



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:58 PM UTC

PDB ID : 9YPB / pdb_00009ypb
EMDB ID : EMD-73292
Title : Fab-14/SARS-CoV-2 D614G spike complex, Mode IV, subgroup II conformation
Authors : Wang, Y.; Hu, Y.; Leiman, P.; Xie, X.
Deposited on : 2025-10-13
Resolution : 3.50 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:

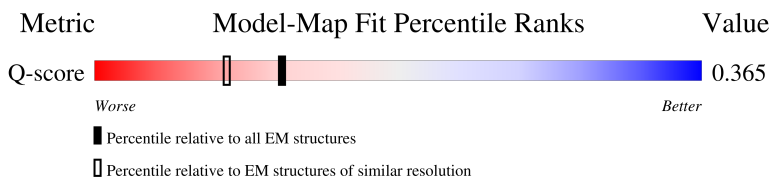
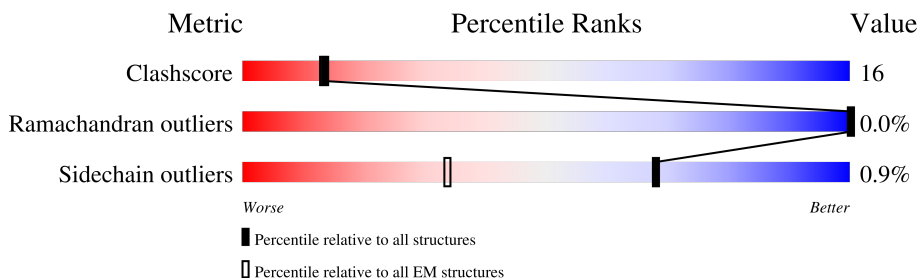
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	D	235	
1	F	235	
2	E	213	
2	G	213	

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Mol	Chain	Length	Quality of chain
3	A	1288	
3	B	1288	
3	C	1288	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29858 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 Fab-14 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	211	Total	C	N	O	S	0	0
			1622	1022	274	320	6		
1	F	193	Total	C	N	O	S	0	0
			1502	949	252	295	6		

- Molecule 2 is a protein called Fab-14 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	212	Total	C	N	O	S	0	0
			1575	985	261	324	5		
2	G	210	Total	C	N	O	S	0	0
			1551	967	259	320	5		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1013	Total	C	N	O	S	0	0
			7918	5066	1318	1498	36		
3	B	973	Total	C	N	O	S	0	0
			7595	4859	1254	1448	34		
3	C	992	Total	C	N	O	S	0	0
			7745	4951	1282	1477	35		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
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C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
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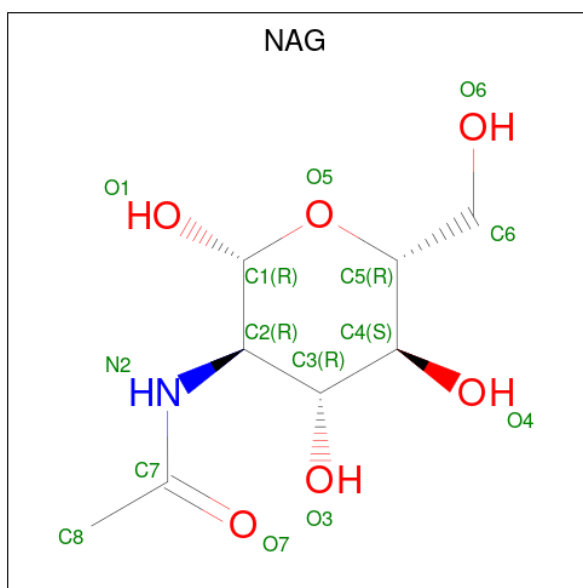
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 4 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
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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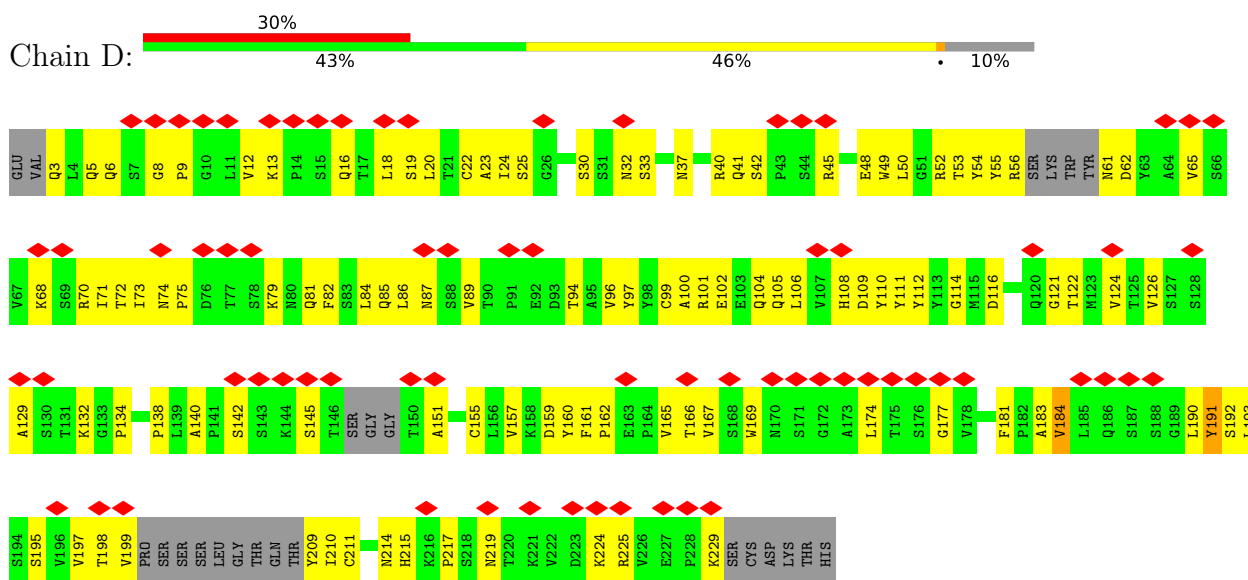
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

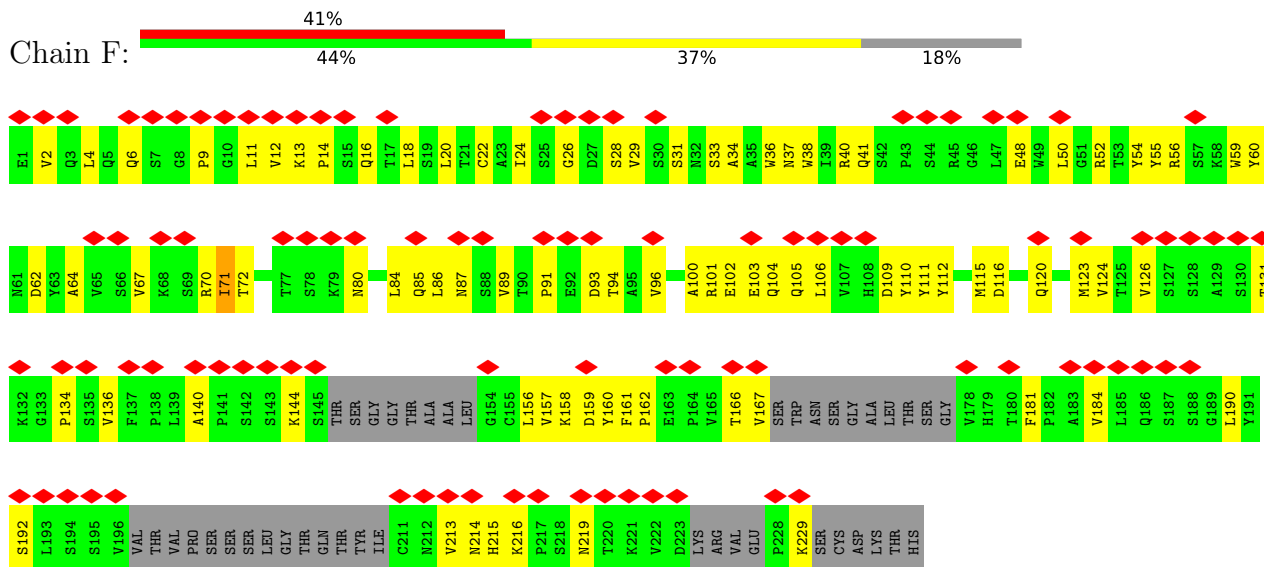
3 Residue-property plots

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.

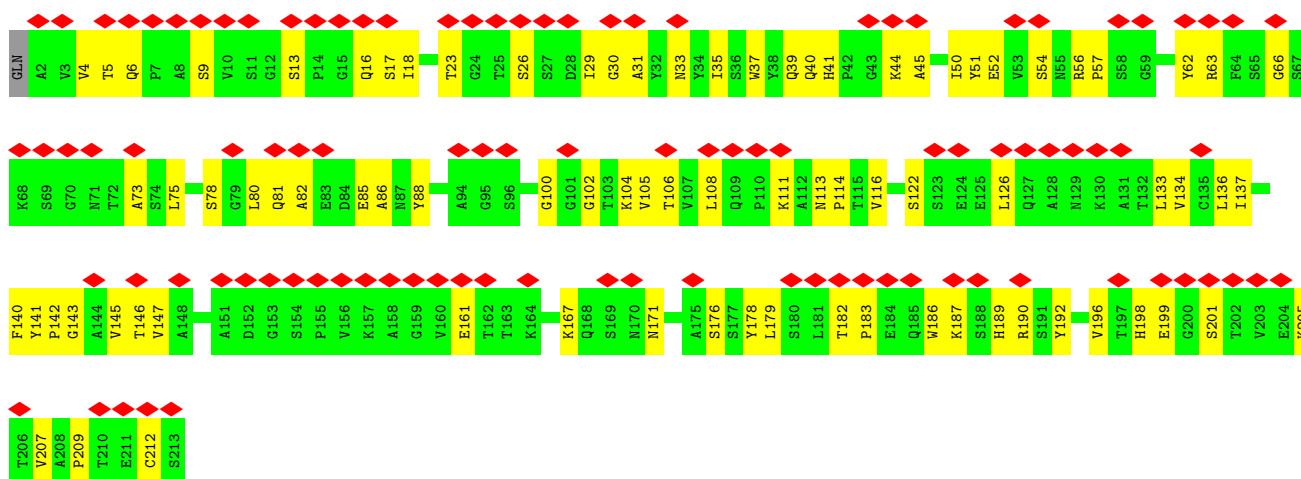
• Molecule 1: Fab-14 heavy chain



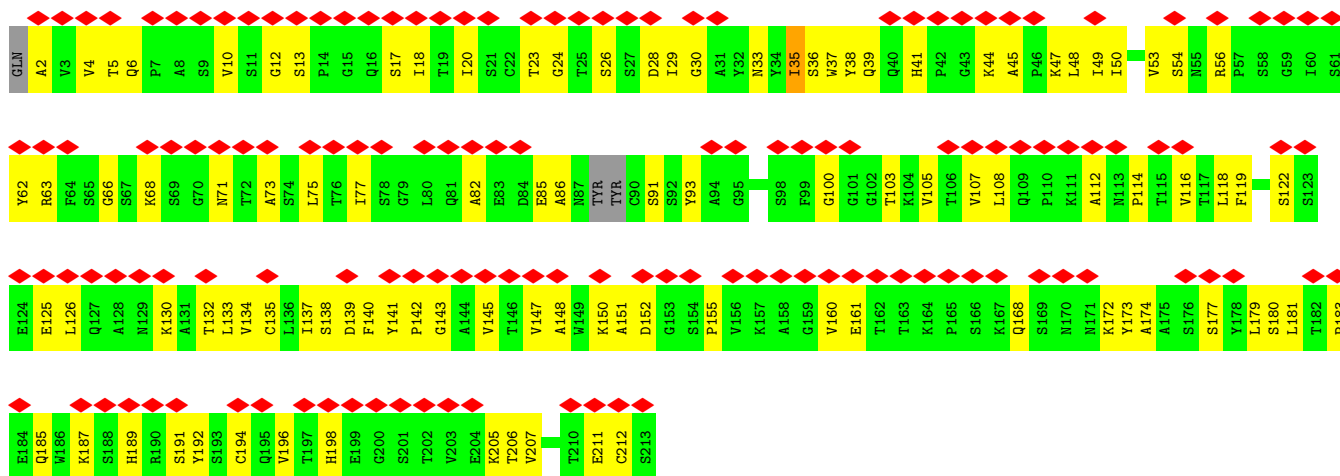
• Molecule 1: Fab-14 heavy chain



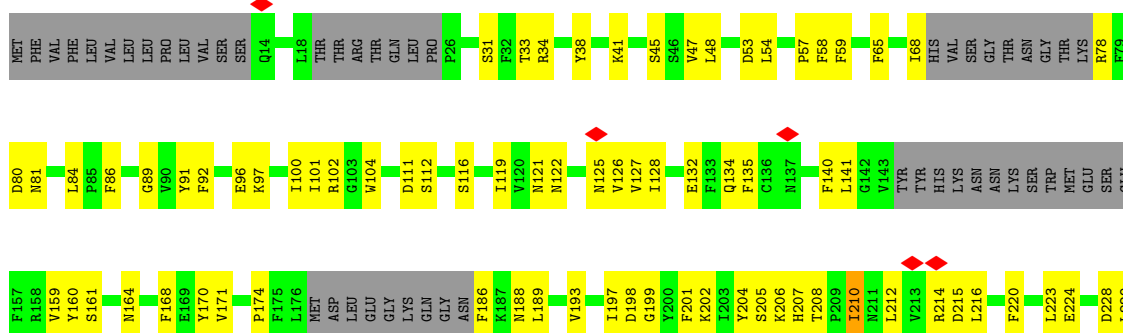
• Molecule 2: Fab-14 light chain

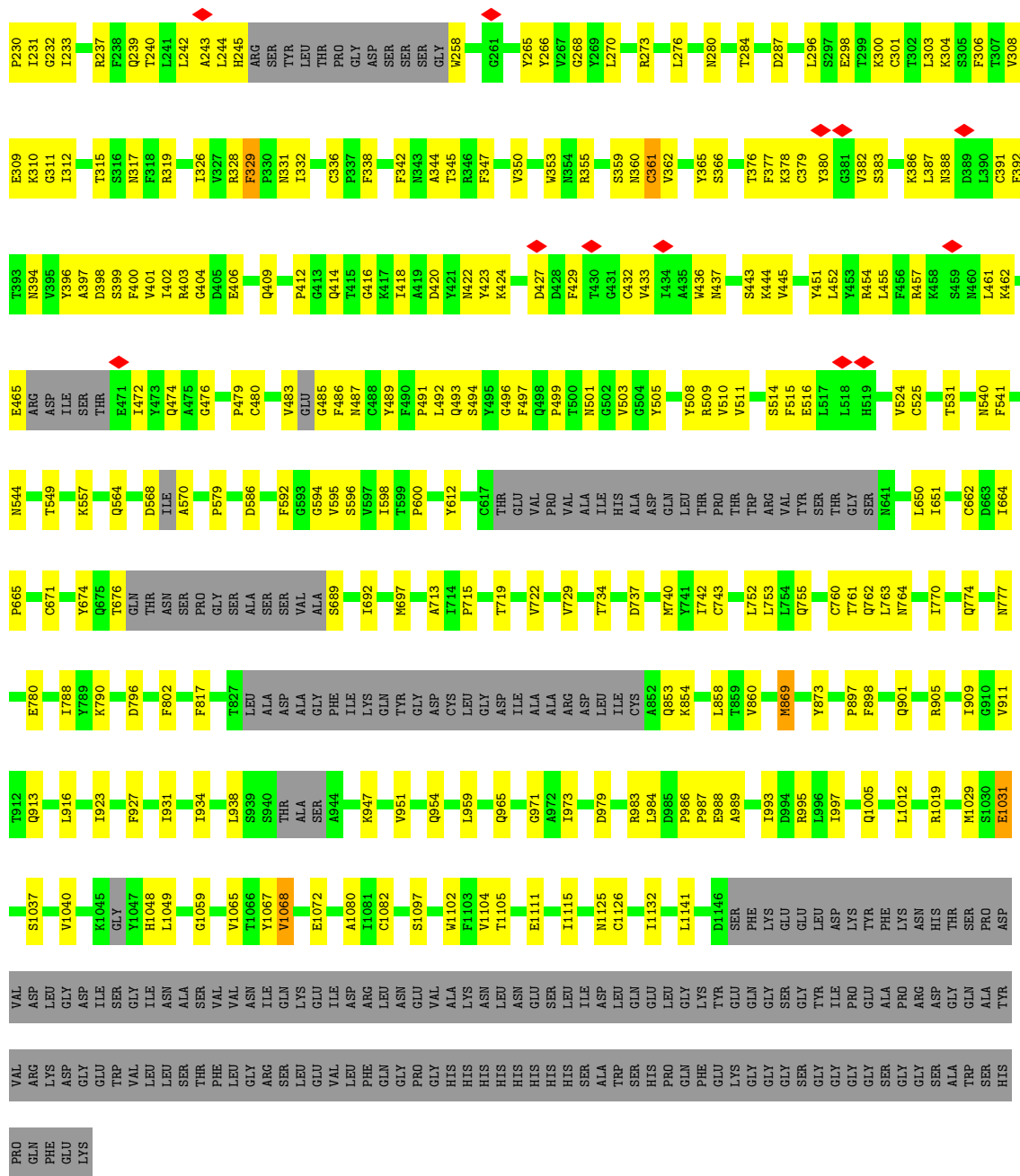


• Molecule 2: Fab-14 light chain



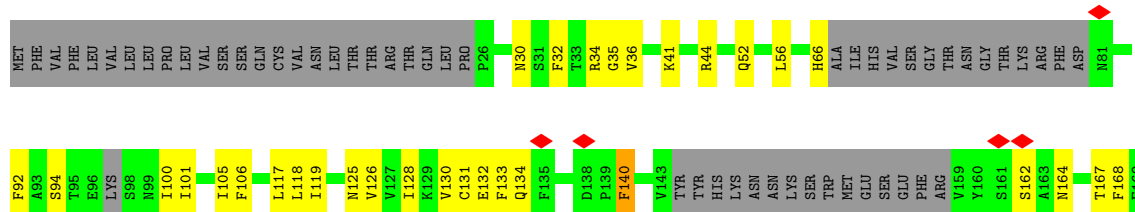
• Molecule 3: Spike glycoprotein





• Molecule 3: Spike glycoprotein

Chain B:



LYS	GLY	GLU	ASP	T1006	LYS	T732	VAL	V534	D442	V362	V369	GLY	E169
TRP	TRP	TRP	ILE	Q1010	F855	V736	PRO	V534	S443	A363	N370	MET	Y170
VAL	VAL	VAL	GLY	Q1011	L858	D737	ALA	C538	S443	D364	S371	ASP	Q173
LEU	LEU	LEU	ILE	L1012	T859	M740	ILE	V539	K444	Y365	A372	LEU	L176
LEU	LEU	LEU	ASN	L1034	V860	E748	HIS	N540	N448	Y369	S373	GLY	Q173
SER	SER	SER	ALA	R1039	M869	D745	ALA	F541	Y449	N370	F374	TRP	L176
THR	THR	THR	SER	V1040	Y873	E748	ASP	N542	N450	S371	F374	THR	Q173
PHE	PHE	PHE	VAL	D1041	L878	L752	GLN	F543	Y453	A372	F374	ALA	Q173
LEU	LEU	LEU	ASN	C1043	L894	L754	LEU	N544	R454	S373	F374	GLY	Q173
GLN	GLN	GLN	LYS	G1044	P897	G757	THR	T547	R455	F377	F374	LYS	Q173
LEU	LEU	LEU	GLU	K1045	M900	S758	ARG	V551	F456	K378	F377	GLN	Q173
VAL	VAL	VAL	ILE	H1048	R905	L763	THR	L552	R457	C379	F377	GLY	Q173
ARG	ARG	ARG	ASN	L1049	M900	S758	THR	T553	K458	TTR	F377	ASN	Q173
LEU	LEU	LEU	LEU	M1050	R905	L763	GLY	F554	R466	G381	F377	PHE	Q173
ASN	ASN	ASN	ASN	Q1054	F927	V781	SER	S555	D467	V382	F377	LYS	Q173
GLY	GLY	GLY	GLY	V1065	Y931	I788	THR	F562	I472	S383	F377	GLY	Q173
HIS	HIS	HIS	ALA	T1077	Y934	I806	SER	N641	Y473	P384	F377	GLY	Q173
HIS	HIS	HIS	LYS	A1078	Y934	I806	GLY	C662	Q475	T385	F377	GLY	Q173
HIS	HIS	HIS	LEU	K1086	S940	K814	THR	D663	A475	N388	F377	GLY	Q173
HIS	HIS	HIS	ASN	R1091	THR	R815	ASN	Q675	N481	D389	F377	GLY	Q173
ILE	ILE	ILE	ILE	N1119	SER	S816	GLN	T676	N481	L390	F377	GLY	Q173
ASP	ASP	ASP	ASP	T1120	A944	E819	THR	I584	N481	L390	F377	GLY	Q173
LEU	LEU	LEU	LEU	F1121	L948	T827	THR	I587	N481	L390	F377	GLY	Q173
GLN	GLN	GLN	GLN	V1122	V951	L827	ASN	T588	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	L1141	N955	LEU	PRO	P889	N481	L390	F377	GLY	Q173
LYS	LYS	LYS	LYS	D1146	L966	ASP	GLY	S891	N481	L390	F377	GLY	Q173
TYR	TYR	TYR	TYR	SER	G971	ASP	GLY	G593	N481	L390	F377	GLY	Q173
GLU	GLU	GLU	GLU	PHE	L977	GLN	VAL	G594	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	GLY	L977	TYR	ALA	S689	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	LEU	L977	GLY	ALA	V597	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	ASP	R983	ASP	ASP	I598	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	LYS	L984	ASP	ASP	T599	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	TYR	D985	CYS	LEU	P600	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	PHE	P986	LEU	GLY	S704	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	LYS	P987	GLY	ASP	S805	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	ASN	E988	ASP	ASP	N606	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	HIS	A999	ILE	ILE	V610	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	THR	A999	ALA	ALA	L611	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	SER	I993	ALA	ALA	Y612	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	PRO	D994	ASP	ASP	V615	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	ASP	R995	LEU	LEU	N616	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	VAL	L996	ILE	ILE	T723	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	ARG	L1004	CYS	CYS	C617	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	LYS	Q1005	ALA	ALA	THR	N481	L390	F377	GLY	Q173
GLY	GLY	GLY	GLY	GLY	Q1005	GLN	GLN	GLU	N481	L390	F377	GLY	Q173

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66402	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.17	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	10500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	369.11603, 369.11603, 369.11603	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8389001, 0.8389001, 0.8389001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	D	0.27	0/1660	0.46	0/2264
1	F	0.12	0/1539	0.37	0/2095
2	E	0.11	0/1613	0.30	0/2199
2	G	0.13	0/1586	0.35	0/2160
3	A	0.29	0/8095	0.44	0/11006
3	B	0.25	0/7761	0.41	0/10551
3	C	0.28	0/7919	0.41	0/10771
All	All	0.26	0/30173	0.41	0/41046

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1622	0	1575	99	0
1	F	1502	0	1449	84	0
2	E	1575	0	1524	61	0
2	G	1551	0	1505	83	0
3	A	7918	0	7719	253	0
3	B	7595	0	7389	210	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	7745	0	7540	216	0
4	A	126	0	117	0	0
4	B	140	0	130	0	0
4	C	84	0	78	0	0
All	All	29858	0	29026	942	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 16.

All (942) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:TYR:OH	3:C:515:PHE:CZ	1.90	1.21
3:A:1072:GLU:OE2	3:B:892:ALA:HB3	1.39	1.16
3:A:715:PRO:HA	3:A:1072:GLU:HA	1.31	1.12
3:C:365:TYR:OH	3:C:515:PHE:HZ	1.25	1.06
3:C:365:TYR:CZ	3:C:515:PHE:HZ	1.81	0.97
3:A:1072:GLU:OE2	3:B:892:ALA:CB	2.19	0.90
3:B:439:ASN:HD22	3:B:506:GLN:HG2	1.39	0.87
1:F:37:ASN:HB2	1:F:100:ALA:HB3	1.55	0.87
3:A:1072:GLU:HG2	3:B:894:LEU:HD21	1.58	0.86
3:B:132:GLU:HB2	3:B:164:ASN:HB2	1.57	0.85
3:A:355:ARG:HA	3:A:397:ALA:O	1.77	0.84
1:D:159:ASP:OD1	1:D:190:LEU:HD13	1.79	0.83
1:D:73:ILE:HG22	1:D:75:PRO:HD3	1.61	0.82
1:D:53:THR:HG21	1:D:75:PRO:HG3	1.63	0.80
3:A:391:CYS:HB2	3:A:525:CYS:HA	1.64	0.80
3:B:702:GLU:HB3	3:C:788:ILE:HD11	1.62	0.80
3:C:83:VAL:HG23	3:C:237:ARG:HD3	1.62	0.79
3:A:1072:GLU:HG2	3:B:894:LEU:CD2	2.12	0.79
3:C:538:CYS:SG	3:C:590:CYS:HB2	2.23	0.79
3:B:350:VAL:HG11	3:B:418:ILE:HD12	1.64	0.78
3:C:363:ALA:HB2	3:C:524:VAL:HG12	1.63	0.78
1:D:33:SER:HB2	1:D:104:GLN:HB3	1.66	0.78
3:A:715:PRO:HG3	3:A:1072:GLU:HG3	1.64	0.78
3:A:230:PRO:O	3:C:357:ARG:NH1	2.15	0.78
3:A:376:THR:HB	3:A:437:ASN:HD21	1.48	0.78
2:E:85:GLU:HA	2:E:105:VAL:O	1.82	0.78
3:A:53:ASP:OD1	3:A:54:LEU:N	2.17	0.77
3:C:402:ILE:HD11	3:C:418:ILE:HG12	1.65	0.77
3:A:134:GLN:HB2	3:A:161:SER:HB3	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:699:LEU:HD21	3:C:869:MET:HG2	1.66	0.76
3:A:92:PHE:CE2	3:A:240:THR:HG21	2.20	0.76
2:E:85:GLU:HG3	2:E:106:THR:HA	1.68	0.75
1:F:123:MET:HA	1:F:123:MET:HE3	1.69	0.75
3:C:732:THR:OG1	3:C:955:ASN:ND2	2.18	0.75
3:A:398:ASP:O	3:A:511:VAL:HA	1.86	0.75
1:D:40:ARG:HH11	1:D:70:ARG:HH22	1.35	0.74
3:C:442:ASP:O	3:C:448:ASN:ND2	2.19	0.74
3:A:422:ASN:ND2	3:A:454:ARG:O	2.20	0.74
3:C:64:TRP:HE1	3:C:264:ALA:HA	1.53	0.74
2:G:37:TRP:HB2	2:G:50:ILE:HB	1.69	0.73
3:A:474:GLN:HG2	3:A:479:PRO:HA	1.70	0.73
2:G:85:GLU:HA	2:G:105:VAL:O	1.89	0.73
3:A:452:LEU:HB3	3:A:492:LEU:HD12	1.71	0.73
2:G:17:SER:HA	2:G:77:ILE:O	1.89	0.72
2:G:33:ASN:OD1	2:G:68:LYS:NZ	2.23	0.72
2:E:18:ILE:HG12	2:E:80:LEU:HD21	1.72	0.71
1:F:94:THR:HG22	1:F:126:VAL:H	1.55	0.71
1:F:96:VAL:HG22	1:F:123:MET:HE1	1.71	0.71
1:D:37:ASN:HA	1:D:52:ARG:HB3	1.72	0.71
3:C:365:TYR:CE2	3:C:515:PHE:HZ	2.08	0.71
3:A:135:PHE:HA	3:A:160:TYR:HA	1.73	0.71
3:A:104:TRP:HD1	3:A:240:THR:HG22	1.55	0.70
3:A:229:LEU:HB3	3:A:231:ILE:HG12	1.73	0.70
3:C:1086:LYS:HB2	3:C:1122:VAL:CG2	2.21	0.70
3:A:91:TYR:HD1	3:A:193:VAL:HG22	1.56	0.70
3:B:702:GLU:CB	3:C:788:ILE:HD11	2.20	0.70
2:G:4:VAL:HG12	2:G:29:ILE:HD11	1.73	0.70
3:C:126:VAL:HG23	3:C:128:ILE:HD11	1.72	0.70
1:D:142:SER:HG	1:D:145:SER:HG	1.38	0.70
3:B:763:LEU:HD12	3:B:1008:VAL:HG21	1.74	0.70
3:A:328:ARG:NH1	3:A:531:THR:O	2.25	0.69
3:C:540:ASN:OD1	3:C:540:ASN:O	2.10	0.69
3:A:360:ASN:ND2	3:B:168:PHE:CE1	2.60	0.69
1:F:6:GLN:HB3	1:F:120:GLN:HE21	1.58	0.69
3:A:199:GLY:HA2	3:A:232:GLY:HA2	1.73	0.69
1:D:6:GLN:HE22	1:D:20:LEU:HD22	1.58	0.69
3:A:350:VAL:HA	3:A:400:PHE:HB2	1.75	0.69
3:B:34:ARG:NH2	3:B:191:GLU:OE2	2.25	0.69
3:B:1106:GLN:NE2	3:B:1111:GLU:OE2	2.26	0.69
3:C:365:TYR:OH	3:C:513:LEU:HD13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:HIS:HD2	1:D:217:PRO:HD2	1.57	0.69
1:D:37:ASN:HB2	1:D:100:ALA:HB3	1.75	0.68
1:F:160:TYR:HB2	1:F:215:HIS:HE1	1.57	0.68
3:B:384:PRO:HA	3:B:387:LEU:HD12	1.75	0.68
3:C:105:ILE:HG23	3:C:239:GLN:HB2	1.75	0.68
3:B:131:CYS:HB2	3:B:133:PHE:HE1	1.58	0.68
1:D:3:GLN:NE2	1:D:25:SER:OG	2.27	0.68
3:A:303:LEU:HD23	3:A:308:VAL:HG12	1.76	0.68
3:C:203:ILE:HB	3:C:227:VAL:HG22	1.77	0.68
1:F:144:LYS:NZ	2:G:206:THR:O	2.27	0.67
2:E:114:PRO:HG3	2:E:198:HIS:HB3	1.77	0.67
1:D:134:PRO:HB2	1:D:157:VAL:HB	1.75	0.67
1:F:105:GLN:NE2	1:F:116:ASP:OD2	2.28	0.67
3:A:317:ASN:HA	3:A:594:GLY:HA2	1.76	0.67
3:A:311:GLY:HA2	3:A:664:ILE:HD12	1.77	0.67
3:C:597:VAL:HG22	3:C:610:VAL:HG12	1.76	0.67
3:C:578:ASP:HB3	3:C:581:THR:HG22	1.77	0.67
2:E:198:HIS:O	2:E:201:SER:OG	2.13	0.67
1:D:86:LEU:HD22	1:D:89:VAL:HG22	1.78	0.66
3:C:971:GLY:HA3	3:C:995:ARG:HH21	1.60	0.66
3:C:326:ILE:HD11	3:C:534:VAL:HG12	1.77	0.66
1:F:136:VAL:HG22	1:F:157:VAL:HG12	1.78	0.66
3:C:1086:LYS:HB2	3:C:1122:VAL:HG21	1.77	0.66
1:D:159:ASP:OD1	1:D:190:LEU:CD1	2.43	0.66
3:B:898:PHE:HZ	3:B:1050:MET:HE1	1.60	0.66
3:C:125:ASN:ND2	3:C:127:VAL:HG23	2.11	0.66
3:A:761:THR:OG1	3:A:762:GLN:NE2	2.29	0.65
3:C:989:ALA:O	3:C:993:ILE:HG12	1.96	0.65
2:E:82:ALA:O	2:E:171:ASN:ND2	2.29	0.65
3:B:130:VAL:O	3:B:167:THR:OG1	2.13	0.65
3:C:1119:ASN:OD1	3:C:1120:THR:HG23	1.97	0.65
1:D:184:VAL:HG12	1:D:192:SER:HB2	1.78	0.65
2:G:2:ALA:N	2:G:28:ASP:OD2	2.29	0.65
1:D:6:GLN:OE1	1:D:122:THR:OG1	2.12	0.65
3:B:379:CYS:HB3	3:B:382:VAL:HB	1.79	0.65
3:B:822:LEU:HD23	3:B:1056:ALA:HB2	1.78	0.65
1:D:132:LYS:HD2	1:D:190:LEU:HD21	1.78	0.65
1:F:36:TRP:HZ3	1:F:101:ARG:HD3	1.61	0.65
3:A:127:VAL:HG12	3:A:171:VAL:HG22	1.78	0.65
3:C:663:ASP:OD1	3:C:663:ASP:N	2.30	0.65
3:C:205:SER:HB3	3:C:226:LEU:HG	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:SER:O	3:A:59:PHE:HA	1.97	0.64
3:B:303:LEU:HD12	3:B:308:VAL:HG12	1.80	0.64
1:F:72:THR:HB	1:F:85:GLN:HB2	1.80	0.64
3:A:214:ARG:O	3:A:266:TYR:OH	2.06	0.64
3:B:327:VAL:HG22	3:B:542:ASN:HB3	1.79	0.64
3:B:353:TRP:O	3:B:466:ARG:NH2	2.30	0.64
2:G:133:LEU:HB2	2:G:179:LEU:HB3	1.79	0.64
3:A:722:VAL:HG22	3:A:1065:VAL:HG22	1.80	0.63
3:A:331:ASN:HD22	3:A:332:ILE:HG12	1.63	0.63
3:A:360:ASN:ND2	3:B:168:PHE:HE1	1.95	0.63
3:C:414:GLN:HG3	3:C:415:THR:HG22	1.80	0.63
1:D:132:LYS:HD2	1:D:190:LEU:CD2	2.29	0.63
2:E:88:TYR:O	2:E:102:GLY:HA2	1.99	0.63
3:B:490:PHE:O	3:B:493:GLN:NE2	2.30	0.63
3:B:403:ARG:HB2	3:B:406:GLU:HG2	1.81	0.63
3:B:429:PHE:HE2	3:B:433:VAL:HG13	1.63	0.62
3:A:100:ILE:HG22	3:A:242:LEU:HD11	1.81	0.62
3:A:376:THR:HG23	3:A:378:LYS:HG2	1.81	0.62
3:B:1084:ASP:HB2	3:B:1086:LYS:HE2	1.79	0.62
1:D:229:LYS:NZ	2:E:212:CYS:SG	2.73	0.62
2:G:118:LEU:HD13	2:G:205:LYS:HB3	1.81	0.62
1:D:169:TRP:HZ3	1:D:209:TYR:HB3	1.63	0.62
3:B:92:PHE:HE1	3:B:94:SER:HB2	1.63	0.62
3:A:206:LYS:NZ	3:A:207:HIS:O	2.27	0.62
3:A:416:GLY:O	3:A:420:ASP:N	2.33	0.62
3:B:1086:LYS:HB3	3:B:1122:VAL:HG21	1.81	0.62
3:C:736:VAL:HG22	3:C:858:LEU:CB	2.30	0.62
3:A:544:ASN:HD22	3:A:579:PRO:HG3	1.64	0.62
3:A:983:ARG:HG2	3:C:390:LEU:HD21	1.81	0.62
3:B:319:ARG:HD3	3:C:740:MET:SD	2.40	0.62
3:B:416:GLY:H	3:B:419:ALA:HB3	1.63	0.62
3:B:32:PHE:HB3	3:B:218:GLN:HG3	1.81	0.62
3:A:909:ILE:HD13	3:A:1049:LEU:HD21	1.81	0.61
1:D:159:ASP:HA	1:D:190:LEU:HD13	1.81	0.61
1:F:160:TYR:HB2	1:F:215:HIS:CE1	2.35	0.61
2:G:12:GLY:HA3	2:G:18:ILE:HD11	1.81	0.61
3:B:170:TYR:HE1	3:B:172:SER:HB2	1.64	0.61
3:C:473:TYR:N	3:C:489:TYR:O	2.30	0.61
2:E:56:ARG:HD3	2:E:62:TYR:HA	1.82	0.61
1:D:41:GLN:N	1:D:96:VAL:O	2.30	0.61
1:F:166:THR:HG23	1:F:214:ASN:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:150:LYS:HG2	2:G:155:PRO:HG3	1.81	0.61
3:A:355:ARG:HD2	3:A:396:TYR:HB3	1.81	0.61
3:A:474:GLN:OE1	3:A:487:ASN:ND2	2.33	0.61
3:A:790:LYS:HG2	3:C:704:SER:HB3	1.82	0.61
1:D:13:LYS:NZ	1:D:129:ALA:O	2.34	0.61
1:F:13:LYS:O	1:F:16:GLN:NE2	2.33	0.61
2:G:35:ILE:HD11	2:G:53:VAL:HG22	1.82	0.61
3:A:86:PHE:H	3:A:237:ARG:HA	1.65	0.61
3:A:780:GLU:OE2	3:A:1019:ARG:NH1	2.34	0.61
3:B:119:ILE:HG13	3:B:128:ILE:HG23	1.82	0.61
2:E:182:THR:O	2:E:186:TRP:N	2.31	0.60
2:E:116:VAL:HG22	2:E:137:ILE:HD13	1.82	0.60
1:F:64:ALA:HB3	1:F:67:VAL:HG22	1.81	0.60
1:F:110:TYR:HB3	3:B:487:ASN:H	1.67	0.60
3:A:984:LEU:HD12	3:A:988:GLU:HB2	1.82	0.60
2:E:5:THR:O	2:E:23:THR:N	2.33	0.60
2:E:142:PRO:O	2:E:198:HIS:NE2	2.33	0.60
2:G:133:LEU:HD22	2:G:179:LEU:HD23	1.83	0.60
2:E:44:LYS:NZ	2:E:45:ALA:O	2.33	0.60
3:A:168:PHE:CE2	3:A:170:TYR:HB2	2.36	0.60
3:A:202:LYS:HG2	3:A:204:TYR:CZ	2.37	0.60
3:A:557:LYS:NZ	3:A:586:ASP:OD1	2.35	0.60
3:C:125:ASN:HD21	3:C:127:VAL:HG23	1.67	0.60
1:D:166:THR:OG1	1:D:214:ASN:HB2	2.02	0.60
3:B:497:PHE:CD1	3:B:507:PRO:HD3	2.37	0.60
1:F:52:ARG:NH2	3:B:484:GLU:O	2.35	0.59
3:A:445:VAL:HA	3:A:499:PRO:HG3	1.83	0.59
1:D:161:PHE:HB3	1:D:162:PRO:HD3	1.83	0.59
1:D:215:HIS:O	1:D:219:ASN:N	2.35	0.59
3:B:749:CYS:SG	3:B:997:ILE:HD11	2.42	0.59
3:B:423:TYR:HE1	3:B:464:PHE:HA	1.66	0.59
1:D:56:ARG:HG2	3:A:485:GLY:HA2	1.84	0.59
3:A:916:LEU:HD12	3:A:923:ILE:HD13	1.82	0.59
3:C:203:ILE:HG22	3:C:226:LEU:HB2	1.84	0.59
3:C:448:ASN:OD1	3:C:450:ASN:ND2	2.35	0.59
3:C:128:ILE:HD13	3:C:170:TYR:HB3	1.85	0.59
3:A:869:MET:HG2	3:C:699:LEU:HD21	1.85	0.59
3:A:298:GLU:HB3	3:A:315:THR:HG21	1.83	0.59
2:E:190:ARG:HA	2:E:209:PRO:HD2	1.85	0.58
3:B:289:VAL:HG23	3:B:306:PHE:CZ	2.38	0.58
3:C:736:VAL:HG22	3:C:858:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:927:PHE:O	3:C:931:ILE:HG12	2.04	0.58
1:D:37:ASN:N	1:D:100:ALA:O	2.34	0.58
1:D:160:TYR:CZ	1:D:191:TYR:HB3	2.38	0.58
3:B:342:PHE:HA	3:B:347:PHE:HZ	1.68	0.58
3:B:406:GLU:O	3:B:409:GLN:HB2	2.03	0.58
3:A:476:GLY:HA3	3:A:487:ASN:HD21	1.67	0.58
3:B:439:ASN:CG	3:B:507:PRO:HD2	2.28	0.58
3:B:713:ALA:HB3	3:C:894:LEU:HB3	1.86	0.58
3:C:360:ASN:H	3:C:523:THR:HB	1.68	0.58
3:B:965:GLN:OE1	3:C:758:SER:N	2.33	0.58
3:A:168:PHE:HE2	3:A:170:TYR:HB2	1.67	0.58
3:A:197:ILE:HG22	3:A:198:ASP:N	2.19	0.58
3:A:676:THR:OG1	3:A:689:SER:O	2.21	0.57
3:A:189:LEU:HB2	3:A:208:THR:HB	1.85	0.57
3:A:1037:SER:H	3:A:1048:HIS:HD2	1.52	0.57
3:B:433:VAL:HG12	3:B:512:VAL:HG12	1.86	0.57
3:C:805:ILE:HG22	3:C:878:LEU:HD21	1.86	0.57
3:A:65:PHE:CZ	3:A:84:LEU:HD11	2.39	0.57
3:B:902:MET:HE1	3:B:1050:MET:HE2	1.86	0.57
1:D:94:THR:HG22	1:D:126:VAL:H	1.69	0.57
3:A:345:THR:O	3:A:509:ARG:NH2	2.32	0.57
2:E:37:TRP:HB2	2:E:50:ILE:HB	1.85	0.57
3:A:366:SER:H	3:A:388:ASN:HD21	1.53	0.57
3:A:927:PHE:O	3:A:931:ILE:HG12	2.04	0.57
3:C:391:CYS:SG	3:C:522:ALA:HB1	2.45	0.57
3:C:455:LEU:HD22	3:C:493:GLN:HB3	1.87	0.57
3:C:722:VAL:HG22	3:C:1065:VAL:HG22	1.85	0.57
1:D:106:LEU:HD23	1:D:109:ASP:HB3	1.87	0.57
1:D:134:PRO:HD3	1:D:215:HIS:HD1	1.69	0.57
1:F:67:VAL:HG12	1:F:70:ARG:HH12	1.70	0.57
3:A:201:PHE:HB3	3:A:229:LEU:HB2	1.86	0.57
3:A:455:LEU:HD22	3:A:493:GLN:HB2	1.87	0.57
3:A:474:GLN:NE2	3:A:480:CYS:SG	2.77	0.57
3:B:449:TYR:HD1	3:B:494:SER:HG	1.51	0.57
2:G:140:PHE:HB2	2:G:198:HIS:CE1	2.39	0.57
3:A:501:ASN:HD22	3:A:505:TYR:HB2	1.69	0.57
3:A:600:PRO:HD3	3:A:692:ILE:HD11	1.87	0.57
3:C:983:ARG:O	3:C:983:ARG:HG2	2.04	0.57
2:G:116:VAL:HG22	2:G:137:ILE:HD13	1.87	0.56
3:A:80:ASP:O	3:A:265:TYR:OH	2.20	0.56
3:B:470:THR:HG22	3:B:492:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:LEU:HD11	3:C:237:ARG:HD2	1.87	0.56
1:F:14:PRO:HB3	1:F:91:PRO:HG3	1.87	0.56
1:F:40:ARG:HG3	1:F:48:GLU:HG2	1.88	0.56
3:A:360:ASN:HD21	3:B:168:PHE:HE1	1.52	0.56
3:A:989:ALA:O	3:A:993:ILE:HG12	2.04	0.56
1:F:29:VAL:HG12	1:F:59:TRP:HH2	1.71	0.56
3:A:102:ARG:NH2	3:A:121:ASN:O	2.39	0.56
2:G:63:ARG:HD3	2:G:77:ILE:HG23	1.87	0.56
3:C:600:PRO:HB3	3:C:674:TYR:HB2	1.88	0.56
3:C:736:VAL:HA	3:C:858:LEU:HA	1.87	0.56
1:F:40:ARG:NH1	1:F:93:ASP:OD1	2.39	0.56
3:C:1041:ASP:OD2	3:C:1045:LYS:NZ	2.32	0.56
1:D:37:ASN:ND2	1:D:102:GLU:OE2	2.39	0.56
2:E:147:VAL:HG22	2:E:196:VAL:HG22	1.88	0.56
3:A:379:CYS:HB3	3:A:432:CYS:HA	1.87	0.56
3:A:1031:GLU:OE2	3:C:1039:ARG:NE	2.39	0.56
3:C:327:VAL:HG23	3:C:542:ASN:HB3	1.88	0.56
3:B:950:ASP:O	3:B:954:GLN:HG3	2.06	0.56
3:C:748:GLU:O	3:C:752:LEU:HG	2.06	0.56
2:E:6:GLN:HE22	2:E:100:GLY:HA3	1.71	0.56
3:B:330:PRO:O	3:B:331:ASN:C	2.49	0.55
3:C:729:VAL:CG2	3:C:781:VAL:HG21	2.36	0.55
3:C:1077:THR:OG1	3:C:1078:ALA:N	2.38	0.55
1:D:160:TYR:CE2	1:D:165:VAL:HG21	2.41	0.55
2:G:6:GLN:HE22	2:G:100:GLY:HA3	1.69	0.55
3:A:45:SER:O	3:A:47:VAL:HG23	2.06	0.55
3:A:96:GLU:HG3	3:A:101:ILE:HB	1.88	0.55
3:A:697:MET:SD	3:B:869:MET:HE1	2.46	0.55
3:C:133:PHE:HB3	3:C:160:TYR:HB2	1.88	0.55
3:C:365:TYR:CE2	3:C:515:PHE:CZ	2.93	0.55
3:A:770:ILE:HD11	3:A:1012:LEU:HA	1.87	0.55
3:B:340:GLU:OE2	3:B:340:GLU:N	2.22	0.55
3:B:451:TYR:OH	3:B:497:PHE:HB2	2.06	0.55
1:D:169:TRP:NE1	1:D:211:CYS:SG	2.80	0.55
1:F:24:ILE:O	1:F:80:ASN:ND2	2.39	0.55
1:F:162:PRO:HB2	1:F:215:HIS:HE2	1.71	0.55
1:F:167:VAL:HG22	1:F:213:VAL:HG22	1.89	0.55
2:G:147:VAL:HG22	2:G:196:VAL:HG22	1.88	0.55
3:A:443:SER:OG	3:A:497:PHE:O	2.24	0.55
3:B:374:PHE:HB2	3:B:435:ALA:H	1.72	0.55
2:E:187:LYS:HA	2:E:209:PRO:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:205:SER:HA	3:A:223:LEU:HD23	1.86	0.55
3:A:344:ALA:O	3:A:509:ARG:NH1	2.40	0.55
3:C:303:LEU:HD12	3:C:308:VAL:HG12	1.88	0.55
1:D:167:VAL:HG11	1:D:195:SER:CB	2.37	0.55
2:G:114:PRO:HG3	2:G:198:HIS:HB3	1.87	0.55
3:B:748:GLU:CD	3:B:748:GLU:H	2.15	0.55
3:B:898:PHE:CZ	3:B:1050:MET:HE1	2.40	0.55
1:D:94:THR:HA	1:D:124:VAL:O	2.06	0.55
1:F:131:THR:HA	1:F:161:PHE:HD2	1.70	0.55
3:A:472:ILE:HA	3:A:491:PRO:HD3	1.89	0.55
3:B:126:VAL:HB	3:B:172:SER:HB3	1.89	0.55
3:B:131:CYS:HB2	3:B:133:PHE:CE1	2.39	0.55
3:B:140:PHE:HD1	3:B:241:LEU:HB2	1.72	0.54
3:C:1043:CYS:HB2	3:C:1048:HIS:CD2	2.41	0.54
2:E:111:LYS:HA	2:E:141:TYR:HD2	1.72	0.54
3:A:329:PHE:CD1	3:A:544:ASN:HA	2.42	0.54
3:B:1092:GLU:N	3:B:1092:GLU:OE2	2.40	0.54
2:E:54:SER:OG	2:E:66:GLY:O	2.25	0.54
3:B:273:ARG:NH1	3:B:290:ASP:OD2	2.40	0.54
3:C:334:ASN:O	3:C:362:VAL:N	2.34	0.54
3:C:312:ILE:HA	3:C:598:ILE:HA	1.90	0.54
1:D:42:SER:HB3	1:D:45:ARG:HB2	1.89	0.54
3:B:396:TYR:HB2	3:B:514:SER:HB3	1.90	0.54
3:C:369:TYR:HA	3:C:377:PHE:HE2	1.72	0.54
3:B:44:ARG:O	3:B:283:GLY:HA2	2.06	0.54
3:C:365:TYR:OH	3:C:515:PHE:CE2	2.51	0.54
1:D:65:VAL:HA	1:D:68:LYS:HD3	1.90	0.54
1:F:50:LEU:HG	1:F:71:ILE:HD12	1.90	0.54
3:A:101:ILE:HD12	3:A:242:LEU:HA	1.88	0.54
3:B:877:LEU:O	3:B:881:THR:HG22	2.08	0.54
3:C:34:ARG:HH12	3:C:217:PRO:HG2	1.73	0.54
2:E:183:PRO:HA	2:E:186:TRP:HB3	1.90	0.54
3:B:398:ASP:O	3:B:511:VAL:HA	2.08	0.54
3:C:310:LYS:HG3	3:C:600:PRO:HA	1.90	0.54
3:C:736:VAL:HG12	3:C:737:ASP:O	2.08	0.54
3:B:403:ARG:HG3	3:B:495:TYR:CE2	2.43	0.53
3:B:1086:LYS:HB3	3:B:1122:VAL:CG2	2.38	0.53
2:G:44:LYS:NZ	2:G:45:ALA:O	2.31	0.53
3:A:729:VAL:HG22	3:A:1059:GLY:HA2	1.91	0.53
3:B:190:ARG:HD3	3:B:207:HIS:CD2	2.43	0.53
3:C:855:PHE:HB2	3:C:858:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:LYS:HZ3	1:F:192:SER:HB3	1.73	0.53
3:B:572:THR:OG1	3:B:573:THR:N	2.40	0.53
2:E:4:VAL:HG12	2:E:29:ILE:HD11	1.90	0.53
3:A:436:TRP:HB3	3:A:511:VAL:O	2.08	0.53
3:B:454:ARG:NH1	3:B:469:SER:O	2.41	0.53
3:C:105:ILE:CG2	3:C:239:GLN:HB2	2.38	0.53
3:C:612:TYR:HB3	3:C:615:VAL:HB	1.90	0.53
2:E:146:THR:O	2:E:196:VAL:HA	2.09	0.53
3:A:132:GLU:HB2	3:A:164:ASN:HB3	1.89	0.53
3:C:403:ARG:HB3	3:C:406:GLU:OE1	2.09	0.53
3:B:435:ALA:HB1	3:B:508:TYR:HB3	1.91	0.53
3:A:394:ASN:OD1	3:A:516:GLU:HB2	2.09	0.53
3:A:965:GLN:HE22	3:B:758:SER:N	2.06	0.53
3:C:406:GLU:OE1	3:C:406:GLU:N	2.42	0.53
3:A:403:ARG:HB2	3:A:406:GLU:HG3	1.92	0.53
3:C:1091:ARG:NH2	3:C:1120:THR:O	2.42	0.53
1:D:97:TYR:O	1:D:121:GLY:HA2	2.10	0.52
1:D:151:ALA:O	1:D:198:THR:HA	2.09	0.52
3:A:429:PHE:HE1	3:A:514:SER:HB2	1.74	0.52
3:C:65:PHE:HB2	3:C:265:TYR:CZ	2.44	0.52
1:D:49:TRP:HE1	1:D:52:ARG:HG2	1.74	0.52
1:D:134:PRO:HB3	1:D:160:TYR:CD1	2.44	0.52
2:E:126:LEU:HD22	2:E:183:PRO:HB3	1.90	0.52
1:F:4:LEU:HB3	1:F:22:CYS:SG	2.49	0.52
3:B:378:LYS:HZ1	3:B:429:PHE:HD2	1.57	0.52
3:A:116:SER:HB2	3:A:135:PHE:HE2	1.75	0.52
3:A:719:THR:HB	3:A:1068:VAL:HG23	1.91	0.52
3:B:134:GLN:HB3	3:B:162:SER:H	1.74	0.52
3:B:196:ASN:C	3:B:197:ILE:HD13	2.35	0.52
1:F:110:TYR:CE1	1:F:112:TYR:HB3	2.45	0.52
3:A:170:TYR:HD1	3:A:171:VAL:N	2.08	0.52
3:A:228:ASP:OD1	3:A:229:LEU:N	2.43	0.52
3:C:1006:THR:O	3:C:1010:GLN:HG2	2.09	0.52
1:D:3:GLN:HA	1:D:101:ARG:HH22	1.74	0.52
1:F:115:MET:O	2:G:48:LEU:HD21	2.10	0.52
1:D:79:LYS:NZ	1:D:81:GLN:O	2.43	0.52
1:F:29:VAL:HG12	1:F:59:TRP:CH2	2.45	0.52
3:A:1105:THR:HG1	3:A:1111:GLU:H	1.57	0.52
3:B:35:GLY:HA3	3:B:56:LEU:HB3	1.92	0.52
1:D:53:THR:HA	1:D:61:ASN:HA	1.92	0.52
3:B:350:VAL:HG22	3:B:402:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:365:TYR:CD2	3:B:387:LEU:HB3	2.44	0.52
3:C:129:LYS:HE2	3:C:169:GLU:OE1	2.10	0.52
3:A:159:VAL:HG23	3:A:160:TYR:CD1	2.45	0.51
3:A:715:PRO:CA	3:A:1072:GLU:HA	2.21	0.51
3:B:125:ASN:ND2	3:B:172:SER:O	2.40	0.51
3:C:455:LEU:HD22	3:C:493:GLN:CB	2.40	0.51
2:E:33:ASN:ND2	2:E:52:GLU:OE1	2.43	0.51
3:A:360:ASN:ND2	3:B:168:PHE:CD1	2.79	0.51
2:E:145:VAL:HG12	2:E:198:HIS:HB2	1.92	0.51
1:F:33:SER:HB2	1:F:104:GLN:HB3	1.90	0.51
3:A:31:SER:O	3:A:59:PHE:CA	2.58	0.51
3:A:102:ARG:HG2	3:A:242:LEU:O	2.11	0.51
1:D:30:SER:HA	1:D:55:TYR:CD2	2.46	0.51
2:G:5:THR:O	2:G:23:THR:N	2.38	0.51
3:A:971:GLY:O	3:A:995:ARG:NH1	2.43	0.51
3:C:417:LYS:NZ	3:C:455:LEU:O	2.34	0.51
2:G:142:PRO:HA	2:G:173:TYR:HE2	1.76	0.51
3:A:48:LEU:O	3:A:304:LYS:NZ	2.39	0.51
3:A:947:LYS:O	3:A:951:VAL:HG13	2.10	0.51
1:F:86:LEU:HD22	1:F:89:VAL:HG22	1.92	0.51
1:F:102:GLU:HG3	1:F:112:TYR:CE2	2.46	0.51
2:G:140:PHE:HE1	2:G:143:GLY:HA2	1.75	0.51
3:A:41:LYS:HG3	3:C:562:PHE:HD2	1.75	0.51
3:B:880:GLY:O	3:B:884:SER:OG	2.25	0.51
3:C:280:ASN:OD1	3:C:284:THR:N	2.37	0.51
2:E:85:GLU:O	2:E:167:LYS:NZ	2.44	0.51
3:A:394:ASN:OD1	3:A:516:GLU:OE1	2.29	0.51
2:G:142:PRO:O	2:G:198:HIS:NE2	2.38	0.51
3:B:289:VAL:HG23	3:B:306:PHE:CE2	2.45	0.51
3:B:378:LYS:HE2	3:B:411:ALA:HA	1.93	0.51
2:E:186:TRP:HH2	2:E:207:VAL:HG22	1.76	0.50
2:G:35:ILE:HG21	2:G:73:ALA:HB2	1.93	0.50
3:A:312:ILE:HG23	3:A:312:ILE:O	2.10	0.50
3:A:897:PRO:HA	3:C:707:TYR:HE1	1.76	0.50
3:B:52:GLN:OE1	3:B:274:THR:OG1	2.22	0.50
1:D:167:VAL:HG11	1:D:195:SER:HB2	1.93	0.50
1:F:158:LYS:NZ	1:F:192:SER:HB3	2.27	0.50
2:G:189:HIS:HB2	2:G:192:TYR:CE2	2.47	0.50
3:A:231:ILE:HG22	3:A:233:ILE:HG23	1.92	0.50
3:B:454:ARG:HH11	3:B:492:LEU:HB2	1.77	0.50
3:C:383:SER:HB2	3:C:386:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:189:LEU:HG	3:A:210:ILE:HB	1.93	0.50
3:A:91:TYR:N	3:A:268:GLY:O	2.34	0.50
3:C:334:ASN:HB2	3:C:361:CYS:HA	1.94	0.50
1:F:100:ALA:HB1	1:F:115:MET:HE1	1.92	0.50
1:F:159:ASP:HA	1:F:190:LEU:HB3	1.91	0.50
3:C:538:CYS:SG	3:C:590:CYS:CB	2.99	0.50
1:D:24:ILE:HD12	1:D:24:ILE:O	2.12	0.50
1:D:40:ARG:NH1	1:D:70:ARG:HH22	2.07	0.50
3:A:96:GLU:O	3:A:188:ASN:ND2	2.45	0.50
3:A:141:LEU:O	3:A:244:LEU:HB3	2.11	0.50
3:B:572:THR:O	3:B:573:THR:OG1	2.30	0.50
1:F:41:GLN:HB3	1:F:96:VAL:HB	1.93	0.50
3:C:403:ARG:HG2	3:C:404:GLY:H	1.77	0.50
3:A:338:PHE:HE2	3:A:365:TYR:HE1	1.60	0.49
3:C:329:PHE:O	3:C:580:GLN:NE2	2.45	0.49
3:C:406:GLU:HG2	3:C:418:ILE:HD13	1.94	0.49
1:D:6:GLN:NE2	1:D:20:LEU:HD22	2.24	0.49
3:C:106:PHE:HB3	3:C:235:ILE:HD12	1.93	0.49
1:D:8:GLY:HA3	1:D:20:LEU:HD23	1.95	0.49
1:F:103:GLU:O	1:F:112:TYR:HB2	2.12	0.49
2:G:130:LYS:HZ1	2:G:180:SER:HA	1.76	0.49
3:A:338:PHE:HB3	3:A:342:PHE:HE2	1.77	0.49
3:B:101:ILE:HA	3:B:242:LEU:HA	1.95	0.49
3:B:412:PRO:HG2	3:B:429:PHE:HB2	1.95	0.49
3:C:423:TYR:HE2	3:C:512:VAL:HG21	1.77	0.49
3:B:242:LEU:HD21	3:B:265:TYR:OH	2.11	0.49
3:B:422:ASN:HB2	3:B:454:ARG:H	1.78	0.49
3:C:374:PHE:HA	3:C:436:TRP:HB3	1.95	0.49
1:D:71:ILE:HA	1:D:86:LEU:HA	1.95	0.49
2:G:41:HIS:H	2:G:44:LYS:HZ2	1.61	0.49
2:G:145:VAL:HG12	2:G:198:HIS:HB2	1.93	0.49
3:B:392:PHE:CG	3:B:515:PHE:HB3	2.48	0.49
3:C:353:TRP:HZ3	3:C:355:ARG:HE	1.61	0.49
1:D:40:ARG:HG2	1:D:50:LEU:HB2	1.94	0.49
1:D:160:TYR:CE2	1:D:165:VAL:CG2	2.95	0.49
2:G:126:LEU:HD22	2:G:183:PRO:HB3	1.94	0.49
1:D:54:TYR:CD2	3:A:486:PHE:HB2	2.48	0.49
3:A:41:LYS:HG3	3:C:562:PHE:CD2	2.48	0.49
3:A:244:LEU:HA	3:A:258:TRP:CE3	2.48	0.49
3:B:338:PHE:HZ	3:B:513:LEU:HD13	1.77	0.49
3:B:422:ASN:HB2	3:B:454:ARG:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:363:ALA:N	3:C:525:CYS:O	2.41	0.49
3:C:541:PHE:O	3:C:547:THR:HA	2.13	0.49
3:C:574:ASP:O	3:C:587:ILE:N	2.43	0.49
1:D:5:GLN:HG2	1:D:23:ALA:HB3	1.95	0.49
1:D:155:CYS:SG	1:D:195:SER:HB3	2.53	0.49
3:C:456:PHE:HB2	3:C:491:PRO:HA	1.95	0.49
1:F:106:LEU:HD22	1:F:109:ASP:H	1.77	0.49
3:B:299:THR:OG1	3:B:597:VAL:HG21	2.13	0.49
3:C:444:LYS:HE2	3:C:448:ASN:HA	1.95	0.49
2:G:24:GLY:HA3	2:G:29:ILE:HD13	1.95	0.48
3:A:229:LEU:HD12	3:A:231:ILE:HD11	1.94	0.48
3:B:421:TYR:HB3	3:B:454:ARG:O	2.13	0.48
3:C:438:SER:O	3:C:507:PRO:HG2	2.13	0.48
1:D:18:LEU:HB3	1:D:86:LEU:HB3	1.96	0.48
2:E:142:PRO:HD2	2:E:199:GLU:HG3	1.95	0.48
3:A:57:PRO:HB3	3:A:273:ARG:NH1	2.28	0.48
3:C:421:TYR:CG	3:C:457:ARG:HB3	2.48	0.48
1:D:19:SER:O	1:D:19:SER:OG	2.29	0.48
2:G:39:GLN:HE22	2:G:47:LYS:HE3	1.79	0.48
3:B:101:ILE:HD11	3:B:240:THR:OG1	2.13	0.48
3:B:916:LEU:HD12	3:B:923:ILE:HD12	1.95	0.48
3:C:724:THR:HB	3:C:934:ILE:HD11	1.94	0.48
2:G:54:SER:OG	2:G:66:GLY:O	2.20	0.48
3:B:965:GLN:HE22	3:C:757:GLY:HA3	1.77	0.48
3:C:133:PHE:HB2	3:C:135:PHE:CE1	2.48	0.48
1:D:70:ARG:HG3	1:D:71:ILE:HG23	1.96	0.48
2:E:17:SER:HA	2:E:78:SER:HA	1.96	0.48
2:E:35:ILE:HD12	2:E:73:ALA:HB1	1.95	0.48
2:G:68:LYS:HD2	2:G:73:ALA:HA	1.95	0.48
3:B:428:ASP:N	3:B:428:ASP:OD1	2.46	0.48
3:C:541:PHE:CD2	3:C:552:LEU:HD21	2.47	0.48
1:F:34:ALA:HA	1:F:102:GLU:O	2.14	0.48
2:G:139:ASP:C	2:G:172:LYS:HZ3	2.20	0.48
3:A:1097:SER:HB2	3:A:1102:TRP:CE3	2.48	0.48
3:C:455:LEU:HG	3:C:456:PHE:CD1	2.48	0.48
3:A:91:TYR:HD1	3:A:193:VAL:CG2	2.25	0.48
3:A:111:ASP:O	3:A:112:SER:OG	2.31	0.48
3:A:197:ILE:CG2	3:A:198:ASP:N	2.76	0.48
3:B:1105:THR:HG22	3:B:1112:PRO:HA	1.95	0.48
3:C:93:ALA:HB3	3:C:266:TYR:HD2	1.79	0.48
1:D:20:LEU:O	1:D:84:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ARG:O	1:D:87:ASN:N	2.35	0.48
2:E:40:GLN:O	2:E:86:ALA:HB1	2.14	0.48
2:E:140:PHE:HE2	2:E:143:GLY:HA2	1.78	0.48
1:F:110:TYR:HB3	3:B:487:ASN:N	2.27	0.48
3:A:931:ILE:O	3:A:934:ILE:HG22	2.13	0.48
3:A:1040:VAL:HG21	3:B:1035:GLY:HA3	1.95	0.48
3:C:473:TYR:O	3:C:488:CYS:HA	2.14	0.48
2:E:51:TYR:HD1	2:E:57:PRO:HG3	1.78	0.48
1:F:52:ARG:NE	1:F:62:ASP:OD2	2.47	0.48
3:A:127:VAL:C	3:A:128:ILE:HD13	2.38	0.48
3:B:168:PHE:CE2	3:B:170:TYR:HB2	2.49	0.48
3:C:108:THR:OG1	3:C:234:ASN:O	2.22	0.48
3:C:729:VAL:HG23	3:C:781:VAL:HG21	1.96	0.48
2:E:140:PHE:HB2	2:E:198:HIS:CE1	2.49	0.47
1:F:134:PRO:HD3	1:F:215:HIS:ND1	2.29	0.47
2:G:37:TRP:CD1	2:G:75:LEU:HB2	2.48	0.47
3:A:909:ILE:HG13	3:A:911:VAL:HG23	1.96	0.47
3:A:598:ILE:HG23	3:A:664:ILE:HG21	1.95	0.47
3:B:1116:THR:HA	3:B:1138:TYR:O	2.13	0.47
3:C:428:ASP:CG	3:C:429:PHE:H	2.22	0.47
3:C:121:ASN:OD1	3:C:121:ASN:N	2.47	0.47
3:C:439:ASN:O	3:C:443:SER:OG	2.27	0.47
2:G:140:PHE:CE1	2:G:173:TYR:HB2	2.49	0.47
3:B:355:ARG:NH2	3:B:398:ASP:OD2	2.41	0.47
3:C:393:THR:HG21	3:C:520:ALA:HB3	1.96	0.47
3:C:1086:LYS:HB2	3:C:1122:VAL:HG23	1.94	0.47
1:D:13:LYS:O	1:D:16:GLN:HG2	2.13	0.47
1:D:52:ARG:HG3	1:D:62:ASP:OD1	2.14	0.47
1:D:183:ALA:HB2	1:D:193:LEU:HB2	1.96	0.47
3:B:392:PHE:CD1	3:B:515:PHE:HB3	2.49	0.47
3:B:498:GLN:HB2	3:B:501:ASN:HB2	1.96	0.47
3:C:287:ASP:HB3	3:C:306:PHE:HE2	1.79	0.47
1:F:162:PRO:HD2	1:F:215:HIS:CE1	2.49	0.47
3:A:310:LYS:HE2	3:A:664:ILE:HD11	1.96	0.47
3:A:402:ILE:HD11	3:A:510:VAL:HG21	1.96	0.47
3:B:453:TYR:CZ	3:B:455:LEU:HB2	2.49	0.47
3:B:815:ARG:HB3	3:B:819:GLU:HB3	1.96	0.47
3:C:326:ILE:HG22	3:C:328:ARG:HG2	1.95	0.47
3:C:415:THR:OG1	3:C:416:GLY:N	2.48	0.47
3:C:457:ARG:NH1	3:C:467:ASP:OD2	2.47	0.47
1:D:138:PRO:HG3	1:D:224:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:PRO:HD2	1:D:215:HIS:CE1	2.50	0.47
2:G:141:TYR:H	2:G:198:HIS:CE1	2.33	0.47
3:A:353:TRP:HE3	3:A:355:ARG:H	1.63	0.47
3:B:100:ILE:HG22	3:B:242:LEU:HD23	1.97	0.47
3:B:737:ASP:HB3	3:B:740:MET:HB3	1.96	0.47
2:G:139:ASP:HA	2:G:168:GLN:HE22	1.79	0.47
3:A:986:PRO:N	3:A:987:PRO:HD2	2.30	0.47
3:B:406:GLU:OE1	3:B:409:GLN:NE2	2.47	0.47
2:E:9:SER:HA	2:E:104:LYS:H	1.80	0.47
2:E:113:ASN:OD1	2:E:114:PRO:HD2	2.14	0.47
1:D:74:ASN:H	1:D:85:GLN:HE22	1.61	0.47
2:E:116:VAL:O	2:E:205:LYS:HE3	2.15	0.47
3:A:392:PHE:CG	3:A:515:PHE:HB3	2.50	0.47
3:A:1082:CYS:HB2	3:A:1132:ILE:HG12	1.97	0.47
3:C:126:VAL:HG13	3:C:173:GLN:O	2.14	0.47
3:C:365:TYR:CZ	3:C:515:PHE:CZ	2.73	0.47
3:C:401:VAL:HG22	3:C:509:ARG:HG2	1.95	0.47
2:G:151:ALA:HB1	2:G:189:HIS:CD2	2.49	0.46
3:A:140:PHE:CD1	3:A:244:LEU:HD22	2.50	0.46
1:F:100:ALA:HB1	1:F:115:MET:CE	2.46	0.46
2:G:112:ALA:HB3	2:G:172:LYS:NZ	2.31	0.46
3:A:81:ASN:HB3	3:A:239:GLN:HE21	1.79	0.46
3:A:89:GLY:HA3	3:A:270:LEU:HD12	1.97	0.46
3:A:97:LYS:HD2	3:A:186:PHE:HA	1.96	0.46
3:A:382:VAL:HB	3:A:387:LEU:HD11	1.97	0.46
3:B:359:SER:HA	3:B:524:VAL:HB	1.97	0.46
3:B:475:ALA:HB3	3:B:487:ASN:ND2	2.30	0.46
1:D:40:ARG:HG3	1:D:48:GLU:HG2	1.96	0.46
1:F:55:TYR:HB2	1:F:59:TRP:CZ3	2.50	0.46
3:A:454:ARG:HH21	3:A:457:ARG:HA	1.80	0.46
3:B:478:THR:HG21	3:B:487:ASN:HB3	1.98	0.46
3:B:897:PRO:HG2	3:B:900:MET:HB2	1.97	0.46
3:C:948:LEU:O	3:C:951:VAL:HG12	2.16	0.46
1:D:224:LYS:NZ	1:D:225:ARG:O	2.48	0.46
1:F:70:ARG:HB3	1:F:87:ASN:O	2.15	0.46
2:G:38:TYR:HE2	2:G:91:SER:HB3	1.79	0.46
3:A:612:TYR:HE2	3:A:651:ILE:HD12	1.80	0.46
3:A:951:VAL:HA	3:A:954:GLN:OE1	2.16	0.46
3:B:338:PHE:HE2	3:B:513:LEU:HD11	1.81	0.46
3:B:555:SER:HB3	3:B:586:ASP:N	2.31	0.46
2:G:168:GLN:NE2	2:G:172:LYS:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:817:PHE:HD1	3:A:817:PHE:H	1.62	0.46
3:C:986:PRO:N	3:C:987:PRO:HD2	2.30	0.46
1:F:215:HIS:O	1:F:219:ASN:N	2.49	0.46
3:A:418:ILE:O	3:A:422:ASN:HB2	2.16	0.46
3:B:106:PHE:HB2	3:B:117:LEU:HB3	1.97	0.46
3:A:38:TYR:HE2	3:A:224:GLU:HG3	1.80	0.46
3:A:1141:LEU:HD13	3:C:1141:LEU:HD22	1.97	0.46
3:B:170:TYR:CE1	3:B:172:SER:HB2	2.48	0.46
3:B:449:TYR:HD1	3:B:494:SER:OG	1.97	0.46
3:C:89:GLY:HA2	3:C:194:PHE:O	2.16	0.46
3:C:414:GLN:HG3	3:C:415:THR:N	2.31	0.46
3:C:662:CYS:HB2	3:C:671:CYS:HB3	1.61	0.46
1:D:79:LYS:O	1:D:81:GLN:HG3	2.16	0.46
2:G:56:ARG:HD3	2:G:62:TYR:HA	1.98	0.46
3:A:401:VAL:HG11	3:A:451:TYR:CE2	2.50	0.46
3:C:106:PHE:HA	3:C:238:PHE:HA	1.97	0.46
2:G:133:LEU:HD12	2:G:133:LEU:H	1.80	0.46
3:C:204:TYR:HA	3:C:225:PRO:HA	1.98	0.46
1:D:181:PHE:CD2	2:E:176:SER:HB3	2.51	0.46
3:A:336:CYS:HB3	3:A:361:CYS:HB2	1.38	0.46
3:A:377:PHE:CD1	3:A:436:TRP:HD1	2.34	0.46
3:B:326:ILE:HD11	3:B:552:LEU:HD11	1.98	0.46
3:B:403:ARG:HG2	3:B:497:PHE:CE1	2.51	0.46
3:C:122:ASN:OD1	3:C:123:ALA:N	2.48	0.46
3:C:168:PHE:CE1	3:C:170:TYR:HB2	2.51	0.46
3:C:449:TYR:HA	3:C:494:SER:HB3	1.98	0.46
1:F:106:LEU:HD13	1:F:111:TYR:HB2	1.97	0.45
2:G:125:GLU:CD	2:G:132:THR:H	2.24	0.45
3:A:412:PRO:HB2	3:A:427:ASP:HA	1.97	0.45
3:A:713:ALA:HB2	3:B:895:GLN:HG2	1.98	0.45
3:B:434:ILE:O	3:B:510:VAL:HA	2.16	0.45
3:B:733:LYS:HE3	3:B:771:ALA:HB1	1.97	0.45
3:C:103:GLY:HA3	3:C:241:LEU:HD12	1.98	0.45
3:C:119:ILE:O	3:C:119:ILE:HG23	2.16	0.45
1:D:109:ASP:OD1	1:D:110:TYR:N	2.49	0.45
1:F:94:THR:HA	1:F:124:VAL:O	2.16	0.45
2:G:118:LEU:HD11	2:G:194:CYS:HB2	1.98	0.45
3:A:399:SER:HA	3:A:511:VAL:HG12	1.98	0.45
3:A:763:LEU:HD21	3:A:1005:GLN:HG3	1.98	0.45
3:A:853:GLN:HB2	3:A:858:LEU:HD12	1.99	0.45
3:B:118:LEU:HB3	3:B:133:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:GLN:NE2	1:D:116:ASP:OD2	2.37	0.45
3:C:29:THR:HG23	3:C:62:VAL:HG13	1.98	0.45
3:C:90:VAL:HG13	3:C:267:VAL:HG13	1.97	0.45
3:C:605:SER:OG	3:C:606:ASN:N	2.49	0.45
3:A:422:ASN:N	3:A:422:ASN:HD22	2.13	0.45
3:B:334:ASN:O	3:B:362:VAL:HG22	2.16	0.45
3:B:457:ARG:HH21	3:B:461:LEU:HA	1.81	0.45
3:B:977:LEU:HD12	3:B:978:ASN:N	2.31	0.45
3:C:122:ASN:N	3:C:125:ASN:O	2.50	0.45
2:G:148:ALA:HB1	2:G:155:PRO:HB3	1.98	0.45
3:A:365:TYR:H	3:A:388:ASN:ND2	2.15	0.45
3:A:740:MET:HG2	3:C:592:PHE:HE2	1.82	0.45
3:B:277:LEU:HD13	3:B:285:ILE:HD13	1.99	0.45
3:B:303:LEU:HD11	3:B:313:TYR:CE1	2.52	0.45
3:B:717:ASN:HB3	3:B:1071:GLN:HB2	1.98	0.45
3:B:776:LYS:HA	3:B:776:LYS:HD3	1.81	0.45
3:B:462:LYS:HD2	3:B:462:LYS:HA	1.72	0.45
1:F:2:VAL:HG12	1:F:26:GLY:HA3	1.99	0.45
1:F:52:ARG:NH2	2:G:93:TYR:OH	2.50	0.45
3:A:715:PRO:HG3	3:A:1072:GLU:CG	2.42	0.45
3:A:740:MET:HG2	3:C:592:PHE:CE2	2.52	0.45
3:B:600:PRO:HB3	3:B:674:TYR:HB2	1.99	0.45
3:B:1086:LYS:HE3	3:B:1086:LYS:HB2	1.78	0.45
3:C:290:ASP:O	3:C:297:SER:HB3	2.16	0.45
3:A:650:LEU:HD12	3:A:650:LEU:HA	1.83	0.45
3:A:734:THR:HG22	3:A:860:VAL:HG22	1.99	0.45
3:B:350:VAL:CG2	3:B:401:VAL:O	2.65	0.45
3:B:826:VAL:HB	3:B:1057:PRO:HG2	1.99	0.45
3:C:428:ASP:C	3:C:430:THR:H	2.24	0.45
1:F:29:VAL:HA	1:F:36:TRP:CZ2	2.52	0.45
1:F:156:LEU:HD11	1:F:158:LYS:NZ	2.32	0.45
3:A:309:GLU:HG2	3:A:310:LYS:H	1.82	0.45
3:A:774:GLN:O	3:A:777:ASN:HB2	2.17	0.45
3:B:172:SER:OG	3:B:173:GLN:N	2.50	0.45
1:D:37:ASN:ND2	1:D:52:ARG:HD3	2.31	0.45
3:B:896:ILE:HG13	3:B:897:PRO:HD2	1.99	0.45
1:F:9:PRO:HD2	1:F:20:LEU:HD12	1.99	0.44
2:G:39:GLN:OE1	2:G:39:GLN:N	2.49	0.44
2:G:152:ASP:HA	2:G:191:SER:HB3	1.99	0.44
3:A:122:ASN:OD1	3:A:125:ASN:N	2.50	0.44
3:A:365:TYR:H	3:A:388:ASN:HD21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:716:THR:N	3:B:1071:GLN:O	2.34	0.44
1:D:9:PRO:HB2	1:D:12:VAL:HG12	1.98	0.44
1:D:140:ALA:H	2:E:122:SER:HB3	1.82	0.44
2:E:183:PRO:O	2:E:187:LYS:HG2	2.17	0.44
1:F:184:VAL:HG11	2:G:161:GLU:HG3	1.99	0.44
3:A:404:GLY:HA2	3:A:508:TYR:CE2	2.52	0.44
3:A:424:LYS:HD3	3:A:461:LEU:O	2.16	0.44
3:B:66:HIS:HA	3:B:263:ALA:HB1	1.99	0.44
3:B:309:GLU:CD	3:B:309:GLU:H	2.25	0.44
3:B:1029:MET:HE2	3:B:1029:MET:HB2	1.83	0.44
3:C:900:MET:HE2	3:C:900:MET:HB3	1.77	0.44
1:F:54:TYR:CE1	1:F:60:TYR:HB2	2.51	0.44
3:A:350:VAL:HG22	3:A:423:TYR:HB3	1.98	0.44
3:C:132:GLU:N	3:C:164:ASN:O	2.45	0.44
3:C:350:VAL:HG23	3:C:400:PHE:CD2	2.51	0.44
3:C:931:ILE:O	3:C:934:ILE:HG22	2.17	0.44
1:F:71:ILE:HG13	1:F:84:LEU:HD11	1.99	0.44
2:G:118:LEU:HB3	2:G:207:VAL:HG21	1.99	0.44
3:C:816:SER:N	3:C:819:GLU:OE1	2.37	0.44
3:C:996:LEU:HD23	3:C:996:LEU:HA	1.79	0.44
1:F:18:LEU:HD11	1:F:20:LEU:HD13	1.98	0.44
1:F:31:SER:HB3	1:F:34:ALA:HB3	1.98	0.44
1:F:54:TYR:OH	3:B:483:VAL:HA	2.16	0.44
3:A:362:VAL:HA	3:A:525:CYS:O	2.18	0.44
3:A:671:CYS:SG	3:A:697:MET:HE3	2.57	0.44
3:B:538:CYS:HB2	3:B:590:CYS:HB3	1.58	0.44
3:B:1077:THR:OG1	3:B:1078:ALA:N	2.51	0.44
3:C:93:ALA:O	3:C:265:TYR:HA	2.17	0.44
3:C:121:ASN:HB3	3:C:126:VAL:HG12	1.99	0.44
3:C:814:LYS:HA	3:C:814:LYS:HD2	1.75	0.44
3:A:287:ASP:HB3	3:A:306:PHE:HE2	1.81	0.44
3:A:359:SER:HA	3:A:524:VAL:HB	2.00	0.44
3:A:1080:ALA:HB3	3:A:1132:ILE:HD12	1.99	0.44
3:B:30:ASN:HB3	3:B:32:PHE:CE1	2.52	0.44
3:B:458:LYS:HE2	3:B:458:LYS:HB3	1.84	0.44
3:C:281:GLU:HG2	3:C:282:ASN:OD1	2.17	0.44
3:C:983:ARG:O	3:C:983:ARG:CG	2.66	0.44
3:C:1054:GLN:HE21	3:C:1054:GLN:HA	1.81	0.44
2:E:116:VAL:HG11	2:E:196:VAL:HG21	1.99	0.44
1:F:110:TYR:HE1	1:F:112:TYR:HB3	1.80	0.44
3:B:289:VAL:CG2	3:B:306:PHE:CE2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:822:LEU:HG	3:B:945:LEU:HD21	1.98	0.44
3:C:116:SER:HB2	3:C:135:PHE:HZ	1.83	0.44
3:C:544:ASN:HD21	3:C:579:PRO:HD3	1.82	0.44
1:D:151:ALA:HB3	1:D:199:VAL:O	2.18	0.44
1:F:67:VAL:O	1:F:71:ILE:HG22	2.17	0.44
1:F:162:PRO:HB2	1:F:215:HIS:NE2	2.33	0.44
2:G:36:SER:HB2	2:G:91:SER:OG	2.17	0.44
3:A:65:PHE:HZ	3:A:84:LEU:HD11	1.80	0.44
3:A:662:CYS:HB2	3:A:697:MET:HE2	2.00	0.44
3:B:36:VAL:O	3:B:222:ALA:HA	2.18	0.44
3:C:110:LEU:HA	3:C:135:PHE:CE2	2.52	0.44
2:G:26:SER:HA	2:G:30:GLY:H	1.83	0.44
3:B:227:VAL:CG1	3:B:229:LEU:HG	2.48	0.44
1:F:229:LYS:NZ	2:G:212:CYS:SG	2.91	0.43
3:B:117:LEU:HD12	3:B:118:LEU:H	1.83	0.43
3:B:130:VAL:HG13	3:B:167:THR:OG1	2.18	0.43
3:B:448:ASN:CG	3:B:449:TYR:H	2.26	0.43
3:B:730:SER:O	3:B:1058:HIS:HB3	2.18	0.43
3:B:934:ILE:HD13	3:B:934:ILE:HA	1.88	0.43
3:C:434:ILE:HG22	3:C:511:VAL:HB	2.00	0.43
1:D:82:PHE:HZ	1:D:99:CYS:HB2	1.83	0.43
2:E:186:TRP:CH2	2:E:207:VAL:HG22	2.53	0.43
3:A:34:ARG:HD2	3:A:216:LEU:HD13	2.00	0.43
3:A:474:GLN:NE2	3:A:487:ASN:O	2.42	0.43
3:B:290:ASP:O	3:B:297:SER:HB2	2.18	0.43
3:C:103:GLY:N	3:C:241:LEU:HB2	2.33	0.43
1:D:160:TYR:CD2	1:D:165:VAL:HG21	2.52	0.43
3:A:243:ALA:HB1	3:A:245:HIS:CD2	2.53	0.43
3:A:480:CYS:HB2	3:A:483:VAL:HG22	1.99	0.43
3:C:276:LEU:HD23	3:C:306:PHE:HE1	1.84	0.43
3:C:977:LEU:HD22	3:C:993:ILE:HD12	1.99	0.43
2:E:18:ILE:HD13	2:E:80:LEU:HD11	2.00	0.43
1:F:166:THR:HG22	1:F:216:LYS:NZ	2.33	0.43
2:G:49:ILE:O	2:G:50:ILE:HG12	2.18	0.43
3:A:126:VAL:HG23	3:A:174:PRO:HA	1.99	0.43
3:A:201:PHE:N	3:A:229:LEU:O	2.47	0.43
3:A:600:PRO:HB3	3:A:674:TYR:HB2	1.99	0.43
3:A:979:ASP:OD1	3:A:979:ASP:C	2.61	0.43
3:B:367:VAL:HG23	3:B:368:LEU:HD12	1.99	0.43
3:C:453:TYR:HB3	3:C:495:TYR:CE1	2.54	0.43
3:C:551:VAL:N	3:C:588:THR:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:LEU:HB2	2:E:179:LEU:HB3	2.00	0.43
2:G:160:VAL:HG22	2:G:179:LEU:HD13	2.00	0.43
3:A:101:ILE:HA	3:A:242:LEU:HD12	2.00	0.43
3:A:770:ILE:O	3:A:774:GLN:HG2	2.18	0.43
3:B:425:LEU:HG	3:B:426:PRO:HD2	2.00	0.43
1:D:181:PHE:CZ	2:E:136:LEU:HB3	2.54	0.43
3:A:68:ILE:O	3:A:78:ARG:HB3	2.19	0.43
3:A:1072:GLU:CD	3:B:892:ALA:HB3	2.32	0.43
3:A:1125:ASN:OD1	3:A:1126:CYS:N	2.50	0.43
3:C:353:TRP:HB3	3:C:400:PHE:HB3	2.00	0.43
3:A:737:ASP:HB3	3:A:740:MET:HB3	2.00	0.43
3:B:338:PHE:CE2	3:B:513:LEU:HD11	2.53	0.43
3:B:699:LEU:HD22	3:C:873:TYR:CZ	2.53	0.43
3:C:200:TYR:CE1	3:C:230:PRO:HB3	2.53	0.43
3:C:235:ILE:HD13	3:C:235:ILE:HA	1.87	0.43
3:C:754:LEU:HD23	3:C:754:LEU:HA	1.82	0.43
1:D:106:LEU:O	1:D:108:HIS:N	2.47	0.43
1:D:191:TYR:HD1	1:D:191:TYR:HA	1.77	0.43
1:F:106:LEU:O	1:F:106:LEU:HD23	2.19	0.43
3:A:383:SER:O	3:A:387:LEU:HD22	2.18	0.43
3:A:973:ILE:HD12	3:A:983:ARG:NH2	2.34	0.43
2:G:119:PHE:HB2	2:G:134:VAL:CG2	2.49	0.43
3:B:409:GLN:O	3:B:419:ALA:HB2	2.18	0.43
3:C:328:ARG:NH2	3:C:580:GLN:OE1	2.52	0.43
3:C:402:ILE:HD12	3:C:402:ILE:HA	1.86	0.43
3:C:763:LEU:HD13	3:C:1004:LEU:HG	2.00	0.43
1:D:177:GLY:O	1:D:197:VAL:HA	2.19	0.43
2:E:140:PHE:CE2	2:E:143:GLY:HA2	2.53	0.43
1:F:115:MET:HE3	1:F:116:ASP:N	2.34	0.43
1:F:181:PHE:CE1	2:G:174:ALA:HB1	2.54	0.43
2:G:181:LEU:HB3	2:G:185:GLN:HG2	2.00	0.43
2:G:183:PRO:O	2:G:187:LYS:HG2	2.18	0.43
3:A:212:LEU:HD13	3:A:215:ASP:HB3	2.00	0.43
3:A:380:TYR:HB2	3:A:433:VAL:HG11	2.01	0.43
3:B:44:ARG:HB2	3:B:279:TYR:CD2	2.53	0.43
3:B:759:PHE:CD2	3:B:1001:LEU:HD21	2.54	0.43
3:B:965:GLN:NE2	3:C:757:GLY:HA3	2.34	0.43
1:D:6:GLN:HG2	1:D:22:CYS:HB2	2.01	0.42
2:E:133:LEU:HD13	2:E:179:LEU:HD23	2.01	0.42
2:G:207:VAL:HA	2:G:211:GLU:OE1	2.18	0.42
3:A:92:PHE:HE2	3:A:240:THR:HG21	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:496:GLY:O	3:A:501:ASN:ND2	2.51	0.42
3:A:752:LEU:O	3:A:755:GLN:HG2	2.19	0.42
3:A:1072:GLU:CG	3:B:894:LEU:HD21	2.40	0.42
3:B:105:ILE:HG13	3:B:239:GLN:HB3	2.01	0.42
3:C:105:ILE:HG23	3:C:105:ILE:O	2.18	0.42
3:C:350:VAL:HG21	3:C:402:ILE:HD13	2.01	0.42
3:A:753:LEU:HD21	3:A:760:CYS:SG	2.59	0.42
3:B:336:CYS:N	3:B:362:VAL:O	2.47	0.42
3:B:342:PHE:HA	3:B:342:PHE:HD1	1.71	0.42
3:B:578:ASP:CG	3:B:581:THR:HG22	2.44	0.42
1:F:184:VAL:HG21	2:G:161:GLU:HB2	2.01	0.42
3:A:338:PHE:HE2	3:A:365:TYR:CE1	2.38	0.42
3:B:402:ILE:HD12	3:B:418:ILE:HG21	2.01	0.42
3:B:412:PRO:HB3	3:B:426:PRO:O	2.19	0.42
1:D:5:GLN:N	1:D:5:GLN:OE1	2.52	0.42
1:D:111:TYR:CE1	3:A:476:GLY:HA2	2.54	0.42
2:E:161:GLU:HG3	2:E:178:TYR:HB2	2.01	0.42
3:A:244:LEU:HA	3:A:258:TRP:HE3	1.85	0.42
3:A:319:ARG:HE	3:A:592:PHE:HB2	1.85	0.42
3:A:409:GLN:N	3:A:409:GLN:OE1	2.52	0.42
3:A:568:ASP:O	3:A:570:ALA:N	2.52	0.42
3:C:388:ASN:HB3	3:C:528:LYS:NZ	2.34	0.42
3:C:409:GLN:NE2	3:C:418:ILE:HB	2.34	0.42
3:C:897:PRO:HG2	3:C:900:MET:HG3	2.01	0.42
1:D:56:ARG:HG2	3:A:485:GLY:CA	2.49	0.42
1:F:38:TRP:CG	1:F:84:LEU:HD13	2.55	0.42
3:C:570:ALA:O	3:C:572:THR:HG23	2.20	0.42
1:D:32:ASN:O	1:D:56:ARG:NH2	2.53	0.42
2:E:108:LEU:HD13	2:E:108:LEU:HA	1.92	0.42
1:F:24:ILE:HD13	1:F:29:VAL:HG22	2.02	0.42
1:F:166:THR:HG22	1:F:216:LYS:HZ3	1.85	0.42
3:A:280:ASN:OD1	3:A:284:THR:N	2.51	0.42
3:A:901:GLN:O	3:A:905:ARG:HG2	2.20	0.42
3:C:194:PHE:CD1	3:C:203:ILE:HG13	2.54	0.42
3:C:327:VAL:HA	3:C:542:ASN:HB3	2.01	0.42
1:D:181:PHE:HE2	2:E:136:LEU:HD23	1.84	0.42
2:E:39:GLN:HE22	2:E:41:HIS:HD2	1.65	0.42
1:F:140:ALA:HB2	2:G:122:SER:HA	2.01	0.42
3:A:462:LYS:HG3	3:A:465:GLU:HB2	2.01	0.42
3:B:770:ILE:HD11	3:B:1012:LEU:HA	2.00	0.42
3:C:1012:LEU:HD23	3:C:1012:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:SER:HA	2:E:30:GLY:H	1.84	0.42
2:G:93:TYR:OH	3:B:484:GLU:O	2.34	0.42
3:A:33:THR:HA	3:A:58:PHE:CD1	2.54	0.42
3:B:310:LYS:HG3	3:B:664:ILE:HD11	2.02	0.42
3:B:457:ARG:HE	3:B:461:LEU:HG	1.85	0.42
3:B:599:THR:HG23	3:B:608:VAL:HG12	2.02	0.42
3:C:437:ASN:ND2	3:C:506:GLN:OE1	2.39	0.42
3:C:472:ILE:HG22	3:C:488:CYS:HB3	2.01	0.42
3:C:714:ILE:HD13	3:C:714:ILE:HA	1.90	0.42
2:E:50:ILE:HG13	2:E:75:LEU:HD13	2.02	0.42
3:A:119:ILE:HG12	3:A:128:ILE:HG23	2.02	0.42
3:A:938:LEU:HD23	3:A:938:LEU:HA	1.84	0.42
3:B:581:THR:O	3:B:582:LEU:C	2.63	0.42
2:G:151:ALA:HB1	2:G:189:HIS:CG	2.55	0.42
3:A:210:ILE:HD11	3:A:212:LEU:HB2	2.02	0.42
3:A:540:ASN:HA	3:A:549:THR:HA	2.02	0.42
3:A:780:GLU:CD	3:A:1019:ARG:HH12	2.28	0.42
3:B:409:GLN:NE2	3:B:417:LYS:H	2.18	0.42
3:B:708:SER:HB2	3:B:711:SER:HB2	2.02	0.42
3:C:206:LYS:HD2	3:C:206:LYS:HA	1.87	0.42
3:C:317:ASN:HA	3:C:594:GLY:HA2	2.02	0.42
3:C:555:SER:HB3	3:C:584:ILE:O	2.20	0.42
1:F:156:LEU:HD11	1:F:158:LYS:HZ3	1.84	0.41
2:G:116:VAL:HG11	2:G:196:VAL:HG21	2.02	0.41
2:G:135:CYS:HB3	2:G:177:SER:HB3	2.02	0.41
3:B:715:PRO:HA	3:B:1072:GLU:HA	2.02	0.41
3:B:815:ARG:HD2	3:B:823:PHE:CD2	2.54	0.41
3:B:964:LYS:HE2	3:B:964:LYS:HB2	1.78	0.41
1:F:11:LEU:HD13	1:F:11:LEU:HA	1.94	0.41
3:A:344:ALA:HB3	3:A:347:PHE:HE1	1.85	0.41
3:A:409:GLN:HA	3:A:414:GLN:HG2	2.02	0.41
3:A:568:ASP:OD1	3:A:568:ASP:N	2.52	0.41
3:A:873:TYR:CZ	3:C:699:LEU:HD23	2.55	0.41
3:C:502:GLY:O	3:C:506:GLN:HG3	2.20	0.41
2:E:63:ARG:NH1	2:E:81:GLN:OE1	2.54	0.41
2:G:20:ILE:HD13	2:G:103:THR:HB	2.02	0.41
3:B:1040:VAL:HG11	3:C:1034:LEU:O	2.20	0.41
3:C:200:TYR:CZ	3:C:230:PRO:HB3	2.54	0.41
3:C:475:ALA:HB3	3:C:487:ASN:HB3	2.03	0.41
3:C:966:LEU:HD23	3:C:966:LEU:HA	1.81	0.41
1:D:109:ASP:OD1	3:A:489:TYR:OH	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:SER:OG	1:F:29:VAL:N	2.52	0.41
2:G:41:HIS:CE1	2:G:86:ALA:HB2	2.56	0.41
2:G:71:ASN:OD1	2:G:71:ASN:N	2.52	0.41
2:G:82:ALA:HA	2:G:107:VAL:HG21	2.02	0.41
2:G:150:LYS:HA	2:G:155:PRO:HA	2.03	0.41
3:A:280:ASN:ND2	3:A:284:THR:OG1	2.53	0.41
3:A:742:ILE:HG22	3:A:743:CYS:SG	2.60	0.41
3:A:762:GLN:CD	3:A:762:GLN:H	2.28	0.41
3:B:473:TYR:CE1	3:B:475:ALA:HB2	2.55	0.41
3:C:353:TRP:CE2	3:C:466:ARG:HG3	2.54	0.41
1:D:112:TYR:O	1:D:114:GLY:N	2.53	0.41
1:D:210:ILE:HA	1:D:225:ARG:HA	2.02	0.41
2:E:13:SER:O	2:E:16:GLN:HB2	2.21	0.41
2:G:130:LYS:HD2	2:G:130:LYS:HA	1.62	0.41
3:A:326:ILE:HG13	3:A:541:PHE:HA	2.02	0.41
3:A:402:ILE:HB	3:A:406:GLU:HB2	2.02	0.41
3:A:404:GLY:HA3	3:A:503:VAL:O	2.20	0.41
3:A:564:GLN:HG2	3:B:41:LYS:HD3	2.00	0.41
3:A:722:VAL:HG12	3:A:934:ILE:HD12	2.03	0.41
3:A:817:PHE:CD1	3:A:817:PHE:N	2.87	0.41
1:D:72:THR:HB	1:D:85:GLN:HB2	2.02	0.41
3:B:472:ILE:HG12	3:B:490:PHE:CE1	2.55	0.41
3:C:82:PRO:HB3	3:C:239:GLN:HB3	2.01	0.41
3:C:985:ASP:HB3	3:C:987:PRO:HD2	2.02	0.41
1:D:82:PHE:CZ	1:D:99:CYS:HB2	2.55	0.41
2:E:134:VAL:HG12	2:E:178:TYR:HD1	1.85	0.41
2:G:13:SER:HA	2:G:108:LEU:HB2	2.02	0.41
3:A:796:ASP:OD1	3:A:796:ASP:N	2.53	0.41
3:B:336:CYS:HB2	3:B:363:ALA:HB2	2.02	0.41
3:B:753:LEU:O	3:B:756:TYR:HB2	2.20	0.41
3:B:993:ILE:O	3:B:997:ILE:HG12	2.20	0.41
3:B:1114:ILE:HD13	3:B:1114:ILE:HA	1.88	0.41
3:C:129:LYS:HG2	3:C:169:GLU:HG2	2.03	0.41
3:C:455:LEU:HD23	3:C:491:PRO:O	2.19	0.41
2:E:189:HIS:HB2	2:E:192:TYR:CE1	2.55	0.41
3:A:452:LEU:HD13	3:A:494:SER:HA	2.02	0.41
3:A:1104:VAL:HG23	3:A:1115:ILE:HG12	2.02	0.41
3:B:202:LYS:O	3:B:203:ILE:HD13	2.21	0.41
1:F:55:TYR:C	1:F:56:ARG:HH11	2.29	0.41
2:G:37:TRP:CE2	2:G:75:LEU:HB2	2.56	0.41
3:A:41:LYS:HB2	3:A:41:LYS:HE2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:276:LEU:HD23	3:A:306:PHE:HE1	1.85	0.41
3:A:854:LYS:HA	3:A:858:LEU:O	2.20	0.41
3:A:897:PRO:HD3	3:C:711:SER:O	2.20	0.41
3:A:959:LEU:HD23	3:A:959:LEU:HA	1.71	0.41
3:A:1029:MET:HE2	3:A:1029:MET:HB2	1.91	0.41
3:B:319:ARG:HA	3:B:592:PHE:HB2	2.02	0.41
3:B:948:LEU:O	3:B:951:VAL:HG22	2.20	0.41
3:B:994:ASP:OD1	3:B:994:ASP:C	2.64	0.41
3:C:574:ASP:HA	3:C:587:ILE:HB	2.02	0.41
1:D:157:VAL:HG23	1:D:160:TYR:CE1	2.55	0.41
2:E:26:SER:O	2:E:31:ALA:N	2.52	0.41
3:A:377:PHE:CD1	3:A:436:TRP:CD1	3.09	0.41
3:C:409:GLN:OE1	3:C:417:LYS:N	2.54	0.41
3:C:457:ARG:HG3	3:C:459:SER:H	1.85	0.41
1:F:12:VAL:HB	1:F:16:GLN:HE22	1.86	0.40
3:A:444:LYS:O	3:A:499:PRO:HD3	2.21	0.40
3:B:395:VAL:HG23	3:B:524:VAL:HG11	2.03	0.40
3:C:905:ARG:HD3	3:C:1049:LEU:O	2.22	0.40
2:E:186:TRP:HZ2	2:E:212:CYS:HB2	1.86	0.40
1:F:181:PHE:HE1	2:G:138:SER:HB3	1.86	0.40
3:A:993:ILE:HG22	3:A:997:ILE:HD12	2.03	0.40
3:B:128:ILE:HB	3:B:170:TYR:HB3	2.03	0.40
3:B:537:LYS:O	3:B:539:VAL:HG13	2.21	0.40
3:C:37:TYR:OH	3:C:54:LEU:O	2.22	0.40
1:F:36:TRP:CZ3	1:F:101:ARG:HD3	2.49	0.40
2:G:10:VAL:O	2:G:105:VAL:HA	2.21	0.40
2:G:49:ILE:HD12	2:G:49:ILE:C	2.46	0.40
3:A:398:ASP:HB3	3:A:400:PHE:CE2	2.56	0.40
3:A:788:ILE:O	3:A:788:ILE:HG13	2.22	0.40
3:B:707:TYR:CE1	3:C:897:PRO:HA	2.57	0.40
2:G:39:GLN:NE2	2:G:47:LYS:HB3	2.37	0.40
3:A:188:ASN:OD1	3:A:188:ASN:N	2.54	0.40
3:A:296:LEU:HG	3:A:300:LYS:NZ	2.36	0.40
3:A:383:SER:HB2	3:A:386:LYS:HB2	2.04	0.40
3:A:761:THR:HA	3:A:764:ASN:HD21	1.86	0.40
3:B:353:TRP:H	3:B:353:TRP:CD1	2.39	0.40
3:C:418:ILE:HG13	3:C:422:ASN:OD1	2.21	0.40
3:C:513:LEU:HD23	3:C:513:LEU:HA	1.85	0.40
3:C:1049:LEU:HD23	3:C:1049:LEU:HA	1.91	0.40
1:D:104:GLN:CD	1:D:110:TYR:HA	2.47	0.40
1:D:169:TRP:HB3	1:D:174:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:LEU:HB3	1:F:86:LEU:HB3	2.04	0.40
2:G:141:TYR:H	2:G:198:HIS:HE1	1.68	0.40
3:A:429:PHE:CE1	3:A:514:SER:HB2	2.54	0.40
3:A:665:PRO:HA	3:A:671:CYS:SG	2.62	0.40
3:A:802:PHE:HZ	3:A:898:PHE:CZ	2.40	0.40
3:B:378:LYS:HE3	3:B:378:LYS:HB3	1.74	0.40
3:B:429:PHE:CE2	3:B:433:VAL:HG13	2.49	0.40
3:B:702:GLU:CG	3:C:788:ILE:HD11	2.51	0.40
3:C:36:VAL:HG11	3:C:220:PHE:CZ	2.56	0.40
3:C:105:ILE:HD11	3:C:135:PHE:CE1	2.57	0.40
3:C:388:ASN:HB3	3:C:528:LYS:HZ1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	203/235 (86%)	185 (91%)	18 (9%)	0	100	100
1	F	183/235 (78%)	164 (90%)	19 (10%)	0	100	100
2	E	210/213 (99%)	200 (95%)	10 (5%)	0	100	100
2	G	206/213 (97%)	198 (96%)	8 (4%)	0	100	100
3	A	985/1288 (76%)	914 (93%)	71 (7%)	0	100	100
3	B	939/1288 (73%)	887 (94%)	51 (5%)	1 (0%)	48	79
3	C	968/1288 (75%)	917 (95%)	51 (5%)	0	100	100
All	All	3694/4760 (78%)	3465 (94%)	228 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	331	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	D	186/207 (90%)	184 (99%)	2 (1%)	65	74
1	F	173/207 (84%)	172 (99%)	1 (1%)	78	79
2	E	177/178 (99%)	177 (100%)	0	100	100
2	G	175/178 (98%)	174 (99%)	1 (1%)	78	79
3	A	883/1112 (79%)	871 (99%)	12 (1%)	59	71
3	B	851/1112 (76%)	847 (100%)	4 (0%)	81	80
3	C	867/1112 (78%)	856 (99%)	11 (1%)	61	72
All	All	3312/4106 (81%)	3281 (99%)	31 (1%)	68	76

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	184	VAL
1	D	191	TYR
1	F	71	ILE
2	G	35	ILE
3	A	210	ILE
3	A	220	PHE
3	A	301	CYS
3	A	329	PHE
3	A	361	CYS
3	A	595	VAL
3	A	596	SER
3	A	869	MET
3	A	913	GLN
3	A	1031	GLU
3	A	1067	TYR
3	A	1068	VAL
3	B	140	PHE

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Mol	Chain	Res	Type
3	B	342	PHE
3	B	451	TYR
3	B	1043	CYS
3	C	121	ASN
3	C	131	CYS
3	C	216	LEU
3	C	385	THR
3	C	392	PHE
3	C	489	TYR
3	C	598	ILE
3	C	663	ASP
3	C	860	VAL
3	C	1043	CYS
3	C	1050	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	D	214	ASN
1	D	215	HIS
2	E	33	ASN
1	F	16	GLN
1	F	120	GLN
2	G	109	GLN
2	G	168	GLN
3	A	99	ASN
3	A	115	GLN
3	A	239	GLN
3	A	317	ASN
3	A	360	ASN
3	A	388	ASN
3	A	422	ASN
3	A	487	ASN
3	A	501	ASN
3	A	519	HIS
3	A	544	ASN
3	A	564	GLN
3	A	606	ASN
3	A	655	HIS
3	A	703	ASN
3	A	762	GLN

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Mol	Chain	Res	Type
3	A	992	GLN
3	A	1048	HIS
3	A	1106	GLN
3	B	439	ASN
3	B	501	ASN
3	B	540	ASN
3	B	606	ASN
3	B	655	HIS
3	B	703	ASN
3	B	853	GLN
3	B	901	GLN
3	B	919	ASN
3	B	969	ASN
3	B	1071	GLN
3	B	1083	HIS
3	B	1101	HIS
3	B	1106	GLN
3	B	1113	GLN
3	C	165	ASN
3	C	334	ASN
3	C	481	ASN
3	C	498	GLN
3	C	540	ASN
3	C	751	ASN
3	C	926	GLN
3	C	955	ASN
3	C	1002	GLN
3	C	1011	GLN
3	C	1054	GLN
3	C	1142	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1302	3	14,14,15	0.67	0	17,19,21	0.90	1 (5%)
4	NAG	C	1303	3	14,14,15	0.74	0	17,19,21	0.88	0
4	NAG	A	1306	3	14,14,15	0.70	0	17,19,21	0.80	0
4	NAG	A	1308	3	14,14,15	0.75	0	17,19,21	0.85	0
4	NAG	C	1301	3	14,14,15	0.40	0	17,19,21	0.35	0
4	NAG	B	1308	3	14,14,15	0.75	0	17,19,21	1.11	1 (5%)
4	NAG	A	1307	3	14,14,15	0.75	0	17,19,21	0.86	0
4	NAG	A	1303	3	14,14,15	0.70	0	17,19,21	0.86	1 (5%)
4	NAG	B	1303	3	14,14,15	0.76	0	17,19,21	2.27	2 (11%)
4	NAG	A	1309	3	14,14,15	0.39	0	17,19,21	0.36	0
4	NAG	B	1305	3	14,14,15	0.73	0	17,19,21	0.81	0
4	NAG	A	1305	3	14,14,15	0.74	0	17,19,21	0.86	0
4	NAG	B	1302	3	14,14,15	0.71	0	17,19,21	1.06	1 (5%)
4	NAG	B	1304	3	14,14,15	0.73	0	17,19,21	0.83	0
4	NAG	C	1305	3	14,14,15	0.74	0	17,19,21	0.86	0
4	NAG	B	1306	3	14,14,15	0.76	0	17,19,21	0.90	0
4	NAG	C	1302	3	14,14,15	0.72	0	17,19,21	0.78	0
4	NAG	A	1304	3	14,14,15	0.75	0	17,19,21	0.88	1 (5%)
4	NAG	B	1310	3	14,14,15	0.37	0	17,19,21	0.39	0
4	NAG	B	1307	3	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
4	NAG	B	1309	3	14,14,15	0.73	0	17,19,21	0.79	0
4	NAG	C	1306	3	14,14,15	0.70	0	17,19,21	0.79	0
4	NAG	B	1301	3	14,14,15	0.71	0	17,19,21	0.85	0
4	NAG	A	1301	3	14,14,15	0.73	0	17,19,21	0.93	0
4	NAG	C	1304	3	14,14,15	0.76	0	17,19,21	0.87	1 (5%)

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1303	NAG	C2-N2-C7	8.13	133.80	122.90
4	B	1308	NAG	C1-O5-C5	3.33	116.65	112.19
4	B	1303	NAG	C8-C7-N2	2.79	120.74	116.12
4	B	1302	NAG	C1-O5-C5	2.61	115.68	112.19
4	A	1304	NAG	O5-C1-C2	-2.40	107.57	111.29
4	C	1304	NAG	O5-C1-C2	-2.16	107.95	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1302	NAG	O5-C1-C2	-2.13	107.99	111.29
4	A	1303	NAG	O5-C1-C2	-2.13	108.00	111.29
4	B	1307	NAG	C1-O5-C5	2.11	115.01	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

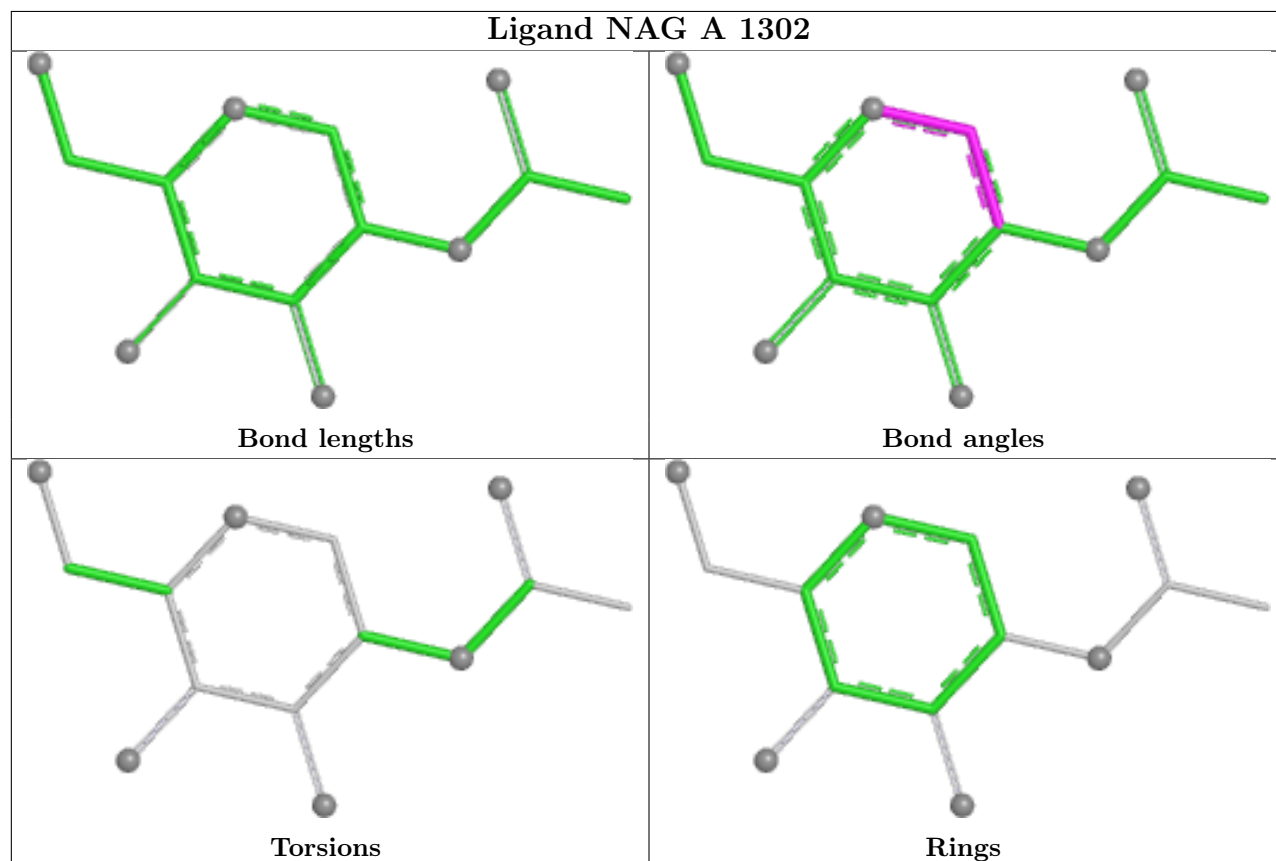
Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	O5-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	A	1303	NAG	C8-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	A	1309	NAG	C8-C7-N2-C2
4	A	1309	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	C	1305	NAG	C4-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	A	1306	NAG	C1-C2-N2-C7
4	B	1303	NAG	C1-C2-N2-C7
4	C	1302	NAG	C1-C2-N2-C7
4	B	1303	NAG	C3-C2-N2-C7

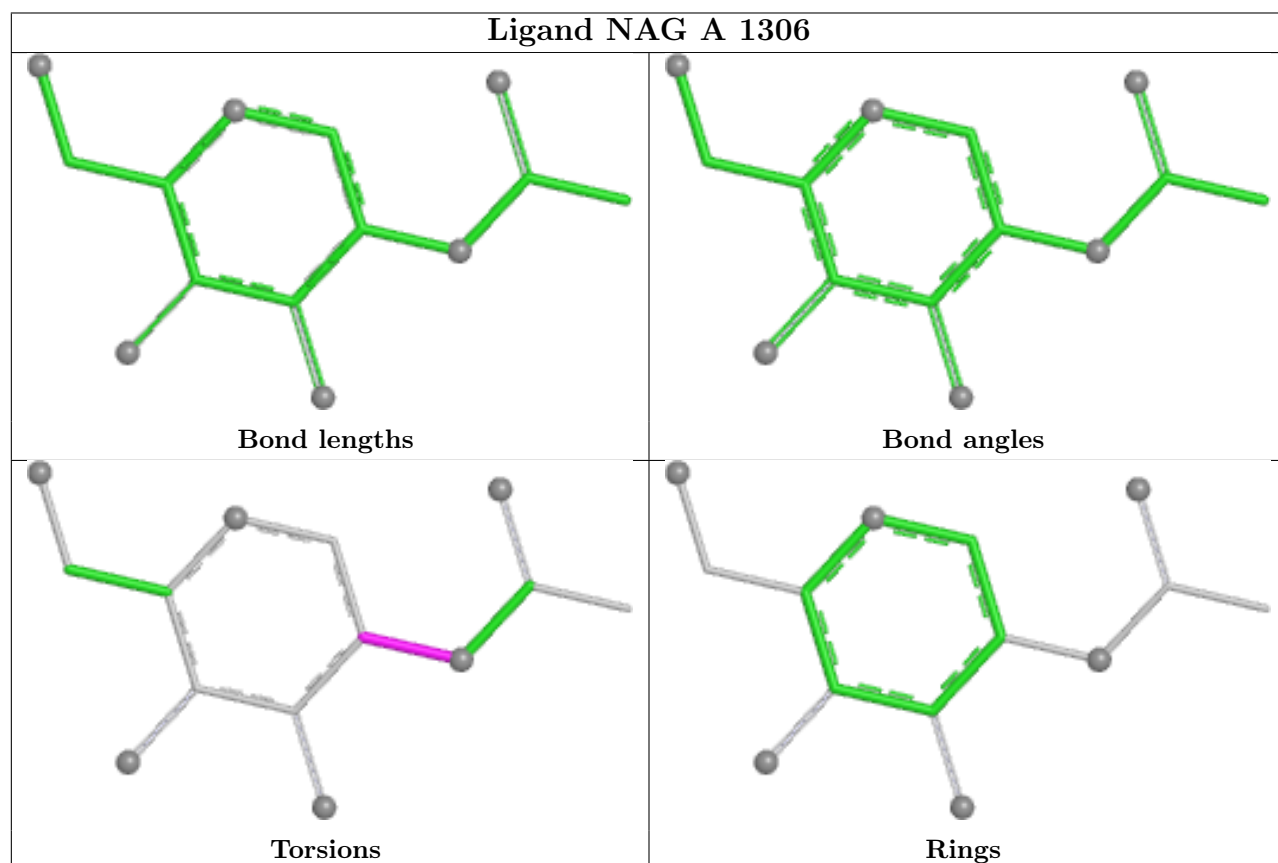
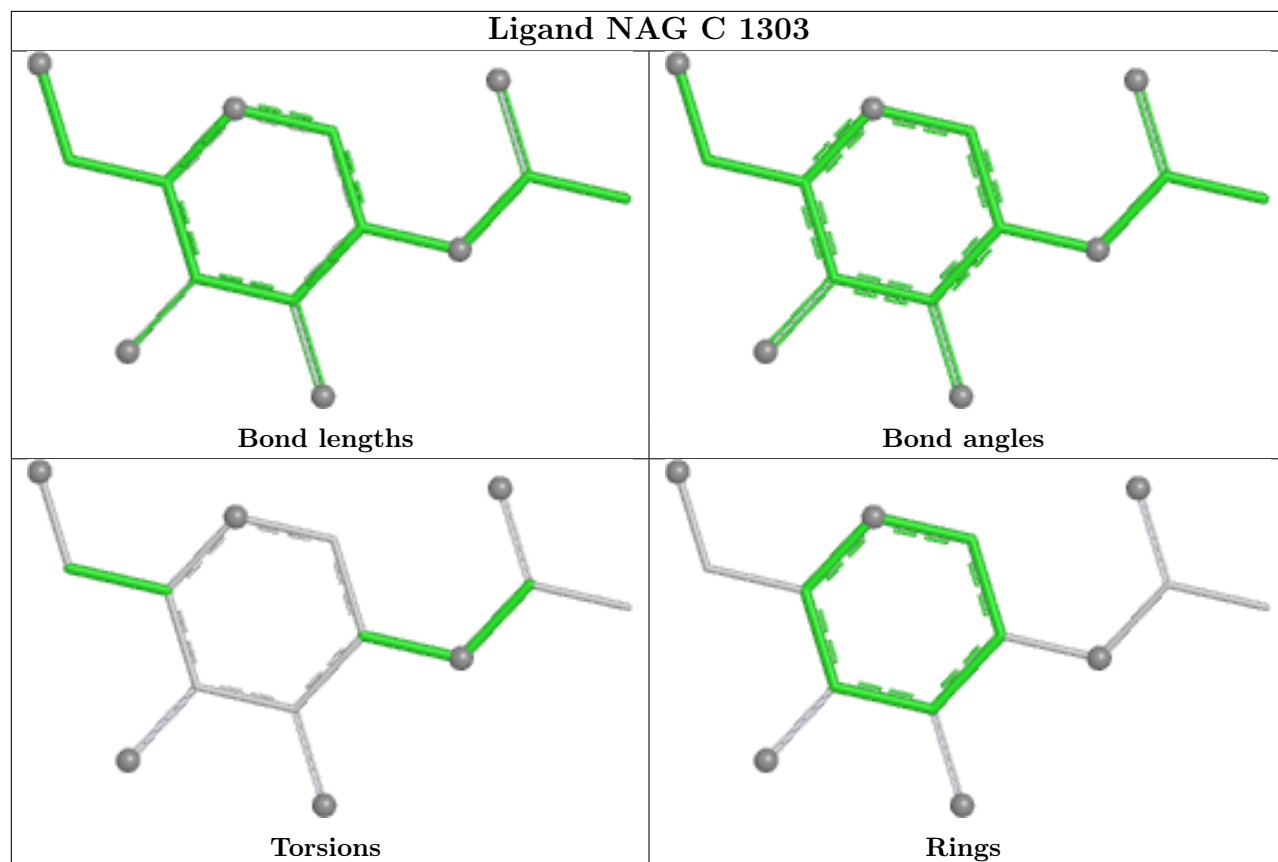
There are no ring outliers.

No monomer is involved in short contacts.

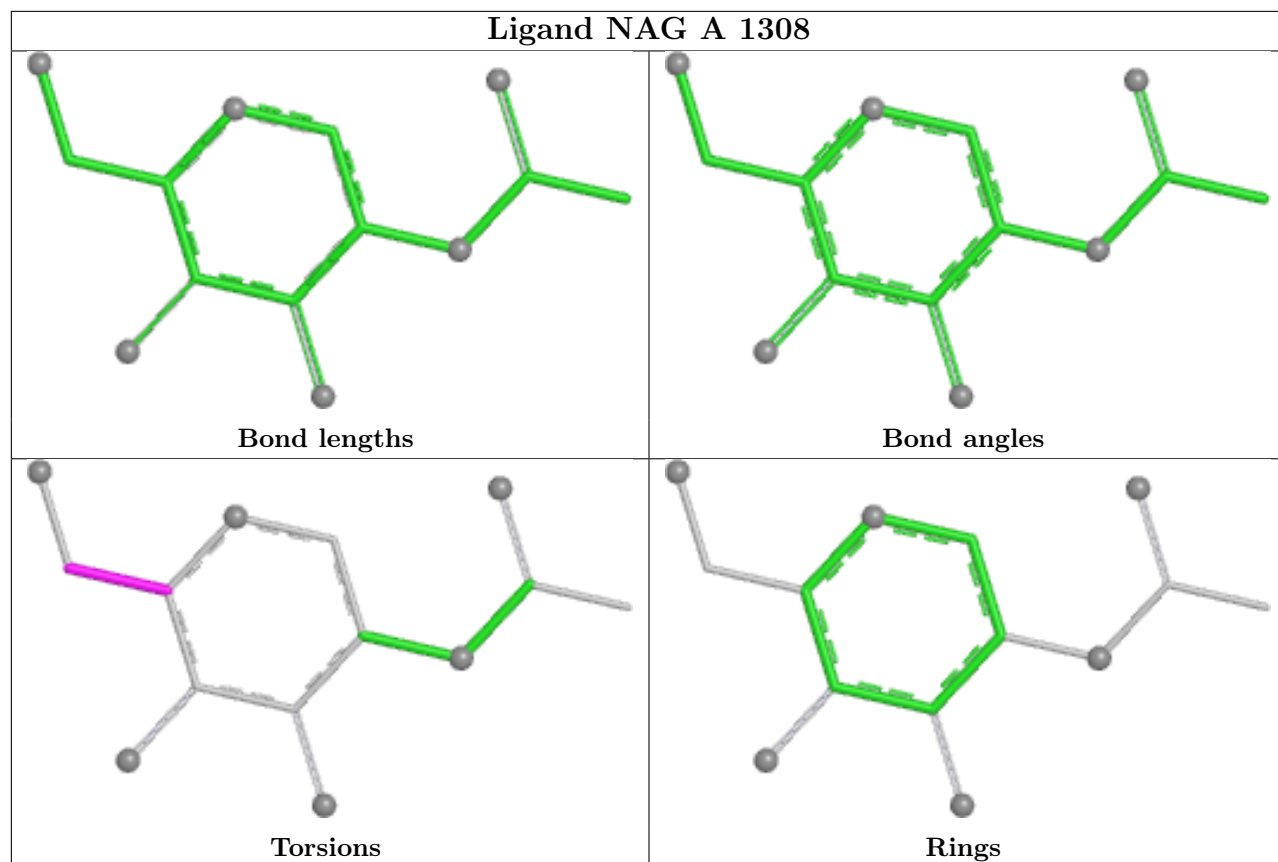
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

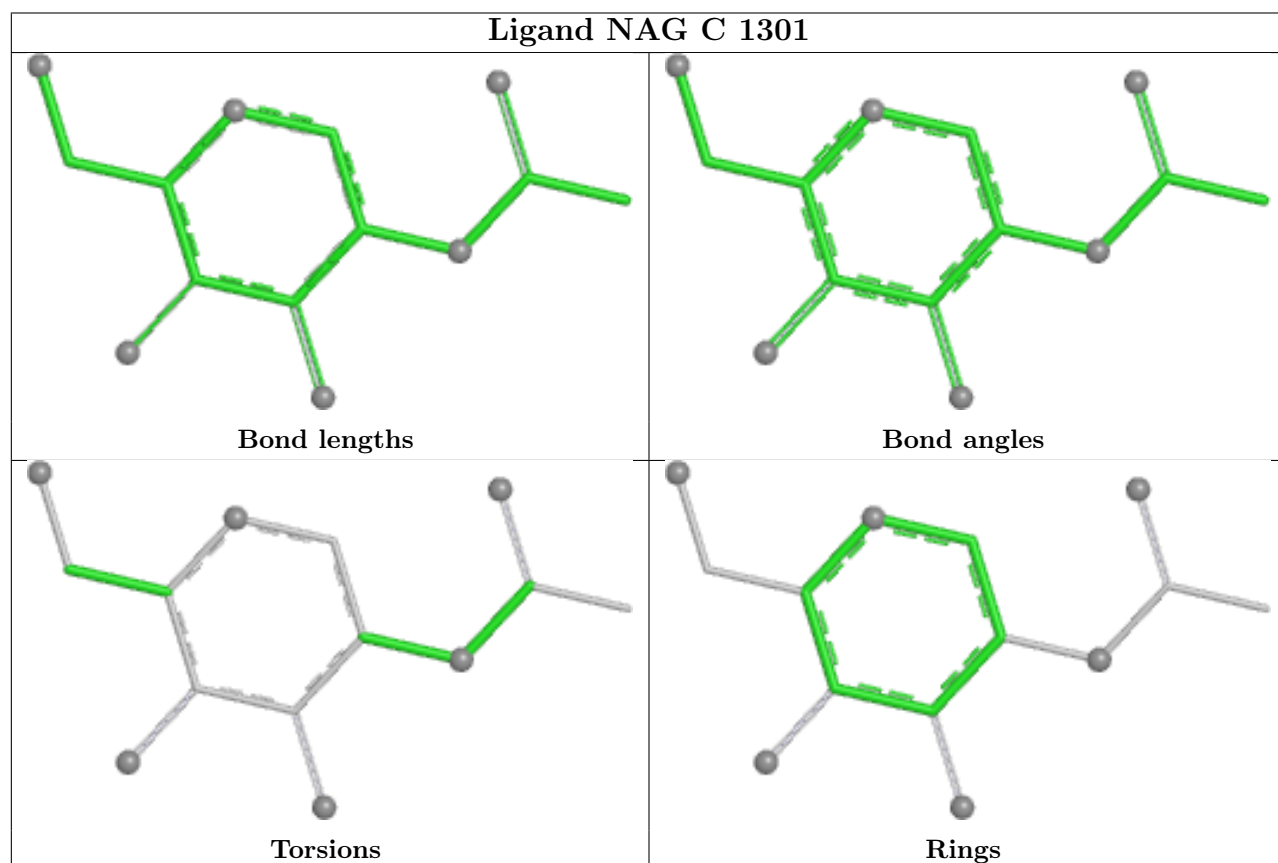


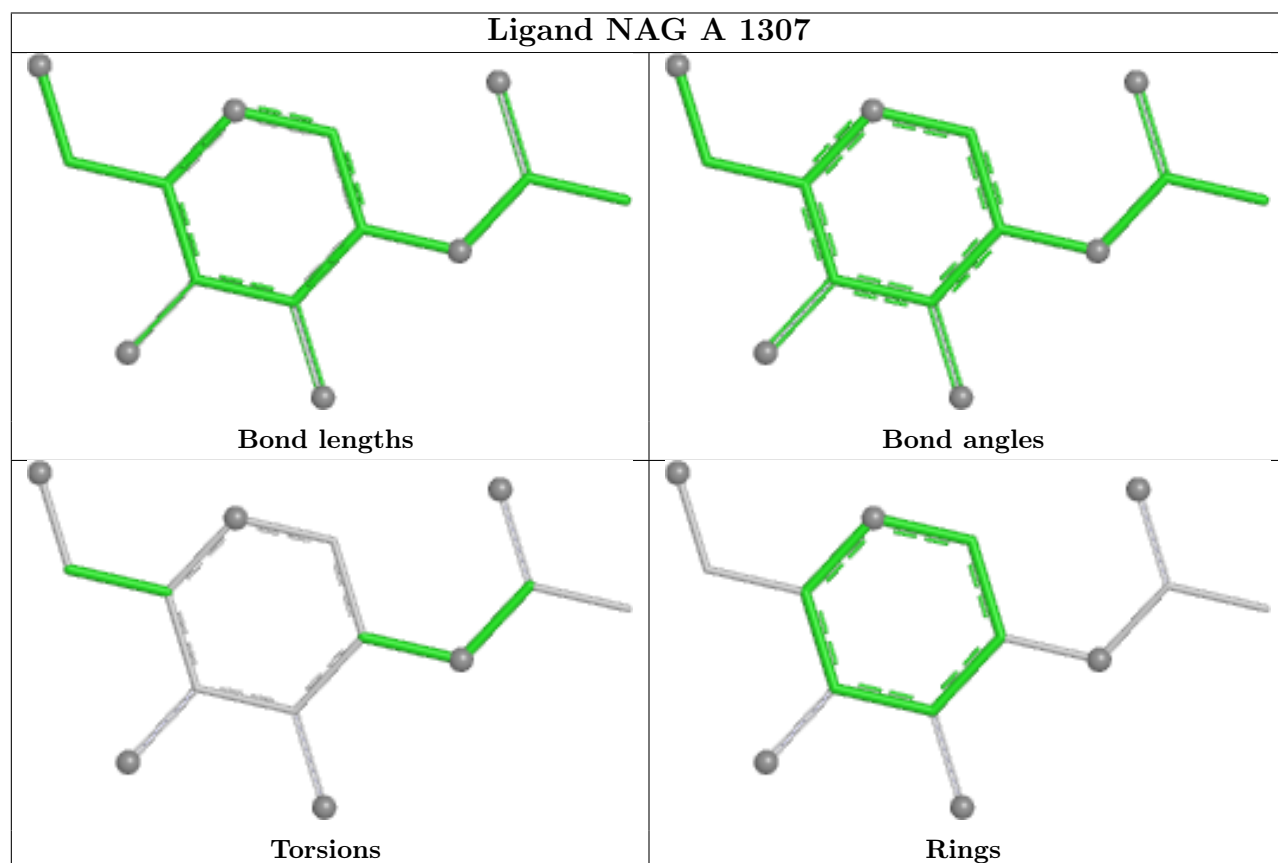
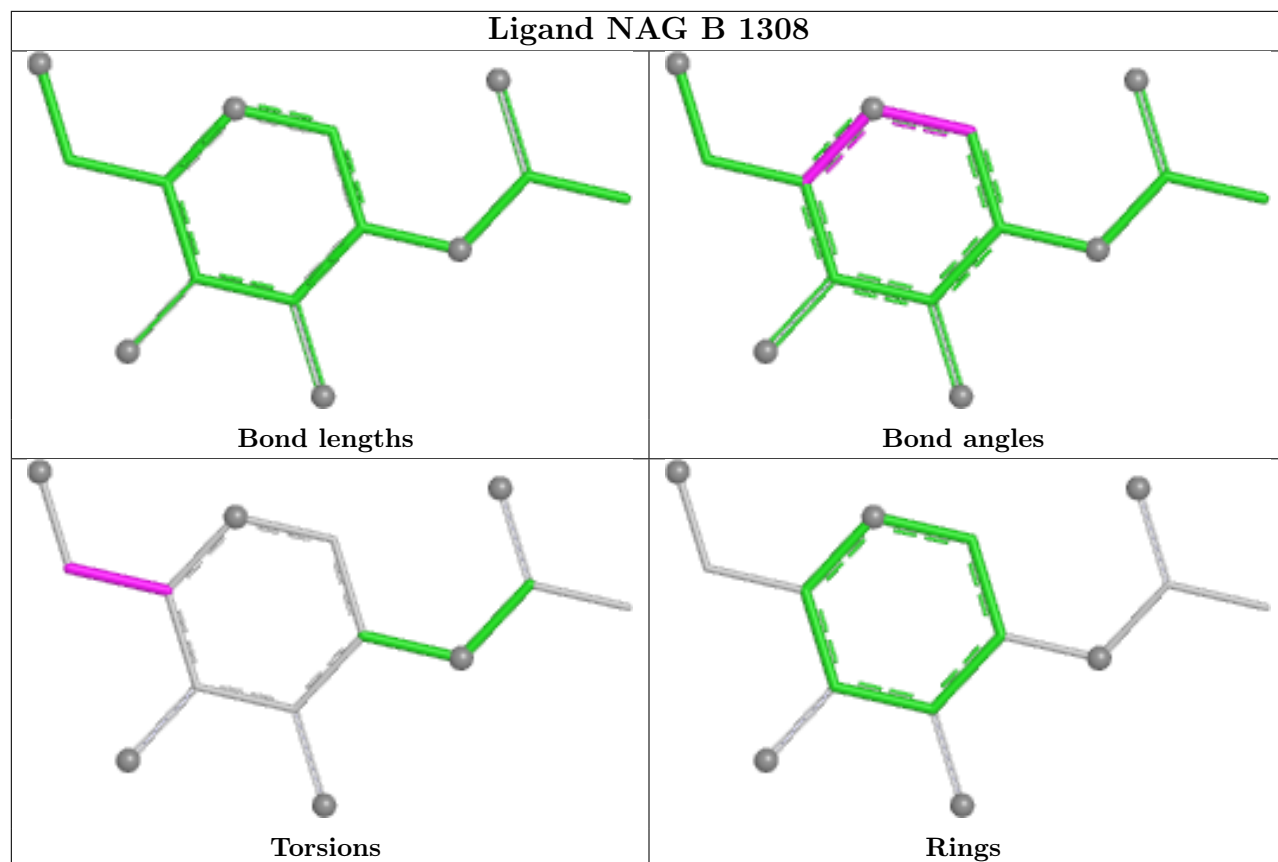


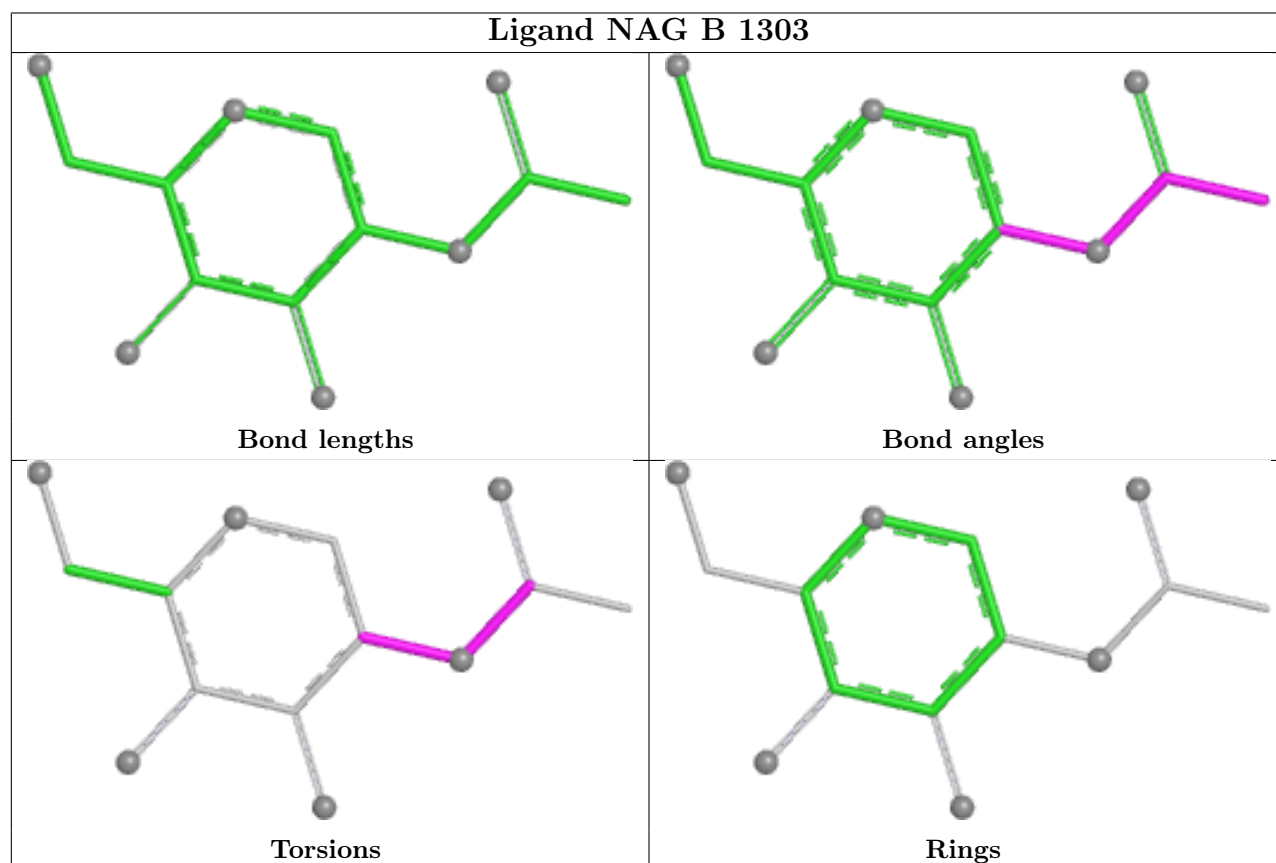
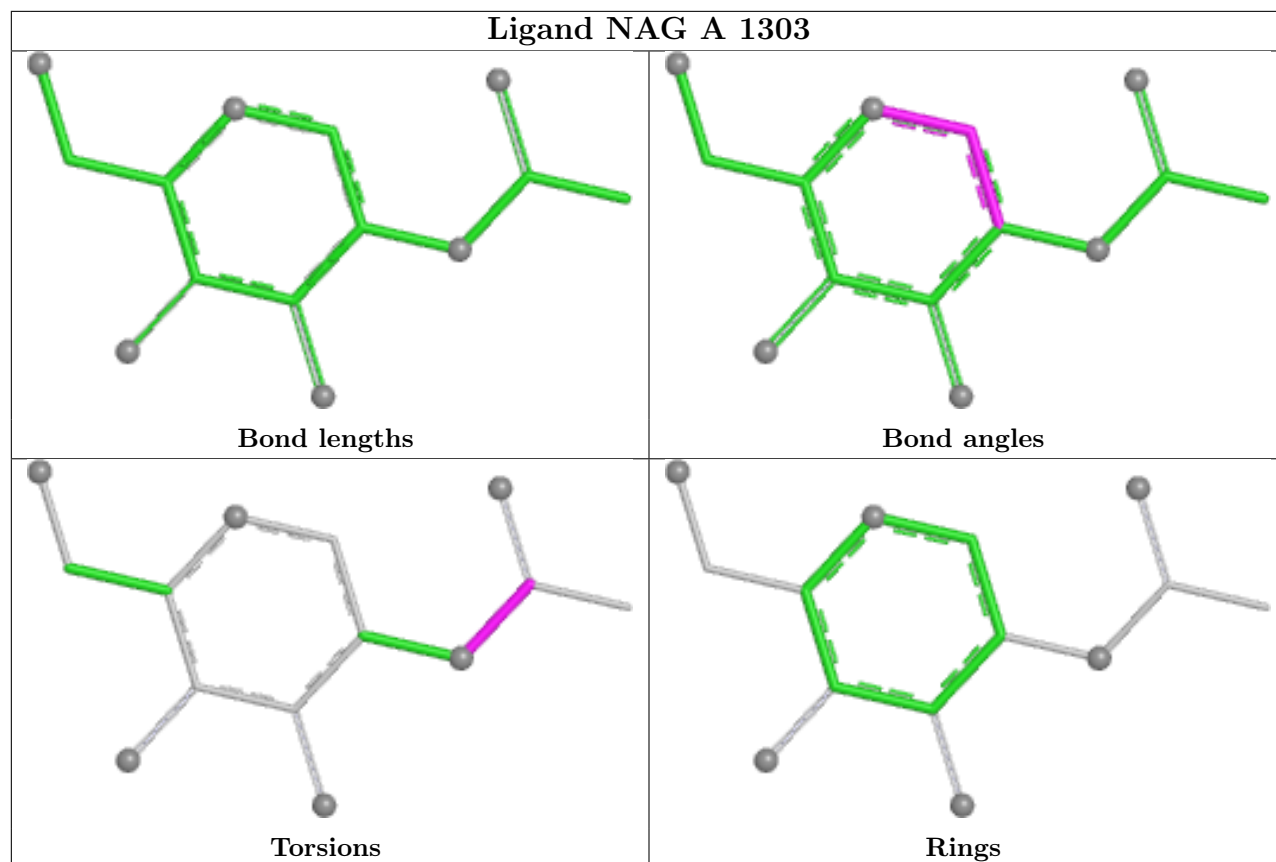
Ligand NAG A 1308



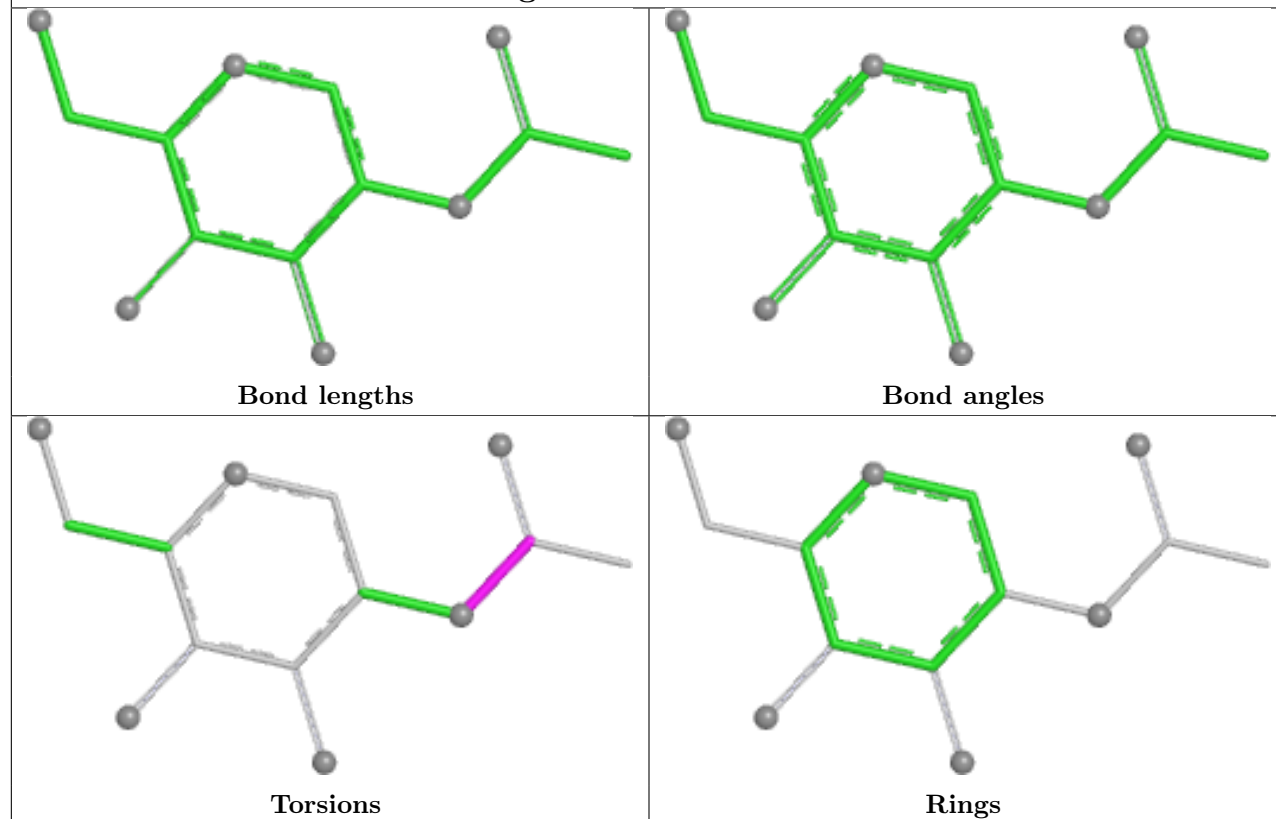
Ligand NAG C 1301



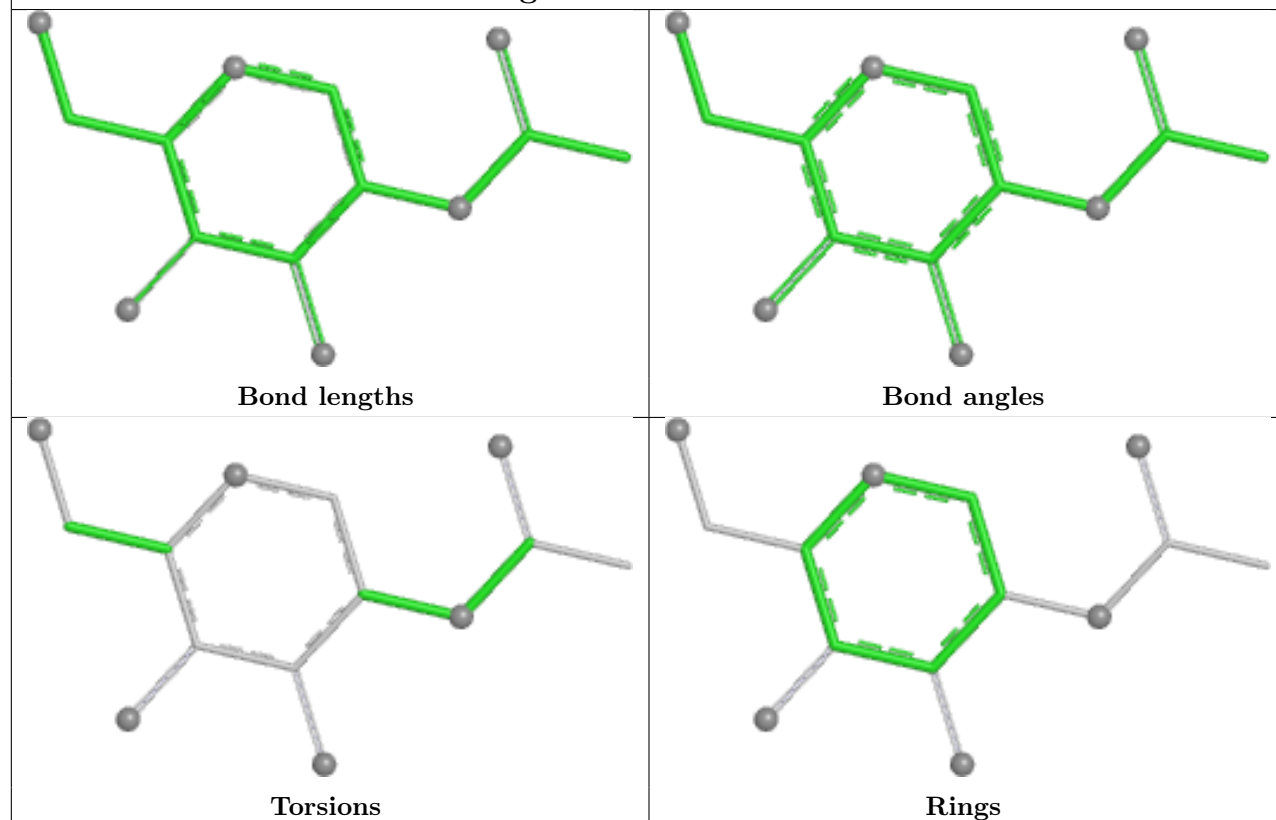




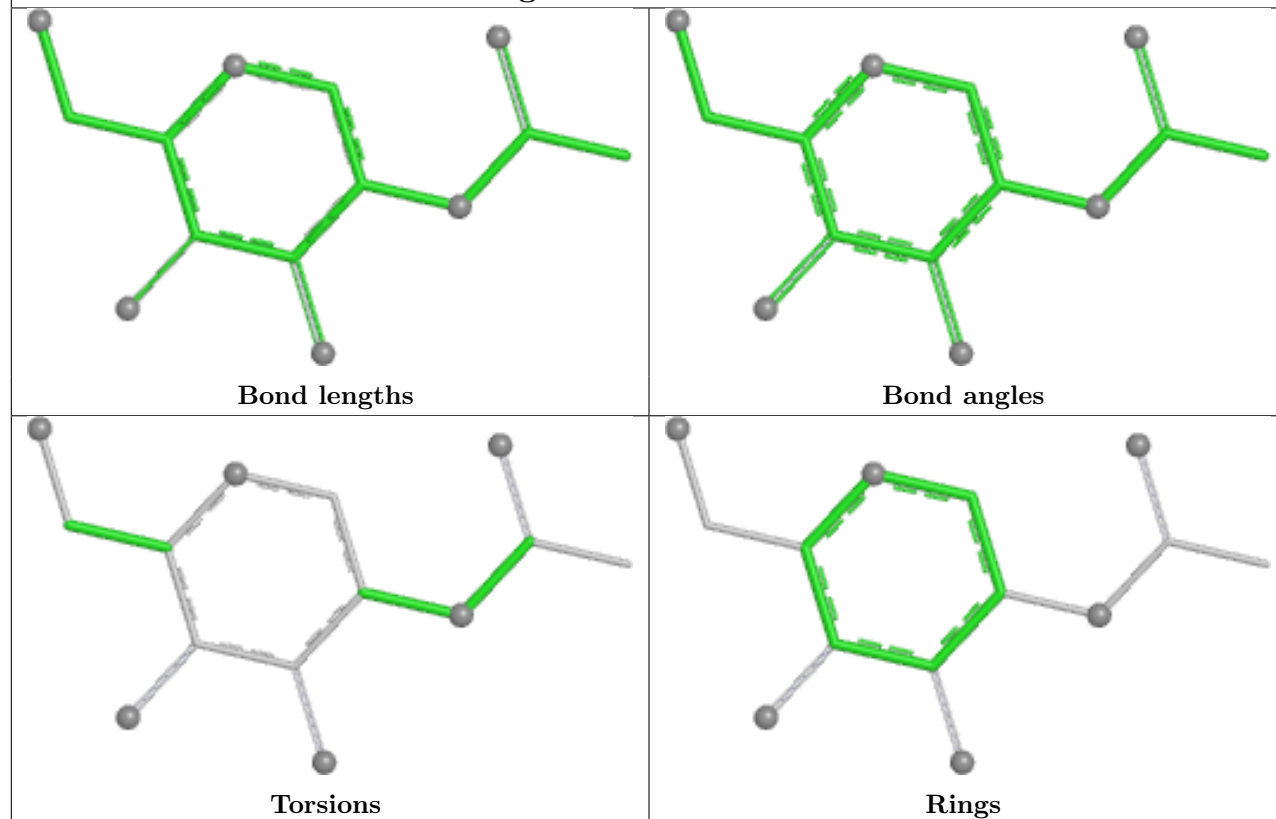
Ligand NAG A 1309



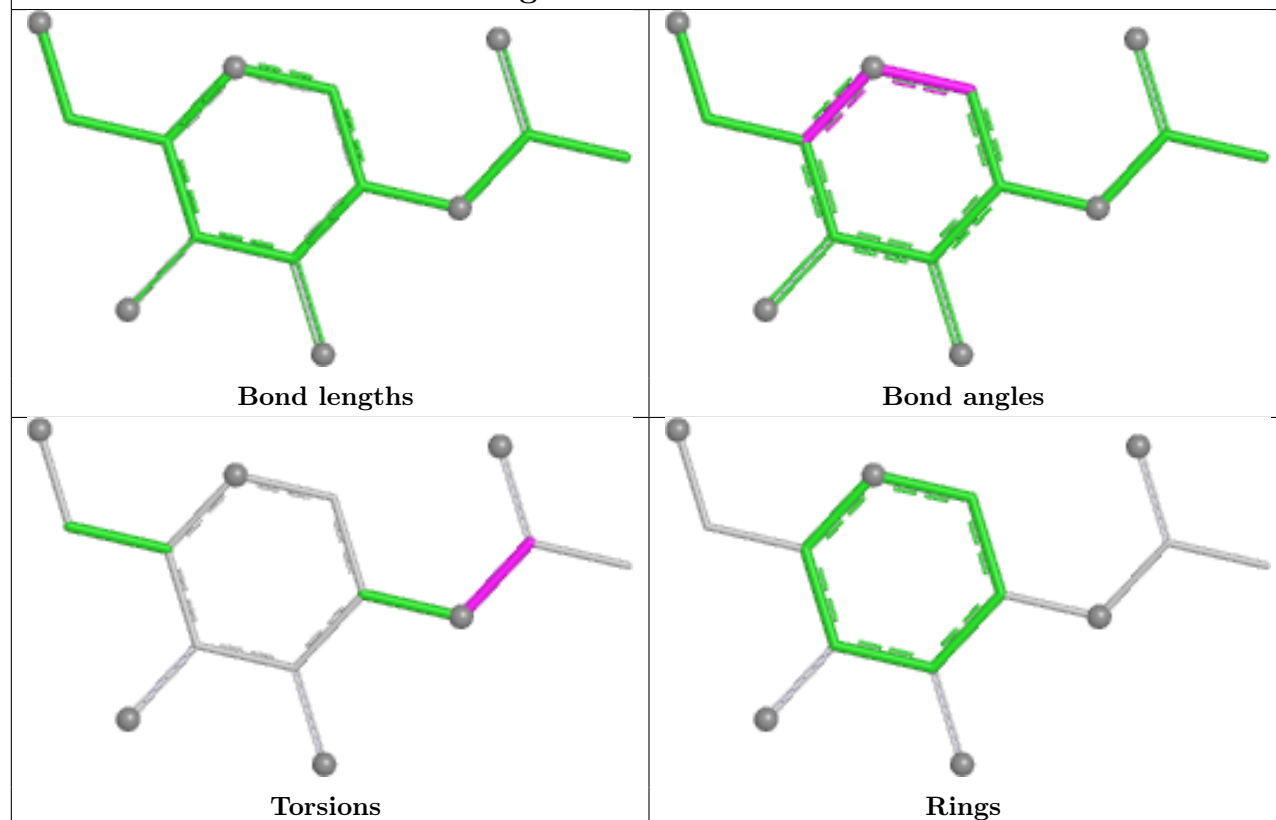
Ligand NAG B 1305

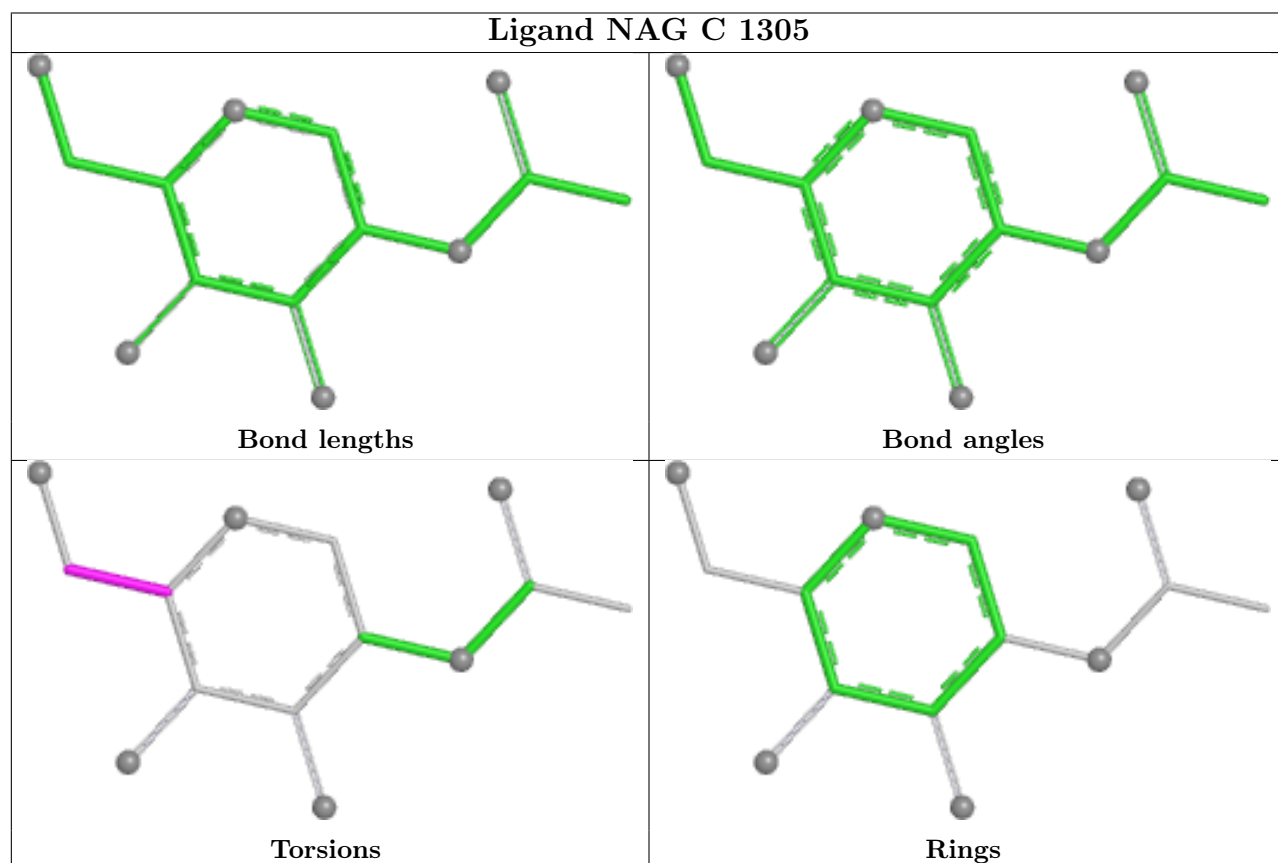
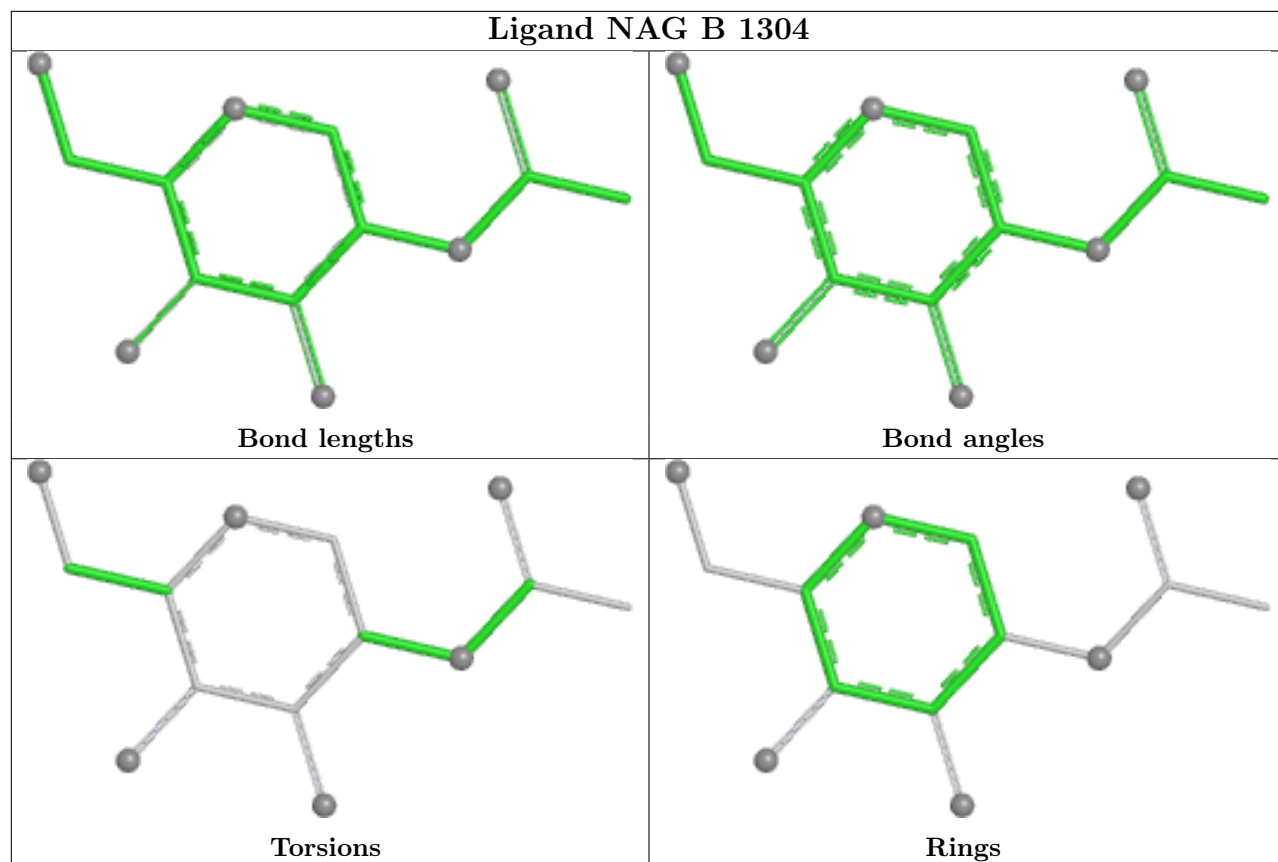


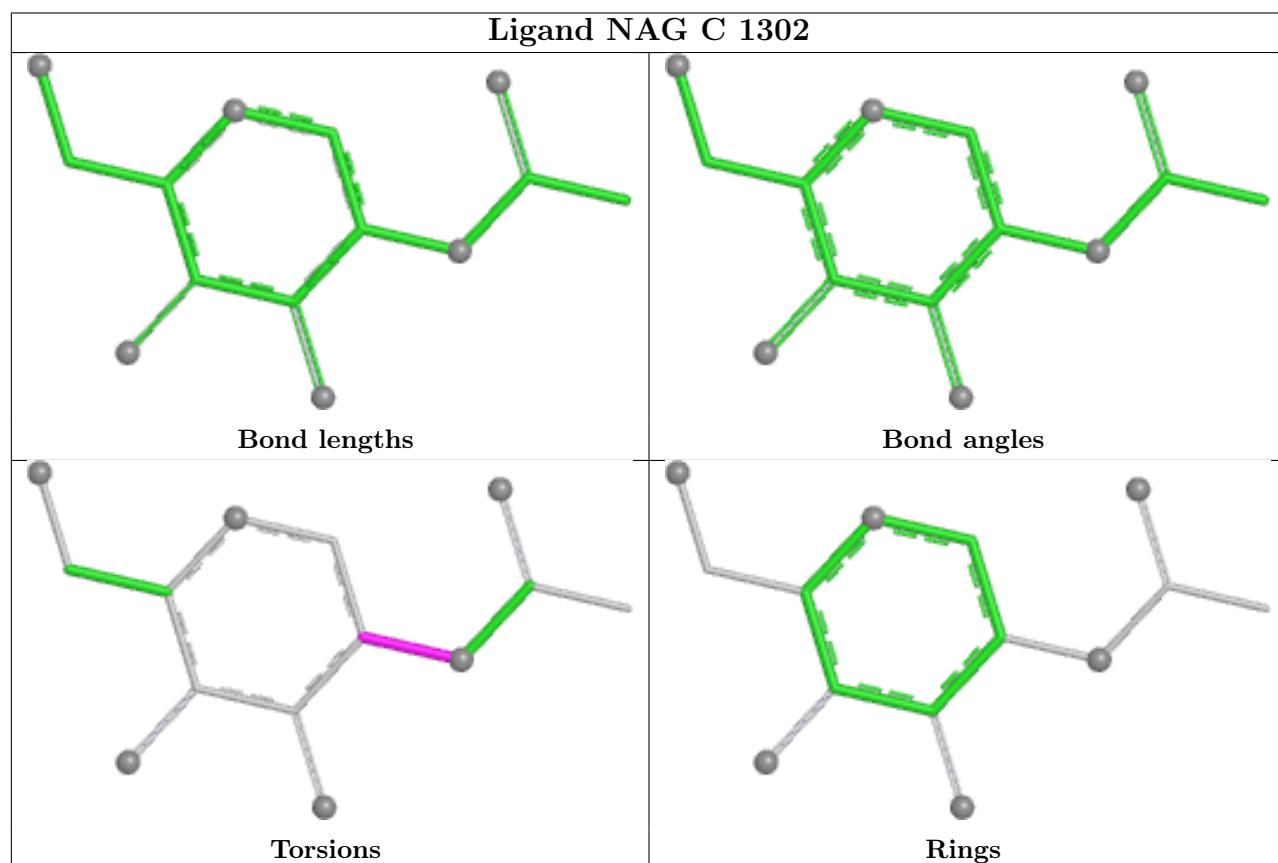
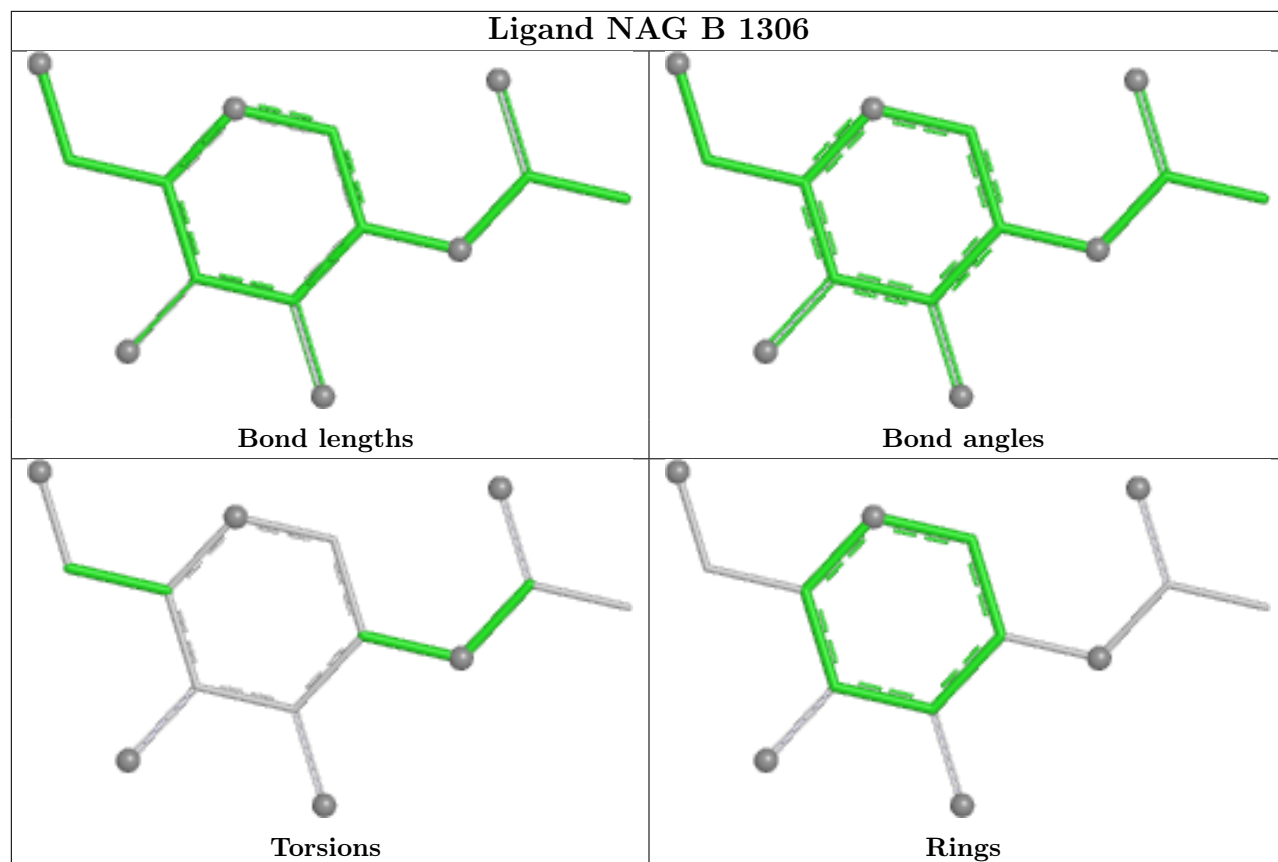
Ligand NAG A 1305



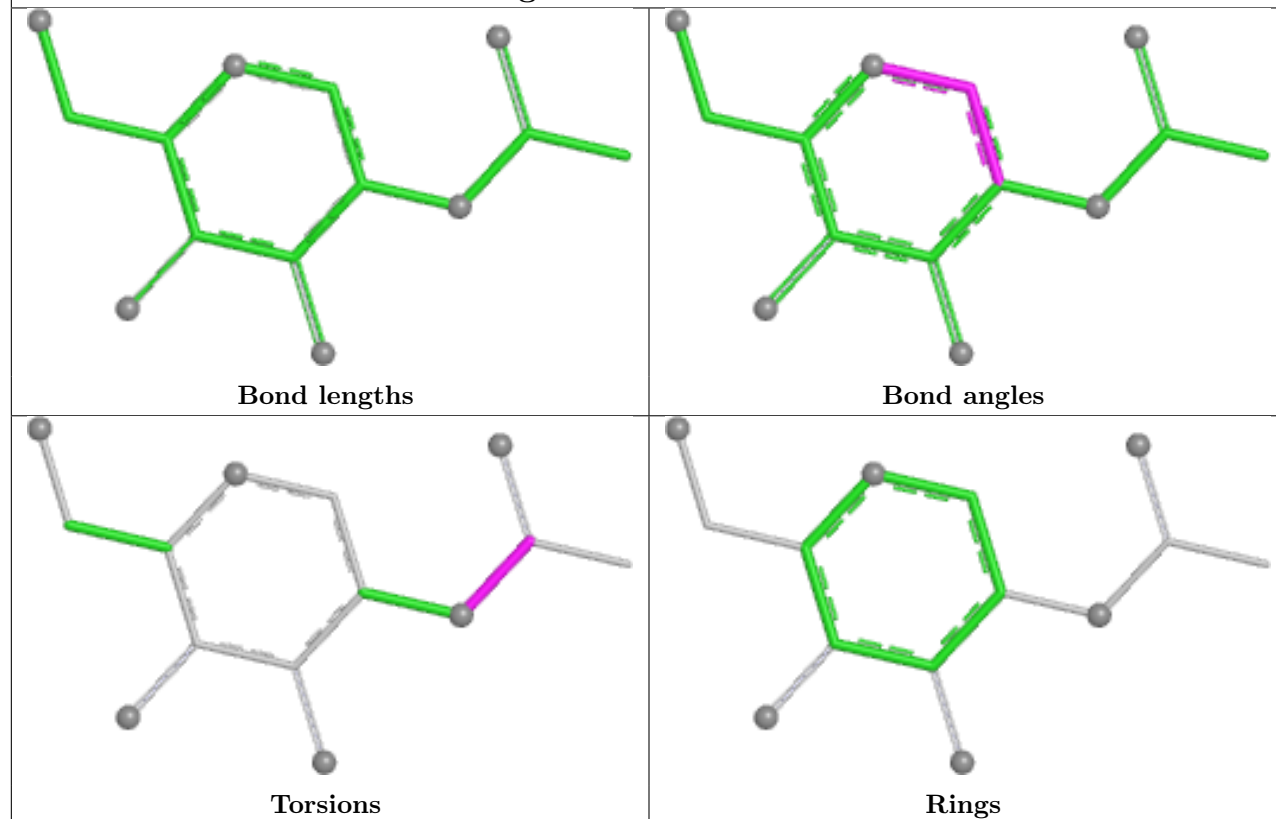
Ligand NAG B 1302



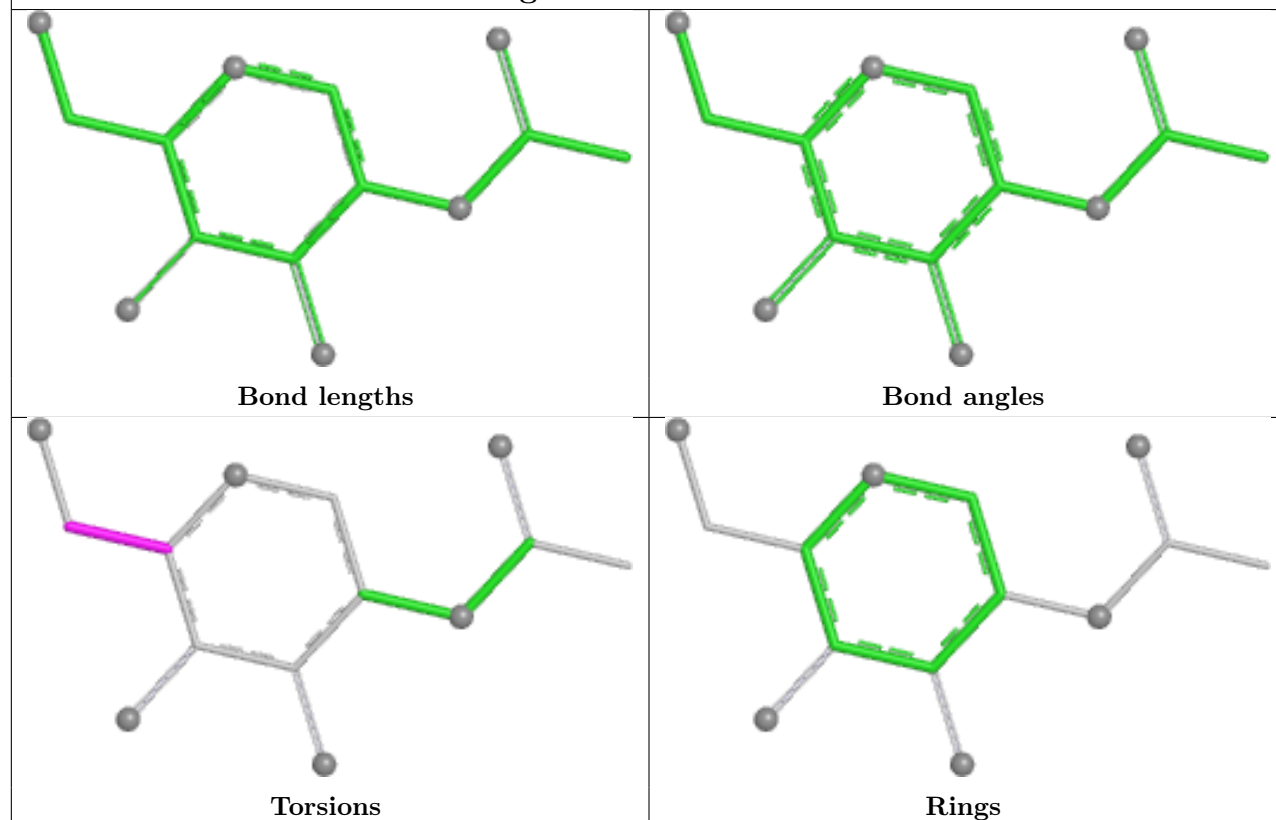


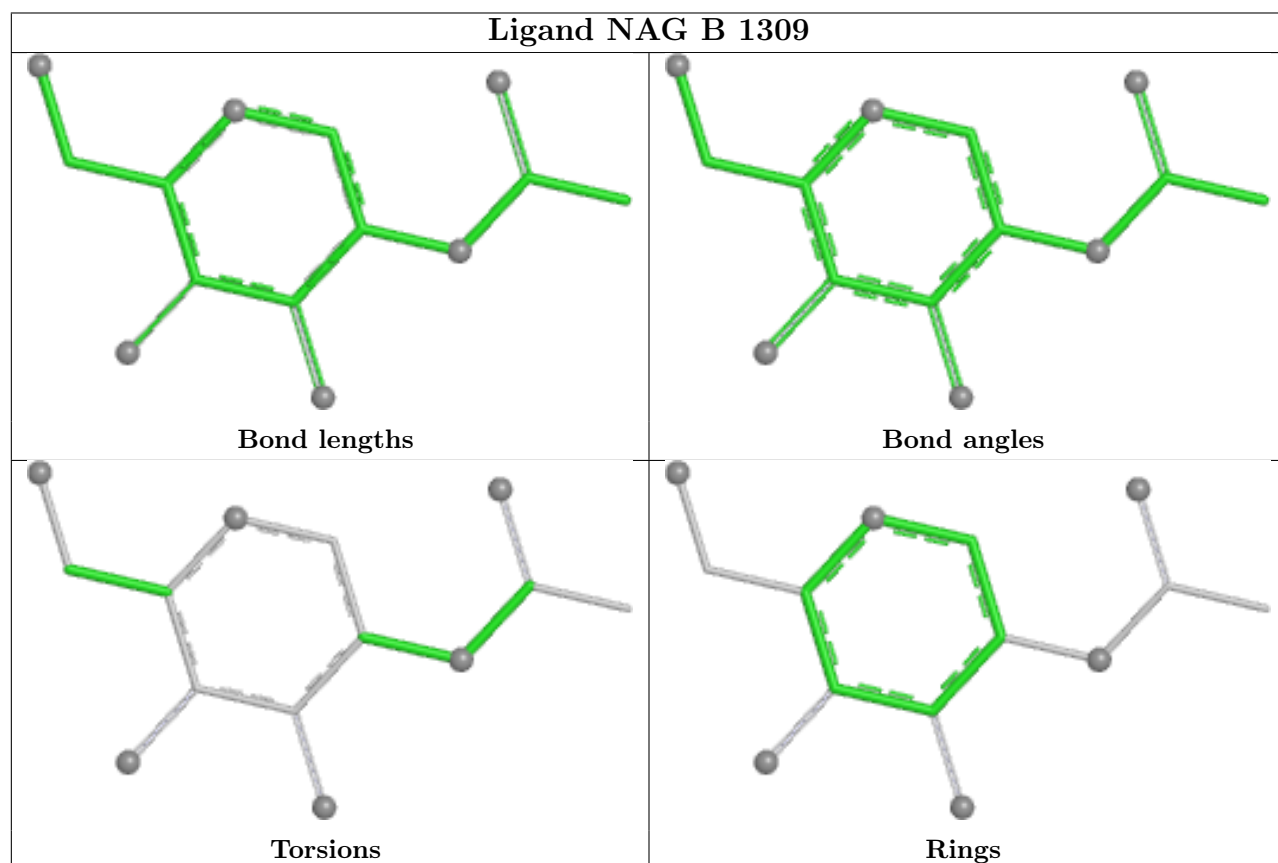
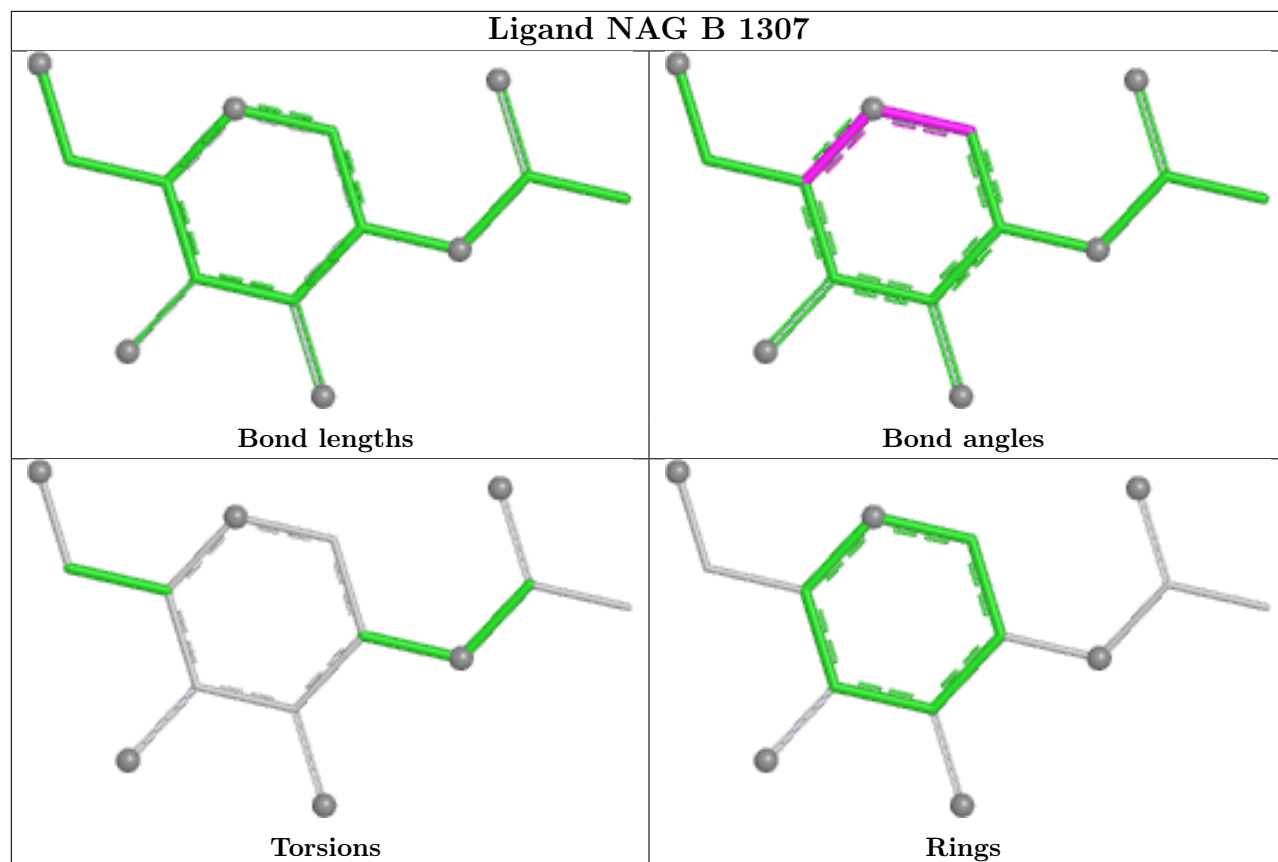


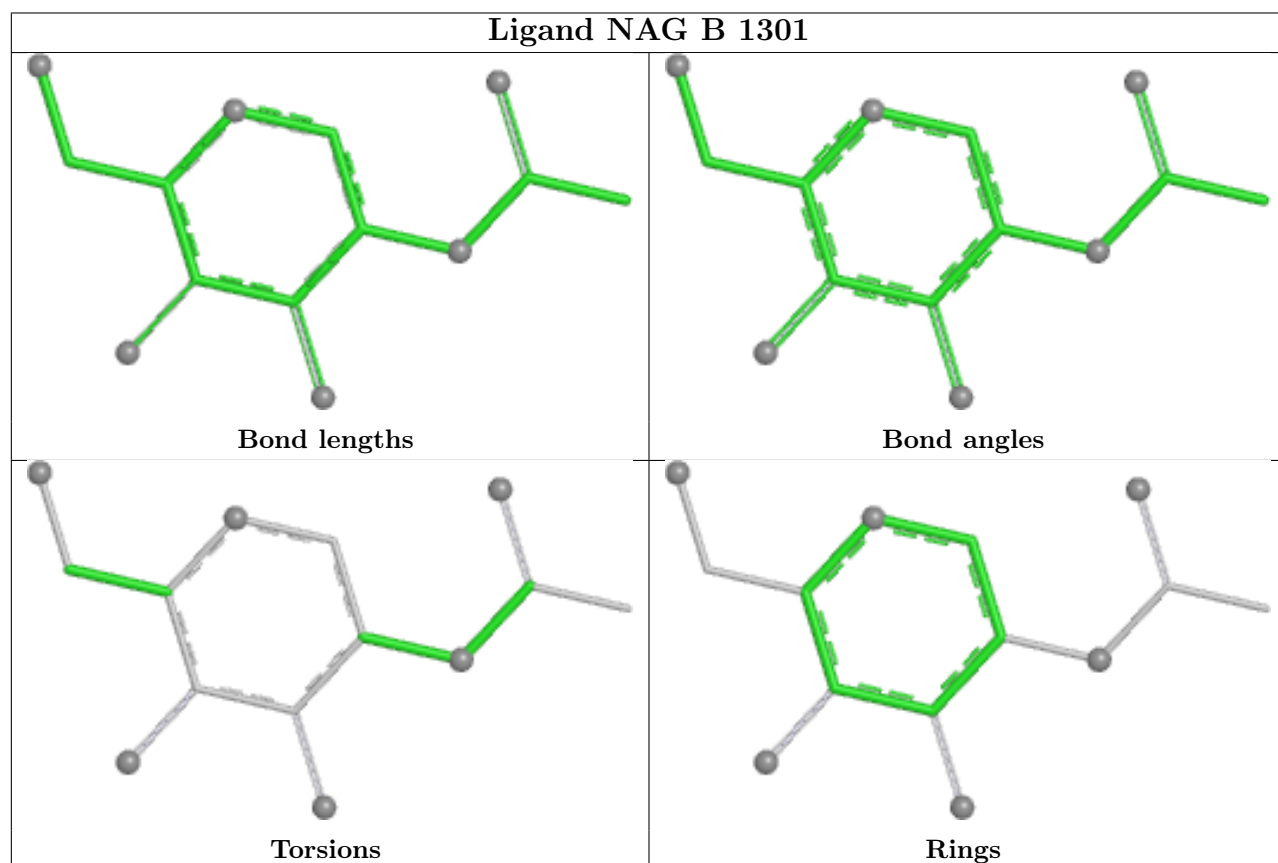
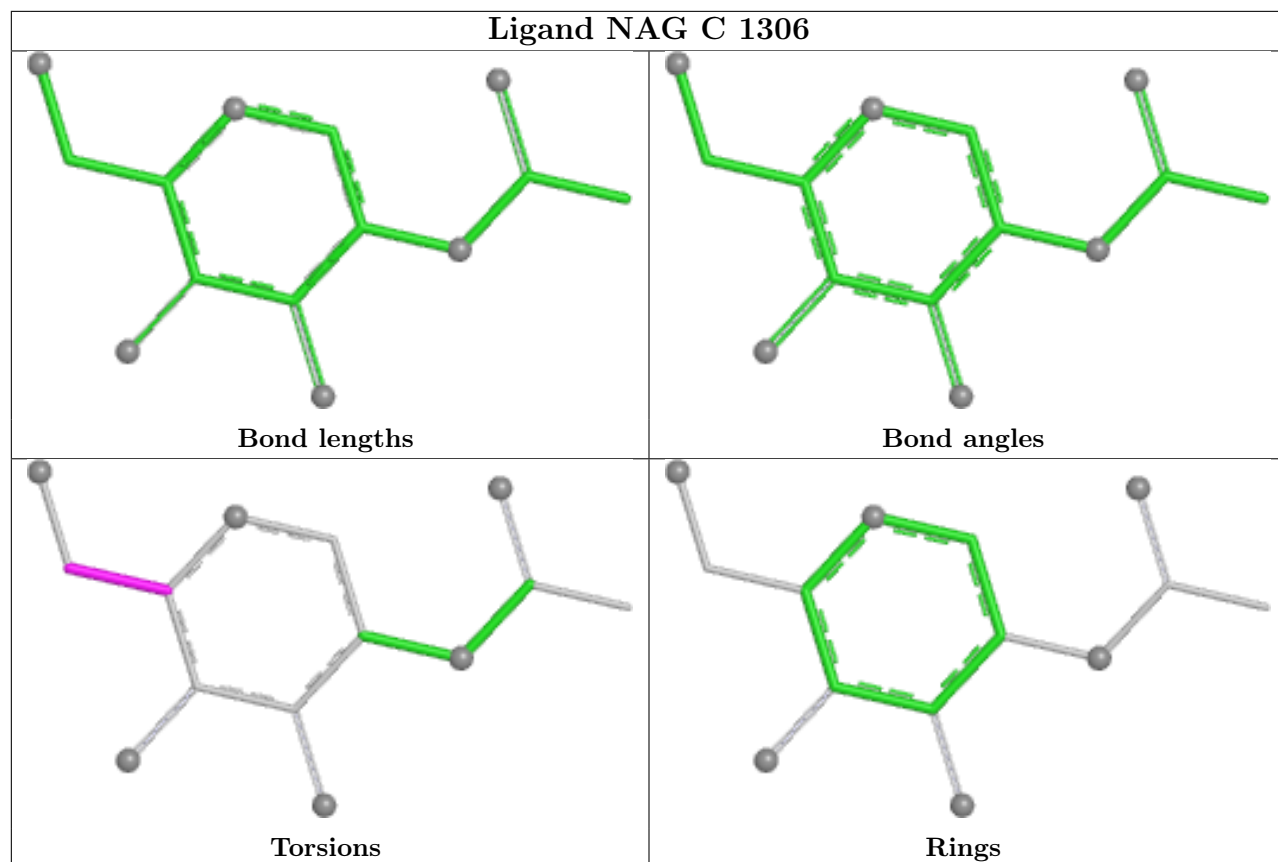
Ligand NAG A 1304



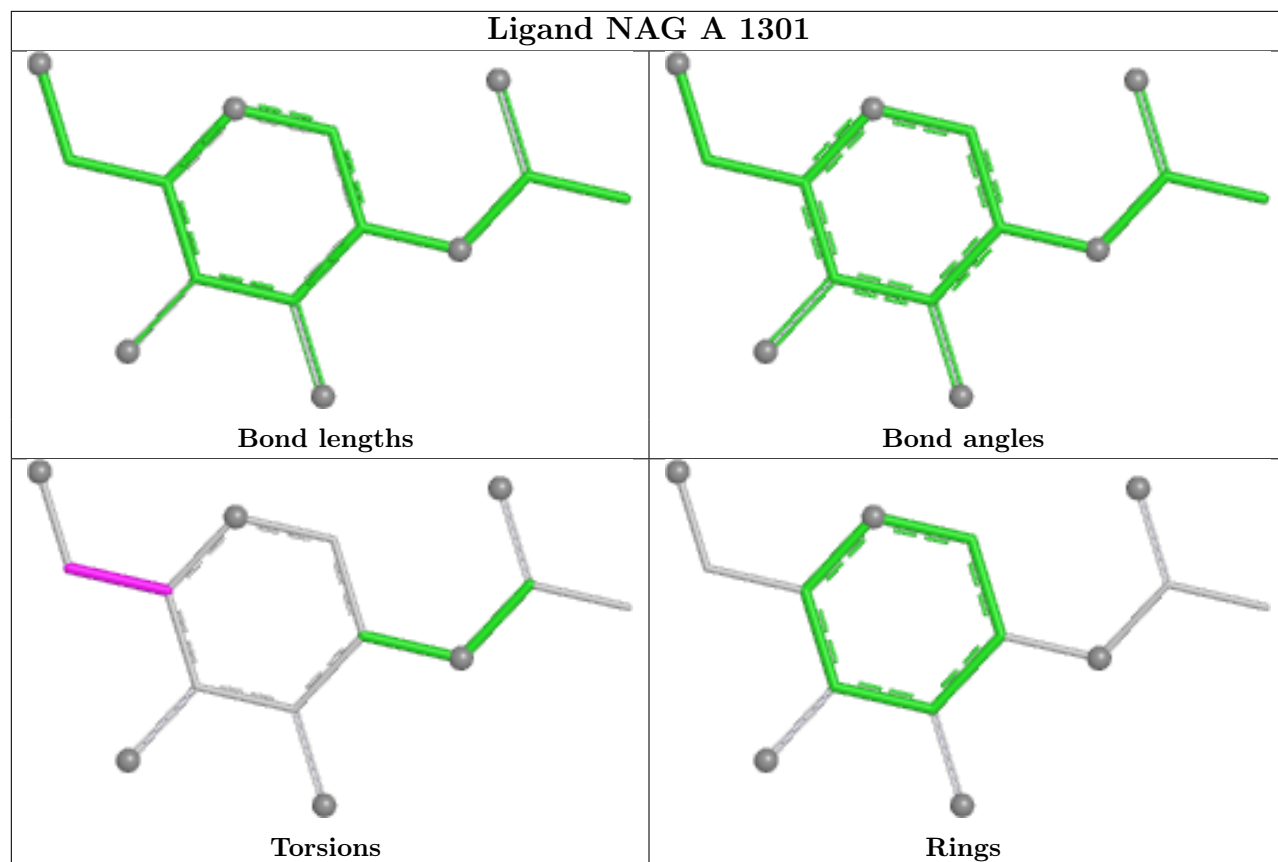
Ligand NAG B 1310



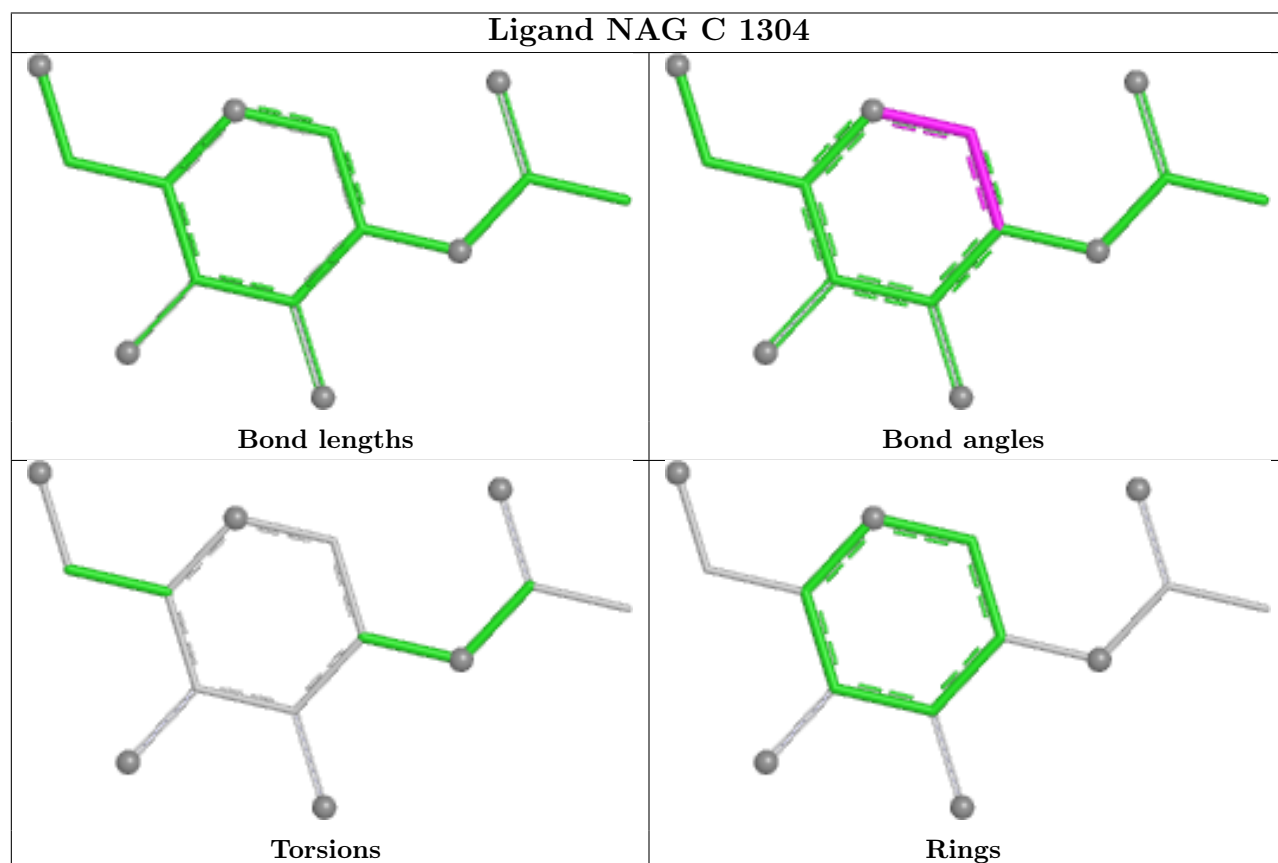




Ligand NAG A 1301



Ligand NAG C 1304



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

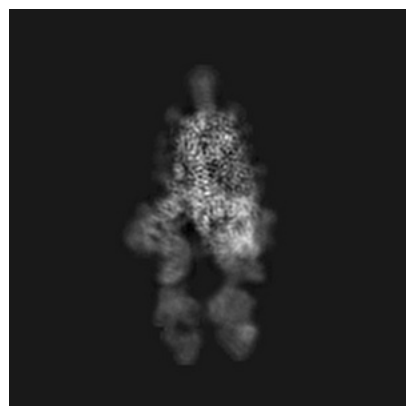
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73292. These allow visual inspection of the internal detail of the map and identification of artifacts.

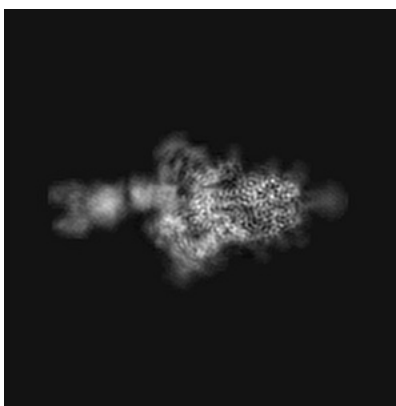
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

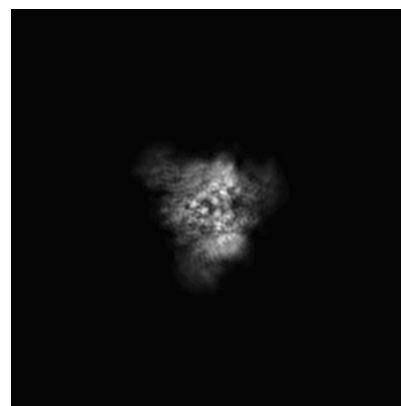
6.1.1 Primary map



X

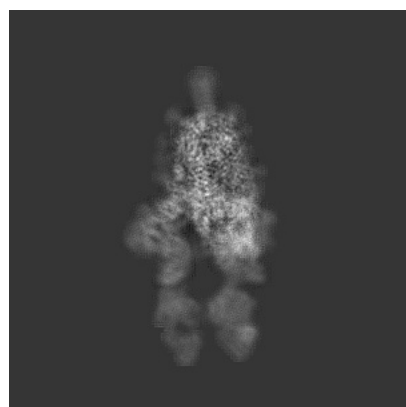


Y

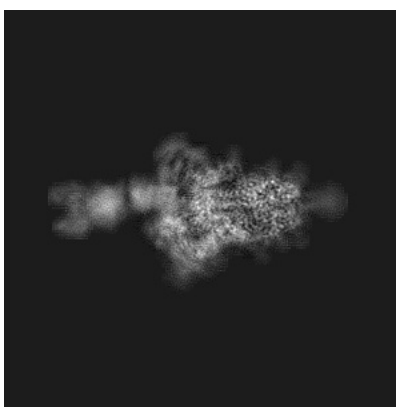


Z

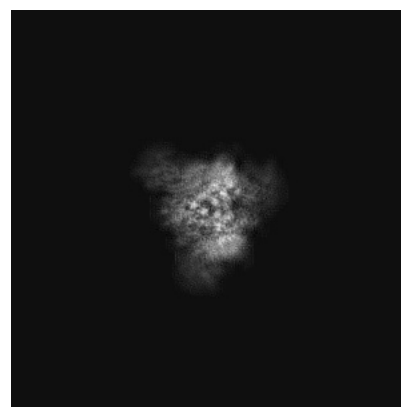
6.1.2 Raw map



X



Y

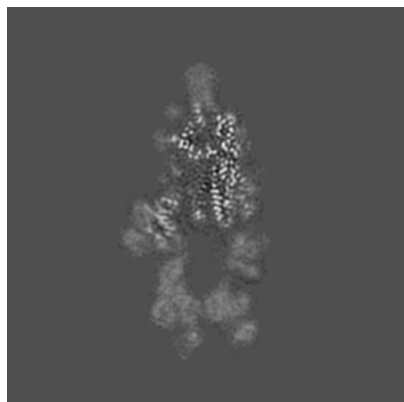


Z

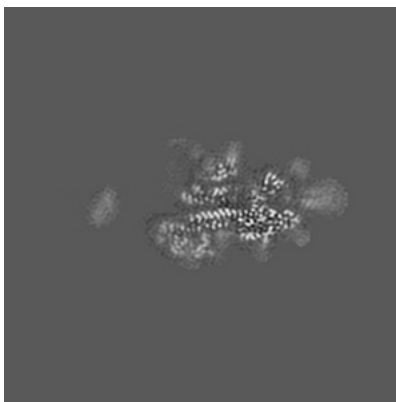
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

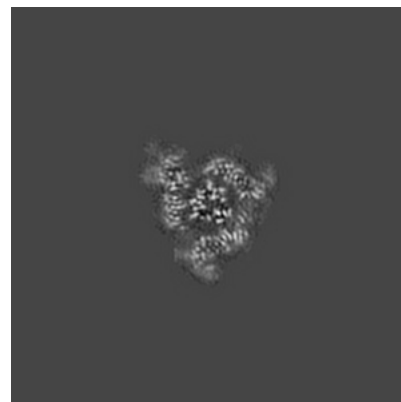
6.2.1 Primary map



X Index: 220

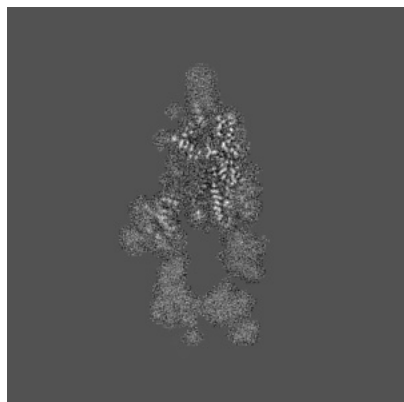


Y Index: 220

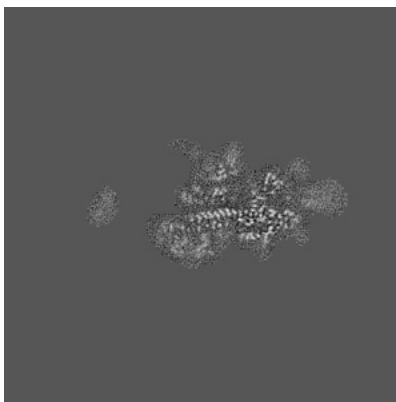


Z Index: 220

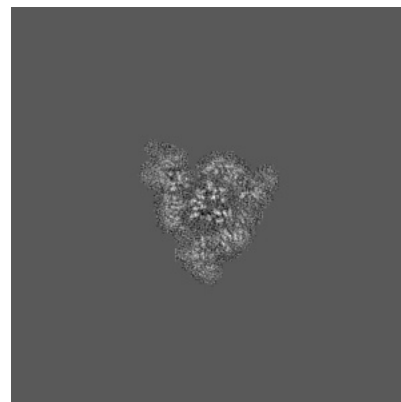
6.2.2 Raw map



X Index: 220



Y Index: 220

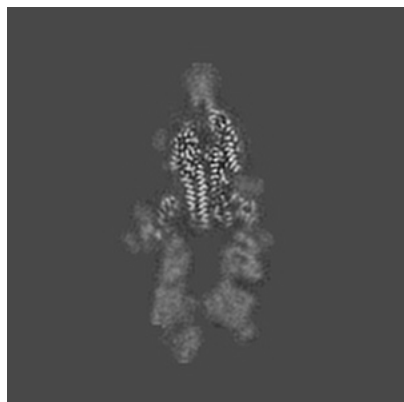


Z Index: 220

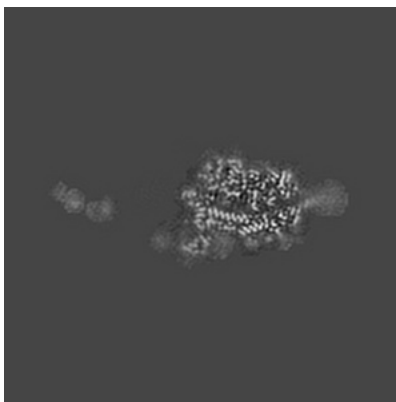
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

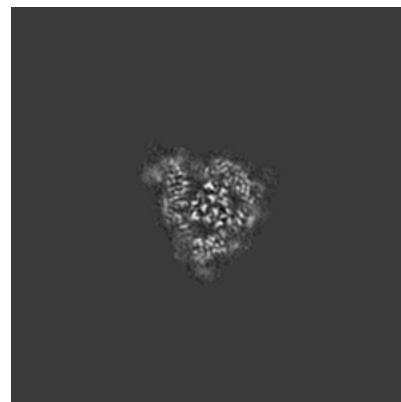
6.3.1 Primary map



X Index: 227

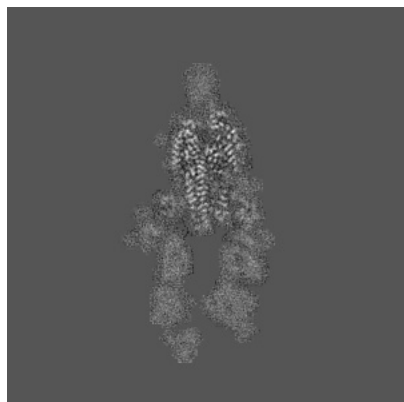


Y Index: 207

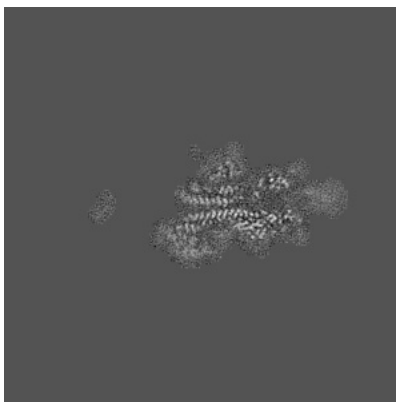


Z Index: 225

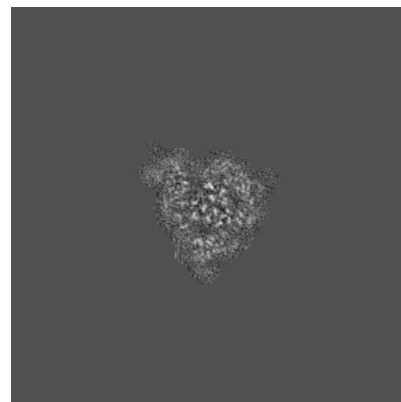
6.3.2 Raw map



X Index: 229



Y Index: 217

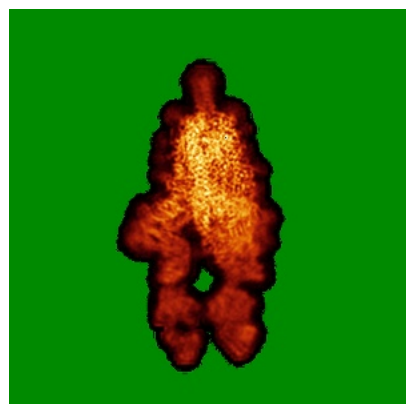


Z Index: 225

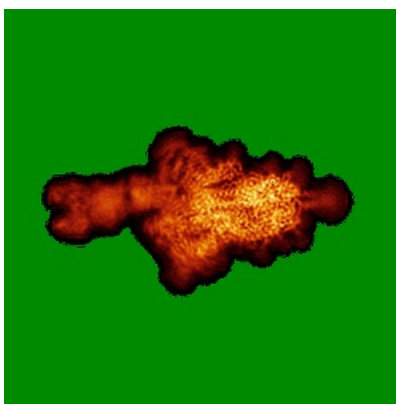
The images above show the largest variance slices of the map in three orthogonal directions.

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

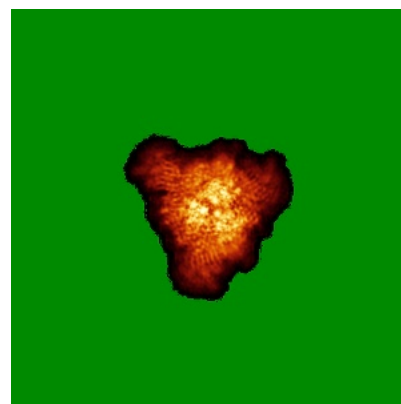
6.4.1 Primary map



X

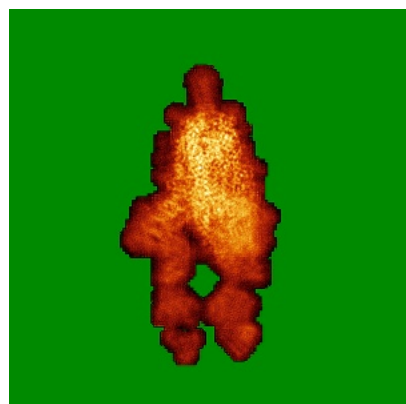


Y

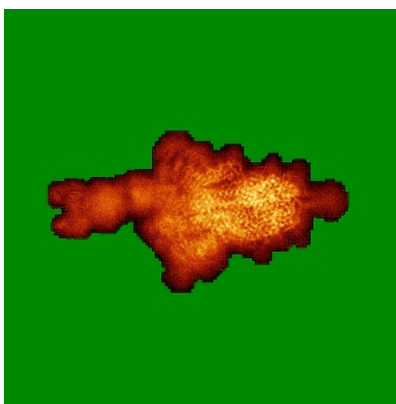


Z

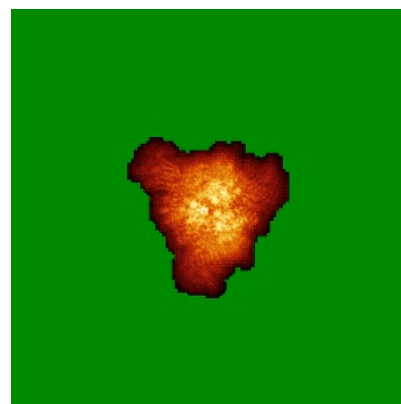
6.4.2 Raw map



X



Y

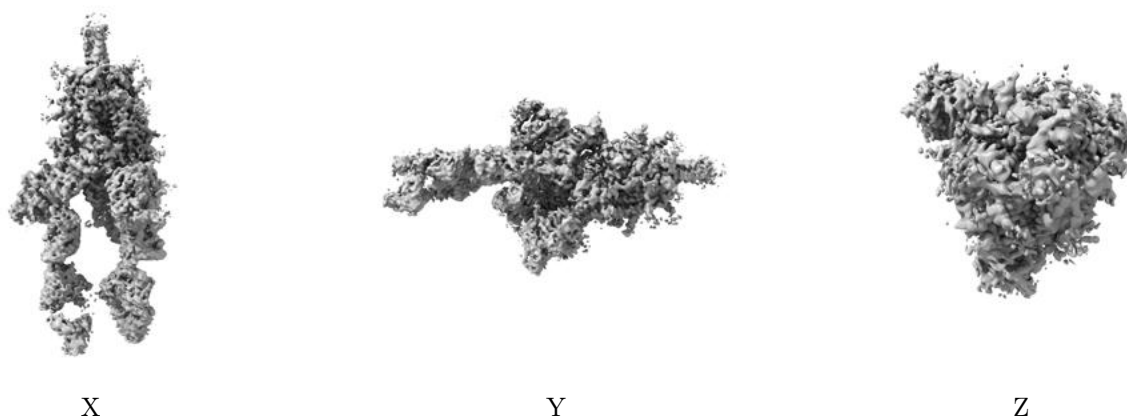


Z

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.

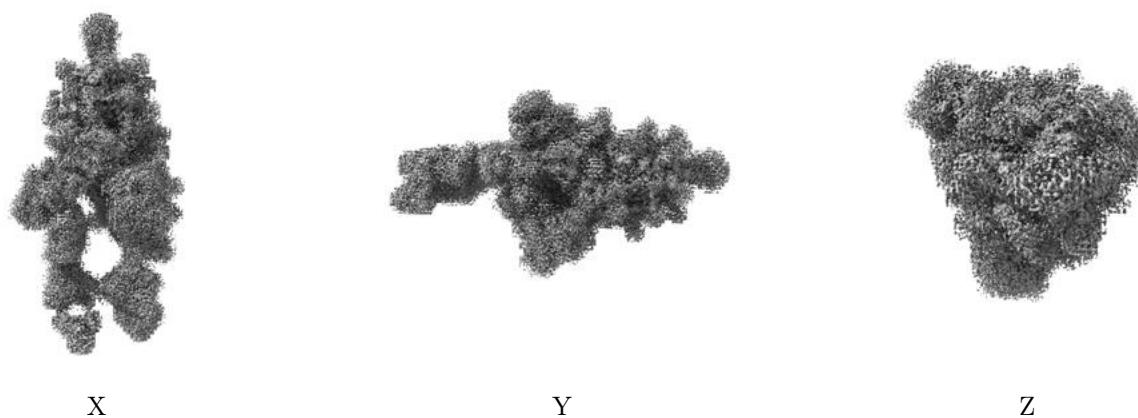
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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



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.

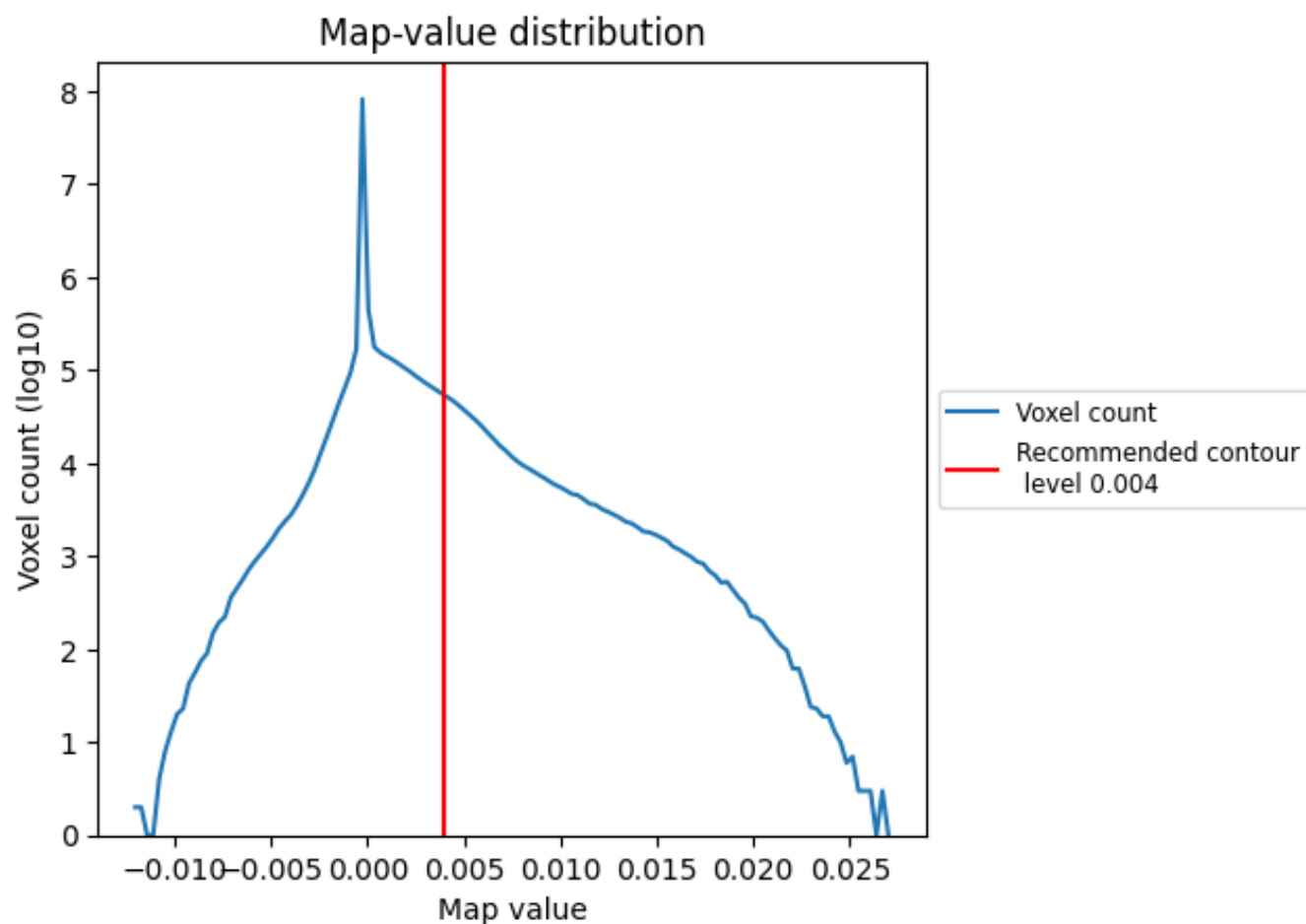
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

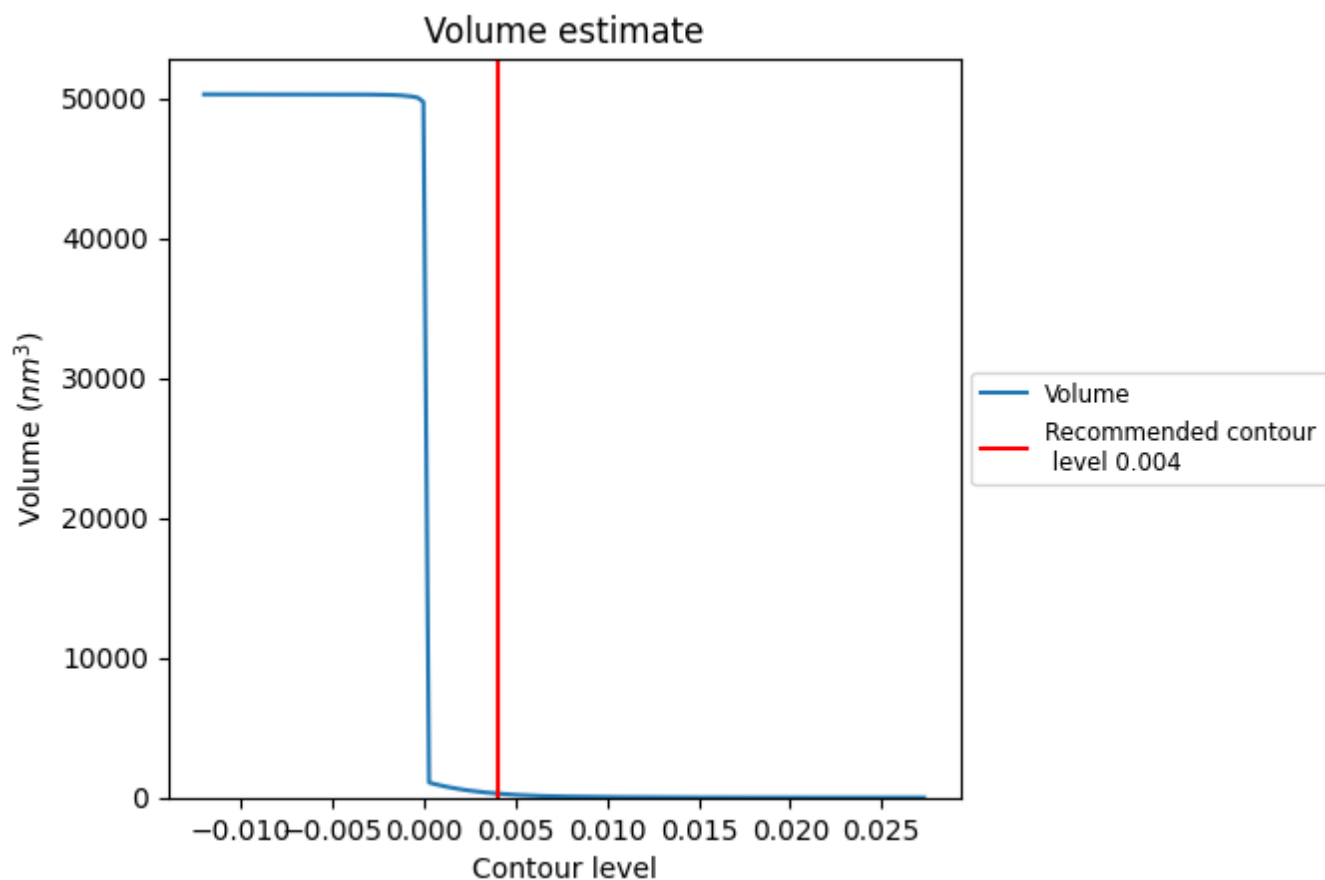
This section contains the results of statistical analysis of the map.

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.

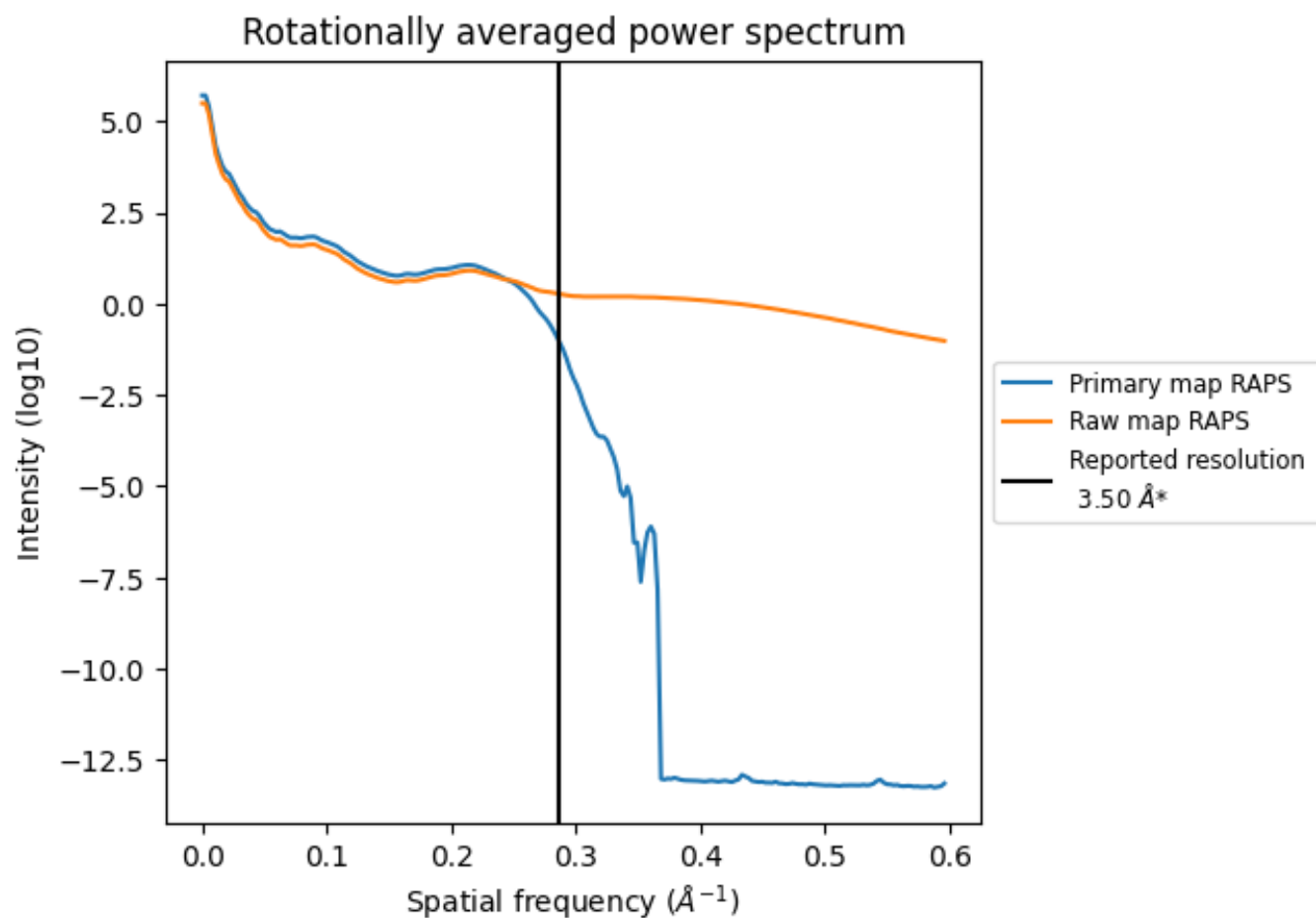
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm³; this corresponds to an approximate mass of 260 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 ⓘ

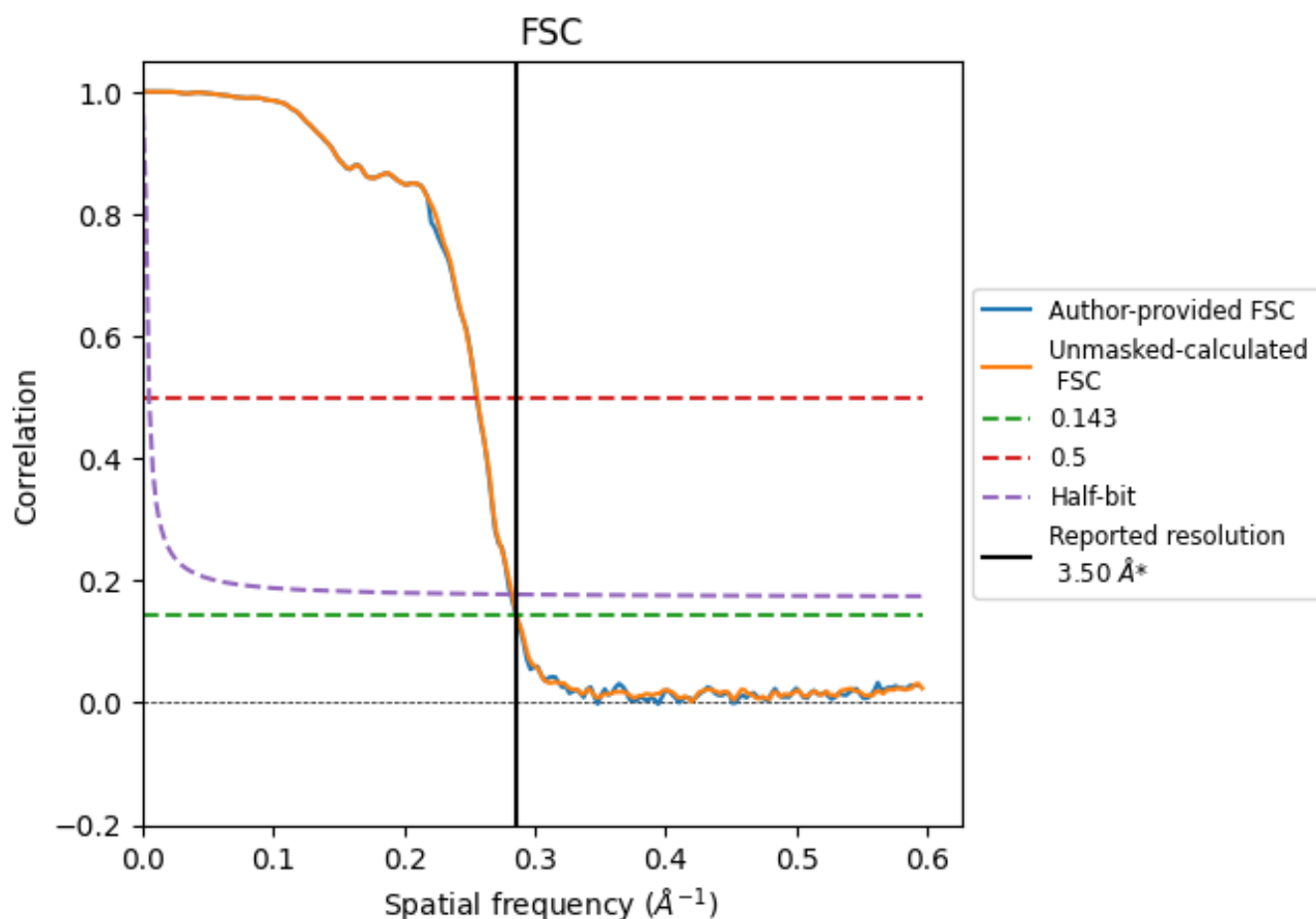


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

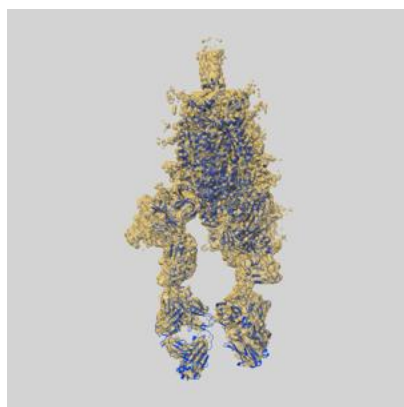
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	3.91	3.55
Unmasked-calculated*	3.49	3.91	3.54

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

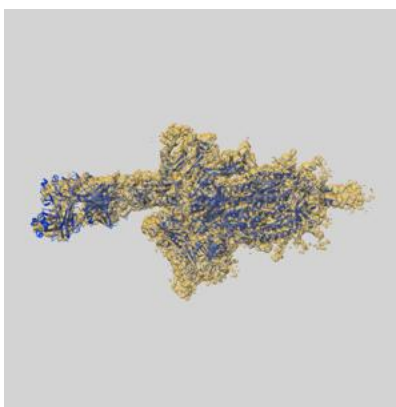
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73292 and PDB model 9YPB. Per-residue inclusion information can be found in section 3 on page 13.

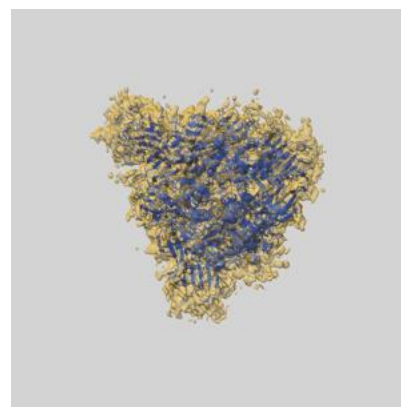
9.1 Map-model overlay [i](#)



X



Y



Z

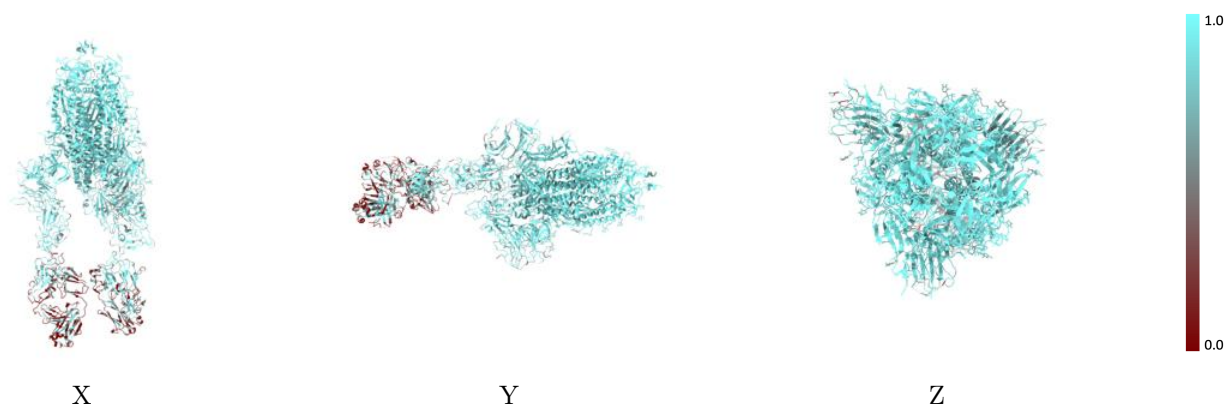
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



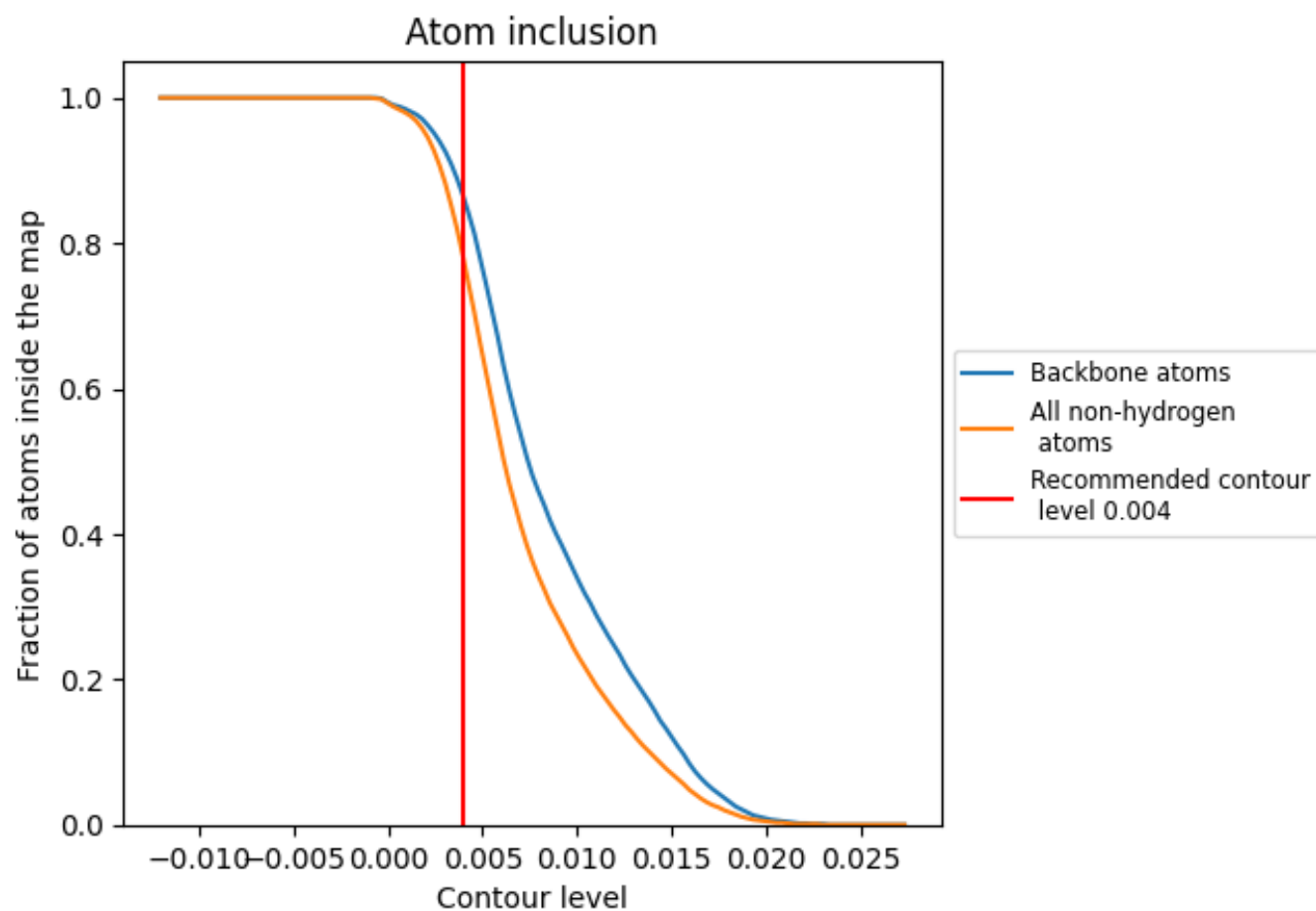
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7780	<div></div> 0.3650
A	<div></div> 0.8640	<div></div> 0.4210
B	<div></div> 0.8470	<div></div> 0.4230
C	<div></div> 0.8840	<div></div> 0.4450
D	<div></div> 0.5630	<div></div> 0.1140
E	<div></div> 0.4700	<div></div> 0.1290
F	<div></div> 0.4410	<div></div> 0.1150
G	<div></div> 0.3240	<div></div> 0.1290

1.0

0.0

<0.0