



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:28 AM UTC

PDB ID : 7YMY / pdb_00007ymy
EMDB ID : EMD-33947
Title : Cryo-EM structure of MERS-CoV spike protein, One RBD-up conformation 1
Authors : Hsu, S.T.D.; Chang, N.E.; Weng, Z.W.; Yang, T.J.; Draczkowski, P.
Deposited on : 2022-07-29
Resolution : 4.96 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:

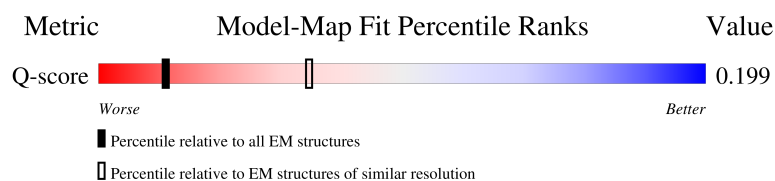
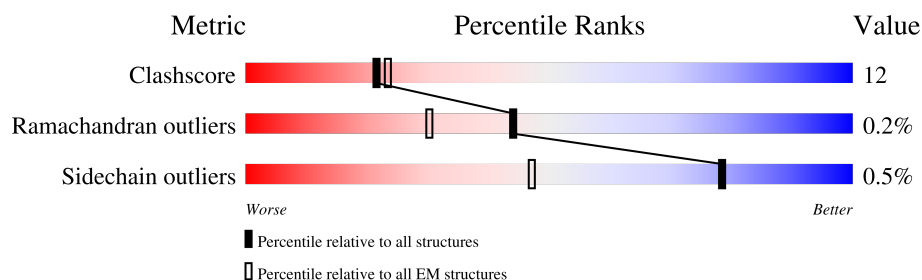
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 4.96 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.



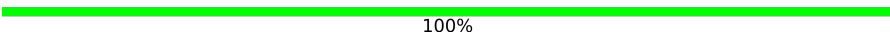
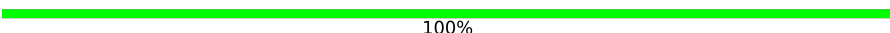
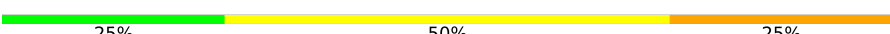
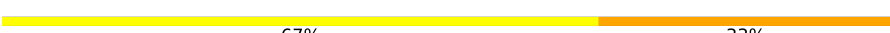
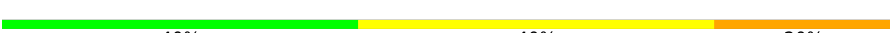
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1045 (4.46 - 5.45)

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	1369	
1	B	1369	
1	C	1369	
2	D	2	

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Mol	Chain	Length	Quality of chain
2	H	2	 50%50%
2	I	2	 100%
2	J	2	 100%
2	K	2	 50%50%
3	E	4	 25%50%25%
4	F	3	 67%33%
5	G	5	 40%40%20%
5	L	5	 20%80%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1166	Total	C	N	O	S	0	0
			9020	5732	1489	1748	51		
1	B	1166	Total	C	N	O	S	0	0
			9020	5732	1489	1748	51		
1	C	1166	Total	C	N	O	S	0	0
			9020	5732	1489	1748	51		

There are 294 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP K0BRG7
A	-1	ASP	-	expression tag	UNP K0BRG7
A	0	SER	-	expression tag	UNP K0BRG7
A	1	TRP	-	expression tag	UNP K0BRG7
A	2	PHE	-	expression tag	UNP K0BRG7
A	3	ILE	-	expression tag	UNP K0BRG7
A	4	LEU	-	expression tag	UNP K0BRG7
A	5	VAL	-	expression tag	UNP K0BRG7
A	6	LEU	-	expression tag	UNP K0BRG7
A	7	LEU	-	expression tag	UNP K0BRG7
A	8	GLY	-	expression tag	UNP K0BRG7
A	9	SER	-	expression tag	UNP K0BRG7
A	10	GLY	-	expression tag	UNP K0BRG7
A	11	LEU	-	expression tag	UNP K0BRG7
A	12	ILE	-	expression tag	UNP K0BRG7
A	13	CYS	-	expression tag	UNP K0BRG7
A	14	VAL	-	expression tag	UNP K0BRG7
A	15	SER	-	expression tag	UNP K0BRG7
A	16	ALA	-	expression tag	UNP K0BRG7
A	748	ALA	ARG	engineered mutation	UNP K0BRG7
A	751	GLY	ARG	engineered mutation	UNP K0BRG7
A	1060	PRO	VAL	engineered mutation	UNP K0BRG7
A	1061	PRO	LEU	engineered mutation	UNP K0BRG7
A	1292	GLU	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1293	PHE	-	expression tag	UNP K0BRG7
A	1294	GLY	-	expression tag	UNP K0BRG7
A	1295	SER	-	expression tag	UNP K0BRG7
A	1296	GLY	-	expression tag	UNP K0BRG7
A	1297	GLY	-	expression tag	UNP K0BRG7
A	1298	TYR	-	expression tag	UNP K0BRG7
A	1299	ILE	-	expression tag	UNP K0BRG7
A	1300	PRO	-	expression tag	UNP K0BRG7
A	1301	GLU	-	expression tag	UNP K0BRG7
A	1302	ALA	-	expression tag	UNP K0BRG7
A	1303	PRO	-	expression tag	UNP K0BRG7
A	1304	ARG	-	expression tag	UNP K0BRG7
A	1305	ASP	-	expression tag	UNP K0BRG7
A	1306	GLY	-	expression tag	UNP K0BRG7
A	1307	GLN	-	expression tag	UNP K0BRG7
A	1308	ALA	-	expression tag	UNP K0BRG7
A	1309	TYR	-	expression tag	UNP K0BRG7
A	1310	VAL	-	expression tag	UNP K0BRG7
A	1311	ARG	-	expression tag	UNP K0BRG7
A	1312	LYS	-	expression tag	UNP K0BRG7
A	1313	ASP	-	expression tag	UNP K0BRG7
A	1314	GLY	-	expression tag	UNP K0BRG7
A	1315	GLU	-	expression tag	UNP K0BRG7
A	1316	TRP	-	expression tag	UNP K0BRG7
A	1317	VAL	-	expression tag	UNP K0BRG7
A	1318	LEU	-	expression tag	UNP K0BRG7
A	1319	LEU	-	expression tag	UNP K0BRG7
A	1320	SER	-	expression tag	UNP K0BRG7
A	1321	THR	-	expression tag	UNP K0BRG7
A	1322	PHE	-	expression tag	UNP K0BRG7
A	1323	LEU	-	expression tag	UNP K0BRG7
A	1324	LYS	-	expression tag	UNP K0BRG7
A	1325	GLY	-	expression tag	UNP K0BRG7
A	1326	GLN	-	expression tag	UNP K0BRG7
A	1327	ASP	-	expression tag	UNP K0BRG7
A	1328	ASN	-	expression tag	UNP K0BRG7
A	1329	SER	-	expression tag	UNP K0BRG7
A	1330	ALA	-	expression tag	UNP K0BRG7
A	1331	ASP	-	expression tag	UNP K0BRG7
A	1332	ILE	-	expression tag	UNP K0BRG7
A	1333	GLN	-	expression tag	UNP K0BRG7
A	1334	HIS	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1335	SER	-	expression tag	UNP K0BRG7
A	1336	GLY	-	expression tag	UNP K0BRG7
A	1337	ARG	-	expression tag	UNP K0BRG7
A	1338	PRO	-	expression tag	UNP K0BRG7
A	1339	LEU	-	expression tag	UNP K0BRG7
A	1340	GLU	-	expression tag	UNP K0BRG7
A	1341	SER	-	expression tag	UNP K0BRG7
A	1342	ARG	-	expression tag	UNP K0BRG7
A	1343	GLY	-	expression tag	UNP K0BRG7
A	1344	PRO	-	expression tag	UNP K0BRG7
A	1345	PHE	-	expression tag	UNP K0BRG7
A	1346	GLU	-	expression tag	UNP K0BRG7
A	1347	GLN	-	expression tag	UNP K0BRG7
A	1348	LYS	-	expression tag	UNP K0BRG7
A	1349	LEU	-	expression tag	UNP K0BRG7
A	1350	ILE	-	expression tag	UNP K0BRG7
A	1351	SER	-	expression tag	UNP K0BRG7
A	1352	GLU	-	expression tag	UNP K0BRG7
A	1353	GLU	-	expression tag	UNP K0BRG7
A	1354	ASP	-	expression tag	UNP K0BRG7
A	1355	LEU	-	expression tag	UNP K0BRG7
A	1356	ASN	-	expression tag	UNP K0BRG7
A	1357	MET	-	expression tag	UNP K0BRG7
A	1358	HIS	-	expression tag	UNP K0BRG7
A	1359	THR	-	expression tag	UNP K0BRG7
A	1360	GLY	-	expression tag	UNP K0BRG7
A	1361	HIS	-	expression tag	UNP K0BRG7
A	1362	HIS	-	expression tag	UNP K0BRG7
A	1363	HIS	-	expression tag	UNP K0BRG7
A	1364	HIS	-	expression tag	UNP K0BRG7
A	1365	HIS	-	expression tag	UNP K0BRG7
A	1366	HIS	-	expression tag	UNP K0BRG7
B	-2	MET	-	initiating methionine	UNP K0BRG7
B	-1	ASP	-	expression tag	UNP K0BRG7
B	0	SER	-	expression tag	UNP K0BRG7
B	1	TRP	-	expression tag	UNP K0BRG7
B	2	PHE	-	expression tag	UNP K0BRG7
B	3	ILE	-	expression tag	UNP K0BRG7
B	4	LEU	-	expression tag	UNP K0BRG7
B	5	VAL	-	expression tag	UNP K0BRG7
B	6	LEU	-	expression tag	UNP K0BRG7
B	7	LEU	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	-	expression tag	UNP K0BRG7
B	9	SER	-	expression tag	UNP K0BRG7
B	10	GLY	-	expression tag	UNP K0BRG7
B	11	LEU	-	expression tag	UNP K0BRG7
B	12	ILE	-	expression tag	UNP K0BRG7
B	13	CYS	-	expression tag	UNP K0BRG7
B	14	VAL	-	expression tag	UNP K0BRG7
B	15	SER	-	expression tag	UNP K0BRG7
B	16	ALA	-	expression tag	UNP K0BRG7
B	748	ALA	ARG	engineered mutation	UNP K0BRG7
B	751	GLY	ARG	engineered mutation	UNP K0BRG7
B	1060	PRO	VAL	engineered mutation	UNP K0BRG7
B	1061	PRO	LEU	engineered mutation	UNP K0BRG7
B	1292	GLU	-	expression tag	UNP K0BRG7
B	1293	PHE	-	expression tag	UNP K0BRG7
B	1294	GLY	-	expression tag	UNP K0BRG7
B	1295	SER	-	expression tag	UNP K0BRG7
B	1296	GLY	-	expression tag	UNP K0BRG7
B	1297	GLY	-	expression tag	UNP K0BRG7
B	1298	TYR	-	expression tag	UNP K0BRG7
B	1299	ILE	-	expression tag	UNP K0BRG7
B	1300	PRO	-	expression tag	UNP K0BRG7
B	1301	GLU	-	expression tag	UNP K0BRG7
B	1302	ALA	-	expression tag	UNP K0BRG7
B	1303	PRO	-	expression tag	UNP K0BRG7
B	1304	ARG	-	expression tag	UNP K0BRG7
B	1305	ASP	-	expression tag	UNP K0BRG7
B	1306	GLY	-	expression tag	UNP K0BRG7
B	1307	GLN	-	expression tag	UNP K0BRG7
B	1308	ALA	-	expression tag	UNP K0BRG7
B	1309	TYR	-	expression tag	UNP K0BRG7
B	1310	VAL	-	expression tag	UNP K0BRG7
B	1311	ARG	-	expression tag	UNP K0BRG7
B	1312	LYS	-	expression tag	UNP K0BRG7
B	1313	ASP	-	expression tag	UNP K0BRG7
B	1314	GLY	-	expression tag	UNP K0BRG7
B	1315	GLU	-	expression tag	UNP K0BRG7
B	1316	TRP	-	expression tag	UNP K0BRG7
B	1317	VAL	-	expression tag	UNP K0BRG7
B	1318	LEU	-	expression tag	UNP K0BRG7
B	1319	LEU	-	expression tag	UNP K0BRG7
B	1320	SER	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1321	THR	-	expression tag	UNP K0BRG7
B	1322	PHE	-	expression tag	UNP K0BRG7
B	1323	LEU	-	expression tag	UNP K0BRG7
B	1324	LYS	-	expression tag	UNP K0BRG7
B	1325	GLY	-	expression tag	UNP K0BRG7
B	1326	GLN	-	expression tag	UNP K0BRG7
B	1327	ASP	-	expression tag	UNP K0BRG7
B	1328	ASN	-	expression tag	UNP K0BRG7
B	1329	SER	-	expression tag	UNP K0BRG7
B	1330	ALA	-	expression tag	UNP K0BRG7
B	1331	ASP	-	expression tag	UNP K0BRG7
B	1332	ILE	-	expression tag	UNP K0BRG7
B	1333	GLN	-	expression tag	UNP K0BRG7
B	1334	HIS	-	expression tag	UNP K0BRG7
B	1335	SER	-	expression tag	UNP K0BRG7
B	1336	GLY	-	expression tag	UNP K0BRG7
B	1337	ARG	-	expression tag	UNP K0BRG7
B	1338	PRO	-	expression tag	UNP K0BRG7
B	1339	LEU	-	expression tag	UNP K0BRG7
B	1340	GLU	-	expression tag	UNP K0BRG7
B	1341	SER	-	expression tag	UNP K0BRG7
B	1342	ARG	-	expression tag	UNP K0BRG7
B	1343	GLY	-	expression tag	UNP K0BRG7
B	1344	PRO	-	expression tag	UNP K0BRG7
B	1345	PHE	-	expression tag	UNP K0BRG7
B	1346	GLU	-	expression tag	UNP K0BRG7
B	1347	GLN	-	expression tag	UNP K0BRG7
B	1348	LYS	-	expression tag	UNP K0BRG7
B	1349	LEU	-	expression tag	UNP K0BRG7
B	1350	ILE	-	expression tag	UNP K0BRG7
B	1351	SER	-	expression tag	UNP K0BRG7
B	1352	GLU	-	expression tag	UNP K0BRG7
B	1353	GLU	-	expression tag	UNP K0BRG7
B	1354	ASP	-	expression tag	UNP K0BRG7
B	1355	LEU	-	expression tag	UNP K0BRG7
B	1356	ASN	-	expression tag	UNP K0BRG7
B	1357	MET	-	expression tag	UNP K0BRG7
B	1358	HIS	-	expression tag	UNP K0BRG7
B	1359	THR	-	expression tag	UNP K0BRG7
B	1360	GLY	-	expression tag	UNP K0BRG7
B	1361	HIS	-	expression tag	UNP K0BRG7
B	1362	HIS	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1363	HIS	-	expression tag	UNP K0BRG7
B	1364	HIS	-	expression tag	UNP K0BRG7
B	1365	HIS	-	expression tag	UNP K0BRG7
B	1366	HIS	-	expression tag	UNP K0BRG7
C	-2	MET	-	initiating methionine	UNP K0BRG7
C	-1	ASP	-	expression tag	UNP K0BRG7
C	0	SER	-	expression tag	UNP K0BRG7
C	1	TRP	-	expression tag	UNP K0BRG7
C	2	PHE	-	expression tag	UNP K0BRG7
C	3	ILE	-	expression tag	UNP K0BRG7
C	4	LEU	-	expression tag	UNP K0BRG7
C	5	VAL	-	expression tag	UNP K0BRG7
C	6	LEU	-	expression tag	UNP K0BRG7
C	7	LEU	-	expression tag	UNP K0BRG7
C	8	GLY	-	expression tag	UNP K0BRG7
C	9	SER	-	expression tag	UNP K0BRG7
C	10	GLY	-	expression tag	UNP K0BRG7
C	11	LEU	-	expression tag	UNP K0BRG7
C	12	ILE	-	expression tag	UNP K0BRG7
C	13	CYS	-	expression tag	UNP K0BRG7
C	14	VAL	-	expression tag	UNP K0BRG7
C	15	SER	-	expression tag	UNP K0BRG7
C	16	ALA	-	expression tag	UNP K0BRG7
C	748	ALA	ARG	engineered mutation	UNP K0BRG7
C	751	GLY	ARG	engineered mutation	UNP K0BRG7
C	1060	PRO	VAL	engineered mutation	UNP K0BRG7
C	1061	PRO	LEU	engineered mutation	UNP K0BRG7
C	1292	GLU	-	expression tag	UNP K0BRG7
C	1293	PHE	-	expression tag	UNP K0BRG7
C	1294	GLY	-	expression tag	UNP K0BRG7
C	1295	SER	-	expression tag	UNP K0BRG7
C	1296	GLY	-	expression tag	UNP K0BRG7
C	1297	GLY	-	expression tag	UNP K0BRG7
C	1298	TYR	-	expression tag	UNP K0BRG7
C	1299	ILE	-	expression tag	UNP K0BRG7
C	1300	PRO	-	expression tag	UNP K0BRG7
C	1301	GLU	-	expression tag	UNP K0BRG7
C	1302	ALA	-	expression tag	UNP K0BRG7
C	1303	PRO	-	expression tag	UNP K0BRG7
C	1304	ARG	-	expression tag	UNP K0BRG7
C	1305	ASP	-	expression tag	UNP K0BRG7
C	1306	GLY	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1307	GLN	-	expression tag	UNP K0BRG7
C	1308	ALA	-	expression tag	UNP K0BRG7
C	1309	TYR	-	expression tag	UNP K0BRG7
C	1310	VAL	-	expression tag	UNP K0BRG7
C	1311	ARG	-	expression tag	UNP K0BRG7
C	1312	LYS	-	expression tag	UNP K0BRG7
C	1313	ASP	-	expression tag	UNP K0BRG7
C	1314	GLY	-	expression tag	UNP K0BRG7
C	1315	GLU	-	expression tag	UNP K0BRG7
C	1316	TRP	-	expression tag	UNP K0BRG7
C	1317	VAL	-	expression tag	UNP K0BRG7
C	1318	LEU	-	expression tag	UNP K0BRG7
C	1319	LEU	-	expression tag	UNP K0BRG7
C	1320	SER	-	expression tag	UNP K0BRG7
C	1321	THR	-	expression tag	UNP K0BRG7
C	1322	PHE	-	expression tag	UNP K0BRG7
C	1323	LEU	-	expression tag	UNP K0BRG7
C	1324	LYS	-	expression tag	UNP K0BRG7
C	1325	GLY	-	expression tag	UNP K0BRG7
C	1326	GLN	-	expression tag	UNP K0BRG7
C	1327	ASP	-	expression tag	UNP K0BRG7
C	1328	ASN	-	expression tag	UNP K0BRG7
C	1329	SER	-	expression tag	UNP K0BRG7
C	1330	ALA	-	expression tag	UNP K0BRG7
C	1331	ASP	-	expression tag	UNP K0BRG7
C	1332	ILE	-	expression tag	UNP K0BRG7
C	1333	GLN	-	expression tag	UNP K0BRG7
C	1334	HIS	-	expression tag	UNP K0BRG7
C	1335	SER	-	expression tag	UNP K0BRG7
C	1336	GLY	-	expression tag	UNP K0BRG7
C	1337	ARG	-	expression tag	UNP K0BRG7
C	1338	PRO	-	expression tag	UNP K0BRG7
C	1339	LEU	-	expression tag	UNP K0BRG7
C	1340	GLU	-	expression tag	UNP K0BRG7
C	1341	SER	-	expression tag	UNP K0BRG7
C	1342	ARG	-	expression tag	UNP K0BRG7
C	1343	GLY	-	expression tag	UNP K0BRG7
C	1344	PRO	-	expression tag	UNP K0BRG7
C	1345	PHE	-	expression tag	UNP K0BRG7
C	1346	GLU	-	expression tag	UNP K0BRG7
C	1347	GLN	-	expression tag	UNP K0BRG7
C	1348	LYS	-	expression tag	UNP K0BRG7

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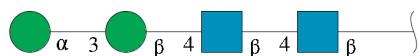
Chain	Residue	Modelled	Actual	Comment	Reference
C	1349	LEU	-	expression tag	UNP K0BRG7
C	1350	ILE	-	expression tag	UNP K0BRG7
C	1351	SER	-	expression tag	UNP K0BRG7
C	1352	GLU	-	expression tag	UNP K0BRG7
C	1353	GLU	-	expression tag	UNP K0BRG7
C	1354	ASP	-	expression tag	UNP K0BRG7
C	1355	LEU	-	expression tag	UNP K0BRG7
C	1356	ASN	-	expression tag	UNP K0BRG7
C	1357	MET	-	expression tag	UNP K0BRG7
C	1358	HIS	-	expression tag	UNP K0BRG7
C	1359	THR	-	expression tag	UNP K0BRG7
C	1360	GLY	-	expression tag	UNP K0BRG7
C	1361	HIS	-	expression tag	UNP K0BRG7
C	1362	HIS	-	expression tag	UNP K0BRG7
C	1363	HIS	-	expression tag	UNP K0BRG7
C	1364	HIS	-	expression tag	UNP K0BRG7
C	1365	HIS	-	expression tag	UNP K0BRG7
C	1366	HIS	-	expression tag	UNP K0BRG7

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



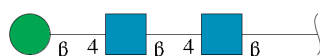
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



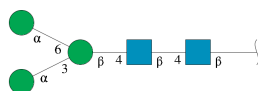
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



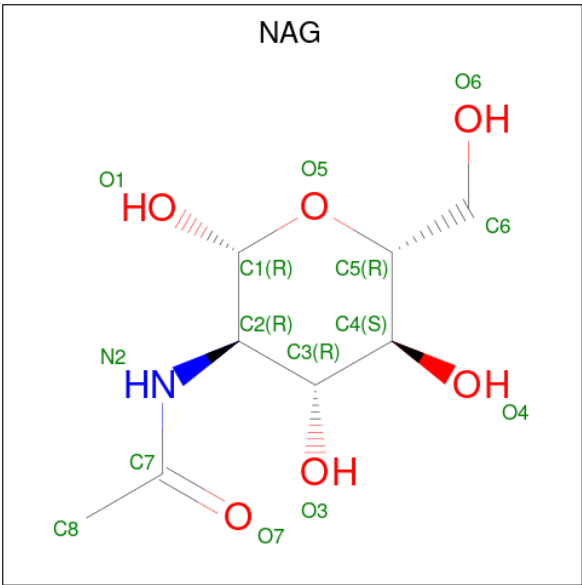
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	G	5	Total	C	N	O	0	0
			61	34	2	25		
5	L	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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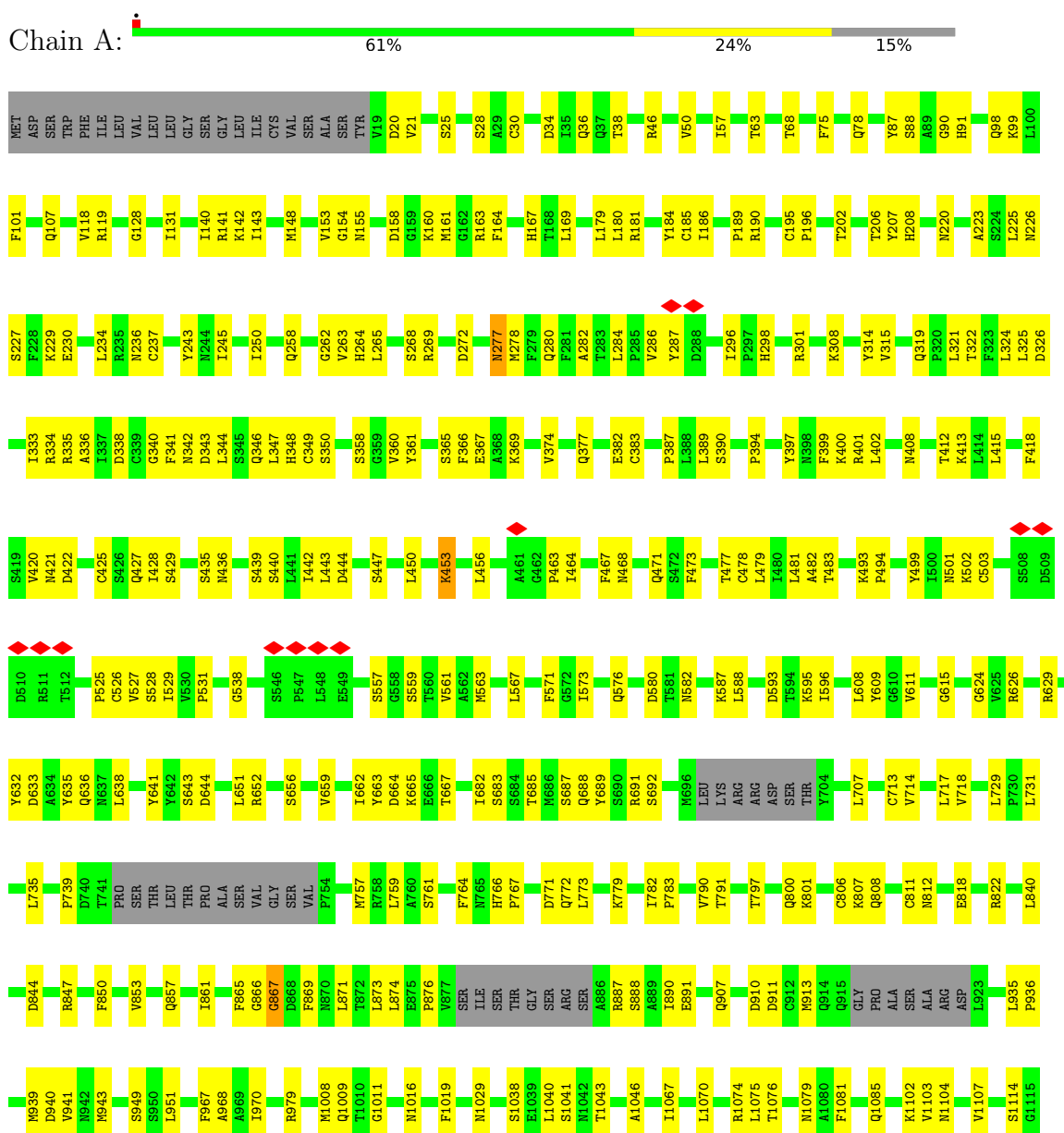
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



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

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

● Molecule 1: Spike glycoprotein

Chain C:  61% 24% 15%

MET	A122	C237	L325	S447	N519	Y606	D740	Q857	A969	S1114	GLY
ASP	A123	T238	D326	S448	A520	R614	I741	L873	T986	C1117	THR
TRP	S126	T242	F327	P449	N521	G615	PRD	L874	S986	S1117	ILE
ILE	G128	V243	D330	M452	Y523	F616	THR	E875	V989	H1122	ASN
LEU	A138	N244	R335	D455	S524	Q628	THR	E876	I987	H1123	VAL
VAL	T139	T245	A336	D455	P525	S643	PRO	S877	K1000	V1124	SER
LEU	T139	T246	D338	S459	C526	S643	ALA	ILE	M1008	S1125	THR
ASN	I140	D248	C339	A460	Y527	D645	VAL	SER	M1008	S1125	ILE
ALA	R141	D248	C339	A461	Y527	D645	GLY	GLY	M1008	S1125	PRO
GLN	K142	V253	L344	A461	S528	D646	SER	SER	M1028	L1134	ALA
SER	N155	Q258	L347	G462	D537	R647	VAL	ARG	S1034	Y1135	THR
ILE	F156	T259	L347	G462	D537	R647	VAL	ARG	S1034	Y1135	VAL
HIS	F156	T259	L347	G462	D537	R647	VAL	ARG	S1034	Y1135	ARG
LYS	M161	Q261	S358	S465	Y540	V659	M757	R887	S1038	H1138	LYS
GLY	G162	Q261	S358	S465	Y540	V659	M757	R887	S1038	H1138	LYS
ASN	R163	V263	V360	Q466	T541	V661	S761	S888	E1039	G1140	THR
PRO	F164	H264	Y361	F467	R542	R660	S761	S888	E1039	G1140	THR
SER	F165	L265	S365	F467	R542	R660	S761	S888	E1039	G1140	THR
TYR	N166	F266	F366	F467	R542	R660	S761	S888	E1039	G1140	THR
GLU	H167	S267	F366	F467	R542	R660	S761	S888	E1039	G1140	THR
ILE	T168	T169	S369	F473	L548	T667	S776	D910	I1043	H1146	THR
LYS	L169	P173	S373	C478	O550	H681	I782	N913	D1053	H1177	THR
GLU	P173	D174	V374	C478	O550	H681	I782	N913	D1053	H1177	THR
GLY	R46	L178	V375	C478	O550	H681	I782	N913	D1053	H1177	THR
ASN	D49	L180	L389	L481	O551	T682	T791	Q915	I1055	ARG	GLY
TYR	SER	R181	N277	A482	O552	S683	Q792	GLY	Q1056	ILE	GLY
GLU	Y184	L188	A282	P485	Y553	S683	Q792	PRO	R1057	VAL	ASP
GLY	G185	L188	L284	P485	Y553	S683	Q792	ALA	L1058	E1183	LEU
SER	N66	L188	P286	L488	S557	S687	T797	ARG	Q1066	E1195	GLN
GLY	T67	E188	V286	L488	S557	S687	T797	ASP	I1067	N1201	VAL
TYR	T68	P189	K291	L488	S557	S687	T797	ASP	I1067	N1201	VAL
PRO	Q78	A197	Y292	L488	S557	S687	T797	ASP	I1067	N1201	VAL
ALA	Q78	A197	Y292	L488	S557	S687	T797	ASP	I1067	N1201	VAL
PRO	D83	T206	L296	L488	S557	S687	T797	ASP	I1067	N1201	VAL
ARG	R84	Y207	R301	L488	S557	S687	T797	ASP	I1067	N1201	VAL
HIS	Y85	H209	S302	L488	S557	S687	T797	ASP	I1067	N1201	VAL
GLY	Y86	H209	S302	L488	S557	S687	T797	ASP	I1067	N1201	VAL
GLN	Y87	Y219	L303	L488	S557	S687	T797	ASP	I1067	N1201	VAL
ALA	L100	Y219	L303	L488	S557	S687	T797	ASP	I1067	N1201	VAL
TYR	R220	R221	R307	L488	S557	S687	T797	ASP	I1067	N1201	VAL
VAL	M104	Y105	A223	L488	S557	S687	T797	ASP	I1067	N1201	VAL
LYS	S106	Q107	S227	L488	S557	S687	T797	ASP	I1067	N1201	VAL
ASP	Q107	S227	S227	L488	S557	S687	T797	ASP	I1067	N1201	VAL
GLY	K110	N233	L234	L488	S557	S687	T797	ASP	I1067	N1201	VAL
TRP	R119	L235	F323	L488	S557	S687	T797	ASP	I1067	N1201	VAL
VAL	R119	L235	F323	L488	S557	S687	T797	ASP	I1067	N1201	VAL
LEU	R119	L235	F323	L488	S557	S687	T797	ASP	I1067	N1201	VAL

MET
HIS
THR
GLY
HIS
HIS
HIS
HIS
HIS

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

Chain D:  100%

NAG1
NAG2

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

Chain H:  50% 50%

NAG1
NAG2

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

Chain I:  100%

NAG1
NAG2

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

Chain J:  100%

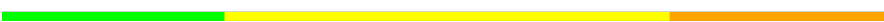
NAG1
NAG2

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

Chain K:  50% 50%

NAG1
NAG2

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

Chain E:  25% 50% 25%

NAG1
NAG2
EMA3
MAN4

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

Chain F:  67% 33%

MAG1
MAG2
BMA3

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  40% 40% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.488	Depositor
Minimum map value	-0.445	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/9230	0.51	4/12557 (0.0%)
1	B	0.31	7/9230 (0.1%)	0.55	5/12557 (0.0%)
1	C	0.32	3/9230 (0.0%)	0.59	7/12557 (0.1%)
All	All	0.29	10/27690 (0.0%)	0.55	16/37671 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	221	ARG	CA-C	-7.76	1.42	1.52
1	B	270	TYR	CA-C	-7.25	1.43	1.52
1	B	268	SER	CA-C	-6.72	1.45	1.53
1	C	220	ASN	CA-C	-6.16	1.44	1.52
1	B	271	VAL	N-CA	-5.36	1.39	1.46
1	B	875	GLU	CA-C	-5.33	1.47	1.53
1	B	272	ASP	CA-C	-5.31	1.45	1.52
1	B	887	ARG	CA-C	-5.14	1.46	1.53
1	B	273	LEU	N-CA	-5.06	1.40	1.46
1	C	184	TYR	CA-C	-5.00	1.47	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ARG	N-CA-C	-9.24	100.13	111.40
1	A	866	GLY	N-CA-C	-8.78	102.29	114.67
1	C	57	ILE	CA-C-N	7.82	132.57	120.68
1	C	57	ILE	C-N-CA	7.82	132.57	120.68
1	A	453	LYS	N-CA-C	6.74	120.37	111.75
1	A	319	GLN	CA-C-N	-5.98	113.62	119.90
1	A	319	GLN	C-N-CA	-5.98	113.62	119.90
1	C	188	GLU	CA-C-N	-5.83	113.75	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	GLU	C-N-CA	-5.83	113.75	119.76
1	C	165	PHE	N-CA-C	5.82	117.70	108.79
1	B	887	ARG	N-CA-C	-5.77	100.66	109.65
1	B	271	VAL	N-CA-C	5.69	117.58	112.17
1	B	270	TYR	CA-C-N	-5.20	114.59	122.76
1	B	270	TYR	C-N-CA	-5.20	114.59	122.76
1	C	43	THR	CA-C-N	5.13	126.80	122.28
1	C	43	THR	C-N-CA	5.13	126.80	122.28

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	9020	0	8705	229	0
1	B	9020	0	8707	209	0
1	C	9020	0	8704	221	0
2	D	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
3	E	50	0	43	1	0
4	F	39	0	34	1	0
5	G	61	0	52	1	0
5	L	61	0	52	0	0
6	A	98	0	91	3	0
6	B	70	0	65	0	0
6	C	98	0	91	2	0
All	All	27677	0	26669	637	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 12.

All (637) 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:497:TYR:HB3	1:B:561:VAL:O	1.76	0.85
1:A:21:VAL:HG12	1:A:237:CYS:H	1.49	0.76
1:B:427:GLN:NE2	1:B:475:ASN:O	2.21	0.73
1:C:169:LEU:HB3	1:C:184:TYR:HD1	1.53	0.72
1:C:237:CYS:SG	1:C:238:THR:N	2.63	0.72
1:A:366:PHE:HB3	1:A:688:GLN:HE21	1.54	0.71
1:B:83:ASP:HB2	1:B:315:VAL:HB	1.73	0.71
1:A:463:PRO:HB3	1:A:501:ASN:HA	1.74	0.70
1:B:271:VAL:HB	1:B:279:PHE:HD2	1.56	0.70
1:C:265:LEU:HB2	1:C:282:ALA:HB3	1.74	0.70
1:B:265:LEU:HB2	1:B:282:ALA:HB3	1.74	0.69
1:A:189:PRO:HB3	1:A:196:PRO:HB2	1.74	0.69
1:A:181:ARG:NH1	4:F:1:NAG:O3	2.25	0.69
1:A:608:LEU:HB2	1:A:611:VAL:HB	1.75	0.69
1:B:401:ARG:HB2	1:B:442:ILE:HD11	1.75	0.69
1:A:180:LEU:HB2	1:A:243:TYR:HB2	1.76	0.68
1:A:68:THR:HA	1:A:325:LEU:O	1.95	0.67
1:A:265:LEU:HB2	1:A:282:ALA:HB3	1.75	0.67
1:A:869:PHE:HB3	1:A:871:LEU:HD21	1.75	0.67
1:A:1081:PHE:O	1:A:1085:GLN:NE2	2.28	0.66
1:C:324:LEU:HD23	1:C:337:ILE:HD11	1.77	0.66
1:C:876:PRO:HA	1:C:888:SER:HA	1.76	0.66
1:A:429:SER:HB3	1:C:510:ASP:HB3	1.78	0.66
1:B:133:SER:HB2	1:B:307:ARG:HH11	1.60	0.65
1:B:736:CYS:SG	1:B:737:ALA:N	2.69	0.65
1:A:767:PRO:HB2	1:B:857:GLN:HA	1.77	0.65
1:B:84:MET:HE1	1:B:312:ALA:HB1	1.79	0.64
1:B:118:VAL:HG22	1:B:315:VAL:HG22	1.79	0.64
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.78	0.64
1:B:607:SER:HA	1:B:611:VAL:O	1.97	0.64
1:B:26:VAL:O	1:B:190:ARG:NH2	2.32	0.63
1:A:344:LEU:O	1:A:348:HIS:ND1	2.32	0.63
1:B:401:ARG:NH1	1:C:286:VAL:O	2.32	0.63
1:C:443:LEU:HA	1:C:572:GLY:O	1.99	0.63
1:C:462:GLY:O	1:C:466:GLN:NE2	2.31	0.63
1:B:1162:THR:HA	1:B:1207:PRO:HG3	1.81	0.62
1:A:593:ASP:H	1:A:595:LYS:HZ1	1.46	0.62
1:B:412:THR:OG1	1:B:413:LYS:NZ	2.32	0.62
1:C:401:ARG:HB3	1:C:442:ILE:HD11	1.82	0.62
1:A:179:LEU:HD23	1:A:181:ARG:HE	1.65	0.62
1:B:797:THR:HG22	1:B:1133:GLY:HA2	1.82	0.62
1:A:797:THR:HG22	1:A:1133:GLY:HA2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LYS:HA	1:B:563:MET:HE1	1.81	0.61
1:C:394:PRO:HG3	1:C:400:LYS:HG3	1.82	0.61
1:A:25:SER:OG	1:A:190:ARG:NH2	2.34	0.61
1:A:358:SER:HA	1:A:663:TYR:O	2.00	0.61
1:C:537:ASP:HA	1:C:559:SER:HA	1.82	0.61
1:A:220:ASN:HB3	1:A:223:ALA:HB2	1.81	0.61
1:C:245:ILE:HG12	1:C:269:ARG:HD2	1.83	0.61
1:B:478:CYS:HB2	1:B:573:ILE:HB	1.82	0.61
1:B:172:LEU:HD22	1:B:225:LEU:HG	1.82	0.61
1:B:524:SER:HB3	1:B:527:VAL:HG23	1.82	0.61
1:B:787:SER:HA	1:B:1000:LYS:HD3	1.83	0.61
1:B:190:ARG:NH1	1:B:229:LYS:O	2.34	0.60
1:B:116:PHE:HA	1:B:318:LEU:HD23	1.83	0.60
1:C:439:SER:N	1:C:576:GLN:O	2.34	0.60
1:A:57:ILE:HA	1:A:278:MET:HB2	1.81	0.60
1:B:449:PRO:HA	1:B:568:GLN:HB2	1.83	0.60
1:B:411:LEU:HA	1:B:414:LEU:HB3	1.83	0.60
1:C:83:ASP:HB2	1:C:315:VAL:HB	1.83	0.60
1:C:366:PHE:HB3	1:C:688:GLN:HE21	1.66	0.60
1:A:333:ILE:O	1:A:334:ARG:NH1	2.34	0.60
1:B:271:VAL:HB	1:B:279:PHE:CD2	2.34	0.60
1:B:1023:GLN:NE2	1:B:1027:ASN:OD1	2.34	0.60
1:A:394:PRO:HG3	1:A:400:LYS:HG3	1.82	0.60
1:A:399:PHE:HB2	1:A:444:ASP:HB2	1.82	0.60
1:C:497:TYR:HB2	1:C:561:VAL:HB	1.84	0.59
1:B:857:GLN:HE21	1:B:967:PHE:HB2	1.66	0.59
1:C:1158:ALA:HA	6:C:1402:NAG:H81	1.84	0.59
1:A:871:LEU:HB3	1:A:874:LEU:HD13	1.84	0.59
1:B:356:VAL:H	1:B:665:LYS:HE3	1.66	0.59
1:C:258:GLN:NE2	1:C:259:THR:O	2.36	0.59
1:C:33:VAL:HG22	1:C:100:LEU:HD12	1.84	0.59
1:A:1011:GLY:O	1:A:1016:ASN:ND2	2.36	0.59
1:C:464:ILE:HA	1:C:468:ASN:HB2	1.85	0.59
1:A:939:MET:HB3	1:A:943:MET:HB2	1.85	0.59
1:A:46:ARG:O	1:A:119:ARG:NH2	2.34	0.59
1:B:1122:HIS:NE2	1:B:1125:SER:OG	2.31	0.59
1:C:691:ARG:NH2	1:C:692:SER:OG	2.36	0.59
1:C:807:LYS:O	1:C:811:CYS:HB3	2.03	0.59
1:C:776:SER:OG	1:C:1212:GLN:NE2	2.36	0.58
1:C:808:GLN:O	1:C:812:ASN:ND2	2.37	0.58
1:C:375:VAL:H	1:C:594:THR:HB	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:O	1:A:298:HIS:ND1	2.36	0.58
1:A:502:LYS:HB3	1:A:557:SER:HB3	1.85	0.58
1:A:869:PHE:O	1:A:871:LEU:HG	2.03	0.58
1:B:500:ILE:HD11	1:B:530:VAL:HG11	1.85	0.58
1:C:831:ILE:HB	1:C:1082:VAL:HG21	1.84	0.58
1:C:169:LEU:HA	1:C:184:TYR:HA	1.85	0.58
1:C:268:SER:OG	1:C:272:ASP:O	2.21	0.58
1:C:540:TYR:HB3	1:C:542:ARG:HH22	1.69	0.58
1:A:245:ILE:HD11	1:A:269:ARG:HG3	1.86	0.58
1:A:979:ARG:NH2	1:A:1123:ILE:O	2.36	0.58
1:A:1114:SER:O	1:B:1104:ASN:ND2	2.36	0.58
1:B:173:PRO:HA	1:B:179:LEU:O	2.03	0.58
1:C:797:THR:HG21	1:C:1134:LEU:HD23	1.86	0.58
1:A:394:PRO:O	1:A:447:SER:N	2.33	0.58
1:C:155:ASN:HA	1:C:161:MET:HA	1.84	0.58
1:B:939:MET:HB3	1:B:943:MET:HB3	1.85	0.58
1:C:104:ASN:HB2	1:C:107:GLN:HB2	1.86	0.58
1:C:253:TRP:HB2	1:C:278:MET:HE3	1.86	0.58
1:C:401:ARG:NH2	1:C:521:ASN:O	2.36	0.57
1:A:538:GLY:H	1:A:559:SER:HA	1.68	0.57
1:C:67:ILE:HG13	1:C:69:ILE:HD11	1.86	0.57
1:C:439:SER:HA	1:C:582:ASN:HA	1.86	0.57
1:A:478:CYS:HB2	1:A:573:ILE:HB	1.86	0.57
1:B:816:LYS:NZ	1:B:1064:ASP:OD1	2.35	0.57
1:C:790:VAL:HG12	1:C:1139:VAL:HG22	1.86	0.57
1:A:425:CYS:HA	1:A:478:CYS:HA	1.86	0.57
1:A:865:PHE:C	1:A:867:GLY:H	2.12	0.57
1:C:269:ARG:O	1:C:269:ARG:NH1	2.37	0.57
1:C:839:ASN:OD1	1:C:842:GLN:NE2	2.37	0.57
1:B:68:THR:HA	1:B:325:LEU:O	2.05	0.57
1:C:123:ALA:HB3	1:C:312:ALA:H	1.69	0.57
1:C:1066:GLN:OE1	1:C:1069:ARG:NH1	2.38	0.57
1:A:141:ARG:HB2	1:A:308:LYS:HZ1	1.70	0.57
1:A:208:HIS:O	1:A:301:ARG:N	2.34	0.57
1:B:168:THR:HG21	1:B:187:LEU:HD23	1.85	0.57
1:C:263:VAL:HG23	1:C:286:VAL:HB	1.86	0.56
1:A:807:LYS:O	1:A:811:CYS:HB3	2.04	0.56
1:A:1102:LYS:NZ	1:A:1116:PHE:O	2.33	0.56
1:A:1127:VAL:HG12	1:A:1136:PHE:HD1	1.70	0.56
1:C:49:ASP:HA	1:C:78:GLN:HE22	1.69	0.56
1:C:389:LEU:HD21	1:C:488:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ILE:HD13	1:A:731:LEU:HD21	1.87	0.56
1:B:139:THR:O	1:B:308:LYS:NZ	2.35	0.56
1:B:208:HIS:O	1:B:301:ARG:N	2.34	0.56
1:B:457:SER:HB3	1:B:460:SER:HB2	1.86	0.56
1:C:64:TYR:HB3	1:C:67:ILE:HD11	1.88	0.56
1:B:212:THR:O	1:B:218:ASN:ND2	2.38	0.56
1:B:222:ASN:HB3	1:B:225:LEU:HB2	1.88	0.56
1:A:346:GLN:O	1:A:350:SER:N	2.38	0.56
1:A:853:VAL:HG22	1:A:951:LEU:HD21	1.88	0.56
1:B:420:VAL:HA	1:B:482:ALA:HA	1.87	0.56
1:A:400:LYS:O	1:A:444:ASP:HA	2.05	0.56
1:B:24:ASP:OD1	1:B:190:ARG:NH1	2.36	0.56
1:C:322:THR:HG1	1:C:339:CYS:HG	1.54	0.56
1:B:521:ASN:ND2	1:C:260:ALA:O	2.40	0.55
1:B:780:LEU:HD13	1:B:1173:ILE:HD11	1.86	0.55
1:A:36:GLN:OE1	1:A:38:THR:OG1	2.25	0.55
1:C:828:CYS:HA	1:C:831:ILE:HG12	1.87	0.55
1:B:66:ASN:N	1:B:327:PHE:O	2.40	0.55
1:A:861:ILE:HG21	1:A:876:PRO:HD2	1.88	0.55
1:B:800:GLN:OE1	1:B:1029:ASN:ND2	2.40	0.55
1:C:910:ASP:HA	1:C:913:MET:HG2	1.89	0.55
1:A:30:CYS:N	1:A:195:CYS:SG	2.79	0.55
1:C:662:ILE:HD13	1:C:731:LEU:HD21	1.88	0.55
1:A:262:GLY:HA2	1:A:286:VAL:HG12	1.88	0.55
1:A:365:SER:HA	1:A:659:VAL:HG22	1.88	0.55
1:B:720:SER:OG	1:B:759:LEU:O	2.23	0.55
1:C:219:TYR:O	1:C:220:ASN:C	2.49	0.55
1:C:394:PRO:HG2	1:C:399:PHE:HA	1.88	0.55
1:C:664:ASP:OD2	1:C:667:THR:OG1	2.25	0.55
1:A:88:SER:HB2	1:A:131:ILE:HD12	1.89	0.55
1:A:397:TYR:OH	1:A:531:PRO:O	2.21	0.55
1:B:119:ARG:NH2	1:B:316:TYR:OH	2.40	0.55
1:C:119:ARG:HG2	1:C:122:ALA:HB2	1.89	0.55
1:C:606:TYR:HB3	1:C:617:PHE:HZ	1.72	0.55
1:A:421:ASN:OD1	1:A:483:THR:OG1	2.23	0.55
1:A:1067:ILE:HD13	1:A:1070:LEU:HD12	1.88	0.55
1:C:681:HIS:NE2	1:C:685:THR:OG1	2.37	0.55
1:A:367:GLU:N	1:A:687:SER:OG	2.35	0.54
1:B:730:PRO:HB2	1:C:938:LEU:HD11	1.88	0.54
1:C:1028:ASN:HB3	1:C:1088:ARG:HH12	1.71	0.54
1:A:808:GLN:O	1:A:812:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:PRO:HA	1:A:888:SER:HA	1.89	0.54
1:B:1160:ASN:ND2	1:B:1163:ASN:OD1	2.39	0.54
1:C:1208:GLN:HB3	1:C:1211:TYR:CZ	2.43	0.54
1:A:873:LEU:HD21	1:A:1009:GLN:HG3	1.89	0.54
1:C:904:GLY:HA3	1:C:908:GLY:HA3	1.90	0.54
1:A:397:TYR:HB2	1:A:527:VAL:HG22	1.88	0.54
1:C:208:HIS:O	1:C:301:ARG:N	2.38	0.54
1:C:939:MET:HE3	1:C:944:GLU:HA	1.90	0.54
1:A:850:PHE:HA	1:A:853:VAL:HG12	1.88	0.54
1:A:346:GLN:HA	1:A:349:CYS:HB2	1.89	0.54
1:A:412:THR:OG1	1:A:413:LYS:NZ	2.41	0.54
1:A:456:LEU:HD11	1:A:481:LEU:HD21	1.90	0.54
1:B:427:GLN:HG2	1:B:476:PRO:HA	1.90	0.54
1:C:234:LEU:O	1:C:235:ARG:NH1	2.35	0.54
1:B:927:GLN:HA	1:B:932:TYR:HB2	1.89	0.54
1:C:142:LYS:NZ	1:C:248:ASP:OD1	2.39	0.54
1:A:873:LEU:HB3	1:A:890:ILE:HB	1.89	0.53
1:B:910:ASP:O	1:B:914:GLN:HB2	2.08	0.53
1:A:142:LYS:NZ	1:A:250:ILE:O	2.37	0.53
1:A:624:GLY:O	1:A:626:ARG:NH1	2.41	0.53
1:A:739:PRO:HB3	1:A:757:MET:HE1	1.91	0.53
1:C:577:TYR:O	1:C:582:ASN:ND2	2.36	0.53
1:C:955:ILE:HA	1:C:958:VAL:HG12	1.90	0.53
1:C:1034:SER:O	1:C:1038:SER:OG	2.26	0.53
1:C:1123:ILE:HD11	1:C:1141:TYR:HB2	1.91	0.53
1:A:1038:SER:O	1:A:1041:SER:OG	2.26	0.53
1:C:404:PHE:HE2	1:C:443:LEU:HB3	1.72	0.53
1:C:1067:ILE:HD13	1:C:1070:LEU:HD21	1.90	0.53
1:A:707:LEU:HB3	6:A:1404:NAG:H81	1.90	0.53
1:B:262:GLY:HA3	1:B:285:PRO:HA	1.89	0.53
1:B:262:GLY:HA2	1:B:286:VAL:HG12	1.90	0.53
1:B:358:SER:HA	1:B:663:TYR:O	2.07	0.53
1:C:1047:ILE:HD11	1:C:1058:LEU:HD21	1.90	0.53
1:A:34:ASP:HB3	1:A:99:LYS:HD3	1.91	0.53
1:A:629:ARG:NH2	1:A:644:ASP:OD1	2.42	0.53
6:A:1401:NAG:H83	1:C:528:SER:HA	1.90	0.53
1:B:717:LEU:HD13	1:B:759:LEU:HB2	1.90	0.53
1:C:245:ILE:HA	1:C:269:ARG:HE	1.73	0.53
1:A:764:PHE:HA	1:B:943:MET:HE1	1.90	0.53
1:C:782:ILE:O	1:C:1146:HIS:HA	2.08	0.53
1:A:20:ASP:OD1	1:A:20:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:GLN:O	1:A:911:ASP:N	2.39	0.53
1:A:790:VAL:HG12	1:A:1139:VAL:HG22	1.89	0.53
1:C:643:SER:OG	1:C:647:ASN:O	2.26	0.53
1:C:857:GLN:HE21	1:C:967:PHE:HB2	1.72	0.53
1:C:997:ILE:HA	1:C:1000:LYS:HD2	1.89	0.53
1:A:615:GLY:HA3	1:A:651:LEU:HD21	1.90	0.52
1:C:169:LEU:HB3	1:C:184:TYR:CD1	2.41	0.52
1:C:358:SER:HB3	1:C:665:LYS:H	1.74	0.52
1:C:615:GLY:HA3	1:C:651:LEU:HD21	1.90	0.52
1:A:935:LEU:HD12	1:A:936:PRO:HD2	1.90	0.52
1:C:206:THR:HG23	1:C:227:SER:HB3	1.90	0.52
1:A:287:TYR:OH	1:C:399:PHE:O	2.26	0.52
1:A:664:ASP:OD2	1:A:667:THR:OG1	2.27	0.52
1:B:525:PRO:O	1:B:528:SER:OG	2.20	0.52
1:C:347:LEU:HD11	1:C:661:VAL:HG11	1.91	0.52
1:B:723:PHE:HB3	1:B:763:ALA:HB2	1.91	0.52
1:B:795:ILE:HG21	1:B:1099:ALA:HB2	1.91	0.52
1:A:418:PHE:HB3	1:A:420:VAL:HG23	1.90	0.52
1:A:439:SER:HA	1:A:582:ASN:HA	1.90	0.52
1:C:399:PHE:O	1:C:523:TYR:OH	2.28	0.52
1:A:456:LEU:HD13	1:A:479:LEU:HB3	1.90	0.52
1:B:399:PHE:O	1:B:523:TYR:OH	2.28	0.52
1:C:181:ARG:NH2	2:K:1:NAG:HN2	2.07	0.52
1:C:1043:THR:HB	1:C:1046:ALA:HB3	1.92	0.52
1:A:347:LEU:HD22	1:A:361:TYR:HD2	1.75	0.52
1:C:207:TYR:HB2	1:C:301:ARG:HG2	1.91	0.52
1:C:263:VAL:HB	1:C:284:LEU:HB2	1.91	0.52
1:A:154:GLY:O	1:A:163:ARG:N	2.43	0.52
1:A:656:SER:OG	1:B:928:TYR:OH	2.27	0.52
1:A:277:ASN:C	1:A:277:ASN:HD22	2.15	0.51
1:A:683:SER:HB3	1:A:691:ARG:HH12	1.74	0.51
1:B:158:ASP:OD2	1:B:160:LYS:NZ	2.41	0.51
1:C:19:VAL:N	1:C:237:CYS:O	2.43	0.51
1:B:988:GLN:NE2	1:B:992:GLU:OE1	2.43	0.51
1:C:373:SER:O	1:C:599:GLN:NE2	2.43	0.51
1:A:818:GLU:O	1:A:822:ARG:NH1	2.43	0.51
1:B:708:GLN:NE2	1:B:712:GLY:O	2.42	0.51
1:B:1038:SER:O	1:B:1041:SER:OG	2.26	0.51
1:C:1068:ASP:O	1:C:1072:ASN:ND2	2.44	0.51
1:A:107:GLN:NE2	1:A:202:THR:O	2.43	0.51
1:A:493:LYS:HB3	1:A:563:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:ASP:HB2	1:A:943:MET:HG3	1.92	0.51
1:B:726:ASP:OD1	1:B:726:ASP:N	2.44	0.51
1:C:66:ASN:CA	1:C:327:PHE:O	2.59	0.51
1:B:819:GLN:HA	1:B:822:ARG:HE	1.76	0.51
1:C:326:ASP:HB3	1:C:335:ARG:HB2	1.93	0.51
1:B:792:GLN:OE1	1:B:1135:TYR:OH	2.29	0.51
1:B:181:ARG:HD3	1:B:240:MET:HG3	1.93	0.51
1:C:876:PRO:HB3	1:C:886:ALA:O	2.11	0.51
1:C:1162:THR:HA	1:C:1207:PRO:HG3	1.93	0.51
1:A:180:LEU:HD11	1:A:245:ILE:HB	1.92	0.50
1:B:401:ARG:NH2	1:C:260:ALA:O	2.43	0.50
1:A:662:ILE:HB	1:A:729:LEU:HD21	1.92	0.50
1:B:365:SER:HB3	1:B:658:PRO:HA	1.93	0.50
1:C:433:ILE:O	1:C:438:TYR:OH	2.23	0.50
1:C:526:CYS:HA	1:C:554:LEU:HD21	1.93	0.50
1:A:587:LYS:HG3	1:A:588:LEU:H	1.77	0.50
1:A:128:GLY:HA3	1:A:140:ILE:HD11	1.93	0.50
1:A:1008:MET:HE3	1:A:1137:MET:HG3	1.92	0.50
1:B:172:LEU:HD13	1:B:225:LEU:HD23	1.93	0.50
1:B:714:VAL:HG21	1:B:717:LEU:HD12	1.94	0.50
1:C:493:LYS:HA	1:C:567:LEU:HD22	1.93	0.50
1:A:800:GLN:OE1	1:A:1029:ASN:ND2	2.39	0.50
1:A:844:ASP:OD1	1:A:847:ARG:NH1	2.37	0.50
1:B:1052:GLY:HA2	1:B:1055:ILE:HG12	1.94	0.50
1:C:189:PRO:HB2	1:C:197:ALA:HB2	1.94	0.50
1:A:456:LEU:HB3	1:A:479:LEU:HD13	1.94	0.50
1:B:691:ARG:HH11	1:B:692:SER:H	1.57	0.50
1:B:46:ARG:O	1:B:119:ARG:NH2	2.42	0.49
1:C:66:ASN:HA	1:C:327:PHE:O	2.12	0.49
1:B:619:ASN:HA	1:B:649:TYR:HD1	1.76	0.49
1:A:154:GLY:N	1:A:163:ARG:O	2.32	0.49
1:B:798:THR:OG1	1:B:842:GLN:OE1	2.24	0.49
1:A:682:ILE:HG22	1:A:683:SER:H	1.78	0.49
1:C:68:THR:HA	1:C:325:LEU:O	2.11	0.49
1:C:873:LEU:HB3	1:C:890:ILE:HB	1.95	0.49
1:A:186:ILE:HG13	1:A:236:ASN:HB2	1.92	0.49
1:A:797:THR:HG21	1:A:1134:LEU:HD23	1.94	0.49
1:A:1043:THR:HB	1:A:1046:ALA:HB3	1.94	0.49
1:B:109:VAL:HG11	1:B:153:VAL:HG11	1.94	0.49
1:A:428:ILE:HG12	1:C:511:ARG:HH11	1.78	0.49
1:A:593:ASP:OD1	1:A:595:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:GLN:NE2	1:B:552:GLY:O	2.45	0.49
1:B:664:ASP:OD2	1:B:667:THR:OG1	2.31	0.49
1:C:740:ASP:OD1	1:C:740:ASP:N	2.45	0.49
1:B:944:GLU:HA	1:B:947:TYR:HB2	1.95	0.49
1:B:850:PHE:HA	1:B:853:VAL:HG22	1.95	0.49
1:C:126:SER:O	1:C:140:ILE:N	2.34	0.49
1:A:360:VAL:HG22	1:A:662:ILE:HG22	1.94	0.49
1:A:383:CYS:N	1:A:408:ASN:O	2.35	0.49
1:A:861:ILE:HD11	1:A:949:SER:HB3	1.95	0.49
1:B:591:ALA:O	1:B:594:THR:OG1	2.28	0.49
1:A:401:ARG:HE	1:A:442:ILE:HD11	1.77	0.49
1:B:174:ASP:OD2	1:B:225:LEU:N	2.40	0.49
1:A:717:LEU:HD22	1:A:759:LEU:HB2	1.94	0.48
1:C:682:ILE:HG22	1:C:683:SER:H	1.78	0.48
1:C:1123:ILE:HG12	1:C:1140:GLY:HA2	1.94	0.48
1:C:1220:PRO:HA	1:C:1223:LEU:HB2	1.95	0.48
1:A:46:ARG:HB2	1:A:314:TYR:CZ	2.48	0.48
1:A:207:TYR:N	1:A:227:SER:OG	2.44	0.48
1:B:187:LEU:HD13	1:B:232:PHE:HE2	1.78	0.48
1:B:629:ARG:NH2	1:B:641:TYR:OH	2.46	0.48
1:B:786:PHE:HB2	1:B:1141:TYR:HE1	1.77	0.48
1:C:643:SER:OG	1:C:645:ASP:OD1	2.21	0.48
1:A:422:ASP:HB3	1:A:481:LEU:HB2	1.95	0.48
1:A:343:ASP:O	1:A:346:GLN:NE2	2.45	0.48
1:C:119:ARG:HB3	1:C:314:TYR:HB2	1.96	0.48
1:C:951:LEU:O	1:C:955:ILE:HG12	2.13	0.48
1:A:148:MET:HE1	1:A:164:PHE:CG	2.49	0.48
1:B:46:ARG:HB2	1:B:314:TYR:CZ	2.48	0.48
1:B:360:VAL:HG22	1:B:662:ILE:HG22	1.96	0.48
1:C:66:ASN:N	1:C:327:PHE:O	2.47	0.48
1:C:265:LEU:HD13	1:C:284:LEU:HD23	1.94	0.48
1:B:151:SER:OG	1:B:289:THR:O	2.26	0.48
1:B:909:TYR:HA	1:B:912:CYS:HB2	1.96	0.48
1:C:396:VAL:HG21	1:C:464:ILE:HD12	1.95	0.48
1:A:440:SER:OG	1:A:576:GLN:OE1	2.31	0.48
1:B:682:ILE:HG22	1:B:683:SER:H	1.79	0.48
1:C:439:SER:OG	1:C:577:TYR:O	2.32	0.48
1:C:470:LYS:O	1:C:521:ASN:N	2.45	0.48
1:A:190:ARG:NH2	1:A:229:LYS:O	2.40	0.48
1:A:450:LEU:HD12	1:A:481:LEU:HD12	1.95	0.48
1:B:280:GLN:NE2	1:B:283:THR:OG1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:HB2	1:C:314:TYR:CZ	2.49	0.48
1:C:220:ASN:O	1:C:221:ARG:C	2.57	0.48
1:C:726:ASP:OD1	1:C:726:ASP:N	2.42	0.48
1:A:326:ASP:OD2	1:A:335:ARG:NH2	2.47	0.48
1:B:1035:LYS:O	1:B:1038:SER:OG	2.28	0.48
1:C:538:GLY:N	1:C:558:GLY:O	2.47	0.48
1:C:839:ASN:O	1:C:842:GLN:NE2	2.47	0.47
1:A:806:CYS:SG	1:A:807:LYS:N	2.86	0.47
1:B:90:GLY:HA2	1:B:101:PHE:HB3	1.96	0.47
1:B:347:LEU:O	1:B:350:SER:OG	2.29	0.47
1:B:383:CYS:N	1:B:408:ASN:O	2.31	0.47
1:B:1174:LYS:HA	1:B:1183:GLU:O	2.14	0.47
1:C:303:ILE:HG13	1:C:306:ASP:H	1.78	0.47
1:A:107:GLN:HE21	1:A:160:LYS:HD2	1.79	0.47
1:C:262:GLY:HA2	1:C:286:VAL:HG12	1.95	0.47
1:C:330:ASP:OD1	1:C:330:ASP:N	2.48	0.47
1:A:782:ILE:O	1:A:1146:HIS:HA	2.14	0.47
1:A:907:GLN:HB3	1:A:910:ASP:HB2	1.96	0.47
1:C:411:LEU:HD13	1:C:414:LEU:HD21	1.96	0.47
1:A:1075:LEU:O	1:A:1079:ASN:ND2	2.47	0.47
1:A:1164:CYS:O	1:A:1205:VAL:N	2.44	0.47
1:A:155:ASN:HA	1:A:161:MET:HA	1.96	0.47
1:A:467:PHE:CD1	1:A:503:CYS:HB3	2.49	0.47
1:A:1126:PHE:HB2	1:A:1137:MET:SD	2.54	0.47
1:B:272:ASP:O	1:B:273:LEU:C	2.57	0.47
1:B:441:LEU:HD13	1:B:575:VAL:HG12	1.97	0.47
1:B:595:LYS:O	1:B:598:SER:OG	2.31	0.47
1:C:44:TRP:O	1:C:314:TYR:OH	2.27	0.47
1:C:605:GLU:HG3	1:C:614:ARG:HB3	1.97	0.47
1:C:667:THR:O	1:C:669:THR:N	2.48	0.47
1:B:208:HIS:HB2	1:B:298:HIS:NE2	2.28	0.47
1:C:57:ILE:HA	1:C:278:MET:HB2	1.96	0.47
1:B:618:GLN:HG3	1:B:652:ARG:HH22	1.78	0.47
1:B:933:LYS:HZ2	1:B:935:LEU:HD13	1.80	0.47
1:C:389:LEU:HA	1:C:491:ILE:HD12	1.97	0.47
1:A:771:ASP:OD1	1:A:772:GLN:N	2.47	0.47
1:B:1129:ASN:OD1	1:B:1130:ALA:N	2.47	0.47
1:B:216:ASP:OD1	1:B:216:ASP:N	2.45	0.46
1:A:342:ASN:HB2	1:A:692:SER:HB2	1.97	0.46
1:A:629:ARG:NH1	1:A:641:TYR:OH	2.47	0.46
1:B:47:PRO:HB2	1:B:79:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG22	1:A:315:VAL:HG22	1.96	0.46
1:A:427:GLN:NE2	1:A:473:PHE:O	2.46	0.46
1:B:1118:GLY:HA3	1:B:1122:HIS:HB2	1.97	0.46
1:C:731:LEU:HD13	1:C:736:CYS:HA	1.97	0.46
1:C:986:THR:HG22	1:C:989:VAL:HG22	1.97	0.46
1:B:74:LEU:HB3	1:B:318:LEU:HD12	1.97	0.46
1:B:816:LYS:HE2	1:B:1063:GLN:HE21	1.81	0.46
1:A:499:TYR:HE1	1:A:561:VAL:HG23	1.80	0.46
1:C:128:GLY:HA3	1:C:140:ILE:HD11	1.96	0.46
1:A:401:ARG:HD2	1:A:444:ASP:HB3	1.98	0.46
1:B:865:PHE:HD2	1:B:871:LEU:HD11	1.79	0.46
1:B:1155:LEU:HD11	1:B:1184:TRP:CD1	2.50	0.46
1:C:188:GLU:HB3	1:C:233:ASN:HD22	1.80	0.46
1:C:493:LYS:HB3	1:C:563:MET:HE2	1.97	0.46
1:C:764:PHE:HB3	1:C:766:HIS:CE1	2.51	0.46
1:C:1117:CYS:HB2	1:C:1138:HIS:CE1	2.51	0.46
1:B:625:VAL:HG12	1:B:628:GLN:H	1.81	0.46
1:B:1170:GLY:HA3	1:B:1187:THR:O	2.16	0.46
1:A:91:HIS:HB3	1:A:98:GLN:HE21	1.81	0.46
1:A:153:VAL:HG12	1:A:161:MET:HE3	1.98	0.46
1:A:167:HIS:HE1	1:A:184:TYR:CD2	2.34	0.46
1:B:396:VAL:HG13	1:B:468:ASN:HB3	1.97	0.46
1:A:1076:THR:HA	1:A:1079:ASN:HD22	1.81	0.45
1:A:1103:VAL:HA	1:A:1107:VAL:HB	1.97	0.45
1:B:690:SER:OG	1:B:691:ARG:N	2.48	0.45
1:B:1120:GLY:HA2	1:C:964:LEU:HD12	1.98	0.45
1:B:1121:THR:HB	1:B:1141:TYR:HB3	1.97	0.45
1:B:142:LYS:NZ	1:B:250:ILE:O	2.46	0.45
1:C:85:TYR:HB3	1:C:105:TYR:CZ	2.51	0.45
1:C:794:TYR:HB2	1:C:1135:TYR:HD1	1.80	0.45
1:C:850:PHE:CE2	1:C:939:MET:HG2	2.52	0.45
1:A:264:HIS:ND1	1:A:280:GLN:OE1	2.49	0.45
1:C:246:THR:OG1	1:C:269:ARG:NH2	2.49	0.45
1:C:291:LYS:HG3	1:C:292:TYR:CD2	2.51	0.45
1:C:735:LEU:HD13	1:C:761:SER:HA	1.99	0.45
1:A:208:HIS:HB2	1:A:298:HIS:CE1	2.52	0.45
1:A:369:LYS:H	1:A:685:THR:HB	1.81	0.45
1:A:377:GLN:HG2	1:A:609:TYR:HB2	1.97	0.45
1:B:44:TRP:O	1:B:314:TYR:OH	2.30	0.45
1:B:401:ARG:NH2	1:B:521:ASN:HD21	2.14	0.45
1:C:449:PRO:HG2	1:C:452:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:HB2	1:A:298:HIS:HE1	1.81	0.45
1:A:258:GLN:HE22	1:A:286:VAL:HG11	1.82	0.45
1:A:420:VAL:HA	1:A:482:ALA:HA	1.98	0.45
1:B:226:ASN:O	1:B:230:GLU:N	2.48	0.45
1:A:439:SER:HB3	1:A:580:ASP:H	1.82	0.45
1:B:468:ASN:ND2	1:B:500:ILE:O	2.40	0.45
1:C:441:LEU:HD11	1:C:573:ILE:HG23	1.98	0.45
1:C:539:ASP:O	1:C:557:SER:HA	2.16	0.45
1:A:707:LEU:O	1:A:713:CYS:HA	2.17	0.45
1:C:245:ILE:HG23	1:C:269:ARG:HG3	1.98	0.45
1:C:1104:ASN:HA	1:C:1108:LYS:HD2	1.97	0.45
1:C:156:PHE:CE2	1:C:162:GLY:HA3	2.52	0.45
1:A:387:PRO:HG2	1:A:402:LEU:HD11	1.97	0.45
1:A:913:MET:HE1	1:C:616:VAL:HG11	1.98	0.45
1:B:330:ASP:OD1	1:B:331:GLY:N	2.49	0.45
1:B:691:ARG:NH1	1:B:692:SER:O	2.50	0.45
1:C:272:ASP:CG	1:C:276:GLY:H	2.24	0.45
1:A:268:SER:OG	1:A:272:ASP:O	2.35	0.45
1:B:771:ASP:HB3	1:B:779:LYS:HD3	1.99	0.45
1:B:46:ARG:O	1:B:316:TYR:OH	2.34	0.44
1:B:270:TYR:HB2	1:B:271:VAL:HG22	1.99	0.44
1:C:422:ASP:HB3	1:C:481:LEU:HB2	1.98	0.44
1:C:478:CYS:HB2	1:C:573:ILE:HB	1.99	0.44
1:A:148:MET:HB3	1:A:296:ILE:HD11	1.99	0.44
1:A:1104:ASN:HB3	1:C:1114:SER:HB3	1.98	0.44
1:B:861:ILE:HD13	1:B:876:PRO:HD2	1.99	0.44
1:C:173:PRO:HA	1:C:179:LEU:O	2.17	0.44
1:C:850:PHE:HA	1:C:853:VAL:HG12	1.99	0.44
1:C:1122:HIS:NE2	1:C:1125:SER:OG	2.32	0.44
1:A:167:HIS:CE1	1:A:184:TYR:CE2	3.06	0.44
1:A:343:ASP:N	1:A:343:ASP:OD1	2.50	0.44
1:A:632:TYR:HA	1:A:638:LEU:HA	1.99	0.44
1:A:1016:ASN:HB2	1:A:1019:PHE:HB2	1.98	0.44
1:C:110:LYS:HE2	1:C:110:LYS:HB2	1.82	0.44
1:A:344:LEU:HD23	1:A:347:LEU:HD12	1.98	0.44
1:A:374:VAL:HG11	1:A:596:ILE:HD13	1.99	0.44
1:B:1067:ILE:HA	1:B:1070:LEU:HG	1.99	0.44
1:C:369:LYS:H	1:C:685:THR:HB	1.83	0.44
1:C:1038:SER:OG	1:C:1039:GLU:OE1	2.33	0.44
1:A:90:GLY:HA2	1:A:101:PHE:HB3	1.99	0.44
1:C:344:LEU:HD23	1:C:347:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ARG:HB3	1:C:555:VAL:HG12	1.99	0.44
1:C:795:ILE:HD11	1:C:1102:LYS:HD2	2.00	0.44
1:C:803:THR:O	1:C:932:TYR:HB2	2.18	0.44
1:A:119:ARG:HB3	1:A:314:TYR:HB2	2.00	0.44
1:A:399:PHE:HE1	1:A:401:ARG:HH11	1.65	0.44
1:A:629:ARG:HH12	1:A:643:SER:HA	1.82	0.44
1:C:174:ASP:OD2	1:C:223:ALA:N	2.50	0.44
1:C:278:MET:HE2	1:C:278:MET:HA	1.99	0.44
1:C:502:LYS:HB3	1:C:557:SER:HB3	1.99	0.44
1:B:187:LEU:HB2	1:B:232:PHE:CD2	2.53	0.43
1:B:344:LEU:HB3	1:B:348:HIS:CE1	2.53	0.43
1:B:1068:ASP:O	1:B:1072:ASN:ND2	2.51	0.43
1:B:1104:ASN:HA	1:B:1108:LYS:HG2	1.99	0.43
1:C:850:PHE:HB3	1:C:947:TYR:HE2	1.82	0.43
1:A:471:GLN:HB3	1:A:477:THR:HG21	2.00	0.43
1:B:207:TYR:HB2	1:B:301:ARG:HG2	2.00	0.43
1:B:548:LEU:HD23	1:B:548:LEU:HA	1.87	0.43
1:B:972:PHE:O	1:B:975:SER:OG	2.25	0.43
1:C:401:ARG:HG2	1:C:444:ASP:HB3	2.00	0.43
1:B:146:ALA:HB3	1:B:296:ILE:HB	1.99	0.43
1:B:463:PRO:HB2	1:B:501:ASN:HA	2.01	0.43
1:A:87:TYR:CE2	1:A:298:HIS:HB3	2.53	0.43
1:A:338:ASP:OD1	1:A:340:GLY:N	2.51	0.43
1:B:436:ASN:ND2	1:C:1056:GLN:OE1	2.39	0.43
1:B:873:LEU:O	1:B:888:SER:OG	2.37	0.43
1:C:178:THR:HG23	1:C:179:LEU:HG	2.00	0.43
1:A:464:ILE:HA	1:A:468:ASN:HB2	1.99	0.43
1:A:633:ASP:CG	1:A:635:TYR:H	2.26	0.43
1:C:420:VAL:HA	1:C:482:ALA:HA	1.99	0.43
1:C:665:LYS:O	1:C:666:GLU:HG3	2.19	0.43
1:A:181:ARG:HG3	1:A:225:LEU:HD11	2.00	0.43
1:B:347:LEU:HD21	1:B:363:VAL:HG12	2.00	0.43
1:B:665:LYS:C	1:B:667:THR:H	2.27	0.43
1:B:725:GLU:OE2	1:B:765:ASN:ND2	2.51	0.43
1:C:360:VAL:HG13	1:C:662:ILE:HG22	2.01	0.43
1:B:684:SER:OG	1:B:685:THR:N	2.50	0.43
1:C:301:ARG:HD2	1:C:301:ARG:HA	1.73	0.43
1:A:415:LEU:HD12	1:A:418:PHE:HD2	1.84	0.43
1:A:714:VAL:HG11	1:A:717:LEU:HD12	2.00	0.43
1:B:483:THR:HG21	1:B:566:GLN:HB3	2.00	0.43
1:C:365:SER:OG	1:C:659:VAL:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1039:GLU:OE1	1:C:1039:GLU:N	2.51	0.43
1:A:435:SER:OG	1:A:436:ASN:ND2	2.52	0.43
1:A:773:LEU:HD11	1:A:779:LYS:HG3	2.00	0.43
1:C:393:PRO:O	1:C:447:SER:OG	2.25	0.43
1:A:593:ASP:N	1:A:595:LYS:HZ1	2.15	0.42
1:B:733:GLN:HG3	1:C:940:ASP:OD2	2.18	0.42
1:C:359:GLY:HA2	1:C:729:LEU:HD22	2.00	0.42
1:C:957:GLY:HA3	1:C:969:ALA:HA	2.00	0.42
1:A:68:THR:HB	1:A:324:LEU:HD11	2.00	0.42
1:A:250:ILE:HG12	3:E:1:NAG:H5	2.01	0.42
1:A:652:ARG:NE	1:B:912:CYS:O	2.52	0.42
1:A:1212:GLN:HA	6:A:1407:NAG:H82	2.00	0.42
1:B:289:THR:O	1:B:291:LYS:NZ	2.49	0.42
1:B:371:SER:N	1:B:603:CYS:O	2.36	0.42
1:B:462:GLY:HA2	1:B:463:PRO:HD3	1.92	0.42
1:C:449:PRO:HA	1:C:568:GLN:HB2	2.02	0.42
1:A:801:LYS:NZ	1:A:936:PRO:O	2.33	0.42
1:B:226:ASN:HA	1:B:229:LYS:HB2	2.00	0.42
1:B:441:LEU:HD21	1:B:443:LEU:HD21	2.00	0.42
1:B:449:PRO:HG2	1:B:452:MET:HE1	2.01	0.42
1:A:87:TYR:HD2	1:A:143:ILE:HD13	1.84	0.42
1:A:263:VAL:HB	1:A:284:LEU:HB2	2.00	0.42
1:A:382:GLU:HA	1:A:408:ASN:H	1.85	0.42
1:A:387:PRO:HA	1:A:390:SER:HB2	2.01	0.42
1:B:189:PRO:HB3	1:B:196:PRO:HB2	2.01	0.42
1:B:253:TRP:HB2	1:B:278:MET:HE3	2.01	0.42
1:B:826:GLN:HG2	1:B:830:LYS:HE2	2.01	0.42
1:C:485:PRO:HG2	1:C:488:LEU:HD13	2.01	0.42
1:B:415:LEU:HA	1:B:418:PHE:CD2	2.55	0.42
1:B:478:CYS:O	1:B:572:GLY:HA2	2.19	0.42
1:B:801:LYS:NZ	1:B:938:LEU:HG	2.34	0.42
1:C:347:LEU:HD22	1:C:361:TYR:HD2	1.84	0.42
1:A:185:CYS:HB2	1:A:234:LEU:HD11	2.02	0.42
1:A:525:PRO:O	1:A:528:SER:OG	2.32	0.42
1:A:632:TYR:HB2	1:B:62:ARG:HD2	2.02	0.42
1:B:397:TYR:HH	1:B:498:SER:HG	1.66	0.42
1:A:636:GLN:OE1	1:B:62:ARG:NH2	2.41	0.42
1:A:791:THR:HG21	1:A:1119:GLN:HB2	2.01	0.42
1:B:354:PHE:O	1:B:665:LYS:NZ	2.33	0.42
1:B:505:ARG:NH1	1:B:507:LEU:HD23	2.35	0.42
1:B:1016:ASN:HB3	1:B:1019:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1170:GLY:CA	1:B:1187:THR:O	2.68	0.42
1:C:496:LYS:HA	1:C:563:MET:HB2	2.00	0.42
1:A:526:CYS:HA	1:A:529:ILE:HG12	2.01	0.42
1:A:735:LEU:HA	1:A:761:SER:HA	2.01	0.42
1:B:1175:THR:OG1	1:B:1176:ASN:N	2.52	0.42
1:C:801:LYS:HB2	1:C:801:LYS:HE3	1.72	0.42
1:A:63:THR:HB	1:C:628:GLN:HG3	2.02	0.42
1:B:183:PHE:HB3	1:B:240:MET:SD	2.59	0.42
1:B:344:LEU:HD23	1:B:347:LEU:HD12	2.01	0.42
1:B:957:GLY:HA3	1:B:967:PHE:CZ	2.55	0.42
1:B:1059:ASP:HB3	1:B:1062:GLU:HG2	2.02	0.42
1:C:220:ASN:CB	1:C:223:ALA:HB2	2.49	0.42
1:C:221:ARG:HA	1:C:221:ARG:HD3	1.69	0.42
1:A:887:ARG:HH22	1:A:941:VAL:HG11	1.85	0.42
1:B:58:TYR:HE1	1:B:333:ILE:HG13	1.85	0.42
1:B:957:GLY:HA2	1:B:968:ALA:C	2.45	0.42
1:C:757:MET:SD	1:C:757:MET:N	2.93	0.42
1:C:1055:ILE:HG13	1:C:1063:GLN:NE2	2.35	0.42
1:A:28:SER:HA	1:A:190:ARG:HD3	2.01	0.41
1:A:169:LEU:HA	1:A:184:TYR:HA	2.01	0.41
1:C:57:ILE:HD13	1:C:266:PHE:CD2	2.55	0.41
1:C:1040:LEU:HD23	1:C:1040:LEU:HA	1.91	0.41
1:A:688:GLN:OE1	1:A:689:TYR:N	2.51	0.41
1:A:343:ASP:HA	1:A:346:GLN:HE21	1.86	0.41
1:B:334:ARG:NE	5:G:4:MAN:O4	2.53	0.41
1:B:519:ASN:N	1:B:522:GLN:OE1	2.53	0.41
1:C:119:ARG:HD3	1:C:253:TRP:CH2	2.55	0.41
1:C:1106:CYS:HB3	1:C:1111:SER:HB3	2.03	0.41
1:A:167:HIS:CE1	1:A:184:TYR:CD2	3.08	0.41
1:B:493:LYS:HD2	1:B:567:LEU:HG	2.02	0.41
1:B:788:PHE:HZ	1:B:980:LEU:HD11	1.85	0.41
1:C:967:PHE:CE2	1:C:969:ALA:HB2	2.55	0.41
1:C:1045:GLY:C	1:C:1069:ARG:HH12	2.29	0.41
1:A:158:ASP:OD2	1:A:160:LYS:NZ	2.48	0.41
1:A:1157:ASP:OD2	1:A:1160:ASN:N	2.53	0.41
1:B:35:ILE:HD12	1:B:104:ASN:HA	2.02	0.41
1:B:334:ARG:HD3	1:B:334:ARG:HA	1.88	0.41
1:B:1102:LYS:NZ	1:B:1116:PHE:O	2.47	0.41
1:C:369:LYS:NZ	1:C:686:MET:H	2.18	0.41
1:C:1128:VAL:HG23	1:C:1135:TYR:HB3	2.03	0.41
1:A:707:LEU:HD11	1:A:718:VAL:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:ARG:HD3	1:A:891:GLU:OE1	2.20	0.41
1:A:1206:ALA:HB3	1:B:987:GLN:NE2	2.36	0.41
1:B:342:ASN:OD1	1:B:345:SER:N	2.52	0.41
1:C:181:ARG:HD3	1:C:242:THR:HG22	2.01	0.41
1:C:696:MET:SD	1:C:696:MET:N	2.93	0.41
1:A:782:ILE:HD12	1:A:783:PRO:HD2	2.01	0.41
1:B:1002:ASN:HA	1:B:1005:LEU:HG	2.01	0.41
1:C:792:GLN:NE2	1:C:1008:MET:HB2	2.35	0.41
1:C:1211:TYR:H	6:C:1402:NAG:HO6	1.68	0.41
1:A:494:PRO:HD2	1:A:567:LEU:HD13	2.03	0.41
1:B:1208:GLN:HB3	1:B:1211:TYR:HE1	1.86	0.41
1:C:138:ALA:HB1	1:C:308:LYS:HD2	2.03	0.41
1:C:501:ASN:ND2	1:C:559:SER:HB3	2.36	0.41
1:A:50:VAL:HG12	1:A:78:GLN:NE2	2.35	0.41
1:A:382:GLU:HA	1:A:408:ASN:HB3	2.02	0.41
1:A:665:LYS:HA	1:A:665:LYS:HD3	1.71	0.41
1:A:735:LEU:HD13	1:A:761:SER:HA	2.03	0.41
1:A:857:GLN:HG3	1:A:967:PHE:HB2	2.02	0.41
1:A:968:ALA:O	1:A:970:ILE:N	2.52	0.41
1:A:1155:LEU:HD23	1:A:1155:LEU:HA	1.95	0.41
1:B:186:ILE:HB	1:B:235:ARG:HB3	2.02	0.41
1:B:711:VAL:HG13	1:B:733:GLN:HB2	2.02	0.41
1:B:799:ILE:HG21	1:B:1088:ARG:HB3	2.01	0.41
1:B:823:GLU:OE1	1:B:823:GLU:N	2.53	0.41
1:B:897:LYS:HD3	1:B:897:LYS:HA	1.93	0.41
1:C:87:TYR:OH	1:C:296:ILE:O	2.22	0.41
1:C:910:ASP:O	1:C:914:GLN:HG3	2.20	0.41
1:A:118:VAL:HA	1:A:314:TYR:O	2.21	0.41
1:A:278:MET:HE2	1:A:278:MET:HA	2.03	0.41
1:A:338:ASP:OD1	1:A:341:PHE:N	2.54	0.41
1:A:807:LYS:HZ1	1:A:822:ARG:HH22	1.68	0.41
1:B:142:LYS:HA	1:B:311:ALA:HB2	2.02	0.41
1:B:266:PHE:CD1	1:B:280:GLN:HA	2.55	0.41
1:B:738:LEU:O	1:B:758:ARG:HB2	2.21	0.41
1:B:1123:ILE:HG12	1:B:1140:GLY:HA2	2.04	0.41
1:C:369:LYS:HE2	1:C:685:THR:HA	2.02	0.41
1:C:597:ALA:HA	1:C:600:LEU:HG	2.02	0.41
1:A:389:LEU:HD21	1:A:418:PHE:HE1	1.86	0.40
1:A:764:PHE:O	1:A:766:HIS:ND1	2.53	0.40
1:B:605:GLU:HA	1:B:613:GLY:O	2.22	0.40
1:A:443:LEU:HD11	1:A:571:PHE:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ASN:HD21	1:B:344:LEU:HB2	1.86	0.40
1:B:369:LYS:HZ1	1:B:685:THR:HA	1.86	0.40
1:B:530:VAL:HG22	1:B:541:TYR:CD2	2.56	0.40
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.91	0.40
1:A:75:PHE:HD2	1:A:321:LEU:HB3	1.86	0.40
1:A:325:LEU:HD13	1:A:336:ALA:HB2	2.03	0.40
1:A:840:LEU:HD23	1:A:840:LEU:HA	1.90	0.40
1:A:1040:LEU:HD12	1:A:1074:ARG:HH21	1.87	0.40
1:B:181:ARG:HA	1:B:241:TYR:O	2.22	0.40
1:B:264:HIS:HD1	1:B:283:THR:HG23	1.87	0.40
1:B:853:VAL:HG12	1:B:1103:VAL:HG11	2.03	0.40
1:C:180:LEU:HB2	1:C:243:TYR:HB2	2.03	0.40
1:C:455:ASP:OD1	1:C:460:SER:OG	2.33	0.40
1:C:1053:ASP:O	1:C:1057:ARG:HG2	2.21	0.40
1:A:857:GLN:HA	1:C:767:PRO:HB2	2.03	0.40
1:B:1119:GLN:HB2	1:B:1142:TYR:OH	2.22	0.40
1:C:439:SER:OG	1:C:580:ASP:O	2.37	0.40
1:C:1074:ARG:O	1:C:1077:THR:OG1	2.34	0.40
1:C:1195:GLU:OE2	1:C:1201:ASN:ND2	2.55	0.40
1:A:226:ASN:O	1:A:230:GLU:N	2.55	0.40
1:C:1063:GLN:O	1:C:1067:ILE:HG12	2.22	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	1154/1369 (84%)	1053 (91%)	100 (9%)	1 (0%)	48	83
1	B	1154/1369 (84%)	1058 (92%)	93 (8%)	3 (0%)	36	72
1	C	1154/1369 (84%)	1046 (91%)	106 (9%)	2 (0%)	43	77
All	All	3462/4107 (84%)	3157 (91%)	299 (9%)	6 (0%)	44	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	ASP
1	C	220	ASN
1	A	867	GLY
1	B	876	PRO
1	C	218	ASN
1	B	218	ASN

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	1003/1180 (85%)	1000 (100%)	3 (0%)	86	84
1	B	1003/1180 (85%)	999 (100%)	4 (0%)	84	83
1	C	1003/1180 (85%)	995 (99%)	8 (1%)	73	78
All	All	3009/3540 (85%)	2994 (100%)	15 (0%)	78	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	322	THR
1	A	453	LYS
1	B	268	SER
1	B	271	VAL
1	B	273	LEU
1	B	877	VAL
1	C	163	ARG
1	C	167	HIS
1	C	168	THR
1	C	186	ILE
1	C	188	GLU
1	C	221	ARG
1	C	875	GLU
1	C	877	VAL

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

Mol	Chain	Res	Type
1	A	107	GLN
1	A	167	HIS
1	A	277	ASN
1	A	346	GLN
1	A	398	ASN
1	A	516	GLN
1	A	602	ASN
1	A	832	ASN
1	A	907	GLN
1	A	981	ASN
1	A	987	GLN
1	A	1066	GLN
1	A	1079	ASN
1	A	1085	GLN
1	A	1097	GLN
1	A	1129	ASN
1	B	36	GLN
1	B	208	HIS
1	B	226	ASN
1	B	410	ASN
1	B	521	ASN
1	B	670	HIS
1	B	733	GLN
1	B	765	ASN
1	B	766	HIS
1	B	772	GLN
1	B	812	ASN
1	B	915	GLN
1	B	981	ASN
1	B	988	GLN
1	B	1016	ASN
1	B	1063	GLN
1	B	1066	GLN
1	C	218	ASN
1	C	233	ASN
1	C	427	GLN
1	C	466	GLN
1	C	475	ASN
1	C	582	ASN
1	C	836	HIS
1	C	842	GLN

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Mol	Chain	Res	Type
1	C	999	ASN
1	C	1002	ASN
1	C	1079	ASN
1	C	1208	GLN
1	C	1212	GLN

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 ⓘ

27 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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.32	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	E	1	1,3	14,14,15	0.37	0	17,19,21	0.91	1 (5%)
3	NAG	E	2	3	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
3	BMA	E	3	3	11,11,12	0.66	0	15,15,17	0.84	0
3	MAN	E	4	3	11,11,12	0.78	1 (9%)	15,15,17	1.34	2 (13%)
4	NAG	F	1	4,1	14,14,15	1.34	2 (14%)	17,19,21	1.31	3 (17%)
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	1.05	2 (11%)
4	BMA	F	3	4	11,11,12	0.60	0	15,15,17	1.06	1 (6%)
5	NAG	G	1	5,1	14,14,15	1.47	2 (14%)	17,19,21	1.31	2 (11%)
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.53	0
5	BMA	G	3	5	11,11,12	0.87	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	G	4	5	11,11,12	0.93	0	15,15,17	1.13	2 (13%)
5	MAN	G	5	5	11,11,12	0.70	0	15,15,17	0.92	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.94	1 (7%)	17,19,21	0.80	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.35	0
2	NAG	I	1	2,1	14,14,15	0.31	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	J	1	2,1	14,14,15	0.32	0	17,19,21	0.51	0
2	NAG	J	2	2	14,14,15	0.35	0	17,19,21	0.44	0
2	NAG	K	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	0.99	0
2	NAG	K	2	2	14,14,15	0.39	0	17,19,21	0.46	0
5	NAG	L	1	5,1	14,14,15	0.93	1 (7%)	17,19,21	1.06	2 (11%)
5	NAG	L	2	5	14,14,15	0.26	0	17,19,21	0.95	2 (11%)
5	BMA	L	3	5	11,11,12	0.51	0	15,15,17	0.88	0
5	MAN	L	4	5	11,11,12	0.97	0	15,15,17	1.13	2 (13%)
5	MAN	L	5	5	11,11,12	0.62	0	15,15,17	1.09	2 (13%)

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
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	1/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
5	NAG	L	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
5	MAN	L	4	5	-	2/2/19/22	1/1/1/1
5	MAN	L	5	5	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	NAG	O5-C1	-4.89	1.35	1.43
4	F	1	NAG	O5-C1	-3.80	1.37	1.43
2	H	1	NAG	C1-C2	3.32	1.56	1.52
5	L	1	NAG	O5-C1	-3.07	1.38	1.43
4	F	1	NAG	C1-C2	2.74	1.56	1.52
3	E	4	MAN	C1-C2	2.37	1.57	1.52
2	K	1	NAG	O5-C1	-2.08	1.40	1.43
5	G	1	NAG	C1-C2	-2.04	1.49	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C3-C4-C5	3.93	117.36	110.23
3	E	4	MAN	C1-O5-C5	3.69	117.13	112.19
4	F	1	NAG	C4-C3-C2	3.47	116.10	111.02
5	G	4	MAN	C1-O5-C5	3.29	116.59	112.19
5	L	4	MAN	C1-O5-C5	3.13	116.38	112.19
4	F	2	NAG	O4-C4-C5	-3.05	101.81	109.32
5	L	5	MAN	C1-O5-C5	3.00	116.21	112.19
4	F	3	BMA	C1-O5-C5	2.97	116.17	112.19
4	F	1	NAG	C2-N2-C7	2.59	126.36	122.90
5	L	1	NAG	C3-C4-C5	2.59	114.92	110.23
3	E	1	NAG	C2-N2-C7	2.54	126.30	122.90
5	L	2	NAG	C2-N2-C7	2.53	126.30	122.90
3	E	4	MAN	O2-C2-C3	-2.33	105.33	110.15
5	G	5	MAN	C1-O5-C5	2.31	115.28	112.19
3	E	2	NAG	C1-O5-C5	2.26	115.21	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C4-C3-C2	2.25	114.32	111.02
5	L	4	MAN	O2-C2-C3	-2.24	105.50	110.15
5	L	5	MAN	O2-C2-C3	-2.17	105.65	110.15
5	G	4	MAN	O2-C2-C3	-2.10	105.80	110.15
4	F	2	NAG	C3-C4-C5	2.07	113.98	110.23
4	F	1	NAG	C3-C4-C5	2.06	113.96	110.23
5	L	1	NAG	O4-C4-C5	-2.02	104.34	109.32
5	L	2	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
5	L	1	NAG	C8-C7-N2-C2
5	L	1	NAG	O7-C7-N2-C2
5	L	4	MAN	O5-C5-C6-O6
5	G	4	MAN	C4-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	L	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
5	L	4	MAN	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
5	L	2	NAG	C1-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
2	J	1	NAG	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6

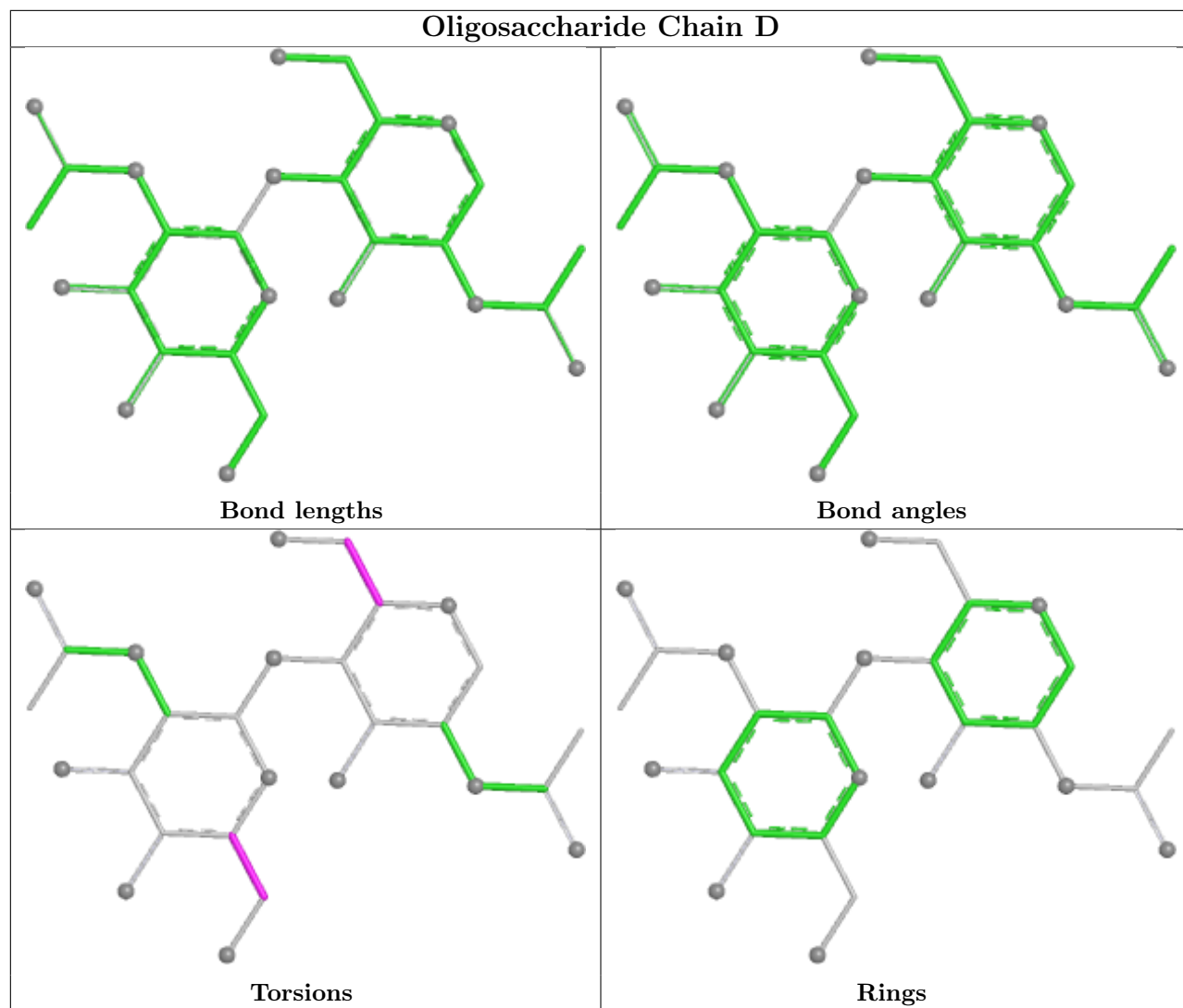
All (2) ring outliers are listed below:

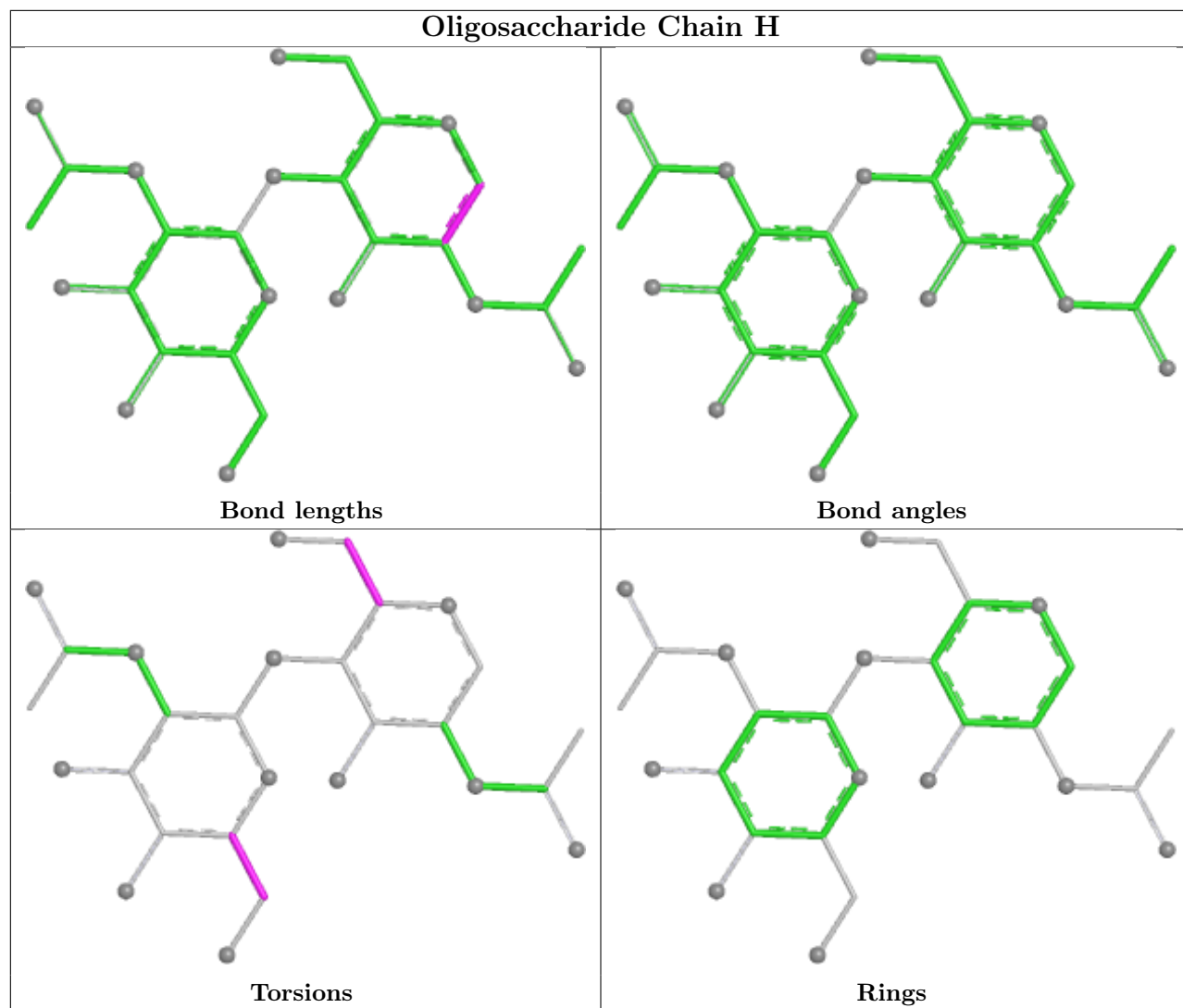
Mol	Chain	Res	Type	Atoms
5	G	4	MAN	C1-C2-C3-C4-C5-O5
5	L	4	MAN	C1-C2-C3-C4-C5-O5

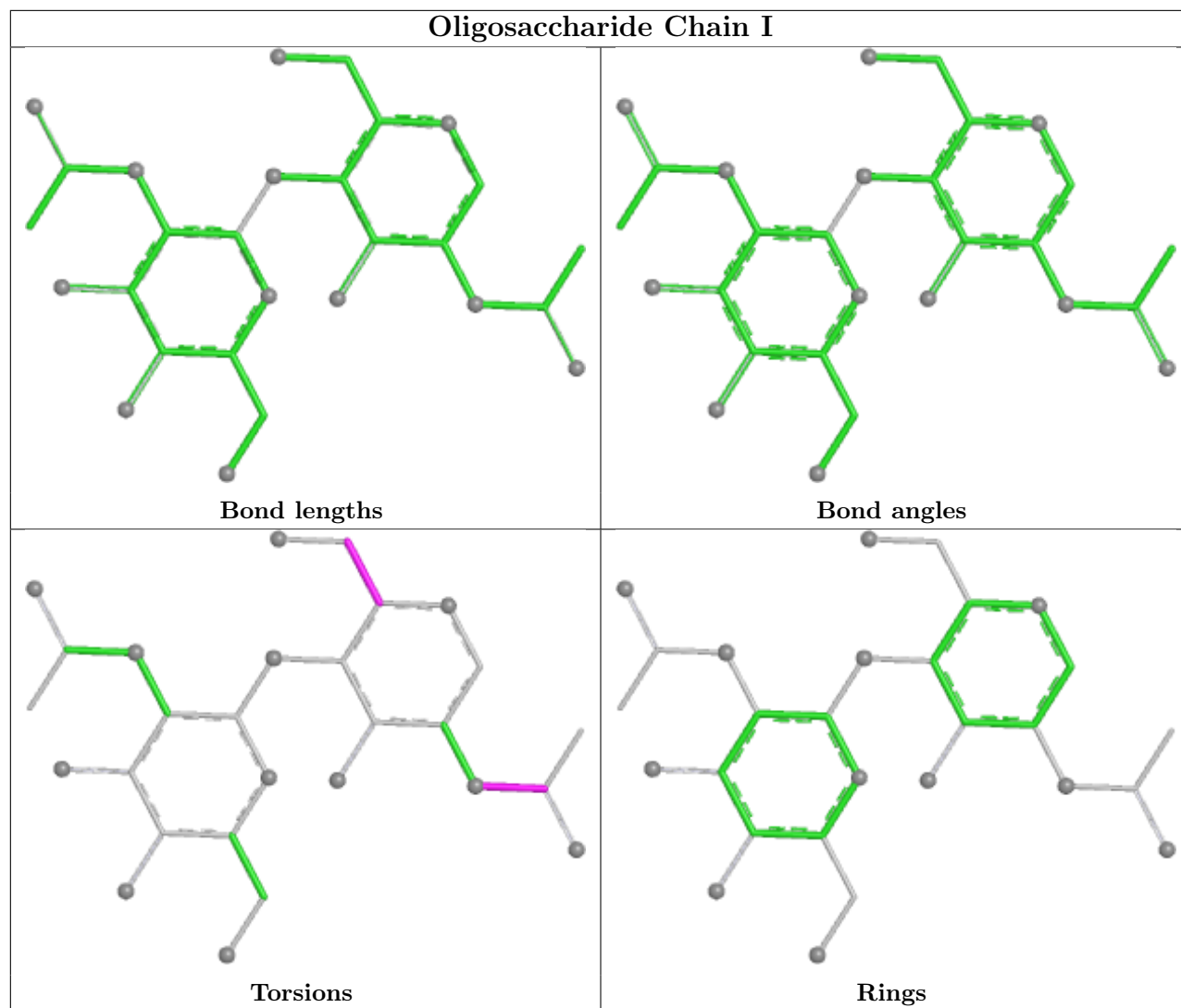
4 monomers are involved in 4 short contacts:

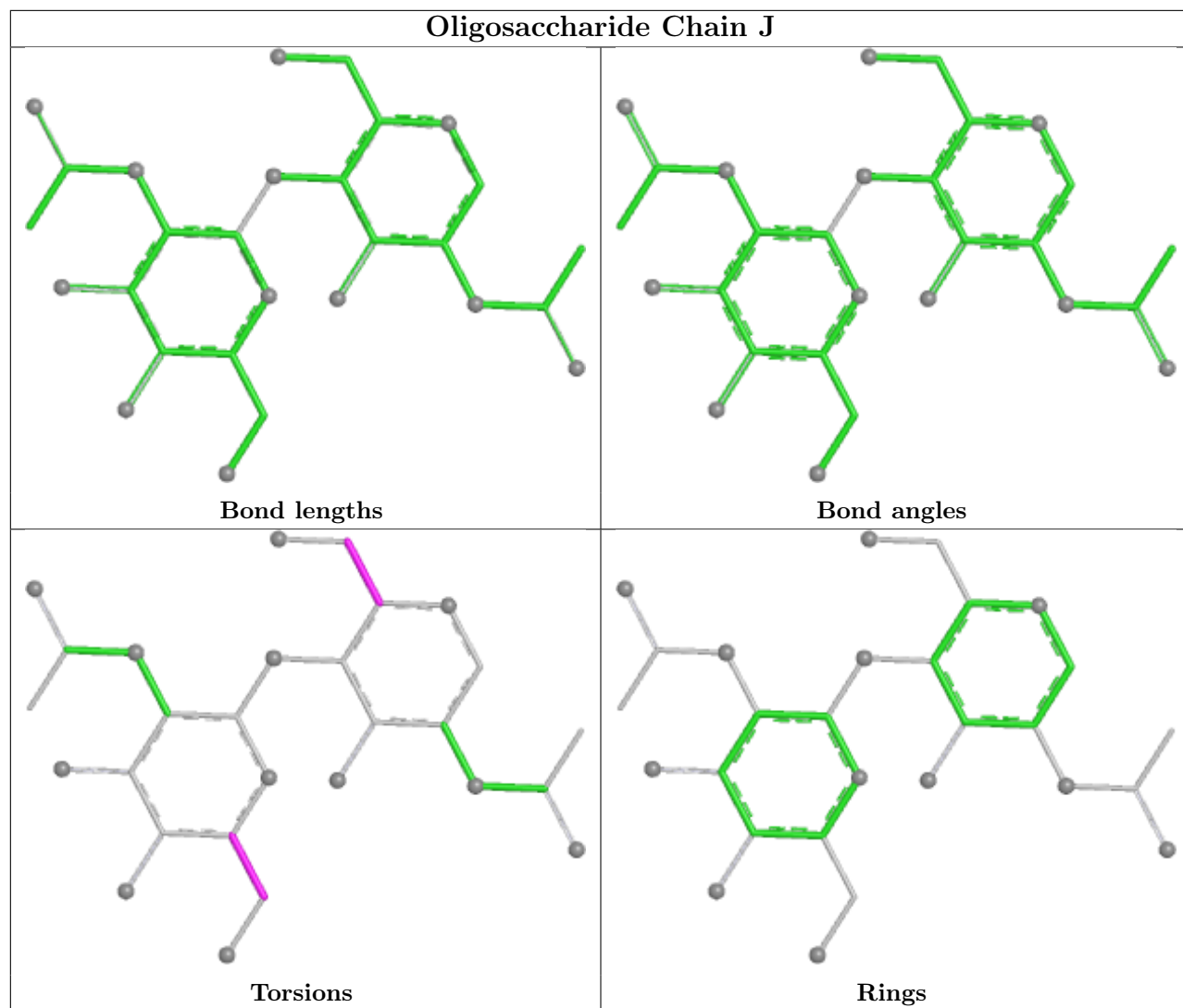
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	1	0
5	G	4	MAN	1	0
3	E	1	NAG	1	0
4	F	1	NAG	1	0

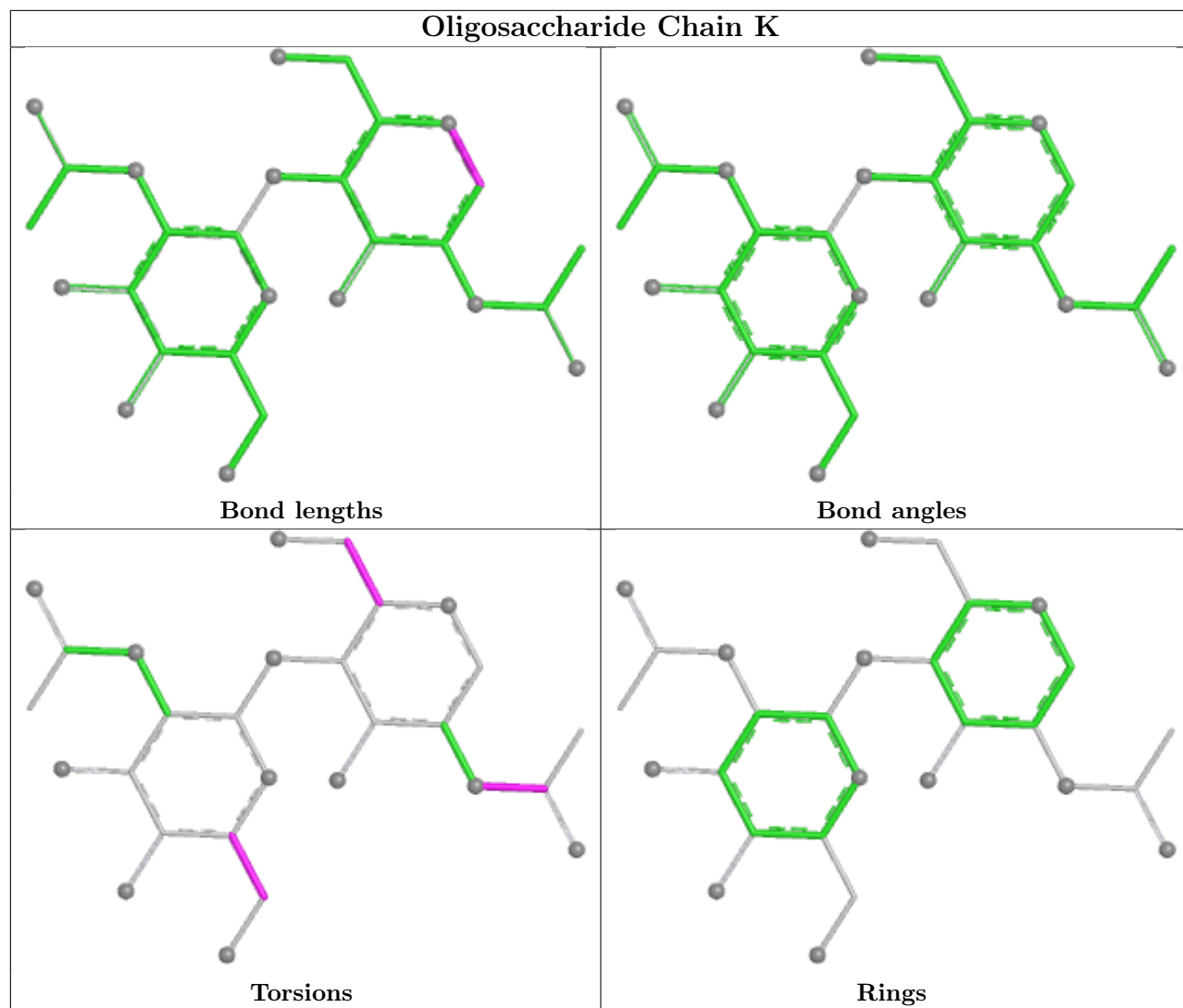
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

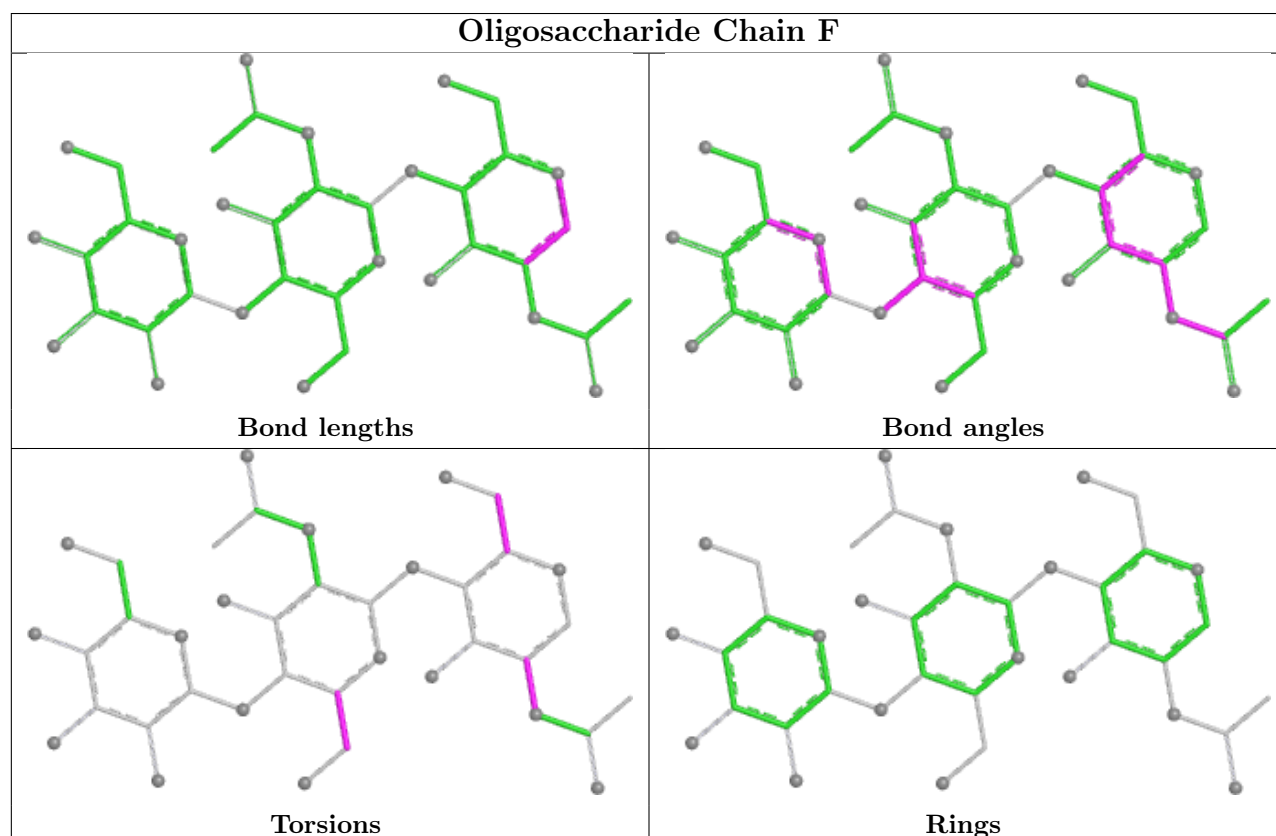
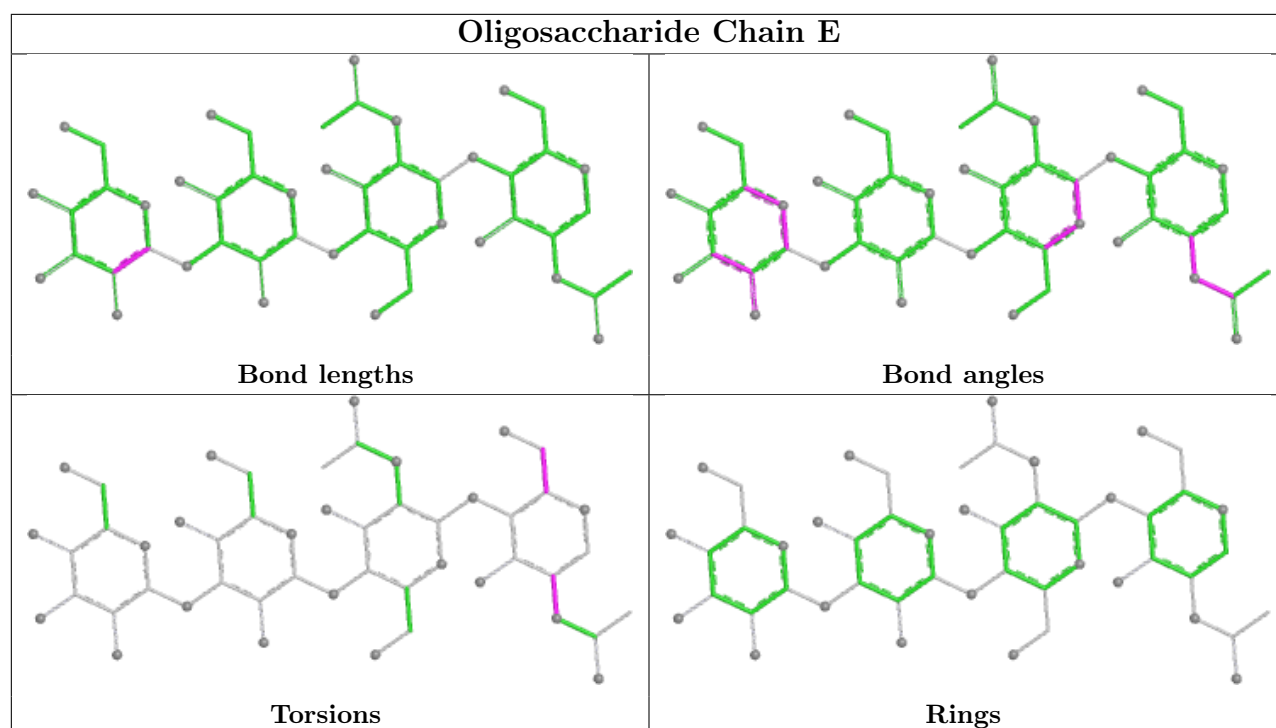


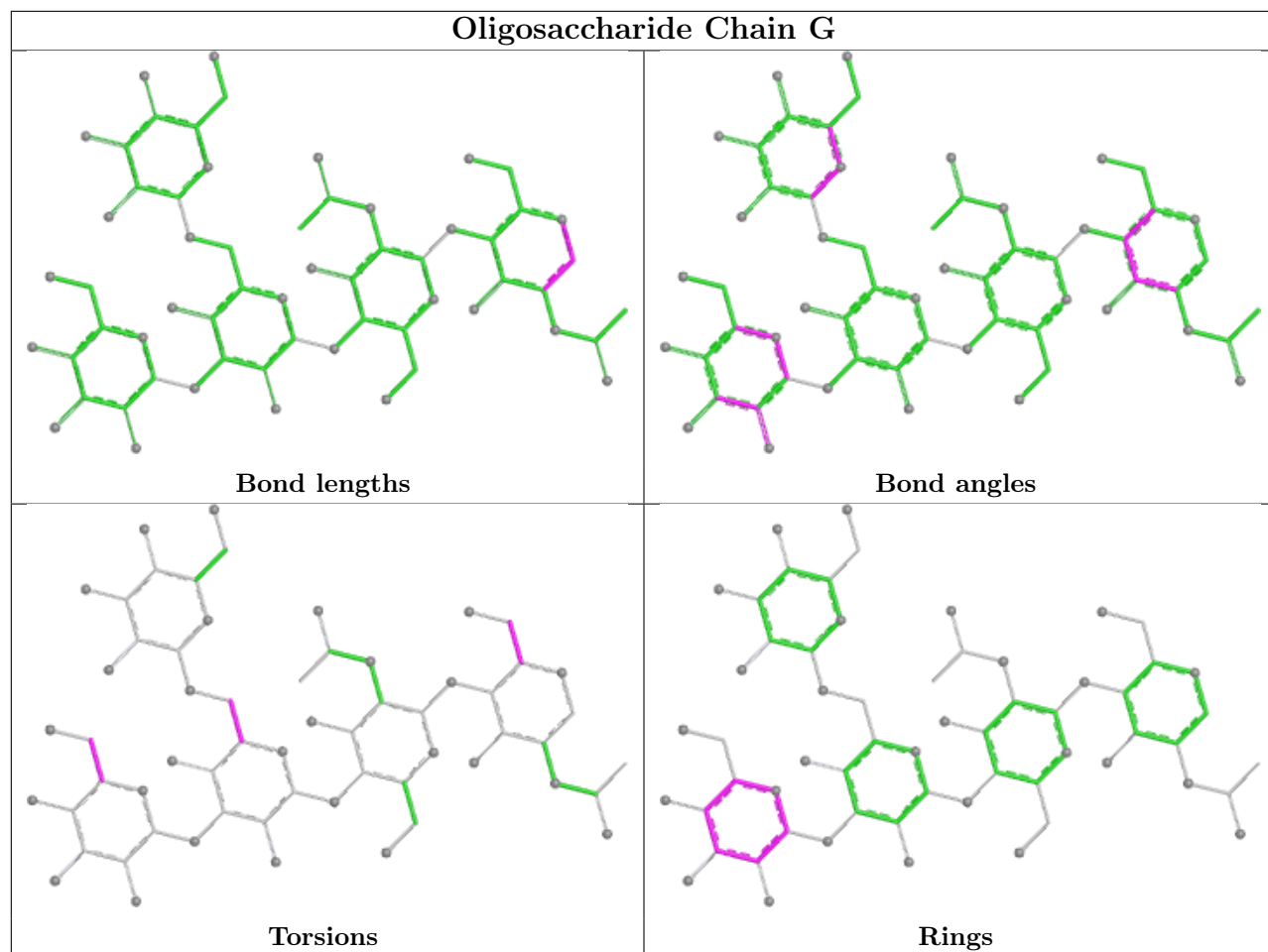


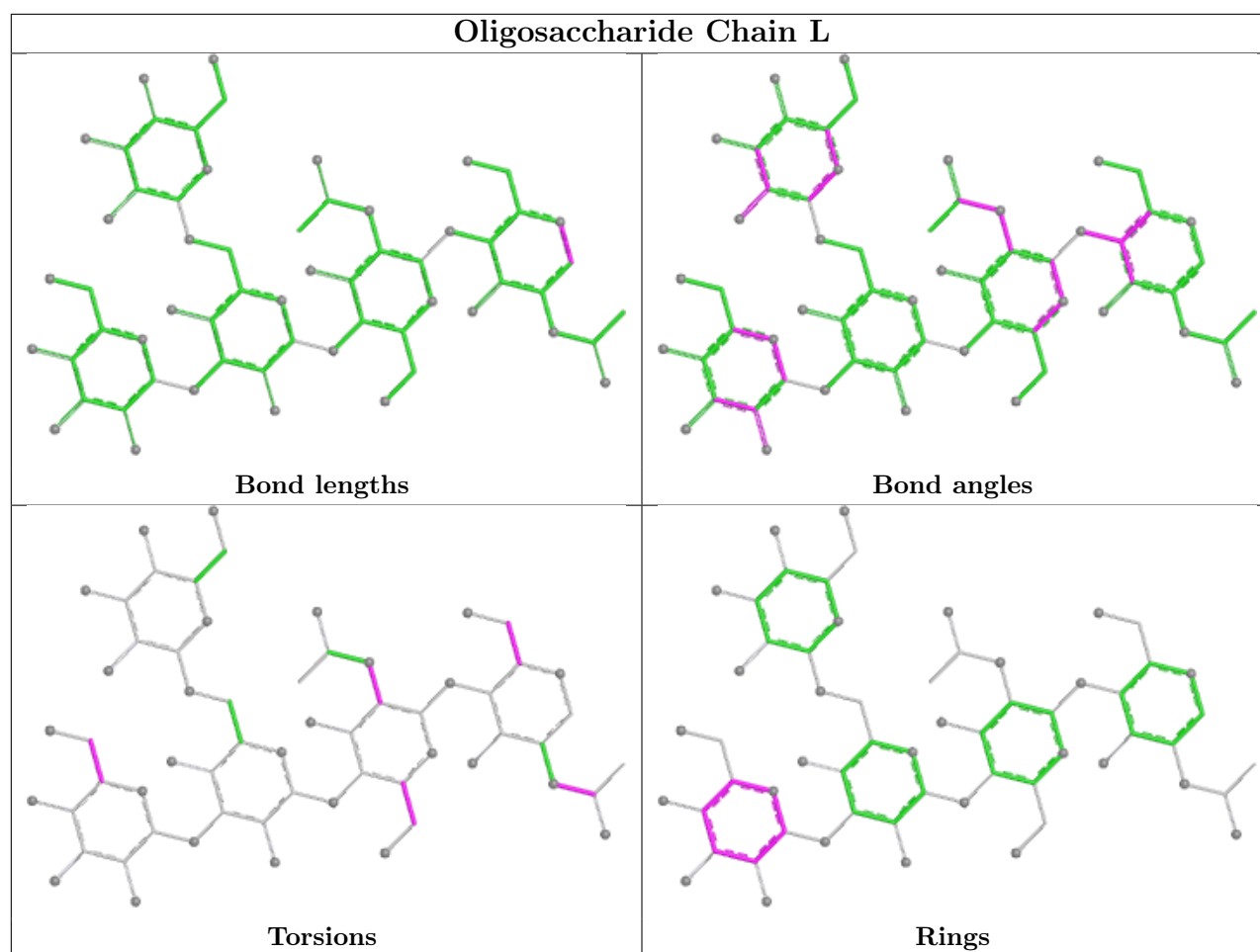












5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
6	NAG	C	1405	1	14,14,15	0.18	0	17,19,21	0.55	0
6	NAG	B	1402	1	14,14,15	0.17	0	17,19,21	0.50	0
6	NAG	A	1402	1	14,14,15	0.38	0	17,19,21	0.52	0
6	NAG	C	1401	1	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	C	1406	1	14,14,15	0.18	0	17,19,21	0.41	0
6	NAG	A	1404	1	14,14,15	0.21	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1403	1	14,14,15	0.31	0	17,19,21	0.53	0
6	NAG	A	1403	1	14,14,15	0.26	0	17,19,21	0.48	0
6	NAG	C	1404	1	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	C	1403	1	14,14,15	0.90	2 (14%)	17,19,21	1.05	2 (11%)
6	NAG	A	1407	1	14,14,15	0.43	0	17,19,21	0.70	1 (5%)
6	NAG	A	1401	1	14,14,15	0.37	0	17,19,21	0.41	0
6	NAG	B	1405	1	14,14,15	0.35	0	17,19,21	0.41	0
6	NAG	B	1401	1	14,14,15	0.28	0	17,19,21	0.52	0
6	NAG	C	1407	1	14,14,15	0.19	0	17,19,21	0.54	0
6	NAG	A	1405	1	14,14,15	0.27	0	17,19,21	0.55	0
6	NAG	B	1404	1	14,14,15	0.39	0	17,19,21	0.43	0
6	NAG	C	1402	1	14,14,15	0.34	0	17,19,21	0.40	0
6	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.47	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
6	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1403	NAG	O5-C1	2.33	1.47	1.43
6	C	1403	NAG	C1-C2	2.31	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1403	NAG	C2-N2-C7	3.03	126.96	122.90
6	A	1407	NAG	C1-O5-C5	2.30	115.27	112.19
6	C	1403	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1403	NAG	C4-C5-C6-O6
6	A	1406	NAG	C4-C5-C6-O6
6	C	1404	NAG	C4-C5-C6-O6
6	B	1401	NAG	O5-C5-C6-O6
6	C	1405	NAG	O5-C5-C6-O6
6	B	1402	NAG	C4-C5-C6-O6
6	A	1405	NAG	O5-C5-C6-O6
6	C	1407	NAG	O5-C5-C6-O6
6	A	1406	NAG	O5-C5-C6-O6
6	C	1403	NAG	O5-C5-C6-O6
6	C	1404	NAG	O5-C5-C6-O6
6	A	1404	NAG	C4-C5-C6-O6
6	B	1401	NAG	C4-C5-C6-O6
6	A	1401	NAG	O5-C5-C6-O6
6	A	1405	NAG	C4-C5-C6-O6
6	C	1405	NAG	C4-C5-C6-O6
6	C	1407	NAG	C4-C5-C6-O6
6	C	1406	NAG	C8-C7-N2-C2
6	C	1406	NAG	O7-C7-N2-C2
6	B	1402	NAG	O5-C5-C6-O6
6	A	1404	NAG	O5-C5-C6-O6
6	C	1406	NAG	O5-C5-C6-O6
6	C	1402	NAG	C4-C5-C6-O6
6	B	1403	NAG	C4-C5-C6-O6
6	C	1402	NAG	O5-C5-C6-O6
6	A	1401	NAG	C4-C5-C6-O6
6	C	1403	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	B	1403	NAG	O5-C5-C6-O6
6	C	1404	NAG	C1-C2-N2-C7

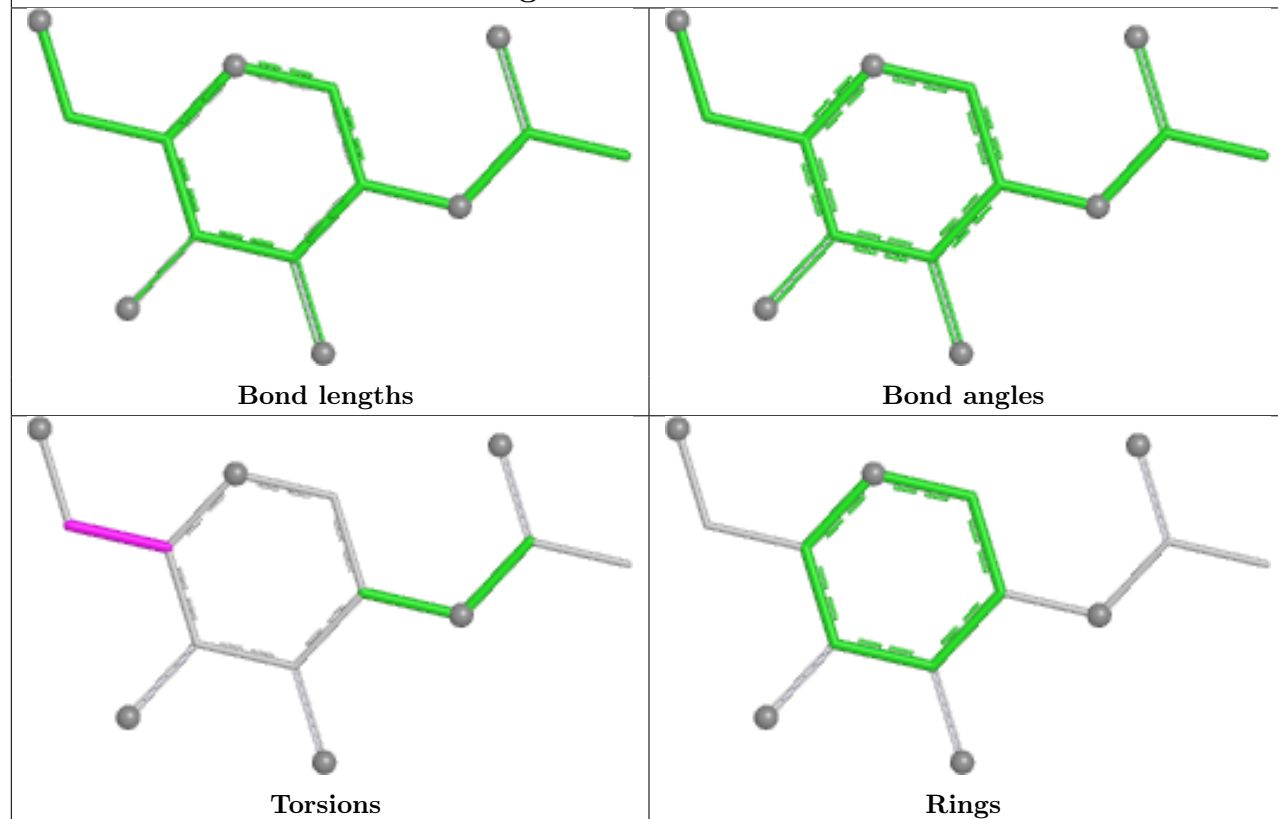
There are no ring outliers.

4 monomers are involved in 5 short contacts:

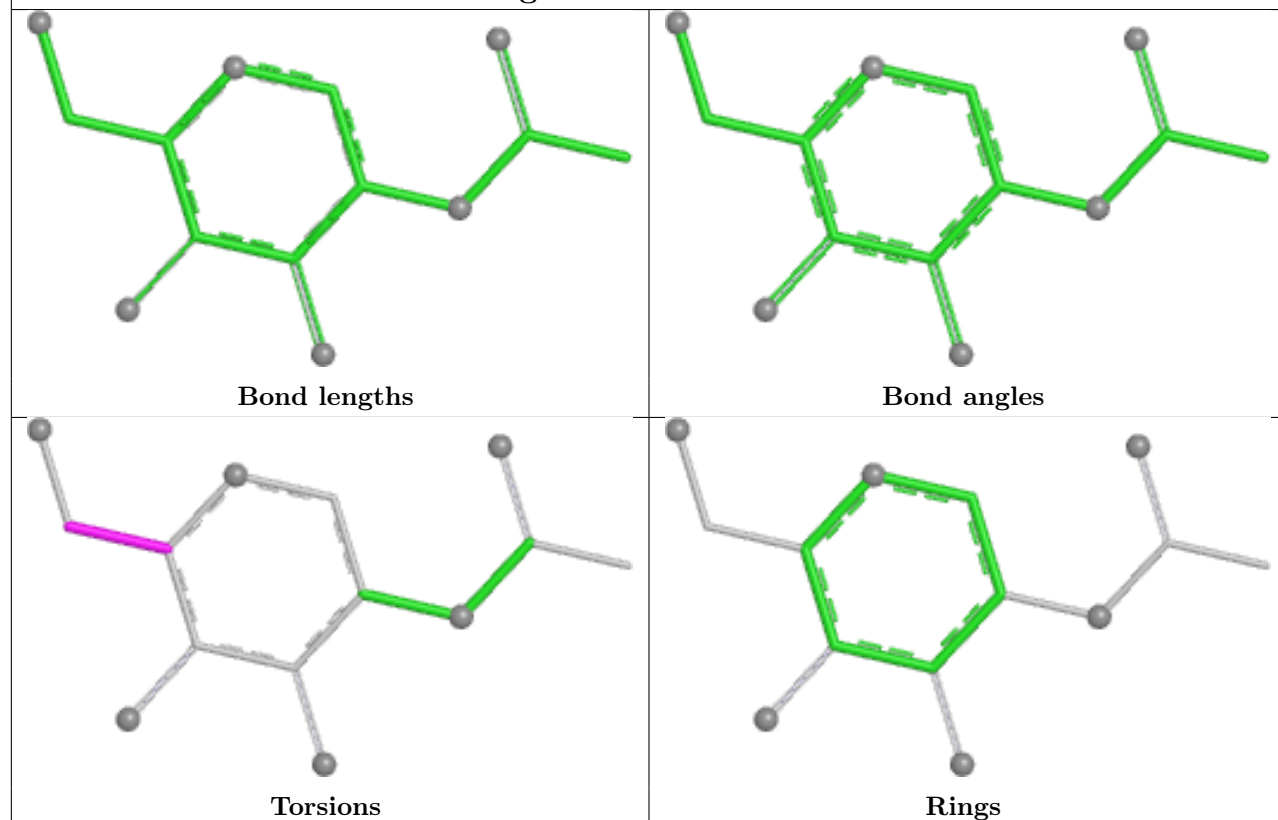
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1404	NAG	1	0
6	A	1407	NAG	1	0
6	A	1401	NAG	1	0
6	C	1402	NAG	2	0

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.

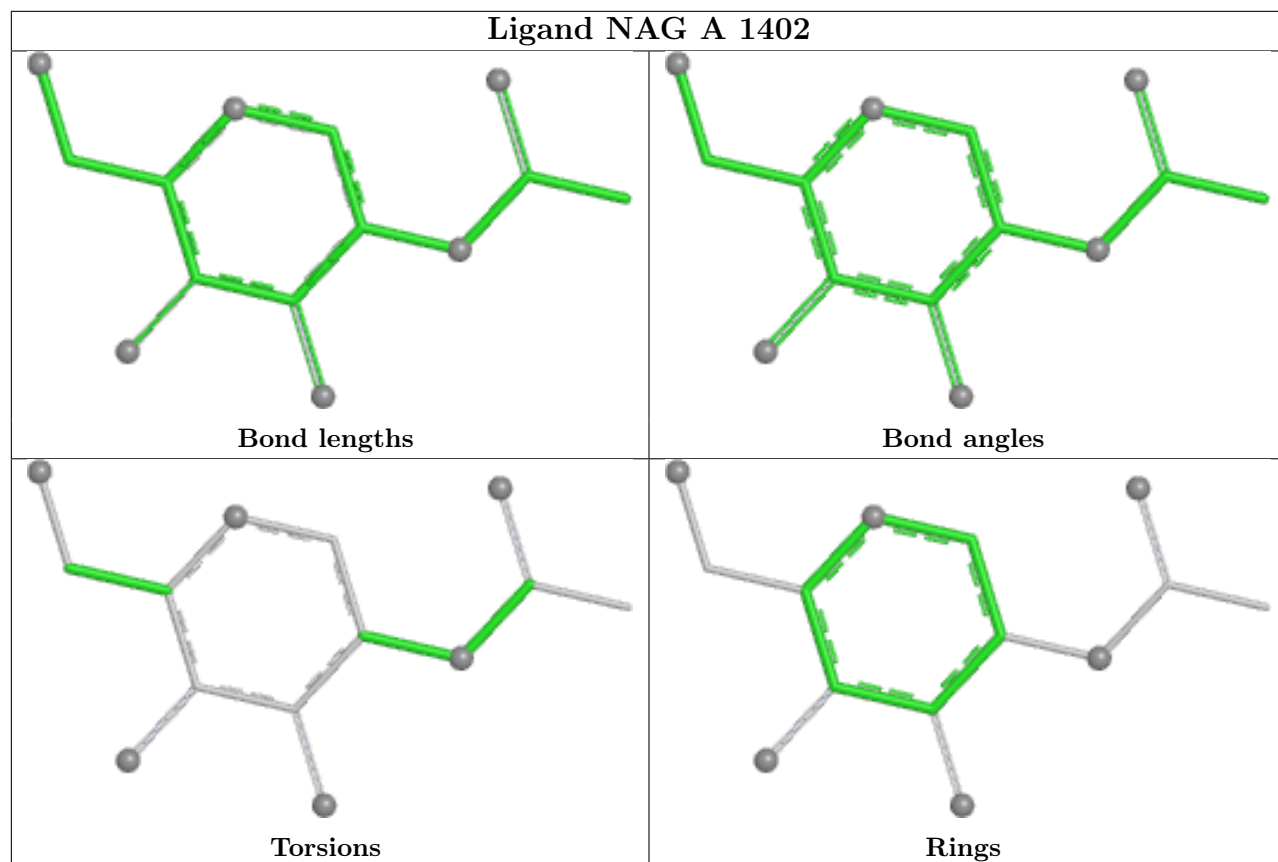
Ligand NAG C 1405



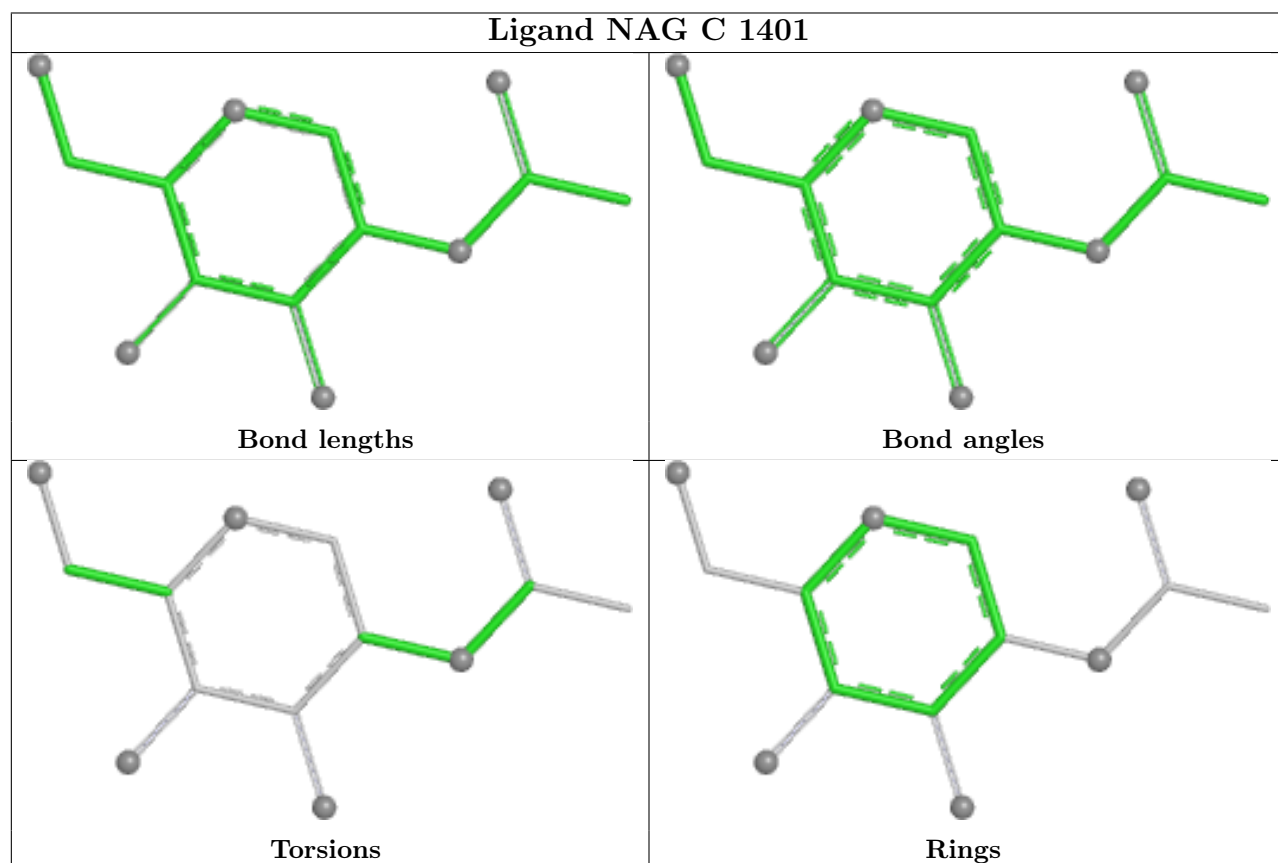
Ligand NAG B 1402



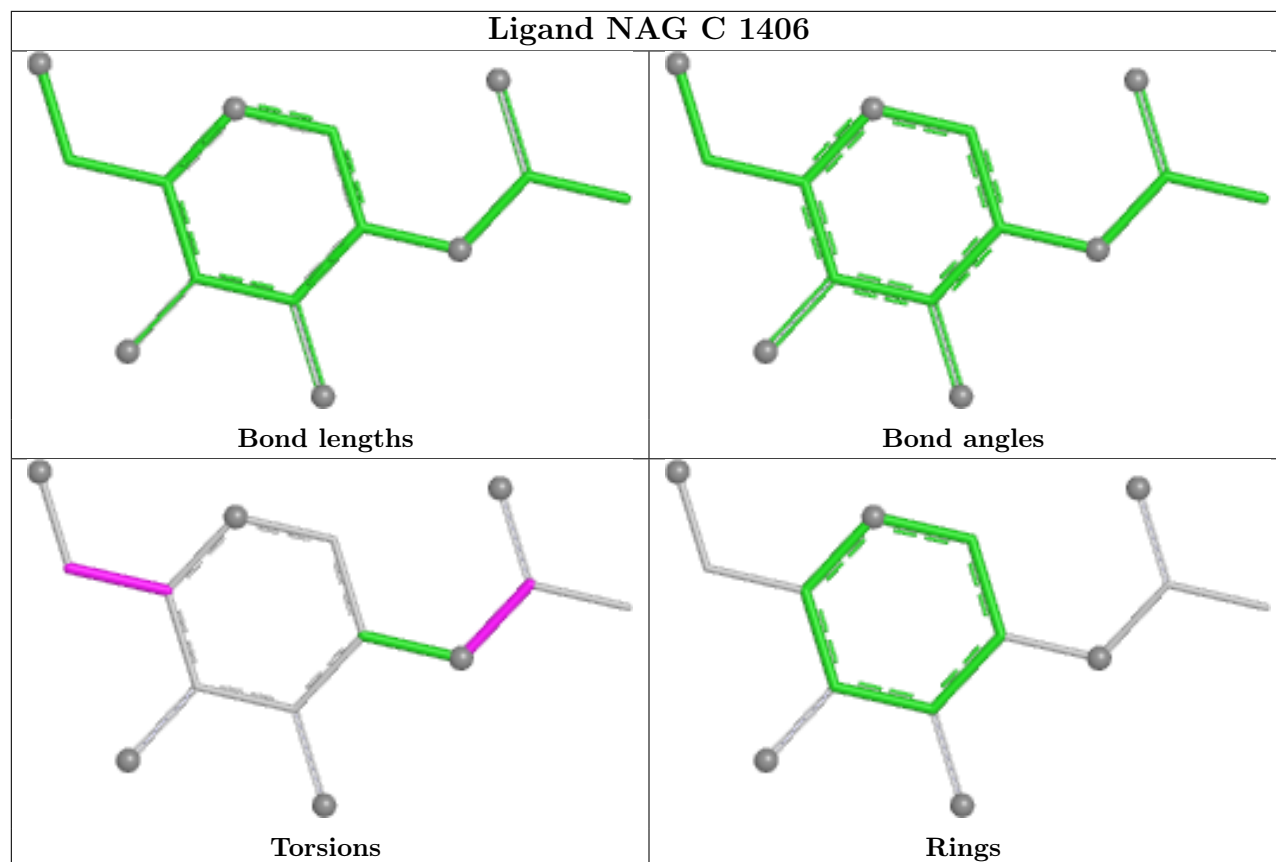
Ligand NAG A 1402



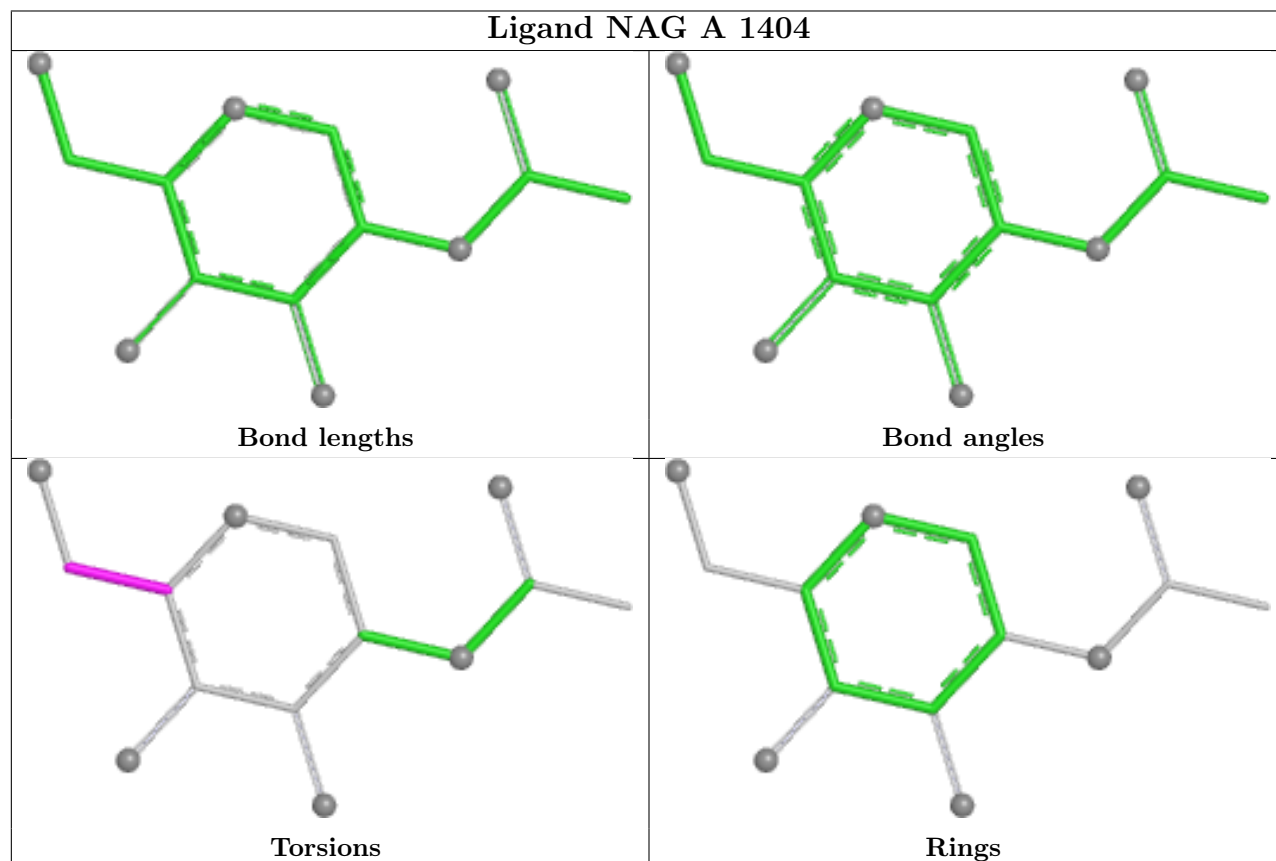
Ligand NAG C 1401



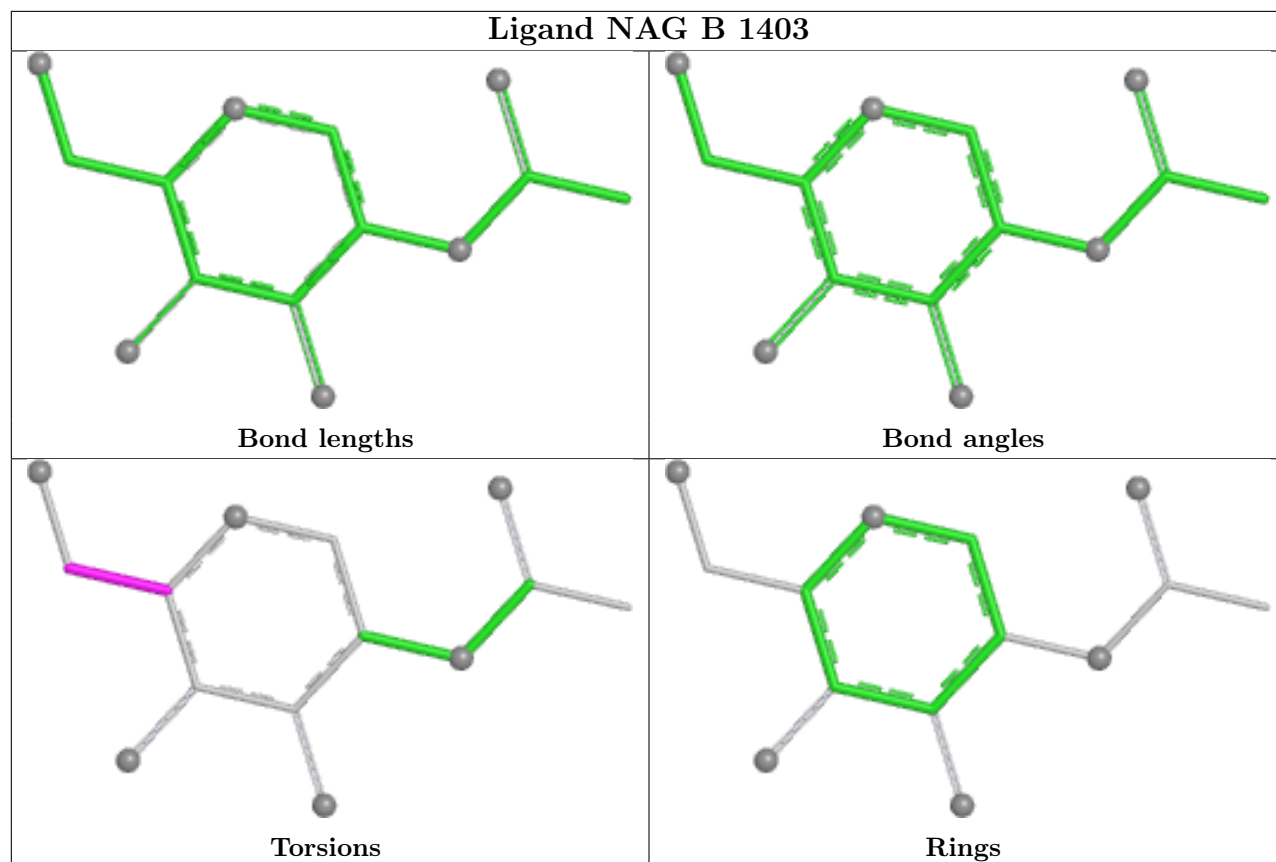
Ligand NAG C 1406



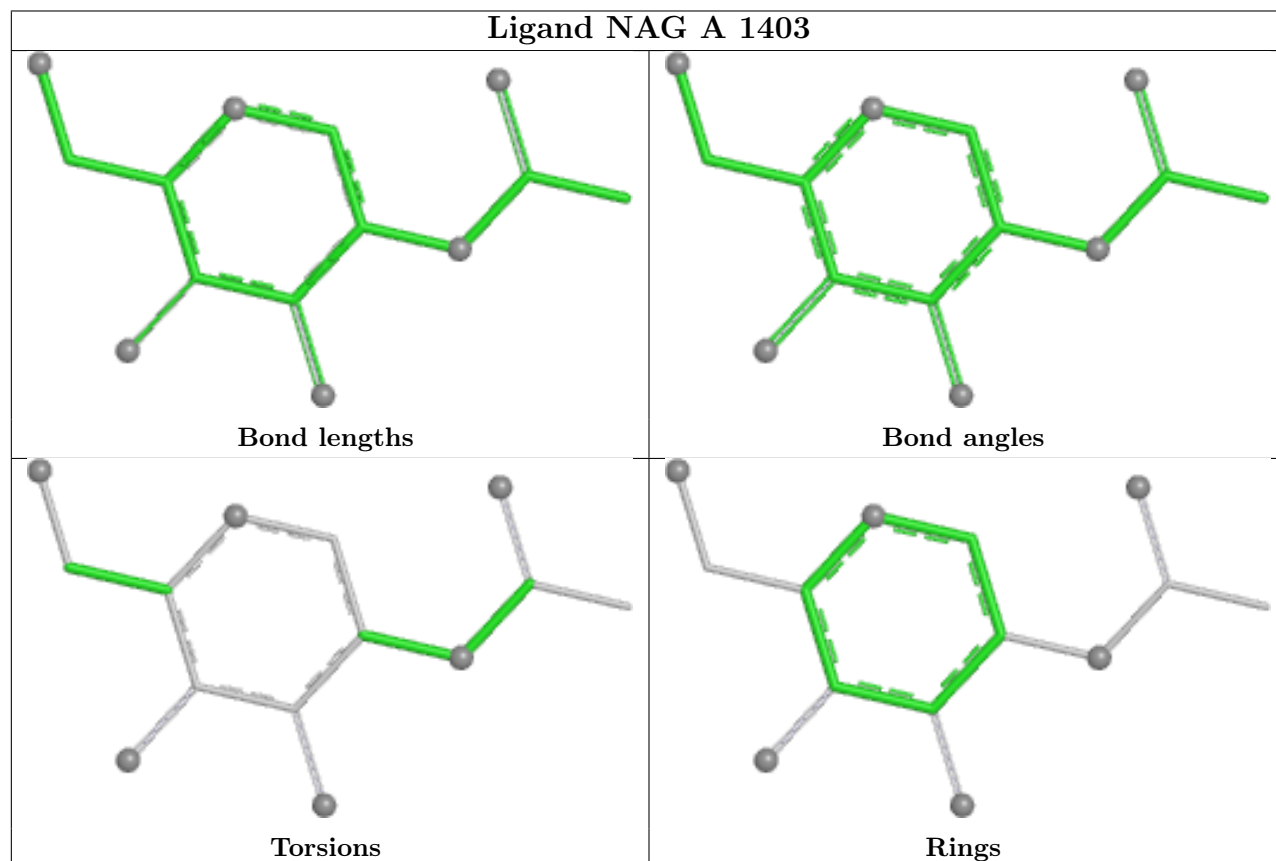
Ligand NAG A 1404

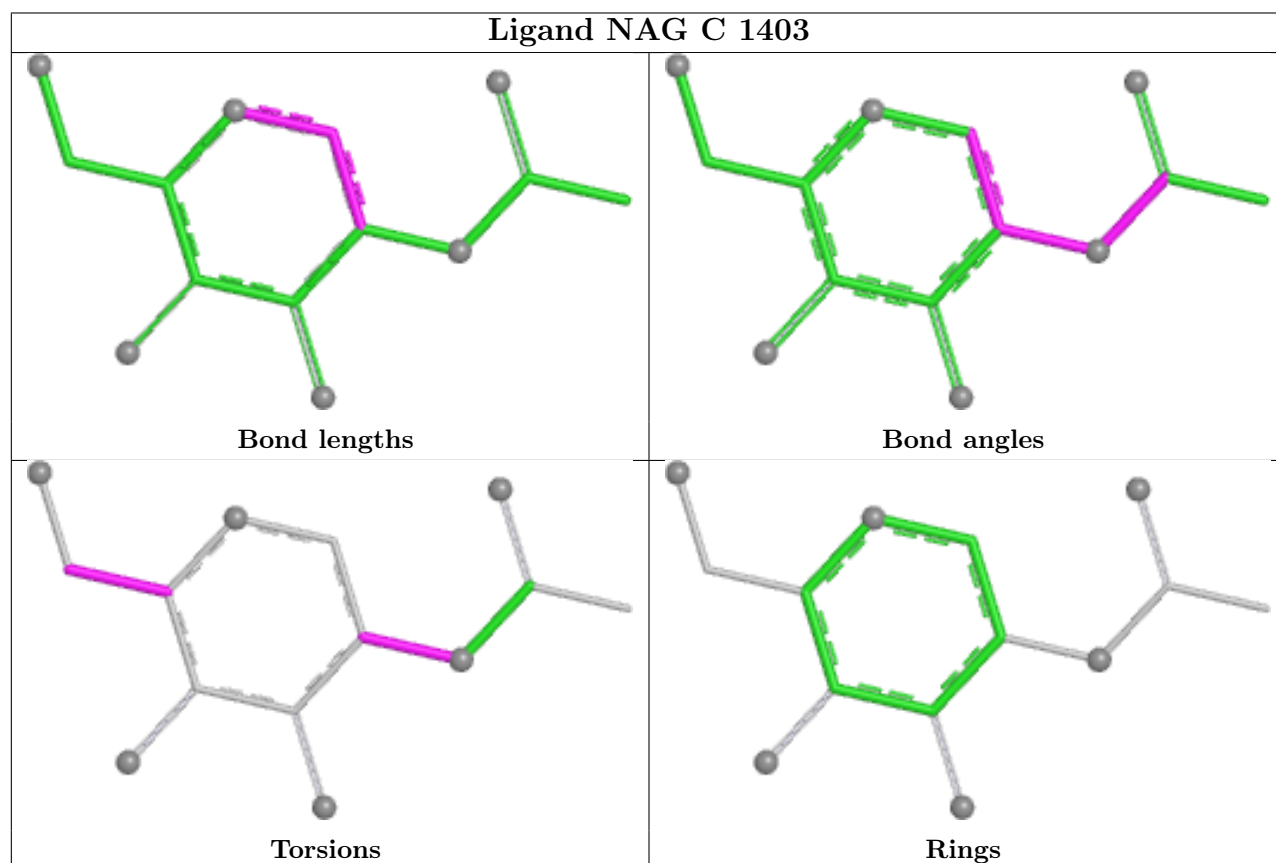
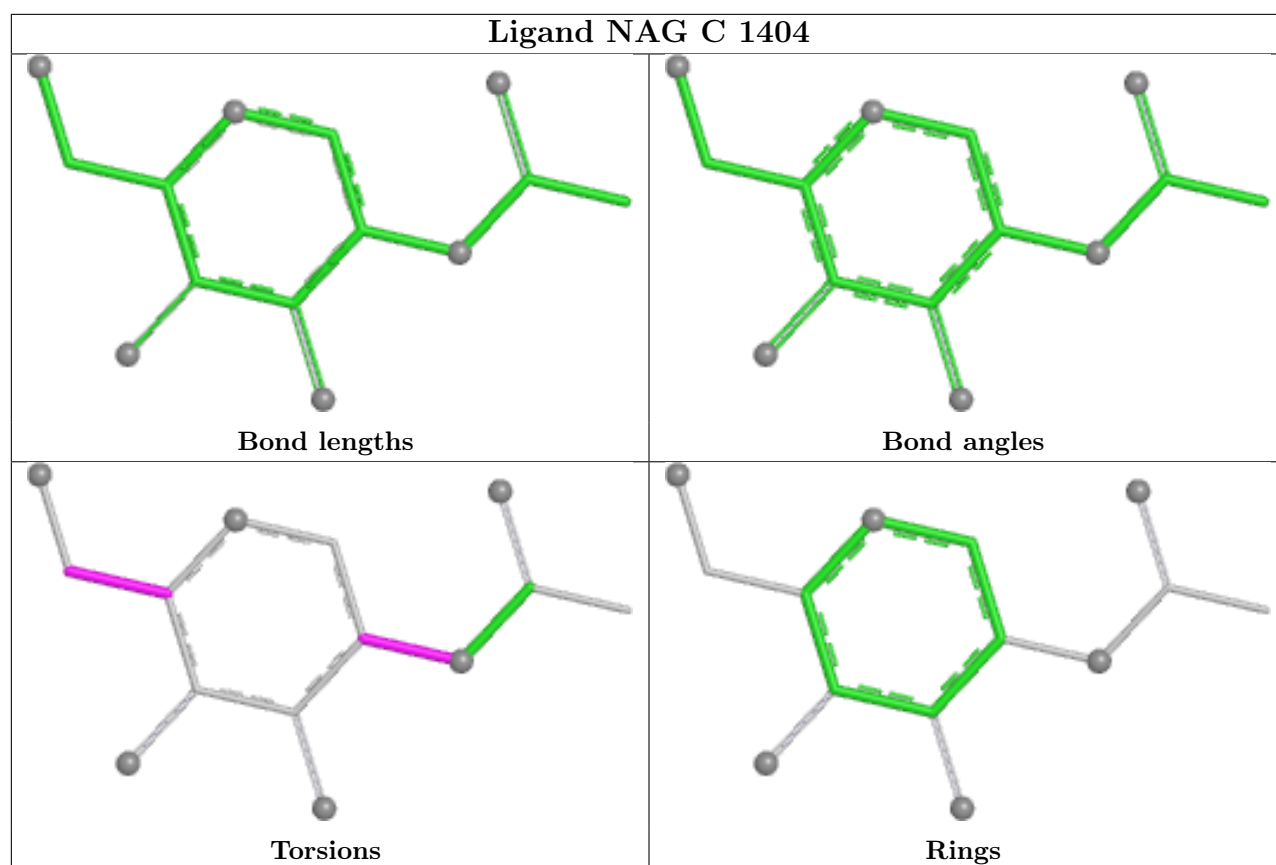


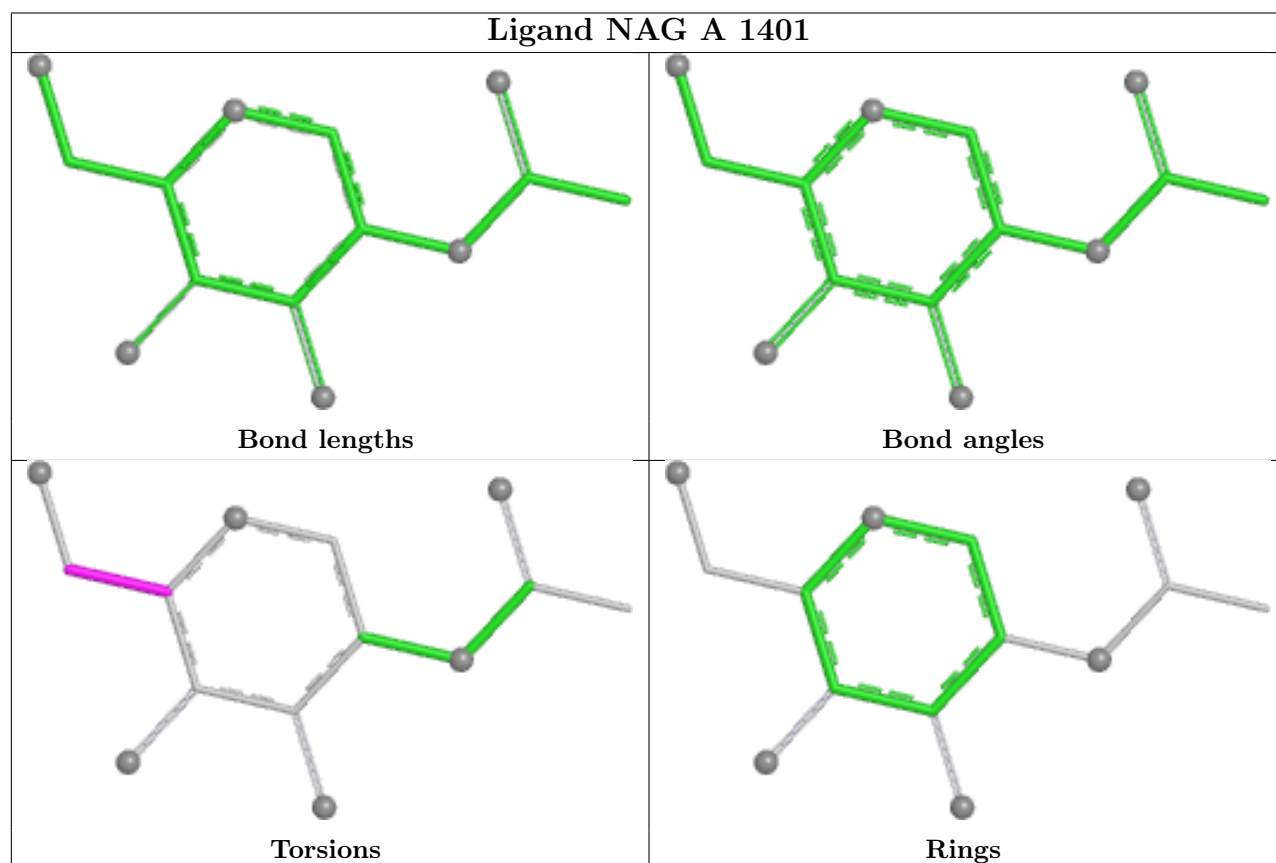
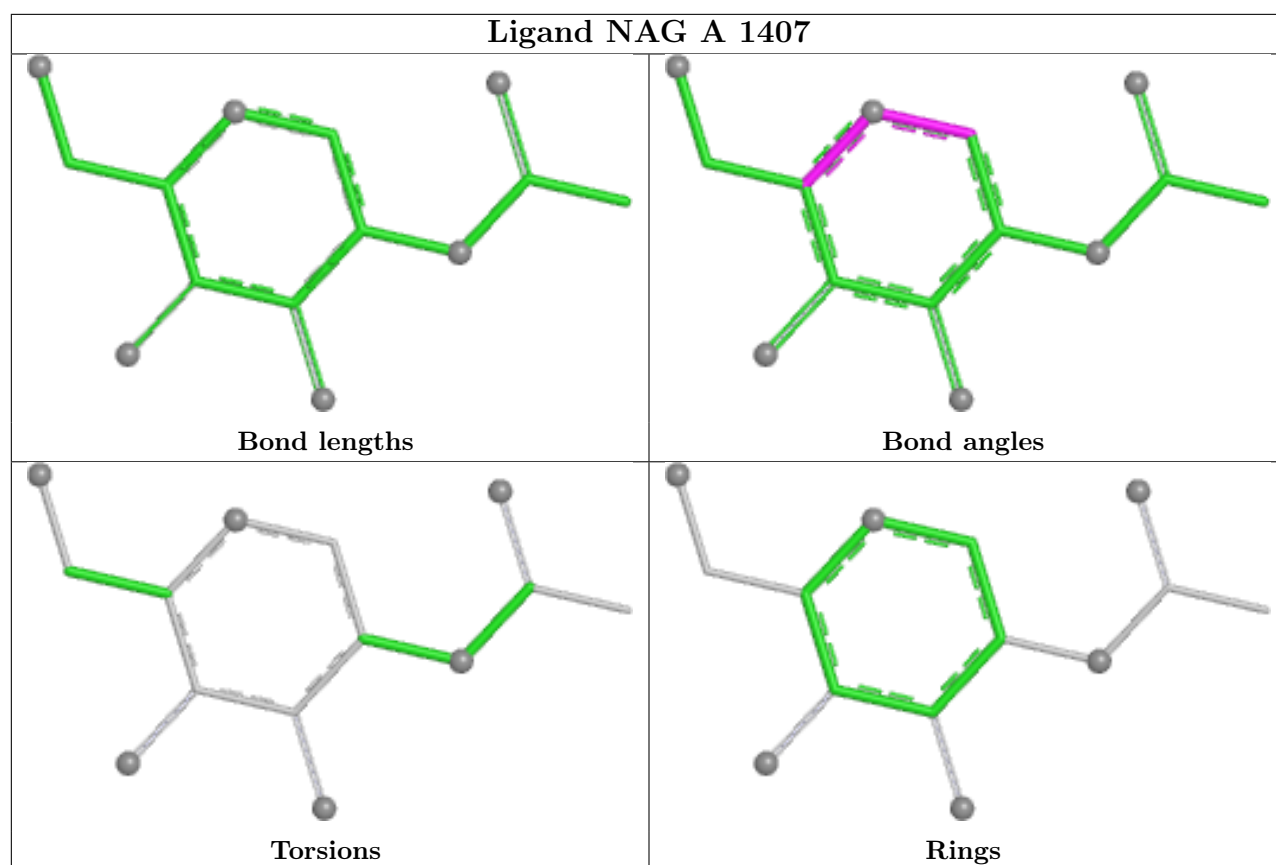
Ligand NAG B 1403

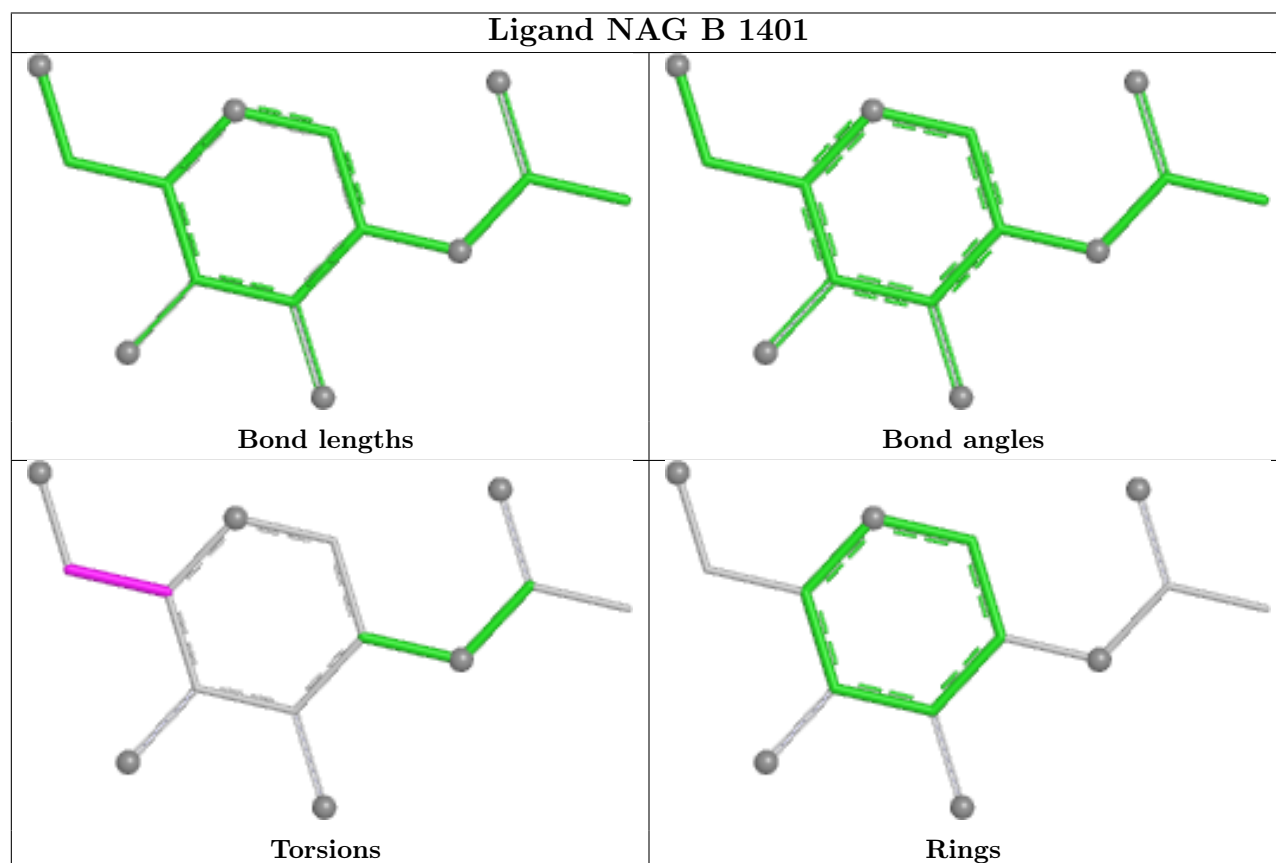
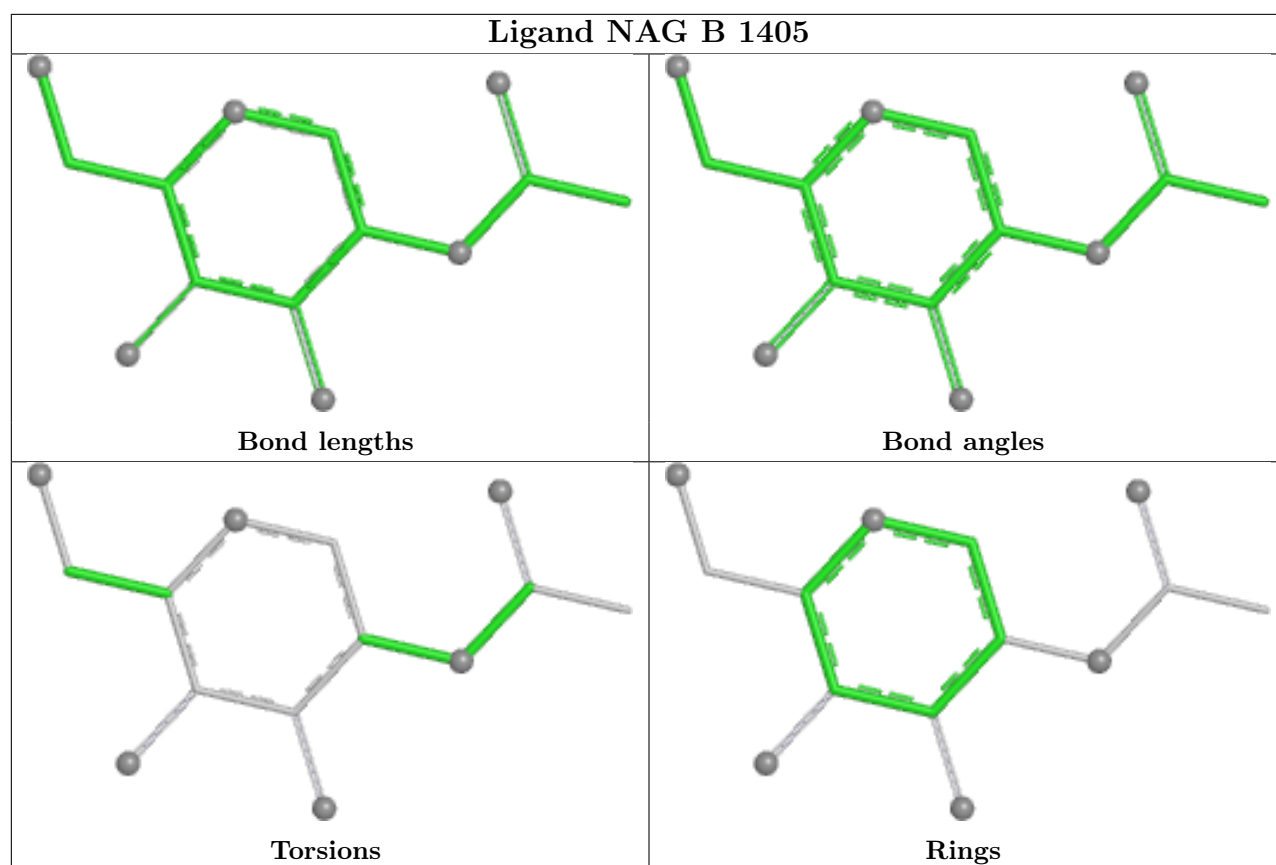


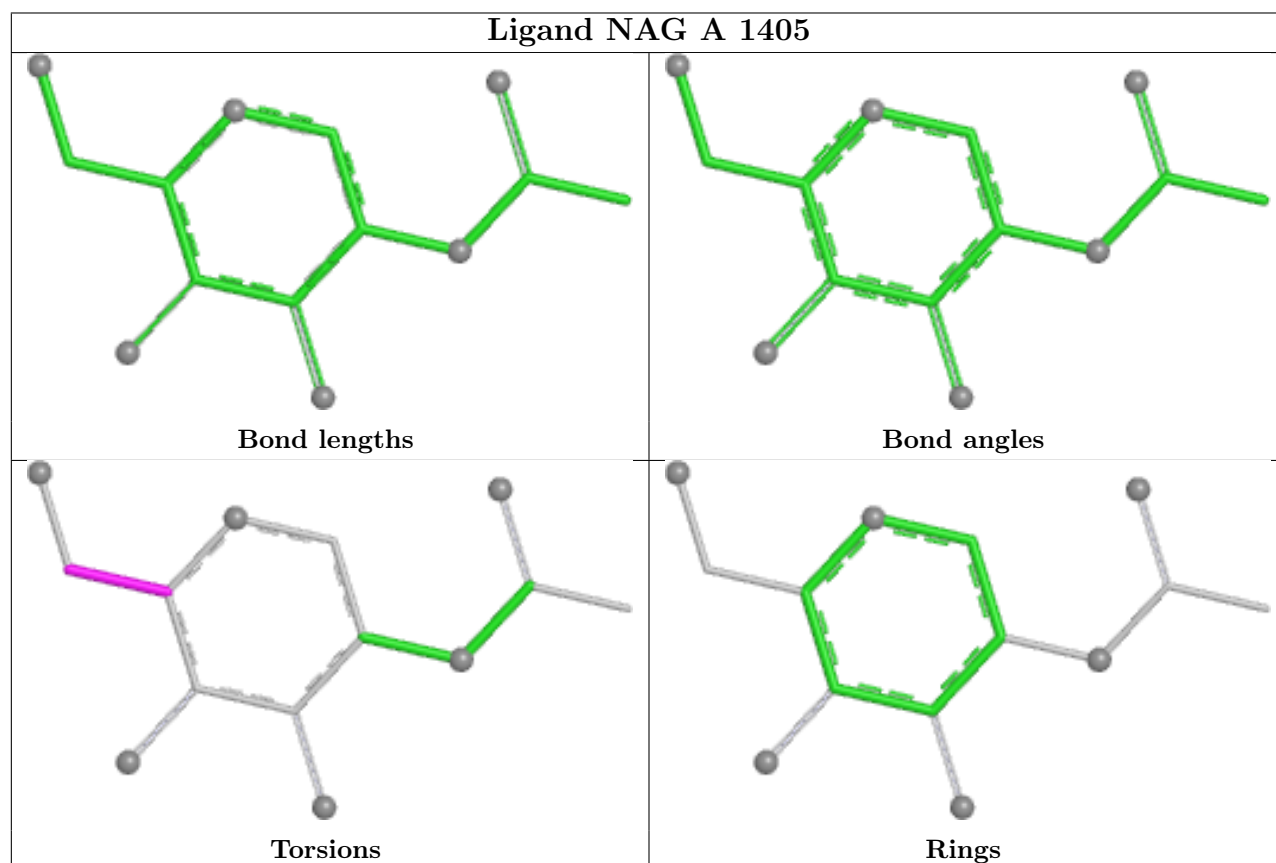
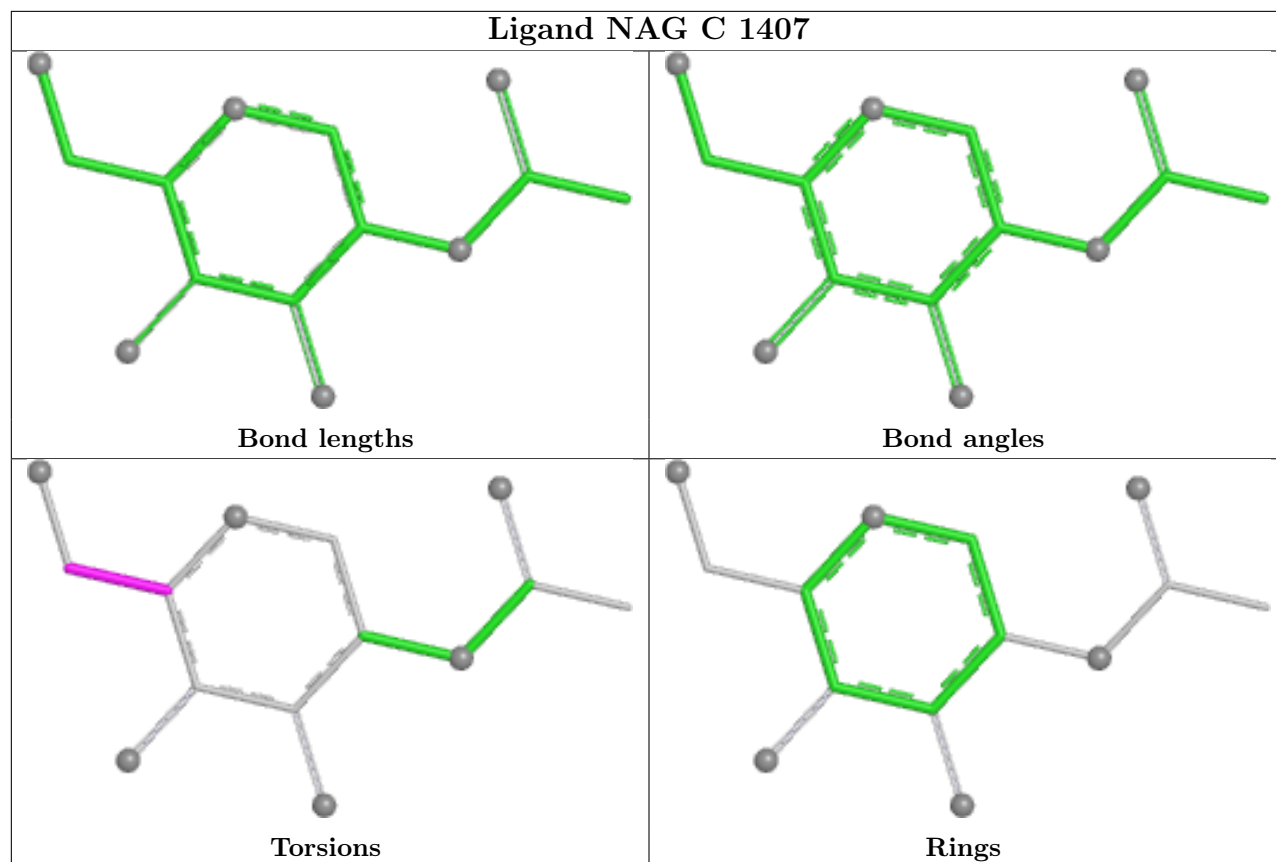
Ligand NAG A 1403

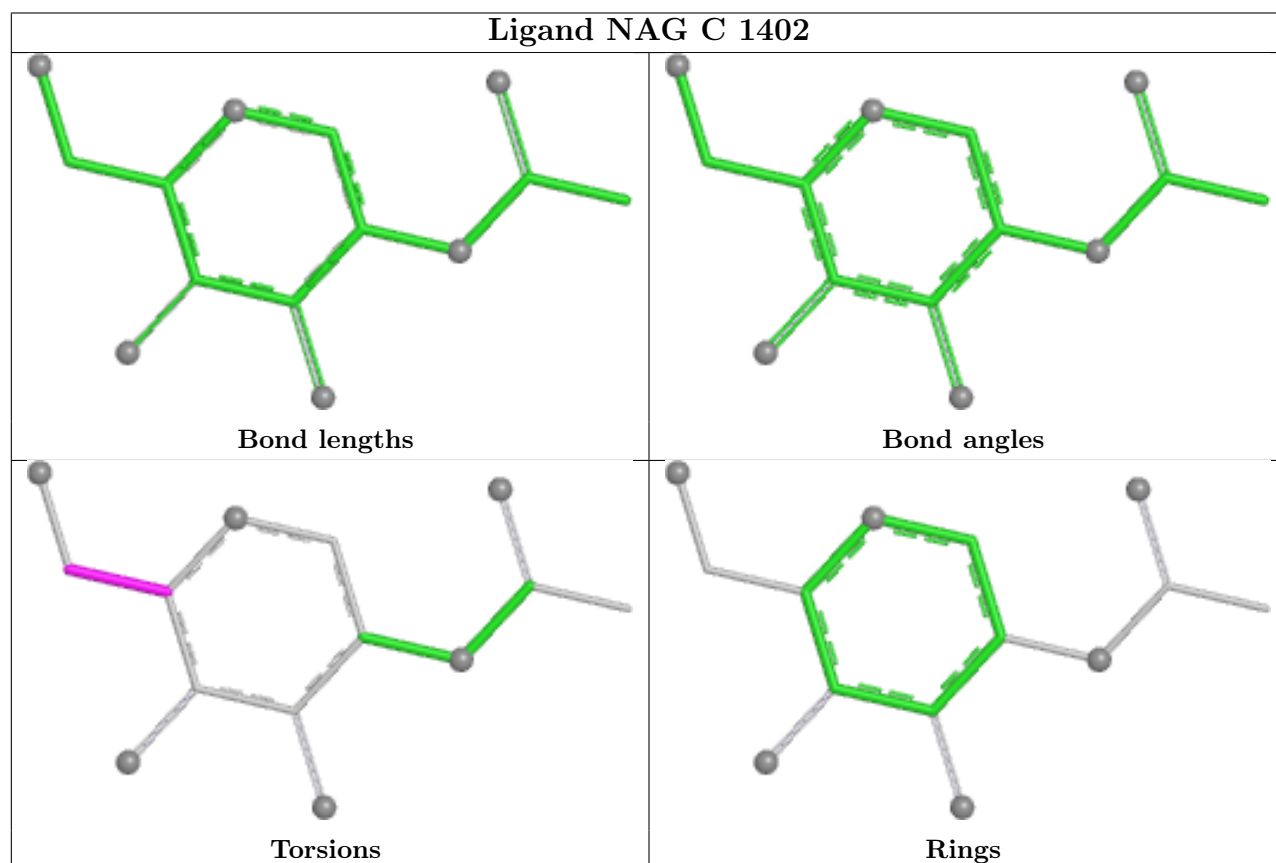
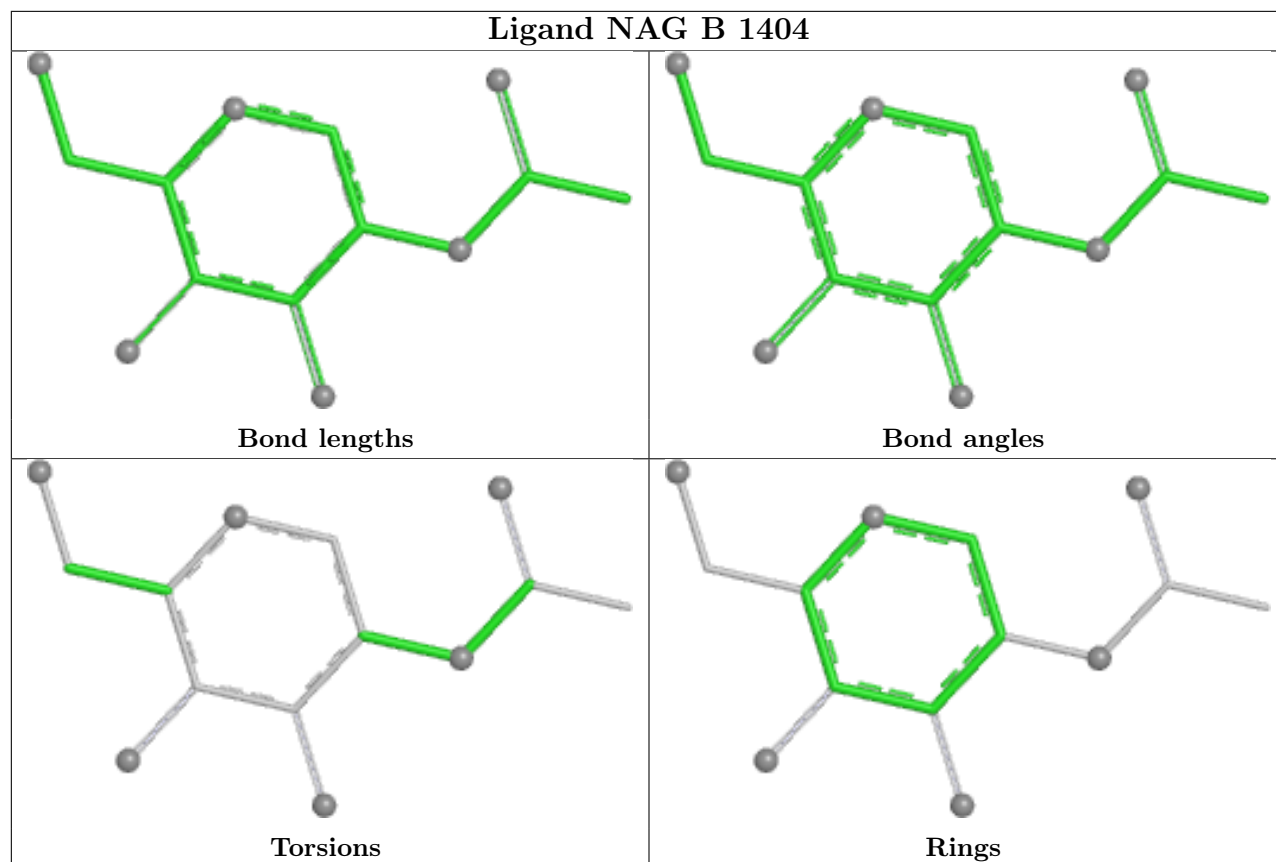


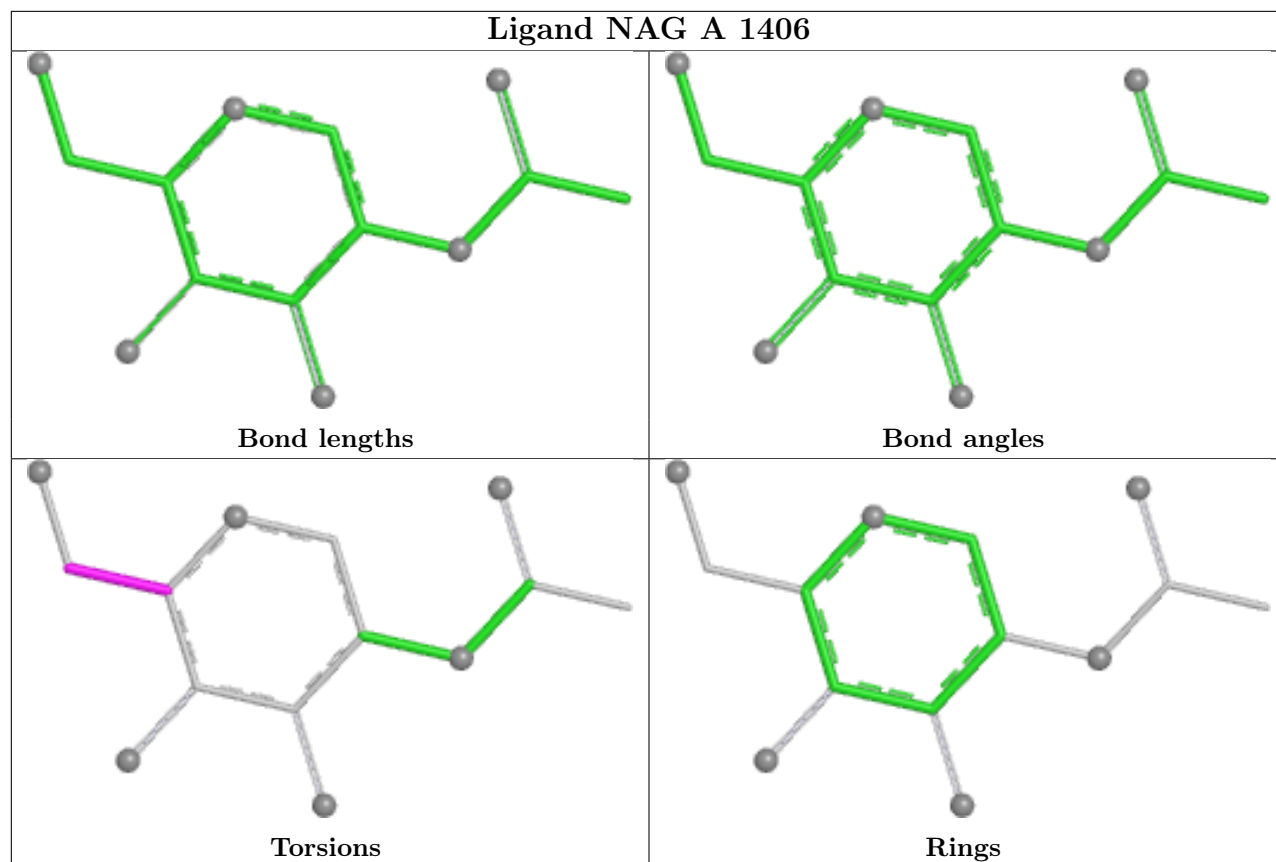












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

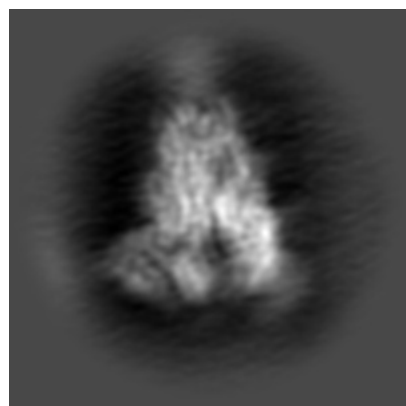
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33947. These allow visual inspection of the internal detail of the map and identification of artifacts.

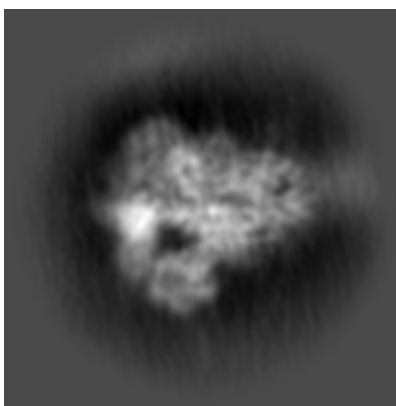
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

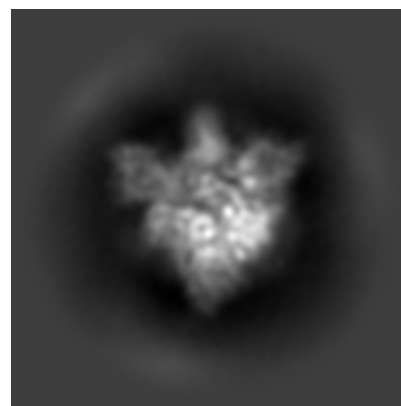
6.1.1 Primary map



X

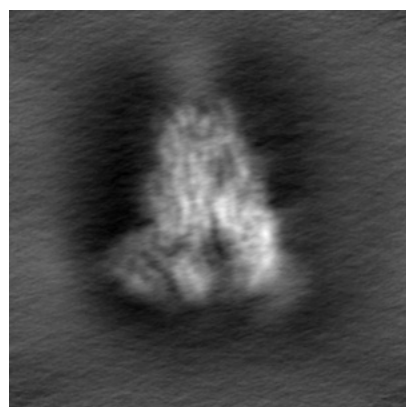


Y

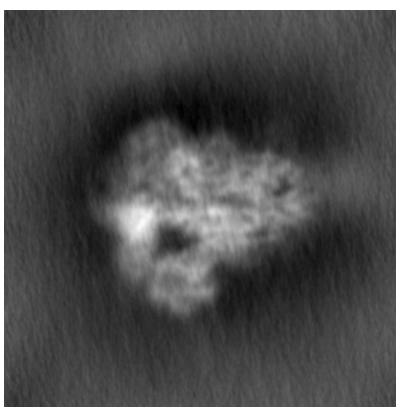


Z

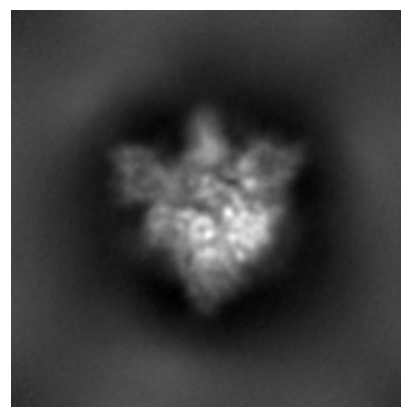
6.1.2 Raw map



X



Y

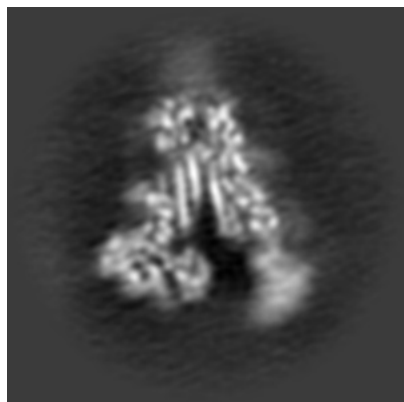


Z

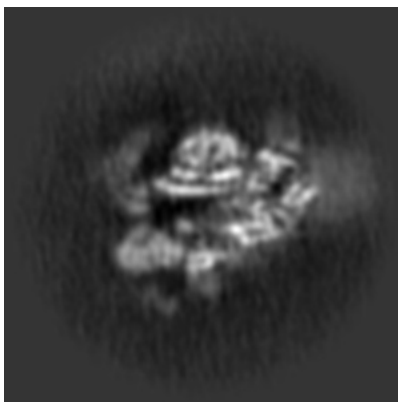
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

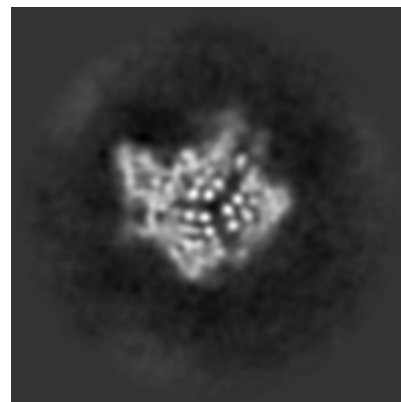
6.2.1 Primary map



X Index: 128

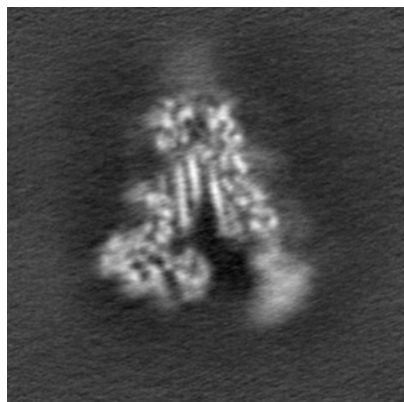


Y Index: 128

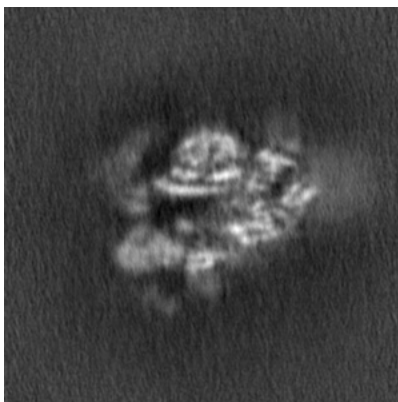


Z Index: 128

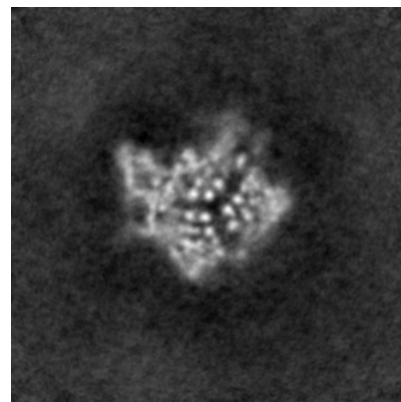
6.2.2 Raw map



X Index: 128



Y Index: 128

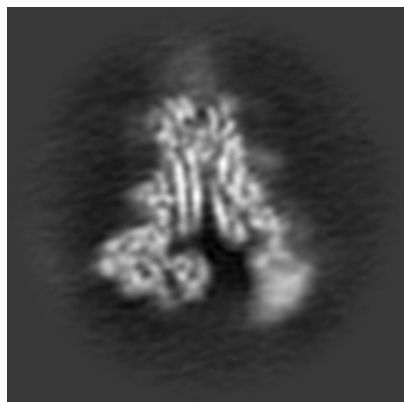


Z Index: 128

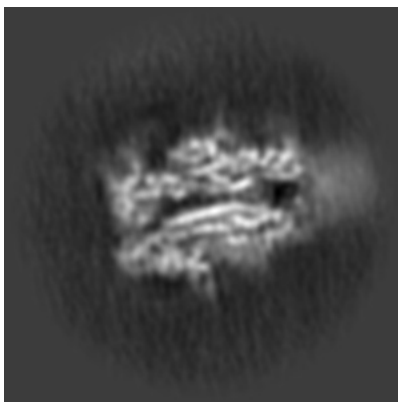
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

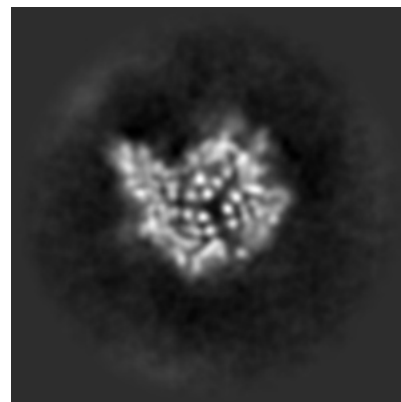
6.3.1 Primary map



X Index: 125

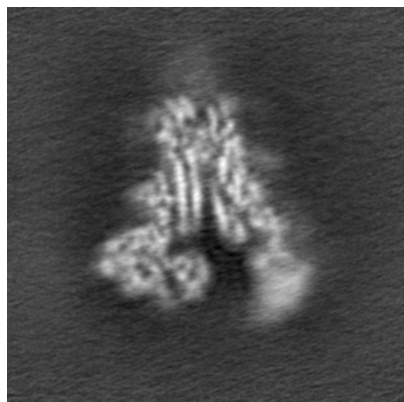


Y Index: 121

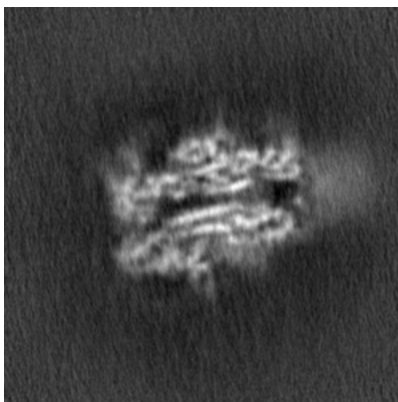


Z Index: 124

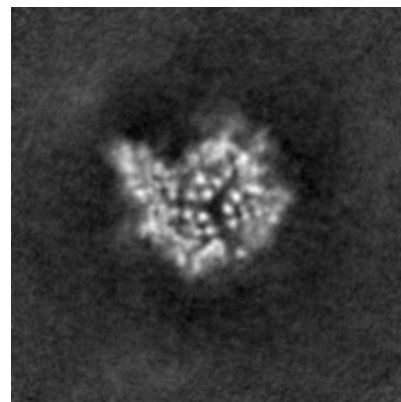
6.3.2 Raw map



X Index: 125



Y Index: 122

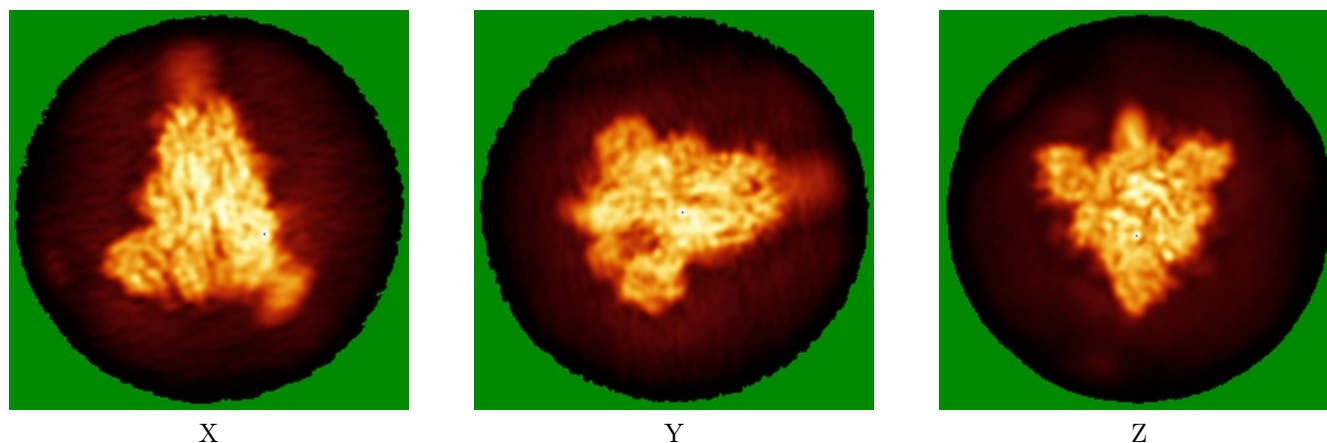


Z Index: 124

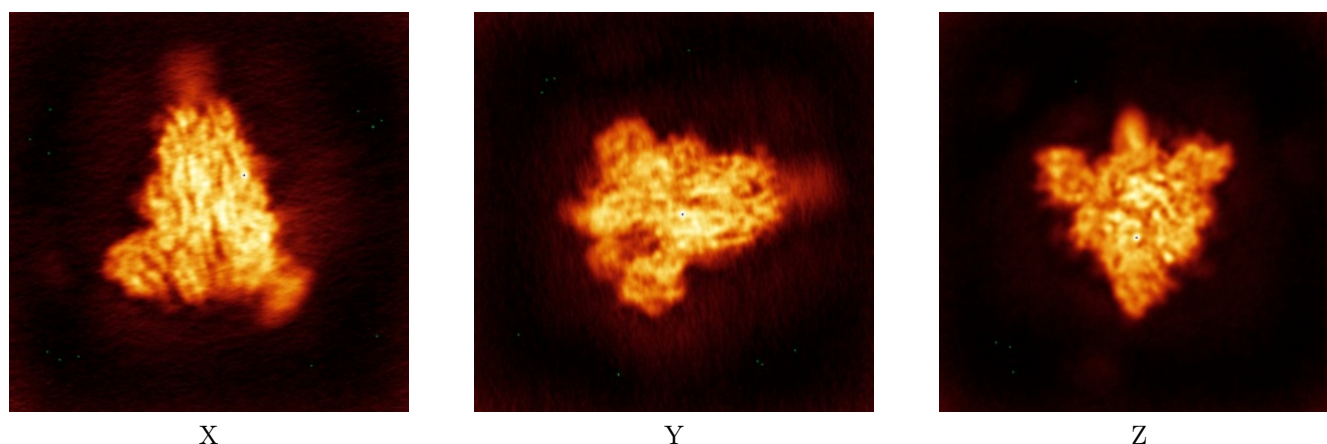
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

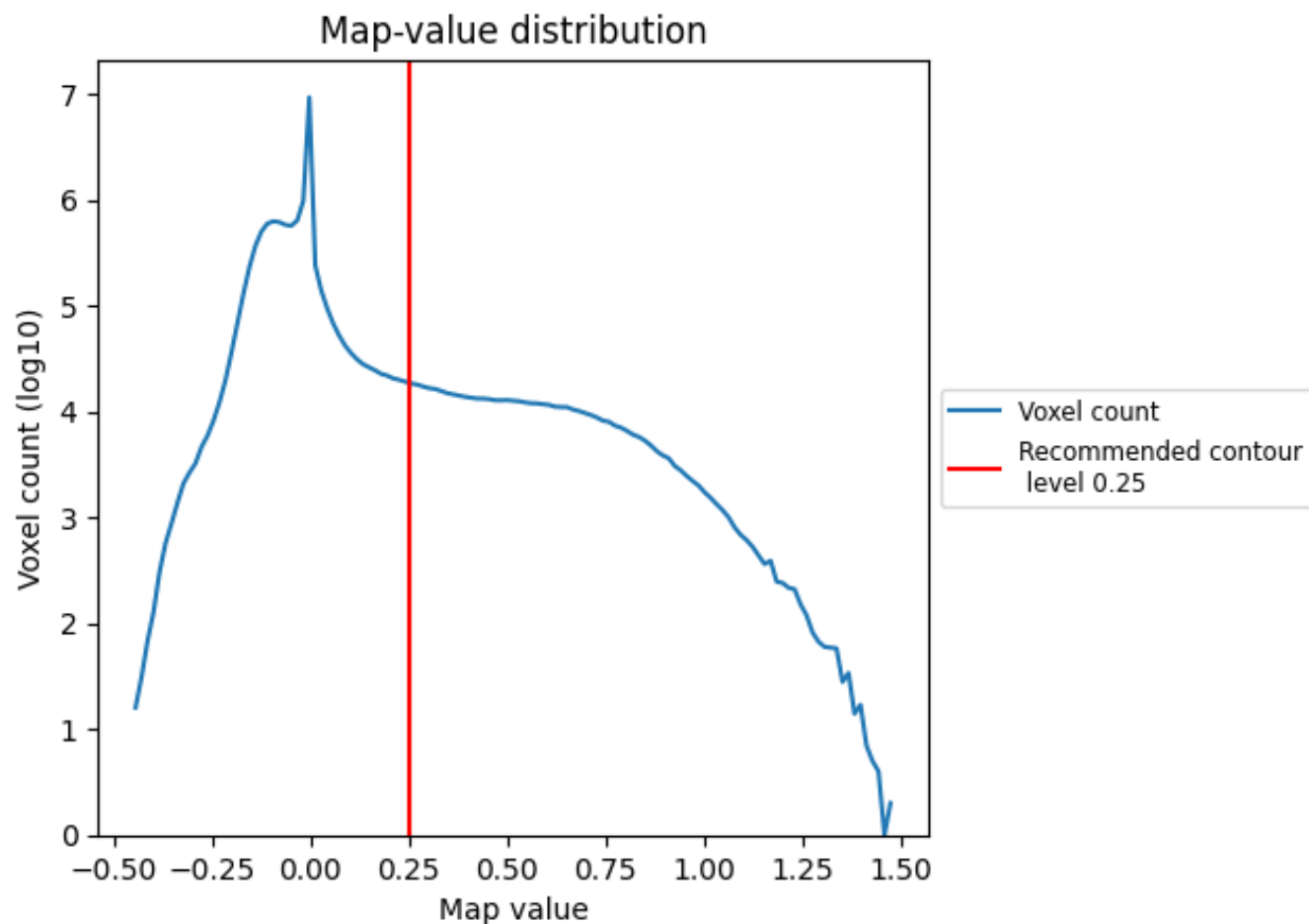
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

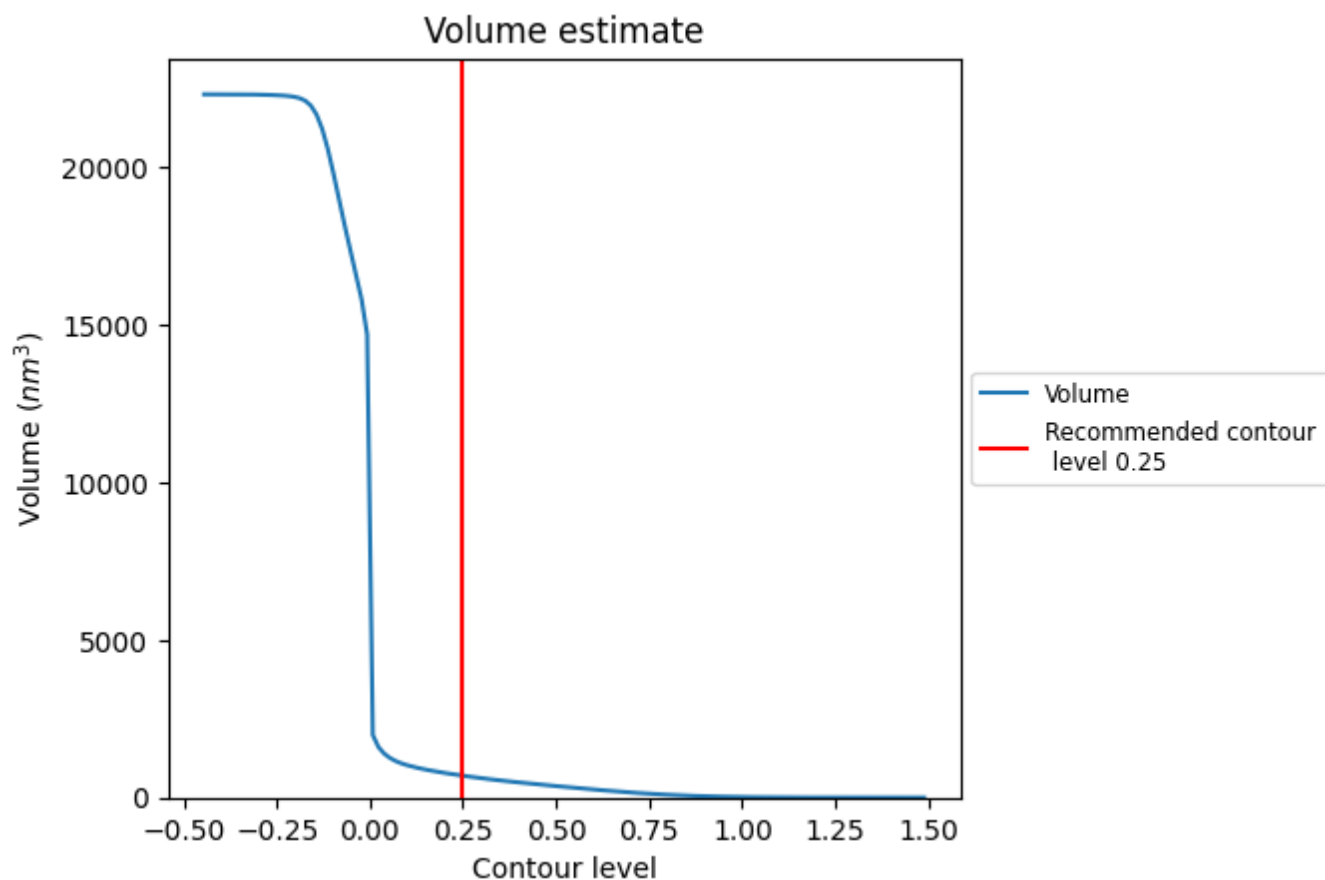
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

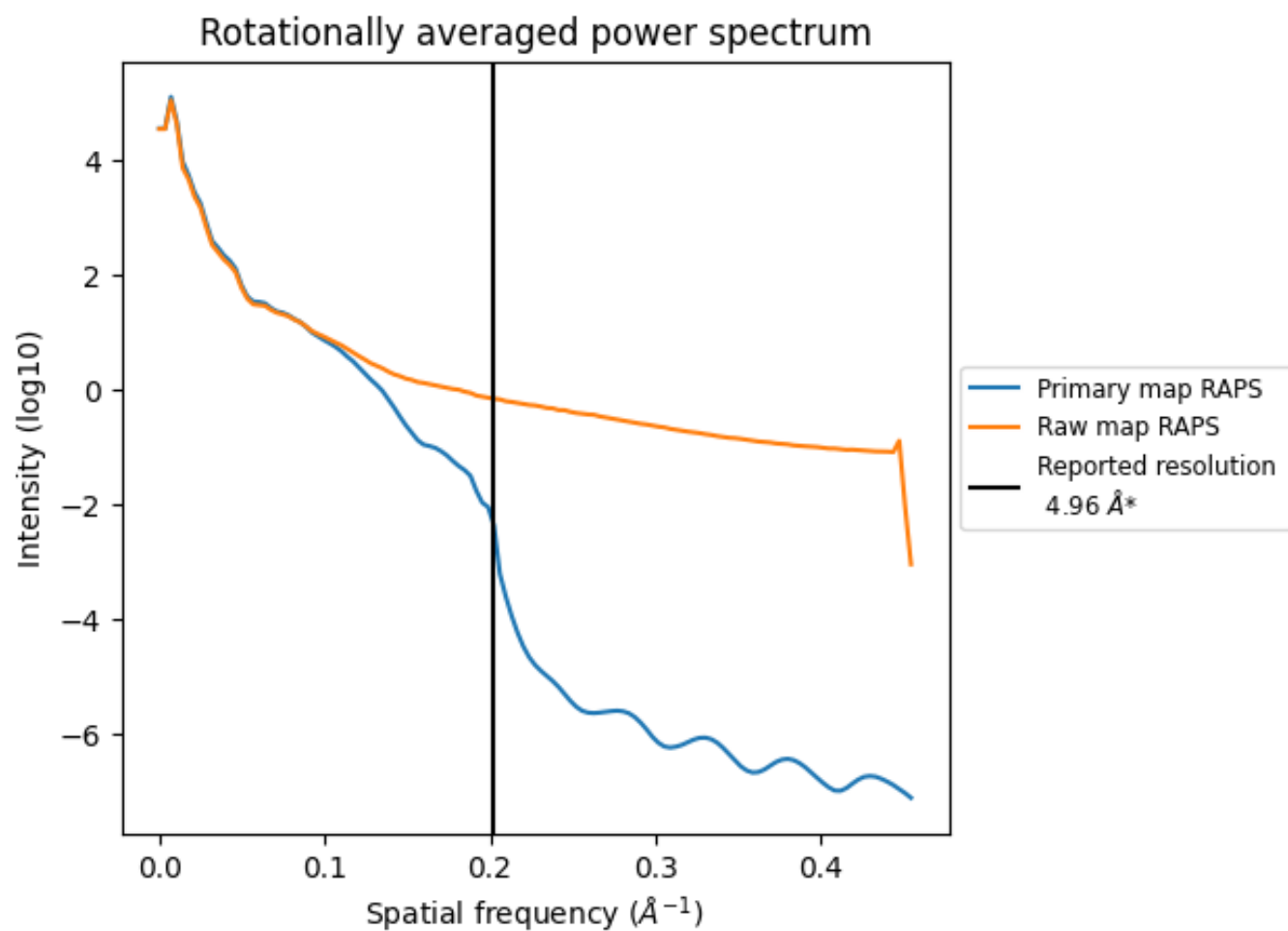
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 693 nm^3 ; this corresponds to an approximate mass of 626 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 ⓘ

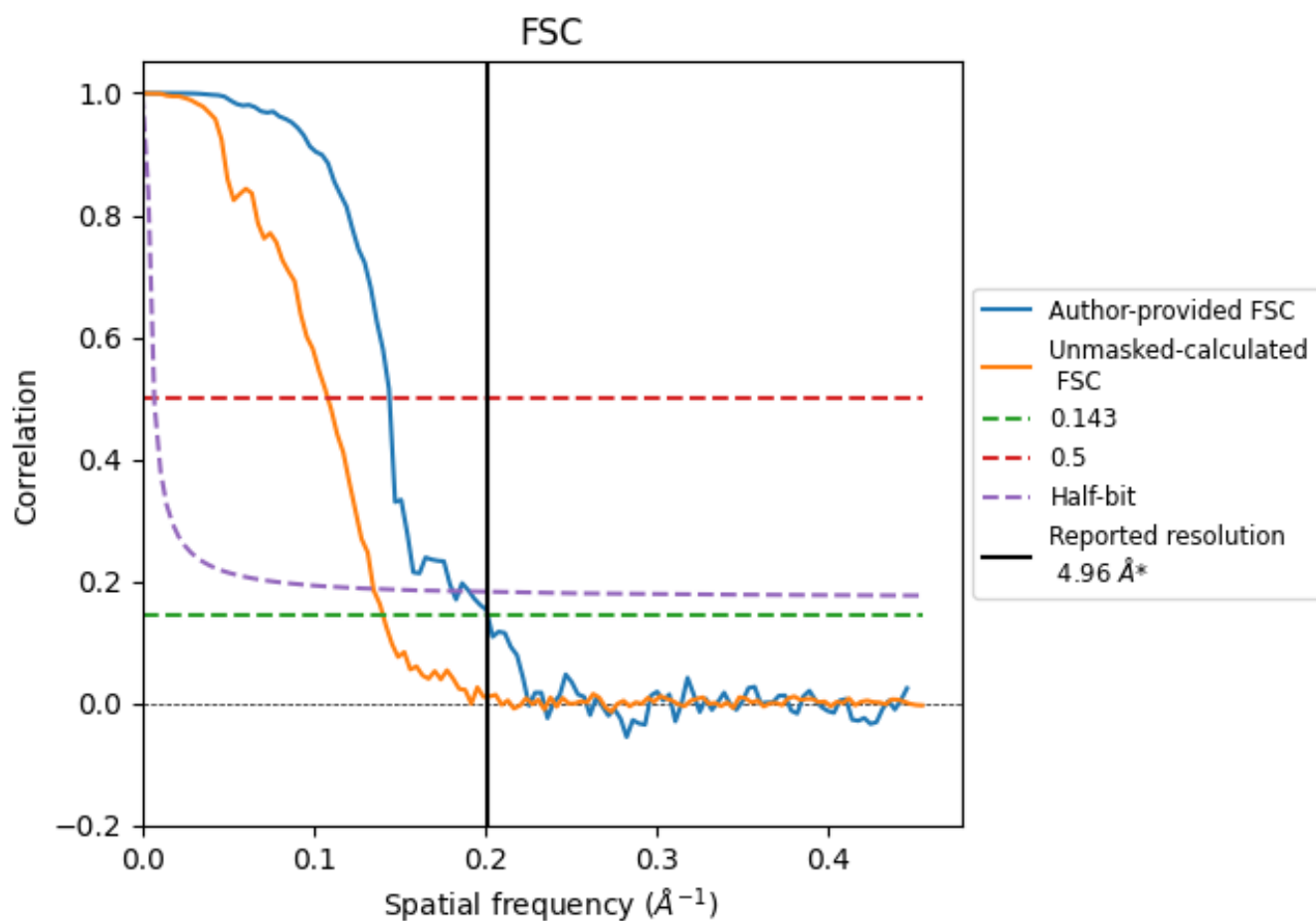


*Reported resolution corresponds to spatial frequency of 0.202 Å⁻¹

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 0.202 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

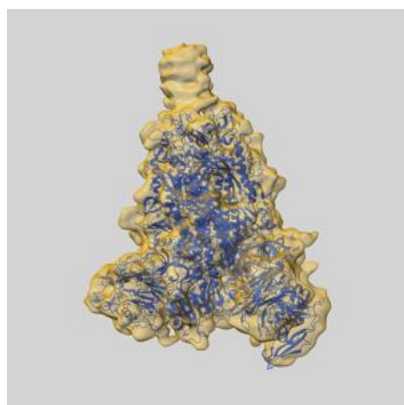
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.96	-	-
Author-provided FSC curve	4.97	6.94	5.52
Unmasked-calculated*	7.12	9.24	7.42

*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 7.12 differs from the reported value 4.96 by more than 10 %

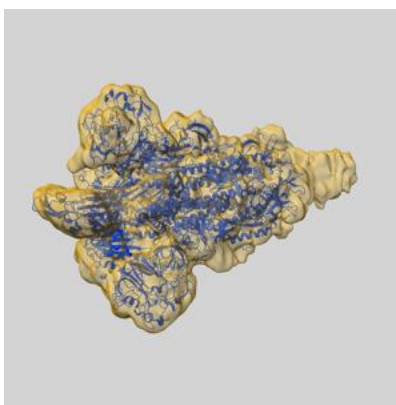
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33947 and PDB model 7YMY. Per-residue inclusion information can be found in section [3](#) on page [15](#).

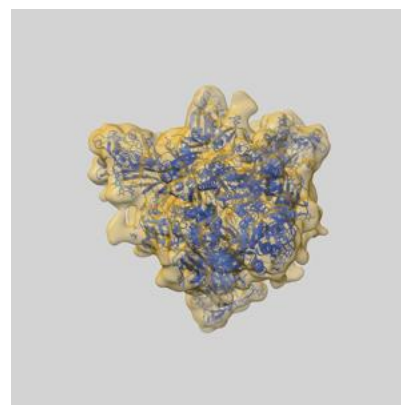
9.1 Map-model overlay [i](#)



X



Y



Z

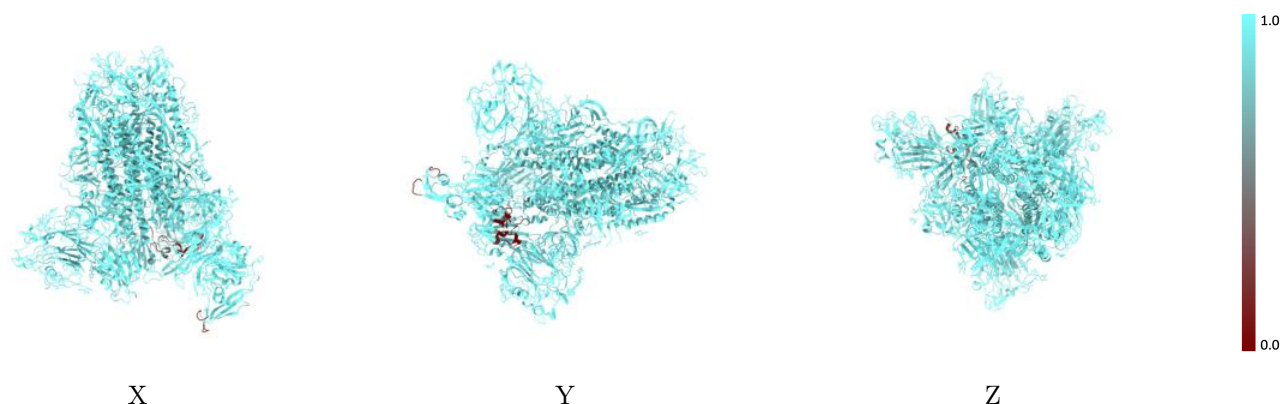
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



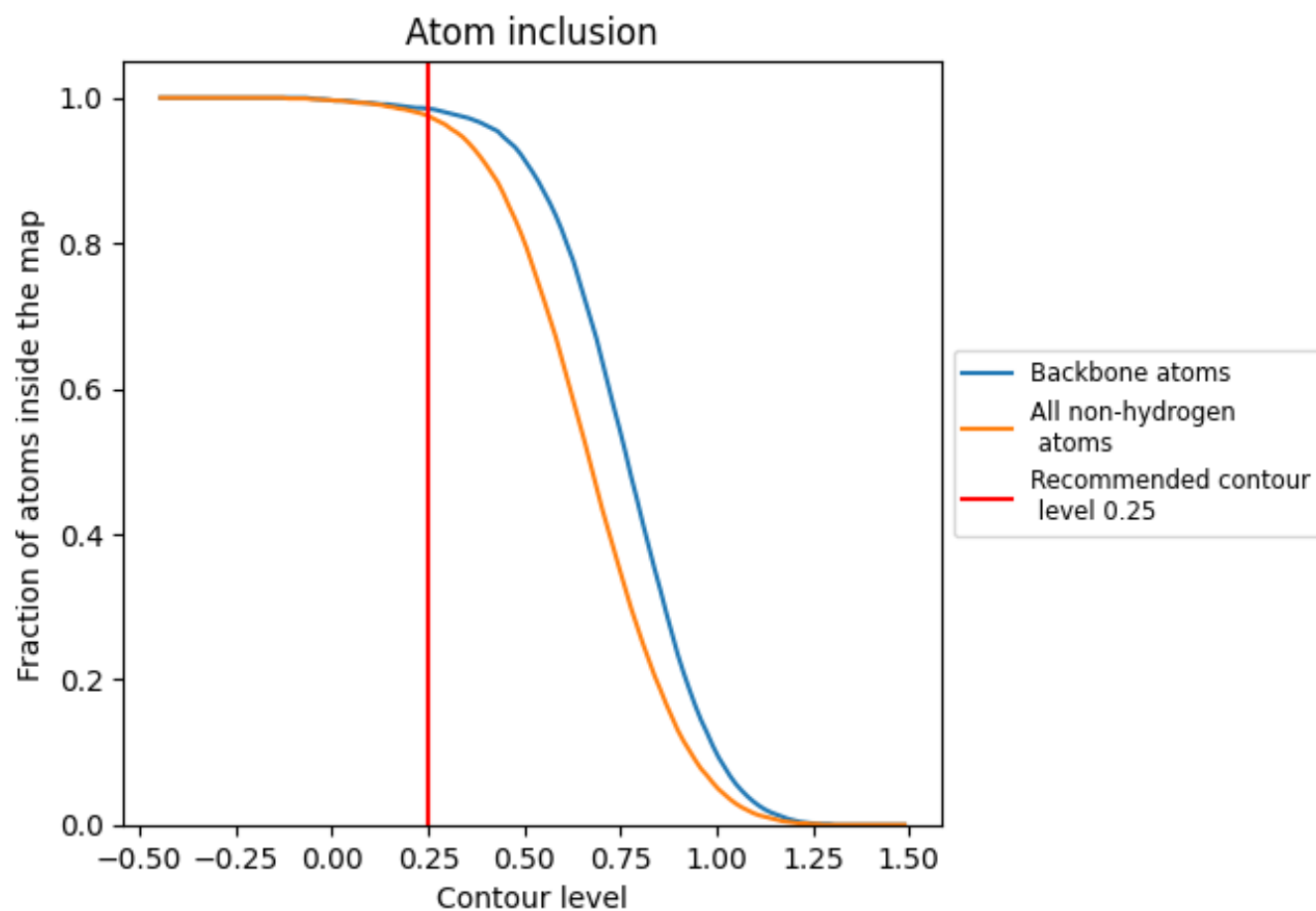
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.1990
A	0.9800	0.1900
B	0.9880	0.2050
C	0.9560	0.1970
D	1.0000	0.3880
E	1.0000	0.2970
F	1.0000	0.2910
G	1.0000	0.2420
H	1.0000	0.2630
I	1.0000	0.3320
J	1.0000	0.3930
K	1.0000	0.2460
L	1.0000	0.3190

1.0

0.0

<0.0