Full wwPDB EM Validation Report ⓘ

Jan 15, 2022 – 08:30 am GMT

PDB ID	:	7Q9P
EMDB ID	:	EMD-13875
Title	:	Beta-06 fab in complex with SARS-CoV-2 beta-Spike glycoprotein
Authors	:	Duyvesteyn, H.M.E.; Ren, J.; Stuart, D.I.
Deposited on	:	2021-11-12
Resolution	:	4.50 Å(reported)
Based on initial model	:	7PRY

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

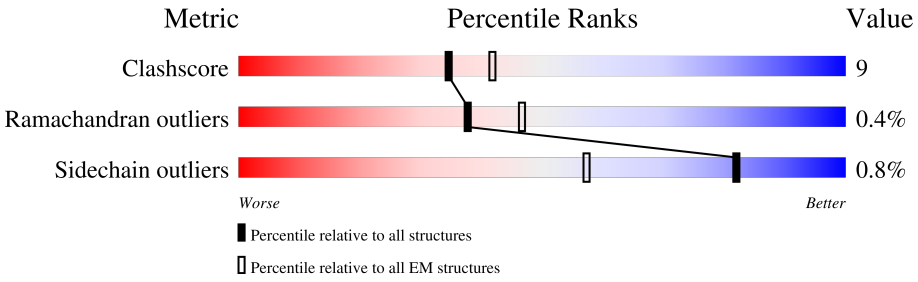
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 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 >=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	62% 19% 19%
1	B	1285	65% 15% 19%
1	C	1285	64% 17% 19%
2	E	228	28% 42% 12% 46%
2	H	228	19% 41% 12% 46%
2	J	228	13% 41% 12% 46%
3	F	215	36% 41% 7% 50%
3	K	215	8% 41% 7% 50%

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Mol	Chain	Length	Quality of chain
3	L	215	27% 42% 7% 50%
4	D	2	100%
4	G	2	100%
4	I	2	100%
4	M	2	100%
4	N	2	100%
4	O	2	100%
4	P	2	50% 50%
4	Q	2	100%
4	R	2	100%
4	S	2	100%
4	T	2	100%
4	U	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30494 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	B	1040	Total	C	N	O	S	0	0
			8148	5207	1357	1547	37		
1	C	1036	Total	C	N	O	S	0	0
			8118	5186	1352	1543	37		
1	A	1041	Total	C	N	O	S	0	0
			8154	5210	1358	1549	37		

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	243	ILE	ARG	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	481	LYS	GLU	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	698	VAL	ALA	variant	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1203	TYR	-	expression tag	UNP P0DTC2
B	1204	GLU	-	expression tag	UNP P0DTC2
B	1205	GLN	-	expression tag	UNP P0DTC2
B	1206	GLY	-	expression tag	UNP P0DTC2
B	1207	SER	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1210	ILE	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ALA	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	ASP	-	expression tag	UNP P0DTC2
B	1217	GLY	-	expression tag	UNP P0DTC2
B	1218	GLN	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	TYR	-	expression tag	UNP P0DTC2
B	1221	VAL	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	LYS	-	expression tag	UNP P0DTC2
B	1224	ASP	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	GLU	-	expression tag	UNP P0DTC2
B	1227	TRP	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	LEU	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	SER	-	expression tag	UNP P0DTC2
B	1232	THR	-	expression tag	UNP P0DTC2
B	1233	PHE	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	ARG	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	PRO	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	GLY	-	expression tag	UNP P0DTC2
B	1256	SER	-	expression tag	UNP P0DTC2
B	1257	ALA	-	expression tag	UNP P0DTC2
B	1258	TRP	-	expression tag	UNP P0DTC2
B	1259	SER	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	PRO	-	expression tag	UNP P0DTC2
B	1262	GLN	-	expression tag	UNP P0DTC2
B	1263	PHE	-	expression tag	UNP P0DTC2
B	1264	GLU	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	SER	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	SER	-	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	ALA	-	expression tag	UNP P0DTC2
B	1278	TRP	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
B	1281	PRO	-	expression tag	UNP P0DTC2
B	1282	GLN	-	expression tag	UNP P0DTC2
B	1283	PHE	-	expression tag	UNP P0DTC2
B	1284	GLU	-	expression tag	UNP P0DTC2
B	1285	LYS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	243	ILE	ARG	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	481	LYS	GLU	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	698	VAL	ALA	variant	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1203	TYR	-	expression tag	UNP P0DTC2
C	1204	GLU	-	expression tag	UNP P0DTC2
C	1205	GLN	-	expression tag	UNP P0DTC2
C	1206	GLY	-	expression tag	UNP P0DTC2
C	1207	SER	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	TYR	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ALA	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	ASP	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	GLN	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	TYR	-	expression tag	UNP P0DTC2
C	1221	VAL	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	LYS	-	expression tag	UNP P0DTC2
C	1224	ASP	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	TRP	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	LEU	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	SER	-	expression tag	UNP P0DTC2
C	1232	THR	-	expression tag	UNP P0DTC2
C	1233	PHE	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	PRO	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	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	GLY	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	ALA	-	expression tag	UNP P0DTC2
C	1258	TRP	-	expression tag	UNP P0DTC2
C	1259	SER	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	PRO	-	expression tag	UNP P0DTC2
C	1262	GLN	-	expression tag	UNP P0DTC2
C	1263	PHE	-	expression tag	UNP P0DTC2
C	1264	GLU	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	SER	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	SER	-	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	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1278	TRP	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	PRO	-	expression tag	UNP P0DTC2
C	1282	GLN	-	expression tag	UNP P0DTC2
C	1283	PHE	-	expression tag	UNP P0DTC2
C	1284	GLU	-	expression tag	UNP P0DTC2
C	1285	LYS	-	expression tag	UNP P0DTC2
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	243	ILE	ARG	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	481	LYS	GLU	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	698	VAL	ALA	variant	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1203	TYR	-	expression tag	UNP P0DTC2
A	1204	GLU	-	expression tag	UNP P0DTC2
A	1205	GLN	-	expression tag	UNP P0DTC2
A	1206	GLY	-	expression tag	UNP P0DTC2
A	1207	SER	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	TYR	-	expression tag	UNP P0DTC2
A	1210	ILE	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ALA	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	ASP	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	GLN	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	TYR	-	expression tag	UNP P0DTC2
A	1221	VAL	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	LYS	-	expression tag	UNP P0DTC2
A	1224	ASP	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2
A	1227	TRP	-	expression tag	UNP P0DTC2
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	LEU	-	expression tag	UNP P0DTC2
A	1230	LEU	-	expression tag	UNP P0DTC2
A	1231	SER	-	expression tag	UNP P0DTC2
A	1232	THR	-	expression tag	UNP P0DTC2
A	1233	PHE	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	PRO	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	HIS	-	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	GLY	-	expression tag	UNP P0DTC2
A	1256	SER	-	expression tag	UNP P0DTC2
A	1257	ALA	-	expression tag	UNP P0DTC2
A	1258	TRP	-	expression tag	UNP P0DTC2
A	1259	SER	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	GLN	-	expression tag	UNP P0DTC2
A	1263	PHE	-	expression tag	UNP P0DTC2
A	1264	GLU	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	SER	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	SER	-	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	ALA	-	expression tag	UNP P0DTC2
A	1278	TRP	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	PRO	-	expression tag	UNP P0DTC2
A	1282	GLN	-	expression tag	UNP P0DTC2
A	1283	PHE	-	expression tag	UNP P0DTC2
A	1284	GLU	-	expression tag	UNP P0DTC2
A	1285	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Beta-06 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total	C	N	O	S	0	0
			946	603	153	186	4		
2	E	122	Total	C	N	O	S	0	0
			946	603	153	186	4		
2	J	122	Total	C	N	O	S	0	0
			946	603	153	186	4		

- Molecule 3 is a protein called Beta-06 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			836	524	144	165	3		
3	F	108	Total	C	N	O	S	0	0
			836	524	144	165	3		

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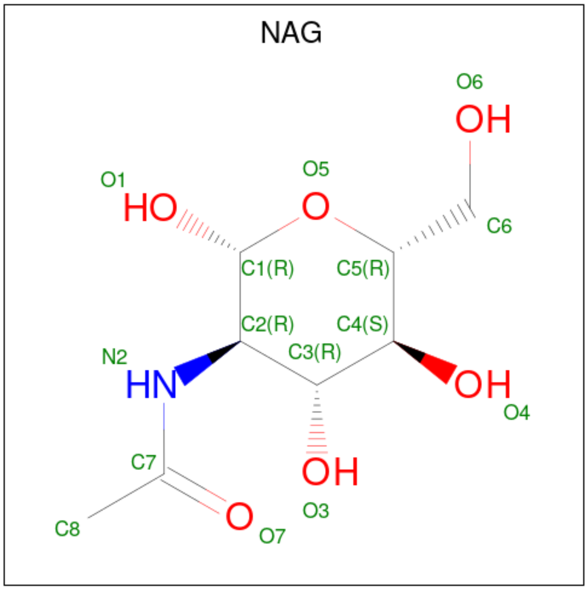
Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	108	Total	C	N	O	S	0	0
			836	524	144	165	3		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-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	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	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	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	B	1	Total C N O 140 80 10 50	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0

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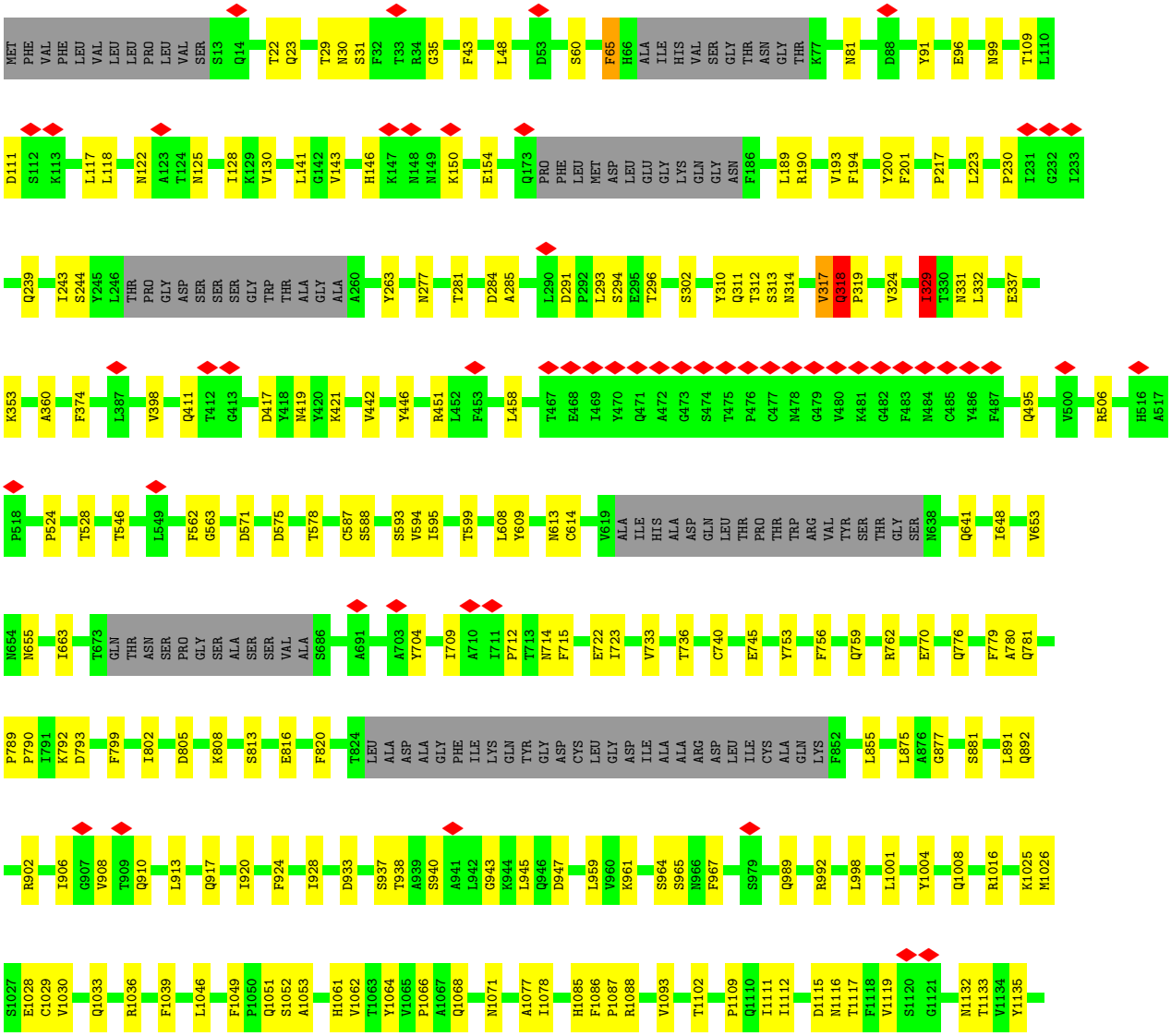
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1	Total 140	C 80	N 10	O 50	0
5	A	1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

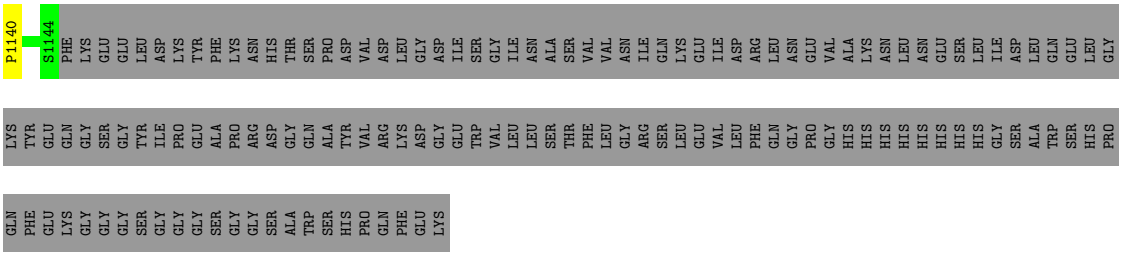
3 Residue-property plots (i)

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

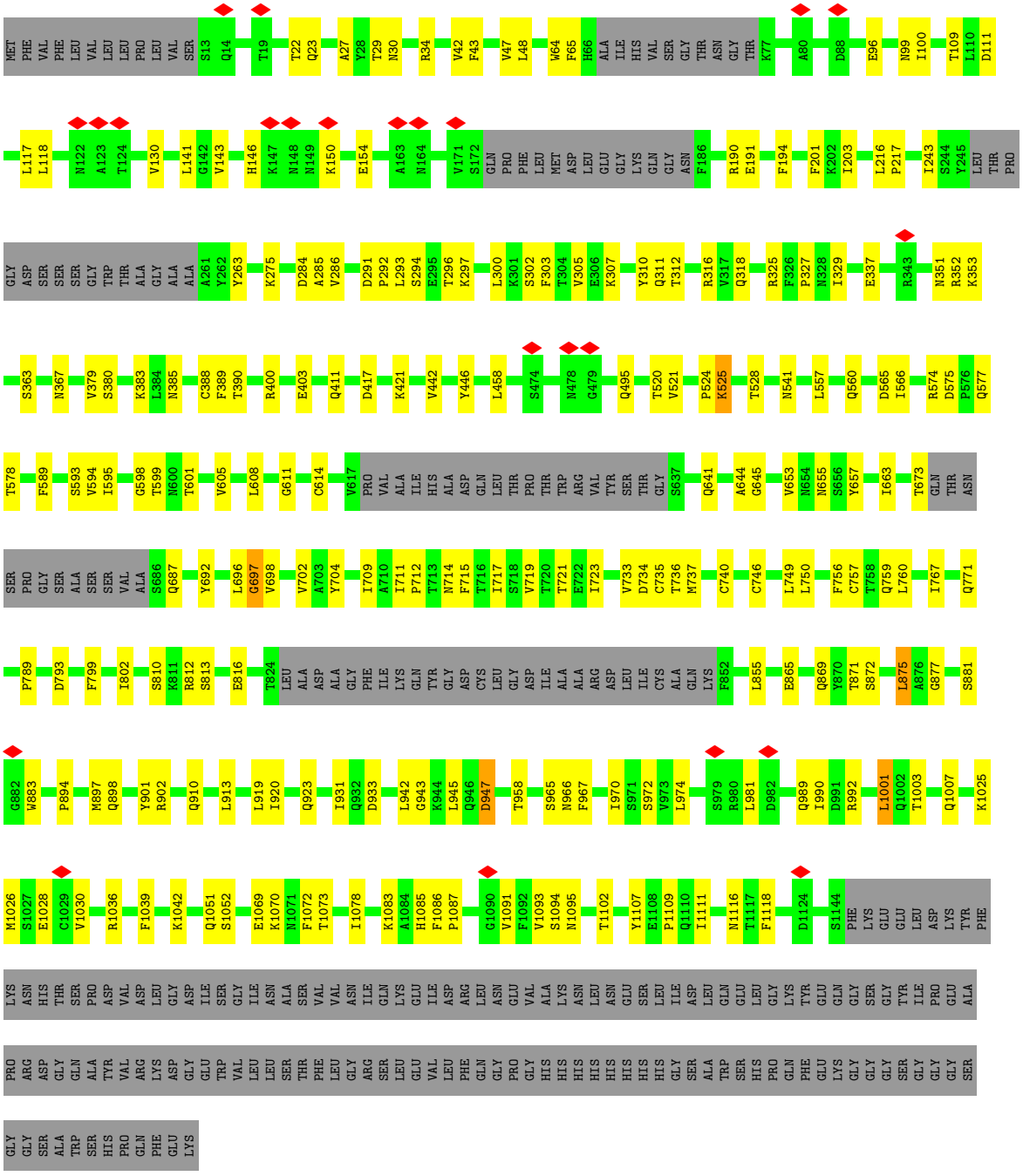
Chain B:





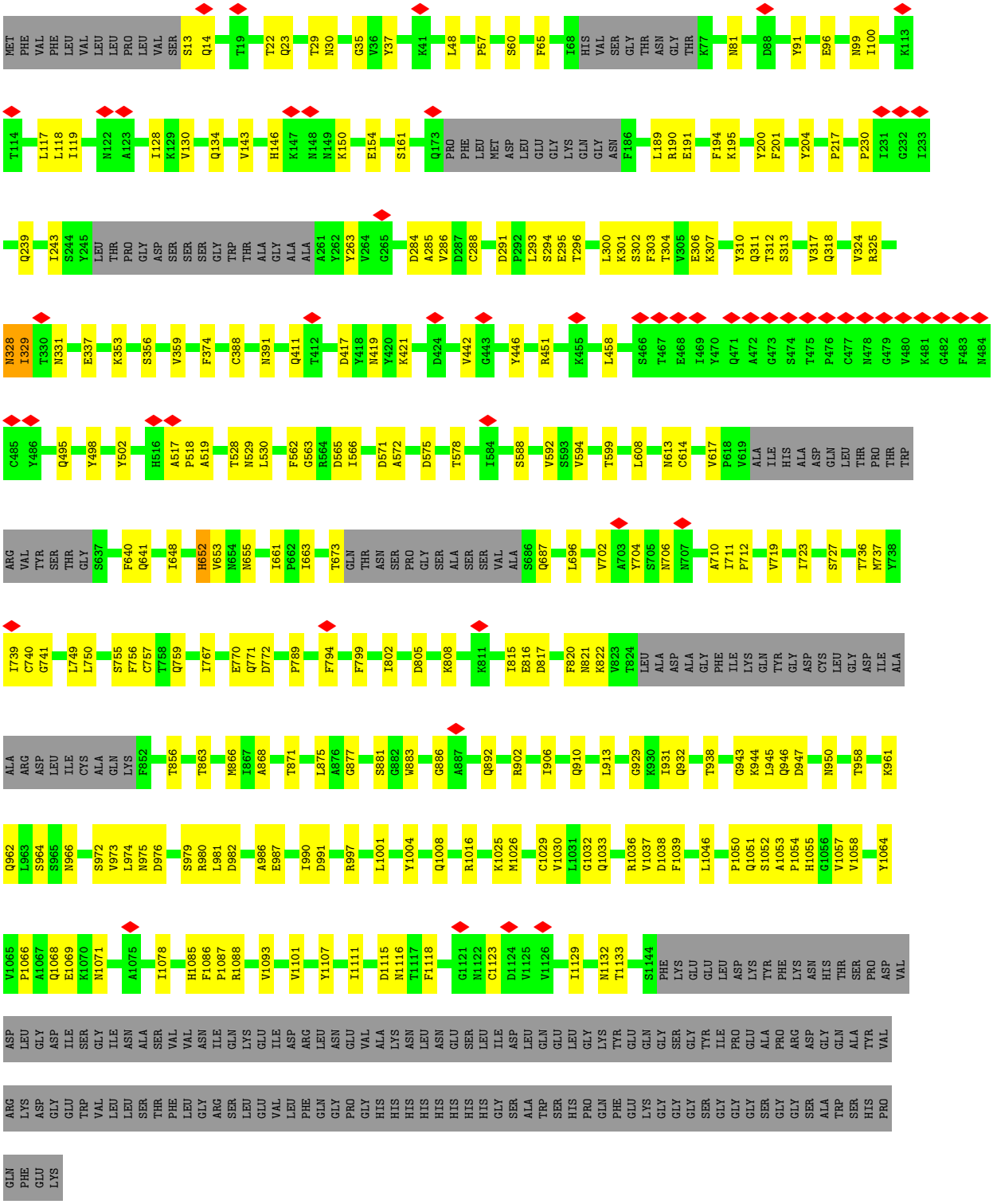
• Molecule 1: Spike glycoprotein

Chain C:



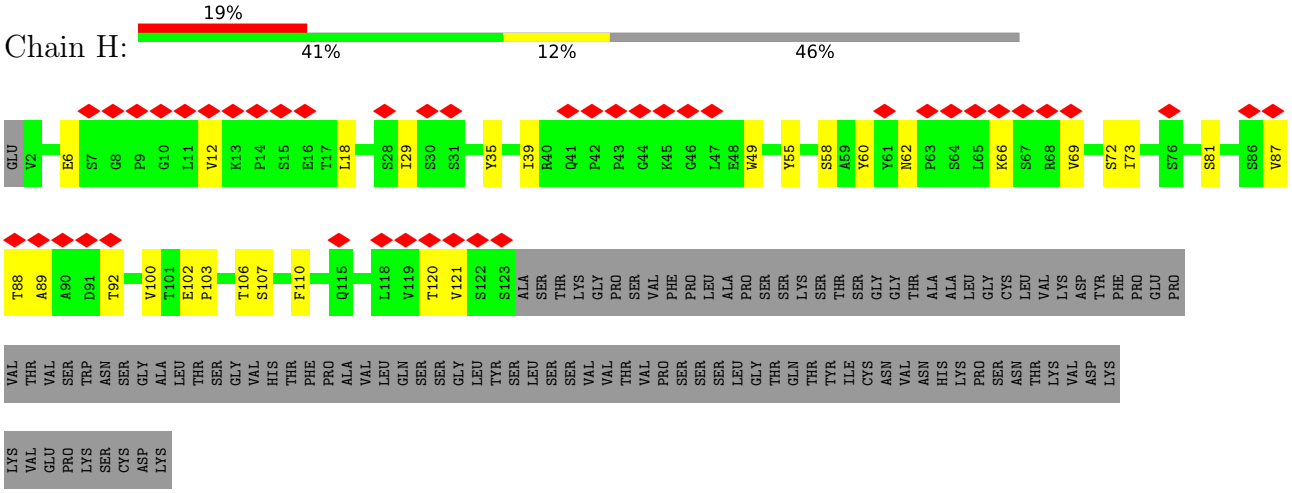
• Molecule 1: Spike glycoprotein

Chain A:



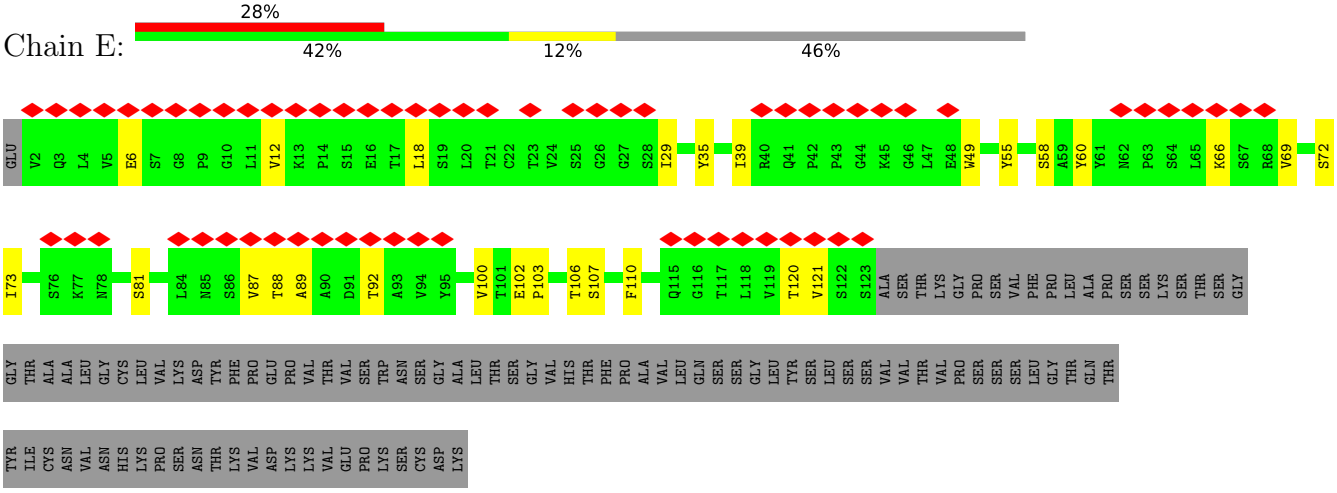
• Molecule 2: Beta-06 heavy chain

Chain H:



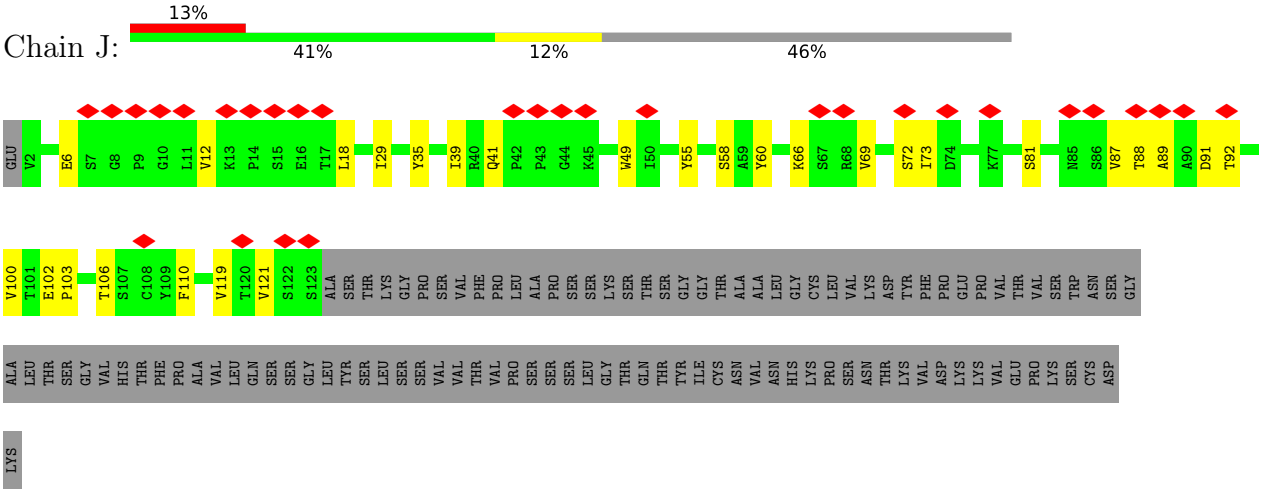
• Molecule 2: Beta-06 heavy chain

Chain E:



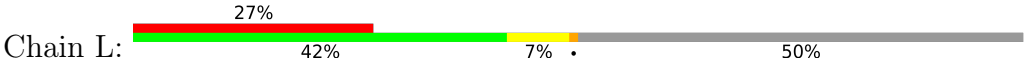
• Molecule 2: Beta-06 heavy chain

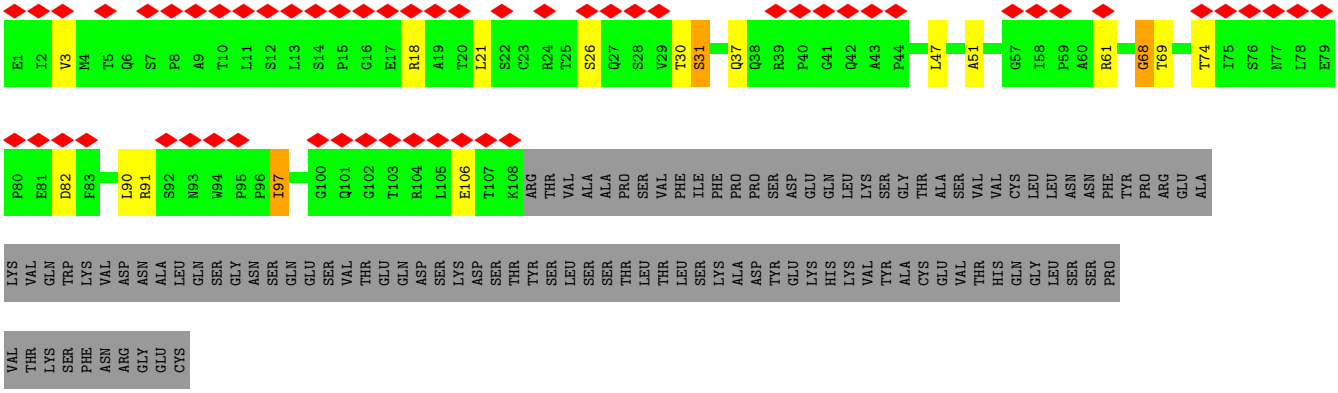
Chain J:



• Molecule 3: Beta-06 light chain

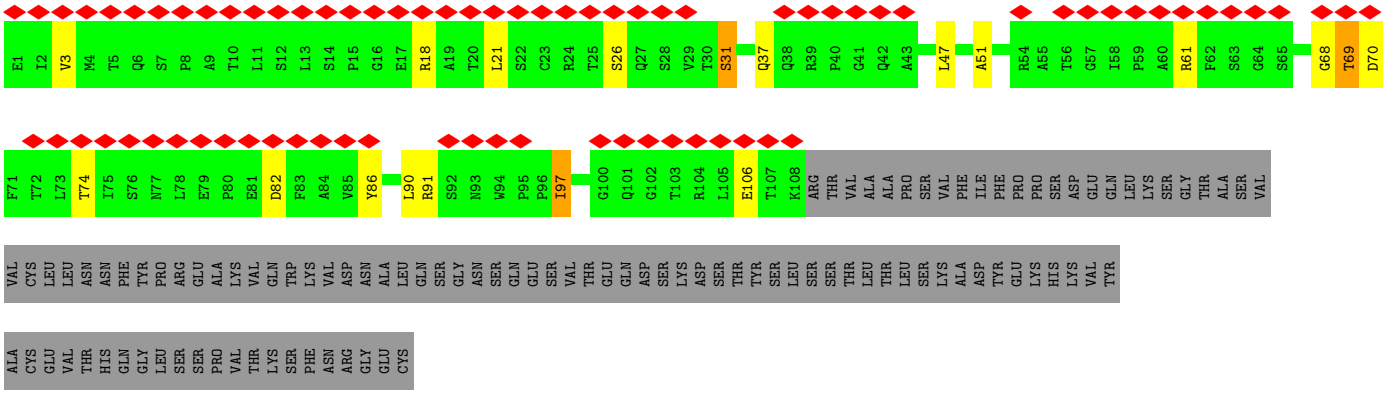
Chain L:





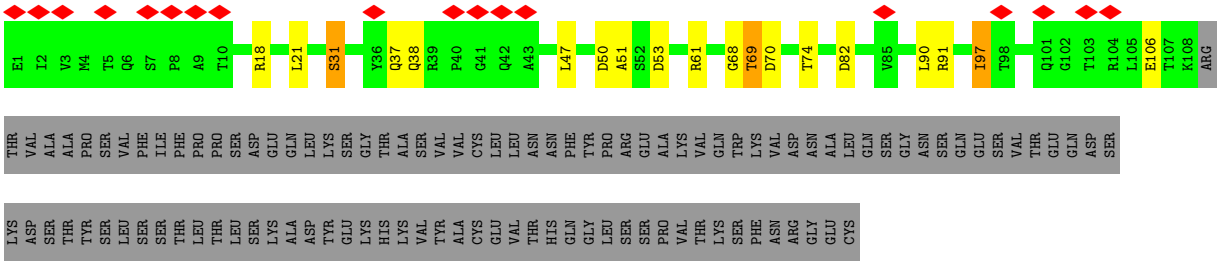
• Molecule 3: Beta-06 light chain

Chain F:



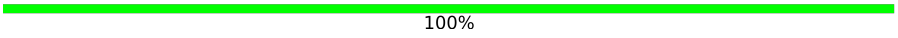
• Molecule 3: Beta-06 light chain

Chain K:



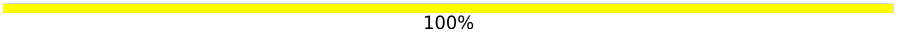
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain G:

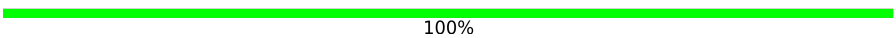


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

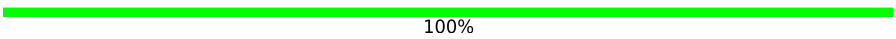
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



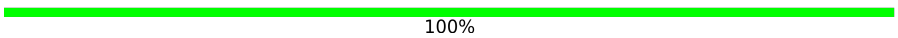
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain O:

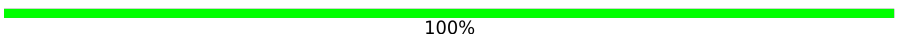


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

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

Chain Q:



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

Chain R: 100%

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

Chain S: 100%

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

Chain T: 100%

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

Chain U: 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79744	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 ($e^-/Å^2$)	40.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.125	Depositor
Minimum map value	-0.512	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.119	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.32	0/8344	0.50	0/11355
1	B	0.30	0/8338	0.52	3/11347 (0.0%)
1	C	0.32	0/8307	0.50	2/11303 (0.0%)
2	E	0.26	0/973	0.50	0/1329
2	H	0.27	0/973	0.50	0/1329
2	J	0.28	0/973	0.50	0/1329
3	F	0.26	0/856	0.54	0/1167
3	K	0.27	0/856	0.54	0/1167
3	L	0.26	0/856	0.60	1/1167 (0.1%)
All	All	0.31	0/30476	0.51	6/41493 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	F	0	1
3	K	0	1
3	L	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	VAL	N-CA-C	-13.00	75.90	111.00
1	B	318	GLN	N-CA-CB	10.06	128.71	110.60
1	B	318	GLN	N-CA-C	-9.42	85.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	69	THR	N-CA-CB	-7.19	96.64	110.30
1	C	698	VAL	N-CA-C	-6.88	92.42	111.00
1	C	698	VAL	N-CA-CB	5.36	123.29	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	696	LEU	Peptide
3	F	51	ALA	Peptide
3	K	51	ALA	Peptide
3	L	51	ALA	Peptide

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	8154	0	7942	162	0
1	B	8148	0	7937	134	0
1	C	8118	0	7904	151	0
2	E	946	0	909	24	0
2	H	946	0	909	25	0
2	J	946	0	909	35	0
3	F	836	0	812	12	0
3	K	836	0	812	13	0
3	L	836	0	812	10	0
4	D	28	0	25	0	0
4	G	28	0	25	1	0
4	I	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	28	0	25	0	0
5	A	140	0	130	3	0
5	B	140	0	130	1	0
5	C	112	0	104	0	0
All	All	30494	0	29610	529	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 9.

All (529) 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:B:1025:LYS:NZ	1:B:1039:PHE:O	1.89	1.04
1:A:816:GLU:OE2	1:A:1052:SER:N	2.01	0.93
2:J:87:VAL:HG11	2:J:121:VAL:HG11	1.54	0.89
1:B:816:GLU:OE2	1:B:1052:SER:N	2.06	0.88
1:B:293:LEU:HD11	1:B:599:THR:HG22	1.53	0.88
2:J:92:THR:HG22	2:J:121:VAL:H	1.39	0.86
1:A:1025:LYS:NZ	1:A:1039:PHE:O	2.08	0.85
2:J:87:VAL:CG1	2:J:121:VAL:HG11	2.09	0.82
2:E:87:VAL:HG11	2:E:121:VAL:HG11	1.59	0.82
1:B:337:GLU:OE1	1:B:353:LYS:NZ	2.13	0.81
1:C:560:GLN:O	1:C:574:ARG:NH2	2.13	0.81
1:A:337:GLU:OE1	1:A:353:LYS:NZ	2.15	0.80
1:C:767:ILE:O	1:C:771:GLN:NE2	2.13	0.80
1:A:614:CYS:N	1:A:641:GLN:OE1	2.14	0.79
2:H:87:VAL:HG11	2:H:121:VAL:HG11	1.61	0.79
1:A:96:GLU:N	1:A:96:GLU:OE1	2.16	0.79
1:A:739:ILE:O	1:A:974:LEU:HD11	1.82	0.79
1:C:1025:LYS:NZ	1:C:1039:PHE:O	2.15	0.78
1:C:96:GLU:OE1	1:C:96:GLU:N	2.16	0.78
1:C:293:LEU:HD11	1:C:599:THR:HG22	1.66	0.77
2:J:106:THR:HG23	3:K:91:ARG:O	1.85	0.77
1:A:987:GLU:O	1:A:991:ASP:N	2.19	0.76
1:C:1069:GLU:N	1:C:1069:GLU:OE1	2.19	0.75
2:J:72:SER:OG	2:J:81:SER:OG	2.04	0.75
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.70	0.74
1:C:380:SER:N	1:A:980:ARG:O	2.21	0.74
1:A:1071:ASN:OD1	5:A:1308:NAG:N2	2.21	0.73
2:H:72:SER:OG	2:H:81:SER:OG	2.06	0.73
1:A:750:LEU:HD21	1:A:757:CYS:SG	2.28	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:GLU:HG3	5:A:1308:NAG:C8	2.18	0.73
2:H:106:THR:HG23	3:L:91:ARG:O	1.89	0.73
1:C:696:LEU:O	1:C:697:GLY:O	2.07	0.73
2:E:106:THR:HG23	3:F:91:ARG:O	1.88	0.73
1:C:989:GLN:OE1	1:C:992:ARG:NH1	2.21	0.73
1:A:1050:PRO:O	1:A:1051:GLN:NE2	2.21	0.73
1:A:312:THR:OG1	1:A:592:VAL:O	2.07	0.72
2:E:87:VAL:CG1	2:E:121:VAL:HG11	2.18	0.72
1:C:608:LEU:HD22	1:C:663:ILE:HG23	1.69	0.72
1:B:99:ASN:OD1	1:B:190:ARG:NH2	2.22	0.72
2:E:92:THR:HG23	2:E:120:THR:HA	1.72	0.72
2:E:72:SER:OG	2:E:81:SER:OG	2.08	0.71
2:H:87:VAL:CG1	2:H:121:VAL:HG11	2.19	0.71
1:A:293:LEU:HD11	1:A:599:THR:HG22	1.71	0.70
1:B:96:GLU:N	1:B:96:GLU:OE1	2.25	0.70
2:J:18:LEU:HB2	2:J:87:VAL:HG21	1.74	0.69
1:C:524:PRO:O	1:C:525:LYS:CB	2.40	0.69
1:C:1042:LYS:NZ	1:A:886:GLY:O	2.26	0.69
2:H:92:THR:HG23	2:H:120:THR:HA	1.72	0.69
1:C:524:PRO:O	1:C:525:LYS:HB3	1.92	0.69
1:C:99:ASN:OD1	1:C:190:ARG:NH2	2.27	0.68
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.06	0.68
2:J:88:THR:O	2:J:121:VAL:HG21	1.93	0.68
1:B:891:LEU:HD23	1:A:1069:GLU:OE1	1.93	0.68
1:C:735:CYS:SG	1:C:736:THR:N	2.66	0.68
1:B:723:ILE:HG22	1:B:945:LEU:HD13	1.75	0.67
1:A:802:ILE:HG22	1:A:815:ILE:HD12	1.75	0.67
2:J:92:THR:CG2	2:J:121:VAL:HG22	2.25	0.67
1:B:81:ASN:O	1:B:239:GLN:NE2	2.28	0.67
1:B:877:GLY:O	1:B:881:SER:OG	2.13	0.66
1:C:363:SER:OG	1:C:385:ASN:ND2	2.28	0.66
2:J:29:ILE:CG2	2:J:73:ILE:HD11	2.26	0.66
1:B:1071:ASN:OD1	5:B:1308:NAG:N2	2.29	0.66
1:B:722:GLU:OE1	1:B:1061:HIS:NE2	2.29	0.66
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.07	0.65
2:J:92:THR:HG23	2:J:121:VAL:HG22	1.79	0.65
2:J:12:VAL:HB	2:J:121:VAL:HG12	1.79	0.65
2:E:29:ILE:CG2	2:E:73:ILE:HD11	2.28	0.64
1:A:29:THR:HG22	1:A:30:ASN:H	1.63	0.64
1:C:711:ILE:HD12	1:C:1093:VAL:HG11	1.80	0.64
1:A:563:GLY:O	1:A:571:ASP:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:ILE:CG2	2:H:73:ILE:HD11	2.29	0.63
1:A:284:ASP:OD1	1:A:285:ALA:N	2.31	0.63
1:A:719:VAL:O	1:A:931:ILE:HD11	1.99	0.63
1:A:1025:LYS:O	1:A:1029:CYS:N	2.32	0.63
1:B:1025:LYS:O	1:B:1029:CYS:N	2.28	0.63
1:A:805:ASP:OD2	1:A:808:LYS:N	2.30	0.63
2:H:88:THR:O	2:H:121:VAL:HG21	1.99	0.62
1:B:1087:PRO:O	1:C:910:GLN:NE2	2.33	0.62
2:E:88:THR:O	2:E:121:VAL:HG21	1.99	0.62
1:C:383:LYS:HB3	1:A:979:SER:O	2.00	0.61
1:C:325:ARG:NH2	1:C:528:THR:O	2.34	0.60
3:K:68:GLY:O	3:K:70:ASP:N	2.35	0.60
1:B:776:GLN:O	1:B:780:ALA:N	2.34	0.60
3:K:18:ARG:HH21	3:K:74:THR:HG21	1.67	0.60
1:A:712:PRO:O	1:A:1107:TYR:N	2.33	0.60
2:E:18:LEU:HB2	2:E:87:VAL:HG21	1.83	0.60
1:B:805:ASP:OD2	1:B:808:LYS:N	2.30	0.59
1:B:1132:ASN:ND2	1:B:1133:THR:O	2.36	0.59
2:H:18:LEU:HB2	2:H:87:VAL:HG21	1.83	0.59
3:F:68:GLY:O	3:F:70:ASP:N	2.36	0.59
1:A:902:ARG:NH1	1:A:1046:LEU:O	2.36	0.59
1:B:770:GLU:OE2	1:B:1016:ARG:NH1	2.35	0.59
1:C:286:VAL:HG23	1:C:303:PHE:CE2	2.38	0.59
1:A:417:ASP:O	1:A:458:LEU:N	2.33	0.58
1:C:813:SER:OG	1:C:1051:GLN:OE1	2.13	0.58
1:C:495:GLN:NE2	2:J:102:GLU:OE1	2.35	0.58
2:J:39:ILE:HD11	2:J:110:PHE:CE2	2.38	0.58
1:C:1036:ARG:NH1	1:C:1039:PHE:CZ	2.71	0.58
3:F:18:ARG:HH21	3:F:74:THR:HG21	1.68	0.58
1:B:419:ASN:OD1	1:B:451:ARG:N	2.33	0.58
2:J:49:TRP:CE2	3:K:97:ILE:HD12	2.38	0.58
1:A:972:SER:O	1:A:997:ARG:NH2	2.36	0.57
1:B:117:LEU:HD13	1:B:130:VAL:HG22	1.86	0.57
1:A:81:ASN:O	1:A:239:GLN:NE2	2.37	0.57
1:C:1036:ARG:CZ	1:C:1039:PHE:CE1	2.87	0.57
1:A:324:VAL:O	1:A:528:THR:OG1	2.23	0.57
1:C:733:VAL:HG13	1:C:855:LEU:HD23	1.87	0.57
1:A:868:ALA:O	1:A:871:THR:OG1	2.21	0.57
1:B:799:PHE:CD1	1:B:802:ILE:HD11	2.40	0.56
1:B:799:PHE:HD1	1:B:802:ILE:HD11	1.70	0.56
2:E:29:ILE:HG21	2:E:73:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:ASP:HB3	1:B:578:THR:O	2.05	0.56
1:A:303:PHE:O	1:A:304:THR:OG1	2.18	0.56
1:C:877:GLY:O	1:C:881:SER:OG	2.21	0.56
1:A:329:ILE:O	1:A:329:ILE:HD13	2.06	0.56
1:A:711:ILE:HD12	1:A:1093:VAL:HG11	1.87	0.56
1:A:1132:ASN:ND2	1:A:1133:THR:O	2.39	0.56
2:H:29:ILE:HG21	2:H:73:ILE:HD11	1.88	0.56
2:J:29:ILE:HG21	2:J:73:ILE:HD11	1.87	0.56
1:C:869:GLN:O	1:C:872:SER:OG	2.24	0.56
1:A:57:PRO:O	1:A:60:SER:OG	2.11	0.56
1:C:297:LYS:HG2	1:C:305:VAL:HG23	1.87	0.56
1:C:417:ASP:O	1:C:458:LEU:N	2.37	0.56
1:C:966:ASN:OD1	1:C:972:SER:N	2.39	0.56
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.88	0.56
1:C:575:ASP:OD2	1:C:578:THR:OG1	2.21	0.55
1:A:1069:GLU:HG3	5:A:1308:NAG:H81	1.87	0.55
1:B:563:GLY:O	1:B:571:ASP:N	2.38	0.55
1:A:306:GLU:O	1:A:310:TYR:OH	2.17	0.55
1:A:419:ASN:OD1	1:A:451:ARG:N	2.34	0.55
1:C:1111:ILE:O	1:C:1116:ASN:ND2	2.39	0.55
1:B:1078:ILE:O	1:B:1085:HIS:N	2.35	0.55
1:C:291:ASP:OD1	1:C:294:SER:N	2.29	0.55
1:B:311:GLN:NE2	1:B:313:SER:O	2.37	0.55
1:B:756:PHE:CD2	1:B:998:LEU:HD21	2.42	0.55
1:A:1111:ILE:O	1:A:1116:ASN:ND2	2.39	0.55
1:A:608:LEU:HD22	1:A:663:ILE:HG23	1.88	0.54
1:C:312:THR:HG21	1:C:594:VAL:HG23	1.88	0.54
1:A:723:ILE:HG22	1:A:945:LEU:HD13	1.88	0.54
1:A:750:LEU:HD11	1:A:757:CYS:SG	2.48	0.54
1:A:146:HIS:O	1:A:150:LYS:N	2.40	0.54
1:A:99:ASN:OD1	1:A:190:ARG:NH2	2.40	0.54
1:A:975:ASN:O	1:A:979:SER:OG	2.21	0.54
1:C:47:VAL:HG22	1:C:48:LEU:N	2.23	0.54
1:A:575:ASP:OD2	1:A:578:THR:OG1	2.17	0.54
1:B:277:ASN:OD1	1:B:281:THR:N	2.41	0.54
1:C:293:LEU:HD11	1:C:599:THR:CG2	2.37	0.54
1:C:293:LEU:O	1:C:296:THR:OG1	2.20	0.54
1:A:727:SER:O	1:A:1055:HIS:HB3	2.08	0.53
1:C:363:SER:O	1:C:367:ASN:ND2	2.41	0.53
1:A:442:VAL:HG21	2:H:58:SER:HB2	1.90	0.53
1:C:736:THR:O	1:C:740:CYS:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:VAL:HB	2:E:121:VAL:HG12	1.90	0.53
1:B:961:LYS:O	1:B:964:SER:OG	2.24	0.53
2:H:49:TRP:CE2	3:L:97:ILE:HD12	2.43	0.53
1:B:117:LEU:HD12	1:B:118:LEU:H	1.72	0.53
1:B:790:PRO:O	1:B:792:LYS:NZ	2.38	0.53
1:B:943:GLY:O	1:B:947:ASP:N	2.33	0.53
1:B:1026:MET:O	1:B:1030:VAL:HB	2.08	0.53
1:A:946:GLN:NE2	1:A:950:ASN:OD1	2.42	0.53
3:L:18:ARG:HH21	3:L:74:THR:HG21	1.74	0.53
1:C:565:ASP:OD1	1:C:566:ILE:N	2.36	0.53
1:C:816:GLU:OE2	1:C:1052:SER:N	2.37	0.53
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.27	0.53
1:A:1026:MET:O	1:A:1030:VAL:HB	2.09	0.53
1:B:417:ASP:O	1:B:458:LEU:N	2.35	0.52
1:B:442:VAL:HG21	2:E:58:SER:HB2	1.91	0.52
1:A:495:GLN:NE2	2:H:102:GLU:OE1	2.41	0.52
1:A:820:PHE:CE1	1:A:1053:ALA:HA	2.44	0.52
1:B:1111:ILE:O	1:B:1116:ASN:ND2	2.42	0.52
1:C:442:VAL:HG21	2:J:58:SER:HB2	1.91	0.52
1:A:312:THR:HG21	1:A:594:VAL:HG23	1.91	0.52
1:A:737:MET:O	1:A:741:GLY:N	2.42	0.52
2:E:66:LYS:HA	2:E:69:VAL:HG12	1.92	0.52
1:C:714:ASN:OD1	1:C:715:PHE:N	2.38	0.52
1:B:146:HIS:O	1:B:150:LYS:N	2.43	0.52
1:A:329:ILE:HA	1:A:359:VAL:HG21	1.92	0.52
1:C:48:LEU:CD1	1:C:302:SER:HA	2.40	0.52
2:J:66:LYS:HA	2:J:69:VAL:HG12	1.90	0.52
1:B:329:ILE:HG12	1:B:329:ILE:O	2.10	0.52
1:B:189:LEU:HD22	1:B:217:PRO:HG3	1.92	0.52
2:H:12:VAL:HB	2:H:121:VAL:HG12	1.91	0.52
1:B:789:PRO:HG3	1:A:704:TYR:HB3	1.92	0.51
1:A:1123:CYS:SG	1:A:1129:ILE:HD13	2.51	0.51
2:E:39:ILE:HD11	2:E:110:PHE:CE2	2.46	0.51
2:E:49:TRP:CE2	3:F:97:ILE:HD12	2.44	0.51
1:B:31:SER:OG	1:B:60:SER:N	2.40	0.51
1:B:331:ASN:OD1	1:B:332:LEU:N	2.43	0.51
1:C:400:ARG:NH1	1:C:403:GLU:OE2	2.43	0.51
1:A:863:THR:O	1:A:866:MET:N	2.43	0.51
2:H:60:TYR:OH	2:H:102:GLU:OE2	2.28	0.51
1:B:733:VAL:HG11	1:B:1001:LEU:HD21	1.93	0.51
2:J:92:THR:HG23	2:J:121:VAL:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.40	0.51
1:B:317:VAL:HG12	1:B:588:SER:O	2.11	0.51
1:C:325:ARG:NH2	1:C:577:GLN:OE1	2.44	0.51
1:B:43:PHE:HB3	1:A:562:PHE:O	2.11	0.51
1:B:820:PHE:CE1	1:B:1053:ALA:HA	2.47	0.51
1:A:194:PHE:HB3	1:A:201:PHE:CZ	2.47	0.50
1:A:913:LEU:C	1:A:913:LEU:HD13	2.31	0.50
1:A:143:VAL:HG12	1:A:154:GLU:HA	1.92	0.50
1:A:293:LEU:O	1:A:296:THR:OG1	2.22	0.50
1:A:356:SER:OG	1:A:391:ASN:OD1	2.17	0.50
2:J:55:TYR:HA	2:J:73:ILE:HD13	1.93	0.50
1:C:390:THR:O	1:C:520:THR:OG1	2.21	0.50
1:A:529:ASN:OD1	1:A:530:LEU:N	2.44	0.50
1:C:958:THR:HG23	1:A:755:SER:OG	2.11	0.50
2:H:66:LYS:HA	2:H:69:VAL:HG12	1.92	0.50
2:J:6:GLU:N	2:J:6:GLU:OE1	2.45	0.50
1:B:143:VAL:HG12	1:B:154:GLU:HA	1.93	0.50
1:A:799:PHE:HD2	1:A:802:ILE:HD11	1.77	0.50
2:E:60:TYR:OH	2:E:102:GLU:OE2	2.24	0.50
2:H:39:ILE:HD11	2:H:110:PHE:CE2	2.47	0.49
1:C:146:HIS:O	1:C:150:LYS:N	2.45	0.49
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.93	0.49
1:C:965:SER:HB2	1:C:967:PHE:CE2	2.48	0.49
1:C:641:GLN:NE2	1:C:645:GLY:O	2.45	0.49
1:C:756:PHE:CG	1:C:757:CYS:N	2.80	0.49
1:A:311:GLN:NE2	1:A:313:SER:O	2.44	0.49
4:G:1:NAG:O4	4:G:2:NAG:O7	2.30	0.49
1:C:1078:ILE:O	1:C:1085:HIS:N	2.45	0.49
1:B:495:GLN:NE2	2:E:102:GLU:OE1	2.41	0.49
1:C:337:GLU:OE2	1:C:353:LYS:NZ	2.38	0.49
1:B:906:ILE:HG13	1:B:908:VAL:HG23	1.94	0.49
1:A:288:CYS:O	1:A:295:GLU:HG3	2.12	0.49
1:A:723:ILE:HG22	1:A:945:LEU:CD1	2.43	0.49
1:A:770:GLU:OE2	1:A:1016:ARG:NH1	2.38	0.49
1:A:943:GLY:O	1:A:947:ASP:N	2.37	0.49
1:B:723:ILE:CG2	1:B:945:LEU:HD13	2.43	0.49
1:C:749:LEU:HD12	1:C:990:ILE:HG21	1.94	0.48
1:C:947:ASP:OD1	1:C:947:ASP:N	2.46	0.48
1:A:563:GLY:N	1:A:572:ALA:O	2.45	0.48
1:A:772:ASP:N	1:A:772:ASP:OD1	2.45	0.48
3:L:61:ARG:NE	3:L:82:ASP:OD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASP:OD1	1:B:285:ALA:N	2.46	0.48
1:C:865:GLU:OE1	1:C:865:GLU:N	2.38	0.48
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.24	0.48
1:A:517:ALA:HB1	1:A:518:PRO:HD2	1.93	0.48
2:H:102:GLU:HA	2:H:107:SER:O	2.14	0.48
1:A:286:VAL:HG23	1:A:303:PHE:CE2	2.48	0.48
1:A:291:ASP:OD1	1:A:291:ASP:N	2.45	0.48
1:C:702:VAL:HG12	1:A:892:GLN:HB3	1.95	0.48
1:A:1078:ILE:O	1:A:1085:HIS:N	2.47	0.48
1:C:383:LYS:CB	1:A:979:SER:O	2.61	0.47
1:B:1036:ARG:HB3	1:C:1028:GLU:OE2	2.13	0.47
1:C:29:THR:HG22	1:C:30:ASN:N	2.29	0.47
1:C:913:LEU:C	1:C:913:LEU:HD13	2.34	0.47
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.47	0.47
2:J:18:LEU:CB	2:J:87:VAL:HG21	2.43	0.47
1:A:702:VAL:O	1:A:704:TYR:N	2.47	0.47
3:K:61:ARG:NE	3:K:82:ASP:OD2	2.46	0.47
1:B:989:GLN:OE1	1:B:992:ARG:NH1	2.48	0.47
1:C:300:LEU:HD22	1:C:305:VAL:HG13	1.96	0.47
2:J:89:ALA:HA	2:J:121:VAL:HG23	1.97	0.47
1:A:817:ASP:O	1:A:821:ASN:ND2	2.46	0.47
2:J:92:THR:HG22	2:J:121:VAL:HG22	1.96	0.47
1:A:328:ASN:OD1	1:A:328:ASN:N	2.47	0.47
2:H:106:THR:HG21	3:L:31:SER:OG	2.15	0.47
2:J:92:THR:HG22	2:J:121:VAL:N	2.19	0.47
1:B:906:ILE:HG23	1:B:1033:GLN:NE2	2.30	0.47
1:C:919:LEU:HD11	1:C:923:GLN:NE2	2.30	0.47
1:B:293:LEU:O	1:B:296:THR:OG1	2.23	0.47
1:C:1086:PHE:HB2	1:C:1118:PHE:CZ	2.50	0.47
1:A:317:VAL:HG12	1:A:588:SER:O	2.15	0.47
1:A:712:PRO:HA	1:A:1068:GLN:O	2.14	0.47
1:C:351:ASN:OD1	1:C:352:ARG:N	2.48	0.47
1:A:767:ILE:O	1:A:771:GLN:HG2	2.15	0.47
1:B:813:SER:OG	1:B:1051:GLN:OE1	2.28	0.46
1:C:696:LEU:O	1:C:697:GLY:C	2.53	0.46
1:B:313:SER:OG	1:B:314:ASN:N	2.48	0.46
1:B:614:CYS:N	1:B:641:GLN:OE1	2.49	0.46
1:A:293:LEU:HD11	1:A:599:THR:CG2	2.43	0.46
2:H:121:VAL:HG23	2:H:121:VAL:O	2.15	0.46
2:E:106:THR:HG21	3:F:31:SER:OG	2.15	0.46
2:J:106:THR:HG21	3:K:31:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASP:OD2	1:B:293:LEU:HB3	2.15	0.46
1:B:1064:TYR:CE1	1:B:1066:PRO:HD3	2.51	0.46
1:C:756:PHE:O	1:C:759:GLN:HG2	2.15	0.46
2:E:102:GLU:HA	2:E:107:SER:O	2.15	0.46
1:B:1064:TYR:HE1	1:B:1066:PRO:HG3	1.80	0.46
1:C:201:PHE:HE2	1:C:203:ILE:HD11	1.80	0.46
1:C:589:PHE:HE2	1:A:856:THR:HG22	1.80	0.46
1:A:325:ARG:NH1	1:A:575:ASP:OD2	2.48	0.46
1:A:736:THR:O	1:A:740:CYS:HB2	2.16	0.46
1:B:296:THR:CG2	1:B:594:VAL:HG11	2.46	0.46
1:B:745:GLU:OE1	1:B:745:GLU:N	2.39	0.46
1:B:1085:HIS:CE1	1:B:1119:VAL:HG12	2.51	0.46
3:F:21:LEU:N	3:F:21:LEU:HD12	2.31	0.46
2:J:121:VAL:HG23	2:J:121:VAL:O	2.15	0.46
1:B:29:THR:HG22	1:B:30:ASN:N	2.30	0.46
1:A:617:VAL:HG11	1:A:648:ILE:HD11	1.98	0.46
1:B:704:TYR:HB3	1:C:789:PRO:HG3	1.97	0.46
1:B:293:LEU:HD11	1:B:599:THR:CG2	2.36	0.46
1:C:1102:THR:HB	1:C:1109:PRO:HA	1.97	0.46
2:H:55:TYR:HA	2:H:73:ILE:HD13	1.98	0.46
3:L:21:LEU:HD12	3:L:21:LEU:N	2.30	0.46
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.51	0.46
1:C:48:LEU:HD23	1:C:275:LYS:HA	1.96	0.46
1:C:719:VAL:O	1:C:931:ILE:HD11	2.16	0.46
1:B:902:ARG:NH1	1:B:1046:LEU:O	2.49	0.46
1:A:307:LYS:HG3	1:A:661:ILE:HD11	1.98	0.46
1:A:892:GLN:OE1	1:A:892:GLN:N	2.37	0.46
3:K:21:LEU:N	3:K:21:LEU:HD12	2.31	0.46
1:B:35:GLY:HA2	1:B:91:TYR:CD1	2.51	0.45
1:A:976:ASP:O	1:A:980:ARG:HG3	2.17	0.45
1:A:117:LEU:HD12	1:A:118:LEU:H	1.80	0.45
1:B:575:ASP:C	1:B:575:ASP:OD1	2.54	0.45
1:A:96:GLU:OE2	1:A:190:ARG:NH1	2.44	0.45
3:L:3:VAL:HG12	3:L:26:SER:HB3	1.98	0.45
1:B:595:ILE:HD12	1:B:595:ILE:H	1.81	0.45
1:C:100:ILE:HA	1:C:243:ILE:HG22	1.98	0.45
1:C:942:LEU:N	1:C:942:LEU:HD22	2.32	0.45
2:E:121:VAL:HG23	2:E:121:VAL:O	2.16	0.45
1:B:117:LEU:HD11	1:B:128:ILE:HG23	1.98	0.45
1:B:141:LEU:O	1:B:244:SER:N	2.43	0.45
1:C:611:GLY:N	1:C:644:ALA:O	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:LEU:HD11	1:C:756:PHE:CZ	2.52	0.45
1:A:749:LEU:HD11	1:A:987:GLU:HG2	1.98	0.45
1:C:411:GLN:O	1:C:421:LYS:NZ	2.50	0.45
1:A:565:ASP:OD1	1:A:566:ILE:N	2.40	0.45
1:B:291:ASP:OD1	1:B:294:SER:OG	2.22	0.45
1:C:1036:ARG:HD3	1:C:1039:PHE:CD2	2.51	0.45
1:A:312:THR:HG21	1:A:594:VAL:CG2	2.47	0.45
1:A:929:GLY:HA2	1:A:932:GLN:OE1	2.17	0.45
1:A:961:LYS:O	1:A:964:SER:OG	2.28	0.45
1:B:924:PHE:CE1	1:B:928:ILE:HD11	2.52	0.45
1:A:411:GLN:O	1:A:421:LYS:NZ	2.50	0.45
1:A:1037:VAL:HG12	1:A:1038:ASP:OD1	2.16	0.45
1:B:1049:PHE:HE2	1:B:1062:VAL:HG21	1.82	0.45
1:C:943:GLY:O	1:C:947:ASP:OD1	2.35	0.45
2:J:87:VAL:HG13	2:J:91:ASP:OD2	2.17	0.45
1:C:704:TYR:HB3	1:A:789:PRO:HG3	1.98	0.44
1:C:799:PHE:HD2	1:C:802:ILE:HD11	1.82	0.44
1:A:291:ASP:OD1	1:A:294:SER:OG	2.20	0.44
1:A:613:ASN:OD1	1:A:614:CYS:N	2.50	0.44
2:J:106:THR:HG22	2:J:106:THR:O	2.16	0.44
1:C:29:THR:HG22	1:C:30:ASN:H	1.82	0.44
1:C:117:LEU:HD12	1:C:118:LEU:H	1.81	0.44
1:A:35:GLY:HA2	1:A:91:TYR:CE1	2.52	0.44
1:B:965:SER:HB2	1:B:967:PHE:CE2	2.52	0.44
1:C:898:GLN:O	1:C:902:ARG:HG2	2.17	0.44
1:A:1088:ARG:NH1	1:A:1115:ASP:O	2.48	0.44
2:E:55:TYR:HA	2:E:73:ILE:HD13	1.98	0.44
3:K:68:GLY:C	3:K:69:THR:HG1	2.20	0.44
1:C:1026:MET:O	1:C:1030:VAL:HB	2.17	0.44
1:C:1095:ASN:ND2	4:P:1:NAG:O7	2.50	0.44
1:B:117:LEU:HD12	1:B:118:LEU:N	2.32	0.44
1:C:383:LYS:CG	1:A:979:SER:O	2.65	0.44
1:C:704:TYR:OH	1:A:794:PHE:HD1	2.01	0.44
3:F:82:ASP:O	3:F:86:TYR:OH	2.31	0.44
1:B:595:ILE:HD12	1:B:595:ILE:N	2.33	0.44
1:B:1088:ARG:NH1	1:B:1115:ASP:O	2.51	0.44
1:B:546:THR:HG22	1:B:587:CYS:SG	2.58	0.44
1:A:820:PHE:CD2	1:A:1054:PRO:HG3	2.53	0.44
2:H:6:GLU:N	2:H:6:GLU:OE1	2.51	0.44
1:C:117:LEU:HD12	1:C:118:LEU:N	2.32	0.43
1:C:746:CYS:HB2	1:C:974:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG23	1:B:223:LEU:HD23	2.00	0.43
1:B:200:TYR:CZ	1:B:230:PRO:HB3	2.54	0.43
1:B:913:LEU:O	1:B:917:GLN:N	2.51	0.43
1:B:1112:ILE:HG23	1:B:1117:THR:HG21	1.99	0.43
1:C:27:ALA:HB3	1:C:64:TRP:NE1	2.33	0.43
1:C:883:TRP:CH2	1:C:901:TYR:HB3	2.53	0.43
1:C:1036:ARG:CZ	1:C:1039:PHE:CD1	3.02	0.43
1:B:562:PHE:O	1:C:43:PHE:HB3	2.18	0.43
1:A:317:VAL:HG22	1:A:318:GLN:H	1.83	0.43
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.00	0.43
1:B:793:ASP:OD2	1:A:706:ASN:OD1	2.37	0.43
1:B:855:LEU:HD21	1:B:959:LEU:HD23	2.01	0.43
1:B:1102:THR:HB	1:B:1109:PRO:HA	2.01	0.43
1:C:712:PRO:O	1:C:1107:TYR:N	2.51	0.43
1:C:1003:THR:O	1:C:1007:GLN:HG2	2.18	0.43
2:J:87:VAL:HG13	2:J:91:ASP:HB2	2.01	0.43
1:B:317:VAL:O	1:B:317:VAL:CG1	2.66	0.43
1:B:608:LEU:HD22	1:B:663:ILE:HG23	2.00	0.43
1:A:143:VAL:HG13	1:A:243:ILE:HD11	2.00	0.43
1:A:906:ILE:HG23	1:A:1033:GLN:NE2	2.33	0.43
1:A:1004:TYR:CZ	1:A:1008:GLN:HG3	2.53	0.43
2:J:35:TYR:HB2	2:J:100:VAL:HB	2.00	0.43
1:B:776:GLN:O	1:B:780:ALA:HB3	2.19	0.43
1:A:310:TYR:N	1:A:310:TYR:CD1	2.86	0.43
1:A:1057:VAL:HG22	1:A:1058:VAL:N	2.34	0.43
1:B:324:VAL:O	1:B:528:THR:N	2.49	0.43
1:B:1004:TYR:CZ	1:B:1008:GLN:HG3	2.54	0.43
1:B:1028:GLU:OE2	1:A:1036:ARG:NE	2.36	0.43
2:E:106:THR:HG22	2:E:106:THR:O	2.19	0.43
1:B:310:TYR:O	1:B:312:THR:HG23	2.18	0.43
1:B:360:ALA:O	1:B:524:PRO:HD3	2.18	0.43
1:C:709:ILE:CD1	1:C:1091:VAL:HG21	2.48	0.43
1:A:706:ASN:OD1	1:A:706:ASN:N	2.48	0.43
1:B:65:PHE:CD1	1:B:65:PHE:N	2.87	0.42
1:A:48:LEU:CD1	1:A:302:SER:HA	2.49	0.42
2:H:106:THR:HG22	2:H:106:THR:O	2.19	0.42
3:K:90:LEU:HG	3:K:91:ARG:N	2.34	0.42
1:B:317:VAL:O	1:B:317:VAL:HG13	2.20	0.42
1:B:816:GLU:HG3	1:B:1051:GLN:CD	2.39	0.42
1:C:300:LEU:HD11	1:C:310:TYR:CD2	2.54	0.42
1:C:673:THR:HA	1:C:687:GLN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:HG22	1:C:23:GLN:N	2.35	0.42
1:C:297:LYS:HE2	1:C:599:THR:HG21	2.00	0.42
1:A:300:LEU:HD21	1:A:310:TYR:CE2	2.54	0.42
1:A:906:ILE:HG23	1:A:1033:GLN:HE22	1.83	0.42
1:A:1086:PHE:HB2	1:A:1118:PHE:CZ	2.54	0.42
1:A:1101:VAL:O	1:A:1101:VAL:HG13	2.18	0.42
2:E:6:GLU:N	2:E:6:GLU:OE1	2.52	0.42
2:J:18:LEU:HD11	2:J:119:VAL:HG21	2.01	0.42
1:B:933:ASP:O	1:B:937:SER:N	2.51	0.42
1:C:311:GLN:HA	1:C:593:SER:OG	2.19	0.42
1:C:595:ILE:N	1:C:595:ILE:HD12	2.34	0.42
1:C:614:CYS:N	1:C:641:GLN:OE1	2.52	0.42
1:B:411:GLN:O	1:B:421:LYS:NZ	2.52	0.42
1:C:389:PHE:N	1:C:521:VAL:O	2.45	0.42
1:C:1070:LYS:HB2	1:C:1072:PHE:CE2	2.55	0.42
1:A:877:GLY:O	1:A:881:SER:OG	2.32	0.42
3:F:3:VAL:HG12	3:F:26:SER:HB3	2.01	0.42
1:B:736:THR:O	1:B:740:CYS:N	2.38	0.42
1:B:938:THR:HG22	1:B:940:SER:H	1.84	0.42
1:C:933:ASP:OD1	1:C:933:ASP:N	2.52	0.42
1:C:1083:LYS:O	1:C:1085:HIS:ND1	2.53	0.42
1:B:141:LEU:HD12	1:B:141:LEU:N	2.34	0.42
1:B:715:PHE:CB	1:B:1064:TYR:CE2	3.03	0.42
1:B:779:PHE:O	1:B:781:GLN:N	2.44	0.42
1:C:316:ARG:O	1:C:318:GLN:NE2	2.52	0.42
1:A:822:LYS:NZ	1:A:938:THR:O	2.53	0.42
1:B:892:GLN:NE2	1:A:710:ALA:HB2	2.34	0.42
1:C:194:PHE:HB3	1:C:201:PHE:CZ	2.55	0.42
1:C:284:ASP:OD1	1:C:285:ALA:N	2.53	0.42
1:C:327:PRO:C	1:C:329:ILE:H	2.23	0.42
1:C:598:GLY:O	1:C:601:THR:N	2.47	0.42
1:A:673:THR:HA	1:A:687:GLN:HA	2.00	0.42
2:H:89:ALA:HA	2:H:121:VAL:HG23	2.02	0.42
2:E:89:ALA:HA	2:E:121:VAL:HG23	2.02	0.42
1:B:653:VAL:HG12	1:B:655:ASN:N	2.34	0.42
1:C:388:CYS:HB2	1:C:541:ASN:O	2.19	0.42
1:A:943:GLY:O	1:A:944:LYS:C	2.57	0.42
1:A:981:LEU:HB3	1:A:986:ALA:HB2	2.01	0.42
3:F:68:GLY:C	3:F:69:THR:HG1	2.22	0.42
1:C:657:TYR:O	1:C:692:TYR:HE2	2.02	0.42
1:A:13:SER:OG	1:A:14:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:GLN:HA	1:B:762:ARG:NH1	2.35	0.41
1:C:42:VAL:HG12	1:C:43:PHE:N	2.34	0.41
1:C:793:ASP:OD1	1:C:793:ASP:N	2.52	0.41
1:A:119:ILE:HG12	1:A:128:ILE:HG23	2.02	0.41
1:A:189:LEU:HD22	1:A:217:PRO:HG3	2.02	0.41
3:F:61:ARG:NE	3:F:82:ASP:OD2	2.45	0.41
1:C:557:LEU:O	1:C:574:ARG:NH2	2.44	0.41
1:A:958:THR:O	1:A:962:GLN:HG2	2.20	0.41
1:A:987:GLU:HA	1:A:990:ILE:HB	2.01	0.41
1:B:1077:ALA:HB2	1:B:1086:PHE:CD2	2.56	0.41
1:C:292:PRO:HB2	1:C:605:VAL:HG21	2.02	0.41
1:C:970:ILE:HD13	1:C:981:LEU:HD11	2.02	0.41
1:A:29:THR:HG22	1:A:30:ASN:N	2.33	0.41
1:A:331:ASN:O	1:A:359:VAL:N	2.34	0.41
1:B:311:GLN:HA	1:B:593:SER:OG	2.20	0.41
1:B:753:TYR:HB3	1:B:756:PHE:HD2	1.86	0.41
1:C:141:LEU:N	1:C:141:LEU:HD12	2.36	0.41
1:C:653:VAL:HG12	1:C:655:ASN:N	2.35	0.41
1:C:733:VAL:HG22	1:C:855:LEU:HD22	2.02	0.41
1:A:100:ILE:HA	1:A:243:ILE:HG22	2.02	0.41
3:K:37:GLN:HB2	3:K:47:LEU:HD11	2.02	0.41
1:B:318:GLN:HG3	1:B:319:PRO:HD2	2.02	0.41
1:B:398:VAL:HG22	1:B:506:ARG:HG2	2.03	0.41
1:C:608:LEU:CD2	1:C:663:ILE:HG23	2.45	0.41
1:C:810:SER:O	1:C:812:ARG:N	2.53	0.41
1:C:1026:MET:SD	1:C:1030:VAL:HG21	2.60	0.41
1:A:134:GLN:O	1:A:161:SER:N	2.52	0.41
1:A:498:TYR:HB3	1:A:502:TYR:HB2	2.01	0.41
1:A:973:VAL:HB	1:A:976:ASP:CG	2.40	0.41
1:B:910:GLN:NE2	1:A:1087:PRO:HD2	2.35	0.41
1:B:1004:TYR:CE2	1:B:1008:GLN:HG3	2.55	0.41
1:C:723:ILE:HG21	1:C:945:LEU:HG	2.02	0.41
1:A:48:LEU:HD12	1:A:301:LYS:O	2.20	0.41
1:A:966:ASN:OD1	1:A:966:ASN:N	2.53	0.41
1:A:982:ASP:O	1:A:986:ALA:N	2.32	0.41
3:F:90:LEU:HG	3:F:91:ARG:N	2.36	0.41
1:B:143:VAL:HG13	1:B:243:ILE:HD11	2.03	0.41
1:B:709:ILE:HG21	1:B:1093:VAL:HG12	2.01	0.41
1:A:1038:ASP:OD1	1:A:1038:ASP:N	2.53	0.41
1:A:1064:TYR:HE1	1:A:1066:PRO:HG3	1.86	0.41
2:J:60:TYR:OH	2:J:102:GLU:OE2	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:21:LEU:HD12	3:K:21:LEU:H	1.85	0.41
3:K:50:ASP:HB2	3:K:53:ASP:OD2	2.21	0.41
1:B:296:THR:HG21	1:B:594:VAL:HG11	2.03	0.41
1:C:305:VAL:HB	1:C:599:THR:HG23	2.01	0.41
1:C:379:VAL:HG22	1:C:380:SER:N	2.36	0.41
1:A:200:TYR:CZ	1:A:230:PRO:HB3	2.56	0.41
1:A:883:TRP:HB3	1:A:1032:GLY:HA2	2.03	0.41
1:B:712:PRO:HA	1:B:1068:GLN:O	2.21	0.41
1:B:1077:ALA:HB2	1:B:1086:PHE:CE2	2.56	0.41
1:B:1135:TYR:OH	1:B:1140:PRO:HG3	2.21	0.41
1:C:143:VAL:HG12	1:C:154:GLU:HA	2.02	0.41
1:C:657:TYR:HB2	1:C:692:TYR:CZ	2.55	0.41
1:C:871:THR:O	1:C:875:LEU:HD12	2.20	0.41
1:A:204:TYR:N	1:A:204:TYR:CD1	2.89	0.41
1:C:721:THR:OG1	1:C:931:ILE:HD12	2.21	0.41
1:C:894:PRO:HB2	1:C:897:MET:HG3	2.03	0.41
1:C:1073:THR:HB	1:C:1094:SER:HB3	2.03	0.41
2:H:49:TRP:O	2:H:62:ASN:ND2	2.54	0.41
3:L:90:LEU:HG	3:L:91:ARG:N	2.36	0.41
1:B:613:ASN:OD1	1:B:614:CYS:N	2.54	0.40
1:A:22:THR:HG22	1:A:23:GLN:N	2.36	0.40
1:A:981:LEU:CB	1:A:986:ALA:HB2	2.51	0.40
1:B:122:ASN:OD1	1:B:125:ASN:N	2.43	0.40
1:B:913:LEU:HD22	1:B:920:ILE:HD12	2.02	0.40
1:A:388:CYS:HB3	1:A:519:ALA:HB1	2.02	0.40
3:F:37:GLN:HB2	3:F:47:LEU:HD11	2.04	0.40
1:B:22:THR:HG22	1:B:23:GLN:N	2.36	0.40
1:B:714:ASN:OD1	1:B:715:PHE:N	2.54	0.40
1:B:933:ASP:OD1	1:B:933:ASP:N	2.54	0.40
1:C:734:ASP:OD2	1:C:737:MET:HB2	2.21	0.40
1:A:653:VAL:HG12	1:A:655:ASN:N	2.37	0.40
1:B:48:LEU:CD1	1:B:302:SER:HA	2.51	0.40
1:B:609:TYR:HE2	1:B:648:ILE:HD12	1.86	0.40
1:C:717:ILE:HG13	1:C:920:ILE:HG23	2.03	0.40
1:C:750:LEU:HD21	1:C:756:PHE:HZ	1.87	0.40
1:C:756:PHE:O	1:C:760:LEU:HG	2.22	0.40
1:C:1036:ARG:NH2	1:C:1039:PHE:CE1	2.89	0.40
1:A:652:HIS:ND1	1:A:653:VAL:N	2.69	0.40
1:A:756:PHE:O	1:A:759:GLN:HG2	2.21	0.40
2:H:35:TYR:HB2	2:H:100:VAL:HB	2.03	0.40
3:L:30:THR:HG23	3:L:68:GLY:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:TYR:HB2	2:E:100:VAL:HB	2.03	0.40
2:J:39:ILE:HD12	2:J:39:ILE:N	2.36	0.40
2:J:87:VAL:HG11	2:J:121:VAL:CG1	2.38	0.40
1:C:48:LEU:HD12	1:C:302:SER:HA	2.03	0.40
1:C:575:ASP:HB3	1:C:578:THR:O	2.22	0.40
1:C:733:VAL:HG11	1:C:1001:LEU:HD21	2.03	0.40
1:C:1087:PRO:O	1:A:910:GLN:OE1	2.40	0.40
2:J:41:GLN:NE2	3:K:38:GLN:OE1	2.51	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	1027/1285 (80%)	983 (96%)	44 (4%)	0	100	100
1	B	1026/1285 (80%)	988 (96%)	37 (4%)	1 (0%)	51	85
1	C	1022/1285 (80%)	974 (95%)	46 (4%)	2 (0%)	47	81
2	E	120/228 (53%)	108 (90%)	11 (9%)	1 (1%)	19	60
2	H	120/228 (53%)	108 (90%)	11 (9%)	1 (1%)	19	60
2	J	120/228 (53%)	108 (90%)	11 (9%)	1 (1%)	19	60
3	F	106/215 (49%)	94 (89%)	9 (8%)	3 (3%)	5	33
3	K	106/215 (49%)	94 (89%)	9 (8%)	3 (3%)	5	33
3	L	106/215 (49%)	94 (89%)	9 (8%)	3 (3%)	5	33
All	All	3753/5184 (72%)	3551 (95%)	187 (5%)	15 (0%)	38	72

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	697	GLY
3	F	69	THR
3	K	69	THR
1	B	329	ILE
1	C	525	LYS
3	L	31	SER
3	L	68	GLY
3	F	31	SER
3	K	31	SER
2	E	103	PRO
3	K	97	ILE
2	H	103	PRO
3	L	97	ILE
3	F	97	ILE
2	J	103	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	914/1109 (82%)	904 (99%)	10 (1%)	73	85
1	B	913/1109 (82%)	906 (99%)	7 (1%)	81	89
1	C	910/1109 (82%)	903 (99%)	7 (1%)	81	89
2	E	107/199 (54%)	107 (100%)	0	100	100
2	H	107/199 (54%)	107 (100%)	0	100	100
2	J	107/199 (54%)	107 (100%)	0	100	100
3	F	92/188 (49%)	91 (99%)	1 (1%)	73	85
3	K	92/188 (49%)	91 (99%)	1 (1%)	73	85
3	L	92/188 (49%)	91 (99%)	1 (1%)	73	85
All	All	3334/4488 (74%)	3307 (99%)	27 (1%)	82	89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	PHE
1	B	263	TYR
1	B	318	GLN
1	B	329	ILE
1	B	374	PHE
1	B	446	TYR
1	B	875	LEU
1	C	65	PHE
1	C	263	TYR
1	C	307	LYS
1	C	446	TYR
1	C	875	LEU
1	C	947	ASP
1	C	1001	LEU
1	A	65	PHE
1	A	263	TYR
1	A	328	ASN
1	A	329	ILE
1	A	374	PHE
1	A	446	TYR
1	A	640	PHE
1	A	652	HIS
1	A	875	LEU
1	A	1001	LEU
3	L	106	GLU
3	F	106	GLU
3	K	106	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	962	GLN
1	B	1008	GLN
1	B	1020	ASN
1	B	1085	HIS
1	B	1132	ASN
1	C	328	ASN
1	C	484	ASN
1	C	774	ASN
1	C	898	GLN
1	C	1008	GLN
1	A	577	GLN
1	A	610	GLN

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Mol	Chain	Res	Type
1	A	821	ASN
1	A	898	GLN
1	A	910	GLN
1	A	946	GLN
1	A	950	ASN
1	A	1008	GLN
1	A	1085	HIS
1	A	1116	ASN
1	A	1132	ASN

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

24 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	0.29	0	17,19,21	0.33	0
4	NAG	D	2	4	14,14,15	0.16	0	17,19,21	0.43	0
4	NAG	G	1	4,1	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	G	2	4	14,14,15	0.17	0	17,19,21	0.35	0
4	NAG	I	1	4,1	14,14,15	0.18	0	17,19,21	0.46	0
4	NAG	I	2	4	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	M	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	M	2	4	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	N	1	4,1	14,14,15	0.23	0	17,19,21	0.33	0
4	NAG	N	2	4	14,14,15	0.17	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	O	1	4,1	14,14,15	0.16	0	17,19,21	0.51	0
4	NAG	O	2	4	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	P	1	4,1	14,14,15	0.17	0	17,19,21	0.44	0
4	NAG	P	2	4	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	Q	1	4,1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	Q	2	4	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	R	1	4,1	14,14,15	0.34	0	17,19,21	0.34	0
4	NAG	R	2	4	14,14,15	0.15	0	17,19,21	0.47	0
4	NAG	S	1	4,1	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	S	2	4	14,14,15	0.27	0	17,19,21	0.34	0
4	NAG	T	1	4,1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	T	2	4	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	U	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	U	2	4	14,14,15	0.26	0	17,19,21	0.40	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	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	S	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6

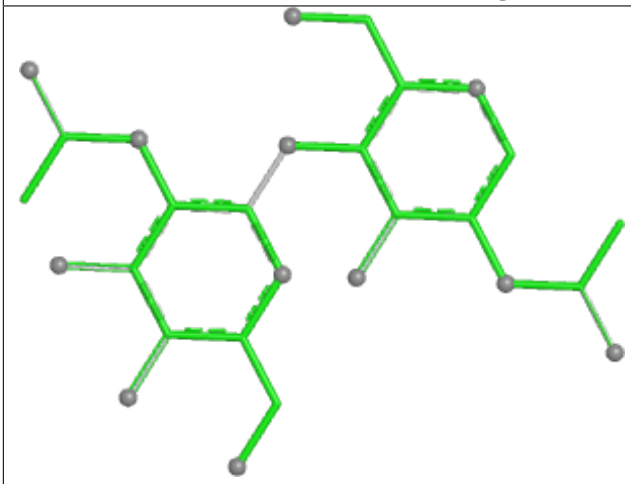
There are no ring outliers.

3 monomers are involved in 2 short contacts:

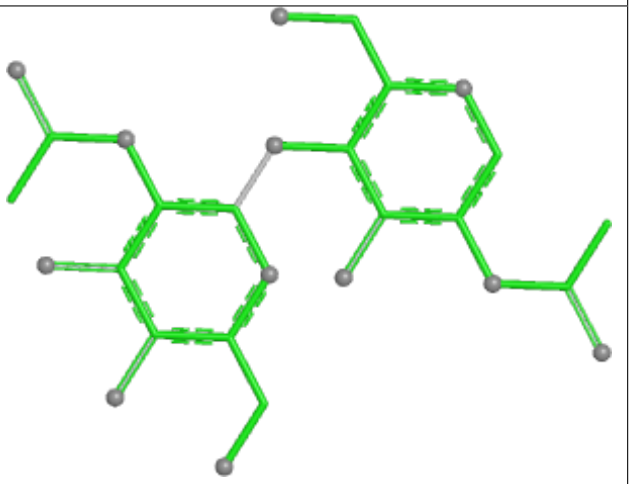
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
4	P	1	NAG	1	0
4	G	2	NAG	1	0

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

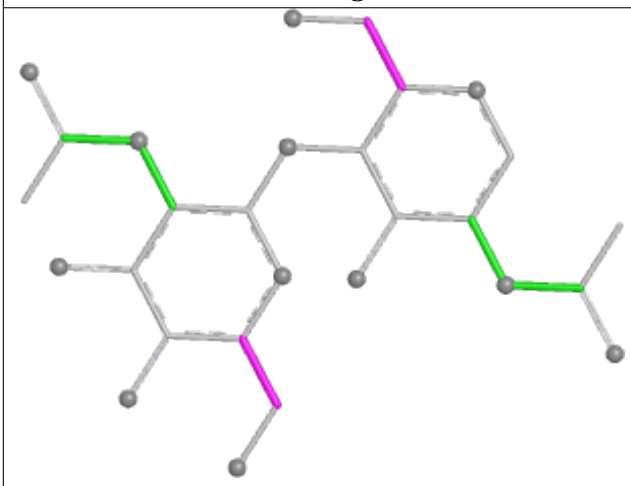
Oligosaccharide Chain D



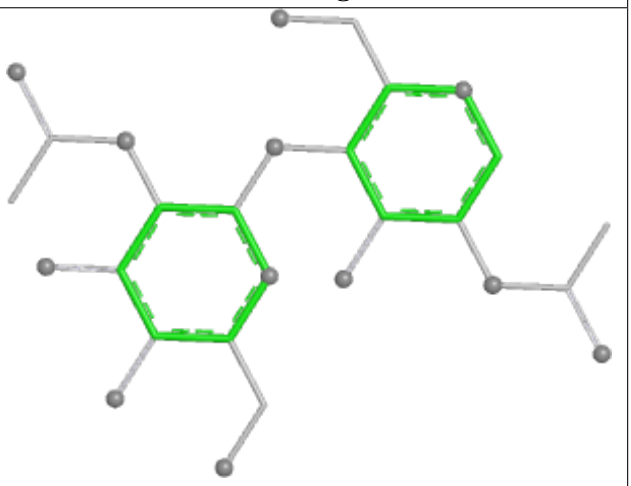
Bond lengths



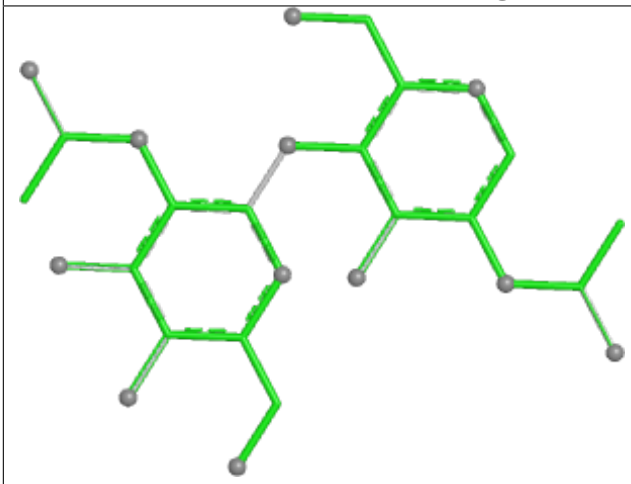
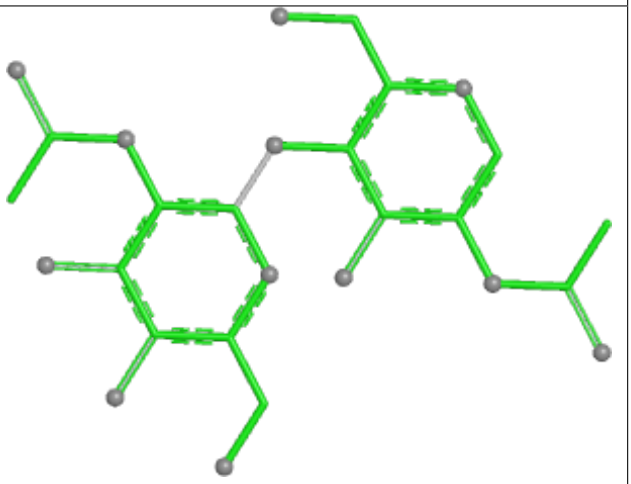
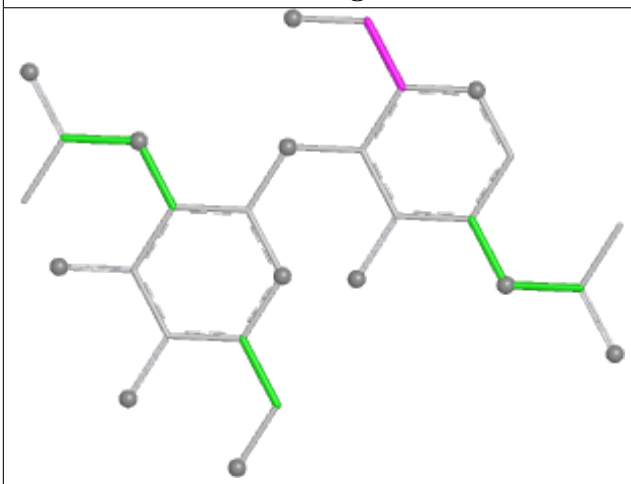
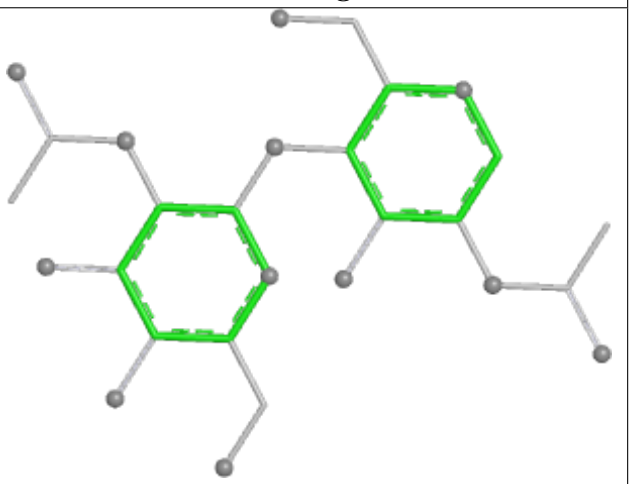
Bond angles

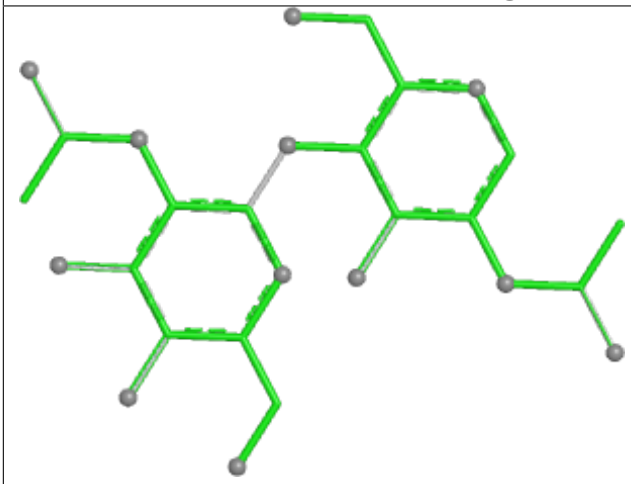
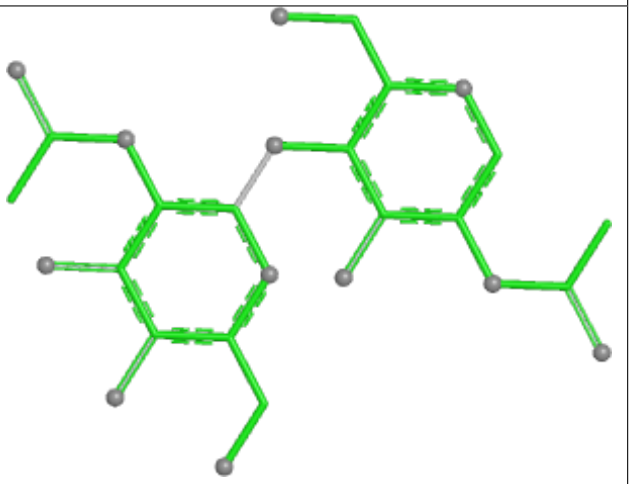
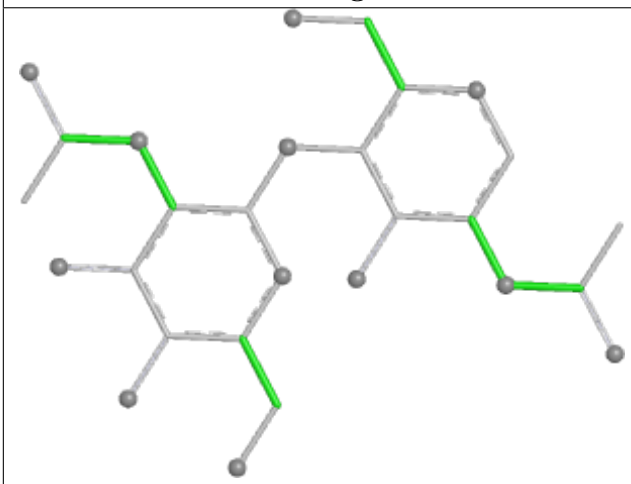
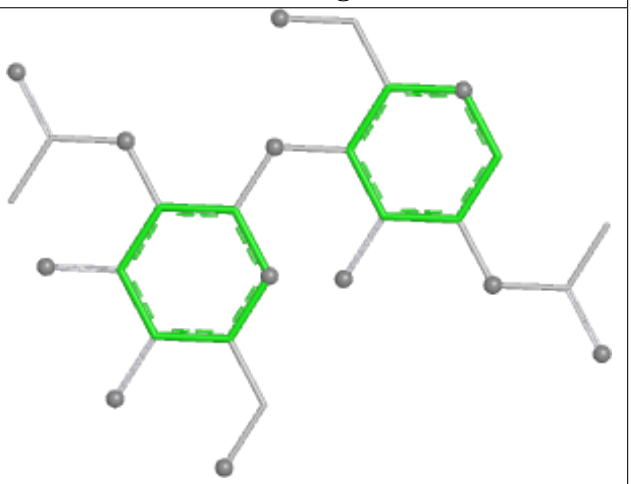


Torsions

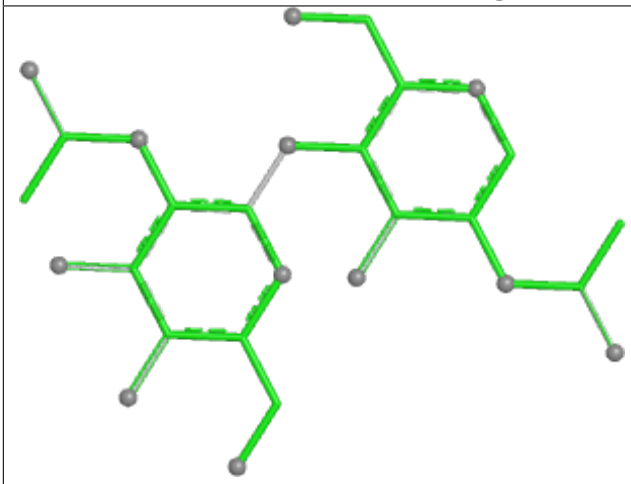


Rings

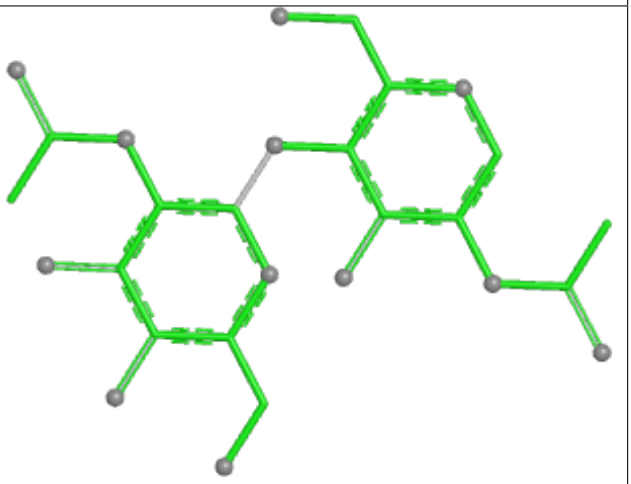
Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain I	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

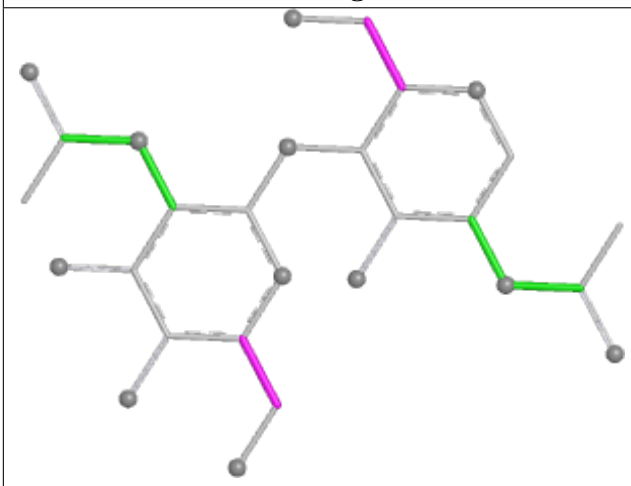
Oligosaccharide Chain M



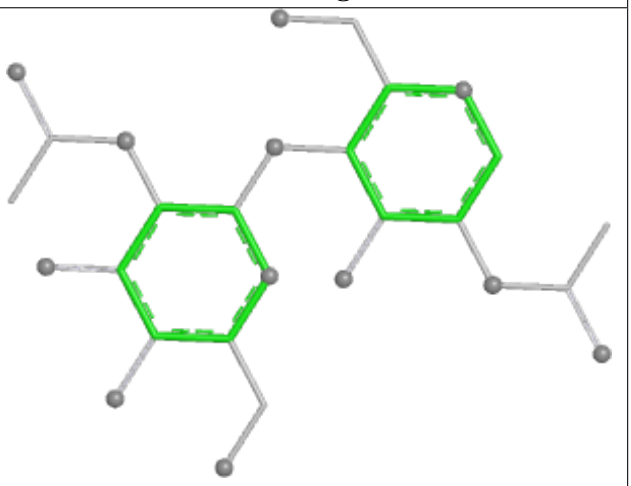
Bond lengths



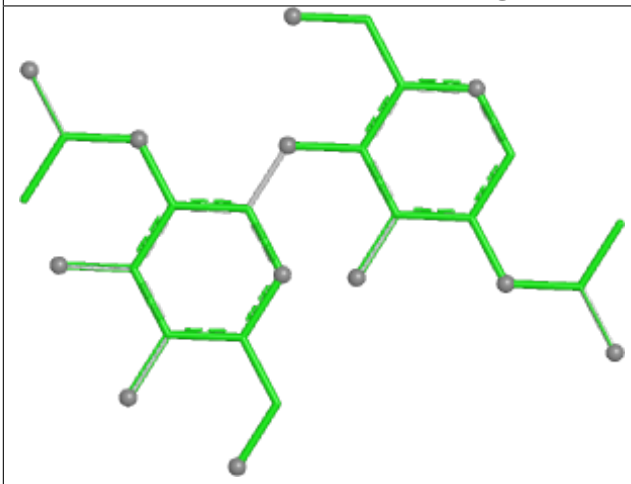
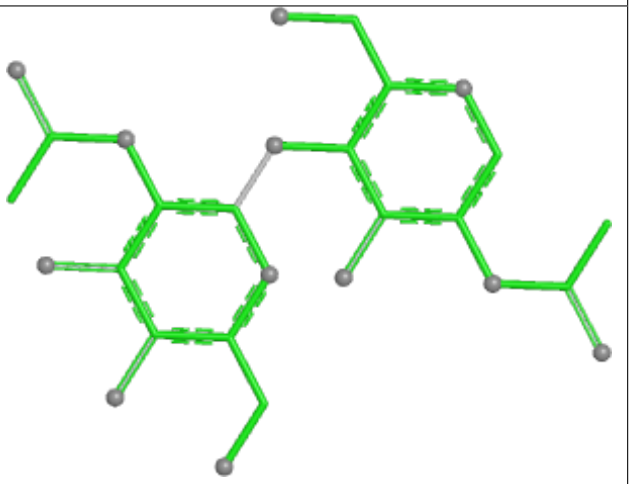
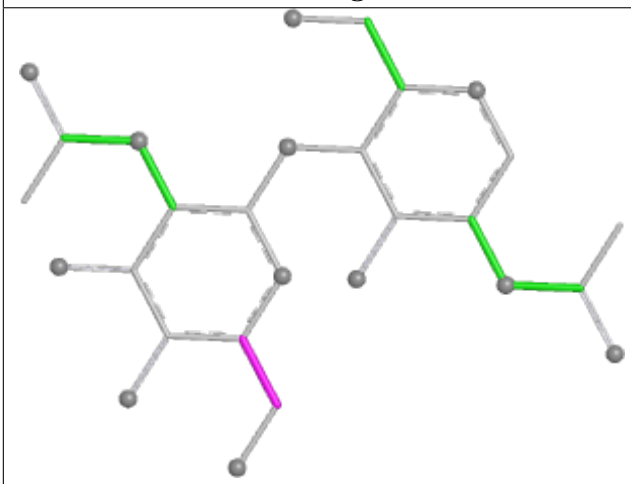
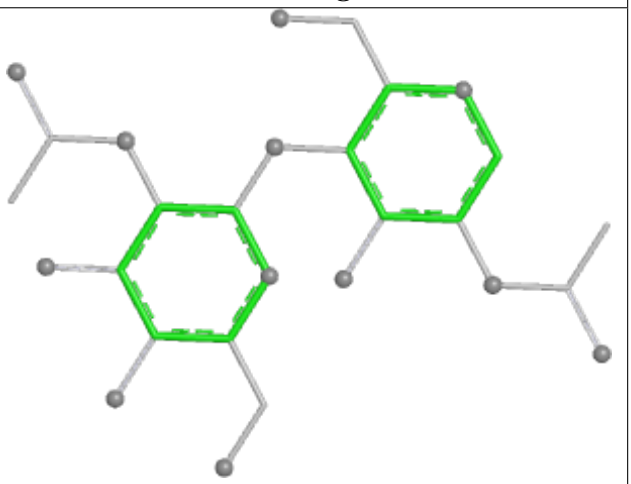
Bond angles



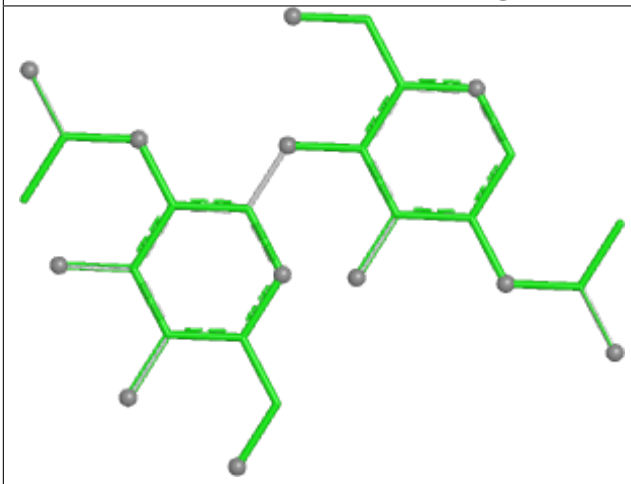
Torsions



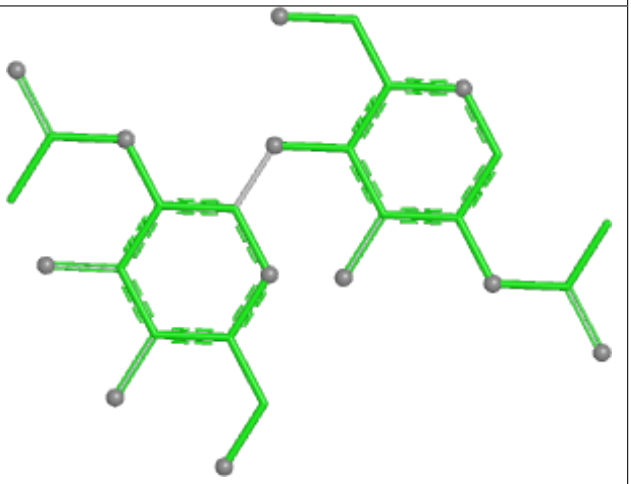
Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

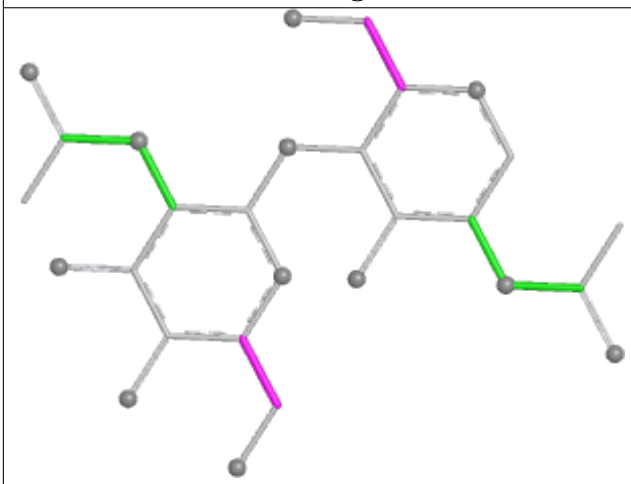
Oligosaccharide Chain O



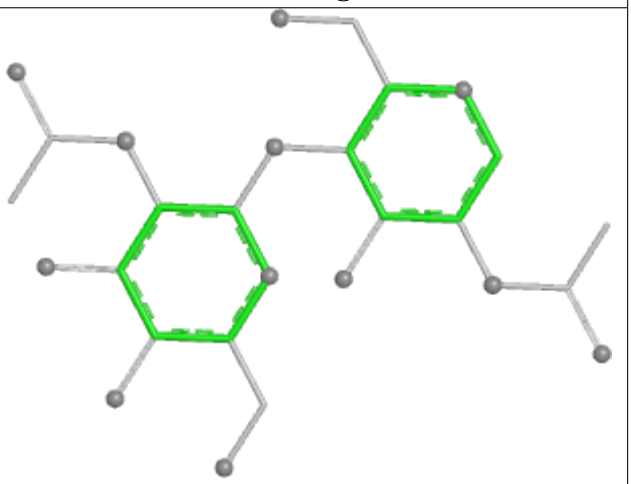
Bond lengths



Bond angles

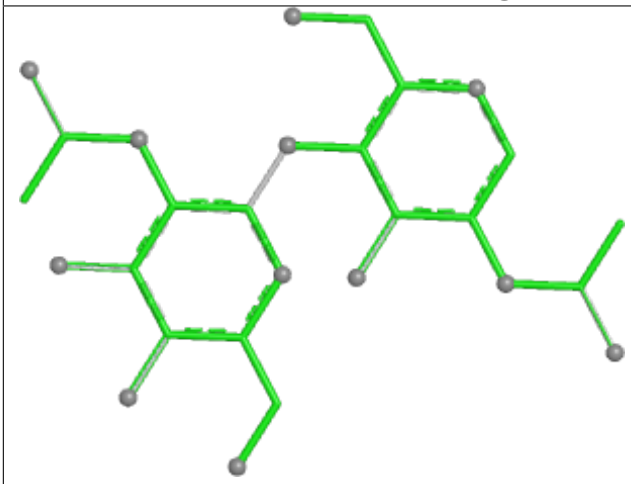


Torsions

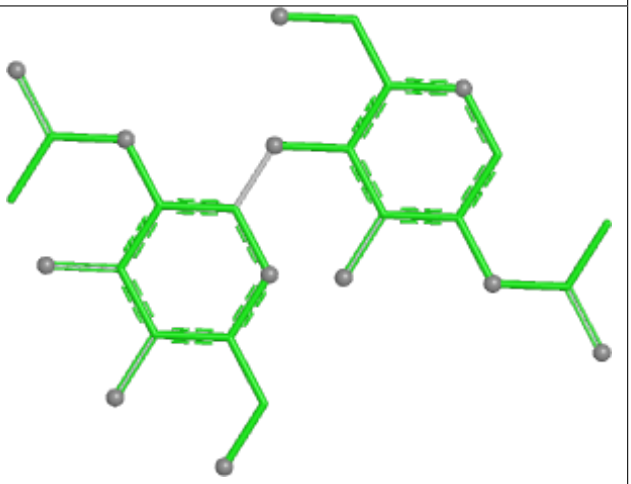


Rings

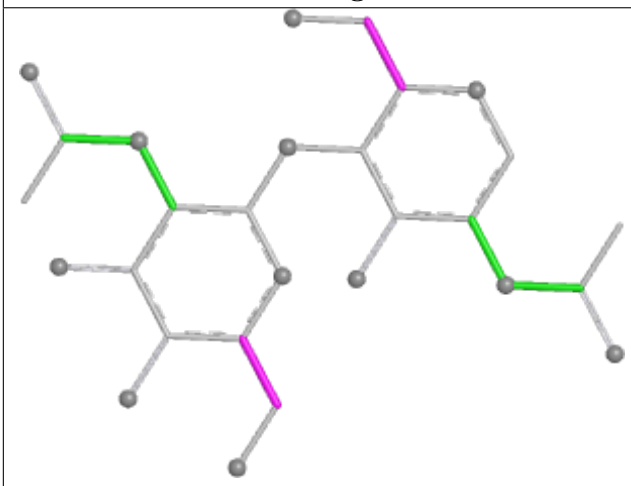
Oligosaccharide Chain P



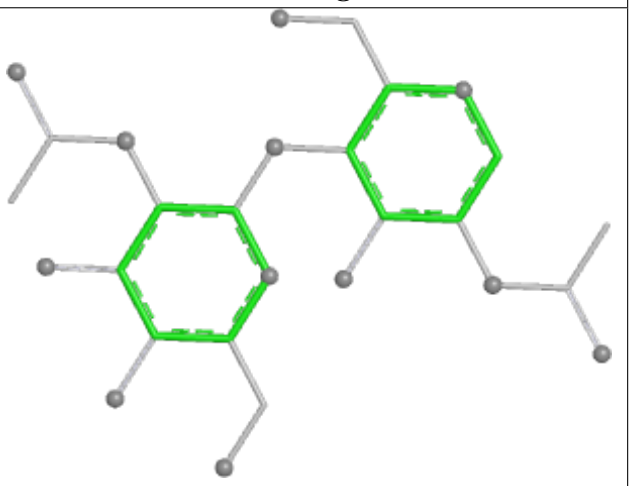
Bond lengths



Bond angles

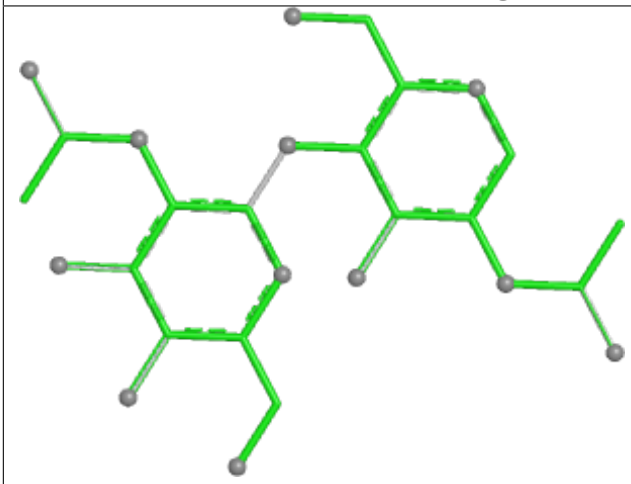


Torsions

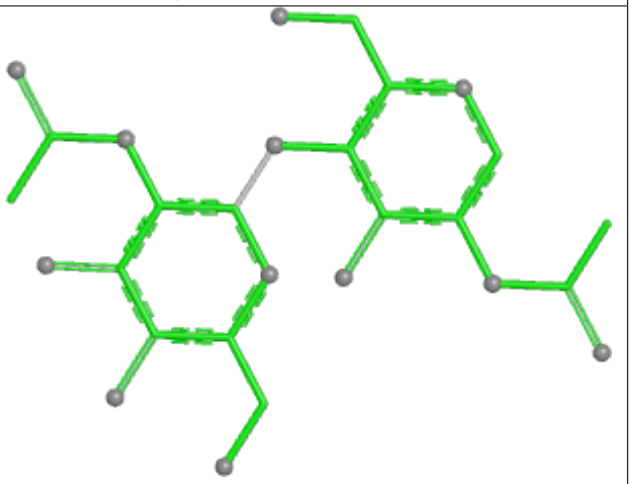


Rings

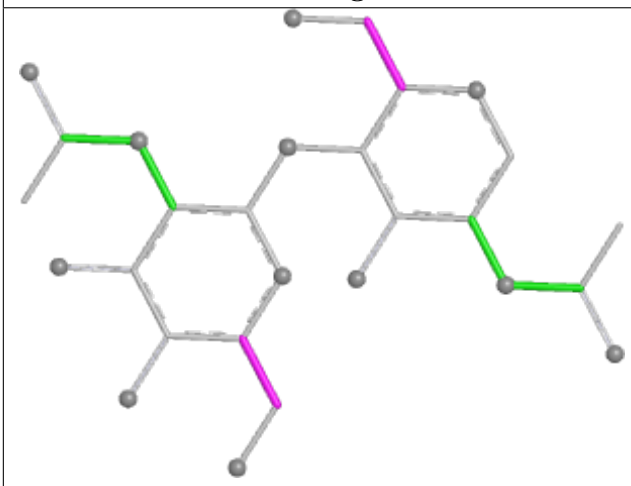
Oligosaccharide Chain Q



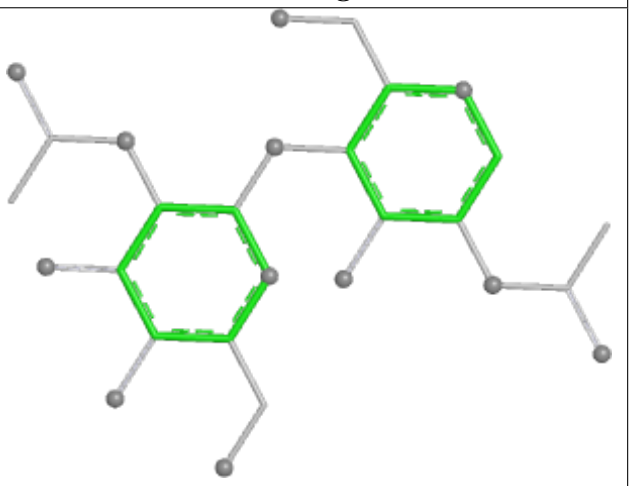
Bond lengths



Bond angles

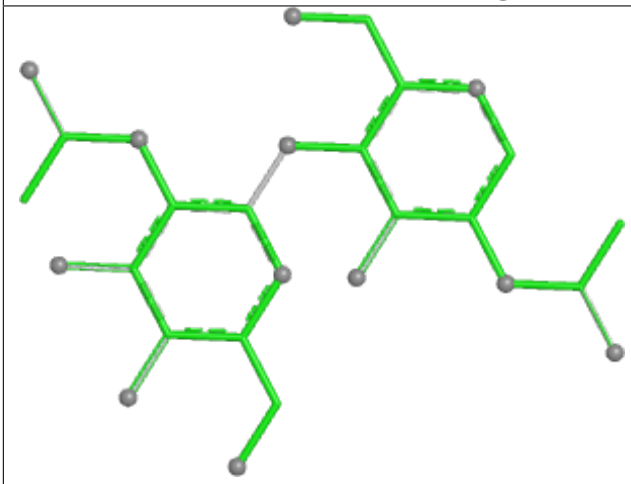


Torsions

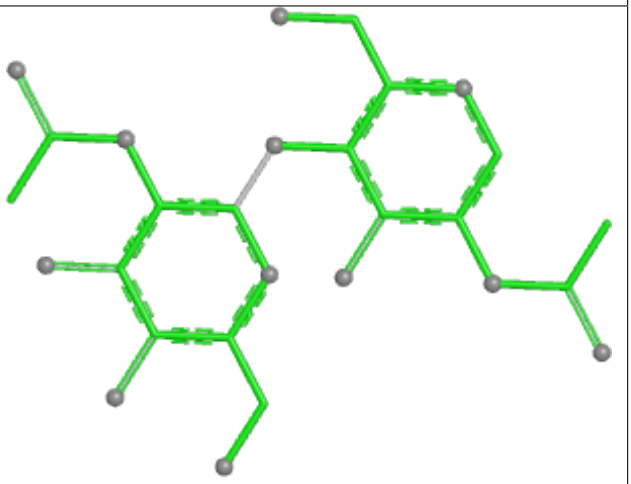


Rings

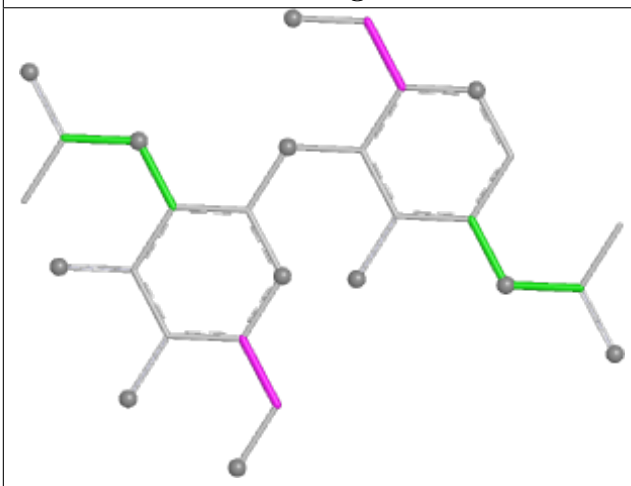
Oligosaccharide Chain R



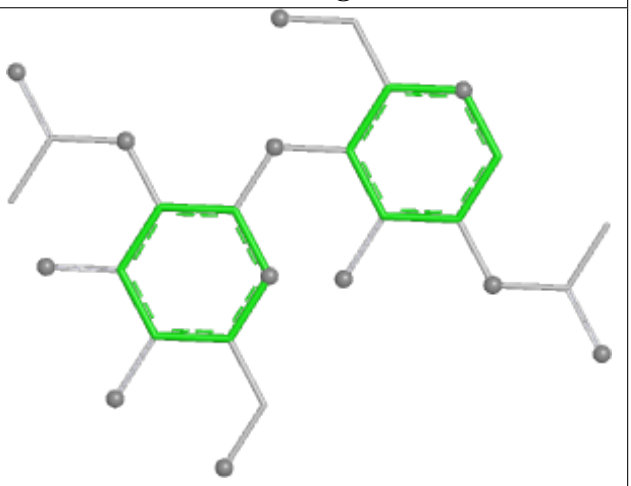
Bond lengths



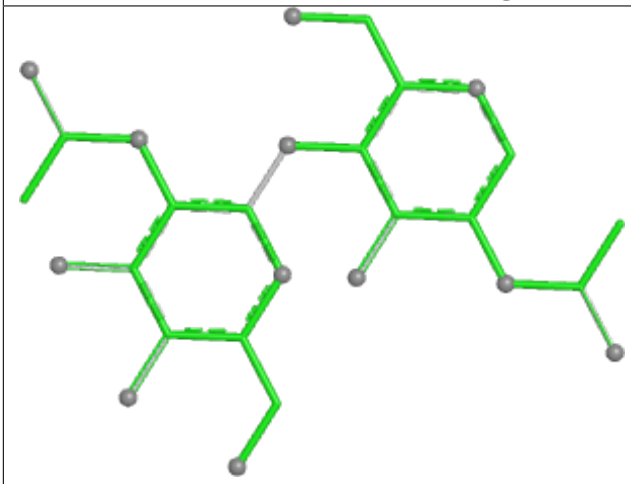
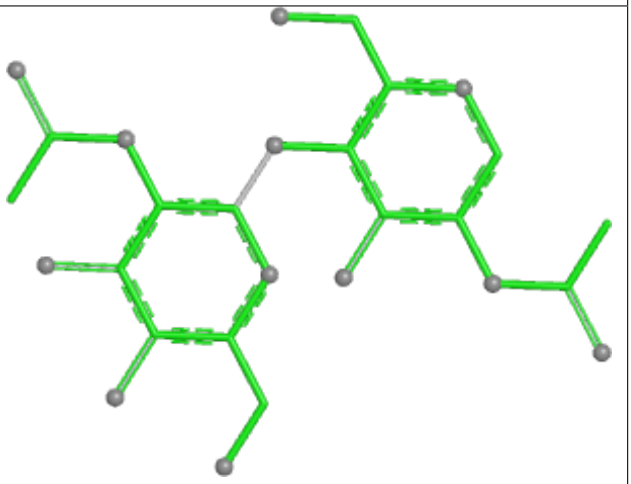
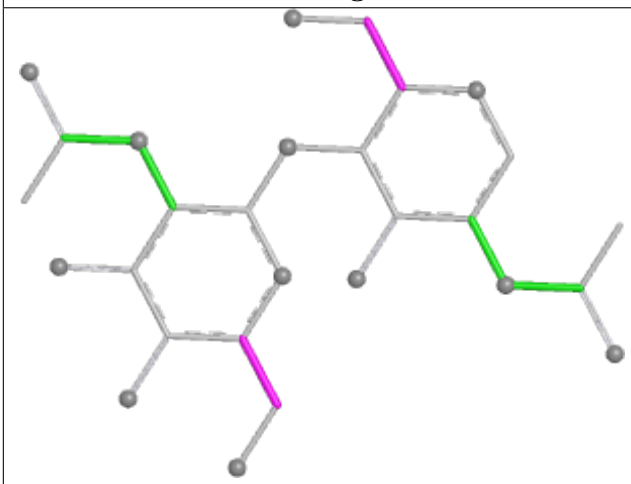
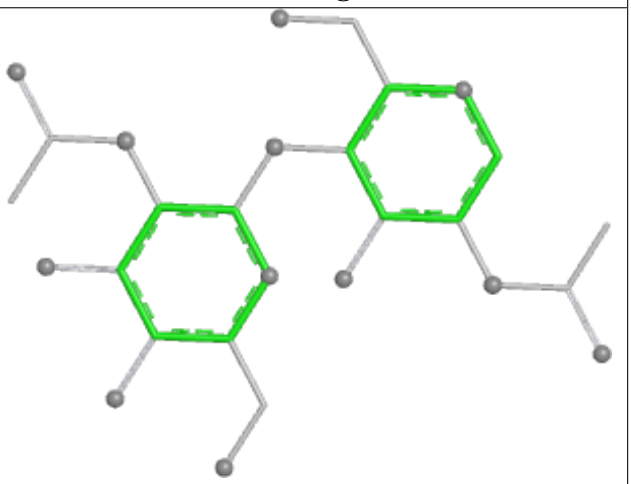
Bond angles

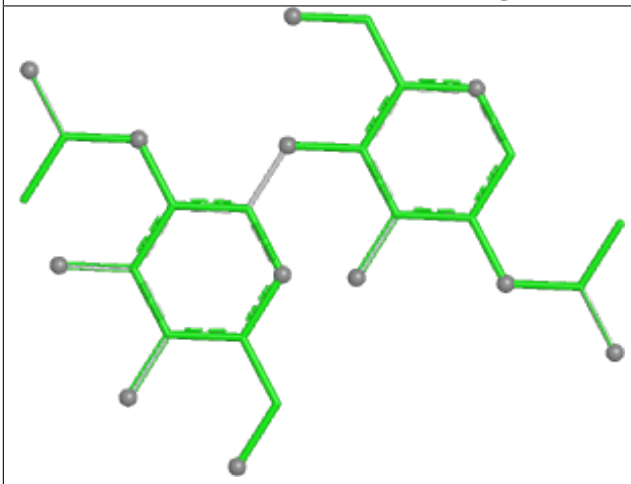
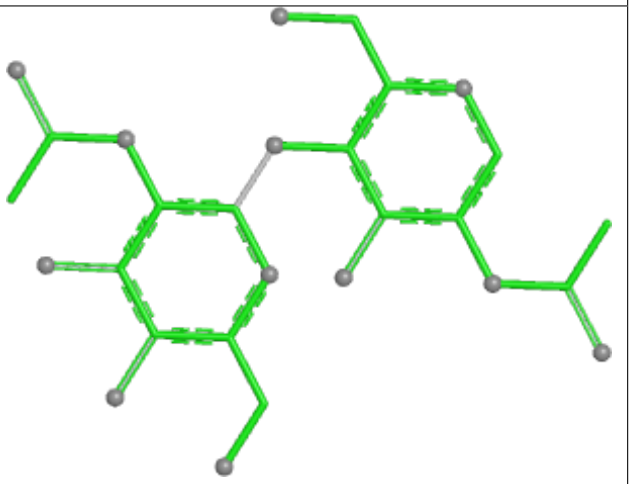
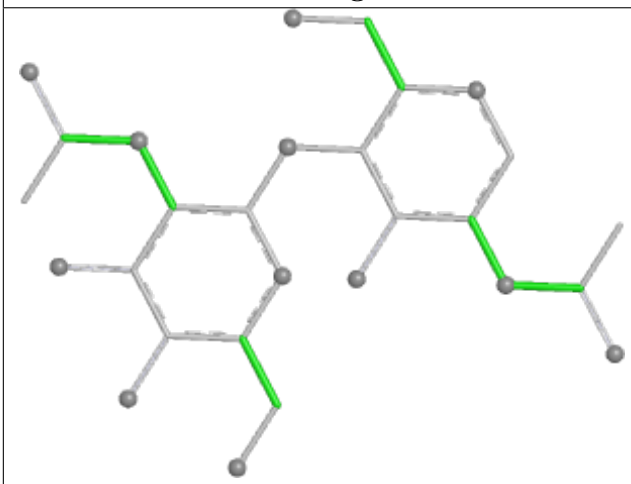
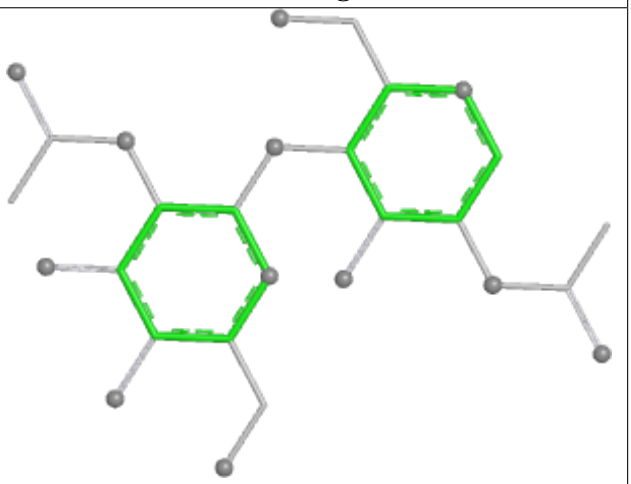


Torsions

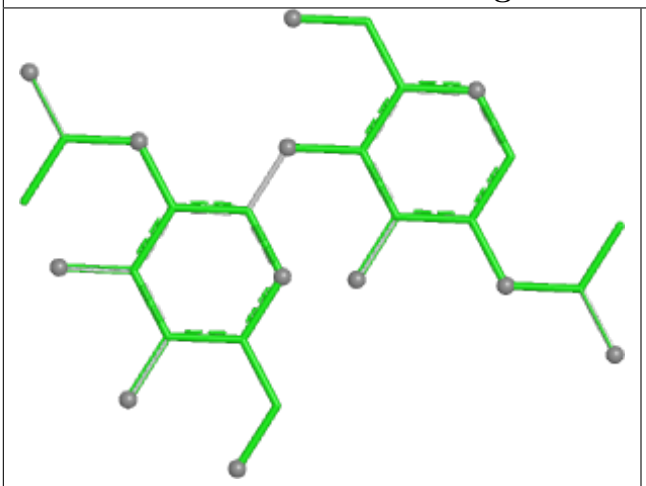


Rings

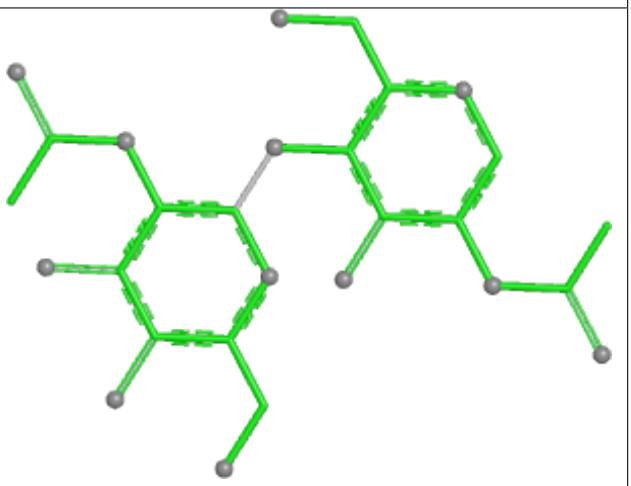
Oligosaccharide Chain S	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain T	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

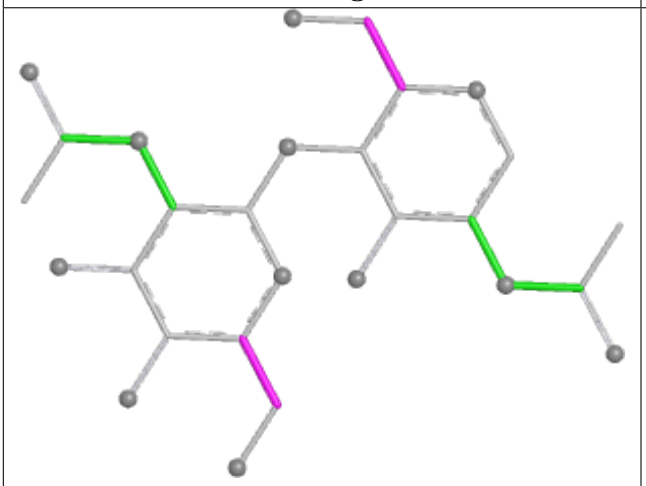
Oligosaccharide Chain U



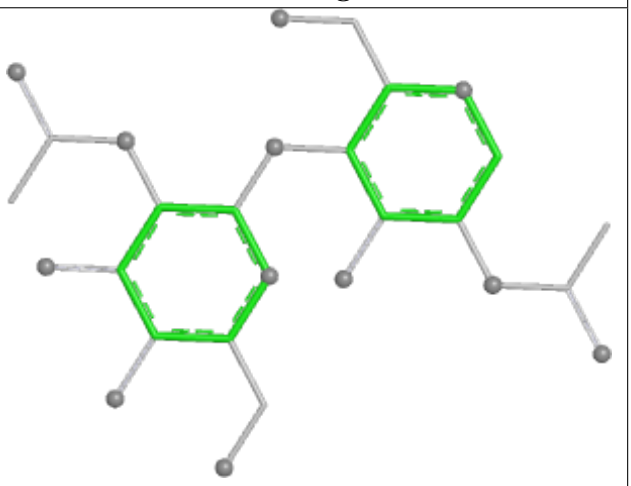
Bond lengths



Bond angles



Torsions



Rings

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	$\#\|Z\| > 2$
5	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	B	1308	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	B	1310	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.38	0
5	NAG	A	1301	1	14,14,15	0.17	0	17,19,21	0.47	0
5	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.36	0
5	NAG	B	1309	1	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.38	0
5	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	B	1304	1	14,14,15	0.17	0	17,19,21	0.47	0
5	NAG	A	1304	1	14,14,15	0.18	0	17,19,21	0.45	0
5	NAG	B	1305	1	14,14,15	0.16	0	17,19,21	0.54	0
5	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.35	0
5	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.47	0
5	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.36	0
5	NAG	B	1303	1	14,14,15	0.40	0	17,19,21	0.55	0
5	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	A	1310	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	C	1301	1	14,14,15	0.18	0	17,19,21	0.46	0
5	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.38	0
5	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.32	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	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1303	NAG	C4-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1301	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	B	1309	NAG	C1-C2-N2-C7
5	A	1309	NAG	C1-C2-N2-C7
5	C	1305	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	1304	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1308	NAG	1	0
5	A	1308	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

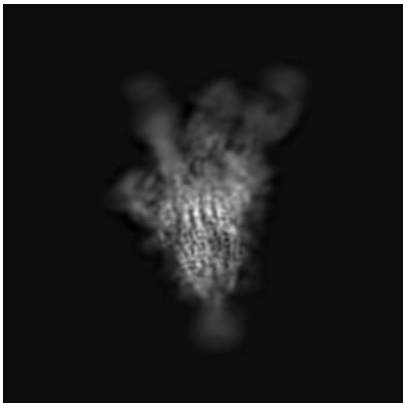
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13875. These allow visual inspection of the internal detail of the map and identification of artifacts.

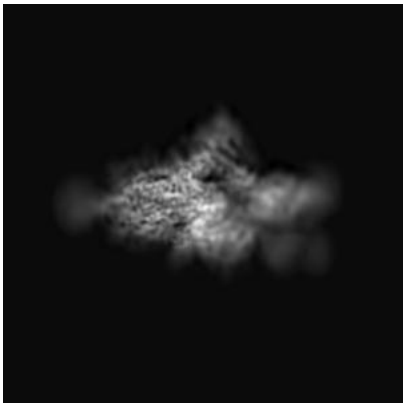
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

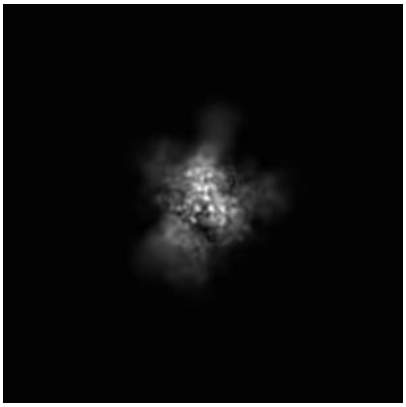
6.1.1 Primary map



X



Y

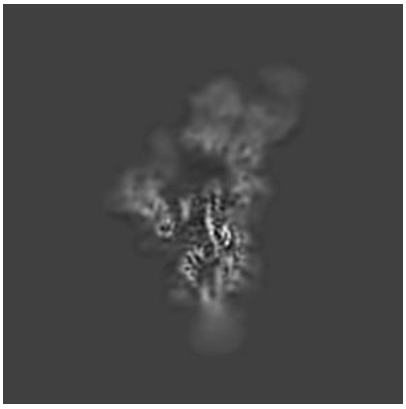


Z

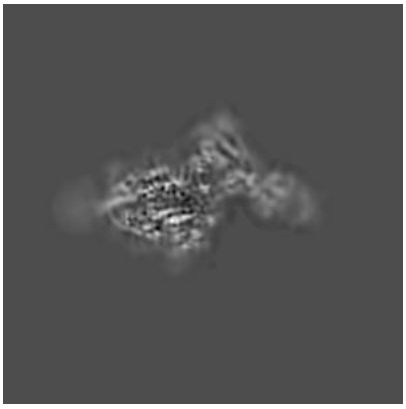
The images above show the map projected in three orthogonal directions.

6.2 Central slices

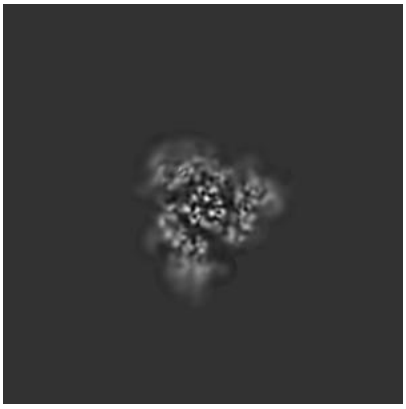
6.2.1 Primary map



X Index: 225



Y Index: 225

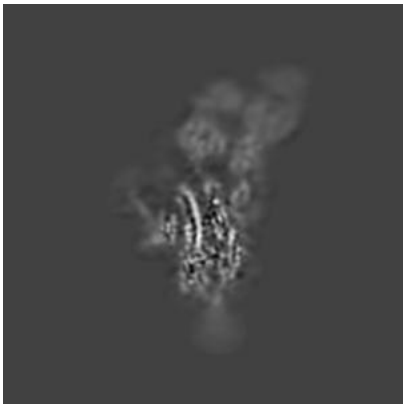


Z Index: 225

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

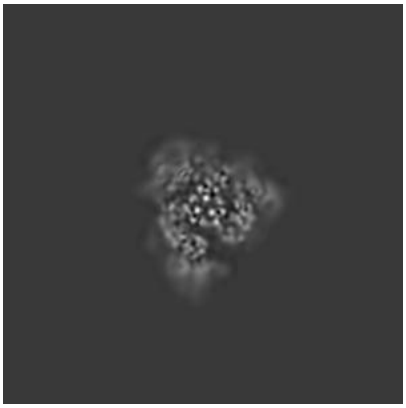
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 234

Y Index: 219

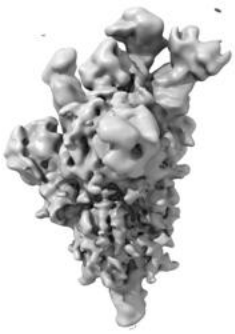


Z Index: 222

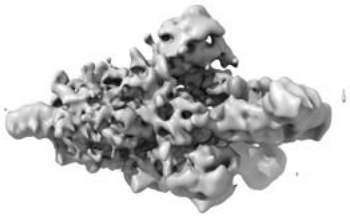
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

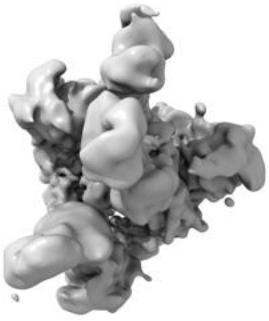
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

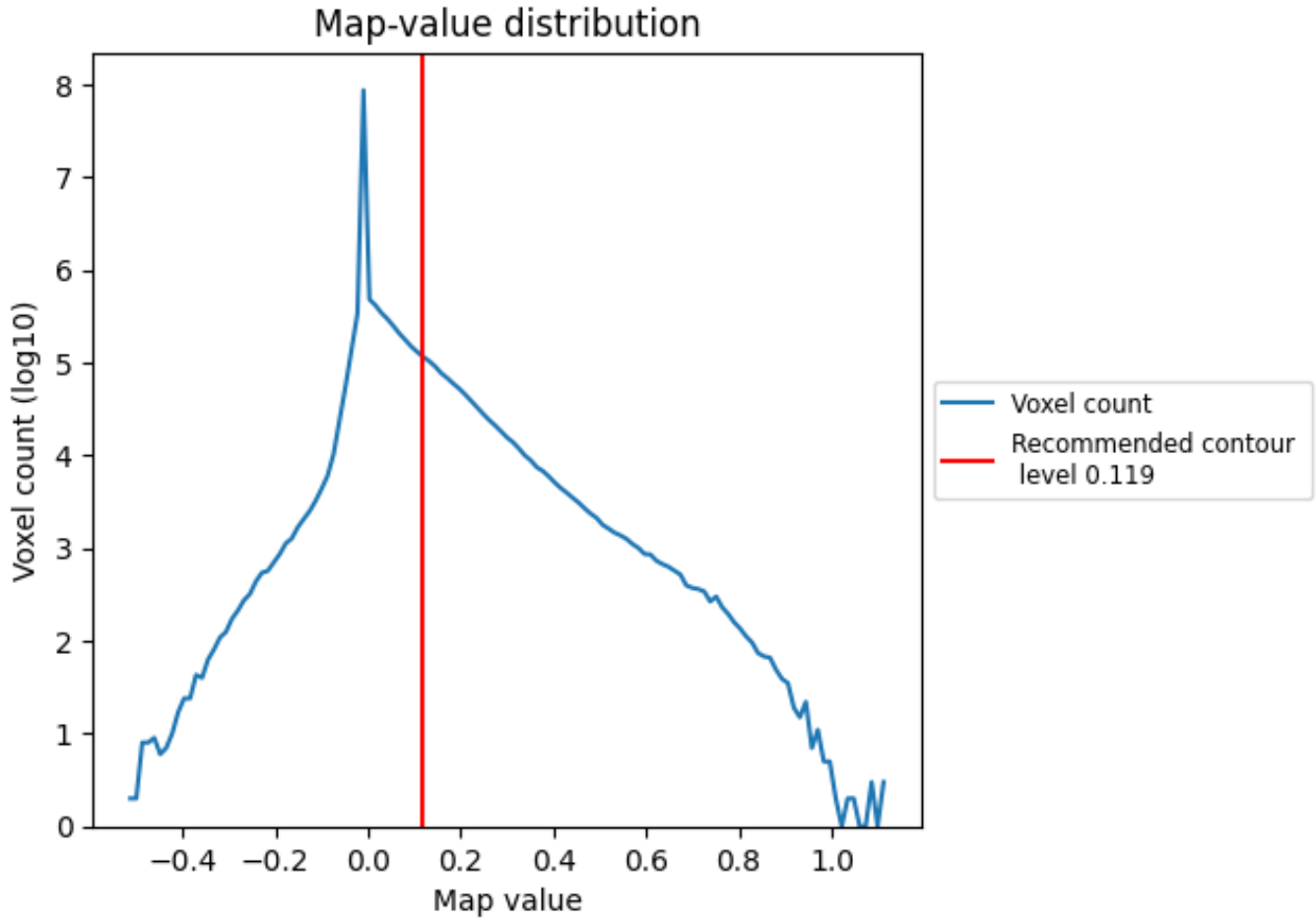
6.5 Mask visualisation (i)

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

7 Map analysis

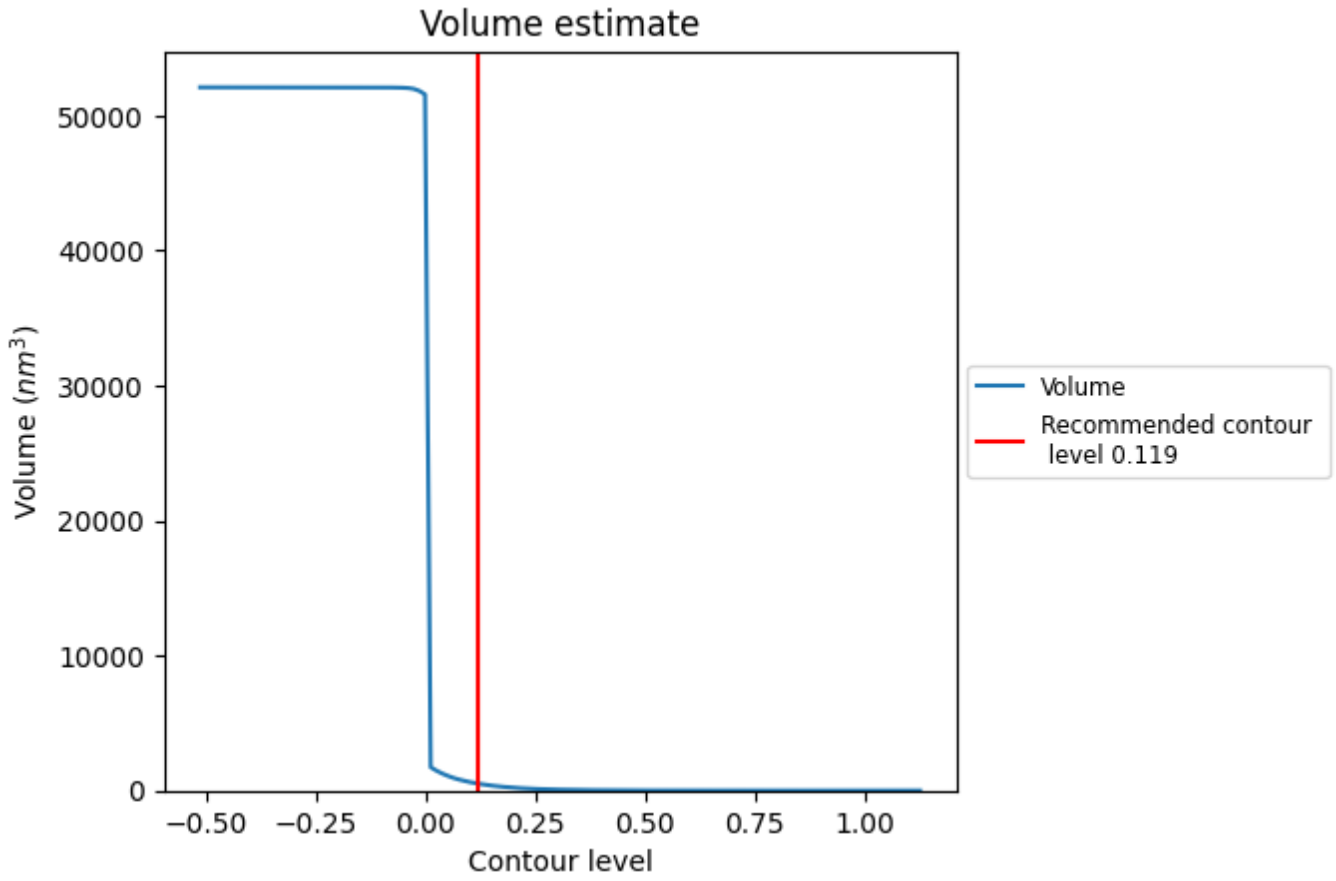
This section contains the results of statistical analysis of the map.

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.

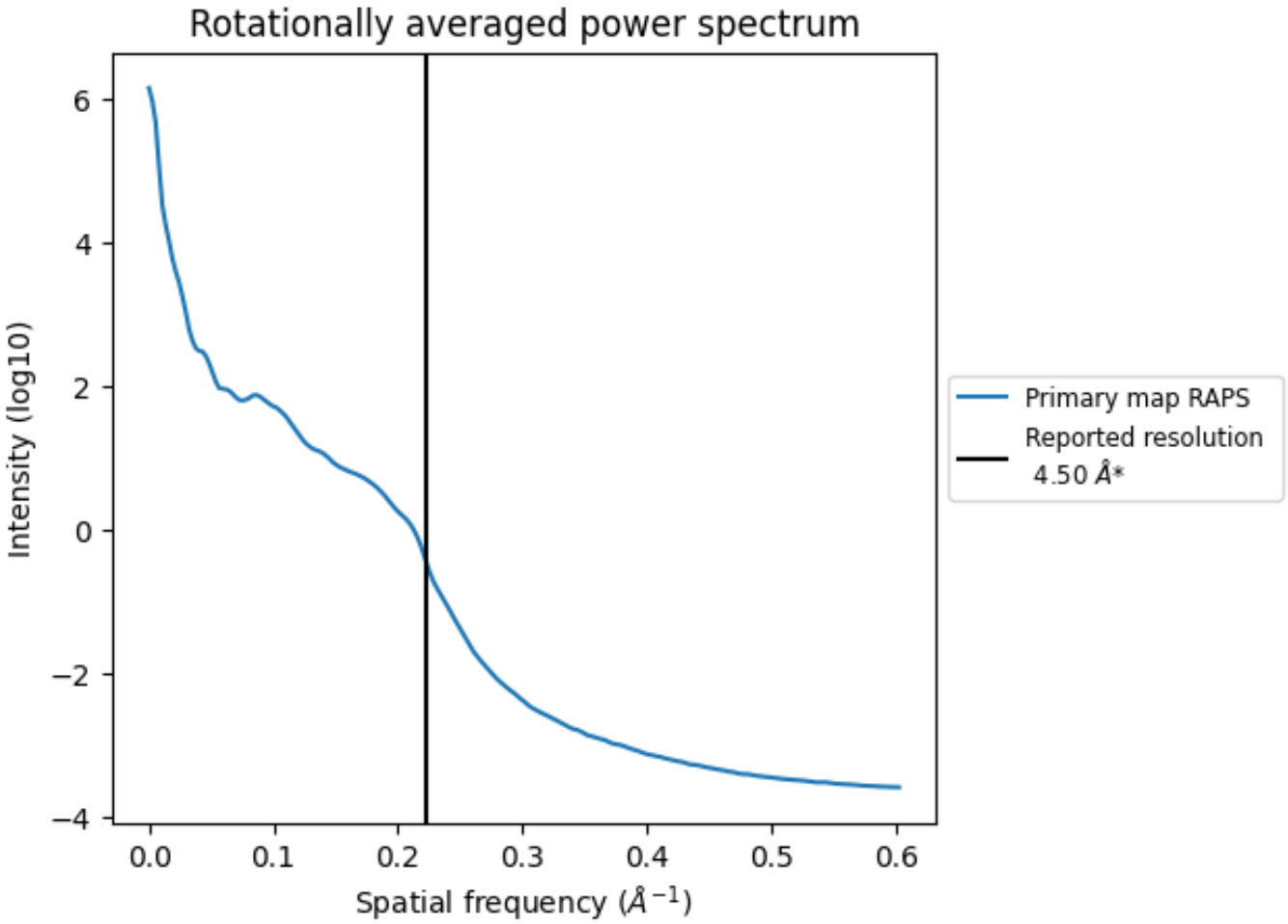
7.2 Volume estimate



The volume at the recommended contour level is 521 nm^3; this corresponds to an approximate mass of 470 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 0.222 Å^{-1}

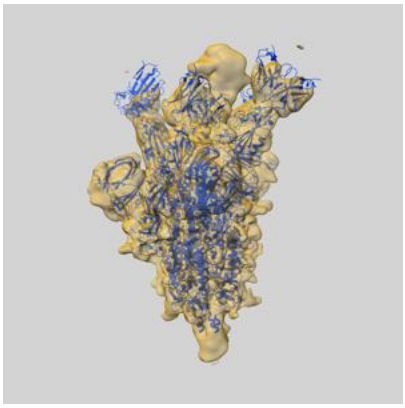
8 Fourier-Shell correlation (i)

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

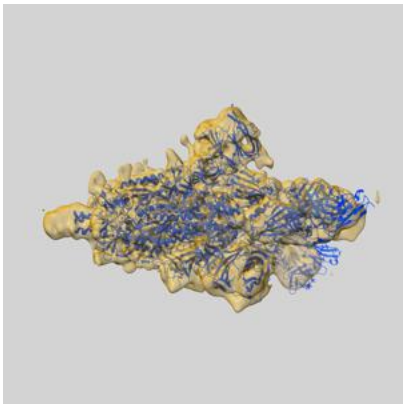
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13875 and PDB model 7Q9P. Per-residue inclusion information can be found in section 3 on page 15.

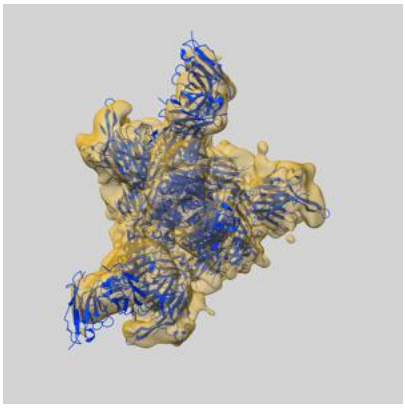
9.1 Map-model overlay



X



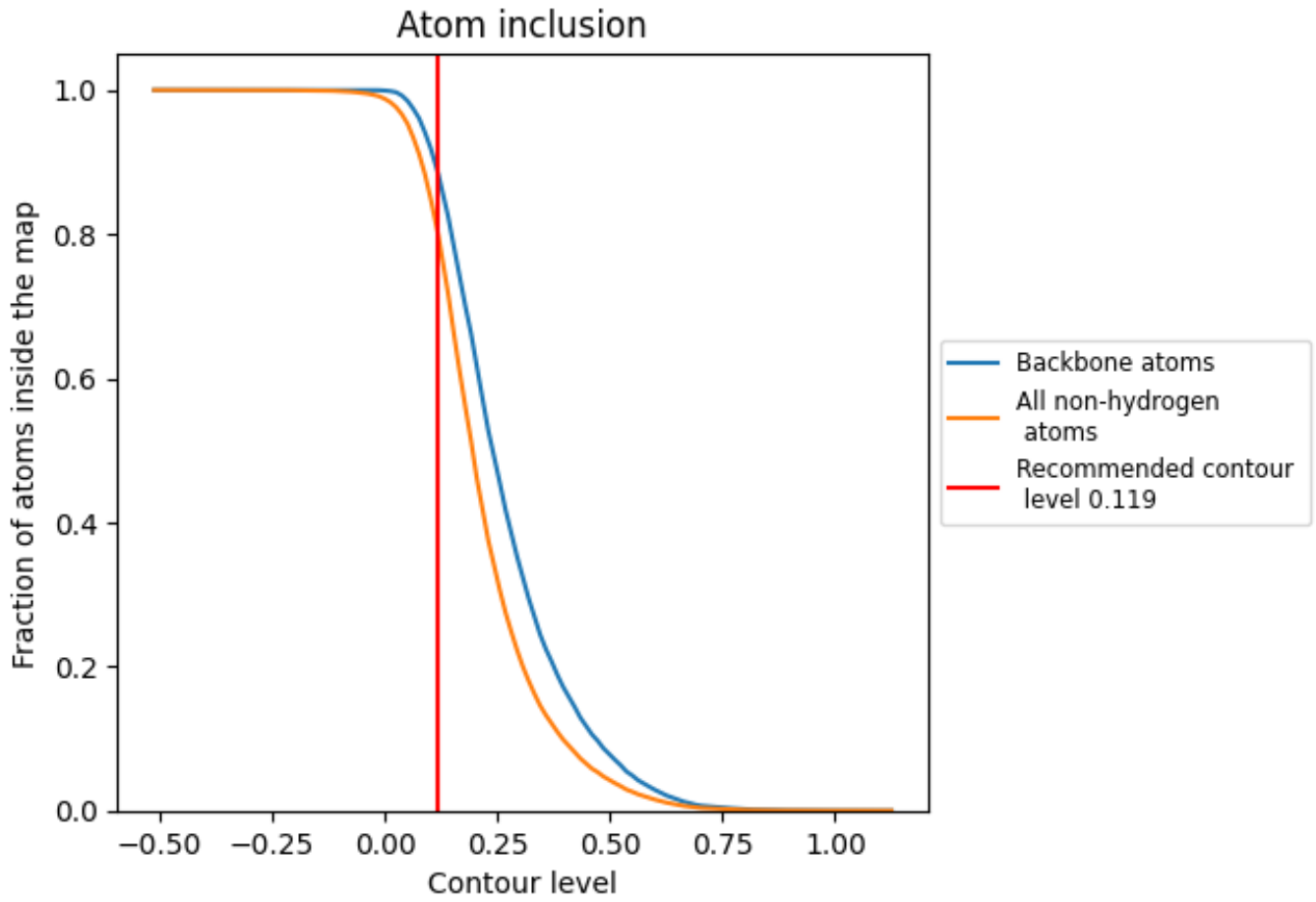
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.119 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 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.