:C:181:GLN:OE1	1:C:182:GLY:N	2.44	0.50
1:C:457:ARG:NH2	1:C:459:SER:O	2.39	0.50
1:A:1030:SER:HB3	1:B:1041:ASP:HB2	1.92	0.50
1:C:65:PHE:HE2	1:C:84:LEU:HD11	1.76	0.50
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.93	0.50
1:C:94:SER:HB2	1:C:188:ARG:HG3	1.93	0.50
3:E:36:TRP:HE1	3:E:78:LEU:HD22	1.76	0.50
1:C:1037:SER:OG	1:C:1043:CYS:SG	2.68	0.50
1:C:350:VAL:HA	1:C:400:PHE:HB2	1.94	0.50
1:A:127:VAL:HG21	4:A:1310:NAG:H81	1.93	0.50
1:A:610:VAL:HG23	1:A:651:ILE:HB	1.94	0.50
1:A:1139:ASP:OD1	1:A:1139:ASP:N	2.45	0.50
1:B:363:ALA:N	1:B:525:CYS:O	2.43	0.50
1:C:67:VAL:HG23	1:C:79:PHE:HA	1.93	0.50
1:A:981:PHE:O	1:B:386:LYS:NZ	2.37	0.50
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.93	0.50
1:B:901:GLN:O	1:B:905:ARG:HG2	2.12	0.49
1:C:409:GLN:NE2	1:C:419:ALA:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:VAL:HG12	1:B:498:ARG:HH12	1.77	0.49
3:F:93:TYR:O	3:F:111:GLY:HA2	2.13	0.49
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.94	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.94	0.49
1:A:1126:CYS:HB2	1:A:1132:ILE:HG12	1.94	0.49
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.46	0.49
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.77	0.49
1:A:328:ARG:HE	1:A:533:LEU:HB2	1.77	0.49
1:A:462:LYS:HB3	1:A:465:GLU:HG3	1.94	0.49
1:C:118:LEU:HD11	1:C:241:LEU:HD11	1.94	0.49
2:H:61:ALA:HB3	2:H:64:VAL:HG22	1.95	0.49
1:A:792:PRO:HG3	1:B:707:TYR:HB3	1.95	0.48
1:B:83:VAL:HG11	1:B:237:ARG:HH11	1.78	0.48
1:B:125:ASN:HD21	4:B:1302:NAG:H3	1.77	0.48
1:C:204:LYS:HB2	1:C:223:LEU:HA	1.95	0.48
2:H:36:TRP:HE1	2:H:79:LEU:HD22	1.78	0.48
1:C:31:SER:HA	1:C:216:LEU:HD12	1.95	0.48
1:C:656:VAL:HG12	1:C:658:ASN:H	1.78	0.48
1:C:393:THR:OG1	1:C:516:GLU:O	2.30	0.48
3:E:39:GLN:HB3	3:E:92:MET:HB2	1.95	0.48
1:A:901:GLN:O	1:A:905:ARG:HG2	2.13	0.48
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	1.96	0.48
2:D:83:MET:HB2	2:D:86:LEU:HD21	1.94	0.48
2:D:87:ARG:HG3	2:D:89:GLU:HG3	1.96	0.48
1:A:516:GLU:HG2	2:H:101:PRO:HB3	1.95	0.48
1:C:853:GLN:HG2	1:C:963:VAL:HG21	1.95	0.48
1:A:472:ILE:HG13	1:A:482:GLY:HA2	1.94	0.48
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.79	0.48
1:A:713:ALA:HB2	1:C:895:GLN:HG2	1.96	0.48
1:C:402:ILE:HD12	1:C:406:GLU:HB3	1.96	0.48
1:C:856:LYS:HD3	1:C:966:LEU:HD12	1.96	0.48
2:D:61:ALA:HB3	2:D:64:VAL:HG22	1.96	0.48
1:B:377:PHE:CE1	1:B:432:CYS:HB3	2.49	0.48
1:B:433:VAL:HG12	1:B:512:VAL:HG22	1.95	0.48
1:C:120:VAL:HB	1:C:127:VAL:HG13	1.96	0.48
3:G:9:GLY:HA2	3:G:114:VAL:HG12	1.96	0.48
1:A:229:LEU:HB3	1:A:231:ILE:HD13	1.96	0.47
1:A:440:LYS:H	1:A:440:LYS:HD2	1.80	0.47
1:B:171:VAL:O	1:B:173:GLN:N	2.47	0.47
1:B:336:CYS:HA	1:B:361:CYS:HB2	1.96	0.47
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:SG	1:A:166:CYS:N	2.88	0.47
1:B:532:ASN:OD1	1:B:533:LEU:N	2.45	0.47
1:B:1126:CYS:HB2	1:B:1132:ILE:HG12	1.96	0.47
1:C:126:VAL:HG21	1:C:176:LEU:HG	1.95	0.47
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.96	0.47
2:H:9:GLY:HA3	2:H:18:LEU:HD11	1.95	0.47
1:B:191:VAL:HG23	1:B:223:LEU:HD22	1.95	0.47
1:C:346:ARG:H	1:C:346:ARG:HD3	1.80	0.47
3:E:73:ASN:ND2	3:E:77:MET:H	2.11	0.47
2:H:40:ALA:HB3	2:H:43:GLN:HE21	1.80	0.47
1:B:185:LYS:HB3	1:B:208:ILE:HG23	1.97	0.47
1:B:302:THR:HG21	1:B:315:THR:HG22	1.97	0.47
1:C:129:LYS:HE3	1:C:169:GLU:HB3	1.96	0.47
2:H:7:SER:OG	2:H:21:SER:O	2.30	0.47
1:C:663:ASP:OD1	1:C:663:ASP:N	2.48	0.47
1:C:905:ARG:HH11	1:C:1036:GLN:HB2	1.79	0.47
3:E:26:ASP:N	3:E:26:ASP:OD1	2.48	0.47
3:F:38:ARG:HE	3:F:46:GLU:HB3	1.79	0.47
3:F:48:ILE:O	3:F:60:ASN:N	2.48	0.47
1:B:612:TYR:HE2	1:B:651:ILE:HD11	1.80	0.47
3:F:14:PRO:HG3	3:F:116:VAL:HG12	1.97	0.47
1:A:97:LYS:HD2	1:A:97:LYS:HA	1.62	0.47
1:B:462:LYS:HD3	1:B:463:PRO:HD2	1.98	0.46
3:E:24:ALA:HB1	3:E:29:PHE:HD2	1.79	0.46
3:G:73:ASN:HD21	3:G:76:ASN:H	1.63	0.46
2:H:67:ARG:NH2	2:H:85:SER:O	2.48	0.46
1:A:209:ILE:H	1:A:209:ILE:HG13	1.41	0.46
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.97	0.46
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.97	0.46
1:B:733:LYS:HD2	1:B:771:ALA:HB1	1.96	0.46
1:A:574:ASP:OD1	1:C:847:ARG:NH2	2.48	0.46
1:B:328:ARG:HE	1:B:533:LEU:HB2	1.80	0.46
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.97	0.46
1:A:727:LEU:HD11	1:A:1028:LYS:HD2	1.97	0.46
3:G:17:SER:OG	3:G:81:GLN:OE1	2.33	0.46
2:H:107:PHE:HB2	2:H:110:TRP:HE1	1.81	0.46
1:A:895:GLN:HG2	1:B:713:ALA:HB2	1.98	0.46
1:A:21:ARG:HD3	1:A:21:ARG:HA	1.69	0.46
1:C:880:GLY:O	1:C:884:SER:OG	2.23	0.46
1:A:229:LEU:HD22	1:A:229:LEU:HA	1.71	0.46
1:A:396:TYR:HB2	1:A:514:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:TYR:OH	1:B:1011:GLN:NE2	2.49	0.46
3:G:19:ARG:HD2	3:G:79:TYR:CD1	2.51	0.46
1:A:388:ASN:HD22	1:A:527:PRO:HD2	1.81	0.46
2:H:87:ARG:HG3	2:H:89:GLU:HG3	1.98	0.46
1:C:1081:ILE:O	1:C:1088:HIS:N	2.42	0.45
1:B:338:PHE:HB3	1:B:368:LEU:HD21	1.98	0.45
1:C:238:PHE:HZ	1:C:267:VAL:HG21	1.80	0.45
1:A:241:LEU:HA	1:A:241:LEU:HD22	1.73	0.45
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.98	0.45
1:C:858:LEU:HD13	1:C:959:LEU:HD22	1.98	0.45
1:C:676:THR:HG22	1:C:690:GLN:HG3	1.99	0.45
3:G:75:GLU:HG2	3:G:76:ASN:H	1.81	0.45
3:G:77:MET:HG2	3:G:79:TYR:CZ	2.50	0.45
1:A:118:LEU:HD11	1:A:120:VAL:HG13	1.99	0.45
1:B:736:VAL:HG11	1:B:1004:LEU:HD11	1.97	0.45
3:G:36:TRP:CD2	3:G:80:LEU:HD22	2.52	0.45
3:G:98:ASN:ND2	3:G:101:SER:OG	2.50	0.45
1:A:100:ILE:H	1:A:100:ILE:HG12	1.43	0.45
1:B:325:SER:HA	1:B:540:ASN:HB2	1.98	0.45
2:D:67:ARG:NH2	2:D:85:SER:O	2.50	0.45
1:A:44:ARG:HE	1:A:44:ARG:HB2	1.58	0.44
1:A:422:ASN:HD21	1:A:454:ARG:H	1.65	0.44
1:C:54:LEU:HD12	1:C:195:ILE:HD11	1.98	0.44
1:C:552:LEU:HD23	1:C:585:LEU:HD13	1.99	0.44
1:A:733:LYS:HD2	1:A:771:ALA:HB1	1.99	0.44
1:C:377:PHE:CG	1:C:434:ILE:HD13	2.52	0.44
2:D:93:LEU:HD22	2:D:95:TYR:CZ	2.53	0.44
3:E:90:THR:HG22	3:E:115:THR:HA	1.98	0.44
1:B:327:VAL:HA	1:B:542:ASN:HB3	1.99	0.44
2:D:39:GLN:HB3	2:D:93:LEU:HB3	1.98	0.44
2:H:67:ARG:HH12	2:H:87:ARG:HE	1.65	0.44
1:C:212:GLU:HB3	1:C:213:PRO:HD2	2.00	0.44
3:F:90:THR:HA	3:F:114:VAL:O	2.18	0.44
3:G:93:TYR:O	3:G:111:GLY:HA2	2.18	0.44
1:C:1081:ILE:HD11	1:C:1115:ILE:HG21	1.98	0.44
1:C:1082:CYS:HB3	1:C:1087:ALA:HA	1.98	0.44
1:A:16:VAL:HB	1:A:158:ARG:HD3	1.99	0.44
1:B:658:ASN:ND2	1:B:660:TYR:OH	2.50	0.44
1:C:906:PHE:HA	1:C:909:ILE:HG12	1.99	0.44
2:D:47:TRP:NE1	2:D:49:SER:O	2.51	0.44
1:A:195:ILE:H	1:A:195:ILE:HG13	1.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:PHE:HA	1:B:592:PHE:HZ	1.83	0.44
1:A:971:GLY:HA3	1:A:995:ARG:HH21	1.82	0.44
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.99	0.44
1:C:339:ASP:OD1	1:C:339:ASP:N	2.50	0.44
1:A:24:LEU:H	1:A:24:LEU:HG	1.52	0.43
1:A:67:VAL:HG13	1:A:80:ASP:H	1.83	0.43
1:C:277:LEU:HD23	1:C:285:ILE:HD13	2.00	0.43
1:A:359:SER:HB2	1:A:394:ASN:ND2	2.32	0.43
1:B:108:THR:HA	1:B:236:THR:HG22	1.99	0.43
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.84	0.43
1:A:641:ASN:HD21	1:A:654:GLU:HA	1.82	0.43
1:C:986:PRO:HA	1:C:989:ALA:HB3	1.99	0.43
3:F:36:TRP:CD2	3:F:80:LEU:HD22	2.53	0.43
1:A:130:VAL:HB	1:A:233:ILE:HG13	2.00	0.43
1:C:126:VAL:CG2	1:C:175:PHE:HA	2.48	0.43
3:E:47:TRP:HH2	3:E:58:TYR:HD2	1.65	0.43
1:B:449:TYR:HB3	3:E:61:PRO:HD2	1.99	0.43
1:C:353:TRP:HB3	1:C:400:PHE:HB3	2.01	0.43
2:H:76:LYS:HE2	2:H:78:THR:HG21	2.01	0.43
1:A:501:TYR:HB3	1:A:505:HIS:HB2	2.00	0.43
1:B:755:GLN:HG3	1:C:969:LYS:HD3	1.99	0.43
3:F:36:TRP:HE1	3:F:78:LEU:HG	1.83	0.43
1:A:53:ASP:HB3	1:A:54:LEU:H	1.60	0.43
1:B:352:ALA:HB1	3:E:101:SER:HB3	2.00	0.43
1:C:201:ILE:HB	1:C:227:VAL:HG22	2.00	0.43
1:C:347:PHE:CE2	1:C:509:ARG:HB3	2.53	0.43
2:D:83:MET:HG3	2:D:86:LEU:HD11	1.99	0.43
1:B:770:ILE:O	1:B:774:GLN:HG2	2.18	0.43
1:B:1081:ILE:HD11	1:B:1115:ILE:HG21	1.99	0.43
1:B:409:GLN:NE2	1:B:418:ILE:H	2.17	0.43
1:B:441:LEU:HD23	1:B:509:ARG:HH22	1.83	0.43
1:C:462:LYS:HZ2	2:D:30:ASP:HB2	1.83	0.43
1:A:176:LEU:HD22	1:A:226:LEU:HD21	2.01	0.43
1:A:139:PRO:HB2	1:A:241:LEU:HD21	2.01	0.42
1:B:226:LEU:HG	1:B:227:VAL:HG13	1.99	0.42
2:D:20:LEU:HB2	2:D:81:LEU:HB3	2.00	0.42
3:G:36:TRP:CG	3:G:80:LEU:HD22	2.54	0.42
1:A:858:LEU:HD21	1:A:962:LEU:HD23	2.01	0.42
1:B:173:GLN:O	1:B:174:PRO:C	2.56	0.42
1:C:430:THR:H	2:D:102:PHE:HD1	1.67	0.42
3:F:38:ARG:HG2	3:F:48:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:19:ARG:HH11	3:G:79:TYR:HB3	1.84	0.42
1:B:341:VAL:HG23	1:B:342:PHE:CD1	2.54	0.42
1:C:244:LEU:HD23	1:C:244:LEU:H	1.83	0.42
1:C:862:PRO:HA	1:C:863:PRO:HD3	1.96	0.42
1:C:599:THR:HB	1:C:608:VAL:HG12	2.01	0.42
1:B:119:ILE:HG23	1:B:128:ILE:HG12	2.01	0.42
1:B:365:TYR:O	1:B:368:LEU:HB2	2.19	0.42
3:F:19:ARG:HD2	3:F:79:TYR:CD1	2.54	0.42
1:B:81:ASN:N	1:B:81:ASN:OD1	2.53	0.42
1:C:993:ILE:HD12	1:C:993:ILE:HA	1.92	0.42
1:C:90:VAL:HG13	1:C:267:VAL:HG23	2.01	0.42
3:F:81:GLN:HE21	3:F:83:ASN:HD21	1.65	0.42
3:G:19:ARG:HD2	3:G:79:TYR:HD1	1.85	0.42
1:C:396:TYR:HB2	1:C:514:SER:OG	2.19	0.42
1:C:421:TYR:CD2	1:C:457:ARG:HG2	2.54	0.42
3:F:40:VAL:HG23	3:F:43:LYS:HB3	2.01	0.42
1:A:1041:ASP:HB2	1:C:1030:SER:HB3	2.02	0.42
1:A:1107:ARG:HH22	1:C:907:ASN:HD22	1.68	0.42
1:B:380:TYR:O	1:B:430:THR:HA	2.20	0.42
1:C:231:ILE:HD12	1:C:231:ILE:HA	1.88	0.42
1:A:106:PHE:HB3	1:A:235:ILE:HD12	2.02	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.02	0.41
1:B:755:GLN:O	1:C:968:SER:OG	2.38	0.41
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.90	0.41
1:C:428:ASP:OD1	1:C:428:ASP:N	2.53	0.41
1:C:125:ASN:HD22	1:C:171:VAL:HG13	1.85	0.41
1:C:788:ILE:HG23	1:C:876:ALA:HB2	2.02	0.41
2:H:39:GLN:HB3	2:H:93:LEU:HB3	2.02	0.41
1:A:326:ILE:HD13	1:A:533:LEU:HA	2.02	0.41
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.02	0.41
1:A:986:PRO:O	1:A:990:GLU:HG2	2.21	0.41
1:C:462:LYS:HE2	2:D:28:TYR:HD2	1.85	0.41
2:H:40:ALA:HA	2:H:92:ALA:HA	2.01	0.41
1:A:368:LEU:HB3	1:A:374:PHE:CE2	2.55	0.41
1:B:490:PHE:HE1	3:E:56:ARG:HB3	1.84	0.41
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	2.01	0.41
2:D:47:TRP:NE1	2:D:50:THR:HG23	2.32	0.41
1:A:444:LYS:O	1:A:498:ARG:NH1	2.52	0.41
1:B:238:PHE:HZ	1:B:267:VAL:HG21	1.85	0.41
1:B:796:TYR:CD2	4:C:1310:NAG:H5	2.55	0.41
1:B:1006:THR:HA	1:B:1009:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ILE:HA	1:C:531:THR:HG21	2.02	0.41
1:C:472:ILE:HD12	1:C:472:ILE:HA	1.96	0.41
2:H:20:LEU:HB2	2:H:81:LEU:HB3	2.02	0.41
1:A:759:PHE:HB3	1:A:1001:LEU:HD11	2.02	0.41
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.85	0.41
3:G:47:TRP:HH2	3:G:58:TYR:HD2	1.68	0.41
1:A:518:LEU:HD21	2:H:50:THR:HB	2.03	0.41
1:A:983:ARG:O	1:B:383:SER:N	2.53	0.41
1:C:733:LYS:HD2	1:C:771:ALA:HB1	2.02	0.41
3:G:30:TYR:CE2	3:G:71:ARG:HD2	2.55	0.41
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.03	0.41
1:A:720:ILE:HG13	1:A:923:ILE:HG23	2.03	0.41
1:A:1006:THR:HA	1:A:1009:THR:HG22	2.03	0.41
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	2.02	0.41
1:B:89:GLY:HA3	1:B:270:LEU:HD12	2.03	0.41
1:B:117:LEU:HD13	1:B:130:VAL:HG13	2.02	0.41
3:G:68:THR:O	3:G:81:GLN:N	2.54	0.41
1:A:502:GLY:O	1:A:506:GLN:HG3	2.21	0.41
1:B:433:VAL:HG12	1:B:512:VAL:HG13	2.02	0.41
1:B:557:LYS:HE2	1:B:559:PHE:HE1	1.85	0.41
1:C:478:LYS:HZ2	1:C:480:CYS:HB3	1.85	0.41
2:D:76:LYS:HE2	2:D:78:THR:HG21	2.01	0.41
1:A:409:GLN:HE22	1:A:417:ASN:H	1.69	0.40
1:B:528:LYS:HE2	1:B:528:LYS:HB3	1.95	0.40
1:C:421:TYR:HD2	1:C:457:ARG:HG2	1.86	0.40
1:C:519:HIS:NE2	2:D:105:TYR:O	2.52	0.40
3:G:73:ASN:HD21	3:G:76:ASN:C	2.24	0.40
1:B:850:ILE:H	1:B:850:ILE:HG13	1.62	0.40
1:B:1076:THR:HB	1:B:1097:SER:HB3	2.03	0.40
1:C:48:LEU:HB3	1:C:276:LEU:HD11	2.03	0.40
1:C:354:ASN:OD1	1:C:399:SER:N	2.34	0.40
1:C:555:SER:OG	1:C:586:ASP:HB2	2.20	0.40
1:A:422:ASN:HA	1:A:454:ARG:HH11	1.86	0.40
1:B:32:PHE:CG	1:B:218:GLN:HG2	2.56	0.40
1:C:903:ALA:HB1	1:C:913:GLN:HG2	2.03	0.40
1:C:969:LYS:NZ	1:C:972:ALA:O	2.36	0.40
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.03	0.40
1:A:191:VAL:HG23	1:A:223:LEU:HD22	2.04	0.40
1:C:26:PRO:HB3	1:C:65:PHE:HE1	1.87	0.40
3:G:36:TRP:HE1	3:G:78:LEU:HB3	1.86	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	1024/1285 (80%)	954 (93%)	66 (6%)	4 (0%)	34	71
1	B	1011/1285 (79%)	972 (96%)	35 (4%)	4 (0%)	34	71
1	C	1027/1285 (80%)	976 (95%)	49 (5%)	2 (0%)	47	81
2	D	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
2	H	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
3	E	115/138 (83%)	105 (91%)	10 (9%)	0	100	100
3	F	114/138 (83%)	98 (86%)	16 (14%)	0	100	100
3	G	114/138 (83%)	99 (87%)	15 (13%)	0	100	100
All	All	3639/4509 (81%)	3426 (94%)	203 (6%)	10 (0%)	44	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	GLU
1	B	172	SER
1	B	292	ALA
1	A	162	SER
1	B	213	PRO
1	C	122	ASN
1	B	174	PRO
1	C	292	ALA
1	A	213	PRO
1	A	139	PRO

### 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	899/1115 (81%)	790 (88%)	109 (12%)	5	20
1	B	886/1115 (80%)	858 (97%)	28 (3%)	39	73
1	C	902/1115 (81%)	866 (96%)	36 (4%)	31	67
2	D	96/97 (99%)	94 (98%)	2 (2%)	53	81
2	H	96/97 (99%)	94 (98%)	2 (2%)	53	81
3	E	100/105 (95%)	98 (98%)	2 (2%)	55	82
3	F	99/105 (94%)	92 (93%)	7 (7%)	14	44
3	G	99/105 (94%)	93 (94%)	6 (6%)	18	51
All	All	3177/3854 (82%)	2985 (94%)	192 (6%)	23	51

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	15	CYS
1	A	17	ASN
1	A	20	THR
1	A	21	ARG
1	A	22	THR
1	A	24	LEU
1	A	30	ASN
1	A	32	PHE
1	A	40	ASP
1	A	41	LYS
1	A	44	ARG
1	A	45	SER
1	A	47	VAL
1	A	50	SER
1	A	51	THR
1	A	52	GLN
1	A	53	ASP
1	A	54	LEU
1	A	60	SER
1	A	62	VAL
1	A	67	VAL
1	A	68	ILE
1	A	78	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	80	ASP
1	A	83	VAL
1	A	84	LEU
1	A	94	SER
1	A	98	SER
1	A	100	ILE
1	A	113	LYS
1	A	115	GLN
1	A	116	SER
1	A	119	ILE
1	A	120	VAL
1	A	126	VAL
1	A	127	VAL
1	A	128	ILE
1	A	129	LYS
1	A	131	CYS
1	A	132	GLU
1	A	135	PHE
1	A	137	ASN
1	A	138	ASP
1	A	141	LEU
1	A	157	PHE
1	A	158	ARG
1	A	159	VAL
1	A	164	ASN
1	A	167	THR
1	A	168	PHE
1	A	169	GLU
1	A	171	VAL
1	A	175	PHE
1	A	177	MET
1	A	185	LYS
1	A	186	ASN
1	A	188	ARG
1	A	193	LYS
1	A	195	ILE
1	A	196	ASP
1	A	198	TYR
1	A	200	LYS
1	A	203	SER
1	A	206	THR
1	A	208	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	209	ILE
1	A	212	GLU
1	A	216	LEU
1	A	218	GLN
1	A	226	LEU
1	A	227	VAL
1	A	229	LEU
1	A	231	ILE
1	A	235	ILE
1	A	236	THR
1	A	238	PHE
1	A	239	GLN
1	A	241	LEU
1	A	242	LEU
1	A	244	LEU
1	A	267	VAL
1	A	270	LEU
1	A	271	GLN
1	A	273	ARG
1	A	277	LEU
1	A	278	LYS
1	A	280	ASN
1	A	281	GLU
1	A	286	THR
1	A	287	ASP
1	A	293	LEU
1	A	294	ASP
1	A	324	GLU
1	A	329	PHE
1	A	340	GLU
1	A	358	ILE
1	A	361	CYS
1	A	369	TYR
1	A	391	CYS
1	A	440	LYS
1	A	445	VAL
1	A	480	CYS
1	A	510	VAL
1	A	581	THR
1	A	850	ILE
1	A	856	LYS
1	A	916	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	993	ILE
1	B	29	THR
1	B	111	ASP
1	B	166	CYS
1	B	169	GLU
1	B	170	TYR
1	B	172	SER
1	B	173	GLN
1	B	176	LEU
1	B	208	ILE
1	B	214	GLU
1	B	299	THR
1	B	301	CYS
1	B	347	PHE
1	B	361	CYS
1	B	377	PHE
1	B	378	LYS
1	B	430	THR
1	B	445	VAL
1	B	455	LEU
1	B	510	VAL
1	B	524	VAL
1	B	525	CYS
1	B	538	CYS
1	B	581	THR
1	B	590	CYS
1	B	847	ARG
1	B	878	LEU
1	B	916	LEU
1	C	19	THR
1	C	127	VAL
1	C	134	GLN
1	C	165	ASN
1	C	169	GLU
1	C	170	TYR
1	C	181	GLN
1	C	184	PHE
1	C	267	VAL
1	C	281	GLU
1	C	293	LEU
1	C	329	PHE
1	C	338	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	346	ARG
1	C	347	PHE
1	C	371	LEU
1	C	377	PHE
1	C	378	LYS
1	C	389	ASP
1	C	390	LEU
1	C	406	GLU
1	C	441	LEU
1	C	445	VAL
1	C	468	ILE
1	C	488	CYS
1	C	516	GLU
1	C	538	CYS
1	C	581	THR
1	C	590	CYS
1	C	617	CYS
1	C	619	GLU
1	C	732	THR
1	C	738	CYS
1	C	849	LEU
1	C	854	LYS
1	C	1068	VAL
2	D	50	THR
2	D	118	VAL
3	E	75	GLU
3	E	95	CYS
3	F	44	THR
3	F	59	ILE
3	F	64	LYS
3	F	73	ASN
3	F	99	TRP
3	F	103	SER
3	F	104	THR
3	G	1	GLU
3	G	26	ASP
3	G	39	GLN
3	G	51	MET
3	G	56	ARG
3	G	90	THR
2	H	50	THR
2	H	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	280	ASN
1	A	314	GLN
1	A	388	ASN
1	A	394	ASN
1	A	409	GLN
1	A	414	GLN
1	A	641	ASN
1	A	690	GLN
1	A	755	GLN
1	A	762	GLN
1	A	784	GLN
1	A	804	GLN
1	A	965	GLN
1	A	1002	GLN
1	A	1048	HIS
1	A	1135	ASN
1	B	125	ASN
1	B	173	GLN
1	B	218	GLN
1	B	314	GLN
1	B	409	GLN
1	B	450	ASN
1	B	487	ASN
1	B	540	ASN
1	B	641	ASN
1	B	658	ASN
1	B	751	ASN
1	B	784	GLN
1	B	965	GLN
1	B	1002	GLN
1	B	1011	GLN
1	B	1106	GLN
1	C	23	GLN
1	C	30	ASN
1	C	121	ASN
1	C	173	GLN
1	C	343	ASN
1	C	394	ASN
1	C	409	GLN
1	C	422	ASN

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Mol	Chain	Res	Type
1	C	450	ASN
1	C	540	ASN
1	C	580	GLN
1	C	641	ASN
1	C	784	GLN
1	C	955	ASN
1	C	965	GLN
1	C	1005	GLN
1	C	1106	GLN
3	E	39	GLN
3	E	73	ASN
3	F	83	ASN
3	G	13	GLN
3	G	73	ASN
3	G	98	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

28 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	C	1307	1	14,14,15	0.46	0	17,19,21	0.92	1 (5%)
4	NAG	C	1310	1	14,14,15	0.31	0	17,19,21	0.88	0
4	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	A	1301	1	14,14,15	0.31	0	17,19,21	1.03	2 (11%)
4	NAG	A	1310	1	14,14,15	0.45	0	17,19,21	1.02	1 (5%)
4	NAG	B	1302	1	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
4	NAG	A	1305	1	14,14,15	0.47	0	17,19,21	0.94	2 (11%)
4	NAG	A	1308	1	14,14,15	0.46	0	17,19,21	0.92	1 (5%)
4	NAG	B	1306	1	14,14,15	0.44	0	17,19,21	0.93	1 (5%)
4	NAG	C	1308	1	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
4	NAG	A	1302	1	14,14,15	0.31	0	17,19,21	0.67	0
4	NAG	C	1303	1	14,14,15	0.46	0	17,19,21	1.59	4 (23%)
4	NAG	A	1309	1	14,14,15	0.29	0	17,19,21	0.67	0
4	NAG	A	1303	1	14,14,15	0.39	0	17,19,21	0.75	0
4	NAG	A	1307	1	14,14,15	0.40	0	17,19,21	1.13	2 (11%)
4	NAG	B	1305	1	14,14,15	0.49	0	17,19,21	0.91	0
4	NAG	C	1302	1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
4	NAG	C	1304	1	14,14,15	0.40	0	17,19,21	0.63	0
4	NAG	B	1301	1	14,14,15	0.33	0	17,19,21	0.73	0
4	NAG	C	1309	1	14,14,15	0.56	0	17,19,21	1.00	0
4	NAG	B	1304	1	14,14,15	0.38	0	17,19,21	0.77	0
4	NAG	C	1305	1	14,14,15	0.35	0	17,19,21	1.69	3 (17%)
4	NAG	A	1306	1	14,14,15	0.30	0	17,19,21	0.72	0
4	NAG	B	1307	1	14,14,15	0.44	0	17,19,21	0.88	0
4	NAG	B	1308	1	14,14,15	0.42	0	17,19,21	0.72	0
4	NAG	B	1303	1	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	C	1306	1	14,14,15	0.44	0	17,19,21	0.79	1 (5%)
4	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1305	NAG	C2-N2-C7	4.29	129.01	122.90
4	C	1303	NAG	C1-O5-C5	3.82	117.37	112.19
4	C	1305	NAG	C1-C2-N2	3.21	115.97	110.49
4	C	1305	NAG	C4-C3-C2	-3.16	106.38	111.02
4	A	1310	NAG	C1-O5-C5	2.93	116.17	112.19
4	C	1302	NAG	C1-O5-C5	2.90	116.11	112.19
4	B	1306	NAG	C1-O5-C5	2.86	116.07	112.19
4	C	1303	NAG	O5-C5-C6	2.69	111.41	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1308	NAG	C1-O5-C5	2.54	115.63	112.19
4	A	1305	NAG	C1-O5-C5	2.54	115.63	112.19
4	A	1304	NAG	C1-O5-C5	2.52	115.61	112.19
4	C	1303	NAG	C2-N2-C7	2.52	126.49	122.90
4	A	1307	NAG	O5-C1-C2	-2.52	107.31	111.29
4	C	1306	NAG	C1-O5-C5	2.50	115.58	112.19
4	B	1302	NAG	C1-O5-C5	2.40	115.45	112.19
4	A	1301	NAG	O5-C1-C2	-2.39	107.52	111.29
4	C	1303	NAG	C6-C5-C4	-2.31	107.61	113.00
4	C	1308	NAG	C1-O5-C5	2.18	115.15	112.19
4	A	1301	NAG	C4-C3-C2	-2.15	107.87	111.02
4	C	1307	NAG	O5-C1-C2	-2.10	107.97	111.29
4	A	1307	NAG	C1-O5-C5	2.07	114.99	112.19
4	A	1305	NAG	O5-C1-C2	-2.01	108.11	111.29

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1304	NAG	C1-C2-N2-C7
4	A	1306	NAG	C8-C7-N2-C2
4	A	1306	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	C	1303	NAG	C3-C2-N2-C7
4	C	1303	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	C	1310	NAG	C8-C7-N2-C2
4	C	1310	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	A	1310	NAG	C8-C7-N2-C2
4	C	1309	NAG	C8-C7-N2-C2
4	C	1309	NAG	O7-C7-N2-C2

*Continued on next page...*

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1310	NAG	1	0
4	A	1310	NAG	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	NAG	1	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.

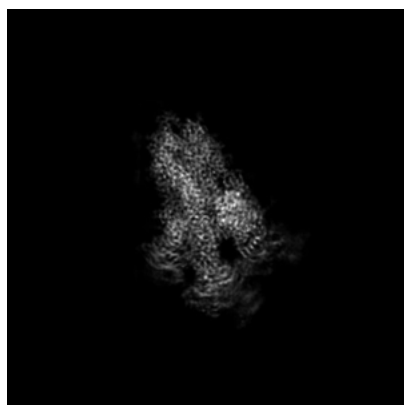
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32503. These allow visual inspection of the internal detail of the map and identification of artifacts.

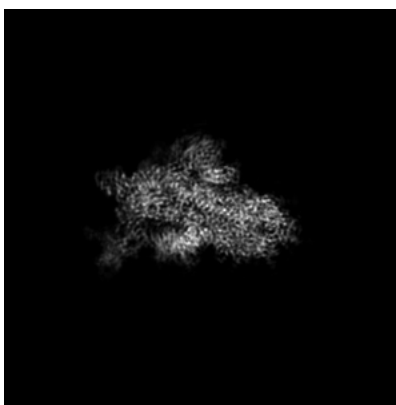
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

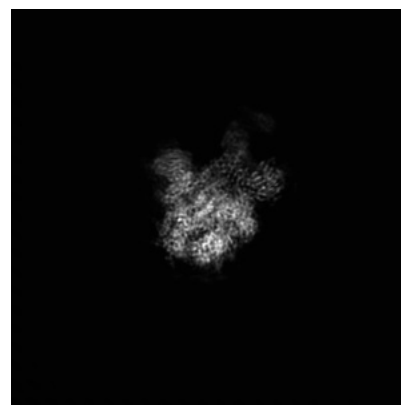
#### 6.1.1 Primary map



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: 160



Y Index: 160



Z Index: 160

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: 135



Y Index: 154



Z Index: 149

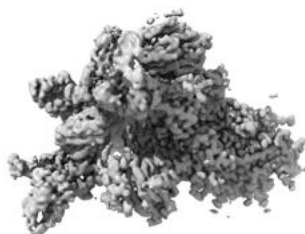
The images above show the largest variance slices of the map in three orthogonal directions.

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

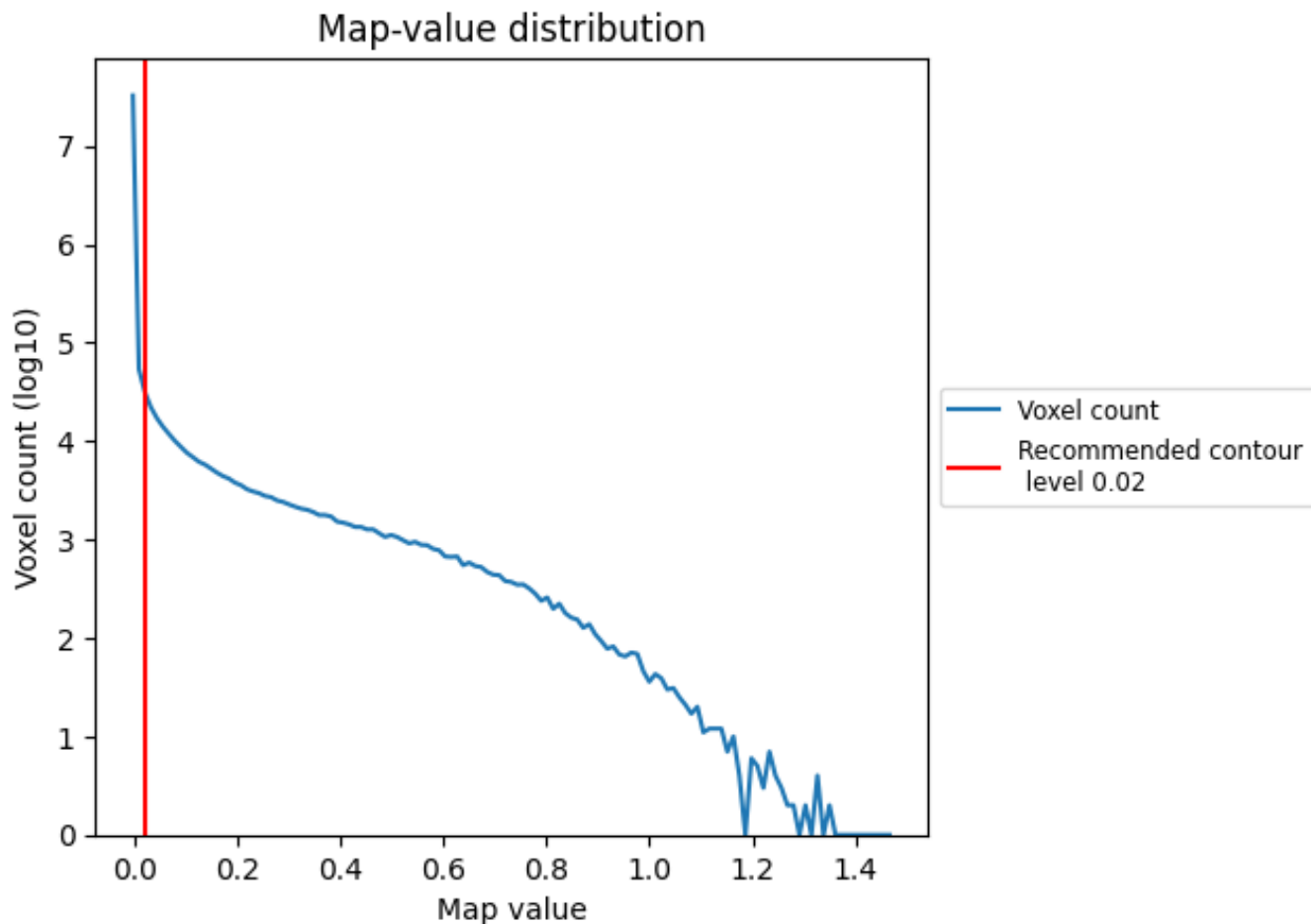
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

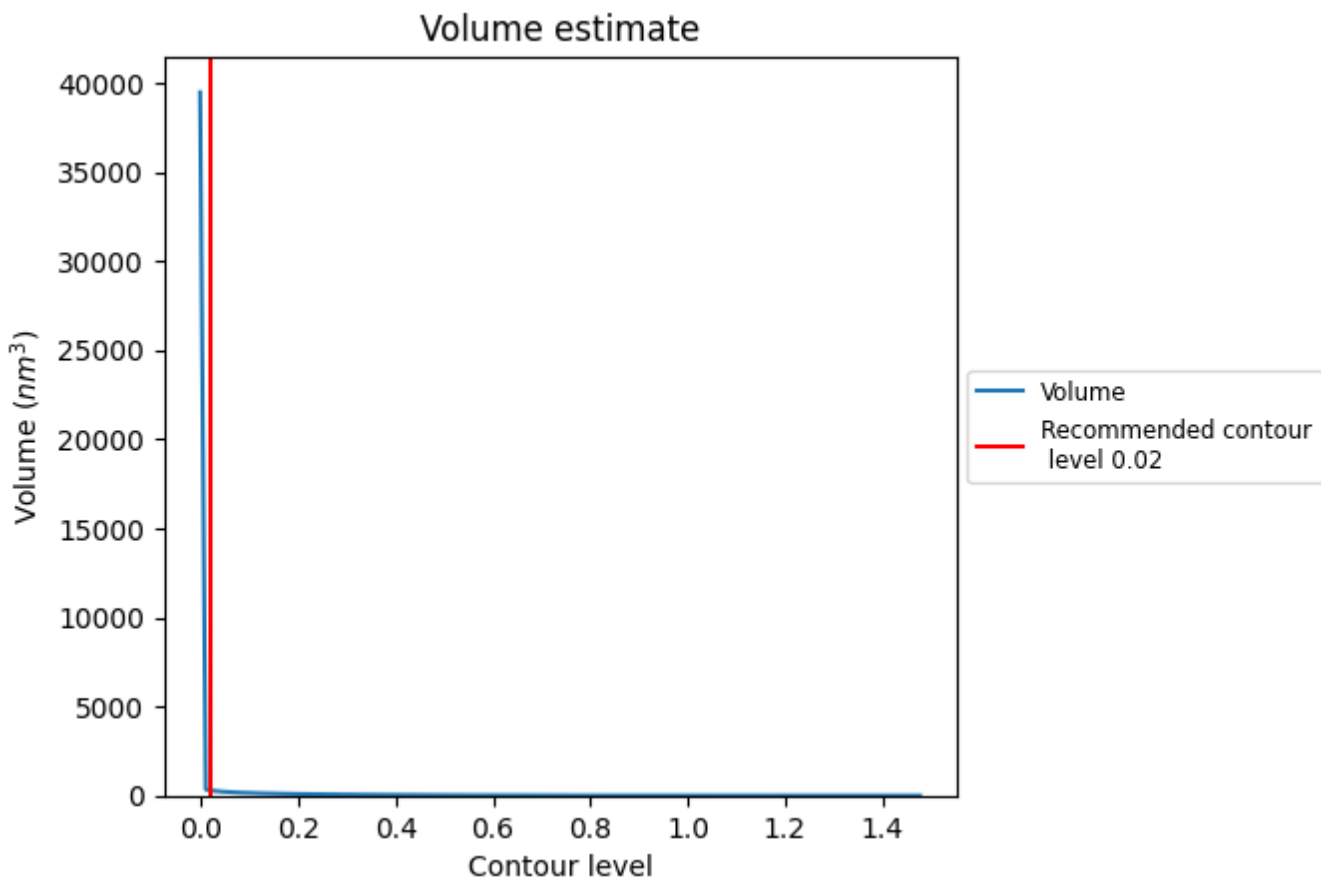
This section contains the results of statistical analysis of the map.

### 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](#)

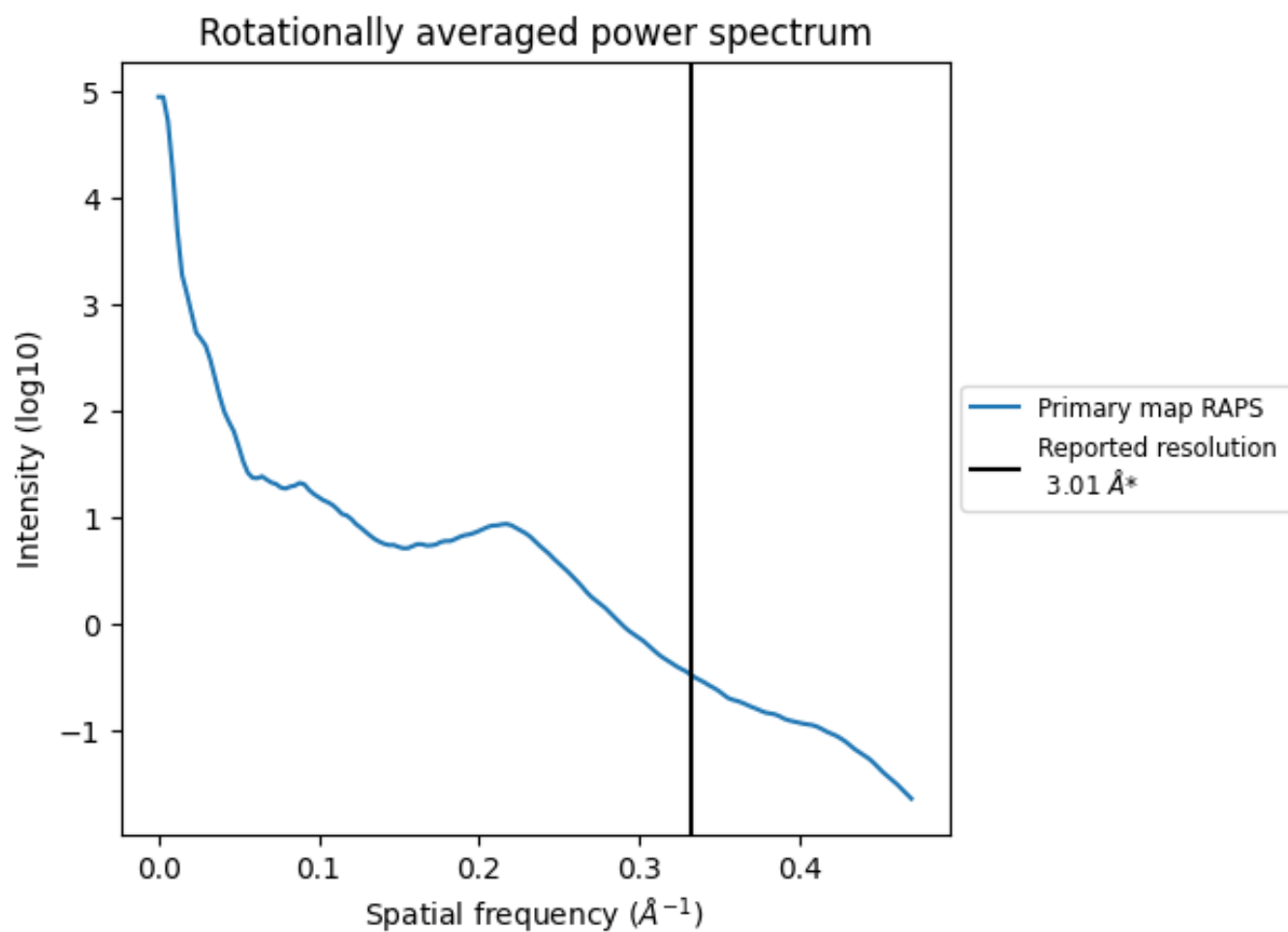


The volume at the recommended contour level is 290 nm<sup>3</sup>; this corresponds to an approximate mass of 262 kDa.

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](#)

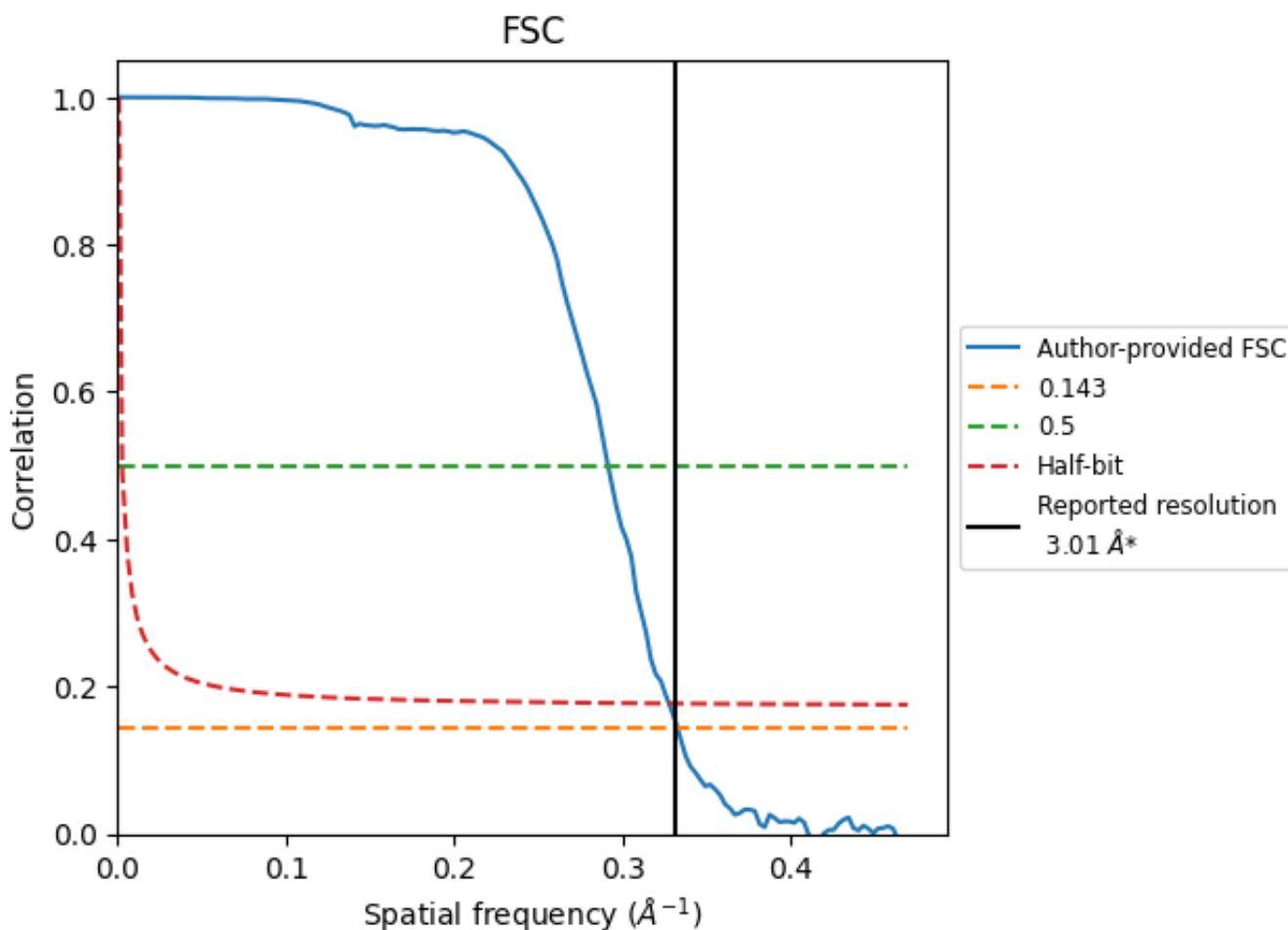


\*Reported resolution corresponds to spatial frequency of  $0.332 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.332 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

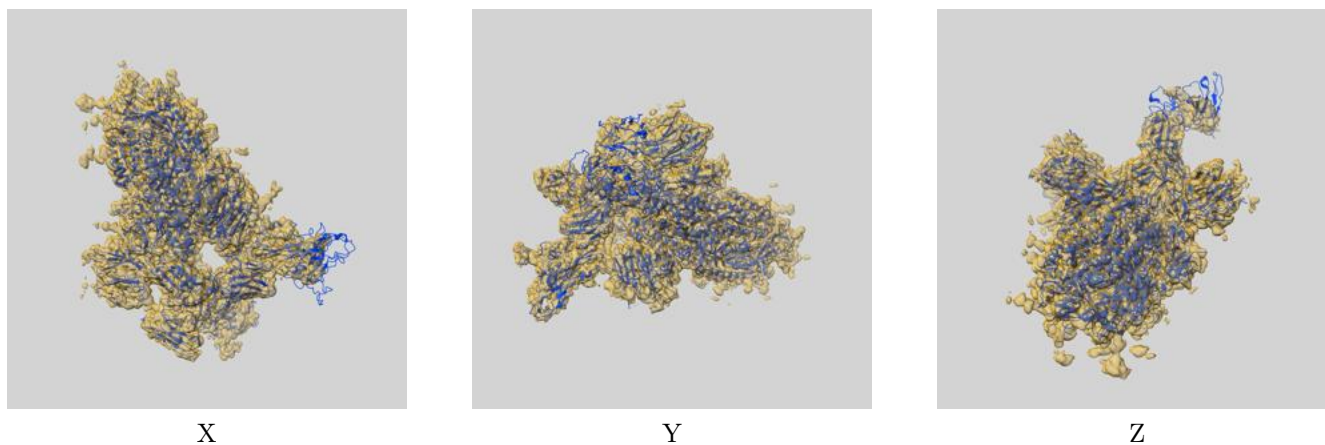
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.00	3.43	3.05
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

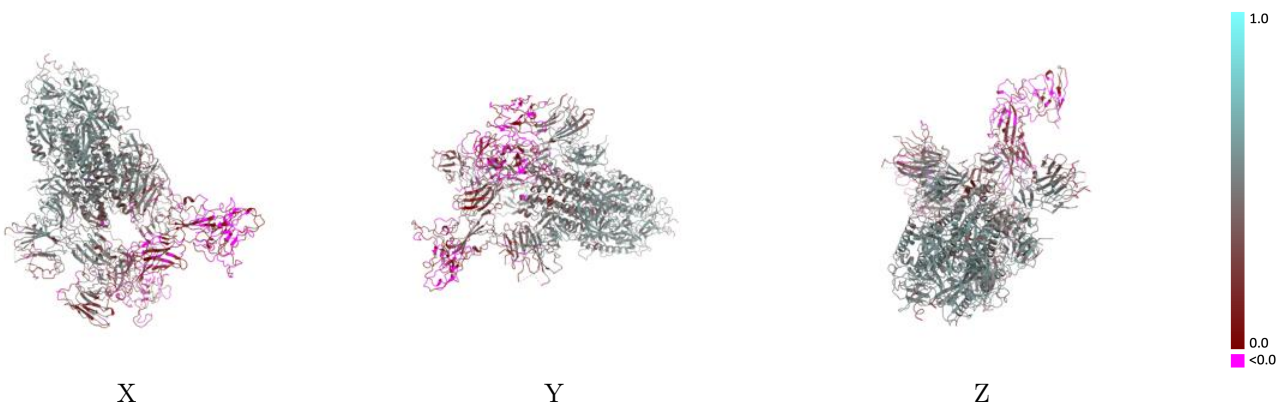
This section contains information regarding the fit between EMDB map EMD-32503 and PDB model 7WHK. Per-residue inclusion information can be found in section 3 on page 15.

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



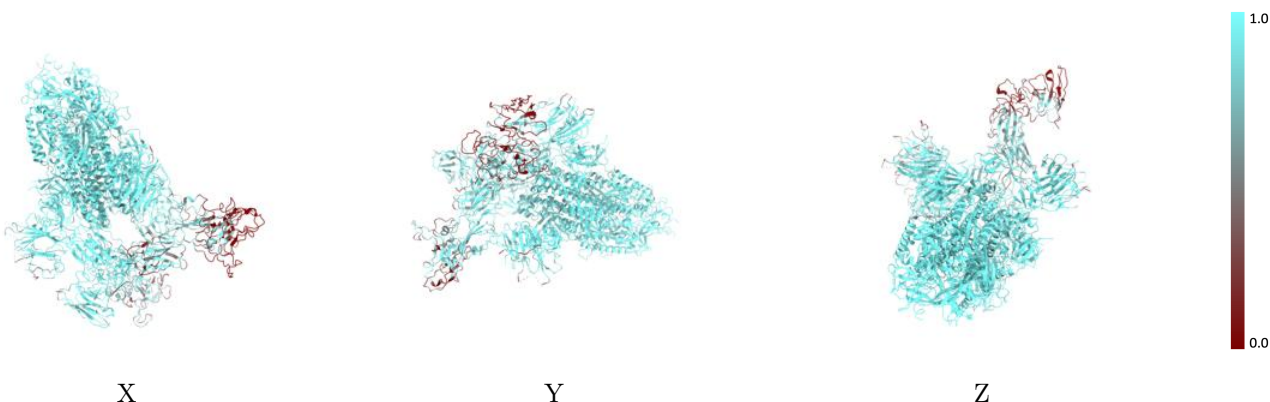
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



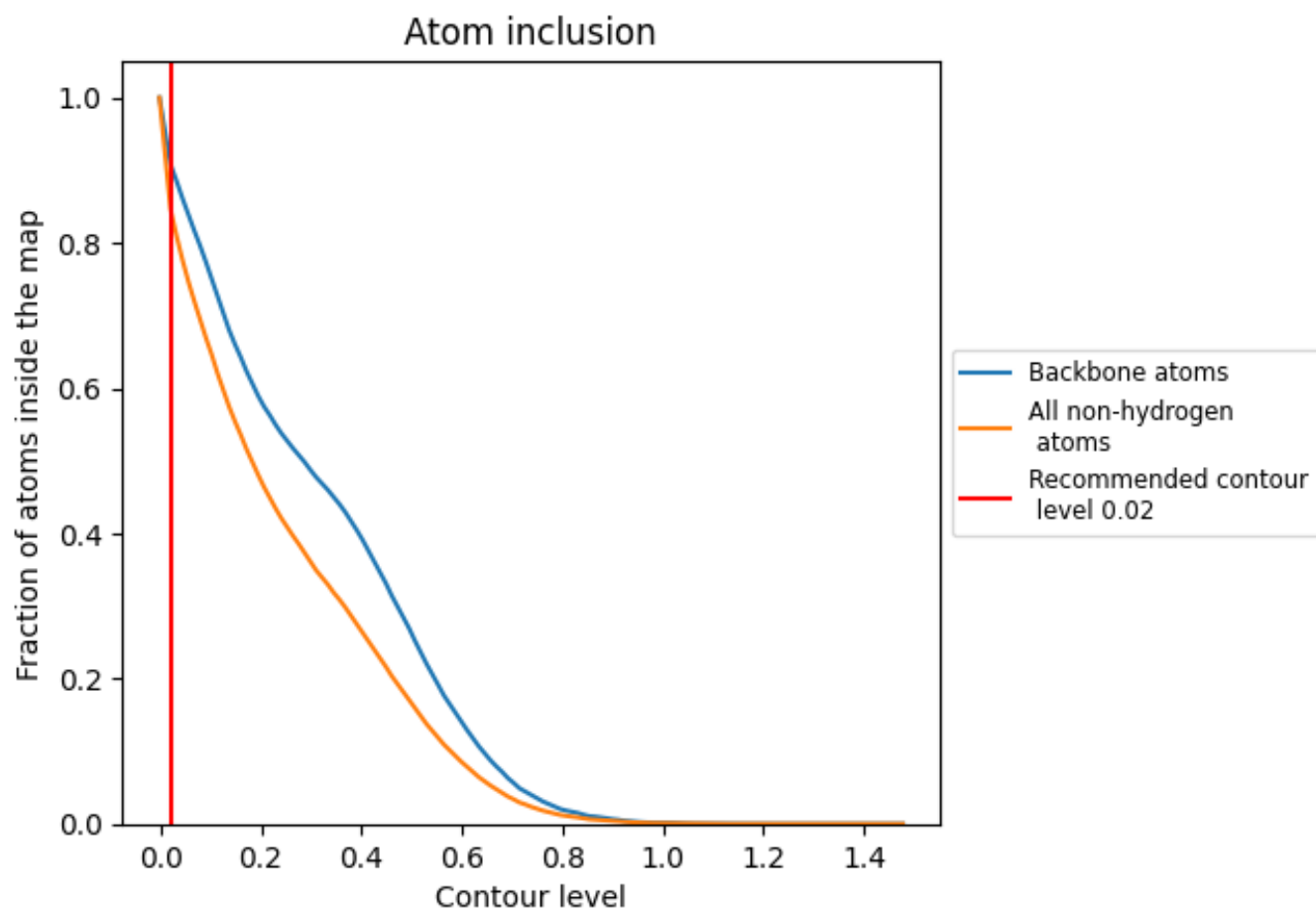
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8476	 0.3700
A	 0.8989	 0.4180
B	 0.9389	 0.4500
C	 0.8356	 0.3740
D	 0.5619	 0.0460
E	 0.8461	 0.2780
F	 0.2870	 0.0390
G	 0.5718	 0.0690
H	 0.7793	 0.2280

