



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:43 PM UTC

PDB ID : 7SB4 / pdb_00007sb4
EMDB ID : EMD-24969
Title : Structure of OC43 spike in complex with polyclonal Fab2 (Donor 1412)
Authors : Bangaru, S.; Antanasijevic, A.; Ward, A.
Deposited on : 2021-09-23
Resolution : 4.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

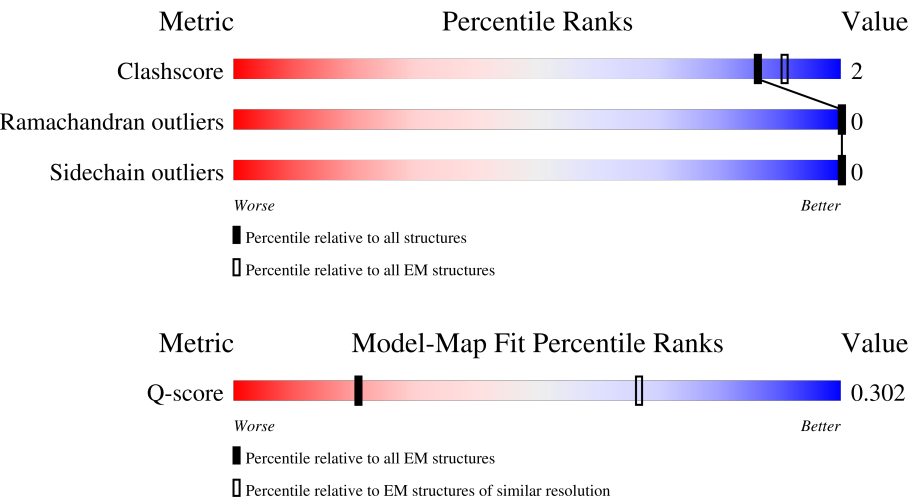
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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

Mol	Chain	Length	Quality of chain
1	A	1367	11% 77% 8% 14%
1	B	1367	11% 81% • 14%
1	C	1367	13% 80% 6% 14%
2	H	113	82% 88% 11% •

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Mol	Chain	Length	Quality of chain
2	L	113	80% 82% 5% 12%
3	D	2	50% 100%
3	F	2	50% 50%
3	G	2	50% 50%
3	I	2	50% 100%
3	J	2	100% 50%
3	M	2	50% 50%
3	N	2	100%
3	O	2	50% 100%
3	P	2	100% 100%
4	E	3	100%
4	K	3	67% 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	2	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29331 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1176	Total	C	N	O	S	0	0
			9151	5834	1504	1750	63		
1	C	1173	Total	C	N	O	S	0	0
			9134	5822	1502	1747	63		
1	B	1180	Total	C	N	O	S	0	0
			9178	5848	1509	1758	63		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	HIS	LEU	conflict	UNP A0A7U1BGV5
A	261	ILE	VAL	conflict	UNP A0A7U1BGV5
A	545	PRO	SER	conflict	UNP A0A7U1BGV5
A	762	ASN	THR	conflict	UNP A0A7U1BGV5
A	1079	PRO	ALA	conflict	UNP A0A7U1BGV5
A	1080	PRO	LEU	conflict	UNP A0A7U1BGV5
A	1217	MET	ILE	conflict	UNP A0A7U1BGV5
A	1269	PHE	LEU	conflict	UNP A0A7U1BGV5
A	1288	GLY	-	expression tag	UNP A0A7U1BGV5
A	1289	SER	-	expression tag	UNP A0A7U1BGV5
A	1290	GLY	-	expression tag	UNP A0A7U1BGV5
A	1291	TYR	-	expression tag	UNP A0A7U1BGV5
A	1292	ILE	-	expression tag	UNP A0A7U1BGV5
A	1293	PRO	-	expression tag	UNP A0A7U1BGV5
A	1294	GLU	-	expression tag	UNP A0A7U1BGV5
A	1295	ALA	-	expression tag	UNP A0A7U1BGV5
A	1296	PRO	-	expression tag	UNP A0A7U1BGV5
A	1297	ARG	-	expression tag	UNP A0A7U1BGV5
A	1298	ASP	-	expression tag	UNP A0A7U1BGV5
A	1299	GLY	-	expression tag	UNP A0A7U1BGV5
A	1300	GLN	-	expression tag	UNP A0A7U1BGV5
A	1301	ALA	-	expression tag	UNP A0A7U1BGV5
A	1302	TYR	-	expression tag	UNP A0A7U1BGV5
A	1303	VAL	-	expression tag	UNP A0A7U1BGV5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1304	ARG	-	expression tag	UNP A0A7U1BGV5
A	1305	LYS	-	expression tag	UNP A0A7U1BGV5
A	1306	ASP	-	expression tag	UNP A0A7U1BGV5
A	1307	GLY	-	expression tag	UNP A0A7U1BGV5
A	1308	GLU	-	expression tag	UNP A0A7U1BGV5
A	1309	TRP	-	expression tag	UNP A0A7U1BGV5
A	1310	VAL	-	expression tag	UNP A0A7U1BGV5
A	1311	LEU	-	expression tag	UNP A0A7U1BGV5
A	1312	LEU	-	expression tag	UNP A0A7U1BGV5
A	1313	SER	-	expression tag	UNP A0A7U1BGV5
A	1314	THR	-	expression tag	UNP A0A7U1BGV5
A	1315	PHE	-	expression tag	UNP A0A7U1BGV5
A	1316	LEU	-	expression tag	UNP A0A7U1BGV5
A	1317	GLY	-	expression tag	UNP A0A7U1BGV5
A	1318	ARG	-	expression tag	UNP A0A7U1BGV5
A	1319	SER	-	expression tag	UNP A0A7U1BGV5
A	1320	LEU	-	expression tag	UNP A0A7U1BGV5
A	1321	GLU	-	expression tag	UNP A0A7U1BGV5
A	1322	VAL	-	expression tag	UNP A0A7U1BGV5
A	1323	LEU	-	expression tag	UNP A0A7U1BGV5
A	1324	PHE	-	expression tag	UNP A0A7U1BGV5
A	1325	GLN	-	expression tag	UNP A0A7U1BGV5
A	1326	GLY	-	expression tag	UNP A0A7U1BGV5
A	1327	PRO	-	expression tag	UNP A0A7U1BGV5
A	1328	GLY	-	expression tag	UNP A0A7U1BGV5
A	1329	HIS	-	expression tag	UNP A0A7U1BGV5
A	1330	HIS	-	expression tag	UNP A0A7U1BGV5
A	1331	HIS	-	expression tag	UNP A0A7U1BGV5
A	1332	HIS	-	expression tag	UNP A0A7U1BGV5
A	1333	HIS	-	expression tag	UNP A0A7U1BGV5
A	1334	HIS	-	expression tag	UNP A0A7U1BGV5
A	1335	HIS	-	expression tag	UNP A0A7U1BGV5
A	1336	HIS	-	expression tag	UNP A0A7U1BGV5
A	1337	SER	-	expression tag	UNP A0A7U1BGV5
A	1338	ALA	-	expression tag	UNP A0A7U1BGV5
A	1339	TRP	-	expression tag	UNP A0A7U1BGV5
A	1340	SER	-	expression tag	UNP A0A7U1BGV5
A	1341	HIS	-	expression tag	UNP A0A7U1BGV5
A	1342	PRO	-	expression tag	UNP A0A7U1BGV5
A	1343	GLN	-	expression tag	UNP A0A7U1BGV5
A	1344	PHE	-	expression tag	UNP A0A7U1BGV5
A	1345	GLU	-	expression tag	UNP A0A7U1BGV5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1346	LYS	-	expression tag	UNP A0A7U1BGV5
A	1347	GLY	-	expression tag	UNP A0A7U1BGV5
A	1348	GLY	-	expression tag	UNP A0A7U1BGV5
A	1349	GLY	-	expression tag	UNP A0A7U1BGV5
A	1350	SER	-	expression tag	UNP A0A7U1BGV5
A	1351	GLY	-	expression tag	UNP A0A7U1BGV5
A	1352	GLY	-	expression tag	UNP A0A7U1BGV5
A	1353	GLY	-	expression tag	UNP A0A7U1BGV5
A	1354	GLY	-	expression tag	UNP A0A7U1BGV5
A	1355	SER	-	expression tag	UNP A0A7U1BGV5
A	1356	GLY	-	expression tag	UNP A0A7U1BGV5
A	1357	GLY	-	expression tag	UNP A0A7U1BGV5
A	1358	SER	-	expression tag	UNP A0A7U1BGV5
A	1359	ALA	-	expression tag	UNP A0A7U1BGV5
A	1360	TRP	-	expression tag	UNP A0A7U1BGV5
A	1361	SER	-	expression tag	UNP A0A7U1BGV5
A	1362	HIS	-	expression tag	UNP A0A7U1BGV5
A	1363	PRO	-	expression tag	UNP A0A7U1BGV5
A	1364	GLN	-	expression tag	UNP A0A7U1BGV5
A	1365	PHE	-	expression tag	UNP A0A7U1BGV5
A	1366	GLU	-	expression tag	UNP A0A7U1BGV5
A	1367	LYS	-	expression tag	UNP A0A7U1BGV5
C	177	HIS	LEU	conflict	UNP A0A7U1BGV5
C	261	ILE	VAL	conflict	UNP A0A7U1BGV5
C	545	PRO	SER	conflict	UNP A0A7U1BGV5
C	762	ASN	THR	conflict	UNP A0A7U1BGV5
C	1079	PRO	ALA	conflict	UNP A0A7U1BGV5
C	1080	PRO	LEU	conflict	UNP A0A7U1BGV5
C	1217	MET	ILE	conflict	UNP A0A7U1BGV5
C	1269	PHE	LEU	conflict	UNP A0A7U1BGV5
C	1288	GLY	-	expression tag	UNP A0A7U1BGV5
C	1289	SER	-	expression tag	UNP A0A7U1BGV5
C	1290	GLY	-	expression tag	UNP A0A7U1BGV5
C	1291	TYR	-	expression tag	UNP A0A7U1BGV5
C	1292	ILE	-	expression tag	UNP A0A7U1BGV5
C	1293	PRO	-	expression tag	UNP A0A7U1BGV5
C	1294	GLU	-	expression tag	UNP A0A7U1BGV5
C	1295	ALA	-	expression tag	UNP A0A7U1BGV5
C	1296	PRO	-	expression tag	UNP A0A7U1BGV5
C	1297	ARG	-	expression tag	UNP A0A7U1BGV5
C	1298	ASP	-	expression tag	UNP A0A7U1BGV5
C	1299	GLY	-	expression tag	UNP A0A7U1BGV5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1300	GLN	-	expression tag	UNP A0A7U1BGV5
C	1301	ALA	-	expression tag	UNP A0A7U1BGV5
C	1302	TYR	-	expression tag	UNP A0A7U1BGV5
C	1303	VAL	-	expression tag	UNP A0A7U1BGV5
C	1304	ARG	-	expression tag	UNP A0A7U1BGV5
C	1305	LYS	-	expression tag	UNP A0A7U1BGV5
C	1306	ASP	-	expression tag	UNP A0A7U1BGV5
C	1307	GLY	-	expression tag	UNP A0A7U1BGV5
C	1308	GLU	-	expression tag	UNP A0A7U1BGV5
C	1309	TRP	-	expression tag	UNP A0A7U1BGV5
C	1310	VAL	-	expression tag	UNP A0A7U1BGV5
C	1311	LEU	-	expression tag	UNP A0A7U1BGV5
C	1312	LEU	-	expression tag	UNP A0A7U1BGV5
C	1313	SER	-	expression tag	UNP A0A7U1BGV5
C	1314	THR	-	expression tag	UNP A0A7U1BGV5
C	1315	PHE	-	expression tag	UNP A0A7U1BGV5
C	1316	LEU	-	expression tag	UNP A0A7U1BGV5
C	1317	GLY	-	expression tag	UNP A0A7U1BGV5
C	1318	ARG	-	expression tag	UNP A0A7U1BGV5
C	1319	SER	-	expression tag	UNP A0A7U1BGV5
C	1320	LEU	-	expression tag	UNP A0A7U1BGV5
C	1321	GLU	-	expression tag	UNP A0A7U1BGV5
C	1322	VAL	-	expression tag	UNP A0A7U1BGV5
C	1323	LEU	-	expression tag	UNP A0A7U1BGV5
C	1324	PHE	-	expression tag	UNP A0A7U1BGV5
C	1325	GLN	-	expression tag	UNP A0A7U1BGV5
C	1326	GLY	-	expression tag	UNP A0A7U1BGV5
C	1327	PRO	-	expression tag	UNP A0A7U1BGV5
C	1328	GLY	-	expression tag	UNP A0A7U1BGV5
C	1329	HIS	-	expression tag	UNP A0A7U1BGV5
C	1330	HIS	-	expression tag	UNP A0A7U1BGV5
C	1331	HIS	-	expression tag	UNP A0A7U1BGV5
C	1332	HIS	-	expression tag	UNP A0A7U1BGV5
C	1333	HIS	-	expression tag	UNP A0A7U1BGV5
C	1334	HIS	-	expression tag	UNP A0A7U1BGV5
C	1335	HIS	-	expression tag	UNP A0A7U1BGV5
C	1336	HIS	-	expression tag	UNP A0A7U1BGV5
C	1337	SER	-	expression tag	UNP A0A7U1BGV5
C	1338	ALA	-	expression tag	UNP A0A7U1BGV5
C	1339	TRP	-	expression tag	UNP A0A7U1BGV5
C	1340	SER	-	expression tag	UNP A0A7U1BGV5
C	1341	HIS	-	expression tag	UNP A0A7U1BGV5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1342	PRO	-	expression tag	UNP A0A7U1BGV5
C	1343	GLN	-	expression tag	UNP A0A7U1BGV5
C	1344	PHE	-	expression tag	UNP A0A7U1BGV5
C	1345	GLU	-	expression tag	UNP A0A7U1BGV5
C	1346	LYS	-	expression tag	UNP A0A7U1BGV5
C	1347	GLY	-	expression tag	UNP A0A7U1BGV5
C	1348	GLY	-	expression tag	UNP A0A7U1BGV5
C	1349	GLY	-	expression tag	UNP A0A7U1BGV5
C	1350	SER	-	expression tag	UNP A0A7U1BGV5
C	1351	GLY	-	expression tag	UNP A0A7U1BGV5
C	1352	GLY	-	expression tag	UNP A0A7U1BGV5
C	1353	GLY	-	expression tag	UNP A0A7U1BGV5
C	1354	GLY	-	expression tag	UNP A0A7U1BGV5
C	1355	SER	-	expression tag	UNP A0A7U1BGV5
C	1356	GLY	-	expression tag	UNP A0A7U1BGV5
C	1357	GLY	-	expression tag	UNP A0A7U1BGV5
C	1358	SER	-	expression tag	UNP A0A7U1BGV5
C	1359	ALA	-	expression tag	UNP A0A7U1BGV5
C	1360	TRP	-	expression tag	UNP A0A7U1BGV5
C	1361	SER	-	expression tag	UNP A0A7U1BGV5
C	1362	HIS	-	expression tag	UNP A0A7U1BGV5
C	1363	PRO	-	expression tag	UNP A0A7U1BGV5
C	1364	GLN	-	expression tag	UNP A0A7U1BGV5
C	1365	PHE	-	expression tag	UNP A0A7U1BGV5
C	1366	GLU	-	expression tag	UNP A0A7U1BGV5
C	1367	LYS	-	expression tag	UNP A0A7U1BGV5
B	177	HIS	LEU	conflict	UNP A0A7U1BGV5
B	261	ILE	VAL	conflict	UNP A0A7U1BGV5
B	545	PRO	SER	conflict	UNP A0A7U1BGV5
B	762	ASN	THR	conflict	UNP A0A7U1BGV5
B	1079	PRO	ALA	conflict	UNP A0A7U1BGV5
B	1080	PRO	LEU	conflict	UNP A0A7U1BGV5
B	1217	MET	ILE	conflict	UNP A0A7U1BGV5
B	1269	PHE	LEU	conflict	UNP A0A7U1BGV5
B	1288	GLY	-	expression tag	UNP A0A7U1BGV5
B	1289	SER	-	expression tag	UNP A0A7U1BGV5
B	1290	GLY	-	expression tag	UNP A0A7U1BGV5
B	1291	TYR	-	expression tag	UNP A0A7U1BGV5
B	1292	ILE	-	expression tag	UNP A0A7U1BGV5
B	1293	PRO	-	expression tag	UNP A0A7U1BGV5
B	1294	GLU	-	expression tag	UNP A0A7U1BGV5
B	1295	ALA	-	expression tag	UNP A0A7U1BGV5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1296	PRO	-	expression tag	UNP A0A7U1BGV5
B	1297	ARG	-	expression tag	UNP A0A7U1BGV5
B	1298	ASP	-	expression tag	UNP A0A7U1BGV5
B	1299	GLY	-	expression tag	UNP A0A7U1BGV5
B	1300	GLN	-	expression tag	UNP A0A7U1BGV5
B	1301	ALA	-	expression tag	UNP A0A7U1BGV5
B	1302	TYR	-	expression tag	UNP A0A7U1BGV5
B	1303	VAL	-	expression tag	UNP A0A7U1BGV5
B	1304	ARG	-	expression tag	UNP A0A7U1BGV5
B	1305	LYS	-	expression tag	UNP A0A7U1BGV5
B	1306	ASP	-	expression tag	UNP A0A7U1BGV5
B	1307	GLY	-	expression tag	UNP A0A7U1BGV5
B	1308	GLU	-	expression tag	UNP A0A7U1BGV5
B	1309	TRP	-	expression tag	UNP A0A7U1BGV5
B	1310	VAL	-	expression tag	UNP A0A7U1BGV5
B	1311	LEU	-	expression tag	UNP A0A7U1BGV5
B	1312	LEU	-	expression tag	UNP A0A7U1BGV5
B	1313	SER	-	expression tag	UNP A0A7U1BGV5
B	1314	THR	-	expression tag	UNP A0A7U1BGV5
B	1315	PHE	-	expression tag	UNP A0A7U1BGV5
B	1316	LEU	-	expression tag	UNP A0A7U1BGV5
B	1317	GLY	-	expression tag	UNP A0A7U1BGV5
B	1318	ARG	-	expression tag	UNP A0A7U1BGV5
B	1319	SER	-	expression tag	UNP A0A7U1BGV5
B	1320	LEU	-	expression tag	UNP A0A7U1BGV5
B	1321	GLU	-	expression tag	UNP A0A7U1BGV5
B	1322	VAL	-	expression tag	UNP A0A7U1BGV5
B	1323	LEU	-	expression tag	UNP A0A7U1BGV5
B	1324	PHE	-	expression tag	UNP A0A7U1BGV5
B	1325	GLN	-	expression tag	UNP A0A7U1BGV5
B	1326	GLY	-	expression tag	UNP A0A7U1BGV5
B	1327	PRO	-	expression tag	UNP A0A7U1BGV5
B	1328	GLY	-	expression tag	UNP A0A7U1BGV5
B	1329	HIS	-	expression tag	UNP A0A7U1BGV5
B	1330	HIS	-	expression tag	UNP A0A7U1BGV5
B	1331	HIS	-	expression tag	UNP A0A7U1BGV5
B	1332	HIS	-	expression tag	UNP A0A7U1BGV5
B	1333	HIS	-	expression tag	UNP A0A7U1BGV5
B	1334	HIS	-	expression tag	UNP A0A7U1BGV5
B	1335	HIS	-	expression tag	UNP A0A7U1BGV5
B	1336	HIS	-	expression tag	UNP A0A7U1BGV5
B	1337	SER	-	expression tag	UNP A0A7U1BGV5

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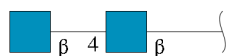
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1338	ALA	-	expression tag	UNP A0A7U1BGV5
B	1339	TRP	-	expression tag	UNP A0A7U1BGV5
B	1340	SER	-	expression tag	UNP A0A7U1BGV5
B	1341	HIS	-	expression tag	UNP A0A7U1BGV5
B	1342	PRO	-	expression tag	UNP A0A7U1BGV5
B	1343	GLN	-	expression tag	UNP A0A7U1BGV5
B	1344	PHE	-	expression tag	UNP A0A7U1BGV5
B	1345	GLU	-	expression tag	UNP A0A7U1BGV5
B	1346	LYS	-	expression tag	UNP A0A7U1BGV5
B	1347	GLY	-	expression tag	UNP A0A7U1BGV5
B	1348	GLY	-	expression tag	UNP A0A7U1BGV5
B	1349	GLY	-	expression tag	UNP A0A7U1BGV5
B	1350	SER	-	expression tag	UNP A0A7U1BGV5
B	1351	GLY	-	expression tag	UNP A0A7U1BGV5
B	1352	GLY	-	expression tag	UNP A0A7U1BGV5
B	1353	GLY	-	expression tag	UNP A0A7U1BGV5
B	1354	GLY	-	expression tag	UNP A0A7U1BGV5
B	1355	SER	-	expression tag	UNP A0A7U1BGV5
B	1356	GLY	-	expression tag	UNP A0A7U1BGV5
B	1357	GLY	-	expression tag	UNP A0A7U1BGV5
B	1358	SER	-	expression tag	UNP A0A7U1BGV5
B	1359	ALA	-	expression tag	UNP A0A7U1BGV5
B	1360	TRP	-	expression tag	UNP A0A7U1BGV5
B	1361	SER	-	expression tag	UNP A0A7U1BGV5
B	1362	HIS	-	expression tag	UNP A0A7U1BGV5
B	1363	PRO	-	expression tag	UNP A0A7U1BGV5
B	1364	GLN	-	expression tag	UNP A0A7U1BGV5
B	1365	PHE	-	expression tag	UNP A0A7U1BGV5
B	1366	GLU	-	expression tag	UNP A0A7U1BGV5
B	1367	LYS	-	expression tag	UNP A0A7U1BGV5

- Molecule 2 is a protein called Human polyclonal Fab model with polyalanine backbone - Heavy chain.

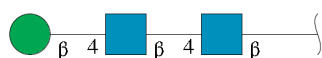
Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	111	Total	C	N	O	0	0
			555	333	111	111		
2	L	99	Total	C	N	O	0	0
			495	297	99	99		

- Molecule 3 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
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



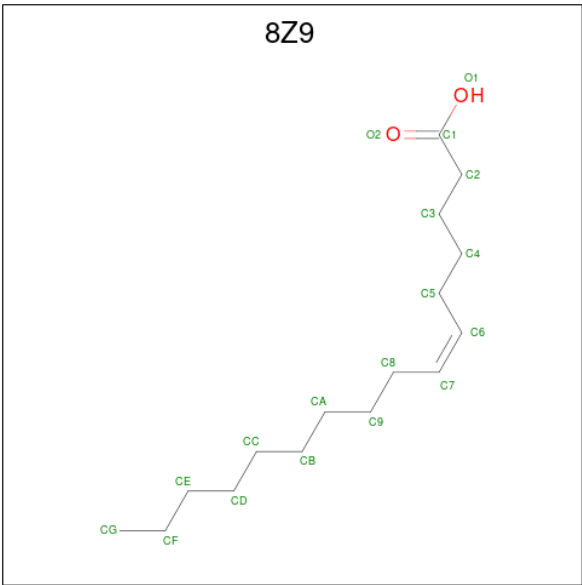
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5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

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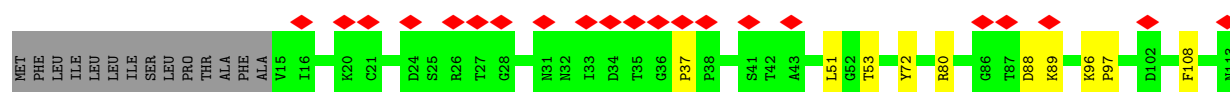
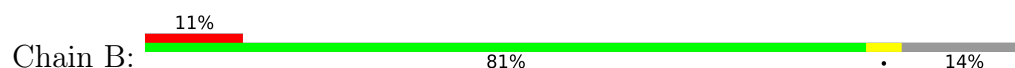
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

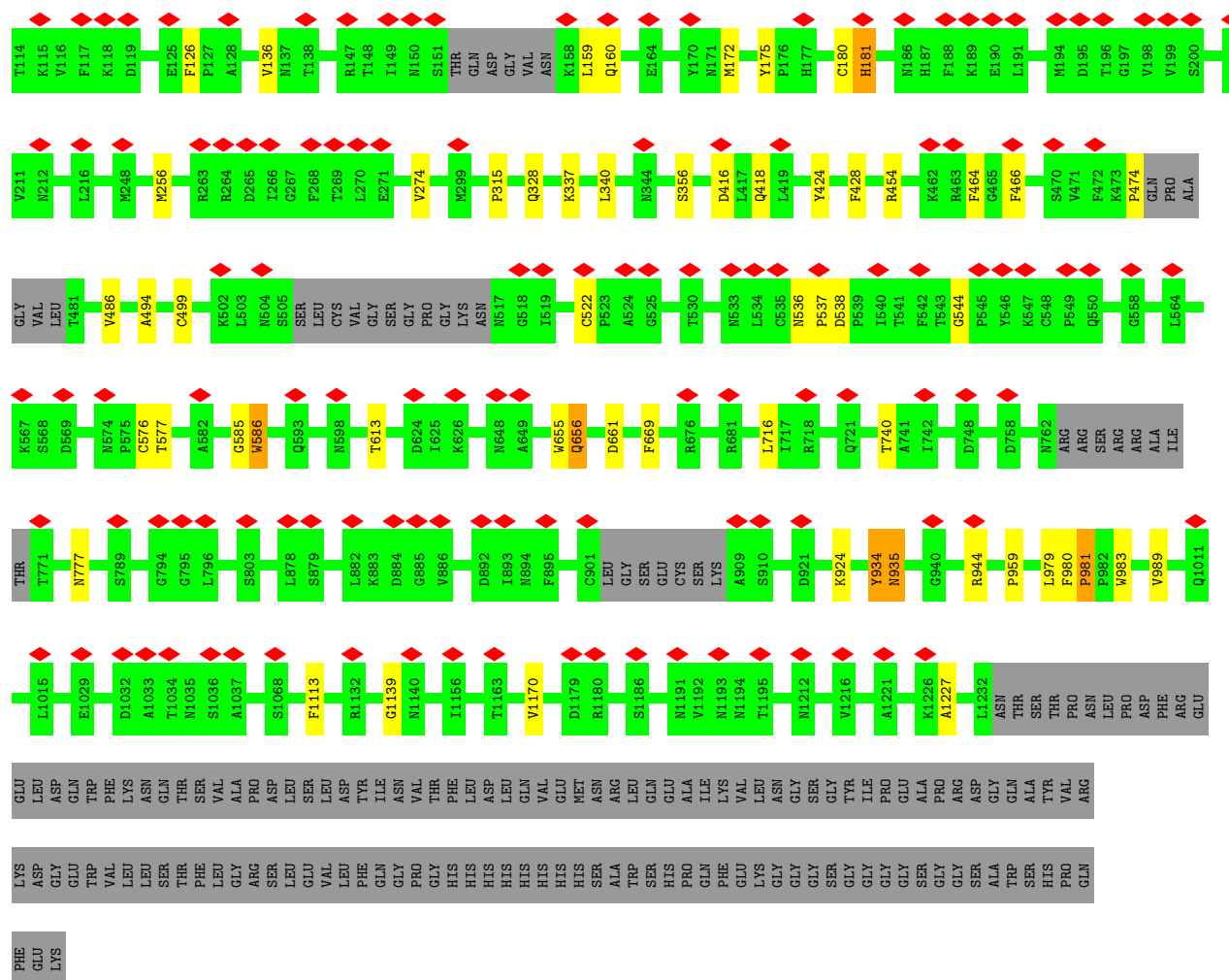
- Molecule 6 is Sapientic acid (CCD ID: 8Z9) (formula: C₁₆H₃₀O₂).



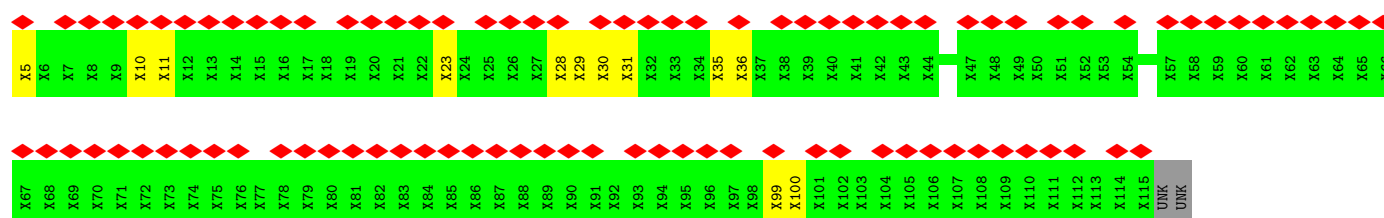
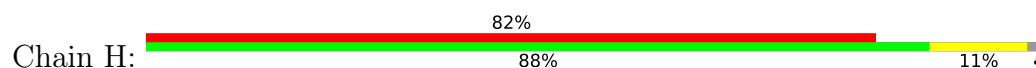
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			18	16	2	
6	B	1	Total	C	O	0
			18	16	2	

Chain C: 

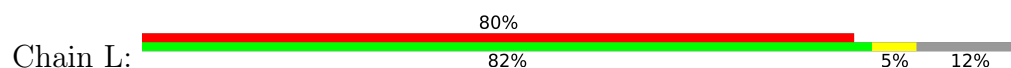


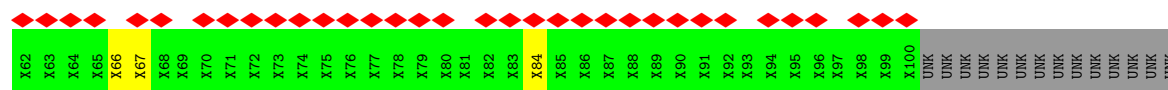


- Molecule 2: Human polyclonal Fab model with polyalanine backbone - Heavy chain



- Molecule 2: Human polyclonal Fab model with polyalanine backbone - Heavy chain





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	350.19998, 350.19998, 350.19998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 8Z9, 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	1.03	3/9364 (0.0%)	1.32	96/12747 (0.8%)
1	B	1.03	1/9391 (0.0%)	1.29	74/12784 (0.6%)
1	C	1.05	2/9344 (0.0%)	1.27	84/12715 (0.7%)
All	All	1.04	6/28099 (0.0%)	1.29	254/38246 (0.7%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	483	HIS	CB-CG	-6.54	1.41	1.50
1	C	219	HIS	CB-CG	-5.96	1.41	1.50
1	A	1213	ASN	CB-CG	-5.73	1.37	1.52
1	A	219	HIS	CB-CG	-5.47	1.42	1.50
1	B	474	PRO	N-CD	5.14	1.54	1.47
1	A	474	PRO	N-CD	5.04	1.54	1.47

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	959	PRO	CA-C-N	9.12	129.06	120.03
1	A	959	PRO	C-N-CA	9.12	129.06	120.03
1	C	959	PRO	CA-C-N	8.90	128.75	120.21
1	C	959	PRO	C-N-CA	8.90	128.75	120.21
1	B	577	THR	N-CA-C	-8.41	96.54	109.24
1	A	37	PRO	CA-C-N	8.34	127.64	118.97
1	A	37	PRO	C-N-CA	8.34	127.64	118.97
1	C	1227	ALA	CA-C-N	8.32	128.04	119.56
1	C	1227	ALA	C-N-CA	8.32	128.04	119.56
1	B	959	PRO	CA-C-N	8.12	128.07	120.03
1	B	959	PRO	C-N-CA	8.12	128.07	120.03
1	C	315	PRO	CA-C-N	8.05	128.00	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	PRO	C-N-CA	8.05	128.00	120.03
1	B	464	PHE	CA-CB-CG	-8.01	105.79	113.80
1	C	544	GLY	CA-C-N	7.98	127.62	119.56
1	C	544	GLY	C-N-CA	7.98	127.62	119.56
1	B	1227	ALA	CA-C-N	7.98	128.17	119.87
1	B	1227	ALA	C-N-CA	7.98	128.17	119.87
1	C	16	ILE	N-CA-C	-7.96	104.05	111.45
1	B	340	LEU	CA-C-N	7.86	127.75	120.21
1	B	340	LEU	C-N-CA	7.86	127.75	120.21
1	A	315	PRO	CA-C-N	7.72	128.16	120.52
1	A	315	PRO	C-N-CA	7.72	128.16	120.52
1	A	356	SER	CA-C-N	7.61	128.30	119.47
1	A	356	SER	C-N-CA	7.61	128.30	119.47
1	B	522	CYS	CA-C-N	7.42	127.37	120.03
1	B	522	CYS	C-N-CA	7.42	127.37	120.03
1	A	544	GLY	CA-C-N	7.29	127.92	120.04
1	A	544	GLY	C-N-CA	7.29	127.92	120.04
1	A	328	GLN	CA-C-N	7.29	127.29	119.78
1	A	328	GLN	C-N-CA	7.29	127.29	119.78
1	A	1227	ALA	CA-C-N	7.21	126.84	119.56
1	A	1227	ALA	C-N-CA	7.21	126.84	119.56
1	C	522	CYS	CA-C-N	7.21	127.20	119.78
1	C	522	CYS	C-N-CA	7.21	127.20	119.78
1	B	315	PRO	CA-C-N	7.17	127.34	120.31
1	B	315	PRO	C-N-CA	7.17	127.34	120.31
1	A	371	ASN	CA-C-N	7.17	130.84	120.38
1	A	371	ASN	C-N-CA	7.17	130.84	120.38
1	C	359	ASN	CA-C-N	-7.15	110.97	121.76
1	C	359	ASN	C-N-CA	-7.15	110.97	121.76
1	C	779	GLU	CA-C-N	7.08	126.72	119.56
1	C	779	GLU	C-N-CA	7.08	126.72	119.56
1	B	1170	VAL	N-CA-C	7.02	118.92	108.46
1	B	37	PRO	CB-CA-C	7.02	119.48	110.92
1	A	378	PHE	CA-CB-CG	-6.97	106.83	113.80
1	C	980	PHE	CA-C-N	6.97	127.56	120.38
1	C	980	PHE	C-N-CA	6.97	127.56	120.38
1	B	585	GLY	CA-C-N	-6.87	113.44	123.05
1	B	585	GLY	C-N-CA	-6.87	113.44	123.05
1	B	980	PHE	CA-C-N	6.81	127.40	120.38
1	B	980	PHE	C-N-CA	6.81	127.40	120.38
1	B	544	GLY	CA-C-N	6.81	127.36	119.47
1	B	544	GLY	C-N-CA	6.81	127.36	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	575	PRO	N-CA-C	-6.79	100.53	111.19
1	B	356	SER	CA-C-N	6.74	126.43	119.56
1	B	356	SER	C-N-CA	6.74	126.43	119.56
1	B	96	LYS	CA-C-N	6.72	127.30	120.38
1	B	96	LYS	C-N-CA	6.72	127.30	120.38
1	B	494	ALA	CA-C-N	6.72	126.68	120.03
1	B	494	ALA	C-N-CA	6.72	126.68	120.03
1	A	416	ASP	CA-CB-CG	6.71	119.31	112.60
1	C	340	LEU	CA-C-N	6.70	126.88	120.31
1	C	340	LEU	C-N-CA	6.70	126.88	120.31
1	B	418	GLN	N-CA-C	6.70	120.41	109.76
1	B	416	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	494	ALA	CA-C-N	6.66	126.62	120.03
1	A	494	ALA	C-N-CA	6.66	126.62	120.03
1	A	275	THR	CA-C-N	6.61	126.53	119.85
1	A	275	THR	C-N-CA	6.61	126.53	119.85
1	B	716	LEU	CA-C-N	6.57	129.75	120.42
1	B	716	LEU	C-N-CA	6.57	129.75	120.42
1	A	579	GLN	CA-C-N	6.53	127.05	119.47
1	A	579	GLN	C-N-CA	6.53	127.05	119.47
1	C	96	LYS	CA-C-N	6.48	127.06	120.38
1	C	96	LYS	C-N-CA	6.48	127.06	120.38
1	C	1079	PRO	N-CA-C	6.48	118.61	110.70
1	C	485	VAL	N-CA-C	6.45	117.20	108.17
1	B	160	GLN	CA-C-N	-6.42	116.43	121.82
1	B	160	GLN	C-N-CA	-6.42	116.43	121.82
1	A	175	TYR	CA-C-N	6.42	126.33	119.85
1	A	175	TYR	C-N-CA	6.42	126.33	119.85
1	A	1172	PRO	N-CA-C	-6.40	101.15	111.14
1	C	356	SER	CA-C-N	6.40	126.10	119.82
1	C	356	SER	C-N-CA	6.40	126.10	119.82
1	B	80	ARG	N-CA-C	6.40	120.48	110.17
1	A	340	LEU	CA-C-N	6.40	126.37	120.03
1	A	340	LEU	C-N-CA	6.40	126.37	120.03
1	B	538	ASP	CA-C-N	6.39	126.88	119.47
1	B	538	ASP	C-N-CA	6.39	126.88	119.47
1	A	538	ASP	CA-C-N	6.38	126.87	119.47
1	A	538	ASP	C-N-CA	6.38	126.87	119.47
1	A	97	PRO	N-CA-C	6.37	118.47	110.70
1	C	494	ALA	CA-C-N	6.34	126.31	120.03
1	C	494	ALA	C-N-CA	6.34	126.31	120.03
1	C	548	CYS	CA-C-N	6.33	126.02	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	CYS	C-N-CA	6.33	126.02	119.56
1	B	97	PRO	N-CA-C	6.33	118.42	110.70
1	C	181	HIS	CA-C-N	6.30	126.78	119.47
1	C	181	HIS	C-N-CA	6.30	126.78	119.47
1	A	96	LYS	CA-C-N	6.30	126.87	120.38
1	A	96	LYS	C-N-CA	6.30	126.87	120.38
1	C	450	VAL	N-CA-C	6.30	117.78	109.21
1	B	181	HIS	CA-C-N	6.29	126.76	119.47
1	B	181	HIS	C-N-CA	6.29	126.76	119.47
1	C	95	PHE	CA-CB-CG	-6.23	107.57	113.80
1	A	1130	SER	N-CA-C	6.22	117.63	108.86
1	A	31	ASN	N-CA-C	6.20	117.30	108.74
1	A	779	GLU	CA-C-N	6.20	125.89	119.56
1	A	779	GLU	C-N-CA	6.20	125.89	119.56
1	A	181	HIS	CA-C-N	6.19	126.65	119.47
1	A	181	HIS	C-N-CA	6.19	126.65	119.47
1	C	935	ASN	N-CA-C	-6.17	100.79	110.36
1	A	698	GLU	CA-C-N	6.17	126.36	120.31
1	A	698	GLU	C-N-CA	6.17	126.36	120.31
1	A	256	MET	CA-C-N	6.14	126.06	119.85
1	A	256	MET	C-N-CA	6.14	126.06	119.85
1	A	980	PHE	CA-C-N	6.08	126.64	120.38
1	A	980	PHE	C-N-CA	6.08	126.64	120.38
1	A	989	VAL	CA-C-N	6.07	126.03	119.78
1	A	989	VAL	C-N-CA	6.07	126.03	119.78
1	B	340	LEU	CB-CA-C	6.05	119.35	109.97
1	C	136	VAL	N-CA-C	-6.02	101.47	108.82
1	B	274	VAL	N-CA-C	6.00	116.51	107.75
1	B	175	TYR	CA-C-N	5.99	125.75	119.76
1	B	175	TYR	C-N-CA	5.99	125.75	119.76
1	B	613	THR	N-CA-C	-5.99	100.09	109.25
1	A	337	LYS	CA-C-N	5.97	126.49	120.04
1	A	337	LYS	C-N-CA	5.97	126.49	120.04
1	C	876	VAL	N-CA-C	5.97	117.37	108.54
1	C	126	PHE	CA-C-N	5.96	125.92	119.78
1	C	126	PHE	C-N-CA	5.96	125.92	119.78
1	B	669	PHE	N-CA-C	5.93	118.89	108.75
1	A	522	CYS	CA-C-N	5.92	125.88	119.78
1	A	522	CYS	C-N-CA	5.92	125.88	119.78
1	C	175	TYR	CA-C-N	5.90	125.66	119.76
1	C	175	TYR	C-N-CA	5.90	125.66	119.76
1	C	489	GLN	N-CA-C	-5.89	106.23	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1078	ASP	CA-C-N	5.86	126.42	120.38
1	C	1078	ASP	C-N-CA	5.86	126.42	120.38
1	A	712	PHE	CA-CB-CG	-5.84	107.95	113.80
1	C	169	GLN	CB-CA-C	-5.83	103.37	112.12
1	C	97	PRO	N-CA-C	5.79	117.76	110.70
1	B	328	GLN	CA-C-N	5.78	125.71	119.76
1	B	328	GLN	C-N-CA	5.78	125.71	119.76
1	A	663	ASN	N-CA-C	-5.77	105.95	112.87
1	B	256	MET	CA-C-N	5.74	125.65	119.85
1	B	256	MET	C-N-CA	5.74	125.65	119.85
1	A	266	ILE	N-CA-C	-5.73	104.75	111.00
1	C	724	ASN	CA-C-N	-5.72	114.94	123.00
1	C	724	ASN	C-N-CA	-5.72	114.94	123.00
1	B	337	LYS	CA-C-N	5.71	126.21	120.04
1	B	337	LYS	C-N-CA	5.71	126.21	120.04
1	A	775	PHE	CA-C-N	5.70	133.30	121.32
1	A	775	PHE	C-N-CA	5.70	133.30	121.32
1	A	371	ASN	CA-CB-CG	-5.68	106.92	112.60
1	A	34	ASP	N-CA-C	5.67	117.68	108.26
1	B	37	PRO	CA-C-N	5.66	126.92	119.84
1	B	37	PRO	C-N-CA	5.66	126.92	119.84
1	C	484	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	269	THR	N-CA-C	-5.64	101.50	109.96
1	A	72	TYR	CA-C-N	5.63	125.58	119.78
1	A	72	TYR	C-N-CA	5.63	125.58	119.78
1	C	936	ASN	CA-CB-CG	5.63	118.23	112.60
1	C	831	GLY	N-CA-C	-5.62	104.56	112.60
1	A	470	SER	N-CA-C	-5.61	105.22	112.68
1	A	300	SER	N-CA-C	5.60	118.15	111.71
1	A	1124	GLU	N-CA-C	5.60	120.24	113.41
1	C	980	PHE	CA-CB-CG	-5.60	108.20	113.80
1	B	172	MET	CA-C-N	5.60	129.73	120.94
1	B	172	MET	C-N-CA	5.60	129.73	120.94
1	A	20	LYS	N-CA-C	5.59	117.37	111.28
1	B	934	TYR	N-CA-C	-5.59	102.64	110.35
1	A	314	ALA	CA-C-N	5.58	126.13	120.38
1	A	314	ALA	C-N-CA	5.58	126.13	120.38
1	B	656	GLN	N-CA-C	5.53	117.42	108.41
1	A	774	ARG	O-C-N	-5.52	116.01	122.96
1	B	981	PRO	N-CA-C	5.52	117.43	110.70
1	C	692	PHE	N-CA-C	5.50	117.86	108.90
1	B	924	LYS	N-CA-C	5.49	117.35	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	ASN	N-CA-C	5.49	117.35	108.34
1	C	698	GLU	CA-C-N	5.49	125.69	120.31
1	C	698	GLU	C-N-CA	5.49	125.69	120.31
1	C	538	ASP	CA-C-N	5.46	125.55	119.32
1	C	538	ASP	C-N-CA	5.46	125.55	119.32
1	B	172	MET	N-CA-C	5.43	117.70	110.53
1	C	26	ARG	CA-C-N	5.43	131.90	121.54
1	C	26	ARG	C-N-CA	5.43	131.90	121.54
1	A	465	GLY	CA-C-N	-5.42	114.98	122.30
1	A	465	GLY	C-N-CA	-5.42	114.98	122.30
1	C	651	TYR	N-CA-C	5.41	119.05	112.23
1	B	428	PHE	N-CA-C	5.40	120.73	114.04
1	A	36	GLY	CA-C-N	5.38	125.93	120.38
1	A	36	GLY	C-N-CA	5.38	125.93	120.38
1	C	218	PHE	CA-CB-CG	5.38	119.18	113.80
1	B	126	PHE	CA-C-N	5.37	125.29	119.76
1	B	126	PHE	C-N-CA	5.37	125.29	119.76
1	A	461	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	979	LEU	N-CA-C	5.36	119.54	112.89
1	A	456	ASN	CA-C-N	5.34	126.38	120.45
1	A	456	ASN	C-N-CA	5.34	126.38	120.45
1	C	371	ASN	CA-C-N	5.33	127.96	120.28
1	C	371	ASN	C-N-CA	5.33	127.96	120.28
1	C	1161	VAL	CA-C-N	5.33	125.27	119.78
1	C	1161	VAL	C-N-CA	5.33	125.27	119.78
1	A	77	SER	N-CA-C	-5.33	103.65	110.53
1	A	79	TYR	CA-CB-CG	5.32	123.48	113.90
1	A	190	GLU	N-CA-C	5.32	116.79	110.19
1	C	456	ASN	CA-C-N	5.32	125.40	119.87
1	C	456	ASN	C-N-CA	5.32	125.40	119.87
1	A	1077	LEU	N-CA-C	5.29	118.34	110.14
1	B	989	VAL	N-CA-C	5.26	113.15	108.63
1	A	794	GLY	N-CA-C	-5.26	107.99	115.30
1	B	424	TYR	N-CA-C	-5.23	105.64	112.23
1	C	409	ILE	N-CA-C	5.22	113.62	107.77
1	B	586	TRP	CA-CB-CG	-5.22	103.69	113.60
1	A	660	TYR	N-CA-C	5.19	118.21	109.95
1	C	125	GLU	N-CA-C	5.18	117.26	109.23
1	A	409	ILE	CB-CA-C	-5.18	104.93	111.04
1	C	409	ILE	CB-CA-C	-5.17	104.83	110.78
1	A	1076	ARG	N-CA-C	5.17	117.00	111.36
1	C	79	TYR	CA-CB-CG	5.16	123.19	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	VAL	N-CA-C	5.16	115.52	107.99
1	A	429	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	126	PHE	CB-CA-C	5.14	117.00	110.22
1	C	1078	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	187	HIS	CA-CB-CG	5.13	118.93	113.80
1	C	314	ALA	CA-C-N	5.13	125.67	120.38
1	C	314	ALA	C-N-CA	5.13	125.67	120.38
1	A	360	TRP	CA-C-N	5.13	129.24	122.42
1	A	360	TRP	C-N-CA	5.13	129.24	122.42
1	C	275	THR	CA-C-N	5.12	125.03	119.76
1	C	275	THR	C-N-CA	5.12	125.03	119.76
1	B	136	VAL	CA-C-O	-5.12	116.45	121.67
1	B	499	CYS	CA-C-N	5.10	124.77	119.56
1	B	499	CYS	C-N-CA	5.10	124.77	119.56
1	C	1183	ALA	N-CA-C	-5.10	103.76	110.39
1	C	464	PHE	CA-CB-CG	-5.09	108.71	113.80
1	C	20	LYS	N-CA-C	5.09	116.83	111.28
1	C	981	PRO	N-CA-C	5.09	116.91	110.70
1	B	136	VAL	N-CA-C	-5.08	101.38	108.80
1	B	1139	GLY	N-CA-C	-5.08	103.78	110.29
1	A	499	CYS	CA-C-N	5.08	125.52	120.04
1	A	499	CYS	C-N-CA	5.08	125.52	120.04
1	A	359	ASN	CA-C-N	-5.05	114.20	121.42
1	A	359	ASN	C-N-CA	-5.05	114.20	121.42
1	C	563	GLY	N-CA-C	5.05	117.80	111.09
1	C	614	CYS	N-CA-C	5.04	117.63	109.06
1	B	935	ASN	CA-C-N	5.04	127.54	120.28
1	B	935	ASN	C-N-CA	5.04	127.54	120.28
1	A	701	LEU	N-CA-C	5.04	116.73	108.52
1	C	42	THR	N-CA-CB	-5.01	104.33	111.00
1	B	576	CYS	N-CA-C	-5.01	100.13	110.80
1	A	428	PHE	CA-CB-CG	-5.00	108.80	113.80

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	9151	0	8841	58	0
1	B	9178	0	8864	26	0
1	C	9134	0	8826	26	0
2	H	555	0	136	6	0
2	L	495	0	120	3	0
3	D	28	0	25	0	0
3	F	28	0	25	3	0
3	G	28	0	25	1	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
3	M	28	0	25	2	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
4	E	39	0	34	0	0
4	K	39	0	34	1	0
5	A	154	0	143	1	0
5	B	140	0	130	2	0
5	C	140	0	130	1	0
6	A	18	0	0	2	0
6	B	18	0	0	2	0
6	C	18	0	0	0	0
All	All	29331	0	27483	121	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 2.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TRP:CD1	1:A:360:TRP:H	2.10	0.67
1:B:486:VAL:HB	1:B:586:TRP:HE1	1.63	0.64
1:A:265:ASP:OD1	1:A:266:ILE:HG13	1.98	0.62
1:A:162:LEU:HB2	1:A:207:PHE:O	1.98	0.62
1:C:142:VAL:HG22	1:C:167:VAL:HG13	1.82	0.61
1:A:775:PHE:O	1:A:775:PHE:CG	2.51	0.60
1:C:149:ILE:HG22	1:C:150:ASN:N	2.18	0.59
1:B:944:ARG:HG2	1:B:944:ARG:O	2.02	0.59
1:C:159:LEU:HD23	1:C:160:GLN:N	2.17	0.59
1:B:454:ARG:HD3	1:B:486:VAL:HG13	1.85	0.58
1:A:348:TRP:HZ3	1:A:404:ILE:CG2	2.19	0.56
1:A:342:ASN:HB3	3:F:1:NAG:H61	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:VAL:CG1	1:B:586:TRP:HE1	2.19	0.56
1:A:162:LEU:C	1:A:162:LEU:HD12	2.30	0.56
1:A:360:TRP:HZ2	1:A:558:GLY:C	2.13	0.56
1:A:430:TYR:HE1	1:A:558:GLY:H	1.55	0.55
1:A:415:VAL:HG11	6:B:1411:8Z9:C5	2.36	0.55
1:B:88:ASP:OD2	1:B:89:LYS:NZ	2.39	0.55
1:A:85:LYS:HD2	1:A:86:GLY:H	1.73	0.54
1:A:119:ASP:OD2	1:A:183:LYS:NZ	2.41	0.54
1:B:51:LEU:HD11	1:B:108:PHE:HZ	1.72	0.54
3:M:2:NAG:O7	3:M:2:NAG:O3	2.24	0.53
1:A:892:ASP:OD2	1:A:1014:LYS:NZ	2.40	0.52
1:A:415:VAL:CG1	6:B:1411:8Z9:C5	2.88	0.52
1:A:19:LEU:HD21	1:A:194:MET:HB3	1.91	0.52
1:C:142:VAL:HG13	1:C:167:VAL:HG22	1.91	0.52
1:C:371:ASN:N	1:C:371:ASN:OD1	2.43	0.52
1:B:454:ARG:HD3	1:B:486:VAL:CG1	2.40	0.51
1:A:193:HIS:CG	1:A:193:HIS:O	2.63	0.51
1:A:38:PRO:O	1:A:39:SER:HB2	2.11	0.50
2:H:28:UNK:C	2:H:30:UNK:N	2.73	0.50
1:C:360:TRP:O	1:C:360:TRP:CE3	2.65	0.50
1:C:241:LEU:HG	1:C:242:PHE:HD1	1.77	0.49
1:B:486:VAL:HB	1:B:586:TRP:NE1	2.27	0.49
1:B:486:VAL:CB	1:B:586:TRP:HE1	2.24	0.49
1:A:360:TRP:CD1	1:A:430:TYR:HB2	2.48	0.49
1:A:149:ILE:HG21	1:A:160:GLN:H	1.78	0.49
1:A:85:LYS:HG3	1:A:86:GLY:O	2.13	0.49
1:A:198:VAL:HG12	1:A:199:VAL:N	2.28	0.49
1:A:159:LEU:C	1:A:159:LEU:HD23	2.38	0.49
1:A:162:LEU:HA	1:A:209:TYR:HD1	1.78	0.48
1:C:196:THR:HB	3:G:2:NAG:O6	2.13	0.48
1:C:723:ILE:HG22	1:C:724:ASN:ND2	2.29	0.48
1:B:51:LEU:CD1	1:B:108:PHE:HZ	2.26	0.48
1:B:159:LEU:HD12	1:B:159:LEU:C	2.39	0.48
1:B:586:TRP:O	1:B:586:TRP:CE3	2.67	0.48
1:A:362:ARG:HG3	1:A:405:ASP:OD1	2.13	0.48
1:B:180:CYS:O	1:B:181:HIS:C	2.55	0.48
1:A:149:ILE:HG21	1:A:160:GLN:C	2.39	0.48
1:B:655:TRP:CE3	1:B:656:GLN:HG3	2.50	0.47
1:C:38:PRO:O	1:C:40:ILE:HG12	2.14	0.47
1:B:586:TRP:CD2	1:B:586:TRP:C	2.88	0.47
2:H:35:UNK:O	2:H:36:UNK:C	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:SER:C	1:A:664:GLY:N	2.71	0.47
2:H:99:UNK:O	2:H:100:UNK:C	2.62	0.47
1:A:348:TRP:CE2	1:A:406:LYS:HE2	2.51	0.46
1:A:265:ASP:OD1	1:A:266:ILE:N	2.48	0.46
1:A:616:THR:O	1:A:616:THR:HG22	2.16	0.46
1:B:934:TYR:O	1:B:935:ASN:HB2	2.15	0.46
1:A:35:THR:O	1:A:36:GLY:C	2.59	0.46
1:C:1222:VAL:HB	5:C:1410:NAG:H82	1.98	0.46
1:A:376:MET:HG2	6:A:1412:8Z9:C5	2.46	0.46
1:A:454:ARG:O	1:A:455:PHE:CD2	2.70	0.46
1:A:1130:SER:OG	1:A:1131:SER:N	2.50	0.45
1:B:466:PHE:CD2	1:B:466:PHE:C	2.94	0.45
1:C:88:ASP:OD2	1:C:89:LYS:NZ	2.46	0.45
1:A:342:ASN:CB	3:F:1:NAG:H61	2.46	0.45
1:A:745:GLN:N	1:A:745:GLN:CD	2.75	0.45
1:C:218:PHE:CE1	1:C:231:PHE:CD1	3.05	0.45
1:B:53:THR:HG23	1:B:72:TYR:HE2	1.82	0.45
1:B:159:LEU:HD11	5:B:1401:NAG:C6	2.47	0.45
1:C:922:LYS:NZ	1:C:1032:ASP:OD2	2.47	0.44
1:B:661:ASP:OD1	1:B:661:ASP:C	2.61	0.44
2:H:10:UNK:O	2:H:11:UNK:C	2.65	0.44
1:C:1192:VAL:HG12	3:J:1:NAG:H82	1.99	0.44
2:H:29:UNK:C	2:H:31:UNK:N	2.78	0.44
1:A:788:ASP:OD1	1:A:788:ASP:N	2.48	0.44
1:C:241:LEU:HD23	1:C:242:PHE:CE1	2.53	0.44
1:A:348:TRP:CD2	1:A:348:TRP:O	2.71	0.44
1:A:616:THR:HG23	1:A:619:GLN:OE1	2.18	0.43
1:A:1113:PHE:HE2	1:B:1113:PHE:HD1	1.65	0.43
1:B:159:LEU:HD11	5:B:1401:NAG:H61	2.00	0.43
1:A:37:PRO:HA	1:A:38:PRO:HD3	1.89	0.43
1:A:161:GLY:H	1:A:211:VAL:HG11	1.83	0.43
1:A:245:TYR:OH	1:C:360:TRP:CH2	2.70	0.43
1:A:348:TRP:CZ2	1:A:406:LYS:HE2	2.53	0.43
1:C:149:ILE:HD11	4:K:1:NAG:O6	2.18	0.43
1:A:272:TYR:C	1:A:272:TYR:CD1	2.94	0.43
1:C:170:TYR:HB2	1:C:193:HIS:CD2	2.54	0.43
1:B:536:ASN:HB2	1:B:537:PRO:HD3	2.00	0.43
2:H:5:UNK:N	2:H:23:UNK:O	2.51	0.43
5:A:1410:NAG:H83	5:A:1410:NAG:H2	1.89	0.43
1:A:96:LYS:HB3	1:A:97:PRO:HD2	2.01	0.43
1:C:218:PHE:CD1	1:C:231:PHE:HD1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TRP:CZ2	1:A:558:GLY:C	2.95	0.42
1:A:522:CYS:HA	1:A:523:PRO:HD3	1.90	0.42
1:A:348:TRP:HZ3	1:A:404:ILE:HG22	1.84	0.42
1:A:376:MET:HG2	6:A:1412:8Z9:C6	2.50	0.42
1:A:1113:PHE:HE1	1:A:1117:GLN:NE2	2.18	0.42
1:C:573:GLY:O	1:C:574:ASN:C	2.63	0.42
3:M:2:NAG:O3	3:M:2:NAG:C7	2.68	0.42
1:A:536:ASN:HB2	1:A:537:PRO:HD3	2.02	0.41
1:A:1198:TYR:CD2	1:A:1198:TYR:C	2.96	0.41
1:C:218:PHE:CD1	1:C:231:PHE:CD1	3.08	0.41
1:C:218:PHE:CZ	1:C:231:PHE:CE1	3.08	0.41
1:B:981:PRO:HA	1:B:983:TRP:CE2	2.56	0.41
1:C:537:PRO:O	1:C:538:ASP:C	2.61	0.41
1:A:537:PRO:O	1:A:538:ASP:C	2.62	0.41
1:B:740:THR:O	1:B:777:ASN:ND2	2.54	0.41
1:A:348:TRP:O	1:A:348:TRP:CE3	2.74	0.41
3:F:1:NAG:H82	3:F:1:NAG:H2	1.93	0.41
1:A:1078:ASP:OD1	1:A:1078:ASP:C	2.64	0.41
1:C:137:ASN:OD1	1:C:137:ASN:C	2.64	0.41
1:A:755:TYR:CD1	1:A:775:PHE:CZ	3.09	0.40
1:C:137:ASN:O	1:C:138:THR:HB	2.22	0.40
2:L:66:UNK:O	2:L:67:UNK:C	2.69	0.40
1:A:162:LEU:HA	1:A:209:TYR:CD1	2.56	0.40
1:B:655:TRP:CH2	1:B:656:GLN:NE2	2.89	0.40
2:L:41:UNK:O	2:L:42:UNK:C	2.66	0.40
2:L:32:UNK:O	2:L:84:UNK:N	2.54	0.40
1:A:297:ASP:OD1	1:A:297:ASP:C	2.64	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	1164/1367 (85%)	1132 (97%)	32 (3%)	0	100	100
1	B	1168/1367 (85%)	1145 (98%)	23 (2%)	0	100	100
1	C	1159/1367 (85%)	1138 (98%)	21 (2%)	0	100	100
All	All	3491/4101 (85%)	3415 (98%)	76 (2%)	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	1023/1182 (86%)	1023 (100%)	0	100	100
1	B	1027/1182 (87%)	1027 (100%)	0	100	100
1	C	1022/1182 (86%)	1022 (100%)	0	100	100
All	All	3072/3546 (87%)	3072 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	858	ASN
1	A	870	ASN
1	A	889	ASN
1	A	1000	ASN
1	A	1042	GLN
1	A	1103	GLN
1	A	1213	ASN
1	C	288	GLN
1	C	342	ASN
1	C	418	GLN
1	C	444	ASN
1	C	517	ASN

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Mol	Chain	Res	Type
1	C	606	HIS
1	C	609	ASN
1	C	724	ASN
1	C	870	ASN
1	C	889	ASN
1	C	1000	ASN
1	B	288	GLN
1	B	387	ASN
1	B	440	GLN
1	B	602	ASN
1	B	606	HIS
1	B	777	ASN
1	B	870	ASN
1	B	994	ASN
1	B	1000	ASN
1	B	1011	GLN
1	B	1042	GLN
1	B	1048	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	$\# Z > 2$
3	NAG	D	1	1,3	14,14,15	2.19	6 (42%)	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	2	3	14,14,15	1.96	6 (42%)	17,19,21	0.96	1 (5%)
4	NAG	E	1	1,4	14,14,15	2.22	6 (42%)	17,19,21	1.01	1 (5%)
4	NAG	E	2	4	14,14,15	2.08	6 (42%)	17,19,21	0.95	1 (5%)
4	BMA	E	3	4	11,11,12	1.94	5 (45%)	15,15,17	0.74	0
3	NAG	F	1	1,3	14,14,15	0.48	0	17,19,21	1.52	2 (11%)
3	NAG	F	2	3	14,14,15	0.39	0	17,19,21	1.08	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.39	0	17,19,21	0.43	0
3	NAG	G	2	3	14,14,15	0.37	0	17,19,21	0.44	0
3	NAG	I	1	1,3	14,14,15	2.12	4 (28%)	17,19,21	1.21	1 (5%)
3	NAG	I	2	3	14,14,15	2.02	6 (42%)	17,19,21	1.04	2 (11%)
3	NAG	J	1	1,3	14,14,15	2.23	7 (50%)	17,19,21	1.24	2 (11%)
3	NAG	J	2	3	14,14,15	2.03	6 (42%)	17,19,21	0.96	1 (5%)
4	NAG	K	1	1,4	14,14,15	2.26	5 (35%)	17,19,21	1.09	1 (5%)
4	NAG	K	2	4	14,14,15	2.09	6 (42%)	17,19,21	0.98	2 (11%)
4	BMA	K	3	4	11,11,12	2.01	6 (54%)	15,15,17	0.62	0
3	NAG	M	1	1,3	14,14,15	0.39	0	17,19,21	0.56	0
3	NAG	M	2	3	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	N	1	1,3	14,14,15	2.13	6 (42%)	17,19,21	1.11	2 (11%)
3	NAG	N	2	3	14,14,15	2.06	5 (35%)	17,19,21	0.92	1 (5%)
3	NAG	O	1	1,3	14,14,15	2.06	4 (28%)	17,19,21	1.25	1 (5%)
3	NAG	O	2	3	14,14,15	2.11	5 (35%)	17,19,21	1.08	2 (11%)
3	NAG	P	1	1,3	14,14,15	2.35	6 (42%)	17,19,21	1.08	1 (5%)
3	NAG	P	2	3	14,14,15	1.99	6 (42%)	17,19,21	0.96	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	0/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	NAG	C1-C2	6.36	1.61	1.52
3	P	1	NAG	C1-C2	6.36	1.61	1.52
4	E	1	NAG	C1-C2	5.99	1.60	1.52
3	I	1	NAG	C1-C2	5.82	1.60	1.52
3	O	1	NAG	C1-C2	5.74	1.60	1.52
3	D	1	NAG	C1-C2	5.61	1.60	1.52
3	J	1	NAG	C1-C2	5.36	1.59	1.52
3	N	1	NAG	C1-C2	5.36	1.59	1.52
3	O	2	NAG	C1-C2	5.25	1.59	1.52
3	N	2	NAG	C1-C2	4.99	1.59	1.52
3	J	2	NAG	C1-C2	4.80	1.58	1.52
4	E	2	NAG	C1-C2	4.74	1.58	1.52
4	K	2	NAG	C1-C2	4.67	1.58	1.52
3	I	2	NAG	C1-C2	4.64	1.58	1.52
3	D	2	NAG	C1-C2	4.59	1.58	1.52
3	P	2	NAG	C1-C2	4.41	1.58	1.52
3	P	2	NAG	O5-C5	3.34	1.49	1.43
4	K	3	BMA	O5-C5	3.29	1.49	1.43
4	K	3	BMA	C2-C3	3.29	1.57	1.52
3	I	2	NAG	O5-C5	3.26	1.49	1.43
4	E	3	BMA	C2-C3	3.22	1.57	1.52
4	K	2	NAG	O5-C5	3.17	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	BMA	O5-C5	3.15	1.49	1.43
3	J	2	NAG	O5-C5	3.12	1.49	1.43
3	D	1	NAG	O5-C5	3.08	1.49	1.43
3	D	2	NAG	O5-C5	3.05	1.49	1.43
3	J	1	NAG	O5-C5	3.04	1.49	1.43
3	O	2	NAG	O5-C5	3.03	1.49	1.43
3	N	2	NAG	O5-C5	3.01	1.49	1.43
4	E	2	NAG	O5-C5	2.99	1.49	1.43
3	P	1	NAG	O5-C5	2.83	1.49	1.43
4	E	1	NAG	O5-C5	2.78	1.48	1.43
4	K	3	BMA	C1-C2	2.73	1.58	1.52
4	E	3	BMA	C1-C2	2.71	1.58	1.52
3	N	1	NAG	O5-C5	2.71	1.48	1.43
3	N	1	NAG	O5-C1	2.66	1.48	1.43
3	J	1	NAG	O5-C1	2.62	1.48	1.43
3	P	1	NAG	C3-C2	2.57	1.57	1.52
3	D	2	NAG	C3-C2	2.57	1.57	1.52
4	K	1	NAG	O5-C5	2.56	1.48	1.43
4	E	2	NAG	C3-C2	2.53	1.57	1.52
4	K	2	NAG	C4-C5	2.52	1.58	1.53
4	K	2	NAG	C3-C2	2.50	1.57	1.52
3	J	2	NAG	C3-C2	2.49	1.57	1.52
3	O	2	NAG	C2-N2	2.49	1.50	1.46
3	I	1	NAG	C3-C2	2.48	1.57	1.52
3	I	1	NAG	O5-C5	2.47	1.48	1.43
3	N	1	NAG	C3-C2	2.47	1.57	1.52
3	J	1	NAG	C2-N2	2.46	1.50	1.46
3	P	2	NAG	C3-C2	2.45	1.57	1.52
3	N	2	NAG	C3-C2	2.44	1.57	1.52
3	O	2	NAG	C3-C2	2.44	1.57	1.52
4	E	3	BMA	C4-C5	2.43	1.58	1.53
3	D	1	NAG	O5-C1	2.42	1.47	1.43
3	P	2	NAG	C4-C5	2.41	1.58	1.53
3	J	2	NAG	C4-C5	2.40	1.58	1.53
3	O	1	NAG	O5-C5	2.40	1.48	1.43
4	K	3	BMA	C4-C5	2.38	1.58	1.53
3	I	2	NAG	C4-C5	2.38	1.58	1.53
3	P	1	NAG	O5-C1	2.37	1.47	1.43
4	E	2	NAG	C4-C3	2.37	1.58	1.52
3	I	2	NAG	C3-C2	2.36	1.57	1.52
3	N	2	NAG	C4-C5	2.34	1.58	1.53
4	K	1	NAG	C3-C2	2.33	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	2	NAG	C2-N2	2.32	1.50	1.46
3	J	1	NAG	C4-C5	2.31	1.58	1.53
4	K	2	NAG	C4-C3	2.31	1.58	1.52
4	E	2	NAG	C2-N2	2.31	1.50	1.46
4	E	2	NAG	C4-C5	2.31	1.57	1.53
3	P	1	NAG	C2-N2	2.29	1.50	1.46
4	K	2	NAG	C2-N2	2.29	1.50	1.46
4	E	1	NAG	O5-C1	2.29	1.47	1.43
4	E	1	NAG	C3-C2	2.29	1.57	1.52
3	D	1	NAG	C3-C2	2.28	1.57	1.52
3	O	2	NAG	C4-C5	2.27	1.57	1.53
3	J	1	NAG	C3-C2	2.26	1.57	1.52
3	D	2	NAG	C4-C5	2.25	1.57	1.53
4	K	1	NAG	C2-N2	2.24	1.50	1.46
3	I	2	NAG	C2-N2	2.23	1.50	1.46
3	O	1	NAG	C3-C2	2.22	1.57	1.52
3	J	1	NAG	C4-C3	2.22	1.58	1.52
3	D	1	NAG	C4-C3	2.20	1.58	1.52
3	D	1	NAG	C4-C5	2.19	1.57	1.53
3	I	1	NAG	O5-C1	2.19	1.47	1.43
3	J	2	NAG	C2-N2	2.18	1.49	1.46
3	P	2	NAG	C2-N2	2.18	1.49	1.46
4	E	1	NAG	C4-C5	2.18	1.57	1.53
4	K	3	BMA	O5-C1	2.14	1.47	1.43
3	I	2	NAG	C4-C3	2.12	1.57	1.52
4	K	1	NAG	O5-C1	2.08	1.47	1.43
3	P	2	NAG	C4-C3	2.08	1.57	1.52
3	J	2	NAG	C4-C3	2.08	1.57	1.52
3	N	1	NAG	C4-C3	2.07	1.57	1.52
3	O	1	NAG	C4-C5	2.07	1.57	1.53
4	K	3	BMA	C4-C3	2.05	1.57	1.52
3	P	1	NAG	C4-C3	2.05	1.57	1.52
4	E	3	BMA	C4-C3	2.05	1.57	1.52
3	D	2	NAG	C2-N2	2.03	1.49	1.46
4	E	1	NAG	C2-N2	2.01	1.49	1.46
3	D	2	NAG	C4-C3	2.01	1.57	1.52
3	N	1	NAG	C4-C5	2.00	1.57	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O4-C4-C3	4.79	121.67	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	C8-C7-N2	3.38	121.72	116.12
3	F	2	NAG	O5-C1-C2	-3.19	106.35	111.29
3	O	2	NAG	C8-C7-N2	2.96	121.03	116.12
3	I	2	NAG	C8-C7-N2	2.75	120.67	116.12
3	I	1	NAG	C1-C2-N2	-2.66	106.25	110.43
3	J	1	NAG	O7-C7-C8	-2.65	117.33	122.05
3	P	1	NAG	C8-C7-N2	2.45	120.19	116.12
4	E	2	NAG	C8-C7-N2	2.45	120.18	116.12
4	K	1	NAG	C8-C7-N2	2.41	120.12	116.12
4	K	2	NAG	C8-C7-N2	2.39	120.09	116.12
3	O	2	NAG	O7-C7-C8	-2.34	117.88	122.05
4	K	2	NAG	O7-C7-C8	-2.33	117.90	122.05
3	P	2	NAG	C8-C7-N2	2.33	119.97	116.12
3	I	2	NAG	O7-C7-C8	-2.26	118.03	122.05
3	N	2	NAG	C8-C7-N2	2.20	119.77	116.12
3	D	2	NAG	C8-C7-N2	2.13	119.66	116.12
3	J	2	NAG	C8-C7-N2	2.13	119.66	116.12
3	O	1	NAG	O4-C4-C3	-2.09	105.45	110.38
3	F	1	NAG	C4-C3-C2	-2.08	107.97	111.02
3	N	1	NAG	C8-C7-N2	2.07	119.56	116.12
3	N	1	NAG	O4-C4-C5	-2.03	104.33	109.32
4	E	1	NAG	C8-C7-N2	2.02	119.47	116.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	2	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C1-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2

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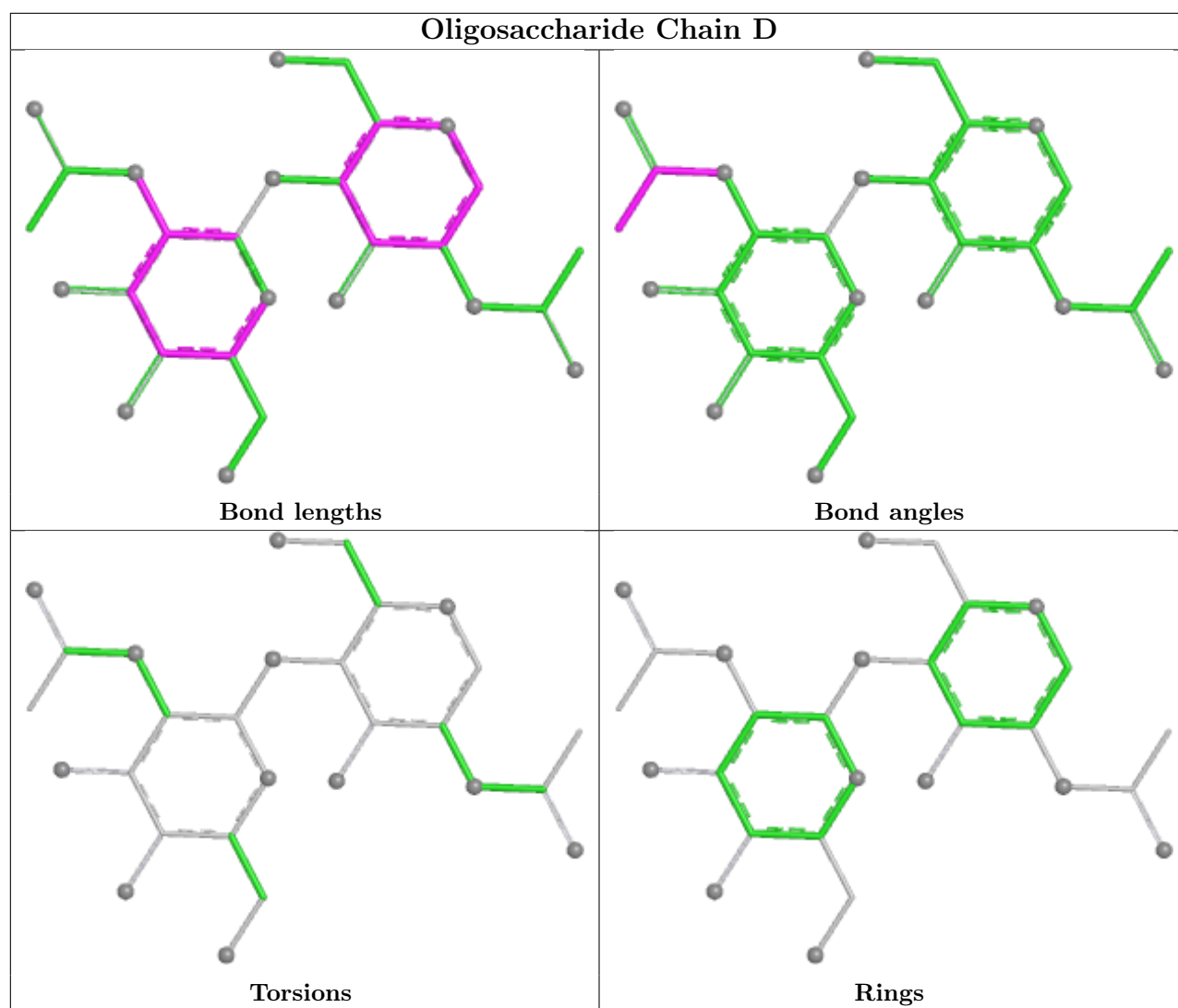
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O7-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C3-C2-N2-C7
3	O	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6

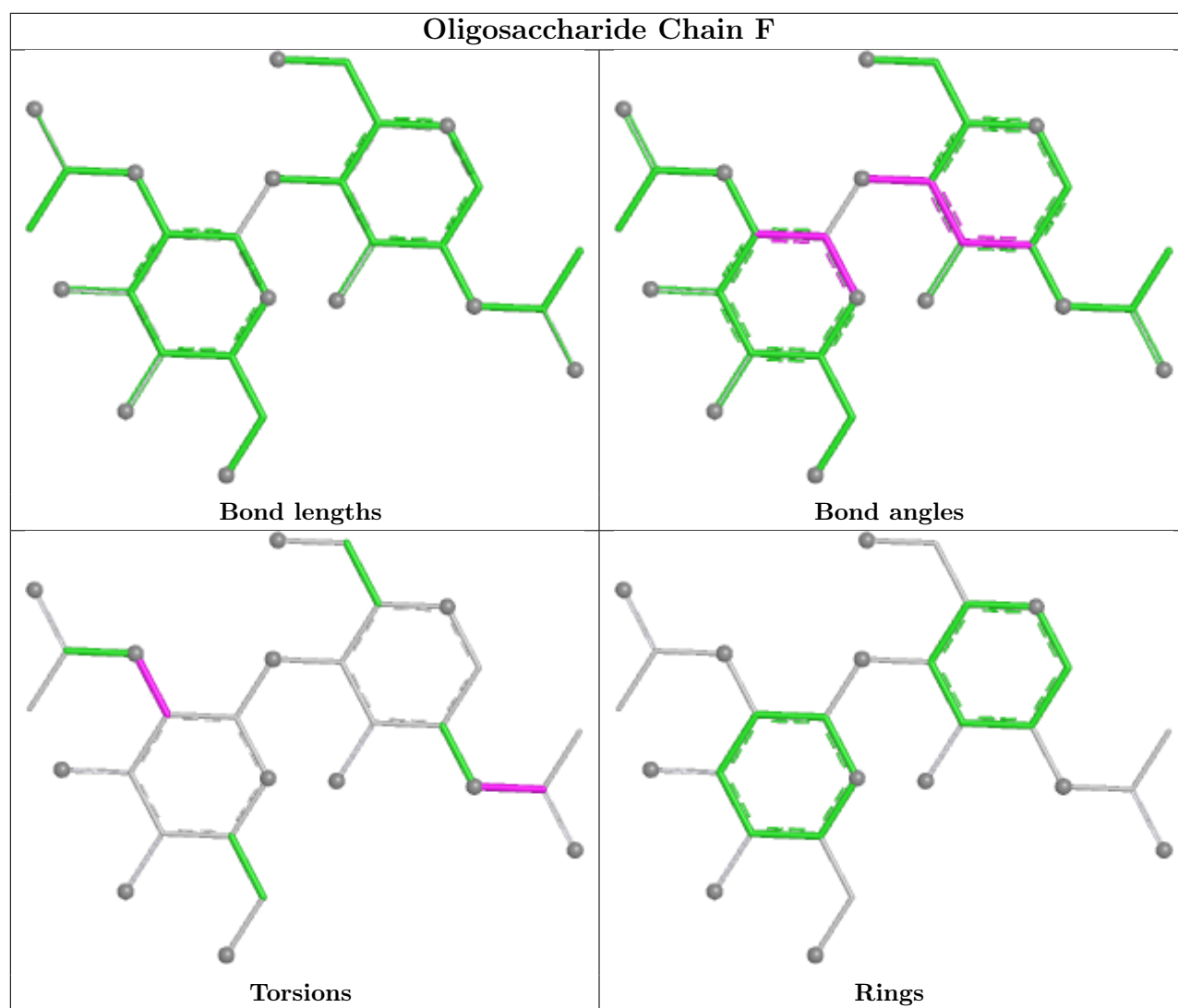
There are no ring outliers.

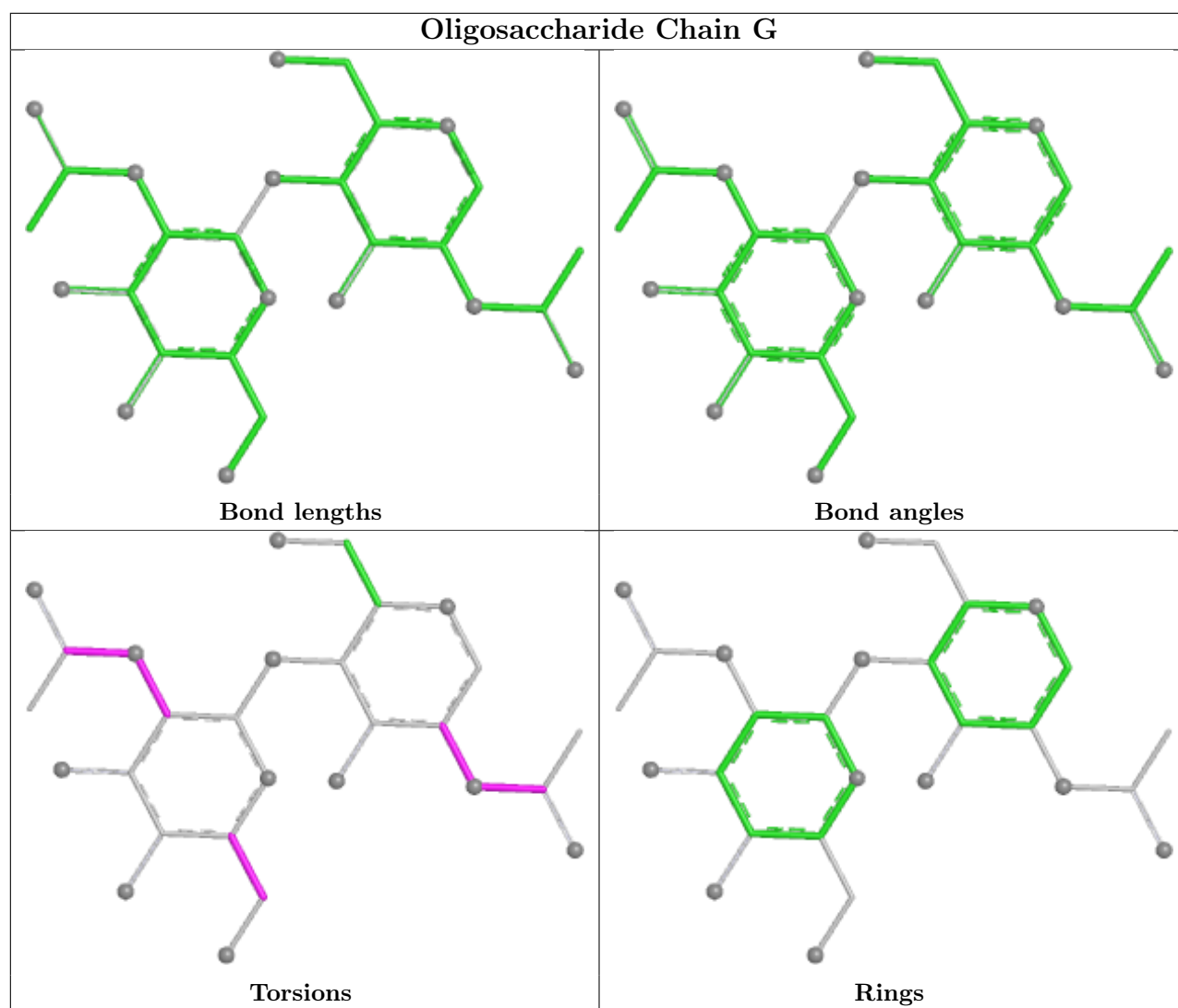
5 monomers are involved in 8 short contacts:

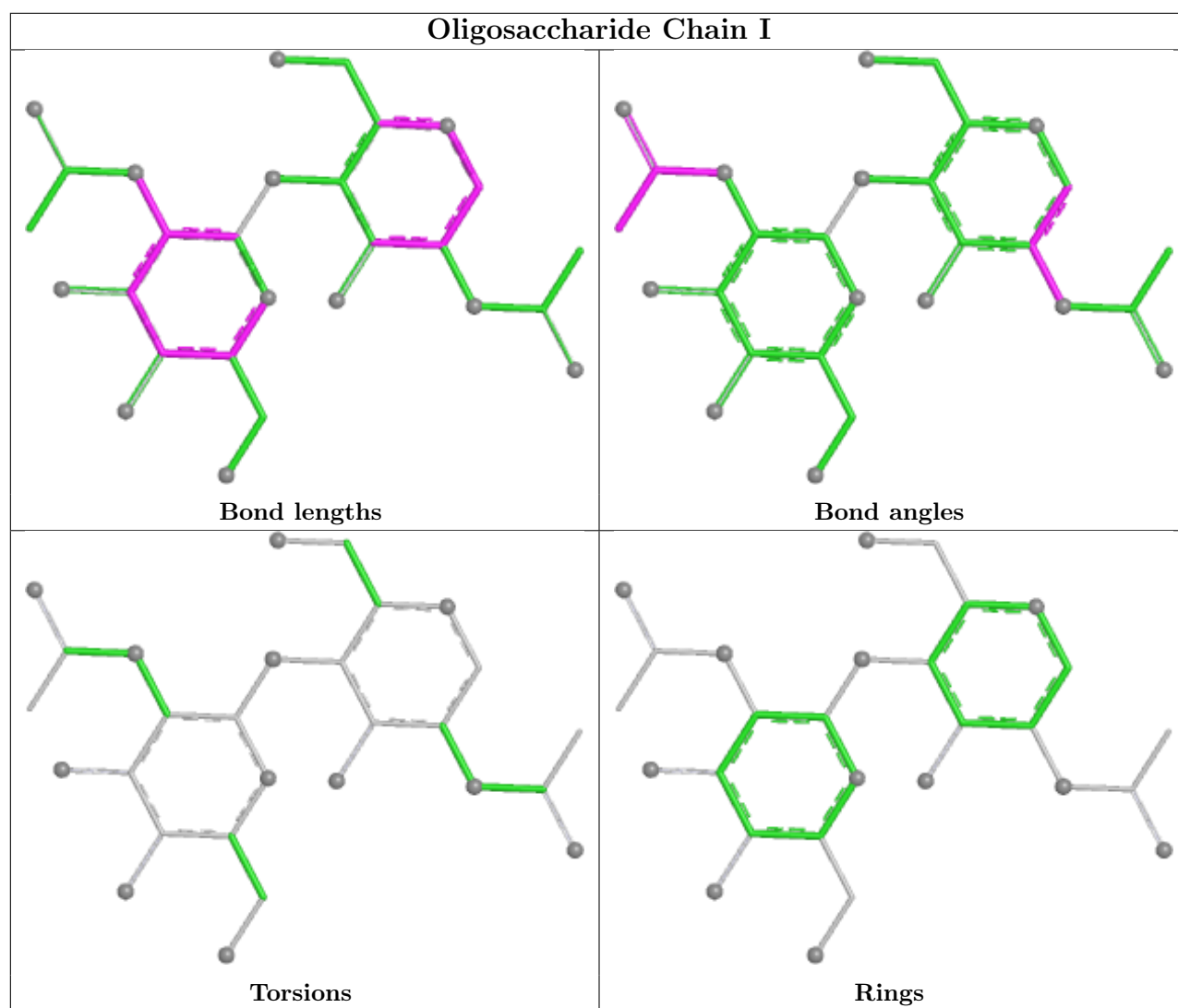
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	1	0
3	F	1	NAG	3	0
3	M	2	NAG	2	0
3	G	2	NAG	1	0
4	K	1	NAG	1	0

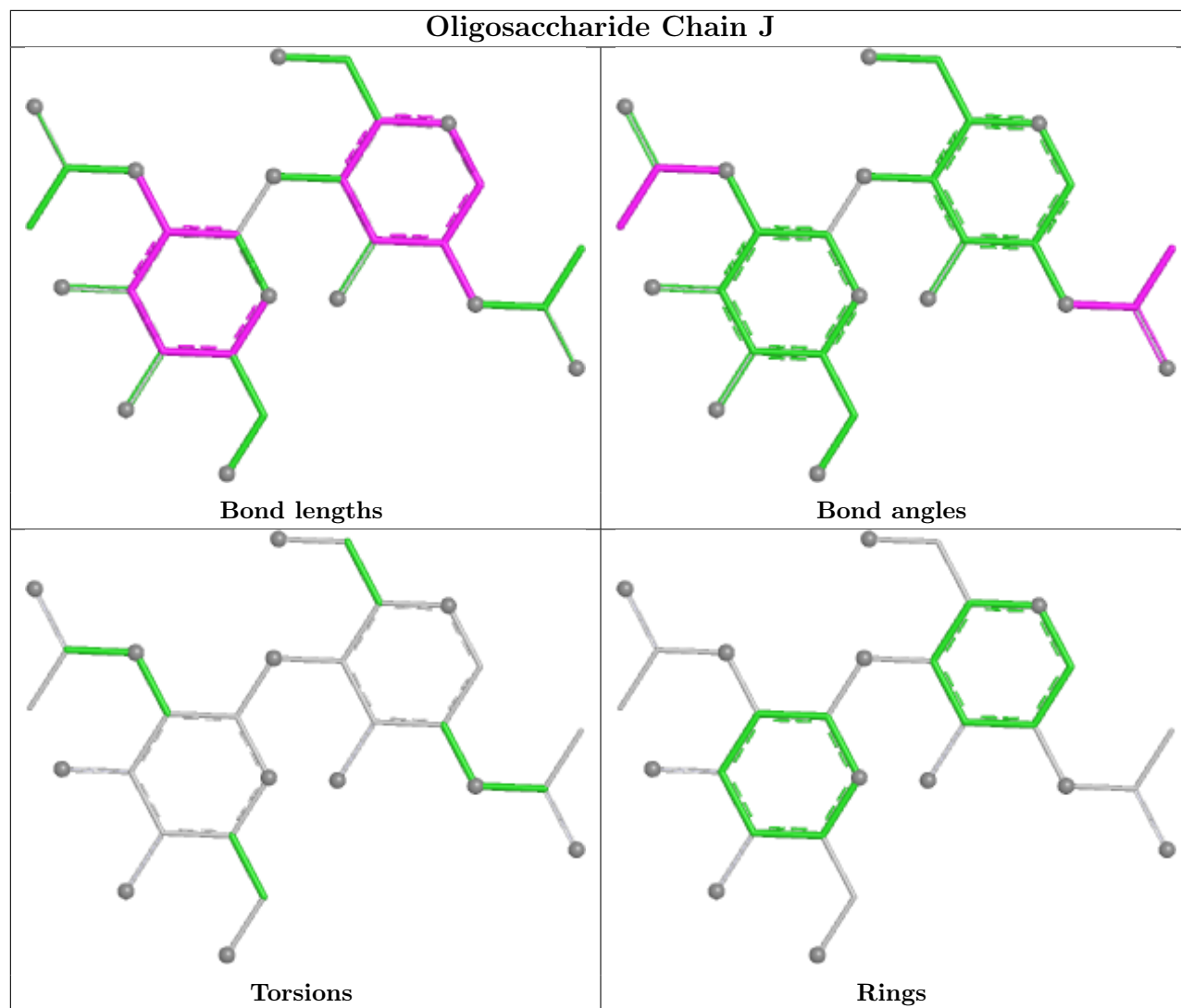
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

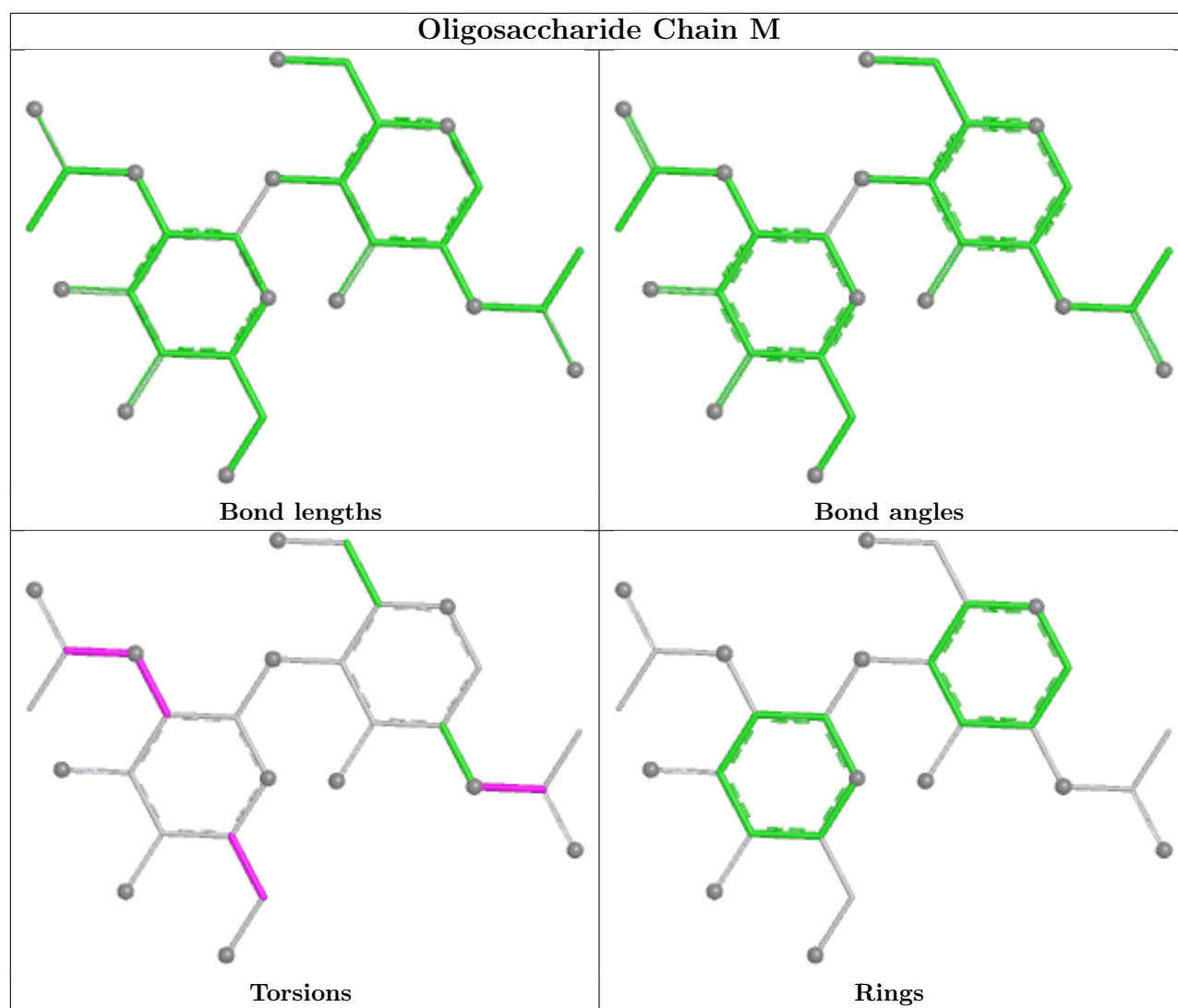


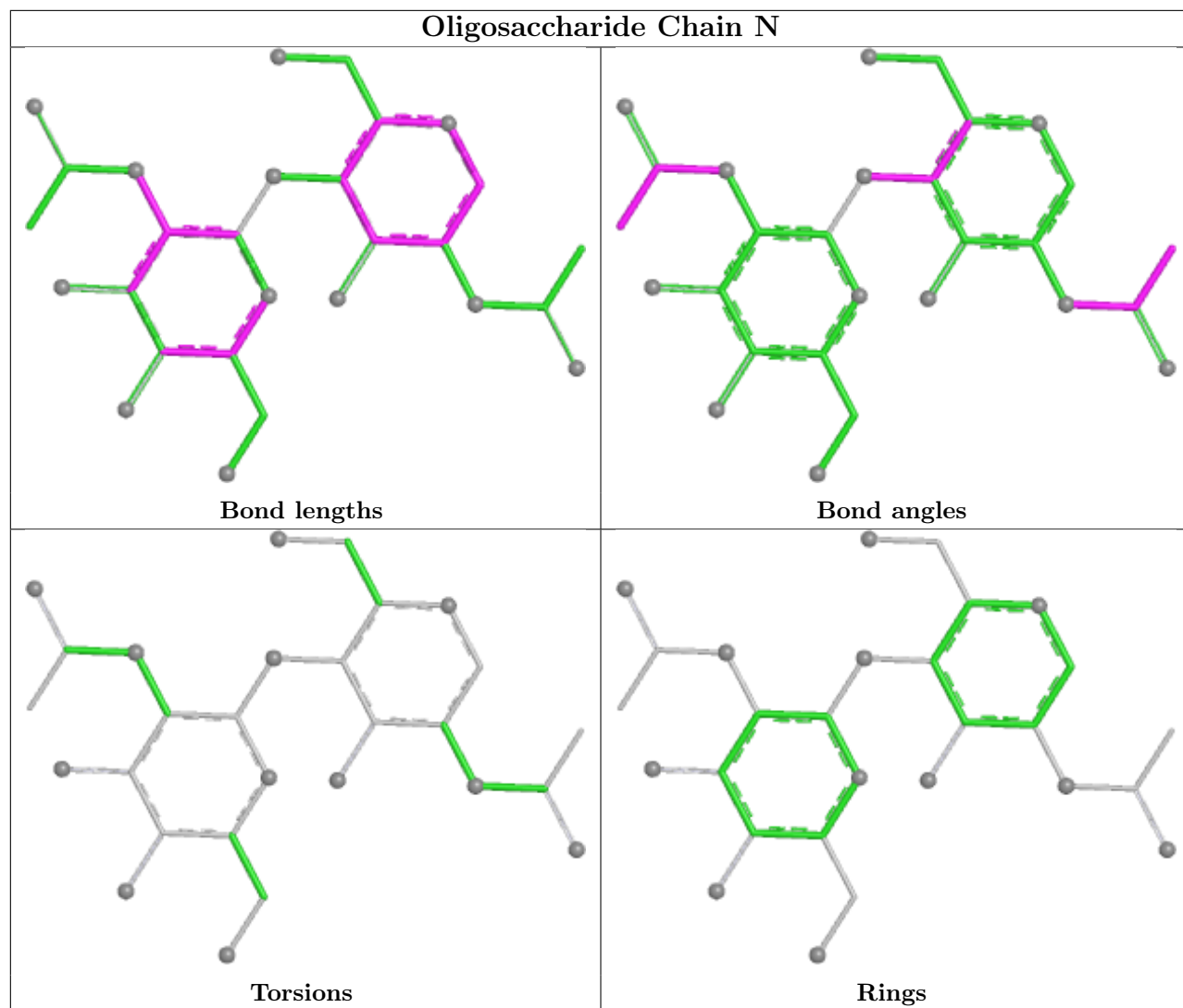


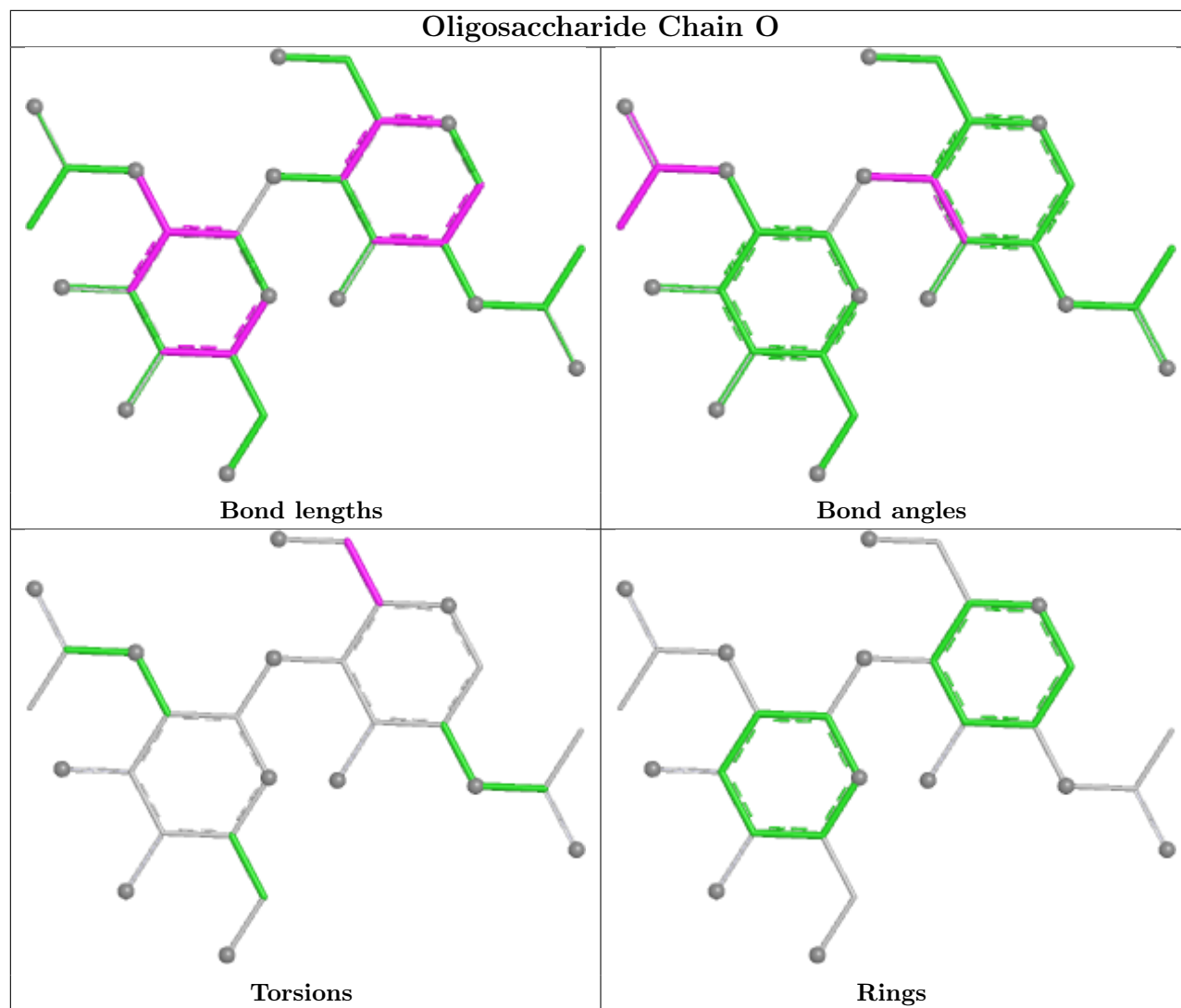


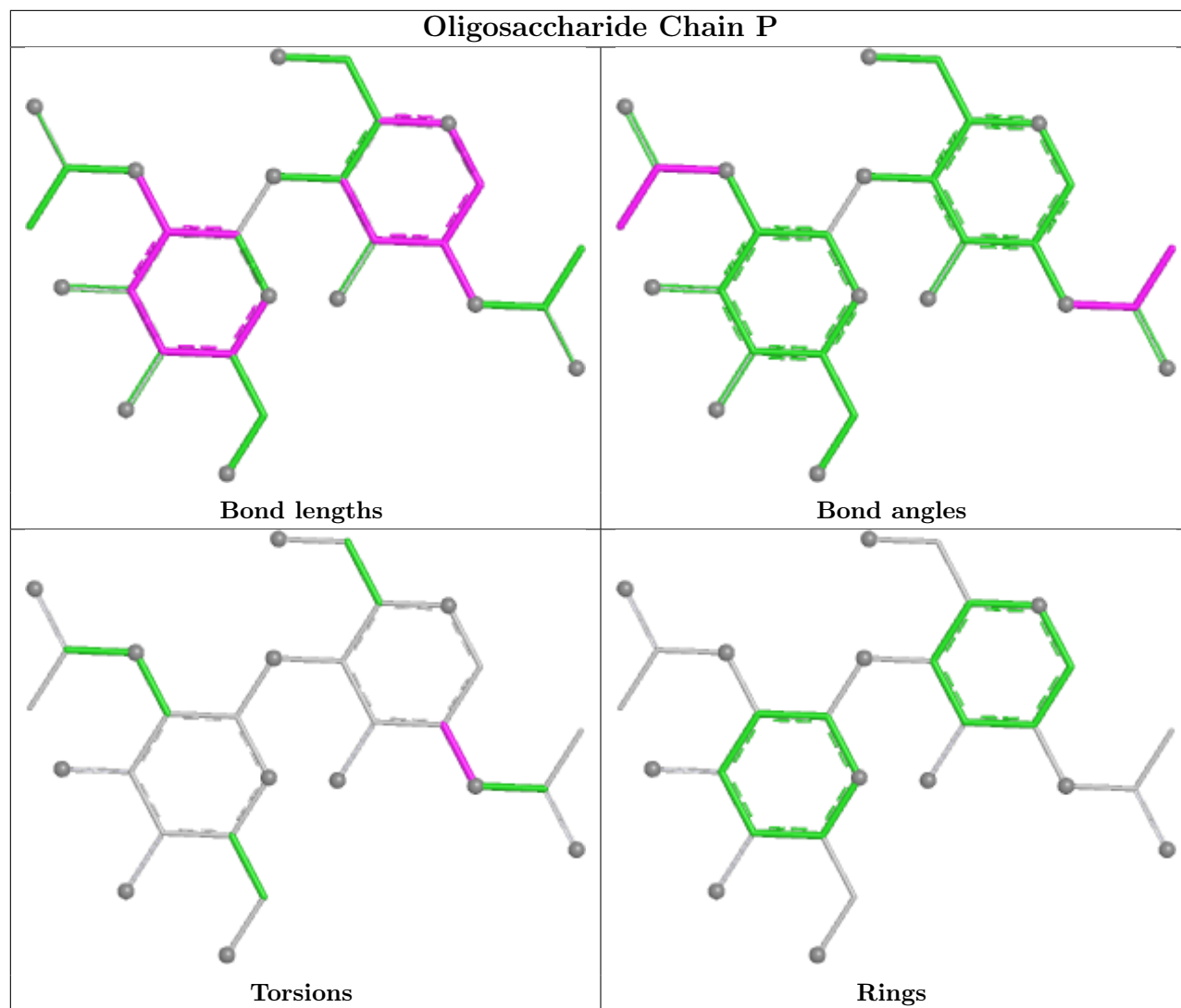


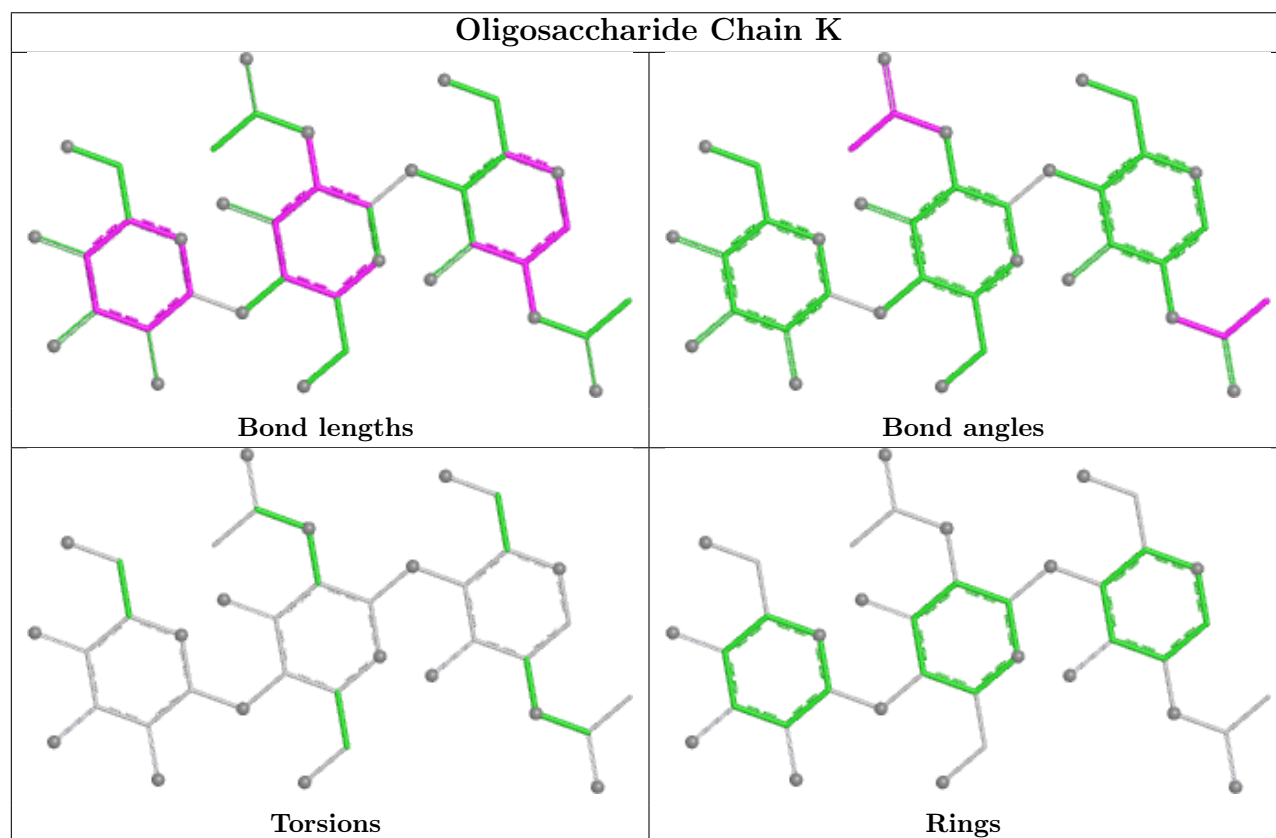
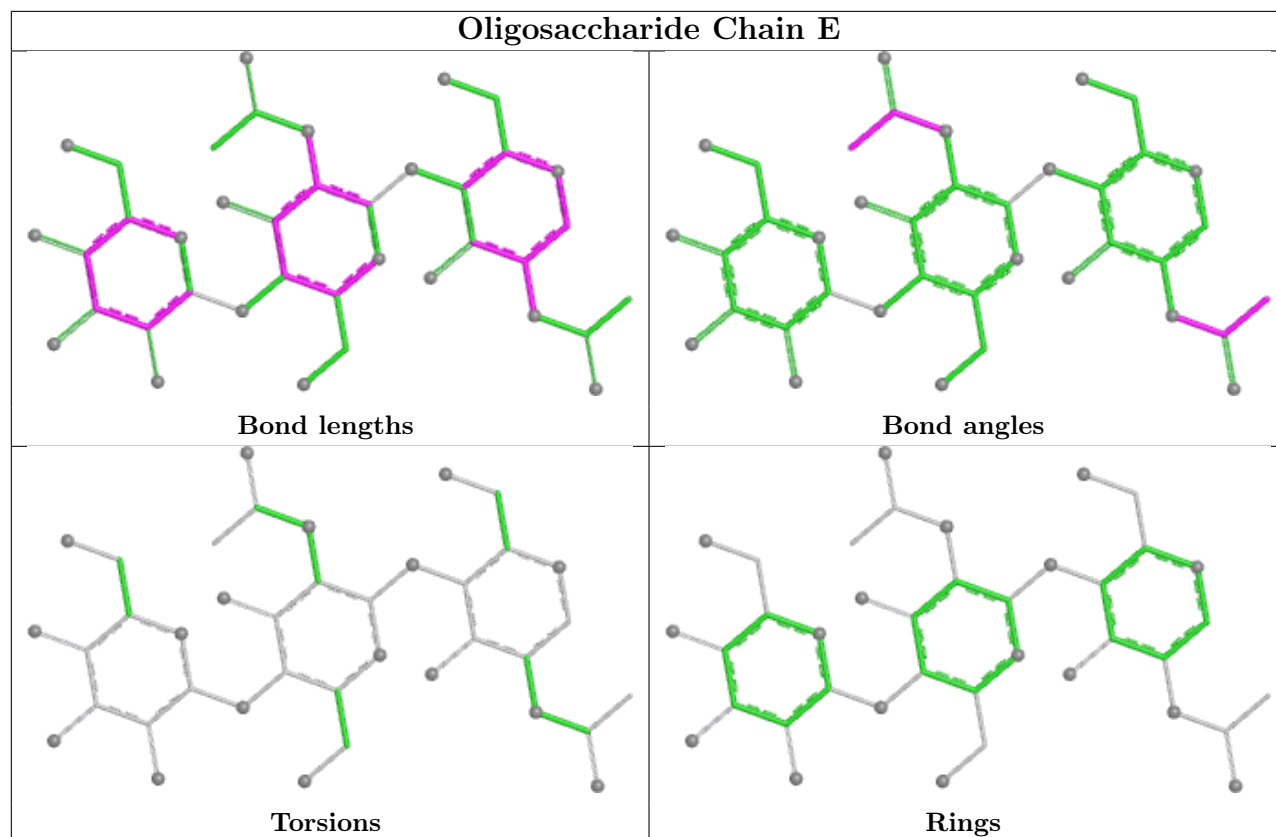












5.6 Ligand geometry

34 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	1405	1	14,14,15	2.11	5 (35%)	17,19,21	1.22	3 (17%)
5	NAG	C	1409	1	14,14,15	0.39	0	17,19,21	0.47	0
5	NAG	A	1406	1	14,14,15	2.30	7 (50%)	17,19,21	1.18	2 (11%)
5	NAG	B	1402	1	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	A	1403	1	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	A	1401	1	14,14,15	0.38	0	17,19,21	0.49	0
5	NAG	A	1402	1	14,14,15	0.43	0	17,19,21	0.46	0
5	NAG	A	1404	1	14,14,15	0.32	0	17,19,21	0.62	0
5	NAG	C	1408	1	14,14,15	2.29	5 (35%)	17,19,21	0.96	1 (5%)
5	NAG	B	1401	1	14,14,15	0.39	0	17,19,21	0.48	0
5	NAG	B	1407	1	14,14,15	0.39	0	17,19,21	0.51	0
5	NAG	B	1410	1	14,14,15	2.36	6 (42%)	17,19,21	1.07	2 (11%)
5	NAG	B	1405	1	14,14,15	2.14	5 (35%)	17,19,21	1.16	2 (11%)
5	NAG	B	1403	1	14,14,15	2.23	6 (42%)	17,19,21	1.02	1 (5%)
5	NAG	B	1408	1	14,14,15	2.23	6 (42%)	17,19,21	0.97	1 (5%)
5	NAG	B	1406	1	14,14,15	2.31	6 (42%)	17,19,21	1.10	2 (11%)
5	NAG	B	1404	1	14,14,15	0.39	0	17,19,21	0.39	0
6	8Z9	A	1412	-	17,17,17	1.29	1 (5%)	17,17,17	0.70	0
5	NAG	A	1409	1	14,14,15	2.24	5 (35%)	17,19,21	1.01	1 (5%)
6	8Z9	C	1411	-	17,17,17	1.33	1 (5%)	17,17,17	0.70	0
5	NAG	A	1408	1	14,14,15	2.27	7 (50%)	17,19,21	1.03	2 (11%)
5	NAG	C	1403	1	14,14,15	2.17	7 (50%)	17,19,21	1.17	2 (11%)
5	NAG	C	1404	1	14,14,15	2.20	5 (35%)	17,19,21	0.95	1 (5%)
5	NAG	C	1406	1	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	C	1410	1	14,14,15	2.33	6 (42%)	17,19,21	1.13	2 (11%)
5	NAG	C	1405	1	14,14,15	2.19	5 (35%)	17,19,21	0.98	2 (11%)
5	NAG	B	1409	1	14,14,15	2.25	5 (35%)	17,19,21	0.96	0
5	NAG	C	1407	1	14,14,15	2.19	5 (35%)	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1411	1	14,14,15	2.28	6 (42%)	17,19,21	0.96	0
5	NAG	A	1407	1	14,14,15	2.23	5 (35%)	17,19,21	0.91	0
5	NAG	C	1402	1	14,14,15	0.39	0	17,19,21	0.50	0
6	8Z9	B	1411	-	17,17,17	1.32	1 (5%)	17,17,17	0.71	0
5	NAG	C	1401	1	14,14,15	0.38	0	17,19,21	0.48	0
5	NAG	A	1410	1	14,14,15	0.40	0	17,19,21	0.55	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	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
6	8Z9	A	1412	-	-	6/15/15/15	-
5	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
6	8Z9	C	1411	-	-	9/15/15/15	-
5	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
6	8Z9	B	1411	-	-	7/15/15/15	-
5	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1410	1	-	2/6/23/26	0/1/1/1

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1410	NAG	C1-C2	6.33	1.61	1.52
5	C	1410	NAG	C1-C2	6.22	1.60	1.52
5	C	1408	NAG	C1-C2	6.13	1.60	1.52
5	B	1409	NAG	C1-C2	5.97	1.60	1.52
5	B	1406	NAG	C1-C2	5.95	1.60	1.52
5	A	1411	NAG	C1-C2	5.95	1.60	1.52
5	A	1409	NAG	C1-C2	5.95	1.60	1.52
5	A	1407	NAG	C1-C2	5.83	1.60	1.52
5	B	1403	NAG	C1-C2	5.82	1.60	1.52
5	A	1406	NAG	C1-C2	5.78	1.60	1.52
5	A	1408	NAG	C1-C2	5.62	1.60	1.52
5	C	1404	NAG	C1-C2	5.60	1.60	1.52
5	B	1408	NAG	C1-C2	5.56	1.59	1.52
5	C	1405	NAG	C1-C2	5.47	1.59	1.52
5	B	1405	NAG	C1-C2	5.31	1.59	1.52
5	A	1405	NAG	C1-C2	5.22	1.59	1.52
5	C	1407	NAG	C1-C2	5.13	1.59	1.52
5	C	1403	NAG	C1-C2	5.11	1.59	1.52
5	C	1407	NAG	O5-C5	3.57	1.50	1.43
5	A	1405	NAG	O5-C5	3.49	1.50	1.43
5	A	1406	NAG	O5-C5	3.47	1.50	1.43
5	C	1405	NAG	O5-C5	3.45	1.50	1.43
5	A	1407	NAG	O5-C5	3.34	1.49	1.43
5	C	1404	NAG	O5-C5	3.33	1.49	1.43
5	C	1403	NAG	O5-C5	3.29	1.49	1.43
5	A	1411	NAG	O5-C5	3.29	1.49	1.43
5	B	1408	NAG	O5-C5	3.28	1.49	1.43
5	B	1409	NAG	O5-C5	3.28	1.49	1.43
5	B	1406	NAG	O5-C5	3.27	1.49	1.43
5	C	1410	NAG	O5-C5	3.26	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1408	NAG	O5-C5	3.24	1.49	1.43
5	C	1408	NAG	O5-C5	3.22	1.49	1.43
5	B	1405	NAG	O5-C5	3.22	1.49	1.43
5	A	1409	NAG	O5-C5	3.18	1.49	1.43
5	B	1403	NAG	O5-C5	3.17	1.49	1.43
6	B	1411	8Z9	C2-C1	3.15	1.57	1.50
6	C	1411	8Z9	C2-C1	3.08	1.57	1.50
5	B	1410	NAG	O5-C5	2.98	1.49	1.43
6	A	1412	8Z9	C2-C1	2.83	1.57	1.50
5	C	1410	NAG	O5-C1	2.79	1.48	1.43
5	C	1407	NAG	O5-C1	2.75	1.48	1.43
5	B	1408	NAG	O5-C1	2.74	1.48	1.43
5	A	1406	NAG	O5-C1	2.73	1.48	1.43
5	B	1406	NAG	O5-C1	2.71	1.48	1.43
5	C	1403	NAG	O5-C1	2.70	1.48	1.43
5	B	1410	NAG	C3-C2	2.69	1.58	1.52
5	A	1408	NAG	O5-C1	2.68	1.48	1.43
5	A	1411	NAG	O5-C1	2.67	1.48	1.43
5	B	1403	NAG	O5-C1	2.65	1.48	1.43
5	C	1404	NAG	O5-C1	2.64	1.48	1.43
5	B	1409	NAG	O5-C1	2.63	1.48	1.43
5	A	1408	NAG	C2-N2	2.62	1.50	1.46
5	A	1405	NAG	O5-C1	2.62	1.48	1.43
5	A	1409	NAG	O5-C1	2.58	1.48	1.43
5	B	1405	NAG	O5-C1	2.56	1.48	1.43
5	C	1408	NAG	O5-C1	2.56	1.48	1.43
5	C	1405	NAG	C3-C2	2.51	1.57	1.52
5	C	1405	NAG	O5-C1	2.51	1.47	1.43
5	B	1410	NAG	O5-C1	2.50	1.47	1.43
5	C	1403	NAG	C2-N2	2.48	1.50	1.46
5	A	1407	NAG	O5-C1	2.47	1.47	1.43
5	B	1410	NAG	C2-N2	2.45	1.50	1.46
5	C	1410	NAG	C3-C2	2.43	1.57	1.52
5	C	1407	NAG	C4-C5	2.42	1.58	1.53
5	C	1408	NAG	C3-C2	2.39	1.57	1.52
5	B	1409	NAG	C3-C2	2.37	1.57	1.52
5	C	1407	NAG	C3-C2	2.37	1.57	1.52
5	A	1406	NAG	C3-C2	2.36	1.57	1.52
5	B	1405	NAG	C3-C2	2.36	1.57	1.52
5	B	1406	NAG	C2-N2	2.36	1.50	1.46
5	A	1408	NAG	C3-C2	2.35	1.57	1.52
5	B	1406	NAG	C3-C2	2.35	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1403	NAG	C3-C2	2.35	1.57	1.52
5	A	1406	NAG	C4-C5	2.31	1.57	1.53
5	A	1411	NAG	C3-C2	2.30	1.57	1.52
5	A	1411	NAG	C4-C5	2.29	1.57	1.53
5	B	1408	NAG	C3-C2	2.28	1.57	1.52
5	B	1403	NAG	C3-C2	2.25	1.57	1.52
5	B	1408	NAG	C2-N2	2.24	1.50	1.46
5	B	1406	NAG	C4-C5	2.23	1.57	1.53
5	A	1408	NAG	C4-C5	2.23	1.57	1.53
5	A	1407	NAG	C3-C2	2.22	1.57	1.52
5	A	1407	NAG	C4-C5	2.22	1.57	1.53
5	A	1405	NAG	C4-C5	2.22	1.57	1.53
5	C	1404	NAG	C4-C5	2.22	1.57	1.53
5	C	1404	NAG	C3-C2	2.20	1.57	1.52
5	C	1403	NAG	C4-C5	2.20	1.57	1.53
5	C	1405	NAG	C4-C5	2.20	1.57	1.53
5	B	1405	NAG	C4-C5	2.18	1.57	1.53
5	A	1409	NAG	C3-C2	2.18	1.57	1.52
5	B	1408	NAG	C4-C5	2.18	1.57	1.53
5	B	1403	NAG	C4-C5	2.15	1.57	1.53
5	A	1405	NAG	C3-C2	2.13	1.57	1.52
5	C	1408	NAG	C4-C5	2.12	1.57	1.53
5	B	1409	NAG	C4-C5	2.12	1.57	1.53
5	A	1406	NAG	C2-N2	2.11	1.49	1.46
5	C	1410	NAG	C4-C5	2.10	1.57	1.53
5	A	1409	NAG	C4-C5	2.10	1.57	1.53
5	C	1410	NAG	C2-N2	2.06	1.49	1.46
5	A	1408	NAG	C4-C3	2.05	1.57	1.52
5	C	1403	NAG	C4-C3	2.03	1.57	1.52
5	B	1410	NAG	C4-C5	2.02	1.57	1.53
5	A	1406	NAG	C4-C3	2.01	1.57	1.52
5	B	1403	NAG	C2-N2	2.01	1.49	1.46
5	A	1411	NAG	C4-C3	2.00	1.57	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1403	NAG	C8-C7-N2	3.23	121.47	116.12
5	A	1406	NAG	C8-C7-N2	3.02	121.12	116.12
5	B	1405	NAG	C8-C7-N2	2.90	120.93	116.12
5	B	1406	NAG	C8-C7-N2	2.78	120.72	116.12
5	A	1408	NAG	C8-C7-N2	2.76	120.69	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1410	NAG	C8-C7-N2	2.75	120.68	116.12
5	B	1410	NAG	C8-C7-N2	2.52	120.30	116.12
5	B	1408	NAG	C8-C7-N2	2.50	120.26	116.12
5	A	1406	NAG	O7-C7-C8	-2.48	117.64	122.05
5	A	1405	NAG	O7-C7-C8	-2.42	117.74	122.05
5	B	1403	NAG	C8-C7-N2	2.37	120.05	116.12
5	C	1407	NAG	C8-C7-N2	2.36	120.03	116.12
5	A	1405	NAG	C1-C2-N2	-2.32	106.77	110.43
5	A	1409	NAG	C8-C7-N2	2.31	119.96	116.12
5	B	1405	NAG	O7-C7-C8	-2.30	117.95	122.05
5	C	1405	NAG	C8-C7-N2	2.28	119.90	116.12
5	A	1405	NAG	C8-C7-N2	2.23	119.82	116.12
5	B	1406	NAG	O7-C7-C8	-2.19	118.15	122.05
5	C	1410	NAG	O7-C7-C8	-2.18	118.17	122.05
5	A	1408	NAG	O7-C7-C8	-2.17	118.19	122.05
5	B	1410	NAG	C1-O5-C5	2.13	115.03	112.19
5	C	1404	NAG	C8-C7-N2	2.13	119.64	116.12
5	C	1403	NAG	O7-C7-C8	-2.11	118.31	122.05
5	C	1408	NAG	C8-C7-N2	2.09	119.58	116.12
5	C	1405	NAG	C1-C2-N2	-2.02	107.26	110.43

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1401	NAG	C8-C7-N2-C2
5	A	1401	NAG	O7-C7-N2-C2
5	A	1402	NAG	C8-C7-N2-C2
5	A	1402	NAG	O7-C7-N2-C2
5	A	1403	NAG	C8-C7-N2-C2
5	A	1403	NAG	O7-C7-N2-C2
5	A	1404	NAG	C8-C7-N2-C2
5	A	1404	NAG	O7-C7-N2-C2
5	A	1410	NAG	C8-C7-N2-C2
5	A	1410	NAG	O7-C7-N2-C2
5	B	1401	NAG	C8-C7-N2-C2
5	B	1401	NAG	O7-C7-N2-C2
5	B	1402	NAG	C8-C7-N2-C2
5	B	1402	NAG	O7-C7-N2-C2
5	B	1407	NAG	C8-C7-N2-C2
5	B	1407	NAG	O7-C7-N2-C2
5	C	1402	NAG	C8-C7-N2-C2

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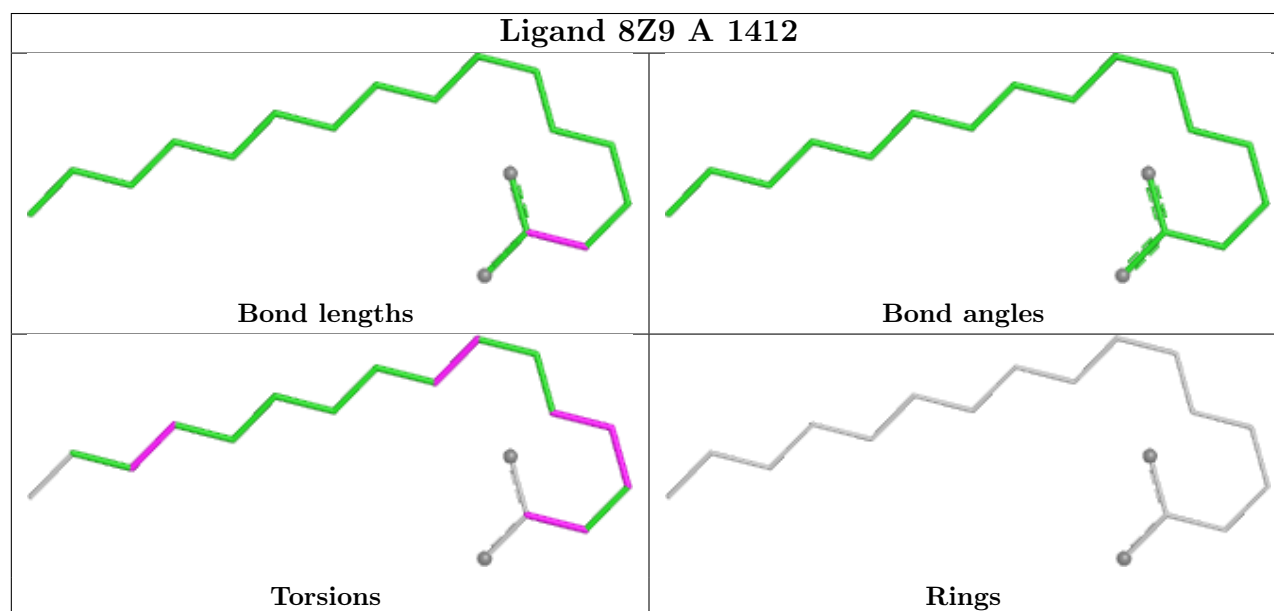
Mol	Chain	Res	Type	Atoms
5	C	1402	NAG	O7-C7-N2-C2
5	A	1404	NAG	O5-C5-C6-O6
6	C	1411	8Z9	CA-CB-CC-CD
5	C	1409	NAG	C8-C7-N2-C2
5	C	1409	NAG	O7-C7-N2-C2
5	B	1404	NAG	C8-C7-N2-C2
5	C	1406	NAG	C8-C7-N2-C2
5	B	1404	NAG	O7-C7-N2-C2
5	C	1406	NAG	O7-C7-N2-C2
6	C	1411	8Z9	C1-C2-C3-C4
6	B	1411	8Z9	C1-C2-C3-C4
5	A	1404	NAG	C4-C5-C6-O6
6	B	1411	8Z9	C9-CA-CB-CC
5	C	1406	NAG	O5-C5-C6-O6
6	B	1411	8Z9	CA-CB-CC-CD
6	B	1411	8Z9	CC-CD-CE-CF
6	B	1411	8Z9	C2-C3-C4-C5
5	B	1407	NAG	C4-C5-C6-O6
6	C	1411	8Z9	C2-C3-C4-C5
5	A	1411	NAG	O5-C5-C6-O6
5	C	1407	NAG	O5-C5-C6-O6
6	A	1412	8Z9	CC-CD-CE-CF
5	C	1410	NAG	O5-C5-C6-O6
6	B	1411	8Z9	C4-C5-C6-C7
5	C	1401	NAG	O5-C5-C6-O6
6	C	1411	8Z9	C7-C8-C9-CA
6	C	1411	8Z9	C9-CA-CB-CC
6	A	1412	8Z9	C3-C4-C5-C6
6	A	1412	8Z9	C2-C3-C4-C5
5	B	1407	NAG	O5-C5-C6-O6
6	C	1411	8Z9	CD-CE-CF-CG
6	B	1411	8Z9	C8-C9-CA-CB
6	A	1412	8Z9	C6-C7-C8-C9
5	B	1408	NAG	C1-C2-N2-C7
6	C	1411	8Z9	CC-CD-CE-CF
6	A	1412	8Z9	O2-C1-C2-C3
6	C	1411	8Z9	O1-C1-C2-C3
6	C	1411	8Z9	O2-C1-C2-C3
6	A	1412	8Z9	O1-C1-C2-C3

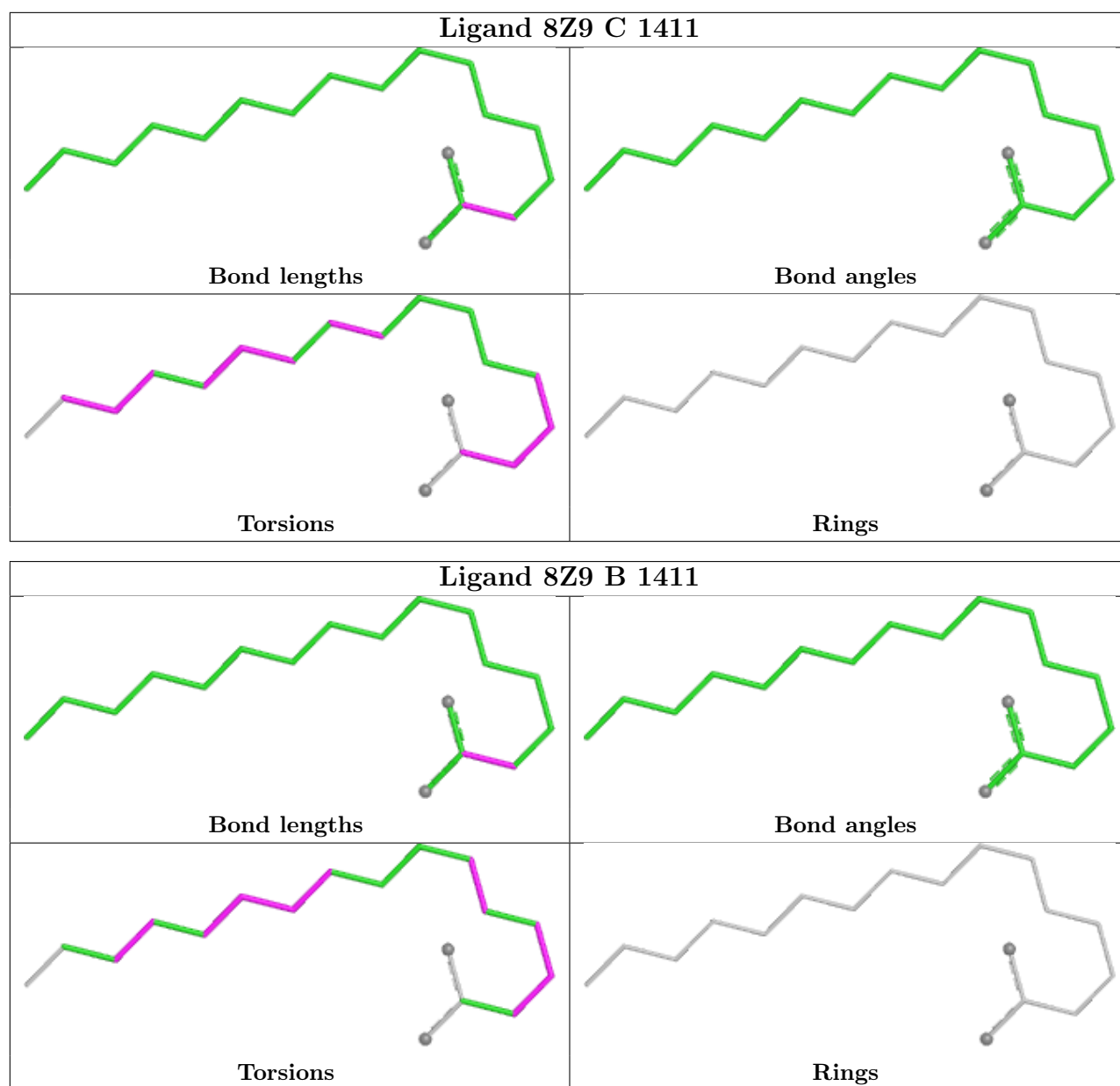
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1401	NAG	2	0
6	A	1412	8Z9	2	0
5	C	1410	NAG	1	0
6	B	1411	8Z9	2	0
5	A	1410	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

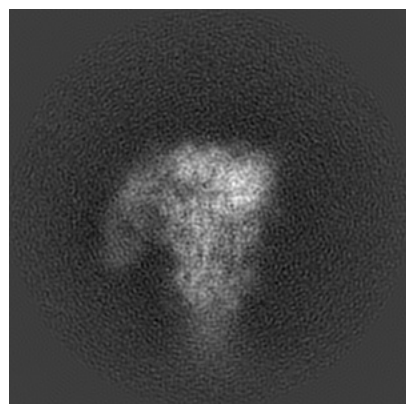
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24969. These allow visual inspection of the internal detail of the map and identification of artifacts.

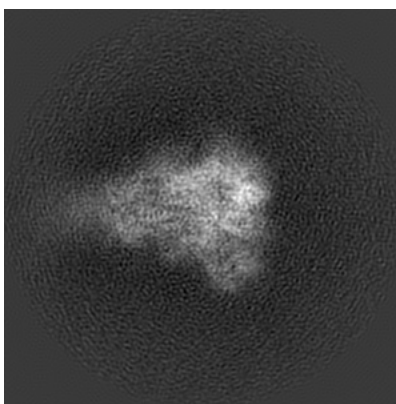
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

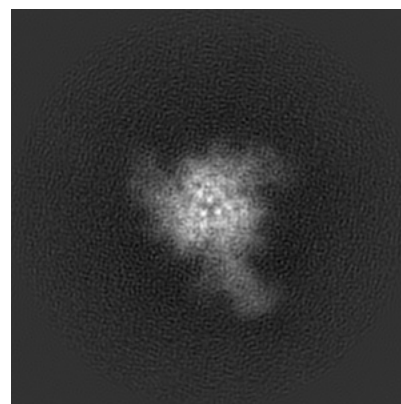
6.1.1 Primary map



X

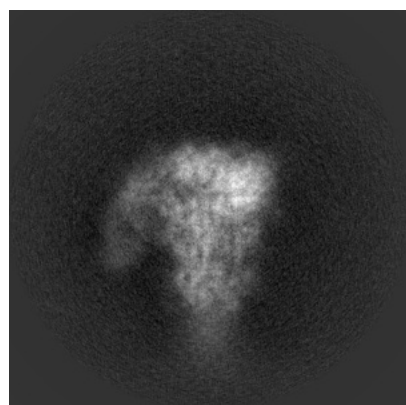


Y

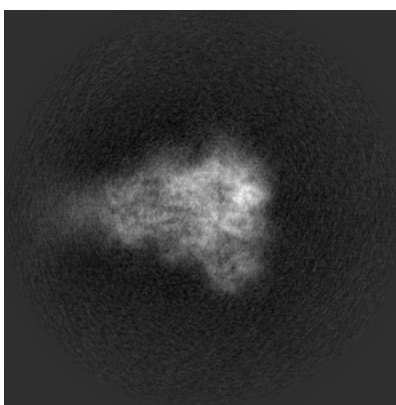


Z

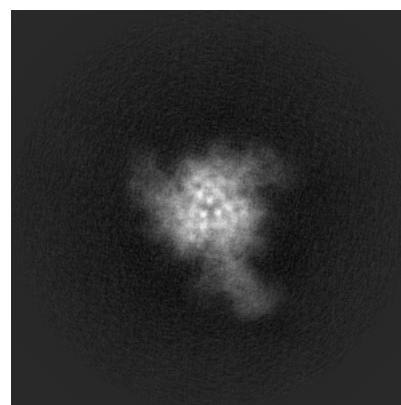
6.1.2 Raw map



X



Y

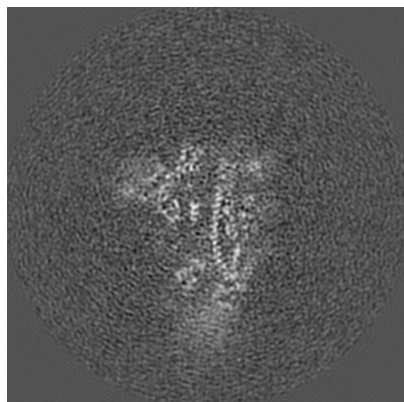


Z

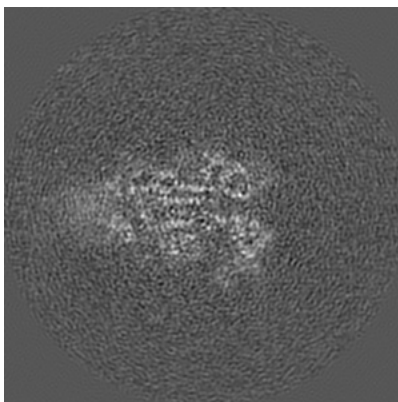
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

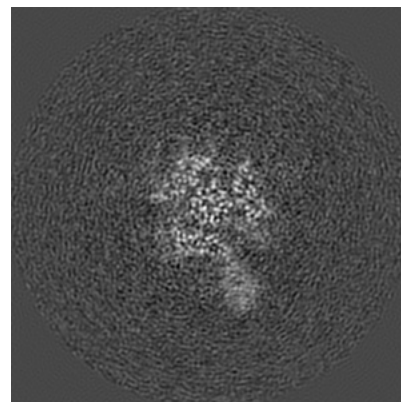
6.2.1 Primary map



X Index: 170

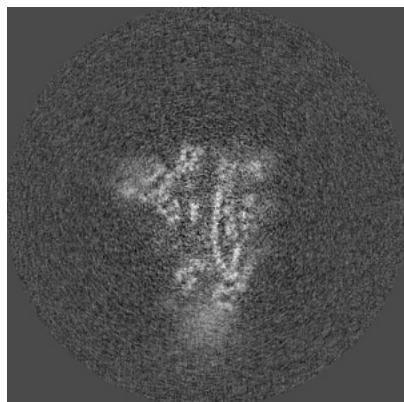


Y Index: 170

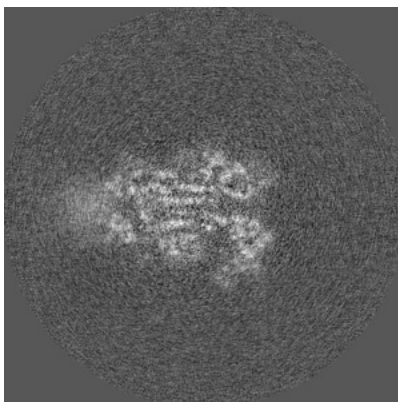


Z Index: 170

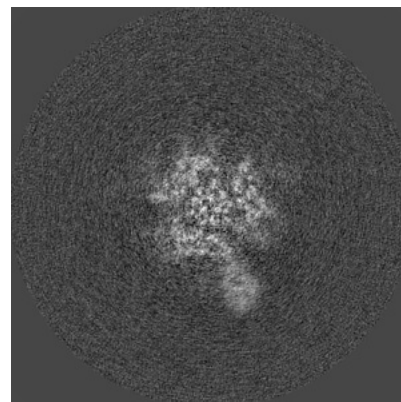
6.2.2 Raw map



X Index: 170



Y Index: 170

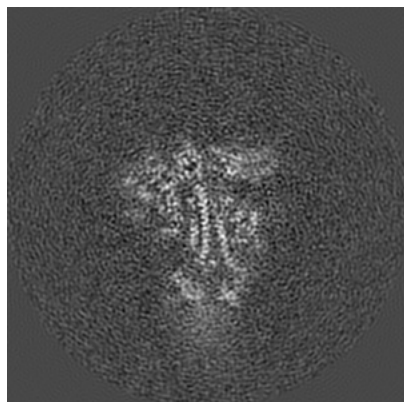


Z Index: 170

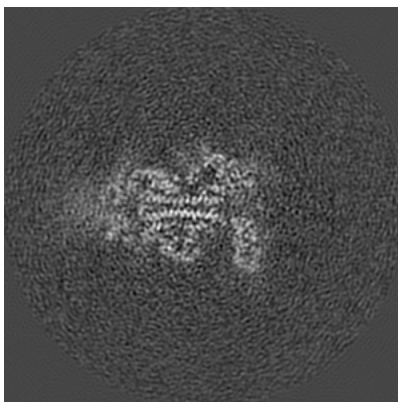
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

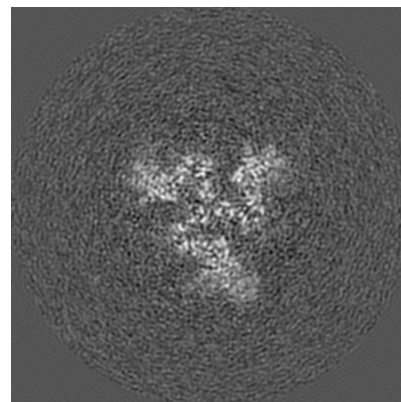
6.3.1 Primary map



X Index: 176

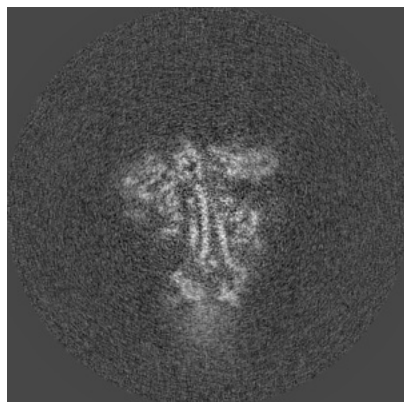


Y Index: 166

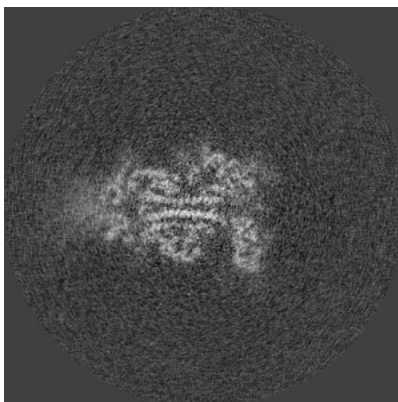


Z Index: 179

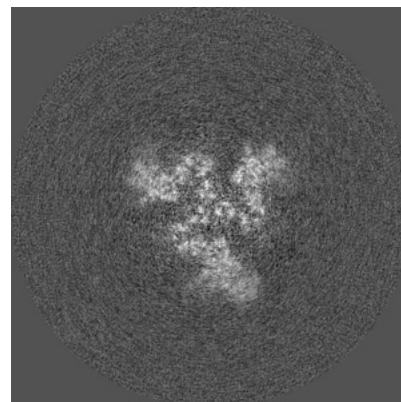
6.3.2 Raw map



X Index: 176



Y Index: 166

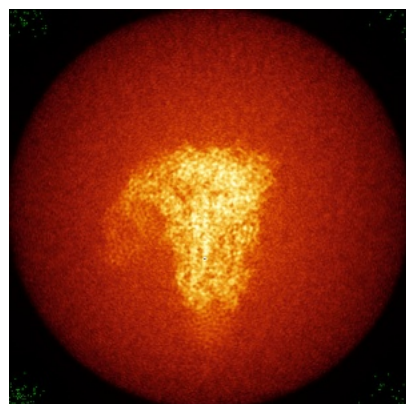


Z Index: 179

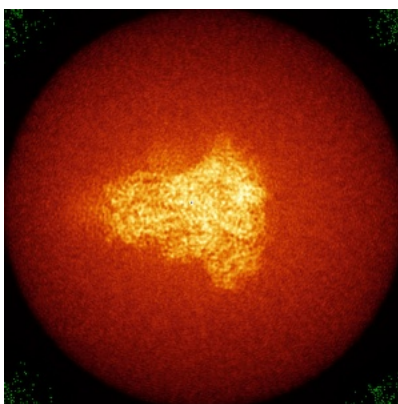
The images above show the largest variance slices of the map in three orthogonal directions.

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

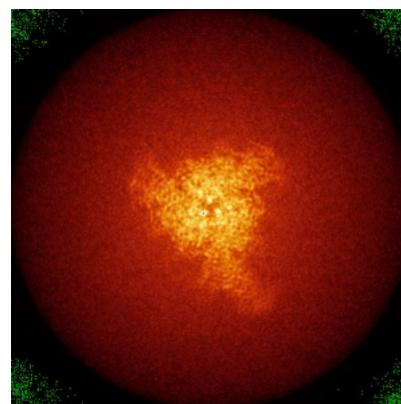
6.4.1 Primary map



X

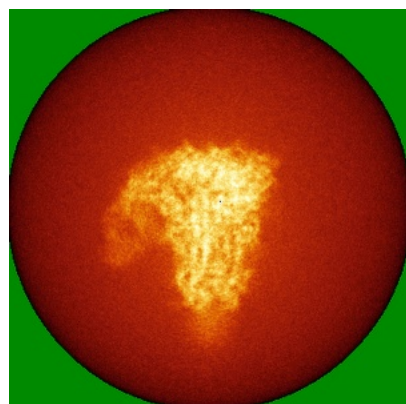


Y

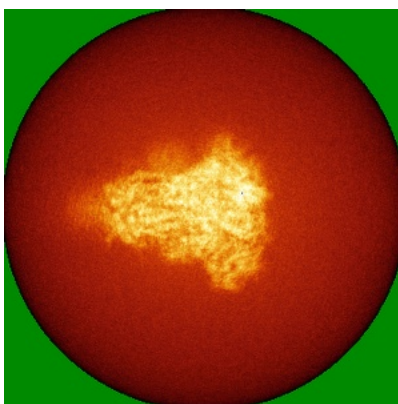


Z

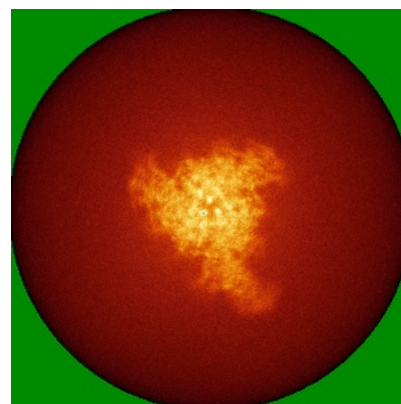
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

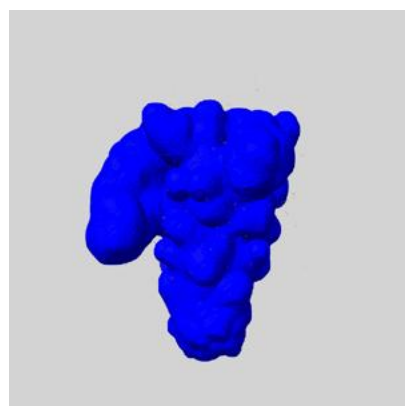
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

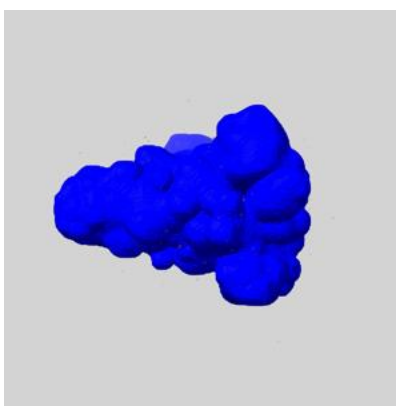
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

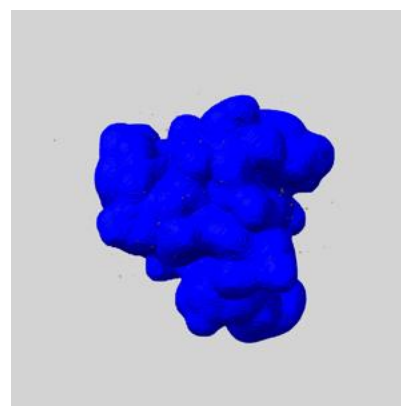
6.6.1 emd_24969_msk_1.map [i](#)



X



Y

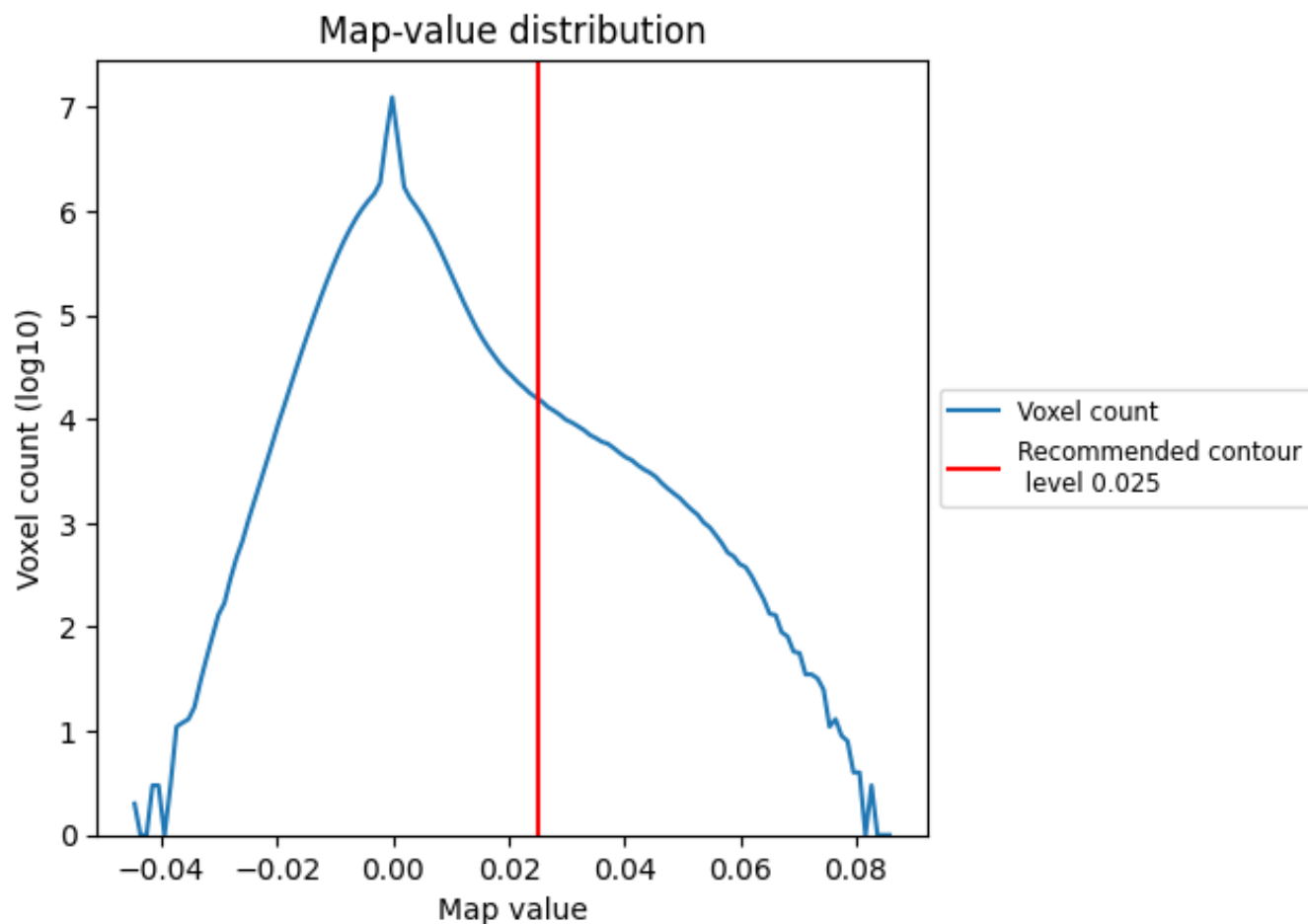


Z

7 Map analysis [i](#)

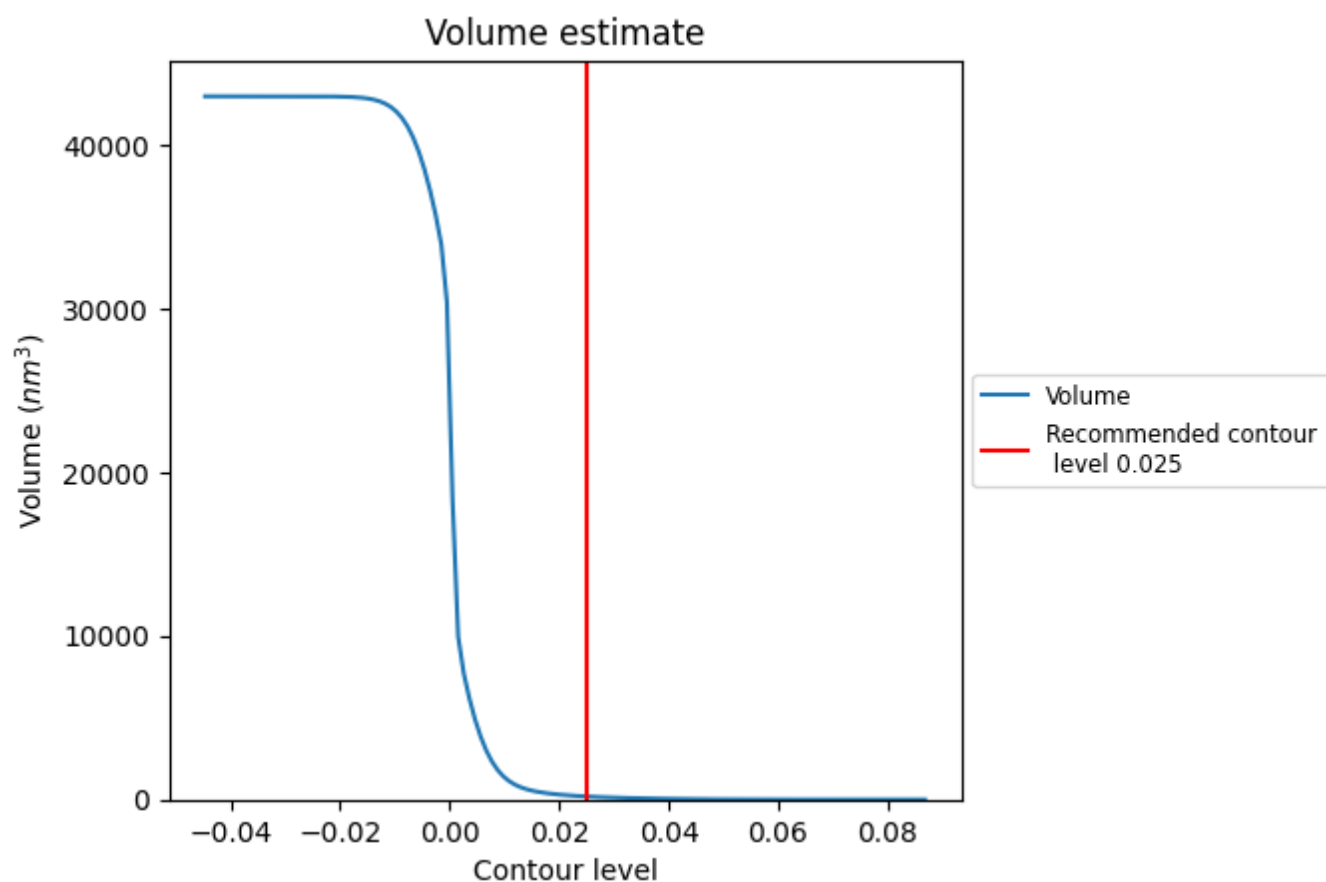
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

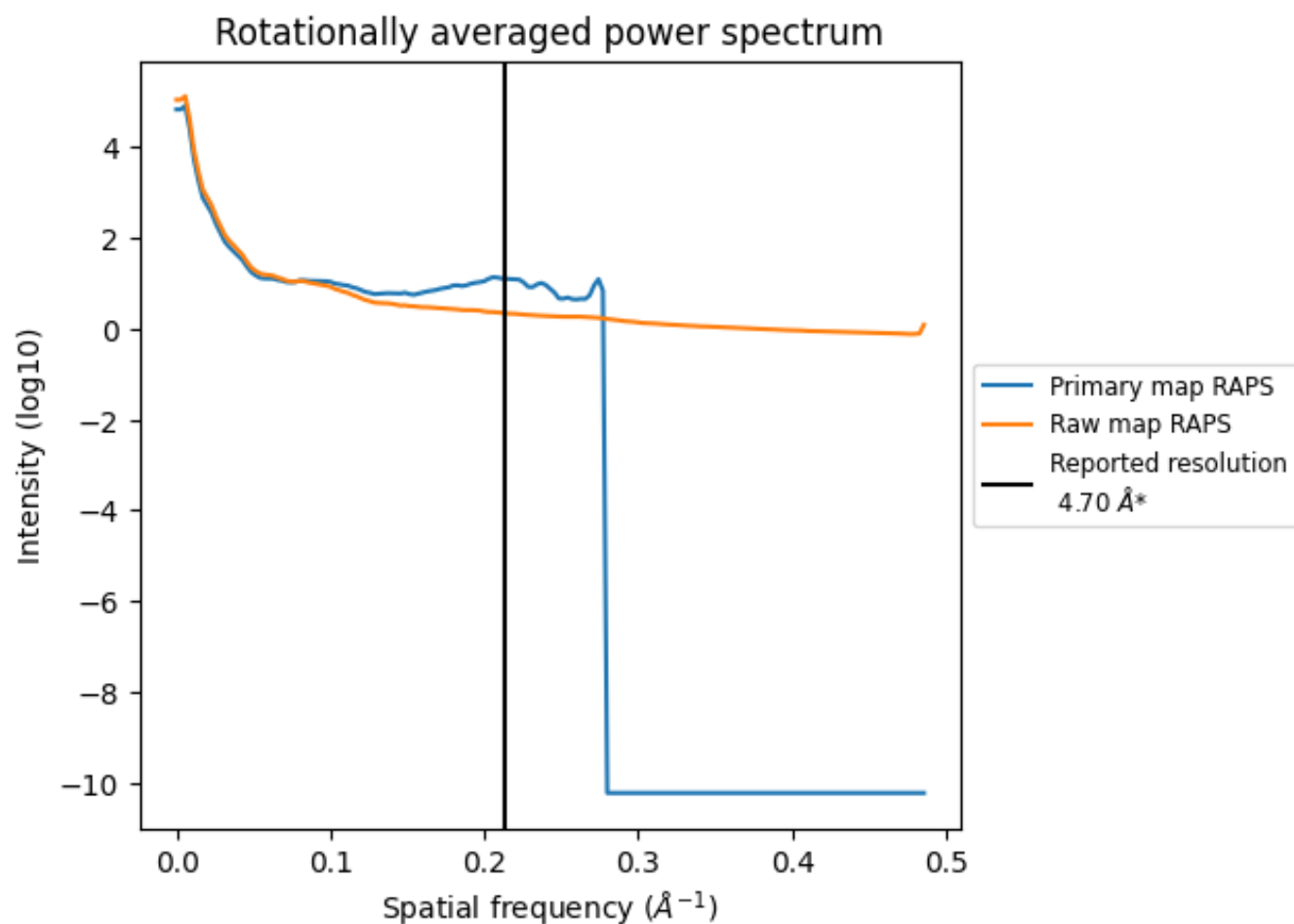
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 170 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

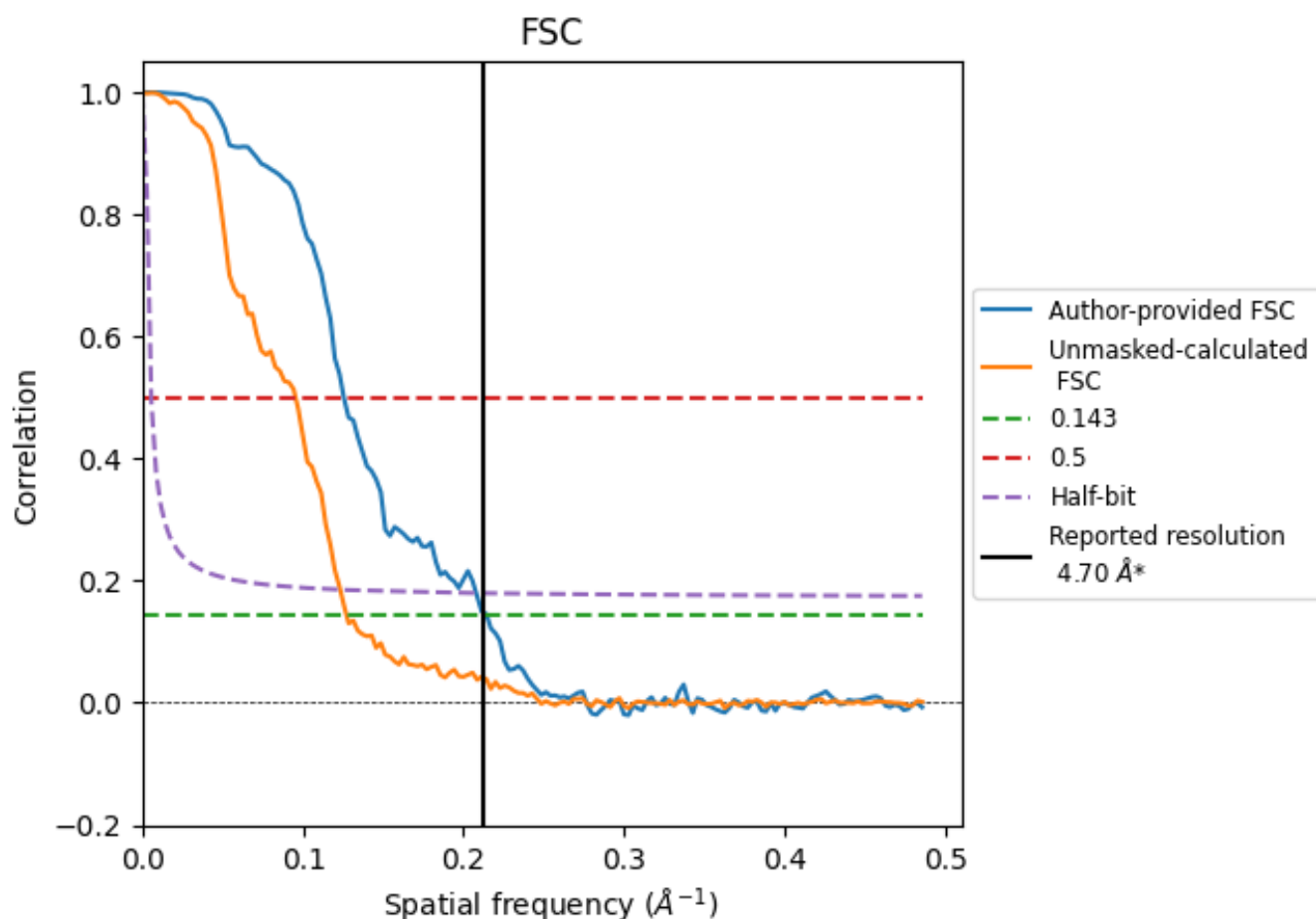


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

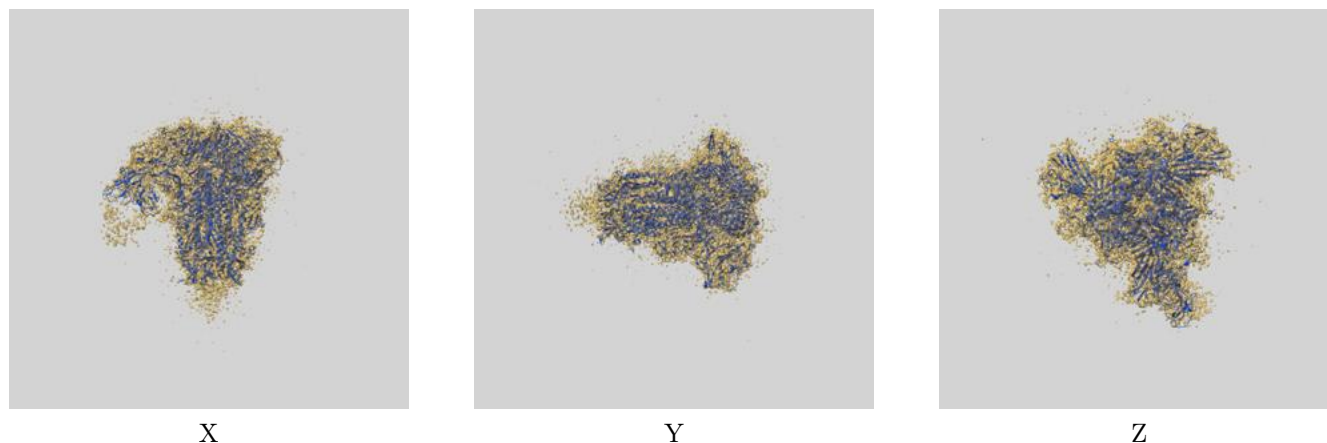
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.66	7.97	4.81
Unmasked-calculated*	7.86	10.48	8.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.86 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

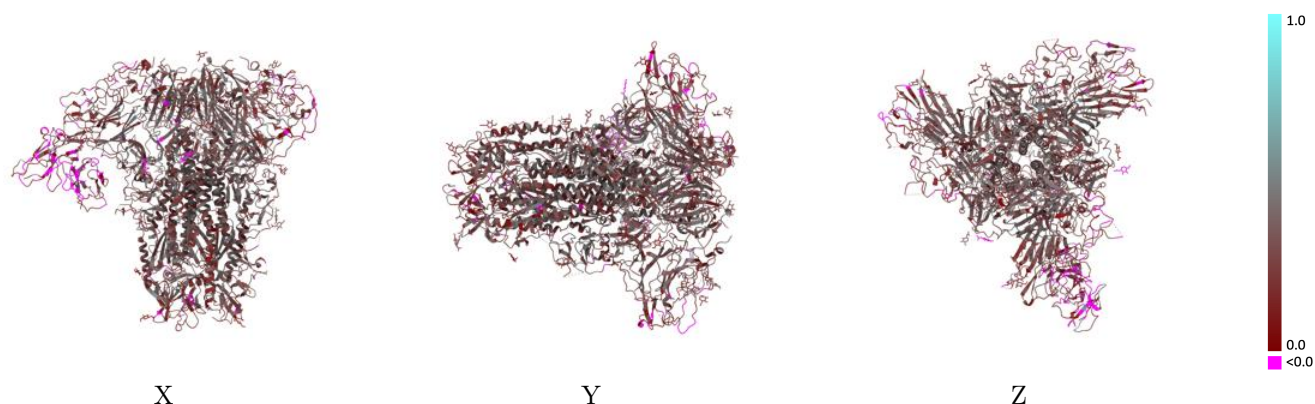
This section contains information regarding the fit between EMDB map EMD-24969 and PDB model 7SB4. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



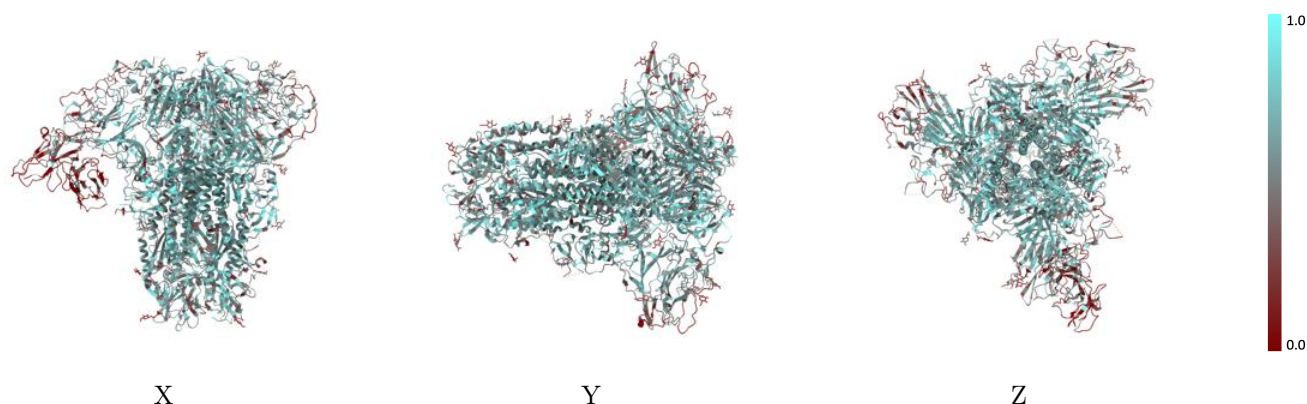
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



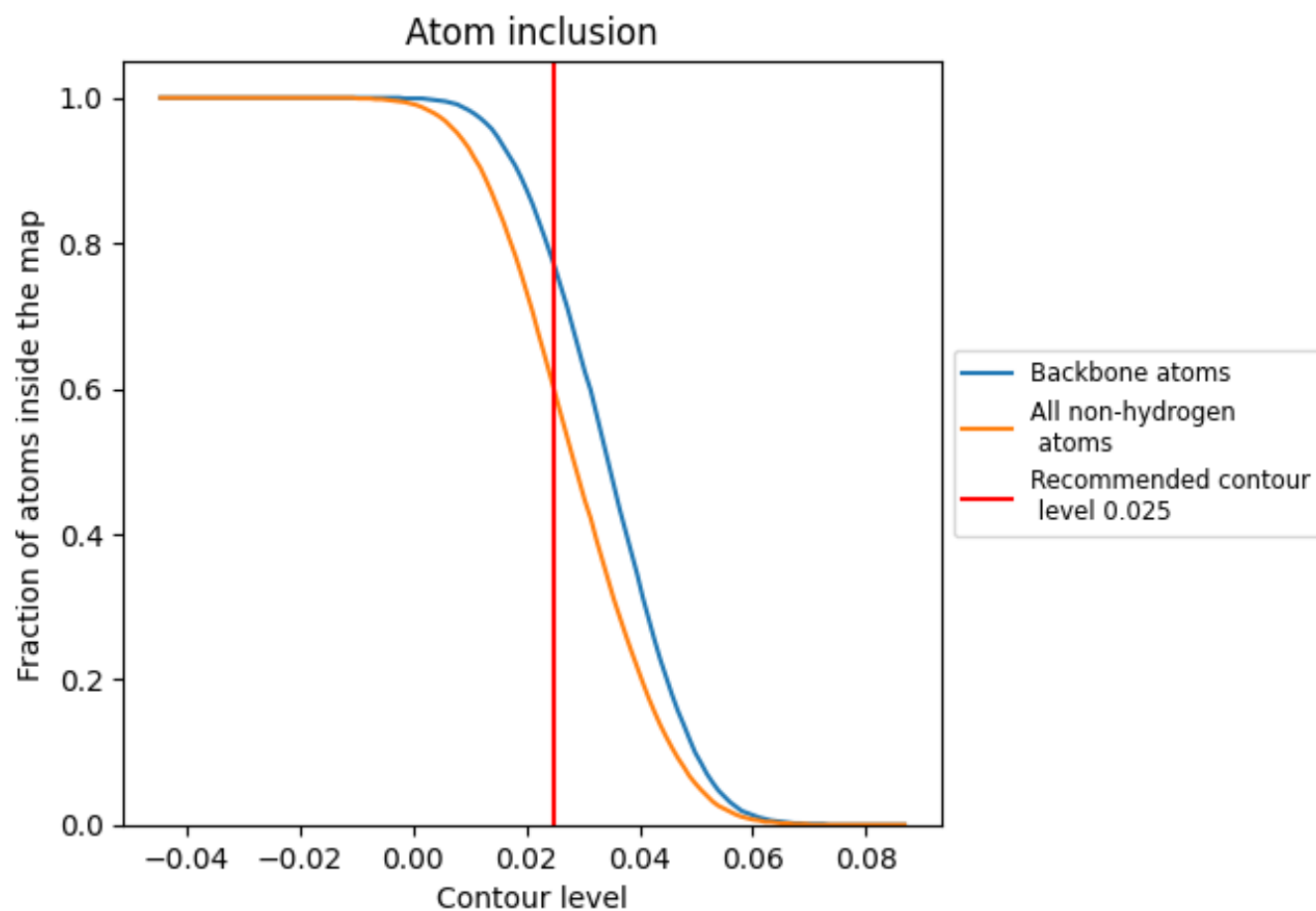
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 60% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5950	 0.3020
A	 0.6090	 0.3080
B	 0.6160	 0.3140
C	 0.6100	 0.3050
D	 0.4640	 0.3170
E	 0.2050	 0.2490
F	 0.5000	 0.1900
G	 0.3570	 0.2400
H	 0.2410	 0.1300
I	 0.3930	 0.1870
J	 0.2500	 0.3000
K	 0.3080	 0.2760
L	 0.1840	 0.1290
M	 0.3930	 0.2380
N	 0.6070	 0.3230
O	 0.5000	 0.3020
P	 0.2860	 0.1910

