WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 03:45 PM JST

PDB ID	:	7WLY
EMDB ID	:	EMD-32594
Title	:	Cryo-EM structure of the Omicron S in complex with 35B5 Fab(1 down- and 2 up RBDs)
Authors	:	Wang, X.; Zhu, Y.
Deposited on	:	2022-01-14
Resolution	:	3.40 Å(reported)

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 3.40 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		1.1%

Worse — *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
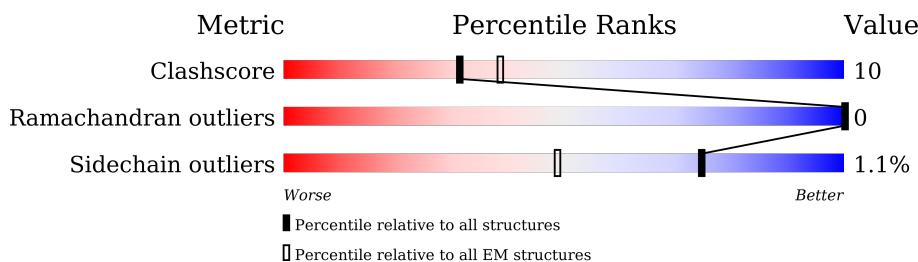
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1285	· 61% 20% · 18%
1	B	1285	12% 63% 18% 19%
1	C	1285	10% 63% 20% 18%
2	P	237	48% 43% 10% 46%
2	Y	237	38% 45% 8% 46%
3	O	219	46% 39% 11% 49%
3	X	219	39% 41% 10% 49%
4	D	2	50% 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	2	50% ▬▬▬▬▬▬ 100%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 28550 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1051	Total	C	N	O	S	0	0
			8196	5255	1356	1548	37		
1	B	1042	Total	C	N	O	S	0	0
			8090	5187	1346	1521	36		
1	C	1058	Total	C	N	O	S	0	0
			8225	5266	1369	1552	38		

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	142	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	212	ILE	LEU	variant	UNP P0DTC2
A	213B	GLU	-	insertion	UNP P0DTC2
A	213C	PRO	-	insertion	UNP P0DTC2
A	214C	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

Continued on next page...

Continued from previous page...

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	engineered mutation	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
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	142	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	212	ILE	LEU	variant	UNP P0DTC2
B	213B	GLU	-	insertion	UNP P0DTC2
B	213C	PRO	-	insertion	UNP P0DTC2
B	214C	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

Continued on next page...

Continued from previous page...

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	engineered mutation	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

Continued on next page...

Continued from previous page...

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	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
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	142	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	212	ILE	LEU	variant	UNP P0DTC2
C	213B	GLU	-	insertion	UNP P0DTC2
C	213C	PRO	-	insertion	UNP P0DTC2
C	214C	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

Continued on next page...

Continued from previous page...

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	engineered mutation	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

Continued from previous page...

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	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2

Continued from previous page...

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

- Molecule 2 is a protein called Heavy chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	127	Total	C	N	O	S	0	0
			962	600	171	185	6		
2	Y	127	Total	C	N	O	S	0	0
			967	605	171	185	6		

- Molecule 3 is a protein called Light chain of 35B5 Fab.

| Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	111	Total	C	N	O	S	0	0
			838	529	139	167	3		
3	X	111	Total	C	N	O	S	0	0
			838	529	139	167	3		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	
5	C	1	Total	C	N	O	0
			126	72	9	45	

3   Residue-property plots ⓘ

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

- Molecule 1: Spike glycoprotein

• Molecule 1: Spike glycoprotein

Chain B:

12%

63% 18% 19%

• Molecule 1: Spike glycoprotein

Chain C:

10%

63%　　　　20%　　　　18%

• Molecule 2: Heavy chain of 35B5 Fab

Chain P:

• Molecule 2: Heavy chain of 35B5 Fab

Chain Y:

• Molecule 3: Light chain of 35B5 Fab

Chain O:

D1 I2 V3 M4 T5 Q6 S7 P8 L9 S10 L11 P12 V13 T14 P15 G16 E17 P18 A19 S20 I21 S22 C23 R24 S25 S26 Q27 S28 L29 L30 H31 S32 N33 G34 Y35 N36 Y37 L38 D39 W40 Y41 L42 Q43 K44 P45 G46 Q47 S48 P49 Q50 L51 L52 I53 Y54 L55 G56 S57 N58 R59 A60

S61 G62 V63 P64 D65 R66 F67 S68 G69 S70 G71 S72 G73 T74 D75 F76 T77 L78 K79 I80 S81 R82 V83 E84 A85 E86 D87 V88 G89 V90 Y91 Y92 C93 M94 Q95 A96 L97 P100 F101 T102 F103 G104 P105 G106 T107 K108 V109 D110 I111 LYS ARG THR VAL ALA ALA PRO SER VAL PHE

ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER

SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

• Molecule 3: Light chain of 35B5 Fab

Chain X:

39%

41%   10%   49%

D1 I2 V3 Q6 S7 P8 L9 S10 L11 P12 V13 T14 P15 G16 E17 P18 A19 S20 I21 S22 C23 R24 S25 S26 Q27 S28 L29 L30 H31 S32 N33 G34 Y35 N36 Y37 L38 L42 Q43 K44 P45 G46 Q47 S48 P49 Q50 L51 L52 I53 Y54 L55 G56 S57 N58 R59 A60 S61 G62 V63

P64 D65 R66 F67 S68 G69 S70 G71 S72 G73 T74 D75 F76 T77 L78 K79 I80 S81 R82 V83 E84 A85 E86 D87 V88 G89 V90 Y91 Y92 C93 M94 Q95 A96 L97 Q98 T99 P100 F101 T102 F103 G104 P105 K108 V109 D110 I111 LYS ARG THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO

PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU

THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

50%

50%   50%

NAG1 NAG2

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

50%

100%

NAG1 NAG2

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91167	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 $(e^-/\text{Å}^2)$	64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.086	Depositor
Minimum map value	-0.499	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	391.40402, 391.40402, 391.40402	wwPDB
Map dimensions	386, 386, 386	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.38	0/8391	0.50	1/11427 (0.0%)
1	B	0.41	0/8282	0.52	0/11277
1	C	0.43	0/8420	0.53	0/11463
2	P	0.30	0/982	0.46	0/1327
2	Y	0.28	0/987	0.47	0/1334
3	O	0.28	0/859	0.44	0/1171
3	X	0.27	0/859	0.45	0/1171
All	All	0.39	0/28780	0.51	1/39170 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ALA	N-CA-CB	-5.49	102.42	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8196	0	7976	181	0
1	B	8090	0	7830	152	0
1	C	8225	0	7956	176	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	962	0	916	17	0
2	Y	967	0	932	13	0
3	O	838	0	805	13	0
3	X	838	0	805	13	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	126	0	117	1	0
5	B	126	0	117	1	0
5	C	126	0	117	1	0
All	All	28550	0	27621	541	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ASN:HD21	2:Y:59:GLY:HA2	1.65	0.62
1:A:48:LEU:HD12	1:A:48:LEU:N	2.14	0.61
1:C:401:VAL:HG11	1:C:451:TYR:CZ	2.36	0.61
1:A:559:PHE:HD2	1:A:584:ILE:HG12	1.65	0.60
1:C:368:LEU:HA	1:C:371:LEU:HD12	1.84	0.60
1:A:393:THR:HB	1:A:522:ALA:HA	1.83	0.60
1:A:1081:ILE:O	1:A:1088:HIS:HB2	2.01	0.60
1:C:822:LEU:HD12	1:C:823:PHE:N	2.16	0.60
1:B:916:LEU:C	1:B:916:LEU:HD23	2.23	0.59
1:A:625:HIS:CD2	1:A:632:THR:HA	2.38	0.59
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.84	0.59
1:C:214(C):GLU:OE1	1:C:264:ALA:HB3	2.05	0.57
1:A:189:LEU:HB2	1:A:208:THR:HB	1.87	0.57
1:A:792:PRO:HG2	1:B:707:TYR:HB3	1.87	0.57
3:O:15:PRO:HA	3:O:83:VAL:HG13	1.87	0.57
1:A:912:THR:O	1:A:915:VAL:HG12	2.04	0.57
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.86	0.57
1:C:118:LEU:O	1:C:128:ILE:HA	2.05	0.57
1:B:267:VAL:HG23	1:B:267:VAL:O	2.05	0.57
1:A:1095:PHE:HE1	1:A:1115:ILE:HD12	1.70	0.56
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.86	0.56
1:B:1009:THR:HA	1:B:1012:LEU:HD12	1.87	0.56
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.88	0.56
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.88	0.56
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.86	0.55
1:B:401:VAL:HG11	1:B:451:TYR:CE2	2.41	0.55
1:C:672:ALA:HA	1:C:694:ALA:HA	1.88	0.55
1:A:671:CYS:SG	1:A:697:MET:HB3	2.46	0.55
1:A:586:ASP:OD1	1:A:587:ILE:N	2.38	0.55
1:A:557:LYS:HD2	1:C:43:PHE:CZ	2.42	0.55
1:A:66:HIS:HA	1:A:264:ALA:HA	1.89	0.54
3:X:15:PRO:HA	3:X:83:VAL:HG13	1.90	0.54
1:A:48:LEU:N	1:A:48:LEU:CD1	2.69	0.54
1:B:1029:MET:O	1:B:1033:VAL:HB	2.08	0.54
1:B:176:LEU:HD22	1:B:190:ARG:HD3	1.89	0.54
1:C:176:LEU:HD21	1:C:192:PHE:HZ	1.73	0.54
1:C:852:ALA:O	1:C:856:LYS:HD3	2.08	0.54
1:A:476:GLY:HA3	1:A:487:ASN:ND2	2.22	0.54
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.87	0.54
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.90	0.54
1:C:206:LYS:HB2	1:C:223:LEU:HG	1.89	0.54
1:C:101:ILE:HA	1:C:242:LEU:HA	1.90	0.54
1:C:676:THR:HG22	1:C:690:GLN:HE22	1.73	0.54
1:B:450:ASN:HB3	2:P:57:THR:HG23	1.90	0.54
1:C:360:ASN:H	1:C:523:THR:HB	1.73	0.54
1:C:537:LYS:O	1:C:539:VAL:HG13	2.07	0.54
1:C:333:THR:HB	1:C:362:VAL:HG21	1.91	0.54
2:P:64:VAL:HG12	2:P:64:VAL:O	2.08	0.53
1:A:120:VAL:HG12	1:A:121:ASN:N	2.22	0.53
1:A:485:GLY:N	1:A:488:CYS:HB2	2.23	0.53
1:A:1126:CYS:HB2	1:A:1132:ILE:HG12	1.90	0.53
1:C:66:HIS:HD2	1:C:78:ARG:HH22	1.55	0.53
2:P:100:VAL:HG23	2:P:116:GLY:O	2.08	0.53
1:A:1082:CYS:N	1:A:1132:ILE:HD11	2.22	0.53
1:A:100:ILE:O	1:A:242:LEU:HD12	2.08	0.53
1:B:911:VAL:CG1	1:B:915:VAL:HG21	2.39	0.53
1:A:328:ARG:HD3	1:A:531:THR:O	2.09	0.53
1:C:33:THR:O	1:C:34:ARG:HD2	2.09	0.53
1:A:800:PHE:HD2	1:A:927:PHE:HD2	1.55	0.53
3:X:95:GLN:HE21	3:X:101:PHE:HA	1.73	0.53
1:A:555:SER:HB3	1:A:584:ILE:HG22	1.90	0.53
1:A:53:ASP:HB2	1:A:55:PHE:HE2	1.74	0.53
1:A:656:VAL:HG12	1:A:658:ASN:H	1.73	0.53
1:B:34:ARG:NH2	1:B:219:GLY:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HB	1:B:395:VAL:HB	1.91	0.53
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.90	0.53
2:Y:29:PHE:CD2	2:Y:74:ASN:HA	2.43	0.53
1:A:563:GLN:HG3	1:C:43:PHE:HB2	1.91	0.53
4:E:1:NAG:H61	4:E:2:NAG:O7	2.09	0.53
1:A:950:ASP:OD1	1:A:951:VAL:N	2.42	0.53
1:A:1048:HIS:NE2	1:A:1050:MET:O	2.42	0.53
1:B:1097:SER:HB3	1:B:1102:TRP:CE3	2.44	0.53
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.43	0.52
1:C:65:PHE:HE1	1:C:84:LEU:HD21	1.74	0.52
1:C:142:ASP:HA	1:C:158:ARG:CZ	2.39	0.52
2:Y:91:THR:O	2:Y:91:THR:HG23	2.09	0.52
1:B:105:ILE:HG23	1:B:239:GLN:HB3	1.91	0.52
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.43	0.52
1:B:917:TYR:HD2	1:C:1089:PHE:CE1	2.27	0.52
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.45	0.52
1:B:884:SER:HB2	1:B:894:LEU:H	1.75	0.52
1:C:989:ALA:O	1:C:993:ILE:HG12	2.10	0.52
1:C:703:ASN:OD1	1:C:704:SER:N	2.42	0.52
1:A:770:ILE:O	1:A:774:GLN:HG2	2.10	0.52
1:C:651:ILE:HG22	1:C:652:GLY:N	2.25	0.52
1:A:569:ILE:HD12	1:A:569:ILE:H	1.73	0.52
1:A:1086:LYS:HA	1:A:1125:ASN:HA	1.92	0.52
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.45	0.51
1:A:989:ALA:O	1:A:993:ILE:HG12	2.10	0.51
1:B:770:ILE:O	1:B:774:GLN:HG2	2.11	0.51
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.92	0.51
1:A:192:PHE:HA	1:A:204:TYR:O	2.10	0.51
1:A:455:LEU:H	1:A:493:ARG:NH2	2.09	0.51
1:B:364:ASP:OD1	1:B:366:SER:OG	2.27	0.51
1:B:917:TYR:HD2	1:C:1089:PHE:HE1	1.58	0.51
1:B:1104:VAL:O	1:B:1104:VAL:HG13	2.10	0.51
1:C:242:LEU:HD23	1:C:242:LEU:H	1.74	0.51
1:C:722:VAL:O	1:C:934:ILE:HD11	2.11	0.51
1:A:625:HIS:CE1	1:A:632:THR:HG23	2.45	0.51
1:A:993:ILE:O	1:A:997:ILE:HG12	2.10	0.51
1:C:589:PRO:HB2	1:C:592:PHE:CE1	2.45	0.51
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.75	0.51
1:C:901:GLN:O	1:C:905:ARG:HG2	2.10	0.51
1:A:327:VAL:H	1:A:531:THR:HG22	1.75	0.51
1:A:676:THR:HA	1:A:690:GLN:HA	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HA	1:C:538:CYS:HB3	1.93	0.51
1:C:977:LEU:HD12	1:C:993:ILE:HD12	1.92	0.51
2:P:40:ALA:HB3	2:P:43:LYS:HB2	1.92	0.51
1:C:767:LEU:HD23	1:C:770:ILE:HD12	1.92	0.51
2:Y:39:GLN:HE21	2:Y:45:LEU:HD23	1.76	0.51
1:B:794:ILE:C	1:B:795:LYS:HD2	2.31	0.50
3:X:6:GLN:NE2	3:X:93:CYS:SG	2.85	0.50
1:B:92:PHE:CZ	1:B:265:TYR:HB2	2.46	0.50
2:P:22:CYS:HB2	2:P:36:TRP:CZ2	2.47	0.50
1:A:316:SER:OG	1:A:317:ASN:N	2.44	0.50
1:A:663:ASP:N	1:A:663:ASP:OD1	2.44	0.50
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.44	0.50
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.93	0.50
1:C:1097:SER:HB3	1:C:1102:TRP:CE2	2.46	0.50
3:X:6:GLN:HE22	3:X:104:GLY:HA3	1.77	0.50
1:A:216:LEU:HD12	1:A:216:LEU:H	1.76	0.50
1:C:134:GLN:HB3	1:C:161:SER:O	2.12	0.50
2:Y:67:ARG:HA	2:Y:84:ARG:NH1	2.27	0.50
1:A:100:ILE:HD13	1:A:263:ALA:HB3	1.92	0.50
1:B:121:ASN:HA	1:B:126:VAL:HG12	1.92	0.50
1:C:642:VAL:O	1:C:642:VAL:HG13	2.12	0.50
2:Y:64:VAL:HG12	2:Y:64:VAL:O	2.12	0.50
3:X:45:PRO:HD3	3:X:89:GLY:HA2	1.94	0.50
1:A:711:SER:HA	1:A:1075:PHE:O	2.11	0.50
1:C:873:TYR:O	1:C:877:LEU:HG	2.12	0.50
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.94	0.50
1:A:665:PRO:HA	1:A:671:CYS:HB3	1.93	0.50
1:B:1106:GLN:HB2	1:B:1109:PHE:O	2.12	0.50
3:O:38:LEU:HD21	3:O:93:CYS:HB2	1.94	0.50
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.47	0.49
1:B:646:ARG:HD3	1:B:668:ALA:HB1	1.94	0.49
1:A:317:ASN:HD22	1:A:319:ARG:NH1	2.09	0.49
1:B:615:VAL:HG12	1:B:617:CYS:H	1.77	0.49
1:A:1106:GLN:HE21	1:A:1109:PHE:HB3	1.77	0.49
1:A:1104:VAL:HG12	1:A:1115:ILE:HD13	1.94	0.49
1:A:553:THR:HB	1:A:586:ASP:HB3	1.95	0.49
1:A:616:ASN:OD1	1:A:617:CYS:N	2.41	0.49
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.95	0.49
1:C:105:ILE:HG12	1:C:241:LEU:HD21	1.95	0.49
1:C:541:PHE:CZ	1:C:587:ILE:HD13	2.47	0.49
1:C:543:PHE:HD2	1:C:576:VAL:HG11	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:879:ALA:O	1:C:883:THR:HG22	2.12	0.49
1:A:340:GLU:O	1:A:344:ALA:HB2	2.13	0.49
1:C:809:PRO:HA	1:C:814:LYS:HE3	1.95	0.49
1:B:33:THR:O	1:B:34:ARG:HD2	2.13	0.49
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.94	0.49
2:P:91:THR:HG22	2:P:128:VAL:H	1.76	0.49
1:A:927:PHE:CZ	1:A:931:ILE:HD11	2.48	0.49
1:C:393:THR:H	1:C:517:LEU:HA	1.78	0.49
1:A:619:GLU:CD	1:A:619:GLU:H	2.17	0.48
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.95	0.48
1:A:758:SER:OG	1:A:761:THR:OG1	2.30	0.48
1:A:833:PHE:HD1	1:A:834:ILE:HG13	1.77	0.48
1:B:607:GLN:CD	1:B:692:ILE:HG13	2.33	0.48
1:B:993:ILE:O	1:B:997:ILE:HG12	2.12	0.48
1:C:329:PHE:CD1	1:C:330:PRO:HD2	2.47	0.48
1:C:516:GLU:N	1:C:516:GLU:CD	2.67	0.48
1:C:598:ILE:HG12	1:C:666:ILE:HD11	1.93	0.48
1:C:961:THR:O	1:C:965:GLN:HG2	2.12	0.48
1:B:200:TYR:CE1	1:B:230:PRO:HB3	2.49	0.48
1:B:911:VAL:HG12	1:B:915:VAL:HG21	1.95	0.48
1:C:766:ALA:O	1:C:770:ILE:HG13	2.14	0.48
1:A:428:ASP:OD1	1:A:428:ASP:N	2.44	0.48
1:B:421:TYR:CD2	1:B:457:ARG:HB3	2.48	0.48
1:A:702:GLU:HG2	1:C:790:LYS:NZ	2.29	0.48
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.95	0.48
1:B:644:GLN:OE1	1:B:649:CYS:HB3	2.13	0.48
1:B:726:ILE:HG23	1:B:1061:VAL:HG12	1.95	0.48
1:C:344:ALA:O	1:C:509:ARG:NH1	2.41	0.48
1:A:159:VAL:HG13	1:A:160:TYR:N	2.28	0.48
1:A:421:TYR:CE1	1:A:457:ARG:HB3	2.49	0.48
1:B:403:ARG:NH2	1:B:406:GLU:OE2	2.46	0.48
1:B:442:ASP:OD1	1:B:451:TYR:OH	2.31	0.48
1:C:134:GLN:O	1:C:161:SER:N	2.45	0.48
1:C:97:LYS:HZ3	1:C:185:ASN:N	2.11	0.48
1:C:984:LEU:HB3	1:C:988:GLU:HG2	1.95	0.48
1:B:326:ILE:HD11	1:B:534:VAL:HG13	1.96	0.48
1:B:559:PHE:CZ	1:B:575:ALA:HB3	2.49	0.48
1:B:712:ILE:O	1:B:1075:PHE:N	2.47	0.48
3:O:44:LYS:H	3:O:50:GLN:HE22	1.60	0.48
1:A:540:ASN:HA	1:A:549:THR:HA	1.96	0.48
1:B:126:VAL:HG21	1:B:175:PHE:CE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:HB2	1:C:117:LEU:HD21	1.95	0.48
1:C:619:GLU:N	1:C:619:GLU:OE1	2.47	0.48
1:C:988:GLU:HG2	1:C:989:ALA:N	2.28	0.48
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.77	0.48
1:A:888:PHE:HA	1:A:892:PRO:O	2.14	0.48
1:B:37:TYR:HB2	1:B:204:TYR:CD2	2.48	0.48
1:B:197:ILE:HG22	1:B:198:ASP:OD2	2.14	0.48
1:C:543:PHE:CD2	1:C:576:VAL:HG11	2.48	0.48
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.95	0.47
1:A:44:ARG:HB3	1:B:567:ARG:HB3	1.95	0.47
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.49	0.47
1:C:949:GLN:HG3	1:C:953:ASN:ND2	2.29	0.47
2:Y:100:VAL:HG12	2:Y:116:GLY:HA3	1.95	0.47
1:C:309:GLU:O	1:C:313:TYR:OH	2.28	0.47
1:C:888:PHE:HB3	1:C:893:ALA:HA	1.96	0.47
1:C:421:TYR:CD2	1:C:457:ARG:HB3	2.48	0.47
1:B:287:ASP:OD1	1:B:288:ALA:N	2.47	0.47
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.50	0.47
1:C:453:TYR:HE2	1:C:455:LEU:HD13	1.79	0.47
1:C:1141:LEU:HG	1:C:1145:LEU:HD11	1.95	0.47
2:P:64:VAL:HG11	2:P:68:PHE:CD2	2.49	0.47
1:A:1101:HIS:ND1	5:A:1309:NAG:H5	2.30	0.47
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.97	0.47
1:B:763:LEU:HD12	1:B:1008:VAL:HG11	1.95	0.47
1:A:174:PRO:HG2	1:A:177:MET:SD	2.55	0.47
1:A:599:THR:HG23	1:A:599:THR:O	2.14	0.47
1:A:927:PHE:CE1	1:A:931:ILE:HD11	2.49	0.47
1:B:1105:THR:HG21	1:B:1110:TYR:CE1	2.50	0.47
3:X:15:PRO:HD3	3:X:111:ILE:HD12	1.97	0.47
1:B:538:CYS:HB3	1:B:549:THR:HG22	1.97	0.47
1:C:316:SER:O	1:C:595:VAL:HB	2.15	0.47
1:C:1087:ALA:O	1:C:1088:HIS:ND1	2.48	0.47
2:P:60:TYR:O	2:P:65:LYS:HE3	2.15	0.47
3:O:95:GLN:NE2	3:O:100:PRO:O	2.48	0.47
1:A:541:PHE:CD1	1:A:543:PHE:HD2	2.33	0.47
1:B:371:LEU:H	1:B:371:LEU:HD22	1.80	0.47
2:P:11:LEU:HA	2:P:127:THR:O	2.15	0.47
1:A:86:PHE:H	1:A:237:ARG:HA	1.80	0.46
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.50	0.46
1:C:324:GLU:HB2	1:C:539:VAL:HG12	1.96	0.46
1:C:401:VAL:HG11	1:C:451:TYR:CE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:VAL:O	1:B:1128:VAL:HG12	2.15	0.46
1:C:220:PHE:HZ	1:C:288:ALA:HB3	1.81	0.46
1:C:822:LEU:HD13	1:C:1056:ALA:HB2	1.97	0.46
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.51	0.46
1:B:559:PHE:HZ	1:B:575:ALA:HB3	1.79	0.46
1:A:38:TYR:OH	1:A:284:THR:HA	2.15	0.46
1:B:322:PRO:HB3	1:B:549:THR:HG21	1.97	0.46
1:B:330:PRO:HA	1:B:580:GLN:HA	1.97	0.46
1:C:1141:LEU:HG	1:C:1145:LEU:CD1	2.45	0.46
3:X:23:CYS:SG	3:X:38:LEU:HD11	2.56	0.46
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.51	0.46
1:A:819:GLU:OE2	1:A:1055:SER:OG	2.28	0.46
1:B:160:TYR:CE1	1:B:162:SER:HA	2.50	0.46
1:B:597:VAL:HB	1:B:608:VAL:CG2	2.45	0.46
1:B:752:LEU:HG	1:B:993:ILE:HD11	1.97	0.46
1:B:1112:PRO:C	1:B:1113:GLN:HG3	2.36	0.46
1:A:328:ARG:NH1	1:A:533:LEU:HD23	2.30	0.46
1:A:901:GLN:O	1:A:905:ARG:HG2	2.16	0.46
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.80	0.46
1:B:1002:GLN:NE2	1:C:1002:GLN:HE22	2.14	0.46
1:B:1043:CYS:HB3	1:B:1048:HIS:CE1	2.51	0.46
1:C:347:PHE:CE2	1:C:509:ARG:HB3	2.50	0.46
1:C:351:TYR:HB2	1:C:454:ARG:NH1	2.31	0.46
3:O:59:ARG:NH1	3:O:67:PHE:O	2.46	0.46
1:A:836:GLN:HE22	1:B:615:VAL:C	2.19	0.46
1:B:802:PHE:HB3	1:B:806:LEU:HD23	1.98	0.46
1:C:340:GLU:HG2	2:Y:104:ARG:HG3	1.97	0.46
1:A:186:PHE:HB3	1:A:210:ILE:O	2.16	0.46
1:A:739:THR:HG23	1:A:740:MET:N	2.31	0.46
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.97	0.46
3:O:45:PRO:HD3	3:O:89:GLY:HA2	1.97	0.46
1:B:650:LEU:HD13	1:B:653:ALA:HB3	1.97	0.46
1:C:941:THR:HG22	1:C:943:SER:H	1.81	0.46
2:P:91:THR:HG22	2:P:127:THR:HA	1.97	0.46
3:X:95:GLN:NE2	3:X:100:PRO:O	2.49	0.46
1:A:344:ALA:HB3	1:A:347:PHE:CE2	2.51	0.45
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.98	0.45
1:A:969:LYS:NZ	1:A:974:SER:HA	2.31	0.45
1:A:1002:GLN:O	1:A:1006:THR:HG22	2.16	0.45
1:C:734:THR:HG22	1:C:860:VAL:HG12	1.98	0.45
1:A:67:VAL:O	1:A:77:LYS:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:HB3	1:A:505:HIS:HB3	1.97	0.45
1:A:58:PHE:CD2	1:A:290:ASP:HB2	2.52	0.45
1:B:736:VAL:HG22	1:B:858:LEU:HD22	1.97	0.45
1:C:196:ASN:OD1	1:C:196:ASN:N	2.48	0.45
1:A:51:THR:HG22	1:A:52:GLN:N	2.31	0.45
1:A:566:GLY:HA2	1:C:43:PHE:HB3	1.99	0.45
1:A:927:PHE:O	1:A:931:ILE:HG13	2.16	0.45
1:B:1061:VAL:HG23	1:B:1061:VAL:O	2.17	0.45
1:C:368:LEU:HD12	1:C:369:TYR:N	2.32	0.45
1:A:44:ARG:HD2	1:A:44:ARG:N	2.31	0.45
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.98	0.45
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.98	0.45
1:B:557:LYS:HG3	1:B:559:PHE:CE1	2.51	0.45
1:B:639:GLY:O	1:B:642:VAL:HG13	2.17	0.45
1:C:497:PHE:CD1	1:C:507:PRO:HG3	2.51	0.45
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.99	0.45
1:C:838:GLY:O	1:C:841:LEU:HG	2.16	0.45
1:A:299:THR:HA	1:A:302:THR:HG22	1.99	0.45
1:A:1049:LEU:HB2	1:A:1065:VAL:O	2.16	0.45
1:B:620:VAL:HG12	1:B:621:PRO:HD3	1.98	0.45
1:C:776:LYS:HE3	1:C:780:GLU:OE1	2.17	0.45
1:A:374:PHE:HD1	1:A:434:ILE:HG21	1.80	0.45
1:B:391:CYS:HA	1:B:524:VAL:O	2.17	0.45
1:C:294:ASP:OD1	1:C:294:ASP:N	2.49	0.45
1:A:727:LEU:HD12	1:A:1062:PHE:HE1	1.82	0.45
1:A:961:THR:O	1:A:965:GLN:HG2	2.16	0.45
1:B:555:SER:OG	1:B:586:ASP:HB2	2.16	0.45
1:B:800:PHE:HD2	1:B:927:PHE:CD1	2.35	0.45
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.17	0.45
1:C:502:GLY:O	1:C:506:GLN:N	2.50	0.45
1:A:86:PHE:N	1:A:236:THR:O	2.50	0.45
1:A:705:VAL:CG1	1:C:883:THR:HG21	2.46	0.45
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.52	0.45
1:A:986:PRO:N	1:A:987:PRO:HD2	2.31	0.45
1:B:636:TYR:O	1:B:651:ILE:HG21	2.16	0.45
2:P:67:ARG:HA	2:P:84:ARG:NH1	2.32	0.45
1:A:197:ILE:HG22	1:A:198:ASP:OD1	2.17	0.44
1:B:328:ARG:HG3	1:B:543:PHE:CE1	2.52	0.44
1:B:560:LEU:HB2	1:B:563:GLN:CD	2.38	0.44
1:C:176:LEU:HD13	1:C:190:ARG:HD3	1.99	0.44
1:C:632:THR:HA	1:C:634:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HG13	1:B:565:PHE:HB2	1.99	0.44
1:B:67:VAL:HG22	1:B:79:PHE:HA	1.98	0.44
1:B:100:ILE:HG23	1:B:243:ALA:O	2.17	0.44
1:B:1101:HIS:HD2	5:B:1308:NAG:H3	1.82	0.44
1:A:909:ILE:HG23	1:A:1036:GLN:HE22	1.82	0.44
1:A:1031:GLU:HA	1:B:1040:VAL:HG22	1.98	0.44
1:A:1094:VAL:HG22	1:C:904:TYR:OH	2.17	0.44
1:B:712:ILE:HG21	1:B:1096:VAL:HG12	2.00	0.44
1:B:822:LEU:O	1:B:826:VAL:HG12	2.17	0.44
1:C:634:ARG:HB3	1:C:634:ARG:NH1	2.32	0.44
2:P:112:ASP:N	2:P:112:ASP:OD1	2.50	0.44
1:A:34:ARG:HH12	1:A:216:LEU:HB3	1.82	0.44
1:B:318:PHE:N	1:B:593:GLY:O	2.50	0.44
1:B:401:VAL:HG11	1:B:451:TYR:CZ	2.52	0.44
1:B:1008:VAL:O	1:B:1012:LEU:HG	2.18	0.44
1:C:126:VAL:O	1:C:171:VAL:HA	2.17	0.44
2:Y:40:ALA:HA	2:Y:92:ALA:CB	2.48	0.44
1:A:201:PHE:N	1:A:229:LEU:O	2.44	0.44
1:B:912:THR:O	1:B:915:VAL:HG22	2.18	0.44
1:B:1082:CYS:HA	1:B:1086:LYS:O	2.17	0.44
1:C:127:VAL:HG13	1:C:127:VAL:O	2.17	0.44
1:C:752:LEU:O	1:C:755:GLN:HG2	2.17	0.44
2:Y:112:ASP:OD1	2:Y:112:ASP:N	2.50	0.44
1:A:896:ILE:HD11	1:A:900:MET:HG3	1.99	0.44
1:B:476:GLY:H	1:B:487:ASN:HB3	1.83	0.44
1:B:800:PHE:HD2	1:B:927:PHE:HD1	1.66	0.44
2:P:39:GLN:HE21	2:P:45:LEU:HD23	1.82	0.44
1:A:485:GLY:H	1:A:488:CYS:HB2	1.82	0.44
1:A:1088:HIS:HB3	1:A:1120:THR:HG21	2.00	0.44
1:B:675:GLN:HB2	1:B:693:ILE:HD11	2.00	0.44
1:B:752:LEU:O	1:B:755:GLN:HG2	2.17	0.44
1:B:904:TYR:OH	1:C:1094:VAL:HB	2.17	0.44
1:A:27:ALA:N	1:A:64:TRP:HB3	2.33	0.44
1:A:41:LYS:HE2	1:A:41:LYS:HB3	1.90	0.44
1:C:1024:LEU:O	1:C:1028:LYS:HG3	2.18	0.44
3:O:6:GLN:HE22	3:O:104:GLY:HA3	1.83	0.44
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.99	0.43
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.50	0.43
1:B:131:CYS:HA	1:B:166:CYS:HA	2.00	0.43
1:C:724:THR:HG23	1:C:934:ILE:HD12	2.00	0.43
3:X:66:ARG:NH2	3:X:87:ASP:OD1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:HA	1:A:432:CYS:HA	1.98	0.43
1:A:1087:ALA:O	1:A:1088:HIS:ND1	2.51	0.43
1:A:128:ILE:O	1:A:169:GLU:HA	2.18	0.43
1:A:419:ALA:HA	1:A:423:TYR:O	2.17	0.43
1:B:796:TYR:HD1	5:C:1304:NAG:HO6	1.66	0.43
1:C:905:ARG:HH11	1:C:1036:GLN:HB2	1.83	0.43
1:C:913:GLN:H	1:C:913:GLN:HG2	1.65	0.43
1:A:445:VAL:HA	1:A:499:PRO:HD2	1.99	0.43
1:A:931:ILE:O	1:A:934:ILE:HG22	2.18	0.43
1:B:242:LEU:HG	1:B:243:ALA:N	2.33	0.43
1:C:726:ILE:HD12	1:C:726:ILE:N	2.34	0.43
3:O:95:GLN:HE21	3:O:101:PHE:HA	1.84	0.43
1:B:36:VAL:HG21	1:B:220:PHE:HE1	1.84	0.43
1:B:994:ASP:O	1:B:998:THR:HG23	2.19	0.43
1:C:642:VAL:HG23	1:C:651:ILE:HD11	2.00	0.43
1:C:838:GLY:HA2	1:C:841:LEU:HG	2.00	0.43
3:X:95:GLN:HG2	3:X:102:THR:H	1.83	0.43
1:A:139:PRO:HG2	1:A:241:LEU:HD22	2.00	0.43
1:B:402:ILE:O	1:B:508:TYR:N	2.50	0.43
3:O:54:TYR:HE1	3:O:60:ALA:HA	1.83	0.43
1:B:102:ARG:H	1:B:242:LEU:HA	1.84	0.43
1:B:244:LEU:O	1:B:245:HIS:CG	2.72	0.43
1:C:741:TYR:HE1	1:C:966:LEU:HD11	1.83	0.43
1:A:120:VAL:CG1	1:A:121:ASN:N	2.80	0.43
1:A:800:PHE:HD2	1:A:927:PHE:CD2	2.35	0.43
1:A:903:ALA:O	1:A:913:GLN:HG2	2.18	0.43
1:C:620:VAL:HB	1:C:621:PRO:HD3	2.00	0.43
1:C:959:LEU:O	1:C:959:LEU:HD23	2.18	0.43
1:A:971:GLY:C	1:A:995:ARG:HH21	2.22	0.43
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.43
1:A:1105:THR:HG22	1:A:1112:PRO:HA	2.00	0.43
1:B:1091:ARG:HB3	1:B:1119:ASN:OD1	2.18	0.43
1:C:927:PHE:O	1:C:931:ILE:HG12	2.19	0.43
3:X:31:HIS:CD2	3:X:32:SER:H	2.37	0.43
1:A:57:PRO:HB3	1:A:273:ARG:NE	2.34	0.43
1:A:705:VAL:HG13	1:C:883:THR:HG21	2.01	0.43
1:B:48:LEU:HD23	1:B:276:LEU:HD21	2.01	0.43
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.54	0.43
1:C:858:LEU:HD12	1:C:858:LEU:N	2.33	0.43
1:C:1029:MET:O	1:C:1034:LEU:HG	2.19	0.43
1:C:1117:THR:HG22	1:C:1140:PRO:HD2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:HB3	1:A:201:PHE:CD2	2.54	0.42
1:B:124:THR:O	1:B:174:PRO:HD3	2.19	0.42
1:B:336:CYS:HA	1:B:337:PRO:HD3	1.90	0.42
1:B:901:GLN:NE2	1:B:905:ARG:HH21	2.16	0.42
1:C:303:LEU:HD12	1:C:308:VAL:HG12	2.01	0.42
1:C:328:ARG:HG2	1:C:579:PRO:HG2	2.00	0.42
1:C:577:ARG:HD3	1:C:582:LEU:HG	2.00	0.42
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.53	0.42
1:A:822:LEU:HD13	1:A:1056:ALA:HB2	2.01	0.42
1:A:833:PHE:CD1	1:A:834:ILE:HG13	2.53	0.42
1:B:1096:VAL:HG21	1:B:1110:TYR:HE1	1.84	0.42
2:P:61:ALA:O	2:P:65:LYS:HG3	2.20	0.42
1:A:567:ARG:HD2	1:C:42:VAL:HG11	2.01	0.42
1:A:627:ASP:OD1	1:A:627:ASP:N	2.52	0.42
1:A:914:ASN:OD1	1:A:915:VAL:N	2.52	0.42
1:C:393:THR:CB	1:C:520:ALA:HB3	2.49	0.42
1:A:1043:CYS:O	1:A:1048:HIS:HD2	2.02	0.42
1:B:384:PRO:HA	1:B:387:LEU:HG	2.01	0.42
1:A:420:ASP:O	1:A:461:LEU:HG	2.20	0.42
1:A:1004:LEU:O	1:A:1008:VAL:HG23	2.19	0.42
1:B:84:LEU:HD13	1:B:267:VAL:HG21	2.01	0.42
1:B:768:THR:O	1:B:772:VAL:HG12	2.20	0.42
1:C:1142:GLN:HA	1:C:1145:LEU:HB2	2.02	0.42
1:A:310:LYS:HG3	1:A:664:ILE:HD11	2.01	0.42
1:A:317:ASN:O	1:A:319:ARG:HG3	2.19	0.42
1:A:556:ASN:ND2	1:C:843:ASP:OD2	2.52	0.42
1:B:101:ILE:HA	1:B:242:LEU:CB	2.50	0.42
1:B:326:ILE:HB	1:B:541:PHE:HA	2.02	0.42
1:B:911:VAL:HG12	1:B:915:VAL:CG2	2.50	0.42
2:P:64:VAL:O	2:P:64:VAL:CG1	2.67	0.42
1:C:568:ASP:CG	1:C:574:ASP:HB2	2.40	0.42
1:C:716:THR:HG22	1:C:1071:GLN:O	2.20	0.42
2:P:62:ASP:N	2:P:62:ASP:OD1	2.52	0.42
3:O:43:GLN:HA	3:O:49:PRO:HA	2.00	0.42
1:A:160:TYR:CG	1:A:161:SER:N	2.88	0.42
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.00	0.42
1:B:818:ILE:O	1:B:822:LEU:HG	2.19	0.42
1:A:738:CYS:O	1:A:742:ILE:HG13	2.20	0.42
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.55	0.42
1:A:874:THR:HG21	1:A:1055:SER:HB3	2.01	0.42
1:A:896:ILE:HD11	1:A:900:MET:CG	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HG12	1:C:128:ILE:HG23	2.02	0.42
1:C:336:CYS:N	1:C:362:VAL:O	2.53	0.42
1:C:976:VAL:HG23	1:C:976:VAL:O	2.19	0.42
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.35	0.42
1:A:122:ASN:HB2	1:A:125:ASN:HB2	2.01	0.42
1:A:442:ASP:OD1	1:A:451:TYR:OH	2.27	0.42
1:A:542:ASN:O	1:A:546:LEU:N	2.53	0.42
1:A:563:GLN:HE21	1:C:43:PHE:HD1	1.68	0.42
1:B:136:CYS:SG	1:B:137:ASN:N	2.93	0.42
1:C:105:ILE:HD11	1:C:118:LEU:HD13	2.02	0.42
1:C:650:LEU:HD23	1:C:650:LEU:H	1.85	0.42
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	2.02	0.42
1:A:1128:VAL:HG13	1:A:1129:VAL:N	2.35	0.41
1:B:854:LYS:HE3	1:B:854:LYS:HB2	1.89	0.41
1:C:85:PRO:HA	1:C:237:ARG:HA	2.03	0.41
1:C:599:THR:HB	1:C:608:VAL:HG12	2.02	0.41
1:A:699:LEU:HD12	1:C:873:TYR:OH	2.20	0.41
1:B:280:ASN:OD1	1:B:284:THR:N	2.52	0.41
1:B:299:THR:OG1	1:B:597:VAL:HG21	2.20	0.41
1:B:727:LEU:HD12	1:B:1062:PHE:HE1	1.85	0.41
1:C:914:ASN:OD1	1:C:914:ASN:N	2.53	0.41
3:O:42:LEU:HD12	3:O:90:VAL:O	2.20	0.41
1:A:295:PRO:HG3	1:A:633:TRP:CD2	2.56	0.41
1:A:398:ASP:O	1:A:511:VAL:HA	2.20	0.41
1:A:854:LYS:HE2	1:A:854:LYS:HB2	1.95	0.41
1:B:294:ASP:N	1:B:294:ASP:OD1	2.53	0.41
1:C:770:ILE:O	1:C:774:GLN:HG2	2.20	0.41
2:Y:29:PHE:HB2	2:Y:77:ASN:CG	2.40	0.41
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.87	0.41
1:B:318:PHE:CE2	1:B:615:VAL:HG21	2.56	0.41
1:C:83:VAL:HB	1:C:237:ARG:NH1	2.35	0.41
1:C:117:LEU:HD12	1:C:117:LEU:C	2.41	0.41
1:C:312:ILE:HA	1:C:597:VAL:O	2.21	0.41
1:C:384:PRO:O	1:C:387:LEU:HG	2.20	0.41
1:C:1049:LEU:HD11	1:C:1067:TYR:HB2	2.01	0.41
1:A:197:ILE:O	1:A:200:TYR:N	2.53	0.41
1:A:321:GLN:NE2	1:A:630:THR:OG1	2.53	0.41
1:A:752:LEU:HD21	1:A:994:ASP:OD1	2.20	0.41
1:B:543:PHE:CD1	1:B:576:VAL:HG11	2.55	0.41
1:C:909:ILE:HG13	1:C:911:VAL:HG22	2.02	0.41
1:A:200:TYR:HA	1:A:230:PRO:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:HD1	1:C:117:LEU:HD11	1.85	0.41
1:C:815:ARG:HB2	1:C:820:ASP:OD1	2.21	0.41
1:C:880:GLY:O	1:C:884:SER:HB3	2.21	0.41
1:A:903:ALA:HB1	1:A:913:GLN:HB3	2.02	0.41
1:B:449:TYR:O	1:B:449:TYR:CD1	2.73	0.41
1:B:535:LYS:HG2	1:B:536:ASN:N	2.35	0.41
1:B:969:LYS:HE3	1:B:974:SER:HA	2.03	0.41
3:O:68:SER:OG	3:O:79:LYS:HB2	2.20	0.41
1:A:122:ASN:N	1:A:125:ASN:O	2.54	0.41
1:A:200:TYR:HB3	1:A:228:ASP:OD2	2.20	0.41
1:B:206:LYS:HE2	1:B:221:SER:OG	2.19	0.41
1:B:230:PRO:HB2	1:C:521:PRO:HG3	2.02	0.41
1:B:901:GLN:O	1:B:905:ARG:HG2	2.21	0.41
1:B:906:PHE:O	1:B:909:ILE:HG12	2.20	0.41
1:A:191:GLU:O	1:A:205:SER:HA	2.21	0.41
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.85	0.41
1:A:911:VAL:CG1	1:A:915:VAL:HG11	2.51	0.41
1:B:86:PHE:HB2	1:B:238:PHE:HD1	1.84	0.41
1:B:244:LEU:HD12	1:B:245:HIS:N	2.36	0.41
1:B:398:ASP:HB2	1:B:512:VAL:HB	2.03	0.41
1:B:557:LYS:HG3	1:B:559:PHE:HE1	1.86	0.41
1:C:121:ASN:HD21	1:C:176:LEU:HB2	1.86	0.41
1:C:214(C):GLU:OE1	1:C:264:ALA:CB	2.69	0.41
1:C:290:ASP:OD2	1:C:291:CYS:N	2.50	0.41
1:C:438:SER:OG	1:C:442:ASP:OD2	2.37	0.41
1:C:537:LYS:C	1:C:551:VAL:HG23	2.41	0.41
1:C:560:LEU:HD23	1:C:562:PHE:HE1	1.85	0.41
1:C:660:TYR:HD2	1:C:695:TYR:CZ	2.39	0.41
1:C:764:LYS:HB3	1:C:764:LYS:HE2	1.86	0.41
1:C:915:VAL:HG11	1:C:1109:PHE:CD2	2.56	0.41
1:C:1135:ASN:ND2	1:C:1136:THR:H	2.18	0.41
3:O:4:MET:HG2	3:O:25:SER:HA	2.03	0.41
3:X:44:LYS:H	3:X:50:GLN:HE22	1.66	0.41
1:A:600:PRO:HG2	1:A:605:SER:HB2	2.03	0.41
1:B:896:ILE:HD11	1:B:900:MET:HG2	2.03	0.41
1:B:984:LEU:N	1:B:984:LEU:HD22	2.36	0.41
1:C:665:PRO:HA	1:C:671:CYS:HB3	2.03	0.41
1:C:834:ILE:HD12	1:C:834:ILE:H	1.85	0.41
1:C:1118:ASP:OD2	1:C:1140:PRO:HG2	2.20	0.41
2:Y:8:GLY:HA3	2:Y:20:LEU:HD23	2.03	0.41
1:A:759:PHE:O	1:A:763:LEU:HG	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:TYR:HB3	1:B:223:LEU:HB3	2.03	0.40
1:C:197:ILE:O	1:C:200:TYR:N	2.54	0.40
1:C:493:ARG:HG2	1:C:494:SER:H	1.86	0.40
1:A:1080:ALA:O	1:A:1132:ILE:HD12	2.21	0.40
1:A:1088:HIS:HB3	1:A:1120:THR:CG2	2.51	0.40
1:B:112:SER:HA	1:B:132:GLU:HB3	2.03	0.40
1:B:1048:HIS:CE1	1:B:1050:MET:O	2.74	0.40
3:X:52:LEU:HD11	3:X:67:PHE:CG	2.56	0.40
1:A:347:PHE:CD1	1:A:399:SER:HB2	2.56	0.40
1:A:630:THR:HB	1:A:631:PRO:HD3	2.02	0.40
1:B:328:ARG:HA	1:B:328:ARG:HD2	1.98	0.40
1:C:121:ASN:ND2	1:C:176:LEU:HB2	2.36	0.40
1:C:287:ASP:OD1	1:C:288:ALA:N	2.54	0.40
1:A:513:LEU:HB3	1:A:515:PHE:CZ	2.57	0.40
1:B:43:PHE:HB3	1:C:565:PHE:O	2.22	0.40
1:B:102:ARG:N	1:B:241:LEU:O	2.50	0.40
1:C:105:ILE:CG1	1:C:241:LEU:HD21	2.51	0.40
1:C:748:GLU:CD	1:C:748:GLU:H	2.25	0.40
1:C:853:GLN:CD	1:C:959:LEU:HD22	2.42	0.40
2:Y:12:VAL:HG11	2:Y:18:LEU:HD11	2.03	0.40
1:A:996:LEU:HA	1:A:996:LEU:HD12	1.72	0.40
1:C:371:LEU:HB2	1:C:374:PHE:HD1	1.86	0.40
1:C:406:GLU:OE2	1:C:418:ILE:CG1	2.69	0.40
1:C:560:LEU:HB2	1:C:563:GLN:HG3	2.03	0.40
2:P:2:VAL:HG12	2:P:27:PHE:HD1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1035/1285 (80%)	959 (93%)	76 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1024/1285 (80%)	937 (92%)	87 (8%)	0	100	100
1	C	1042/1285 (81%)	956 (92%)	86 (8%)	0	100	100
2	P	123/237 (52%)	123 (100%)	0	0	100	100
2	Y	123/237 (52%)	120 (98%)	3 (2%)	0	100	100
3	O	109/219 (50%)	108 (99%)	1 (1%)	0	100	100
3	X	109/219 (50%)	108 (99%)	1 (1%)	0	100	100
All	All	3565/4767 (75%)	3311 (93%)	254 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	910/1116 (82%)	898 (99%)	12 (1%)	69	84
1	B	888/1116 (80%)	877 (99%)	11 (1%)	71	85
1	C	903/1116 (81%)	892 (99%)	11 (1%)	71	85
2	P	98/195 (50%)	98 (100%)	0	100	100
2	Y	100/195 (51%)	100 (100%)	0	100	100
3	O	94/193 (49%)	94 (100%)	0	100	100
3	X	94/193 (49%)	94 (100%)	0	100	100
All	All	3087/4124 (75%)	3053 (99%)	34 (1%)	74	86

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	131	CYS
1	A	169	GLU
1	A	336	CYS
1	A	361	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	408	ARG
1	A	432	CYS
1	A	493	ARG
1	A	671	CYS
1	A	934	ILE
1	A	976	VAL
1	A	1050	MET
1	B	105	ILE
1	B	237	ARG
1	B	244	LEU
1	B	357	ARG
1	B	501	TYR
1	B	617	CYS
1	B	671	CYS
1	B	738	CYS
1	B	888	PHE
1	B	995	ARG
1	B	1049	LEU
1	C	135	PHE
1	C	190	ARG
1	C	501	TYR
1	C	508	TYR
1	C	538	CYS
1	C	559	PHE
1	C	617	CYS
1	C	662	CYS
1	C	749	CYS
1	C	888	PHE
1	C	1105	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	87	ASN
1	A	317	ASN
1	A	321	GLN
1	A	370	ASN
1	A	417	ASN
1	A	625	HIS
1	A	784	GLN
1	A	804	GLN

Continued from previous page...

Mol	Chain	Res	Type
1	A	836	GLN
1	A	1054	GLN
1	A	1058	HIS
1	A	1106	GLN
1	A	1135	ASN
1	B	218	GLN
1	B	239	GLN
1	B	314	GLN
1	B	580	GLN
1	B	779	GLN
1	B	804	GLN
1	B	901	GLN
1	B	913	GLN
1	B	955	ASN
1	B	1002	GLN
1	B	1101	HIS
1	C	360	ASN
1	C	388	ASN
1	C	437	ASN
1	C	450	ASN
1	C	540	ASN
1	C	625	HIS
1	C	690	GLN
1	C	751	ASN
1	C	901	GLN
1	C	935	GLN
1	C	955	ASN
1	C	960	ASN
1	C	965	GLN
1	C	1113	GLN
1	C	1135	ASN
2	P	39	GLN
3	O	31	HIS
3	O	50	GLN
2	Y	13	GLN
2	Y	39	GLN
3	X	31	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides 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	D	1	4,1	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	D	2	4	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	E	2	4	14,14,15	0.25	0	17,19,21	0.71	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	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	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(^{o})	Ideal(^{o})
4	D	2	NAG	C1-O5-C5	2.36	115.39	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
4	E	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
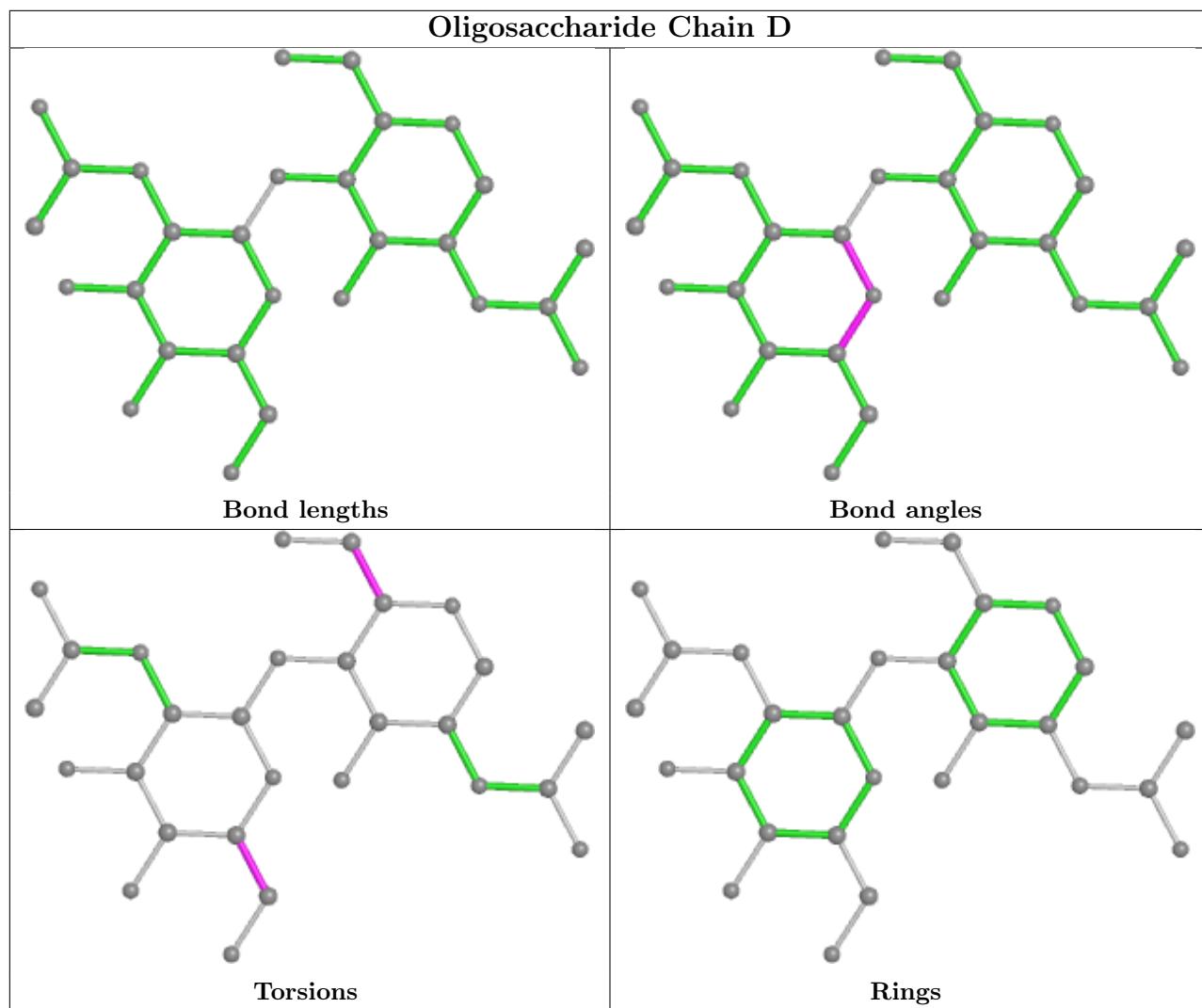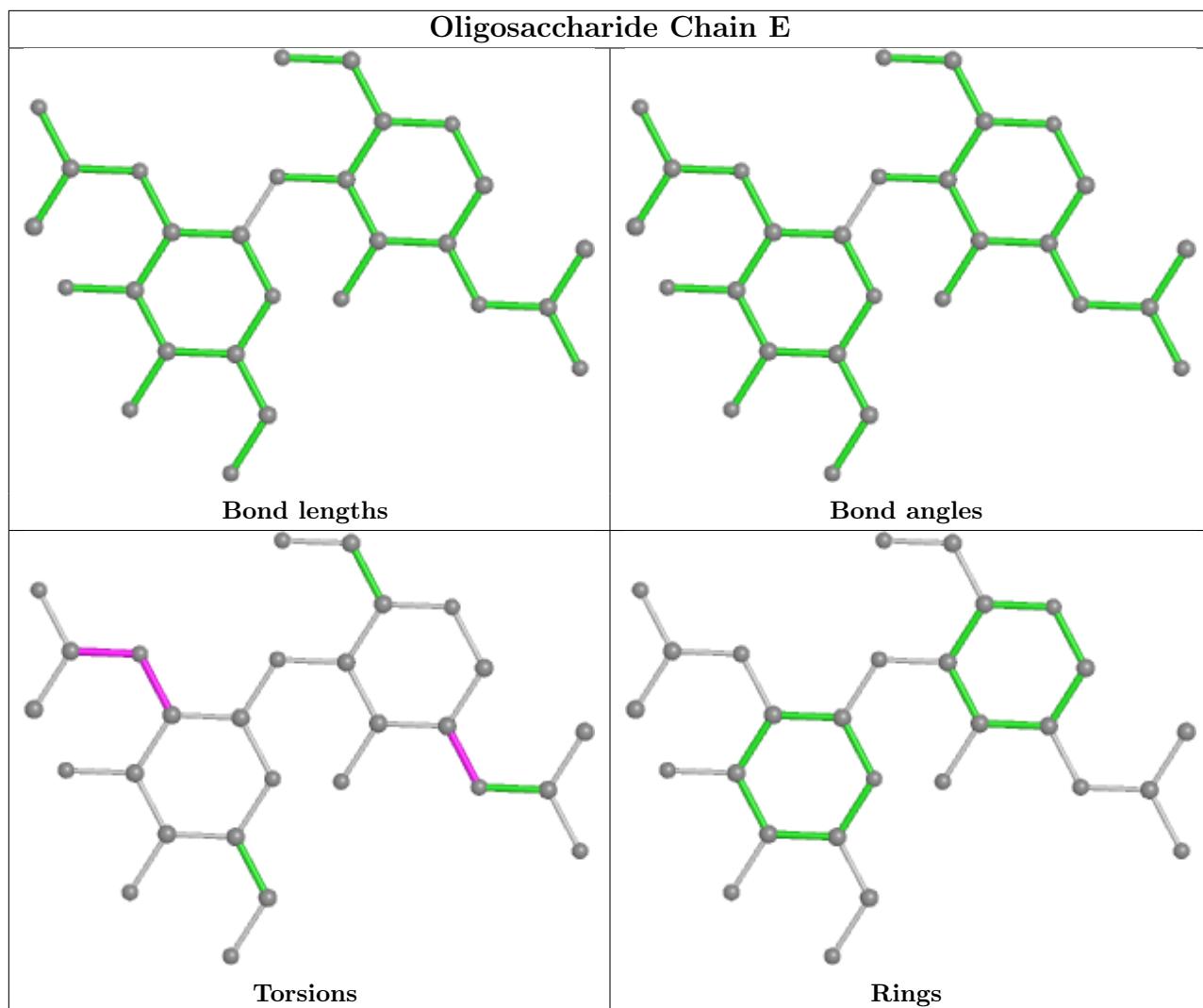
5.6 Ligand geometry (i)

27 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	$\#|Z| > 2$
5	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	C	1306	1	14,14,15	0.54	0	17,19,21	0.36	0
5	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	B	1303	1	14,14,15	0.17	0	17,19,21	0.62	1 (5%)
5	NAG	C	1303	1	14,14,15	0.24	0	17,19,21	0.52	0
5	NAG	A	1301	1	14,14,15	0.30	0	17,19,21	0.60	0
5	NAG	A	1304	1	14,14,15	0.49	0	17,19,21	0.69	1 (5%)
5	NAG	B	1305	1	14,14,15	0.35	0	17,19,21	0.55	0
5	NAG	A	1307	1	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.55	0
5	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.36	0
5	NAG	A	1309	1	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.56	0
5	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	C	1305	1	14,14,15	0.19	0	17,19,21	0.56	0
5	NAG	A	1302	1	14,14,15	0.18	0	17,19,21	0.39	0
5	NAG	B	1309	1	14,14,15	0.30	0	17,19,21	0.61	0
5	NAG	C	1304	1	14,14,15	0.26	0	17,19,21	0.55	0
5	NAG	B	1308	1	14,14,15	0.29	0	17,19,21	0.73	0
5	NAG	B	1301	1	14,14,15	0.29	0	17,19,21	0.64	0
5	NAG	C	1309	1	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	C	1302	1	14,14,15	0.28	0	17,19,21	0.70	0
5	NAG	B	1302	1	14,14,15	0.81	1 (7%)	17,19,21	1.25	1 (5%)
5	NAG	C	1307	1	14,14,15	0.34	0	17,19,21	0.57	0
5	NAG	A	1308	1	14,14,15	0.24	0	17,19,21	0.51	0
5	NAG	B	1306	1	14,14,15	0.59	1 (7%)	17,19,21	0.44	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
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1302	NAG	O5-C1	2.85	1.48	1.43
5	B	1306	NAG	O5-C1	-2.07	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1302	NAG	C1-O5-C5	4.96	118.91	112.19
5	A	1304	NAG	C1-O5-C5	2.25	115.25	112.19
5	B	1303	NAG	C1-O5-C5	2.12	115.06	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1301	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1301	NAG	C8-C7-N2-C2
5	A	1301	NAG	O7-C7-N2-C2
5	A	1305	NAG	C3-C2-N2-C7
5	A	1305	NAG	C8-C7-N2-C2
5	A	1305	NAG	O7-C7-N2-C2
5	B	1301	NAG	C3-C2-N2-C7
5	B	1301	NAG	C8-C7-N2-C2
5	B	1301	NAG	O7-C7-N2-C2
5	B	1308	NAG	C8-C7-N2-C2
5	B	1308	NAG	O7-C7-N2-C2
5	C	1301	NAG	C3-C2-N2-C7
5	C	1301	NAG	C8-C7-N2-C2
5	C	1301	NAG	O7-C7-N2-C2
5	C	1302	NAG	C8-C7-N2-C2
5	C	1302	NAG	O7-C7-N2-C2
5	B	1307	NAG	O5-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	B	1309	NAG	C8-C7-N2-C2
5	B	1309	NAG	O7-C7-N2-C2
5	C	1307	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	B	1308	NAG	C1-C2-N2-C7
5	A	1304	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	A	1305	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1308	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	B	1308	NAG	C3-C2-N2-C7
5	C	1304	NAG	C4-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	C	1301	NAG	C1-C2-N2-C7
5	A	1301	NAG	C1-C2-N2-C7
5	A	1304	NAG	C1-C2-N2-C7
5	C	1307	NAG	C1-C2-N2-C7
5	A	1309	NAG	C3-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7
5	C	1303	NAG	C3-C2-N2-C7
5	A	1306	NAG	C3-C2-N2-C7
5	C	1306	NAG	C3-C2-N2-C7
5	A	1306	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1309	NAG	1	0
5	C	1304	NAG	1	0
5	B	1308	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 ⓘ

This section contains visualisations of the EMDB entry EMD-32594. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

| X | Y | Z |
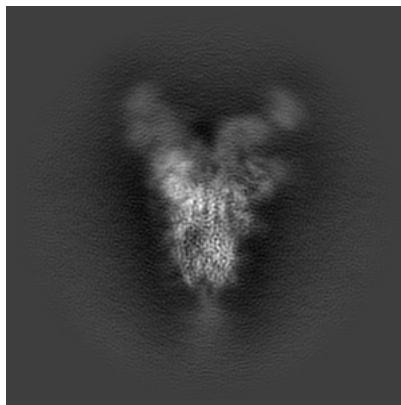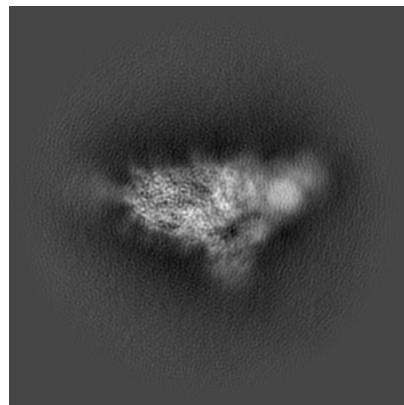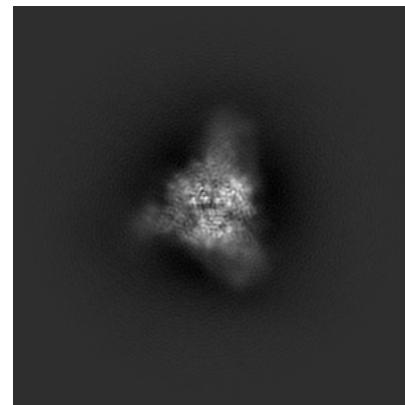
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
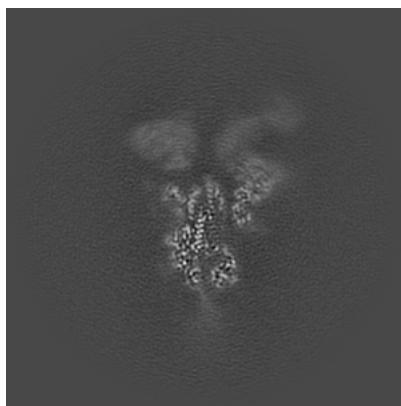
6.2.1 Primary map
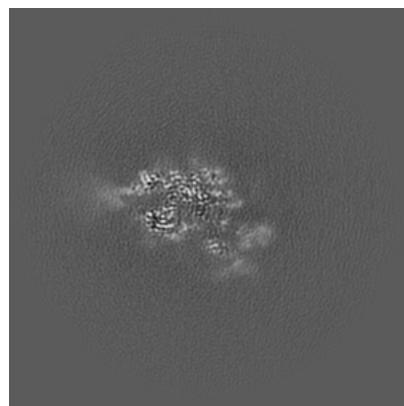
| X Index: 193 | Y Index: 193 | Z Index: 193 |
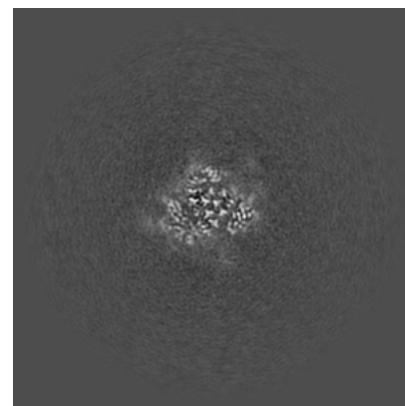
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
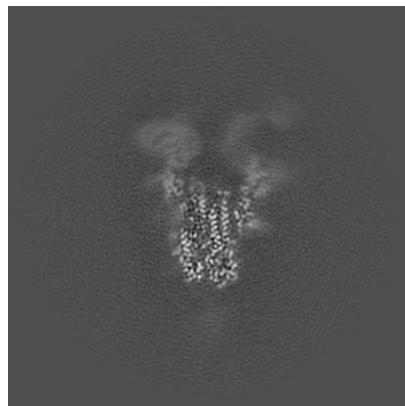
6.3.1 Primary map
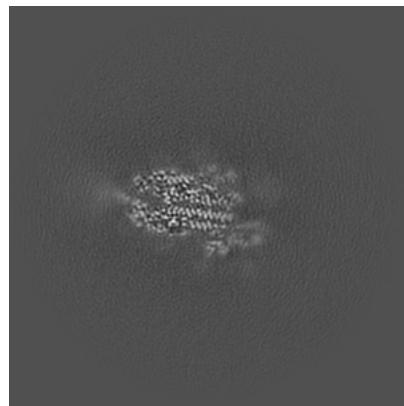
| X Index: 188 | Y Index: 199 | Z Index: 153 |
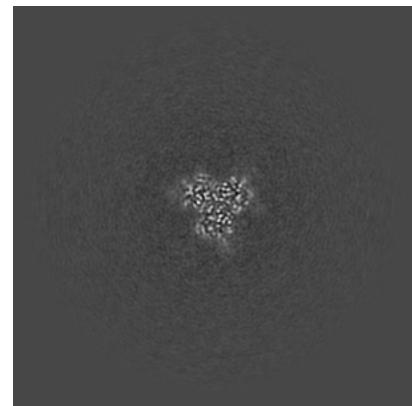
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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 ⓘ

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

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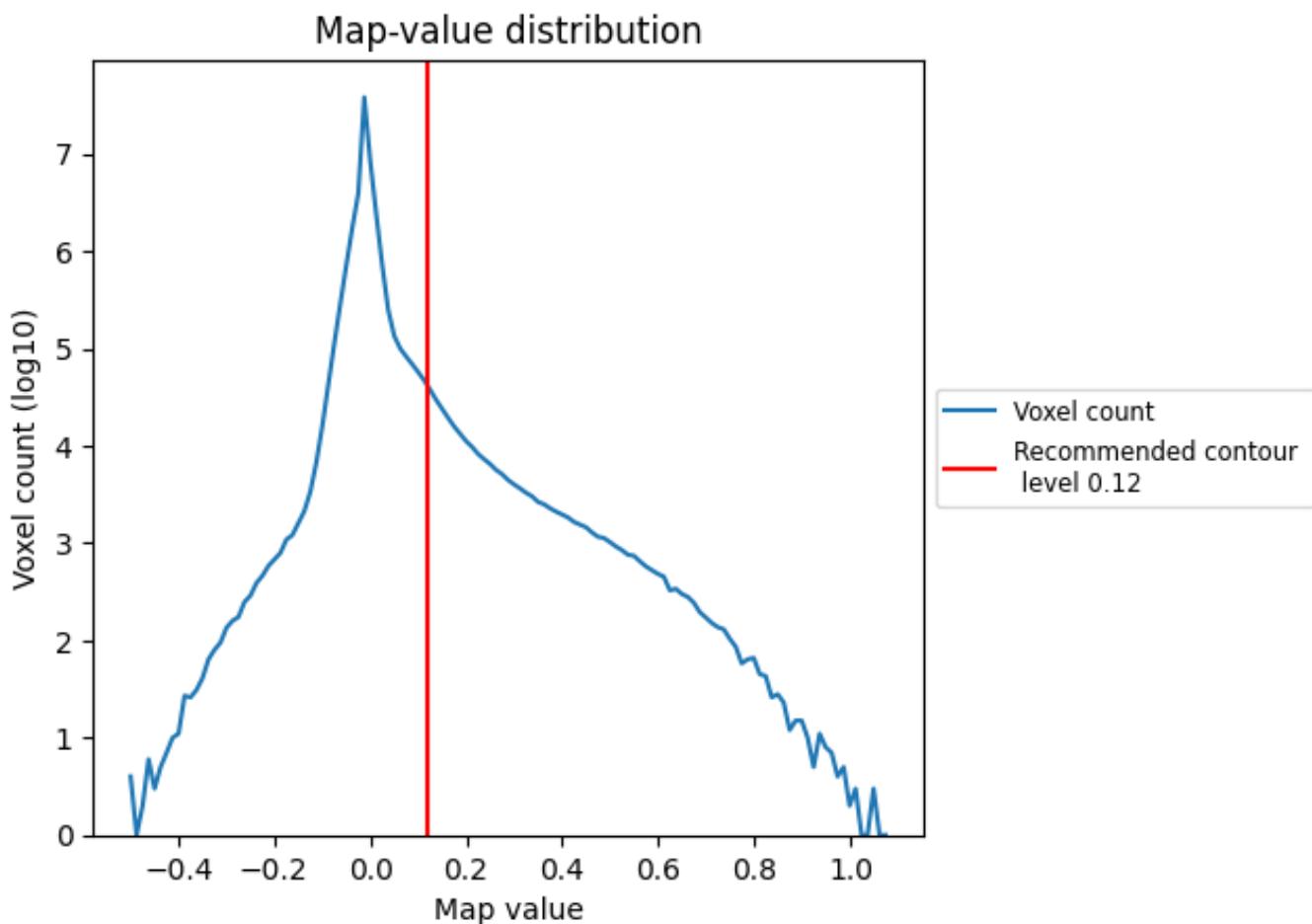
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
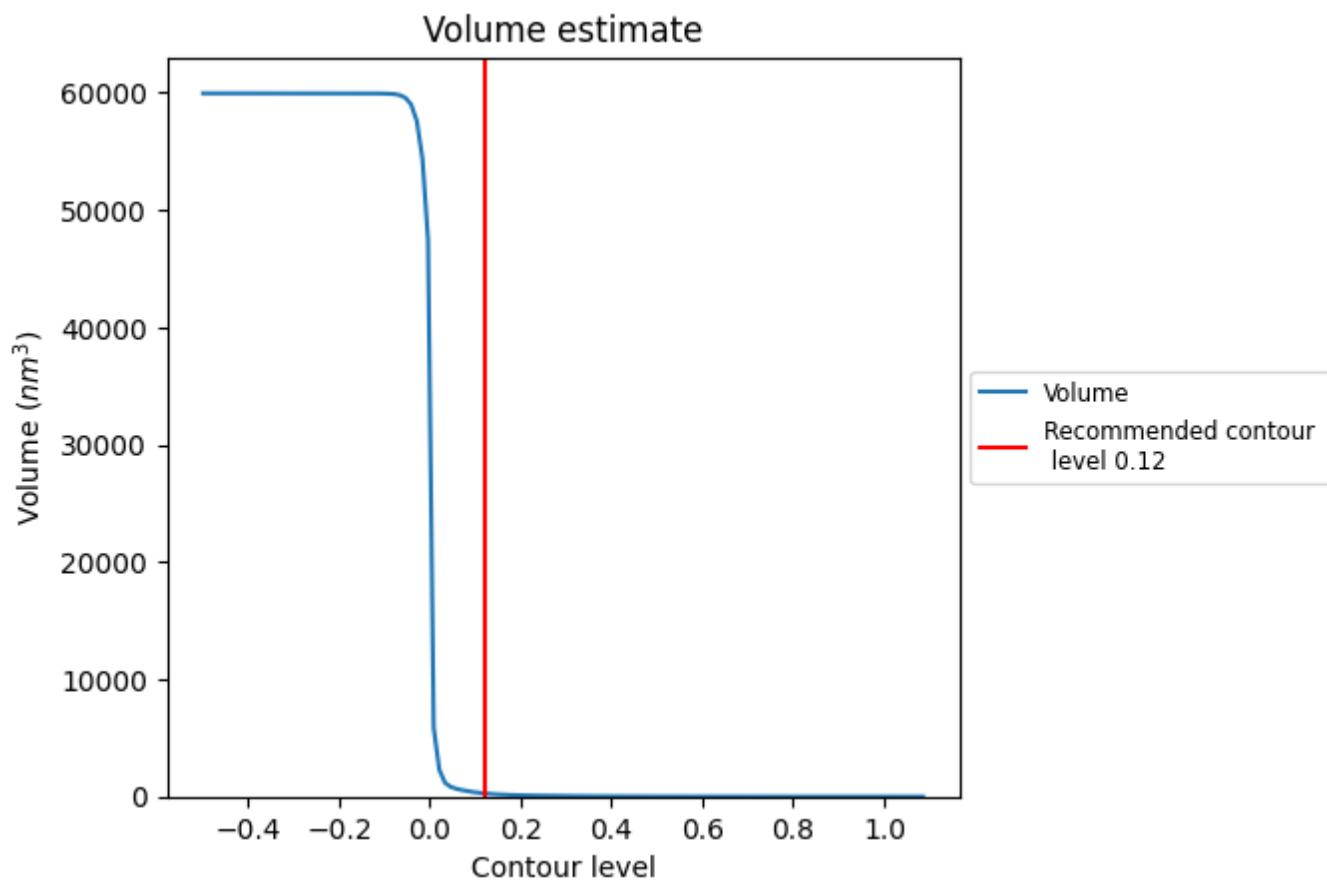
The volume at the recommended contour level is 272 nm^3; this corresponds to an approximate mass of 246 kDa.

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)
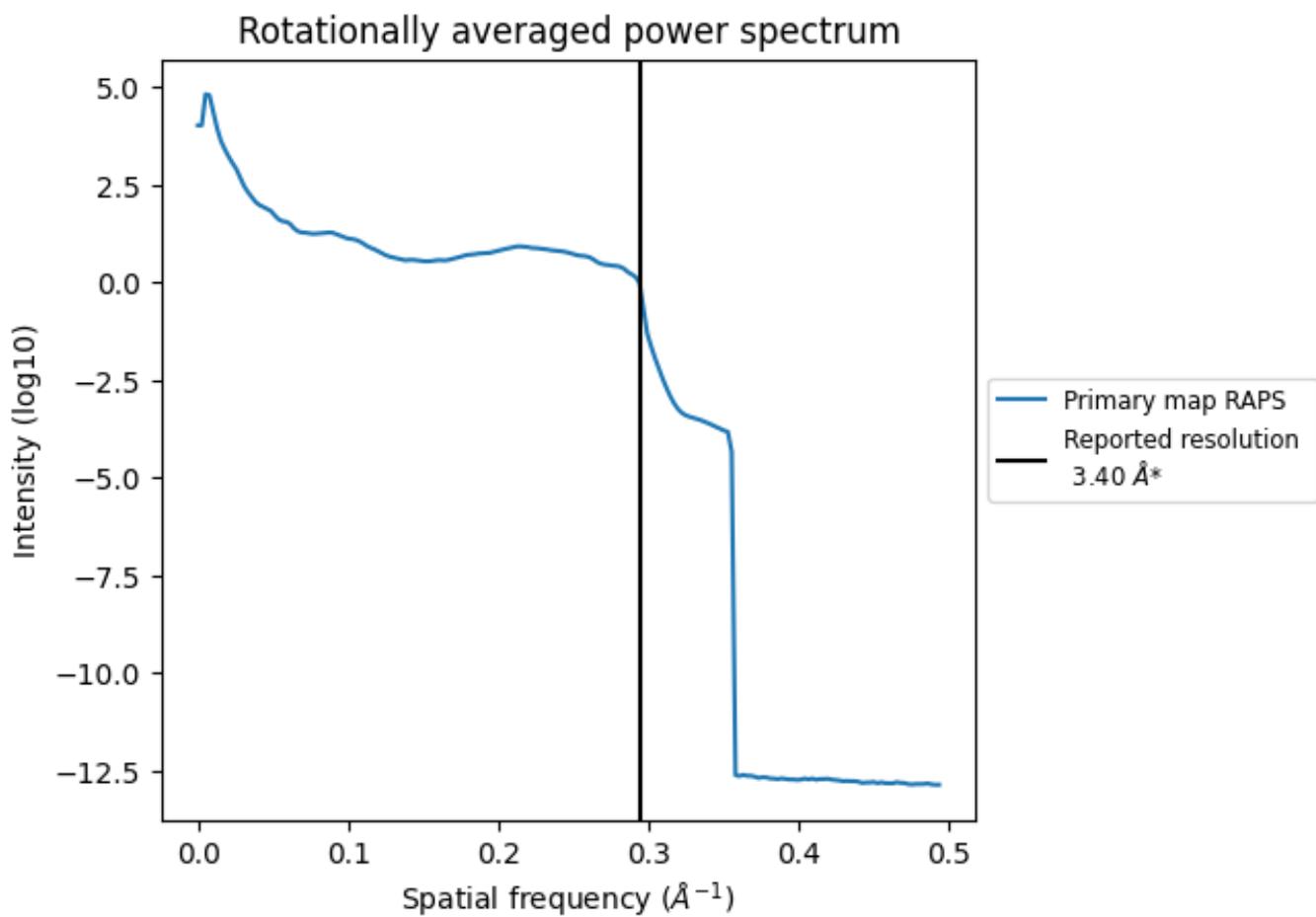
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32594 and PDB model 7WLY. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay ⓘ

| X | Y | Z |
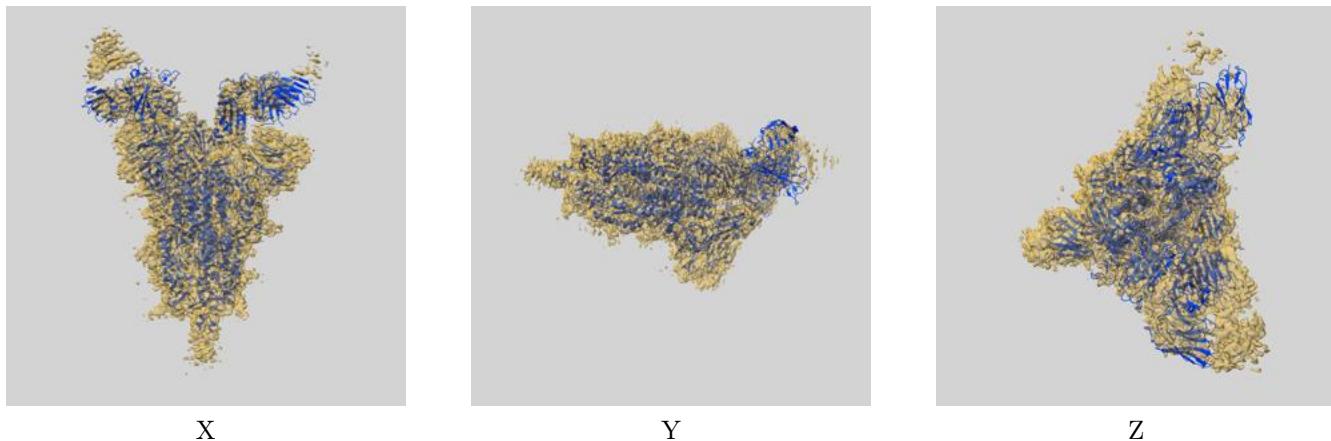
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model　ⓘ

X　　　　　　　　　　　　Y　　　　　　　　　　　　Z
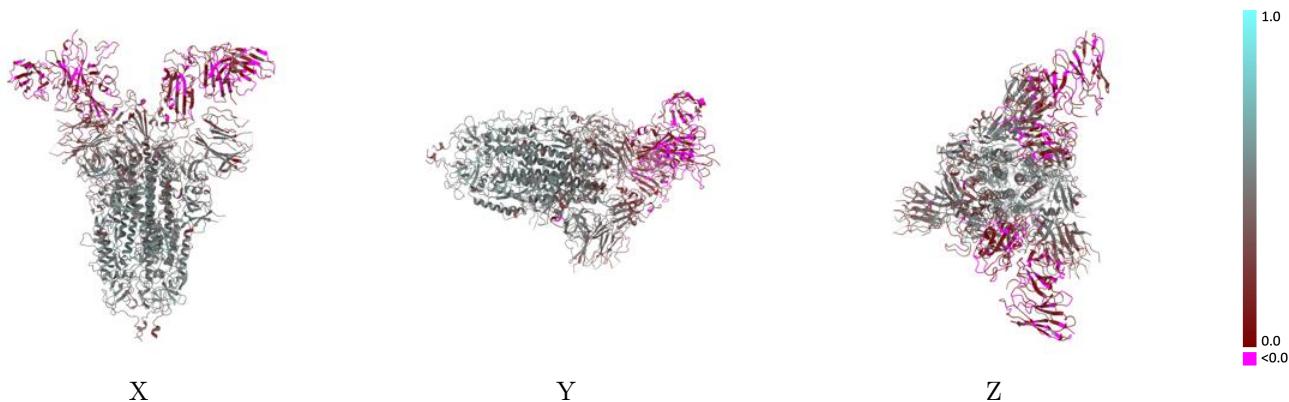
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3　Atom inclusion mapped to coordinate model　ⓘ

X　　　　　　　　　　　　Y　　　　　　　　　　　　Z
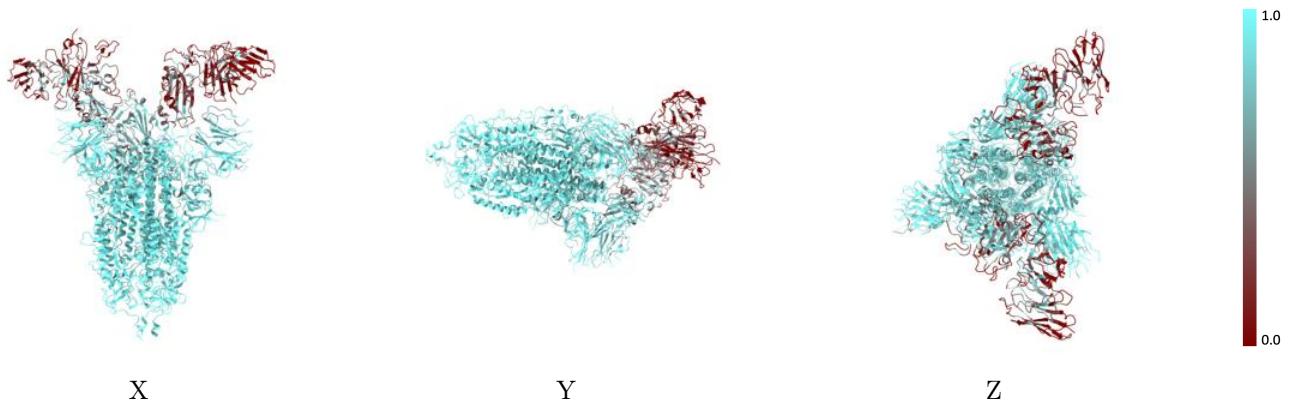
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4   Atom inclusion ⓘ
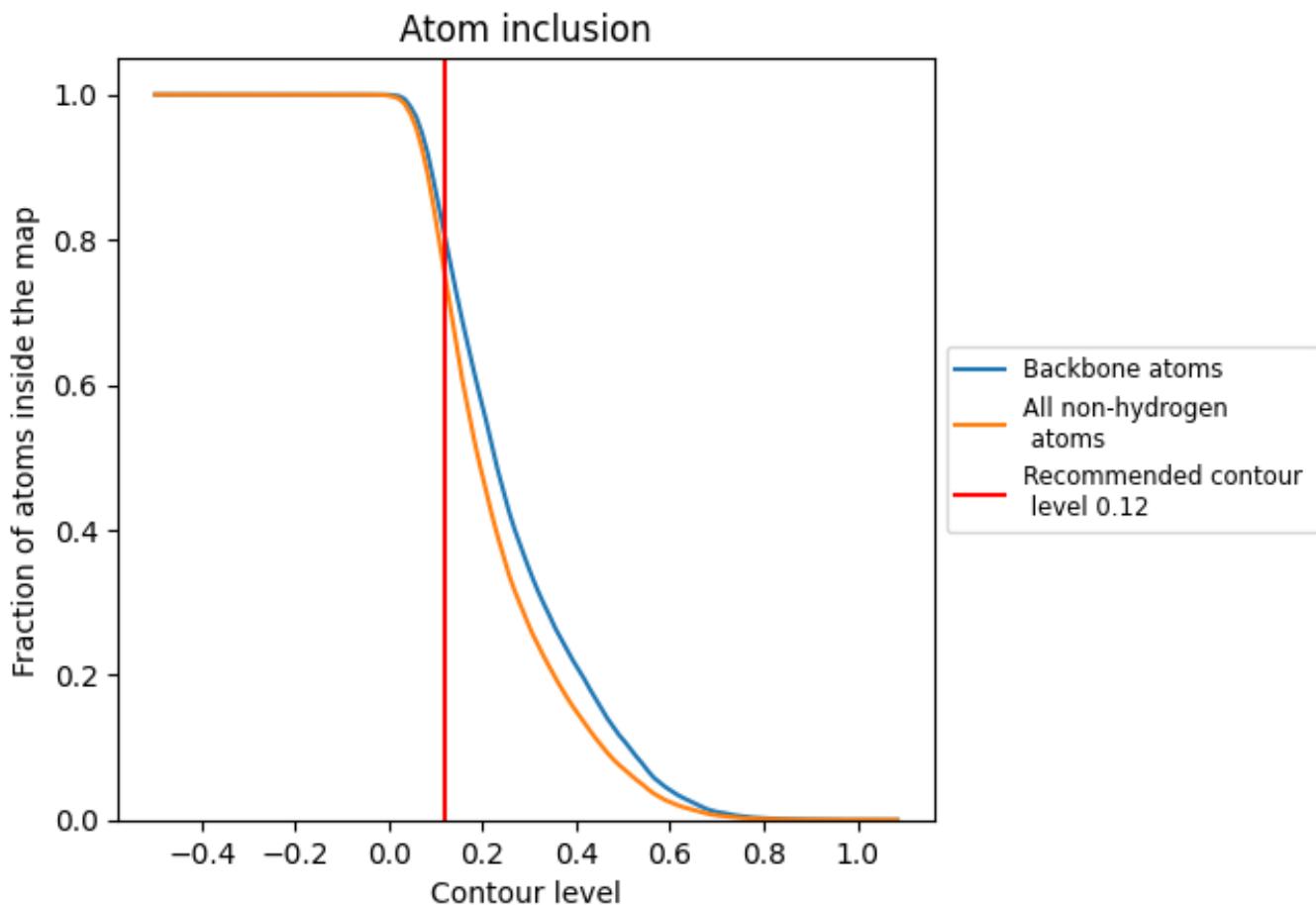
At the recommended contour level, 80% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7494	0.3600
A	0.8755	0.4330
B	0.8003	0.3840
C	0.8096	0.3840
D	0.3571	0.4030
E	0.3929	0.4180
O	0.1227	0.0830
P	0.1667	0.0900
X	0.2394	0.0780
Y	0.2827	0.0770

1.0

0.0
<0.0