



Full wwPDB EM Validation Report ⓘ

Nov 8, 2023 – 12:37 AM EST

PDB ID : 8F4P
EMDB ID : EMD-28856
Title : SARS-CoV-2 spike protein trimer (down conformation) bound with a nanobody
Authors : Laughlin, Z.T.; Patel, A.; Ortlund, E.A.
Deposited on : 2022-11-11
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

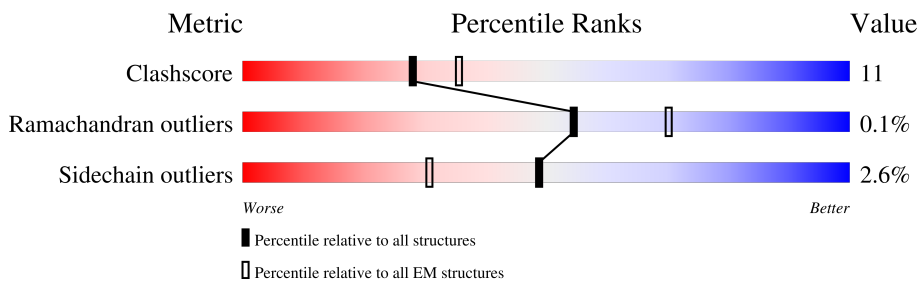
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



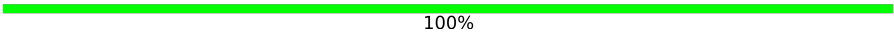

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1136	
1	B	1136	
1	C	1136	
2	D	118	
3	E	2	
3	F	2	
3	G	2	
3	H	2	

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Mol	Chain	Length	Quality of chain
3	I	2	
3	J	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1069	8375	5344	1398	1594	39	2	0
1	B	1088	8524	5441	1422	1623	38	2	0
1	C	1067	8350	5327	1395	1589	39	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called Anti-S1 Nanobody.

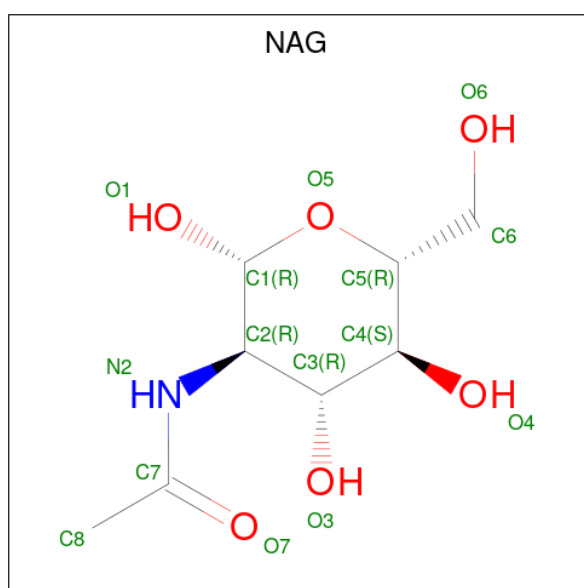
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	118	868	543	147	174	4	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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	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	
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	

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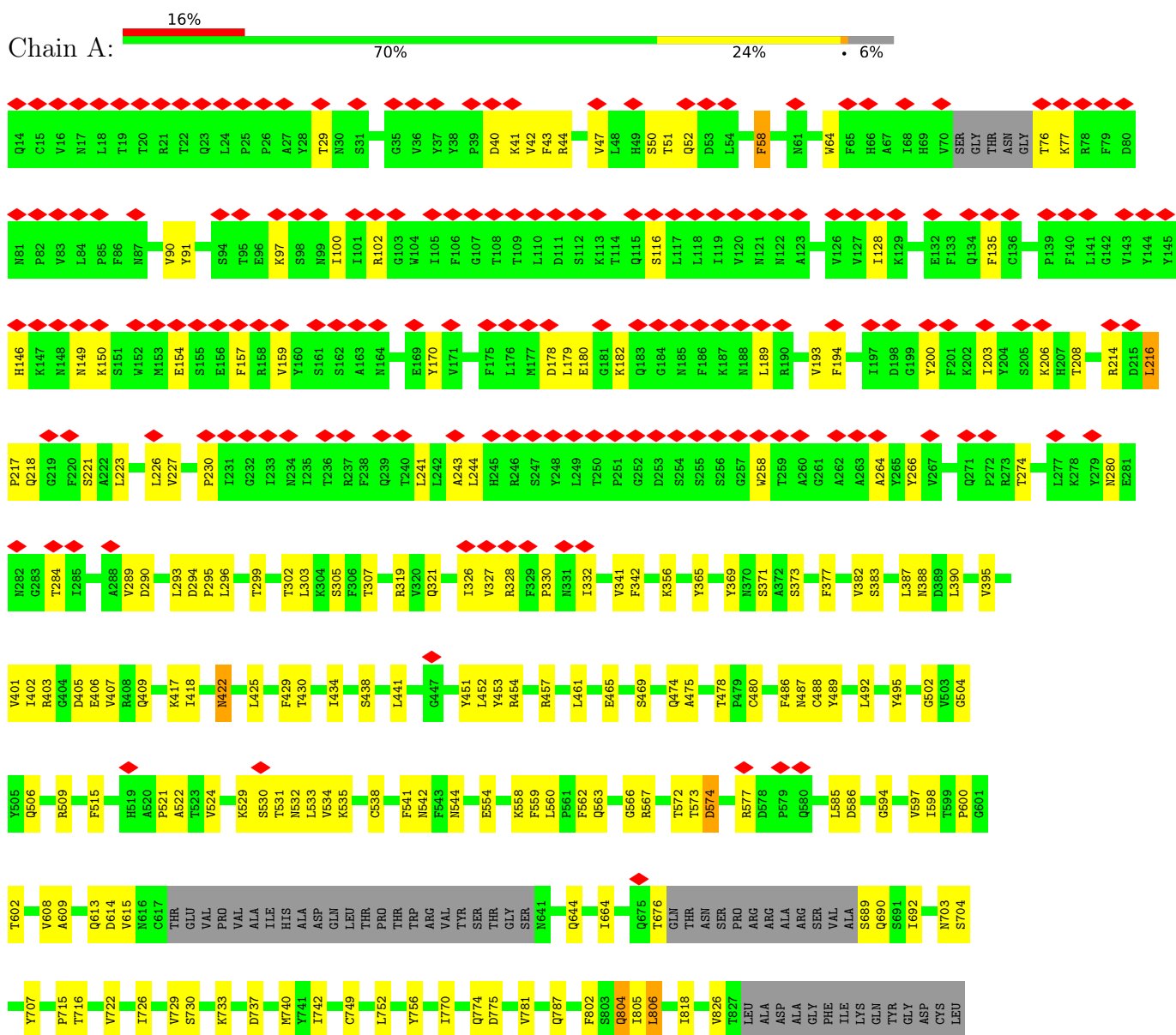
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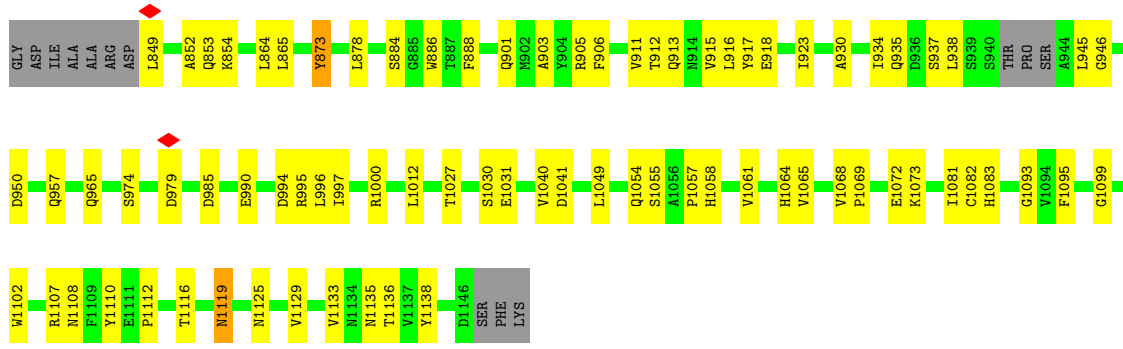
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

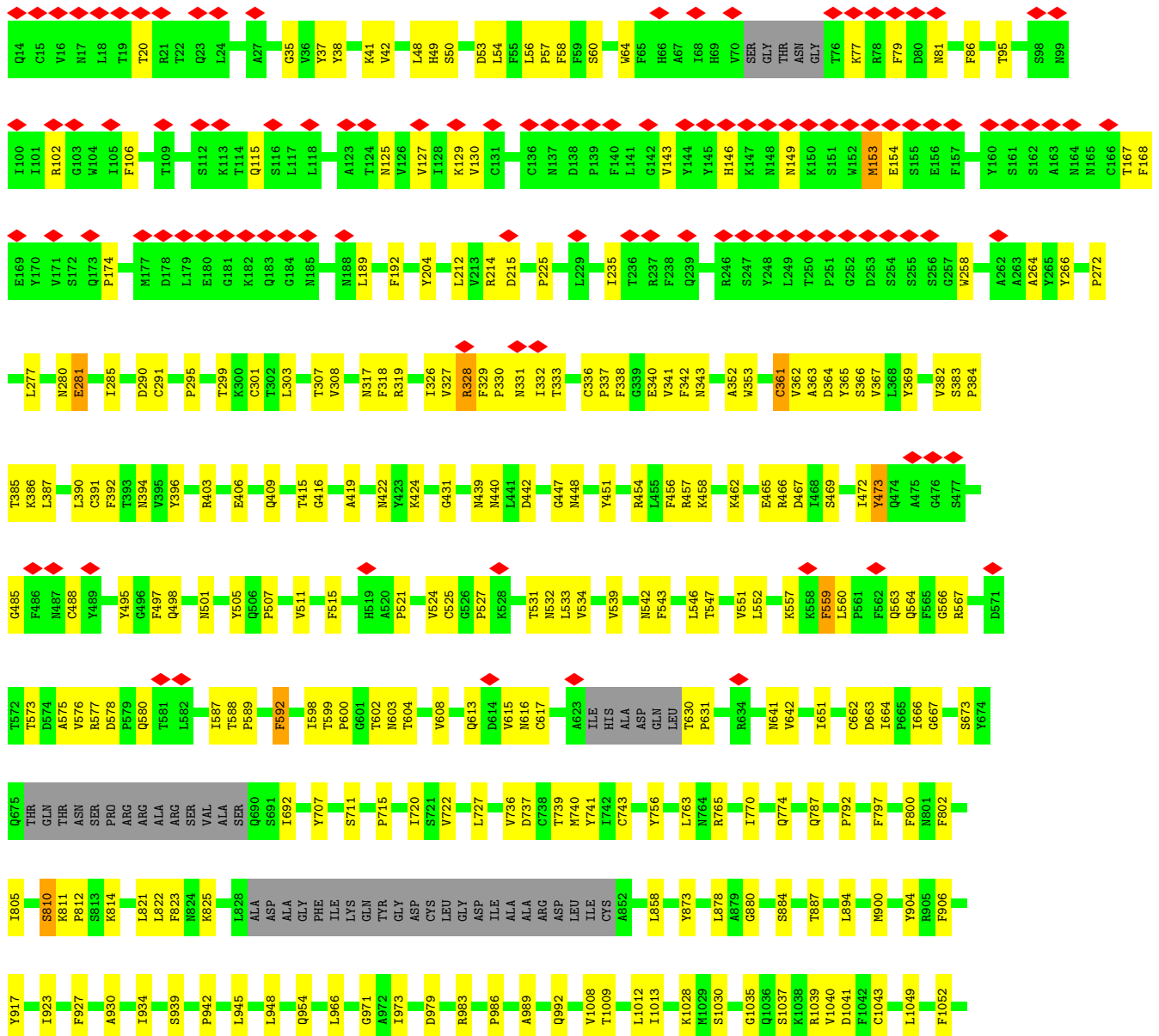
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein



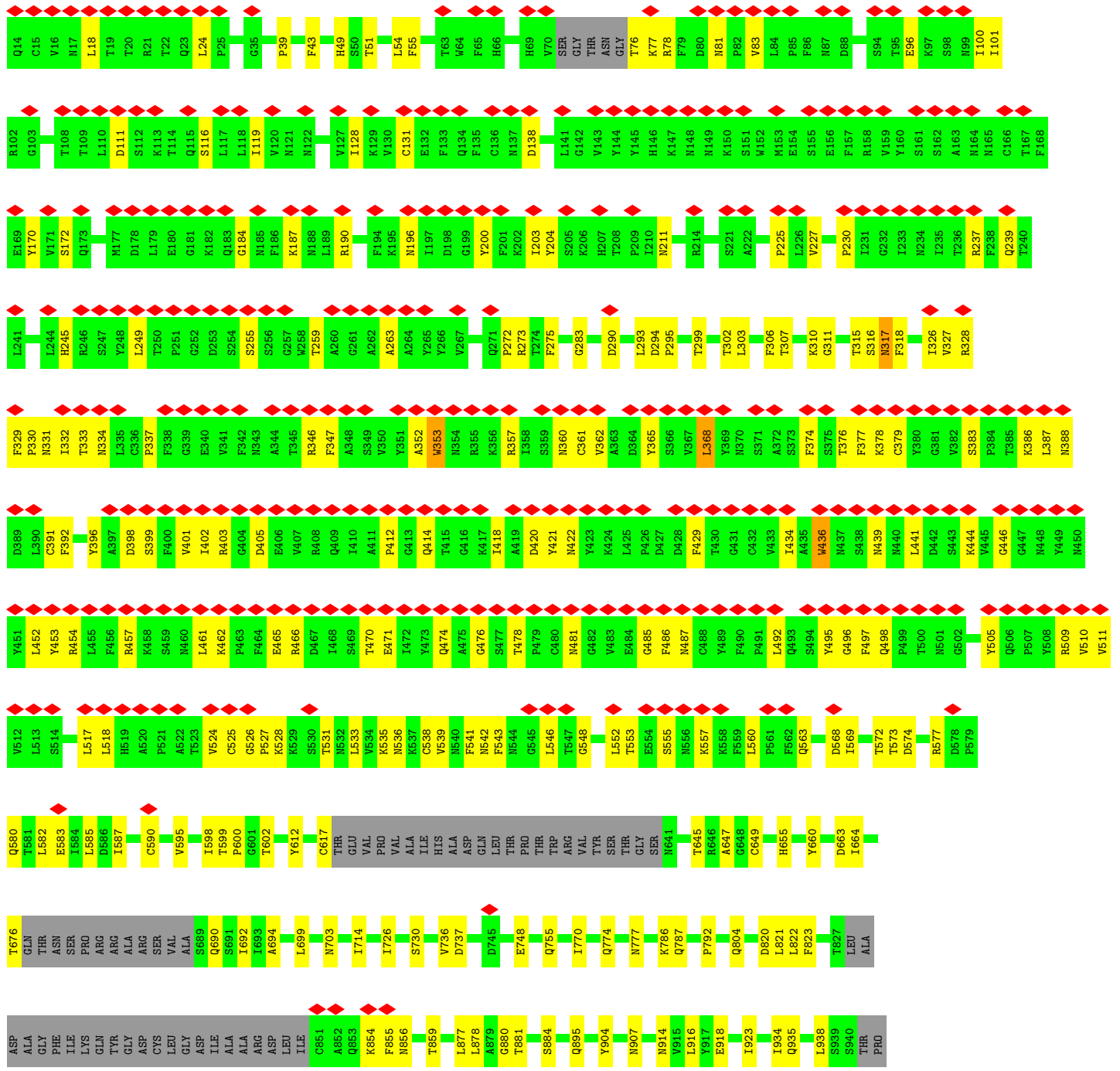


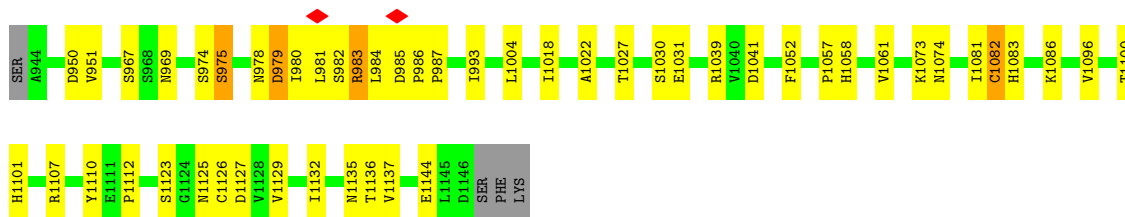
• Molecule 1: Spike glycoprotein



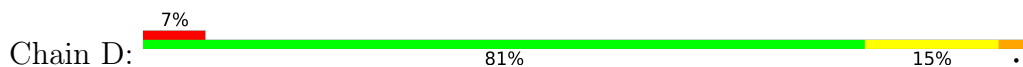


● Molecule 1: Spike glycoprotein





- Molecule 2: Anti-S1 Nanobody



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



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



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



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



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





NAG1
NAG2

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

Chain J: 



NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	489600	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.81	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	115.570	Depositor
Minimum map value	-102.901	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.117	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	444.7456, 444.7456, 444.7456	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0691, 1.0691, 1.0691	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	A	0.27	0/8574	0.49	0/11670
1	B	0.28	0/8731	0.49	0/11890
1	C	0.26	0/8546	0.48	0/11632
2	D	0.31	0/886	0.54	0/1198
All	All	0.27	0/26737	0.49	0/36390

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	A	8375	0	8170	189	0
1	B	8524	0	8326	196	0
1	C	8350	0	8145	193	0
2	D	868	0	831	22	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	1	0
4	A	126	0	117	2	0
4	B	98	0	91	2	0
4	C	126	0	117	0	0
All	All	26635	0	25947	556	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 11.

All (556) 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)
2:D:97:ALA:HB1	2:D:105:PHE:HB2	1.60	0.83
1:A:216:LEU:H	1:A:217:PRO:HD2	1.44	0.82
1:B:547:THR:HG23	1:C:978:ASN:HB3	1.63	0.80
1:A:189:LEU:HB3	1:A:208:THR:O	1.82	0.80
1:A:328:ARG:HA	1:A:530:SER:HA	1.62	0.79
1:C:1100:THR:HG1	1:C:1101:HIS:HD1	1.25	0.79
1:B:337:PRO:HB2	1:B:340:GLU:HB2	1.65	0.78
1:A:521:PRO:HA	1:A:577:ARG:HH12	1.47	0.78
1:A:43:PHE:HD1	1:C:563:GLN:HB3	1.49	0.76
1:B:979:ASP:O	1:B:983:ARG:HB2	1.87	0.74
1:B:391:CYS:CB	1:B:525:CYS:HA	2.20	0.72
1:C:470:THR:HG22	1:C:471:GLU:H	1.52	0.72
1:A:474:GLN:NE2	1:A:488:CYS:SG	2.63	0.72
1:A:522:ALA:H	1:A:577:ARG:HH22	1.38	0.71
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.74	0.69
1:B:391:CYS:HB3	1:B:525:CYS:HA	1.74	0.69
1:B:153:MET:SD	1:B:153:MET:N	2.67	0.68
1:C:401:VAL:HG12	1:C:509:ARG:HA	1.77	0.67
1:C:560:LEU:HD11	1:C:563:GLN:HB2	1.76	0.67
1:B:567:ARG:HA	1:B:573:THR:HA	1.77	0.66
1:B:589:PRO:HG2	1:C:855:PHE:HB3	1.76	0.66
1:C:568:ASP:OD1	1:C:569:ILE:N	2.28	0.66
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.28	0.66
1:B:557:LYS:HE3	1:B:559:PHE:HB2	1.76	0.66
1:C:444:LYS:HG3	1:C:446:GLY:H	1.61	0.66
1:A:403:ARG:HB3	1:A:406:GLU:HG3	1.77	0.66
1:B:125:ASN:HA	1:B:174:PRO:HD3	1.77	0.66
1:C:374:PHE:HE1	1:C:436:TRP:HB3	1.60	0.66
1:C:315:THR:HG22	1:C:316:SER:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PRO:HB3	1:C:361:CYS:SG	2.35	0.65
1:A:864:LEU:HD22	1:A:865:LEU:HD12	1.77	0.65
1:B:599:THR:HB	1:B:608:VAL:HG12	1.79	0.64
1:A:609:ALA:HB2	1:A:692:ILE:HG21	1.77	0.64
1:A:787:GLN:OE1	1:C:703:ASN:ND2	2.30	0.64
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.79	0.64
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.80	0.64
2:D:100:ASP:HB2	2:D:103:LYS:HB3	1.80	0.64
1:C:548:GLY:H	1:C:577:ARG:HH22	1.45	0.64
1:B:454:ARG:NH2	1:B:469:SER:O	2.32	0.63
1:B:20:THR:HG21	1:B:79:PHE:HB3	1.80	0.63
1:B:498:GLN:NE2	1:B:501:ASN:OD1	2.30	0.63
1:A:849:LEU:O	1:A:853:GLN:NE2	2.32	0.63
1:B:95:THR:HG22	1:B:189:LEU:HA	1.81	0.62
1:B:454:ARG:NH1	1:B:467:ASP:O	2.30	0.62
1:A:475:ALA:HB1	2:D:32:ILE:HD11	1.82	0.62
1:C:388:ASN:HB3	1:C:527:PRO:HB3	1.80	0.62
1:C:1125:ASN:ND2	1:C:1127:ASP:OD1	2.33	0.62
1:B:38:TYR:HE1	1:B:285:ILE:HG13	1.64	0.62
1:C:96:GLU:OE2	1:C:190:ARG:NH1	2.32	0.62
1:A:200:TYR:HA	1:A:230:PRO:HA	1.80	0.62
1:A:1107:ARG:HD2	1:B:904:TYR:CZ	2.35	0.62
1:C:326:ILE:HB	1:C:531:THR:HG21	1.81	0.61
1:B:560:LEU:HD13	1:B:563:GLN:HG3	1.83	0.61
1:C:1081:ILE:HG21	1:C:1135:ASN:HB3	1.82	0.61
1:C:950:ASP:OD1	1:C:951:VAL:N	2.33	0.61
2:D:109:GLN:OE1	2:D:109:GLN:N	2.27	0.61
1:C:310:LYS:HA	1:C:599:THR:O	2.01	0.61
1:C:200:TYR:HA	1:C:230:PRO:HA	1.83	0.61
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	1.83	0.61
1:A:567:ARG:HA	1:A:572:THR:HG22	1.82	0.60
1:A:52:GLN:HG3	1:A:274:THR:HG22	1.83	0.60
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.84	0.60
1:C:533:LEU:HB3	1:C:552:LEU:HB3	1.83	0.60
1:C:726:ILE:HD13	1:C:1061:VAL:HG22	1.84	0.60
1:A:395:VAL:HG23	1:A:524:VAL:HG11	1.83	0.60
2:D:17:SER:HA	2:D:83:MET:O	2.01	0.60
1:B:821:LEU:HD11	1:B:939:SER:HB2	1.83	0.60
1:B:146:HIS:HB3	1:B:149:ASN:HB2	1.83	0.60
1:C:462:LYS:HG2	1:C:465:GLU:HB2	1.84	0.60
2:D:7:SER:OG	2:D:21:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:SER:OG	1:A:888:PHE:HB3	2.02	0.59
1:B:534:VAL:HG11	1:B:539:VAL:HG21	1.84	0.59
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	1.84	0.59
1:A:307:THR:HA	1:A:602:THR:HG21	1.84	0.59
1:C:542:ASN:HB2	1:C:577:ARG:NE	2.18	0.59
1:A:722:VAL:HG12	1:A:1065:VAL:HG22	1.83	0.59
1:C:357:ARG:HB3	1:C:396:TYR:HB2	1.85	0.59
1:A:326:ILE:HD12	1:A:533:LEU:HA	1.84	0.59
1:A:726:ILE:HD13	1:A:945:LEU:HD13	1.84	0.59
1:B:317:ASN:ND2	1:C:737:ASP:OD2	2.35	0.59
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.85	0.59
1:C:328:ARG:NH1	1:C:329:PHE:O	2.36	0.59
1:C:362:VAL:HB	1:C:526:GLY:HA3	1.85	0.59
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.33	0.58
1:A:216:LEU:H	1:A:217:PRO:CD	2.14	0.58
1:A:805:ILE:HB	1:A:878:LEU:HD21	1.85	0.58
1:A:934:ILE:HA	1:A:937:SER:HB3	1.86	0.58
1:C:496:GLY:O	1:C:498:GLN:NE2	2.36	0.58
1:C:542:ASN:HB2	1:C:577:ARG:HE	1.67	0.58
1:A:452:LEU:HD22	1:A:492:LEU:HD23	1.84	0.58
1:C:548:GLY:O	1:C:577:ARG:NH2	2.36	0.58
1:C:557:LYS:N	1:C:583:GLU:HB3	2.18	0.58
1:C:333:THR:OG1	1:C:334:ASN:N	2.35	0.58
1:A:146:HIS:O	1:A:150:LYS:N	2.36	0.58
1:A:418:ILE:HA	1:A:422:ASN:ND2	2.18	0.58
1:A:752:LEU:HD11	1:A:990:GLU:HG2	1.85	0.58
1:B:739:THR:O	1:B:743:CYS:HB2	2.04	0.58
1:C:81:ASN:OD1	1:C:239:GLN:NE2	2.38	0.57
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.85	0.57
1:C:533:LEU:HD22	1:C:552:LEU:HD22	1.85	0.57
1:A:985:ASP:OD1	1:A:985:ASP:N	2.38	0.57
1:A:128:ILE:HD12	1:A:170:TYR:HB3	1.87	0.57
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.53	0.57
1:C:119:ILE:HG12	1:C:128:ILE:HG23	1.87	0.57
1:C:914:ASN:O	1:C:918:GLU:HG3	2.05	0.57
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.87	0.56
1:B:1107:ARG:HD3	1:C:904:TYR:CE2	2.40	0.56
1:C:548:GLY:N	1:C:577:ARG:HH12	2.02	0.56
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.87	0.56
1:C:951:VAL:HG21	1:C:1018:ILE:HD11	1.87	0.56
1:A:44:ARG:HG2	1:A:47:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ALA:O	1:C:399:SER:OG	2.22	0.56
1:A:29:THR:HG21	1:A:216:LEU:HD21	1.87	0.56
1:A:42:VAL:O	1:C:563:GLN:NE2	2.33	0.56
1:C:310:LYS:NZ	1:C:663:ASP:OD2	2.29	0.56
1:C:737:ASP:N	1:C:737:ASP:OD1	2.38	0.56
1:C:975:SER:OG	1:C:975:SER:O	2.20	0.56
1:B:822:LEU:HD21	1:B:1061:VAL:HG21	1.87	0.56
1:A:454:ARG:NH2	1:A:469:SER:O	2.36	0.56
1:A:770:ILE:O	1:A:774:GLN:HG2	2.06	0.56
1:C:290:ASP:HB3	1:C:293:LEU:HB2	1.88	0.56
1:C:418:ILE:O	1:C:422:ASN:ND2	2.38	0.56
1:B:215:ASP:HB3	1:B:266:TYR:HE2	1.71	0.56
1:C:83:VAL:HG21	1:C:237:ARG:HE	1.71	0.56
1:B:331:ASN:OD1	1:B:580:GLN:NE2	2.39	0.56
1:A:383:SER:N	1:B:983:ARG:O	2.38	0.56
1:B:736:VAL:HG11	1:B:858:LEU:HD23	1.87	0.56
2:D:98:LYS:C	2:D:105:PHE:HA	2.27	0.56
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.87	0.55
1:A:402:ILE:HD11	1:A:407:VAL:HA	1.88	0.55
1:B:58:PHE:HD1	1:B:290:ASP:HB2	1.70	0.55
1:B:369:TYR:OH	1:B:384:PRO:HB2	2.07	0.55
1:A:326:ILE:HD13	1:A:534:VAL:HG12	1.88	0.55
1:B:143:VAL:HG12	1:B:154:GLU:HB2	1.88	0.55
1:B:722:VAL:HG12	1:B:1065:VAL:HG22	1.89	0.55
1:B:566:GLY:H	1:B:575:ALA:HB3	1.71	0.55
1:C:880:GLY:O	1:C:884:SER:OG	2.24	0.55
1:A:566:GLY:H	1:A:573:THR:HG22	1.72	0.55
1:B:1041:ASP:HB2	1:C:1030:SER:OG	2.06	0.55
1:A:102:ARG:NH2	1:A:154:GLU:OE2	2.39	0.54
1:C:663:ASP:OD1	1:C:663:ASP:N	2.40	0.54
1:C:854:LYS:HE2	1:C:859:THR:HG22	1.88	0.54
1:C:39:PRO:HB3	1:C:51:THR:HG21	1.89	0.54
1:B:385:THR:HG23	1:B:386:LYS:HG2	1.87	0.54
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.72	0.54
1:A:903:ALA:HB1	1:A:913:GLN:HB2	1.90	0.54
1:C:402:ILE:HG12	1:C:510:VAL:HG21	1.90	0.54
1:B:415:THR:OG1	1:B:416:GLY:N	2.40	0.54
1:B:457:ARG:NH1	1:B:467:ASP:OD1	2.40	0.54
1:A:1041:ASP:HB2	1:B:1030:SER:HB3	1.89	0.54
1:A:327:VAL:HG13	1:A:542:ASN:HD21	1.73	0.54
1:A:563:GLN:NE2	1:B:42:VAL:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD13	1:B:587:ILE:HG22	1.89	0.54
1:A:613:GLN:O	1:A:615:VAL:N	2.40	0.54
2:D:97:ALA:HA	2:D:106:ASP:O	2.08	0.53
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.48	0.53
1:A:146:HIS:HB3	1:A:149:ASN:HB2	1.91	0.53
1:A:179:LEU:HD23	1:A:179:LEU:H	1.72	0.53
1:B:382:VAL:HG13	1:C:983:ARG:HB2	1.90	0.53
1:C:1083:HIS:NE2	1:C:1136:THR:HA	2.23	0.53
1:A:58:PHE:HE2	1:A:289:VAL:HA	1.73	0.53
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.89	0.53
1:B:290:ASP:OD1	1:B:291:CYS:N	2.41	0.53
1:C:454:ARG:HD3	1:C:457:ARG:HG3	1.90	0.53
1:C:877:LEU:O	1:C:881:THR:HG22	2.09	0.53
1:C:486:PHE:CD1	1:C:487:ASN:N	2.77	0.53
1:B:319:ARG:HG2	1:B:592:PHE:HB2	1.89	0.53
1:C:486:PHE:HD1	1:C:487:ASN:N	2.07	0.53
1:C:770:ILE:O	1:C:774:GLN:HG2	2.09	0.53
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.90	0.53
1:A:332:ILE:HG12	4:A:1202:NAG:H5	1.91	0.53
1:A:818:ILE:HD13	1:A:934:ILE:HD11	1.90	0.53
1:A:934:ILE:O	1:A:938:LEU:N	2.42	0.52
1:C:353:TRP:O	1:C:466:ARG:NH2	2.42	0.52
1:C:332:ILE:HG13	1:C:333:THR:H	1.74	0.52
1:C:748:GLU:HB2	1:C:981:LEU:HD11	1.92	0.52
1:B:473:TYR:O	1:B:488:CYS:HA	2.09	0.52
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.91	0.52
1:B:547:THR:O	1:C:978:ASN:ND2	2.43	0.52
1:C:1126:CYS:HB2	1:C:1132:ILE:HG12	1.91	0.52
1:A:703:ASN:OD1	1:A:704:SER:N	2.42	0.52
1:B:352:ALA:O	1:B:466:ARG:NH2	2.43	0.52
1:C:361:CYS:SG	1:C:362:VAL:N	2.83	0.52
1:C:555:SER:HA	1:C:583:GLU:HB2	1.92	0.52
1:C:273:ARG:HB3	1:C:275:PHE:CE1	2.44	0.52
1:B:945:LEU:HD12	1:B:948:LEU:HD12	1.92	0.52
1:A:390:LEU:HD22	1:B:983:ARG:CZ	2.40	0.52
1:A:461:LEU:HD23	1:A:465:GLU:HB3	1.91	0.52
1:B:448:ASN:N	1:B:497:PHE:O	2.41	0.52
1:A:729:VAL:HG11	1:A:781:VAL:HG11	1.91	0.52
1:A:562:PHE:O	1:B:41:LYS:NZ	2.35	0.51
1:B:212:LEU:HD23	1:B:214:ARG:H	1.74	0.51
1:B:456:PHE:HB3	1:B:473:TYR:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.92	0.51
1:B:930:ALA:O	1:B:934:ILE:HG22	2.11	0.51
1:C:403:ARG:NH1	1:C:421:TYR:OH	2.44	0.51
1:B:578:ASP:OD2	1:B:580:GLN:N	2.42	0.51
1:C:295:PRO:O	1:C:299:THR:HG23	2.11	0.51
1:C:474:GLN:O	1:C:476:GLY:N	2.44	0.51
1:A:916:LEU:HD12	1:A:923:ILE:HD12	1.91	0.51
1:A:341:VAL:HG21	1:A:356:LYS:HG2	1.92	0.51
1:A:715:PRO:HD3	1:B:894:LEU:HD13	1.93	0.51
1:A:946:GLY:O	1:A:950:ASP:HB2	2.10	0.51
1:C:116:SER:HB2	1:C:131:CYS:O	2.10	0.51
1:B:353:TRP:NE1	1:B:465:GLU:O	2.36	0.51
1:B:367:VAL:HG12	2:D:101:VAL:HG21	1.93	0.51
1:B:1083:HIS:CD2	1:B:1136:THR:HA	2.45	0.51
1:A:319:ARG:NH2	1:B:740:MET:SD	2.80	0.51
1:B:447:GLY:HA2	1:B:498:GLN:HB3	1.93	0.51
1:B:736:VAL:HG12	1:B:858:LEU:HA	1.93	0.51
1:B:810:SER:O	1:B:810:SER:OG	2.27	0.51
1:A:901:GLN:O	1:A:905:ARG:HG2	2.11	0.50
1:A:737:ASP:HB3	1:A:740:MET:HB3	1.93	0.50
1:A:1099:GLY:HA3	4:A:1207:NAG:H82	1.93	0.50
1:B:307:THR:HA	1:B:602:THR:HG21	1.93	0.50
1:B:642:VAL:HA	1:B:651:ILE:HG22	1.93	0.50
1:A:529:LYS:HE3	1:A:530:SER:H	1.77	0.50
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.91	0.50
1:C:365:TYR:HB3	1:C:368:LEU:HD11	1.93	0.50
1:C:821:LEU:HD11	1:C:935:GLN:HE21	1.77	0.50
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.93	0.50
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.94	0.50
1:A:40:ASP:HB3	1:A:42:VAL:HG22	1.94	0.50
1:A:280:ASN:OD1	1:A:284:THR:N	2.45	0.50
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.45	0.50
1:B:394:ASN:HB3	1:B:396:TYR:HE1	1.76	0.50
1:C:361:CYS:O	1:C:524:VAL:HA	2.12	0.50
1:C:55:PHE:HB2	1:C:275:PHE:CE1	2.47	0.50
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.94	0.50
1:C:539:VAL:HG11	1:C:552:LEU:HG	1.93	0.49
1:A:614:ASP:OD1	1:A:614:ASP:N	2.46	0.49
1:B:532:ASN:OD1	1:B:533:LEU:N	2.43	0.49
1:C:1083:HIS:O	1:C:1086:LYS:N	2.46	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LEU:HD22	1:C:272:PRO:HB3	1.93	0.49
2:D:105:PHE:O	2:D:106:ASP:C	2.51	0.49
1:A:994:ASP:OD1	1:A:995:ARG:N	2.45	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.95	0.49
1:C:200:TYR:CZ	1:C:230:PRO:HB3	2.48	0.49
1:C:327:VAL:HB	1:C:543:PHE:HB3	1.95	0.49
1:A:244:LEU:HD23	1:A:258:TRP:CG	2.47	0.49
1:A:418:ILE:HG23	1:A:422:ASN:HD22	1.76	0.49
1:B:212:LEU:HD23	1:B:214:ARG:N	2.27	0.49
1:B:1040:VAL:HG22	1:B:1041:ASP:OD2	2.12	0.49
2:D:73:ASP:O	2:D:77:ASN:N	2.45	0.49
1:A:689:SER:O	1:A:690:GLN:HG3	2.12	0.49
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.48	0.49
1:C:311:GLY:HA2	1:C:664:ILE:HG23	1.94	0.49
1:C:461:LEU:HD22	1:C:465:GLU:HG2	1.93	0.49
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.78	0.49
2:D:97:ALA:HB1	2:D:105:PHE:CB	2.39	0.49
1:B:880:GLY:O	1:B:884:SER:OG	2.27	0.49
1:C:577:ARG:HH11	1:C:577:ARG:HG2	1.78	0.49
1:A:295:PRO:O	1:A:299:THR:HG23	2.13	0.48
1:B:383:SER:HB2	1:C:984:LEU:HA	1.93	0.48
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.76	0.48
1:B:1074:ASN:OD1	1:C:895:GLN:NE2	2.47	0.48
1:A:326:ILE:O	1:A:541:PHE:HB2	2.14	0.48
1:A:854:LYS:HG3	1:C:572:THR:HG22	1.95	0.48
1:B:1081:ILE:O	1:B:1088:HIS:N	2.38	0.48
1:C:398:ASP:OD1	1:C:398:ASP:N	2.45	0.48
1:C:916:LEU:HD12	1:C:923:ILE:HG13	1.96	0.48
2:D:34:MET:SD	2:D:98:LYS:HB2	2.53	0.48
1:B:576:VAL:HG12	1:B:577:ARG:H	1.77	0.48
1:A:342:PHE:HE1	1:A:434:ILE:HG21	1.77	0.48
1:B:77:LYS:NZ	1:B:258:TRP:O	2.45	0.48
1:B:102:ARG:HH22	1:B:143:VAL:HG11	1.78	0.48
1:C:204:TYR:HD2	1:C:225:PRO:HA	1.79	0.48
1:B:365:TYR:CG	1:B:387:LEU:HD23	2.49	0.48
1:B:521:PRO:HB3	1:B:564:GLN:HG2	1.96	0.48
1:C:383:SER:HB3	1:C:386:LYS:HB3	1.95	0.48
1:A:873:TYR:CZ	1:C:699:LEU:HD12	2.48	0.48
1:B:57:PRO:HG2	1:B:60:SER:HB3	1.96	0.48
1:C:273:ARG:HB3	1:C:275:PHE:CZ	2.49	0.48
1:C:495:TYR:HB3	1:C:497:PHE:HD1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	1.95	0.48
1:B:501:ASN:ND2	1:B:505:TYR:HB3	2.29	0.48
1:C:804:GLN:O	1:C:804:GLN:HG3	2.14	0.48
1:B:613:GLN:O	1:B:615:VAL:N	2.46	0.48
1:C:403:ARG:H	1:C:418:ILE:HD11	1.79	0.48
1:A:560:LEU:O	1:A:562:PHE:N	2.40	0.47
1:B:391:CYS:HB2	1:B:524:VAL:O	2.13	0.47
1:A:535:LYS:NZ	1:A:554:GLU:OE2	2.39	0.47
1:B:722:VAL:HA	1:B:1064:HIS:O	2.14	0.47
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.40	0.47
1:B:280:ASN:OD1	1:B:281:GLU:N	2.45	0.47
1:B:456:PHE:HB3	1:B:473:TYR:CE2	2.49	0.47
1:B:543:PHE:CD2	1:B:576:VAL:HG11	2.49	0.47
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.49	0.47
1:B:566:GLY:HA3	1:C:43:PHE:HB3	1.96	0.47
1:C:204:TYR:CD2	1:C:225:PRO:HA	2.50	0.47
1:A:474:GLN:NE2	1:A:478:THR:O	2.47	0.47
1:B:440:ASN:ND2	2:D:75:SER:O	2.25	0.47
1:C:100:ILE:HG21	1:C:263:ALA:HB2	1.95	0.47
1:C:211:ASN:OD1	1:C:211:ASN:N	2.47	0.47
1:C:736:VAL:HG21	1:C:1004:LEU:HD11	1.95	0.47
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.97	0.47
1:B:215:ASP:HB3	1:B:266:TYR:CE2	2.50	0.47
1:B:566:GLY:HA2	1:C:43:PHE:H	1.78	0.47
1:B:1090:PRO:HD3	1:B:1095:PHE:HE2	1.80	0.47
1:B:35:GLY:HA3	1:B:56:LEU:HD21	1.97	0.46
1:B:1141:LEU:HD21	1:C:1144:GLU:HG3	1.97	0.46
1:C:24:LEU:O	1:C:78:ARG:NH2	2.48	0.46
1:C:249:LEU:HD13	1:C:255:SER:HB2	1.97	0.46
1:A:214:ARG:HE	1:A:218:GLN:HB2	1.80	0.46
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.79	0.46
1:A:1125:ASN:N	1:A:1125:ASN:OD1	2.48	0.46
1:B:770:ILE:O	1:B:774:GLN:HG2	2.15	0.46
1:A:194:PHE:HE1	1:A:203:ILE:HG23	1.81	0.46
1:C:557:LYS:H	1:C:583:GLU:HB3	1.79	0.46
1:C:822:LEU:HD21	1:C:938:LEU:HD21	1.98	0.46
1:A:43:PHE:CD1	1:C:563:GLN:HB3	2.39	0.46
1:A:703:ASN:ND2	1:B:787:GLN:OE1	2.46	0.46
1:B:37:TYR:OH	1:B:53:ASP:OD1	2.32	0.46
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.79	0.46
1:C:1083:HIS:CE1	1:C:1137:VAL:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLN:NE2	1:A:480:CYS:SG	2.89	0.46
1:A:805:ILE:HG22	1:A:1054:GLN:HE21	1.80	0.46
1:B:364:ASP:HB3	1:B:527:PRO:HG2	1.98	0.46
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG11	2.50	0.46
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.96	0.46
1:C:294:ASP:OD1	1:C:294:ASP:N	2.47	0.46
1:C:405:ASP:OD1	1:C:405:ASP:N	2.49	0.46
1:A:180:GLU:HG3	1:A:182:LYS:HE3	1.96	0.46
1:A:294:ASP:OD1	1:A:294:ASP:N	2.49	0.46
1:B:1106:GLN:HE21	1:B:1111:GLU:HB3	1.80	0.46
1:C:18:LEU:N	1:C:138:ASP:OD2	2.40	0.46
1:C:362:VAL:HG11	1:C:528:LYS:NZ	2.30	0.46
1:A:371:SER:OG	1:A:373:SER:OG	2.31	0.46
1:B:497:PHE:CD2	1:B:507:PRO:HB3	2.51	0.46
1:B:973:ILE:HG23	1:B:992:GLN:NE2	2.31	0.46
1:A:1102:TRP:CE2	1:A:1133:VAL:HG11	2.51	0.46
1:B:825:LYS:NZ	1:B:942:PRO:HA	2.31	0.46
1:C:1110:TYR:CZ	1:C:1112:PRO:HG3	2.51	0.46
1:B:86:PHE:HD1	1:B:86:PHE:H	1.64	0.46
1:A:328:ARG:HB2	1:A:531:THR:H	1.80	0.46
1:B:811:LYS:HD2	1:B:812:PRO:HD2	1.97	0.46
1:A:328:ARG:O	1:A:544:ASN:N	2.36	0.45
1:A:770:ILE:HD11	1:A:1012:LEU:HA	1.97	0.45
1:A:1040:VAL:HG21	1:B:1035:GLY:HA3	1.97	0.45
1:C:453:TYR:HB3	1:C:495:TYR:CE1	2.51	0.45
1:A:487:ASN:HA	1:A:489:TYR:CE2	2.52	0.45
1:B:81:ASN:N	1:B:81:ASN:OD1	2.49	0.45
1:C:984:LEU:H	1:C:984:LEU:HD23	1.81	0.45
1:A:502:GLY:O	1:A:506:GLN:HG2	2.15	0.45
1:B:462:LYS:N	1:B:465:GLU:OE1	2.50	0.45
1:A:159:VAL:HG11	1:A:241:LEU:HD11	1.97	0.45
1:A:180:GLU:HG2	1:A:182:LYS:H	1.80	0.45
1:A:996:LEU:HD21	1:A:1000:ARG:HH21	1.82	0.45
1:B:403:ARG:HD3	1:B:495:TYR:CD1	2.51	0.45
1:C:353:TRP:HD1	1:C:398:ASP:HB2	1.82	0.45
1:C:546:LEU:N	1:C:577:ARG:HD3	2.30	0.45
2:D:32:ILE:HG22	2:D:100:ASP:HA	1.99	0.45
1:A:76:THR:OG1	1:A:77:LYS:N	2.48	0.45
1:B:431:GLY:HA2	1:B:515:PHE:HD2	1.82	0.45
1:C:980:ILE:HD12	1:C:993:ILE:HD11	1.97	0.45
1:A:574:ASP:HB3	1:A:585:LEU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ASP:OD1	1:A:504:GLY:HA2	2.17	0.45
1:A:1116:THR:OG1	1:A:1119:ASN:OD1	2.34	0.45
1:B:1085:GLY:HA2	1:B:1126:CYS:SG	2.56	0.45
1:C:96:GLU:OE1	1:C:101:ILE:N	2.46	0.45
1:C:331:ASN:OD1	1:C:331:ASN:N	2.50	0.45
1:A:319:ARG:O	1:A:321:GLN:N	2.40	0.45
1:A:486:PHE:HE2	2:D:105:PHE:CD2	2.35	0.45
1:B:331:ASN:ND2	1:B:580:GLN:HG2	2.32	0.45
1:B:457:ARG:HG3	1:B:458:LYS:N	2.31	0.45
1:B:1040:VAL:HG13	1:B:1041:ASP:H	1.82	0.45
1:C:330:PRO:HA	1:C:580:GLN:HB3	1.97	0.45
1:C:347:PHE:CD2	1:C:511:VAL:HG12	2.52	0.45
1:A:957:GLN:HE21	1:B:765:ARG:CZ	2.30	0.44
1:B:295:PRO:O	1:B:299:THR:HG23	2.17	0.44
1:B:1037:SER:OG	1:B:1043:CYS:SG	2.72	0.44
1:C:478:THR:HG21	1:C:487:ASN:HB3	1.98	0.44
1:B:106:PHE:HD2	1:B:235:ILE:HG21	1.82	0.44
1:B:383:SER:HA	1:B:384:PRO:HD3	1.88	0.44
1:B:472:ILE:HD12	1:B:472:ILE:HA	1.85	0.44
1:B:1091:ARG:NH2	1:B:1118:ASP:O	2.50	0.44
1:C:645:THR:HG22	1:C:647:ALA:H	1.82	0.44
1:A:558:LYS:NZ	4:B:1301:NAG:O5	2.49	0.44
1:C:360:ASN:O	1:C:360:ASN:ND2	2.49	0.44
1:A:387:LEU:HD21	1:A:515:PHE:HZ	1.81	0.44
1:A:742:ILE:HA	1:A:1000:ARG:HD2	2.00	0.44
1:B:663:ASP:OD2	1:B:673:SER:OG	2.32	0.44
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.98	0.44
1:A:327:VAL:O	1:A:531:THR:N	2.50	0.44
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.99	0.44
1:A:438:SER:HB3	1:A:509:ARG:HG3	2.00	0.44
1:A:453:TYR:HB3	1:A:495:TYR:HE1	1.83	0.44
1:B:326:ILE:HD13	1:B:534:VAL:HG12	2.00	0.44
1:B:342:PHE:CE1	1:B:511:VAL:HG11	2.53	0.44
1:C:538:CYS:HB2	1:C:590:CYS:HB3	1.40	0.44
1:A:401:VAL:HG11	1:A:451:TYR:CE2	2.53	0.44
1:B:127:VAL:HG12	1:B:129:LYS:HG3	2.00	0.44
1:C:317:ASN:OD1	1:C:317:ASN:N	2.50	0.44
1:C:535:LYS:HZ2	1:C:553:THR:HG21	1.83	0.44
1:A:707:TYR:HB3	1:B:792:PRO:HG3	2.00	0.44
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.99	0.44
1:C:452:LEU:HD12	1:C:452:LEU:HA	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:823:PHE:CD1	1:C:1057:PRO:HD3	2.53	0.44
1:A:388:ASN:N	1:A:388:ASN:OD1	2.51	0.43
1:B:1101:HIS:NE2	3:G:1:NAG:H5	2.32	0.43
1:B:49:HIS:HD2	1:B:50:SER:N	2.15	0.43
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.99	0.43
1:B:439:ASN:HB3	1:B:507:PRO:HD2	2.00	0.43
1:B:1039:ARG:HH12	1:C:1039:ARG:NH1	2.15	0.43
1:C:481:ASN:HB2	1:C:485:GLY:HA2	2.00	0.43
1:C:582:LEU:HD12	1:C:582:LEU:HA	1.84	0.43
1:A:302:THR:HG23	1:A:303:LEU:HD13	1.98	0.43
1:A:707:TYR:HE2	1:B:797:PHE:CE1	2.35	0.43
1:A:849:LEU:N	1:A:852:ALA:O	2.51	0.43
1:A:911:VAL:HG12	1:A:1108:ASN:HB2	2.00	0.43
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.58	0.43
1:A:401:VAL:HG11	1:A:451:TYR:CD2	2.52	0.43
1:A:722:VAL:HA	1:A:1064:HIS:O	2.17	0.43
1:B:737:ASP:OD1	1:B:740:MET:HB3	2.18	0.43
1:B:878:LEU:HD21	1:B:1052:PHE:HB3	2.01	0.43
1:B:983:ARG:HA	1:B:983:ARG:HD3	1.69	0.43
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.50	0.43
1:A:382:VAL:HG23	1:B:983:ARG:HH11	1.83	0.43
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.77	0.43
1:A:521:PRO:HA	1:A:577:ARG:NH1	2.24	0.43
1:B:409:GLN:OE1	1:B:419:ALA:N	2.51	0.43
1:B:727:LEU:HD11	1:B:1028:LYS:HD3	2.01	0.43
1:A:409:GLN:OE1	1:A:418:ILE:N	2.52	0.43
1:B:485:GLY:N	1:B:488:CYS:HB2	2.33	0.43
1:C:777:ASN:HD21	1:C:1022:ALA:HB3	1.82	0.43
1:A:327:VAL:HG22	1:A:542:ASN:HD21	1.84	0.43
1:A:676:THR:HB	1:A:689:SER:N	2.33	0.43
1:B:204:TYR:HE1	1:B:225:PRO:HG3	1.82	0.43
1:B:462:LYS:HB2	1:B:462:LYS:HE2	1.70	0.43
2:D:51:ILE:HG22	2:D:70:ILE:HD11	2.00	0.43
1:A:454:ARG:HD3	1:A:457:ARG:HG2	2.00	0.43
1:A:594:GLY:O	1:A:613:GLN:HG2	2.19	0.43
1:A:597:VAL:HG13	1:A:608:VAL:HG13	2.01	0.43
1:A:995:ARG:HH11	1:A:995:ARG:HG2	1.83	0.43
1:A:1030:SER:OG	1:C:1041:ASP:HB2	2.19	0.43
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.54	0.43
1:B:54:LEU:HA	1:B:272:PRO:HA	2.01	0.43
1:B:551:VAL:HG12	1:B:588:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:971:GLY:HA2	1:C:755:GLN:NE2	2.33	0.43
1:C:387:LEU:HB3	1:C:388:ASN:H	1.56	0.43
1:C:392:PHE:HD1	1:C:517:LEU:HG	1.84	0.43
1:C:466:ARG:HA	1:C:466:ARG:HD3	1.78	0.43
1:A:100:ILE:HG23	1:A:243:ALA:H	1.84	0.43
1:A:403:ARG:HB2	1:A:495:TYR:HE2	1.83	0.43
1:B:592:PHE:CD1	1:B:592:PHE:C	2.92	0.43
1:C:986:PRO:HB2	1:C:987:PRO:HD3	2.00	0.43
1:A:100:ILE:HA	1:A:243:ALA:HB3	2.00	0.42
1:A:403:ARG:HB2	1:A:495:TYR:CE2	2.54	0.42
1:B:711:SER:HB2	4:B:1305:NAG:H83	2.01	0.42
1:B:741:TYR:CE1	1:B:966:LEU:HD11	2.53	0.42
2:D:73:ASP:HB3	2:D:76:LYS:HB2	2.01	0.42
1:B:442:ASP:OD2	1:B:451:TYR:OH	2.29	0.42
1:A:912:THR:O	1:A:915:VAL:HG12	2.19	0.42
1:A:1081:ILE:HG12	1:A:1095:PHE:HE2	1.85	0.42
1:B:54:LEU:HD23	1:B:272:PRO:HB3	2.01	0.42
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.38	0.42
1:C:979:ASP:OD2	1:C:983:ARG:NH2	2.53	0.42
1:A:369:TYR:HE2	1:A:377:PHE:CE2	2.37	0.42
1:A:299:THR:HA	1:A:302:THR:HG22	2.01	0.42
1:B:603:ASN:OD1	1:B:604:THR:N	2.52	0.42
1:C:196:ASN:HA	1:C:200:TYR:O	2.20	0.42
1:B:336:CYS:HB3	1:B:361:CYS:HB3	1.90	0.42
1:B:341:VAL:HG23	1:B:342:PHE:CD1	2.54	0.42
1:C:76:THR:OG1	1:C:77:LYS:N	2.52	0.42
1:A:403:ARG:NH1	1:A:406:GLU:OE2	2.53	0.42
1:A:425:LEU:HD13	1:A:429:PHE:CD2	2.55	0.42
1:C:452:LEU:HG	1:C:492:LEU:HG	2.01	0.42
1:C:676:THR:HG23	1:C:690:GLN:HG3	2.01	0.42
1:A:226:LEU:HG	1:A:227:VAL:HG23	2.02	0.42
1:A:330:PRO:HD3	1:A:544:ASN:CG	2.40	0.42
1:A:487:ASN:HA	1:A:489:TYR:HE2	1.85	0.42
1:B:332:ILE:HG13	1:B:333:THR:H	1.84	0.42
1:C:203:ILE:O	1:C:227:VAL:HB	2.19	0.42
1:C:376:THR:O	1:C:378:LYS:NZ	2.42	0.42
1:A:529:LYS:HD2	1:A:529:LYS:HA	1.92	0.42
1:A:716:THR:HG21	1:A:1073:LYS:HD3	2.00	0.42
1:B:900:MET:HG2	1:B:917:TYR:OH	2.20	0.42
1:C:573:THR:O	1:C:587:ILE:HG13	2.20	0.42
1:C:969:ASN:OD1	1:C:969:ASN:N	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:LYS:HA	1:B:814:LYS:HD2	1.77	0.42
1:C:730:SER:O	1:C:1058:HIS:HB3	2.20	0.42
1:C:1073:LYS:HB3	1:C:1073:LYS:HE2	1.75	0.42
1:A:50:SER:OG	1:A:51:THR:N	2.53	0.41
1:B:934:ILE:HD11	1:B:1063:LEU:HD22	2.01	0.41
1:A:41:LYS:HE3	1:A:41:LYS:HB3	1.89	0.41
1:A:326:ILE:CD1	1:A:533:LEU:HA	2.51	0.41
1:A:409:GLN:OE1	1:A:417:LYS:N	2.53	0.41
1:A:730:SER:O	1:A:1058:HIS:HB3	2.21	0.41
1:B:303:LEU:HD12	1:B:308:VAL:HG12	2.02	0.41
1:B:616:ASN:OD1	1:B:617:CYS:N	2.52	0.41
1:C:541:PHE:CZ	1:C:552:LEU:HD23	2.55	0.41
1:C:543:PHE:O	1:C:577:ARG:HB2	2.19	0.41
1:A:598:ILE:HB	1:A:609:ALA:HB3	2.02	0.41
1:C:307:THR:HA	1:C:602:THR:HG21	2.01	0.41
1:A:598:ILE:HG23	1:A:664:ILE:HD13	2.01	0.41
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.97	0.41
1:B:630:THR:N	1:B:631:PRO:HD2	2.36	0.41
1:B:720:ILE:HD12	1:B:923:ILE:HG23	2.01	0.41
1:C:43:PHE:HE1	1:C:283:GLY:HA3	1.85	0.41
1:A:430:THR:O	1:A:430:THR:OG1	2.33	0.41
1:A:1110:TYR:CZ	1:A:1112:PRO:HG3	2.54	0.41
1:B:439:ASN:HA	1:B:507:PRO:HG2	2.02	0.41
1:B:1009:THR:O	1:B:1013:ILE:HG12	2.19	0.41
1:C:170:TYR:CZ	1:C:172:SER:HB3	2.55	0.41
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.20	0.41
1:A:326:ILE:HD12	1:A:532:ASN:O	2.20	0.41
1:C:985:ASP:CG	1:C:987:PRO:HD2	2.41	0.41
1:C:1100:THR:HG1	1:C:1101:HIS:CE1	2.37	0.41
1:A:1093:GLY:O	1:A:1107:ARG:NH1	2.53	0.41
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG11	2.56	0.41
1:B:327:VAL:CG1	1:B:542:ASN:HB3	2.51	0.41
1:B:641:ASN:OD1	1:B:641:ASN:N	2.52	0.41
1:B:887:THR:HG21	1:B:894:LEU:HD12	2.03	0.41
1:C:655:HIS:HA	1:C:694:ALA:O	2.20	0.41
1:C:974:SER:OG	1:C:975:SER:N	2.53	0.41
1:A:802:PHE:HB3	1:A:806:LEU:HD11	2.03	0.41
1:C:439:ASN:O	1:C:441:LEU:N	2.53	0.41
1:C:934:ILE:HA	1:C:934:ILE:HD12	1.80	0.41
1:A:116:SER:HG	1:A:135:PHE:HZ	1.69	0.41
1:B:361:CYS:SG	1:B:362:VAL:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:TRP:CD1	1:C:398:ASP:HB2	2.55	0.41
1:C:377:PHE:CD2	1:C:379:CYS:HB3	2.55	0.41
1:C:546:LEU:HD12	1:C:546:LEU:HA	1.83	0.41
1:C:595:VAL:HG23	1:C:612:TYR:CD1	2.56	0.41
1:C:1082:CYS:HB2	1:C:1126:CYS:HB3	1.93	0.41
1:A:290:ASP:OD2	1:A:293:LEU:N	2.54	0.41
1:B:343:ASN:HB3	3:J:1:NAG:O5	2.20	0.41
1:B:666:ILE:HG22	1:B:667:GLY:H	1.85	0.41
1:C:245:HIS:O	1:C:259:THR:OG1	2.32	0.41
1:C:434:ILE:O	1:C:510:VAL:HA	2.21	0.41
1:A:206:LYS:NZ	1:A:221:SER:HB2	2.36	0.40
1:A:644:GLN:OE1	1:A:644:GLN:HA	2.21	0.40
1:A:1068:VAL:HA	1:A:1069:PRO:HD3	1.93	0.40
1:B:406:GLU:HB3	1:B:409:GLN:NE2	2.36	0.40
1:C:184:GLY:HA2	1:C:187:LYS:HE2	2.03	0.40
1:C:302:THR:OG1	1:C:303:LEU:N	2.54	0.40
2:D:98:LYS:O	2:D:105:PHE:HA	2.21	0.40
1:A:365:TYR:CG	1:A:387:LEU:HD23	2.56	0.40
1:A:918:GLU:OE2	1:C:1123:SER:OG	2.37	0.40
1:B:390:LEU:HD21	1:C:982:SER:OG	2.21	0.40
1:C:412:PRO:HB3	1:C:429:PHE:CE1	2.57	0.40
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.21	0.40
1:B:366:SER:HA	1:B:369:TYR:HD1	1.85	0.40
1:B:419:ALA:O	1:B:424:LYS:HB2	2.21	0.40
1:B:531:THR:OG1	1:B:532:ASN:N	2.54	0.40
1:C:111:ASP:N	1:C:111:ASP:OD1	2.53	0.40
1:C:391:CYS:N	1:C:525:CYS:SG	2.94	0.40
2:D:17:SER:OG	2:D:84:ASN:OD1	2.28	0.40
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.34	0.40
1:B:328:ARG:HG3	1:B:533:LEU:HD13	2.03	0.40
1:C:951:VAL:CG2	1:C:1018:ILE:HD11	2.50	0.40
2:D:4:LEU:HD11	2:D:106:ASP:HB2	2.02	0.40
1:A:613:GLN:HA	1:A:613:GLN:OE1	2.21	0.40
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	2.03	0.40
1:C:403:ARG:HG2	1:C:505:TYR:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1059/1136 (93%)	985 (93%)	72 (7%)	2 (0%)	47	78
1	B	1080/1136 (95%)	1041 (96%)	39 (4%)	0	100	100
1	C	1055/1136 (93%)	952 (90%)	102 (10%)	1 (0%)	51	83
2	D	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	54
All	All	3310/3526 (94%)	3088 (93%)	218 (7%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
2	D	106	ASP
1	A	90	VAL
1	C	414	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	939/990 (95%)	913 (97%)	26 (3%)	43	67
1	B	956/990 (97%)	933 (98%)	23 (2%)	49	71
1	C	935/990 (94%)	911 (97%)	24 (3%)	46	69
2	D	89/89 (100%)	85 (96%)	4 (4%)	27	57
All	All	2919/3059 (95%)	2842 (97%)	77 (3%)	49	69

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	91	TYR
1	A	97	LYS
1	A	157	PHE
1	A	178	ASP
1	A	266	TYR
1	A	305	SER
1	A	422	ASN
1	A	441	LEU
1	A	538	CYS
1	A	559	PHE
1	A	574	ASP
1	A	586	ASP
1	A	756	TYR
1	A	804	GLN
1	A	806	LEU
1	A	873	TYR
1	A	886	TRP
1	A	965	GLN
1	A	974	SER
1	A	979	ASP
1	A	1055	SER
1	A	1082	CYS
1	A	1083	HIS
1	A	1119	ASN
1	A	1138	TYR
1	B	48	LEU
1	B	115	GLN
1	B	153	MET
1	B	167	THR
1	B	192	PHE
1	B	277	LEU
1	B	281	GLU
1	B	301	CYS
1	B	318	PHE
1	B	328	ARG
1	B	338	PHE
1	B	361	CYS
1	B	392	PHE
1	B	422	ASN
1	B	473	TYR
1	B	559	PHE

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Mol	Chain	Res	Type
1	B	592	PHE
1	B	662	CYS
1	B	756	TYR
1	B	810	SER
1	B	823	PHE
1	B	873	TYR
1	B	954	GLN
1	C	49	HIS
1	C	306	PHE
1	C	317	ASN
1	C	318	PHE
1	C	346	ARG
1	C	353	TRP
1	C	368	LEU
1	C	420	ASP
1	C	436	TRP
1	C	518	LEU
1	C	536	ASN
1	C	574	ASP
1	C	585	LEU
1	C	660	TYR
1	C	820	ASP
1	C	856	ASN
1	C	907	ASN
1	C	967	SER
1	C	975	SER
1	C	979	ASP
1	C	983	ARG
1	C	1074	ASN
1	C	1082	CYS
1	C	1107	ARG
2	D	100	ASP
2	D	101	VAL
2	D	103	LYS
2	D	105	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	474	GLN
1	A	501	ASN

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Mol	Chain	Res	Type
1	B	992	GLN
1	C	66	HIS
1	C	703	ASN
1	C	804	GLN
1	C	935	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	E	2	3	14,14,15	0.45	0	17,19,21	0.75	0
3	NAG	F	1	1,3	14,14,15	0.21	0	17,19,21	0.54	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.51	0
3	NAG	G	1	1,3	14,14,15	0.48	0	17,19,21	0.81	1 (5%)
3	NAG	G	2	3	14,14,15	0.19	0	17,19,21	0.49	0
3	NAG	H	1	1,3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	H	2	3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	I	1	1,3	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.56	0
3	NAG	J	1	1,3	14,14,15	0.35	0	17,19,21	0.71	1 (5%)
3	NAG	J	2	3	14,14,15	0.80	1 (7%)	17,19,21	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	NAG	O5-C1	-2.64	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	2.45	115.51	112.19
3	J	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

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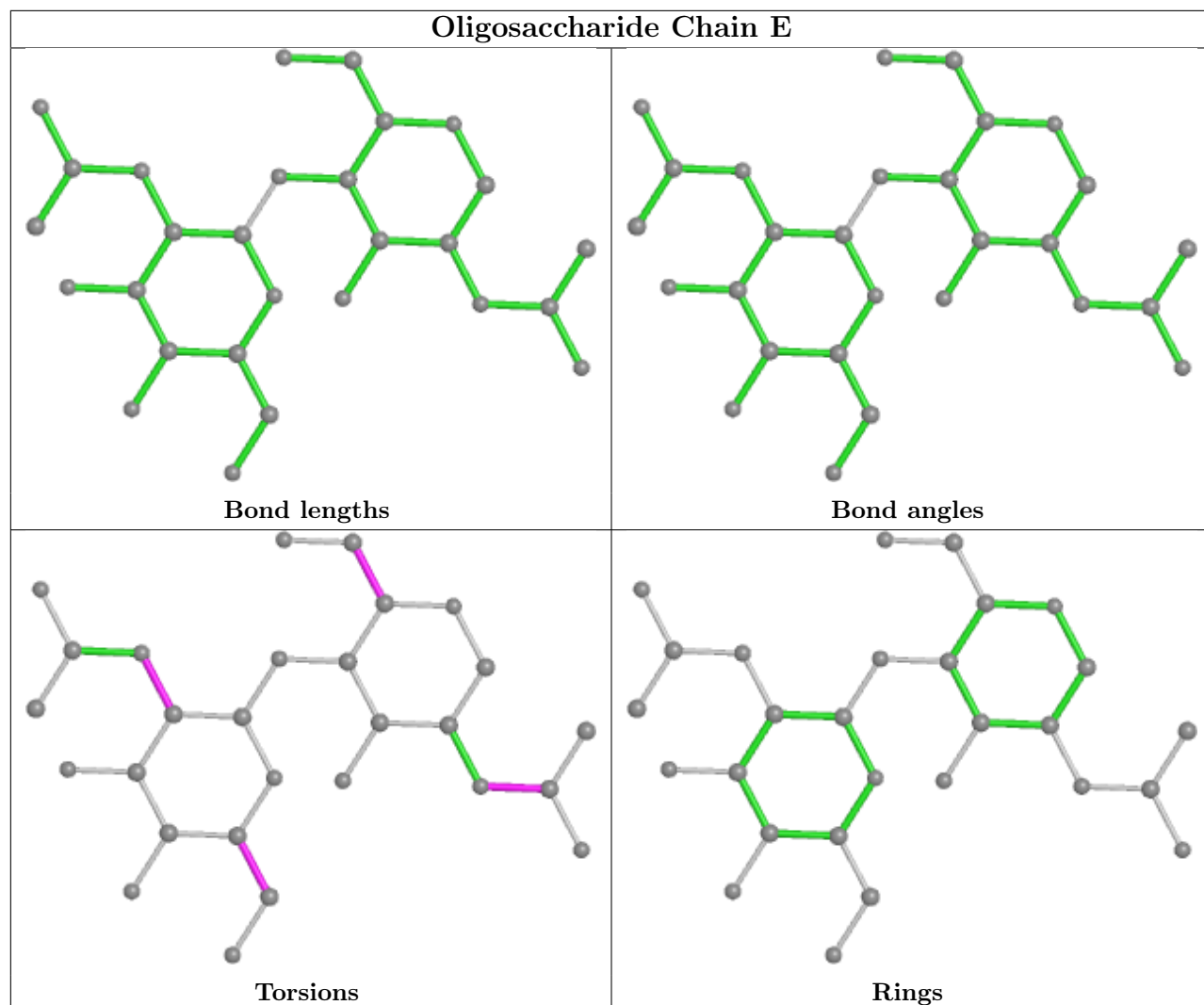
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C1-C2-N2-C7

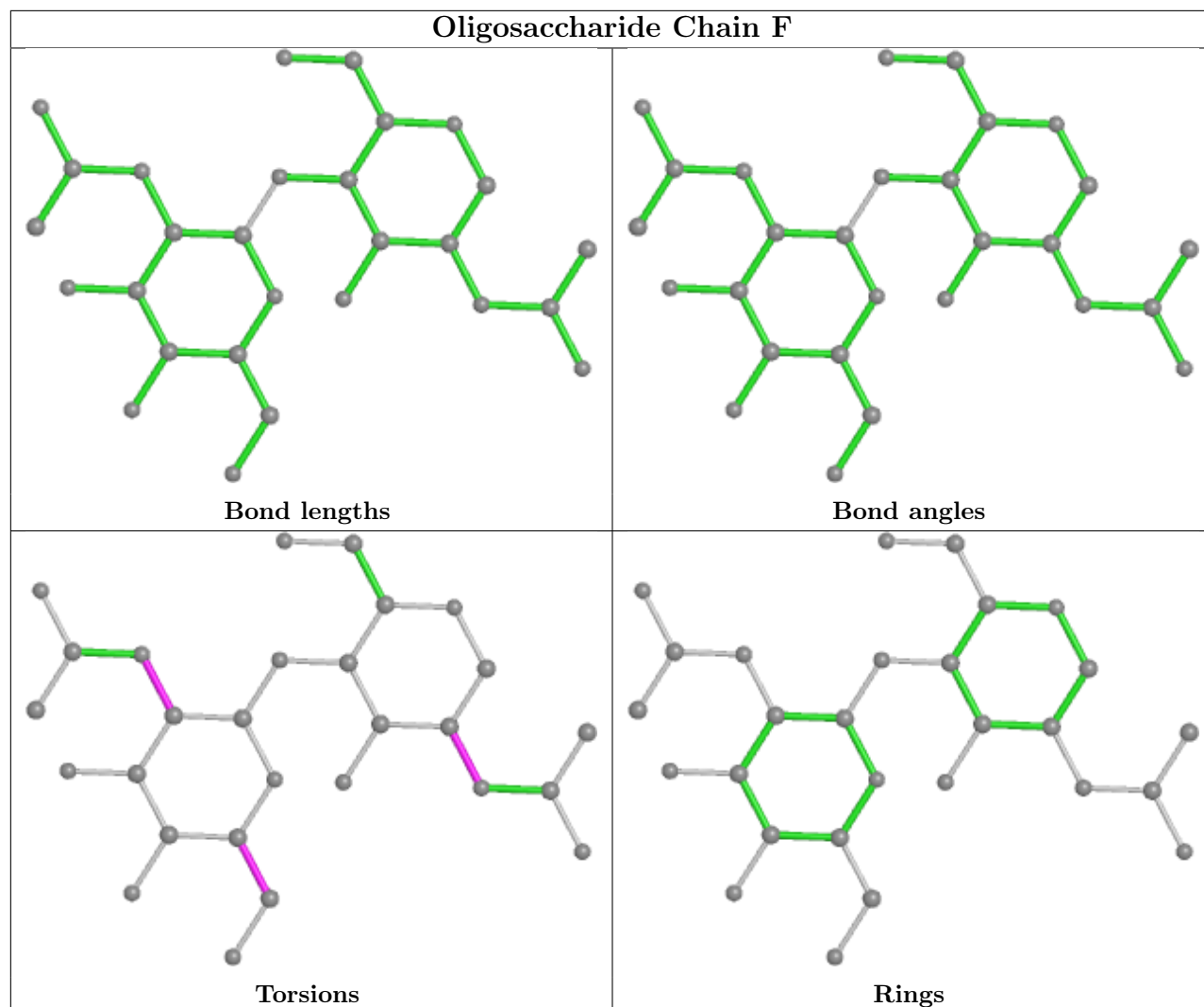
There are no ring outliers.

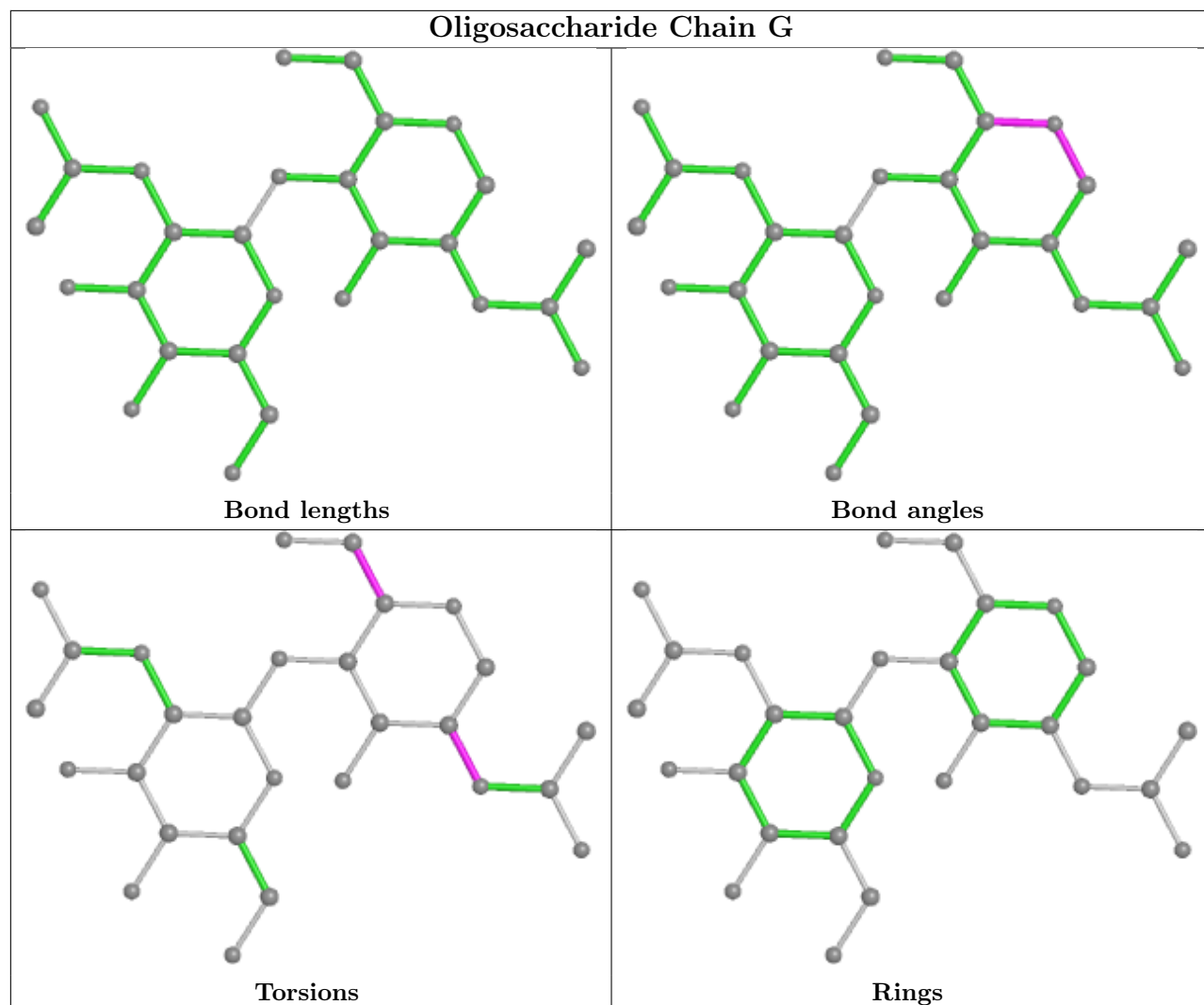
2 monomers are involved in 2 short contacts:

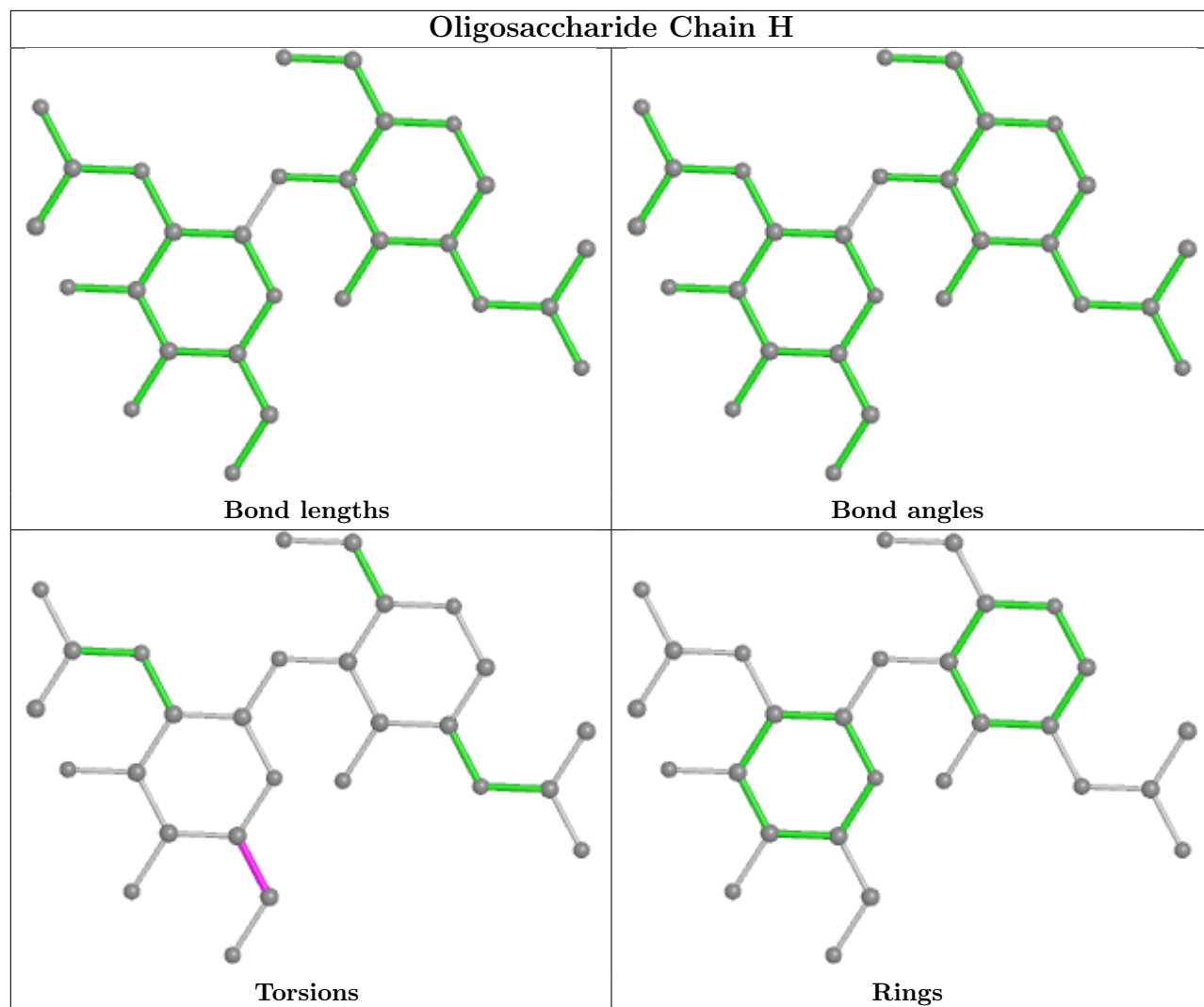
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	J	1	NAG	1	0

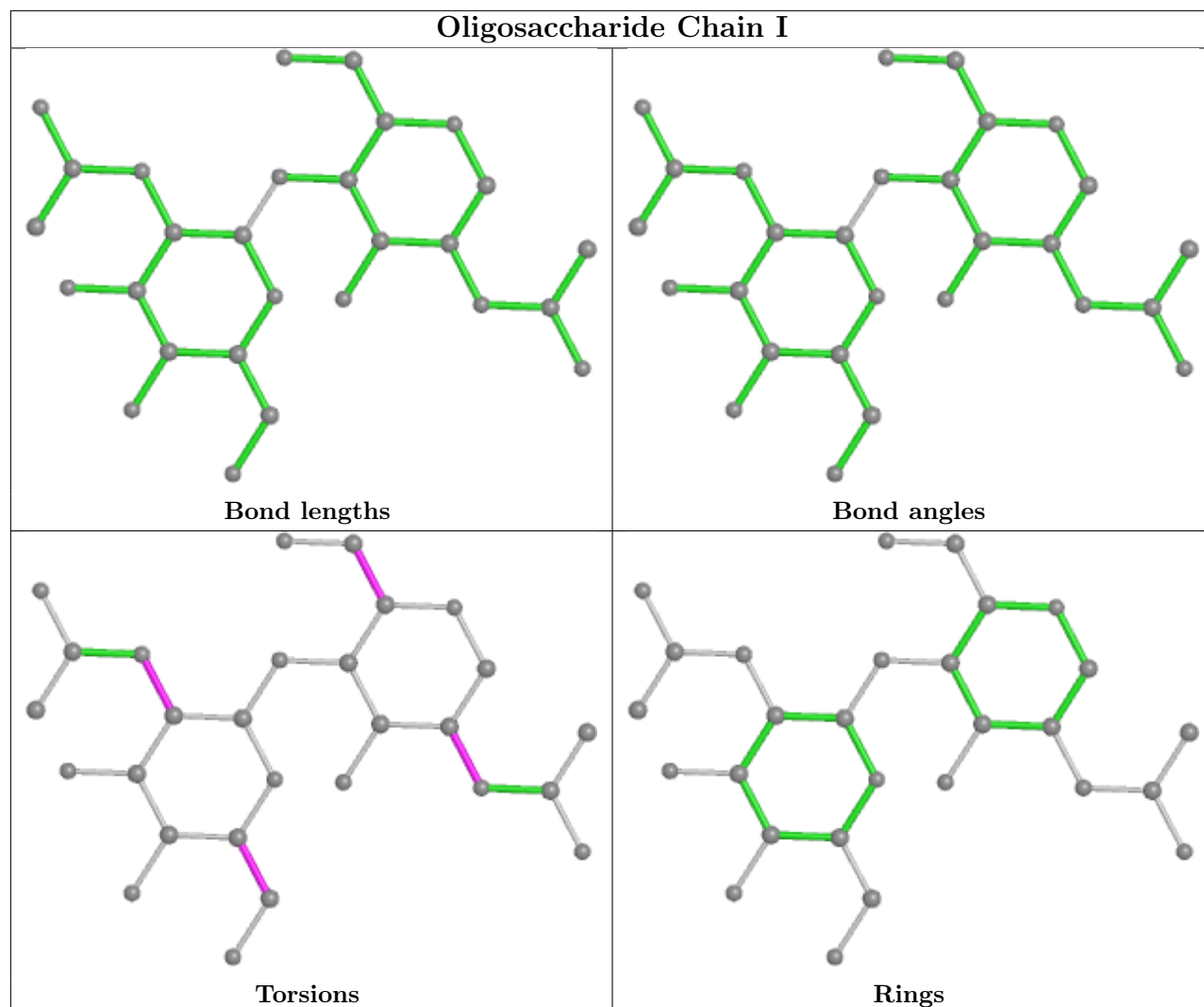
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

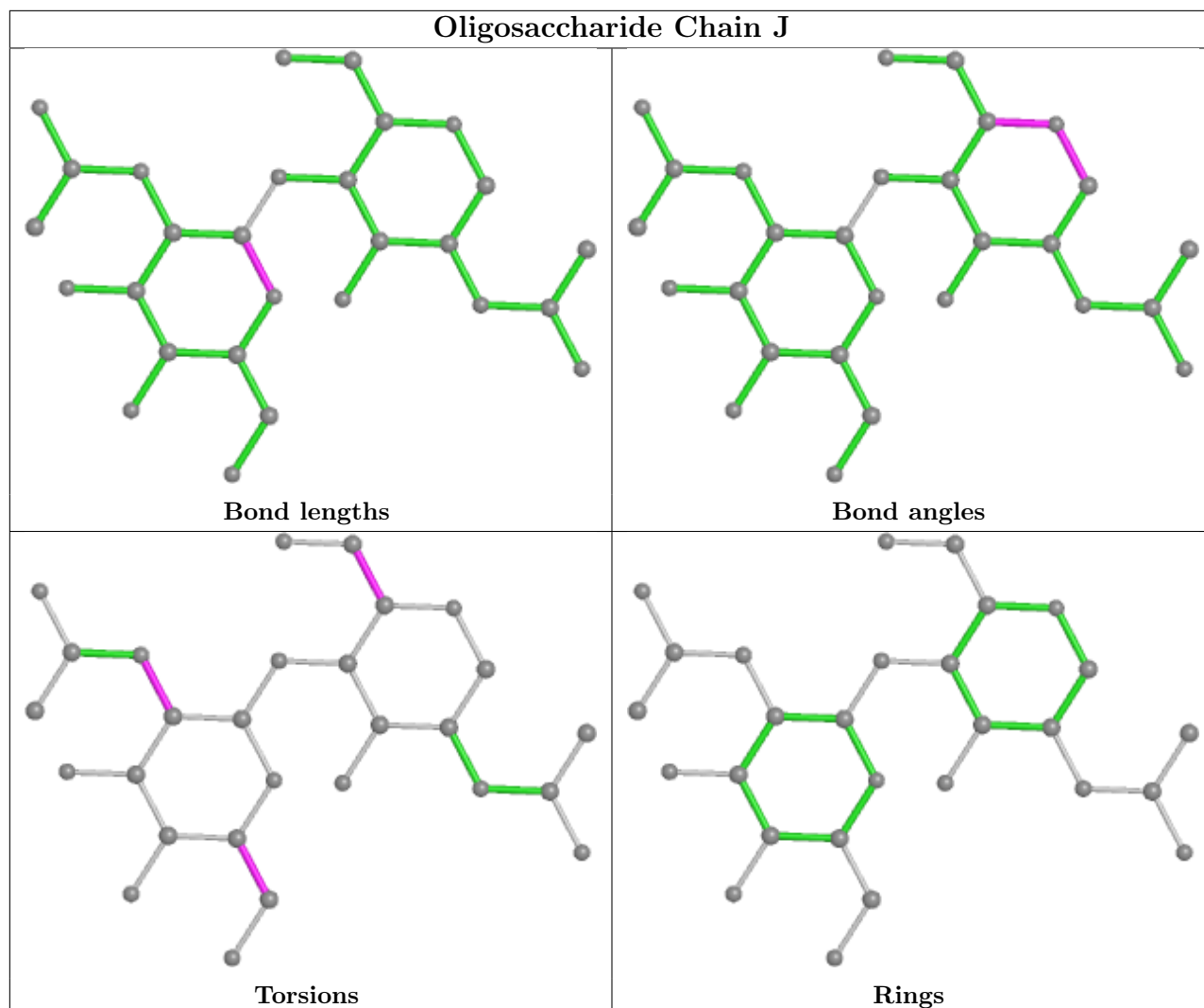












5.6 Ligand geometry [i](#)

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	1206	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	B	1301	1	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	A	1208	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1207	1	14,14,15	0.23	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1204	1	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	A	1203	1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	C	1202	1	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	C	1206	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1205	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1202	1	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	C	1208	1	14,14,15	0.42	0	17,19,21	0.35	0
4	NAG	B	1307	1	14,14,15	0.38	0	17,19,21	0.38	0
4	NAG	C	1203	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	A	1209	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	A	1201	1	14,14,15	0.87	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	C	1209	-	14,14,15	0.42	0	17,19,21	0.85	1 (5%)
4	NAG	B	1305	1	14,14,15	0.34	0	17,19,21	0.57	0
4	NAG	A	1204	1	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.37	0
4	NAG	A	1207	1	14,14,15	0.29	0	17,19,21	0.36	0
4	NAG	C	1205	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	1304	1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	C	1201	1	14,14,15	0.61	1 (7%)	17,19,21	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1206	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1207	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1203	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1206	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1202	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1209	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1201	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1209	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1207	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1201	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1201	NAG	O5-C1	2.82	1.48	1.43
4	C	1201	NAG	O5-C1	-2.07	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1201	NAG	C1-O5-C5	3.91	117.49	112.19
4	C	1209	NAG	C1-O5-C5	2.94	116.17	112.19

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1205	NAG	O5-C5-C6-O6
4	A	1208	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	A	1207	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	C	1205	NAG	C4-C5-C6-O6

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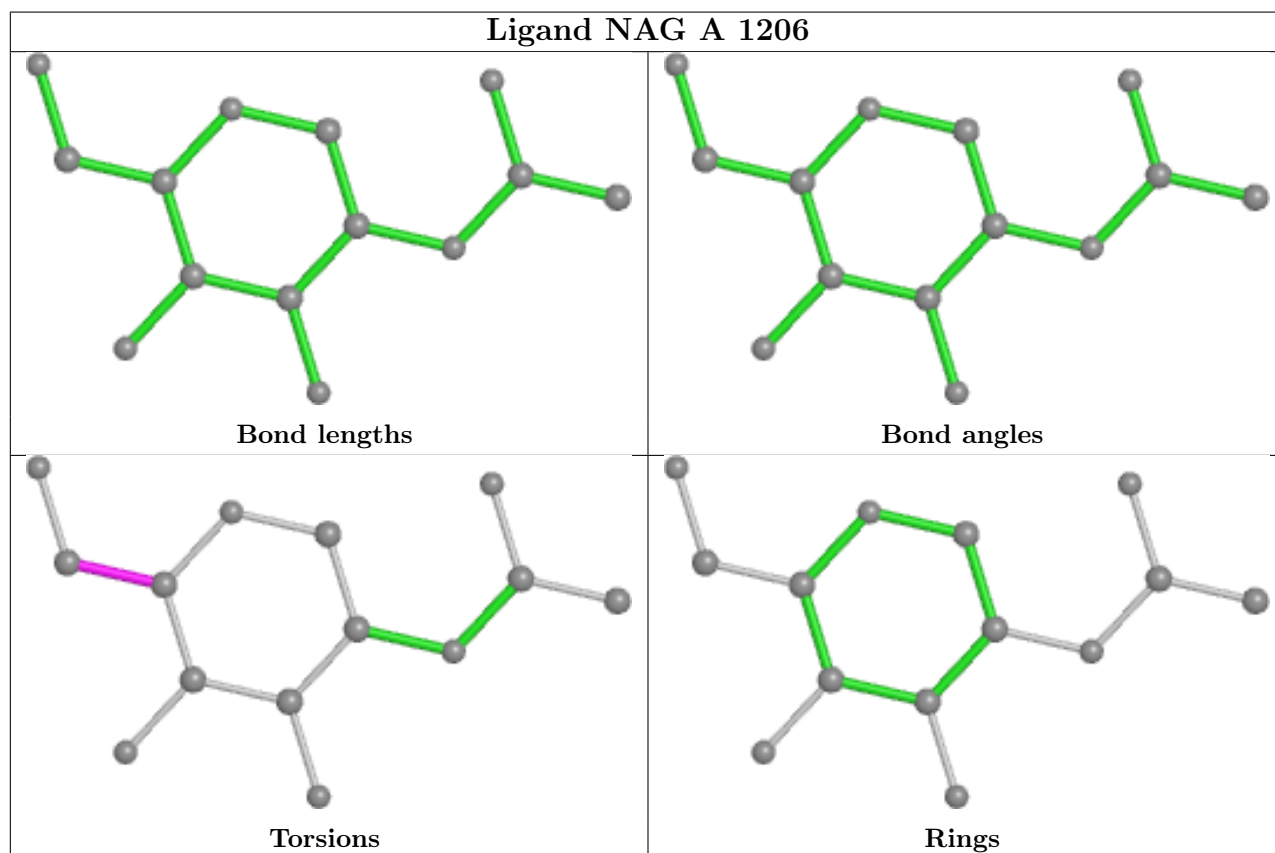
Mol	Chain	Res	Type	Atoms
4	A	1201	NAG	O5-C5-C6-O6
4	C	1207	NAG	O5-C5-C6-O6
4	C	1208	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	C	1209	NAG	C4-C5-C6-O6
4	C	1207	NAG	C4-C5-C6-O6
4	C	1208	NAG	C4-C5-C6-O6
4	A	1208	NAG	C4-C5-C6-O6
4	A	1205	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	A	1203	NAG	C4-C5-C6-O6
4	A	1201	NAG	C4-C5-C6-O6
4	C	1209	NAG	O5-C5-C6-O6
4	A	1204	NAG	O5-C5-C6-O6
4	A	1204	NAG	C4-C5-C6-O6
4	A	1205	NAG	O5-C5-C6-O6
4	A	1207	NAG	C4-C5-C6-O6
4	A	1203	NAG	O5-C5-C6-O6
4	A	1206	NAG	O5-C5-C6-O6
4	C	1206	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1201	NAG	O5-C5-C6-O6
4	A	1201	NAG	C3-C2-N2-C7
4	A	1203	NAG	C3-C2-N2-C7
4	A	1209	NAG	C3-C2-N2-C7
4	B	1302	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	C	1201	NAG	C3-C2-N2-C7
4	C	1202	NAG	C3-C2-N2-C7
4	C	1209	NAG	C3-C2-N2-C7
4	C	1201	NAG	C1-C2-N2-C7
4	B	1306	NAG	C4-C5-C6-O6

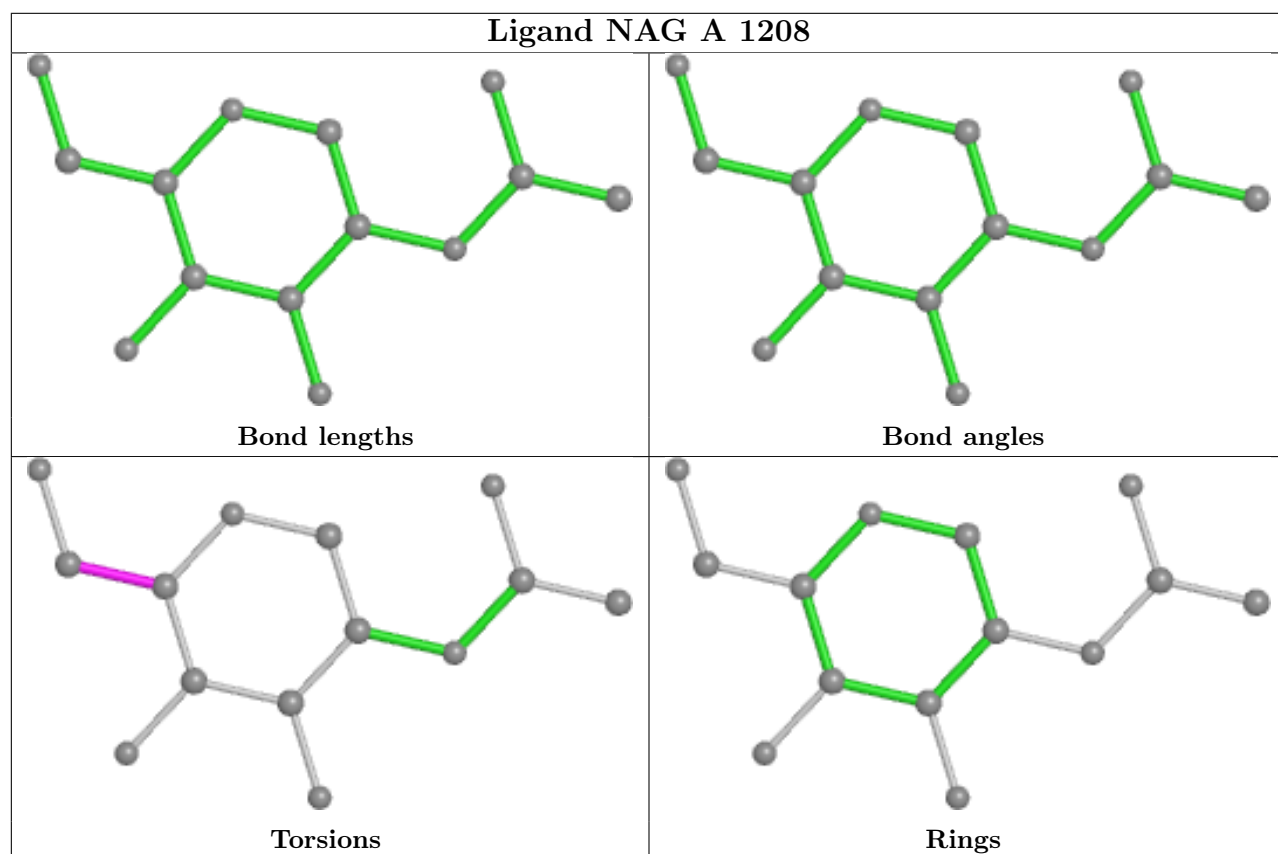
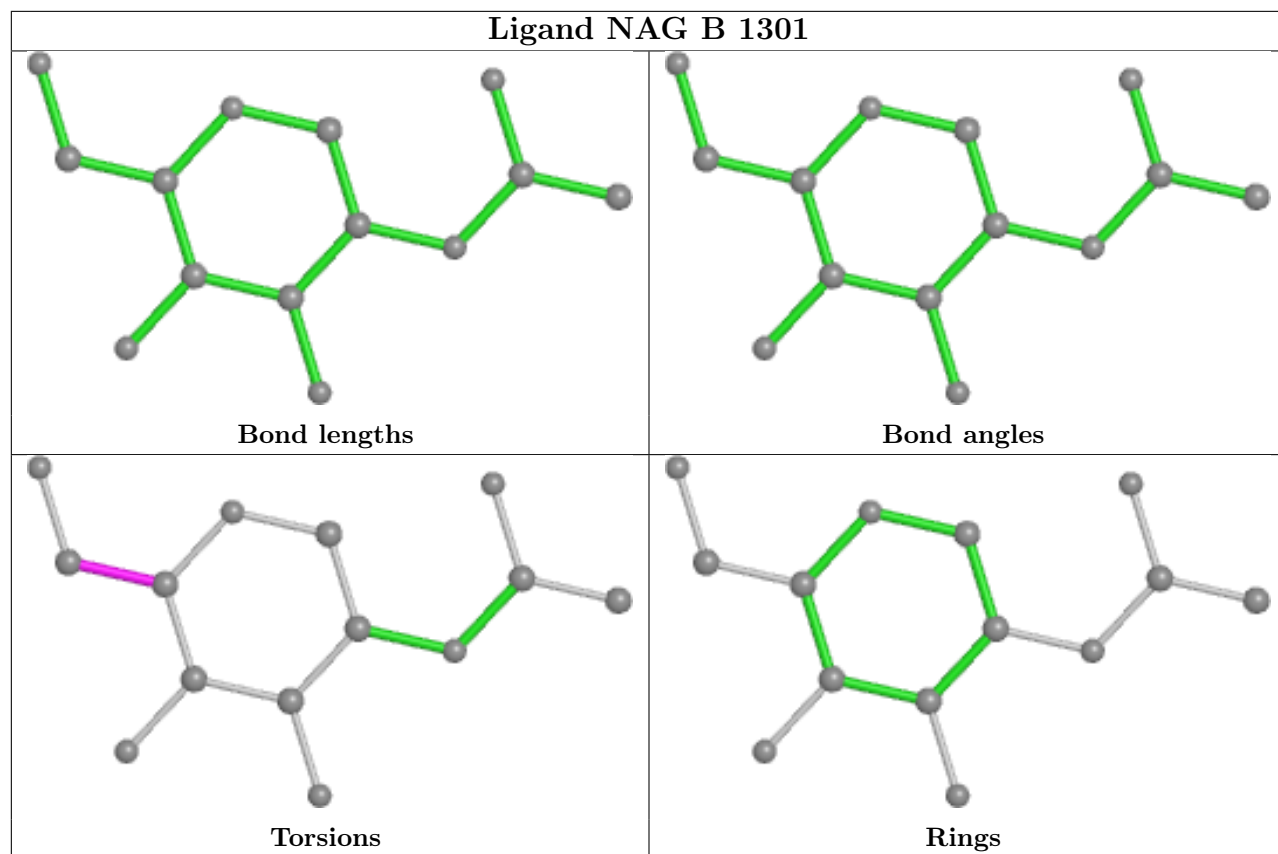
There are no ring outliers.

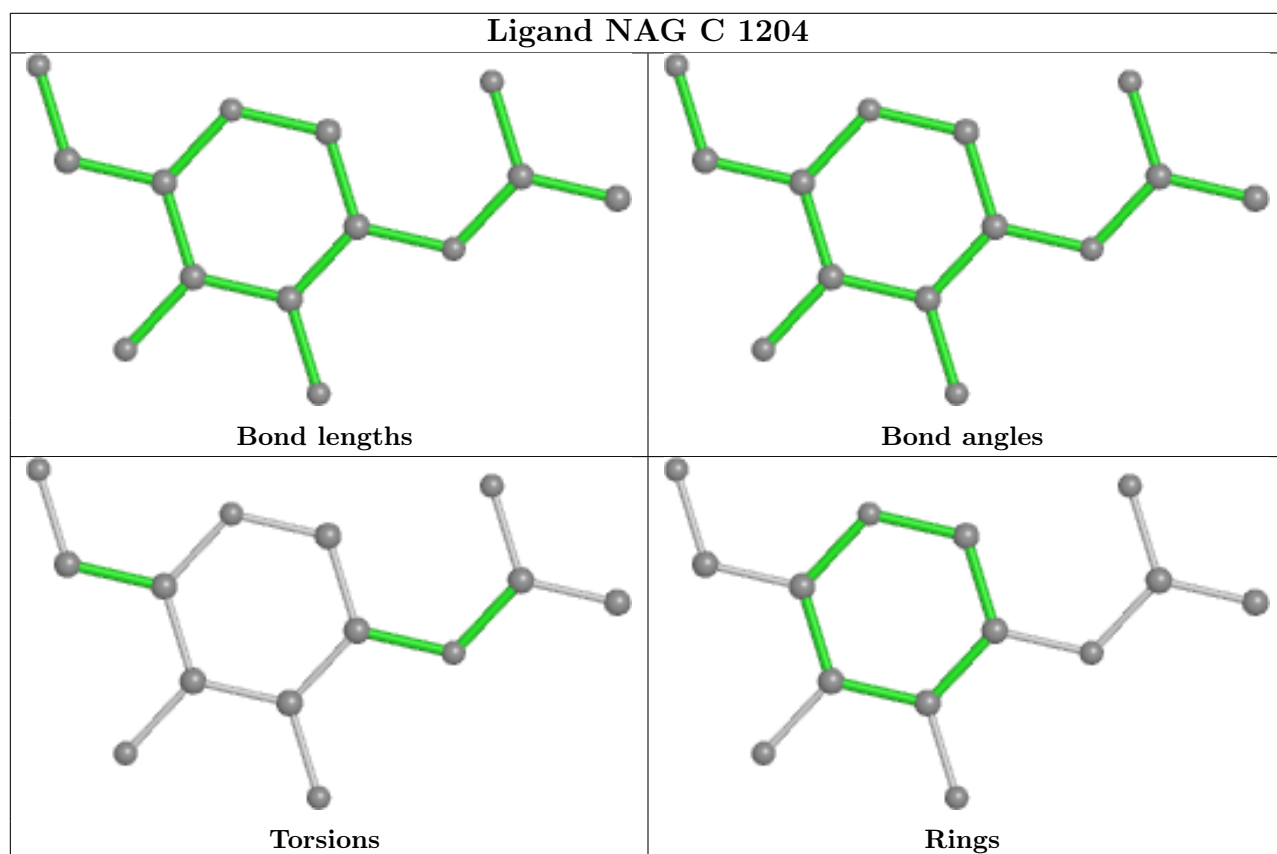
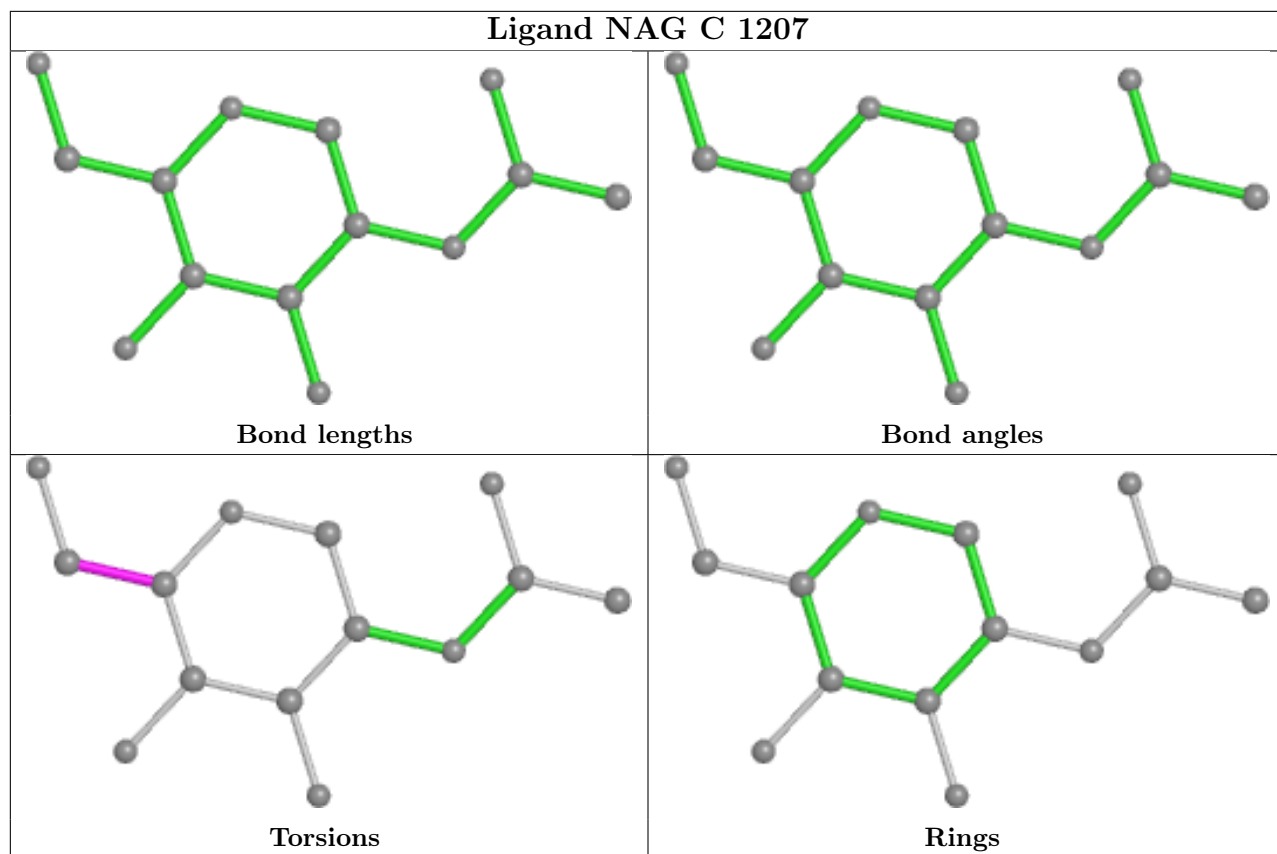
4 monomers are involved in 4 short contacts:

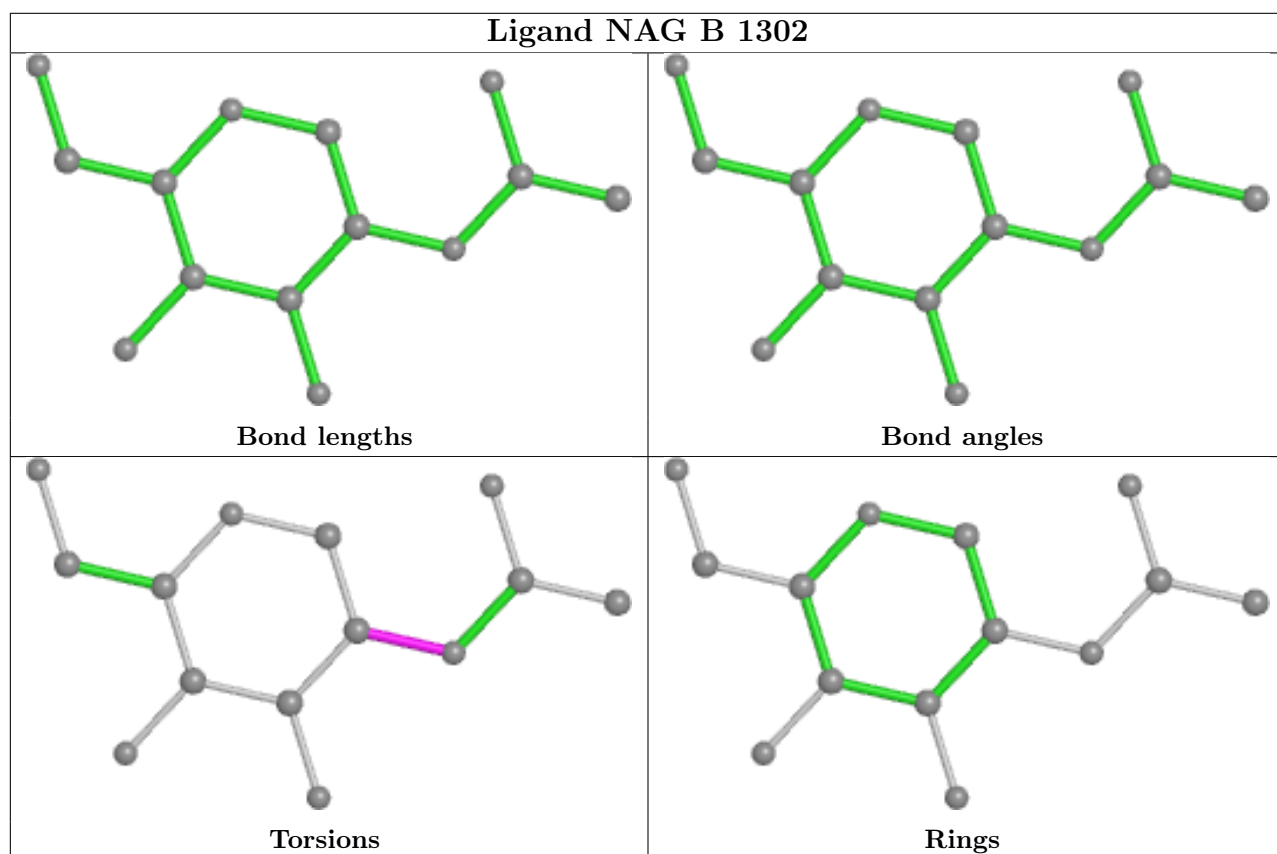
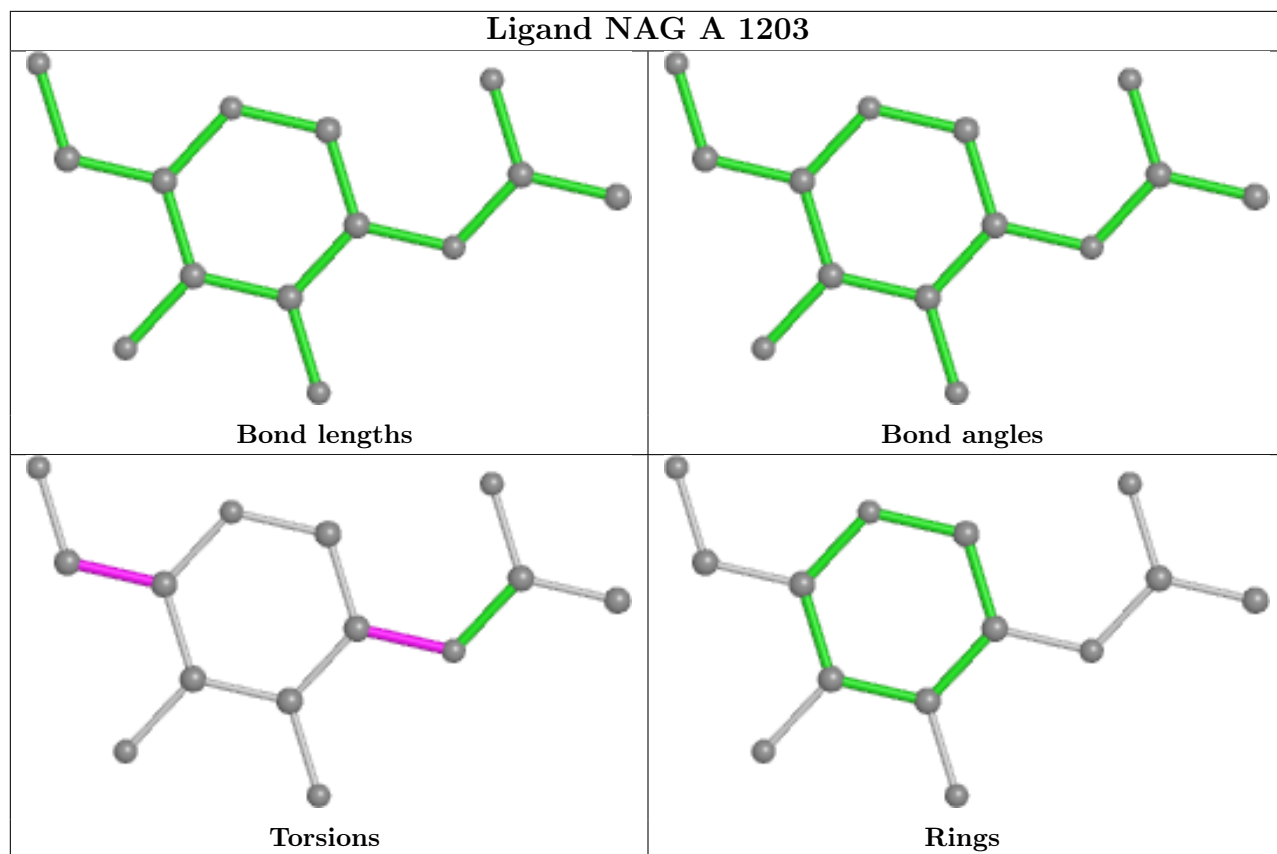
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1301	NAG	1	0
4	A	1202	NAG	1	0
4	B	1305	NAG	1	0
4	A	1207	NAG	1	0

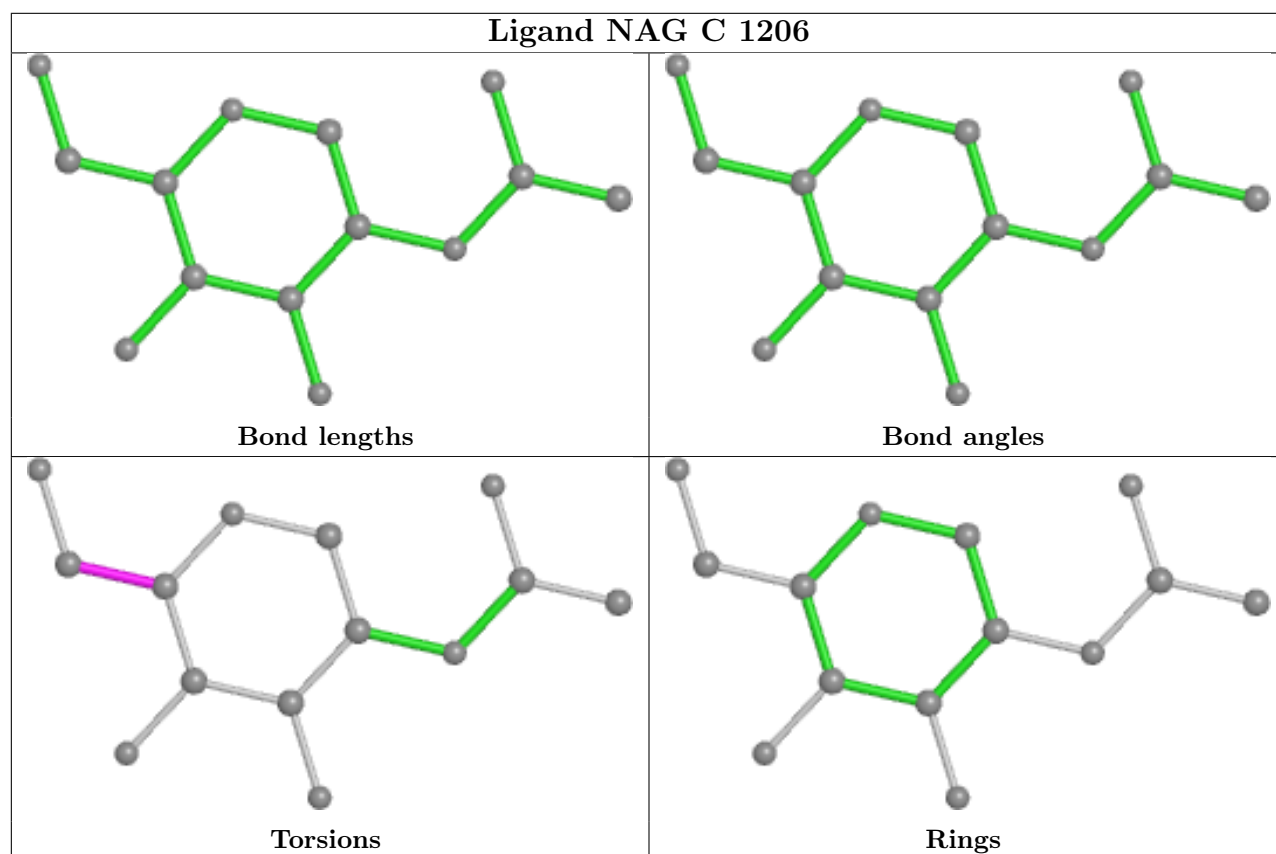
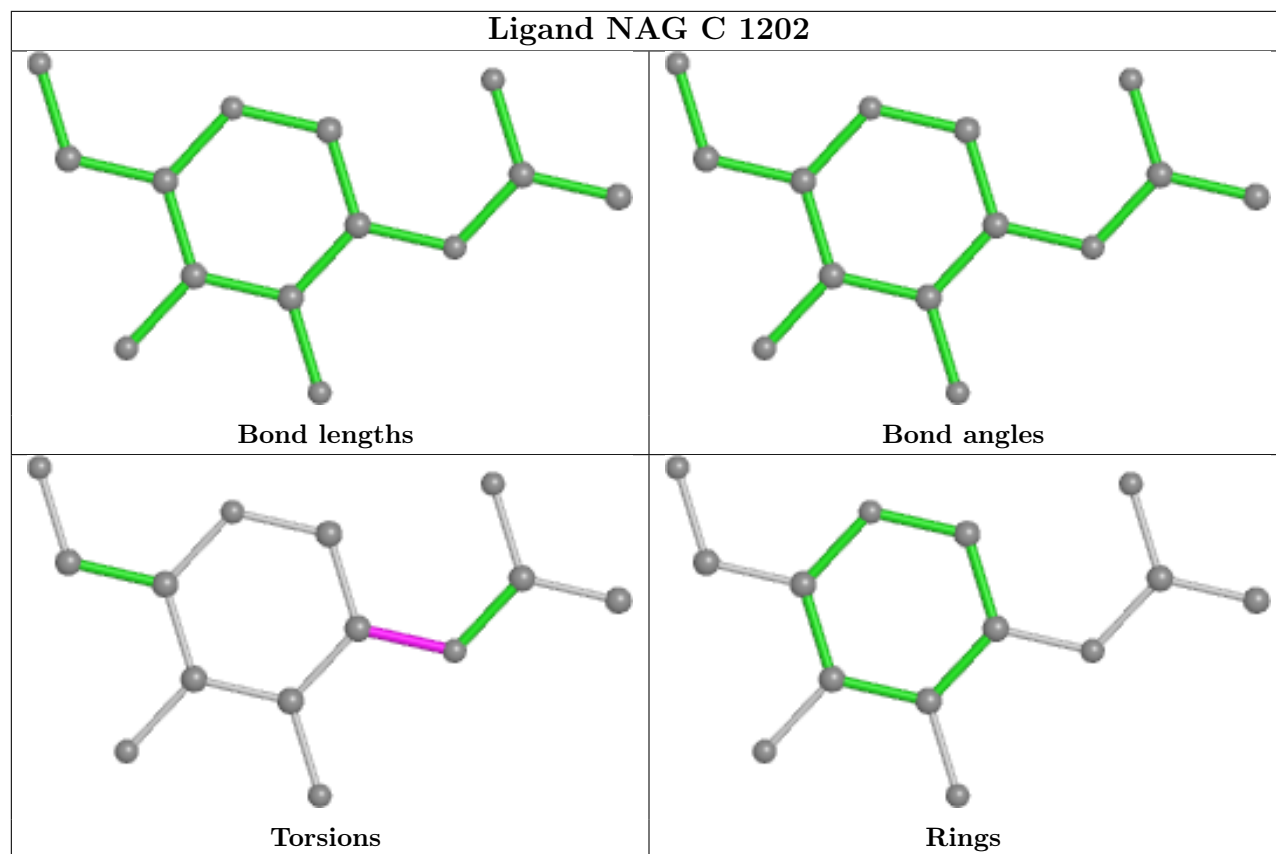
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

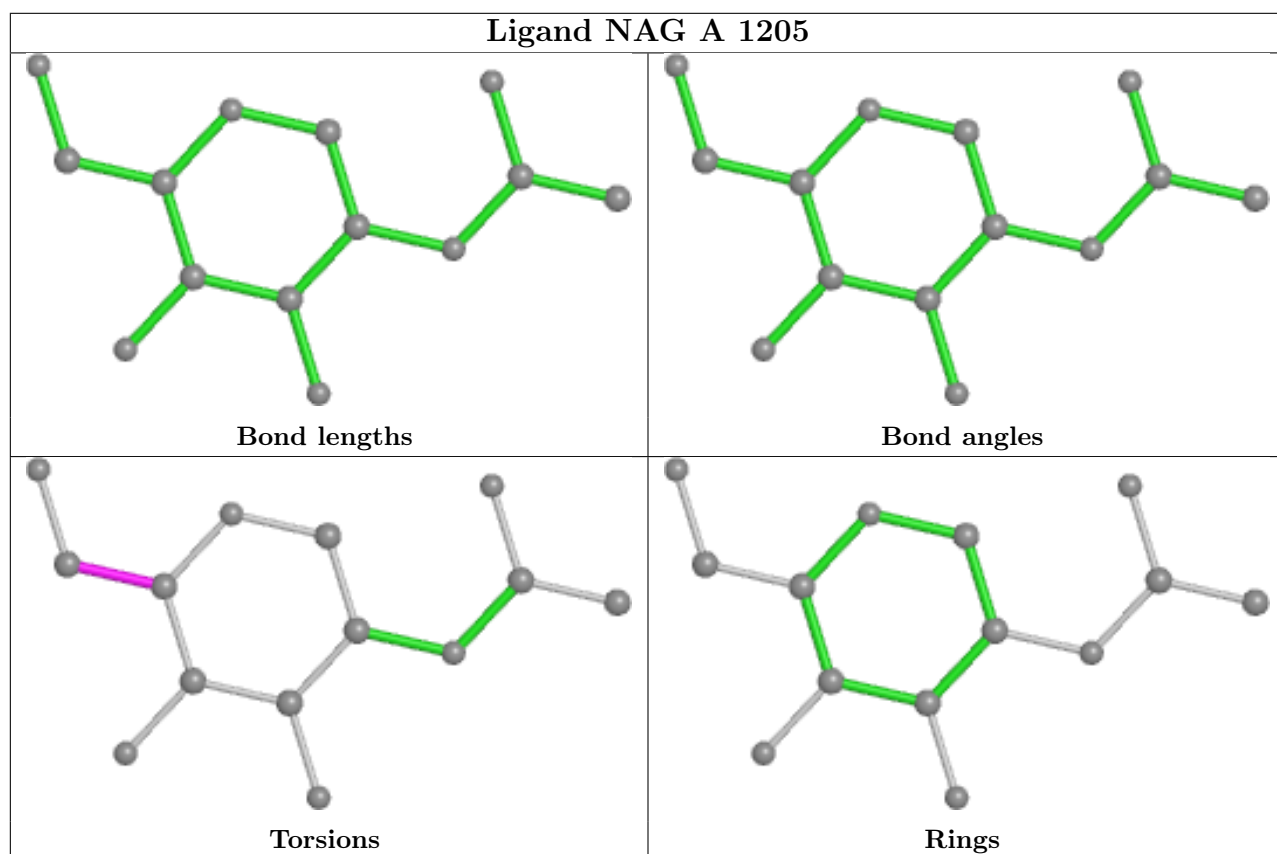
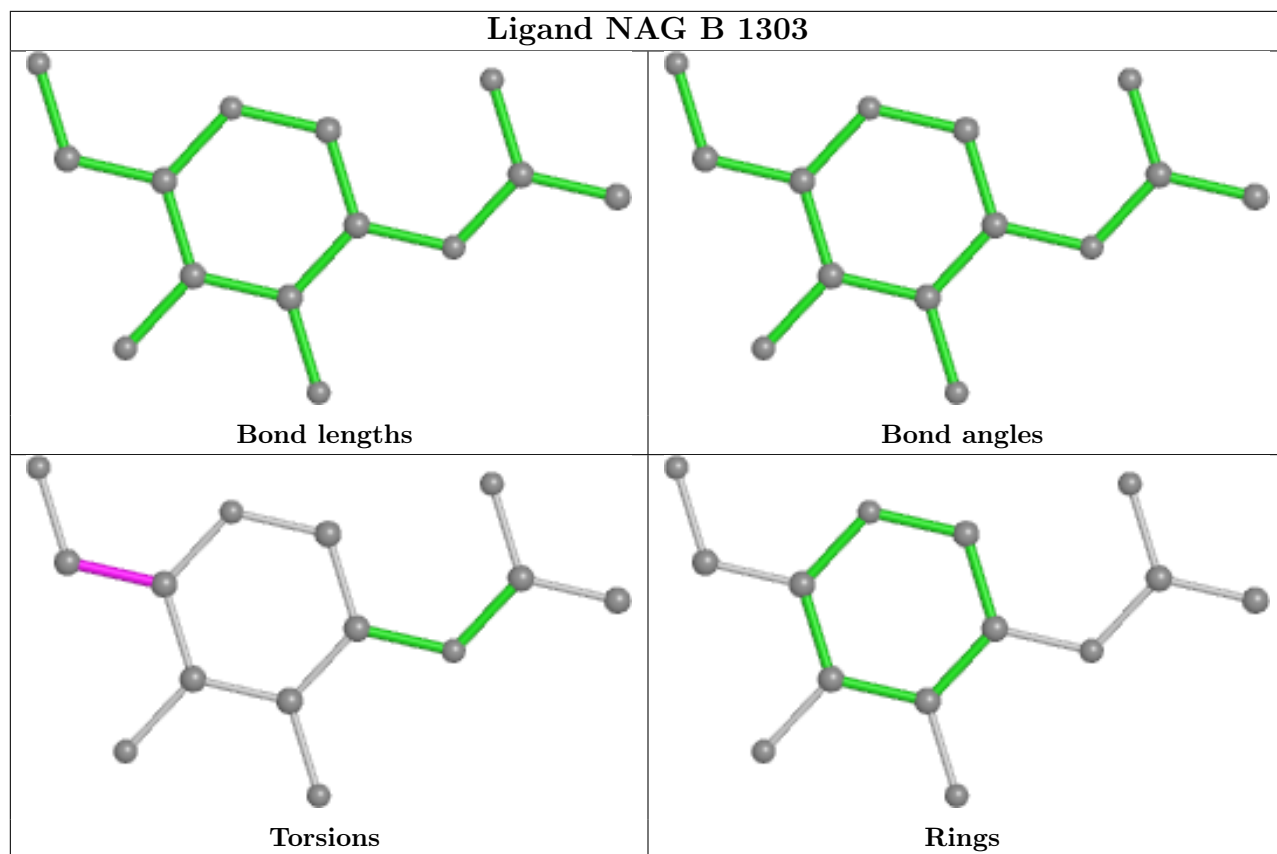


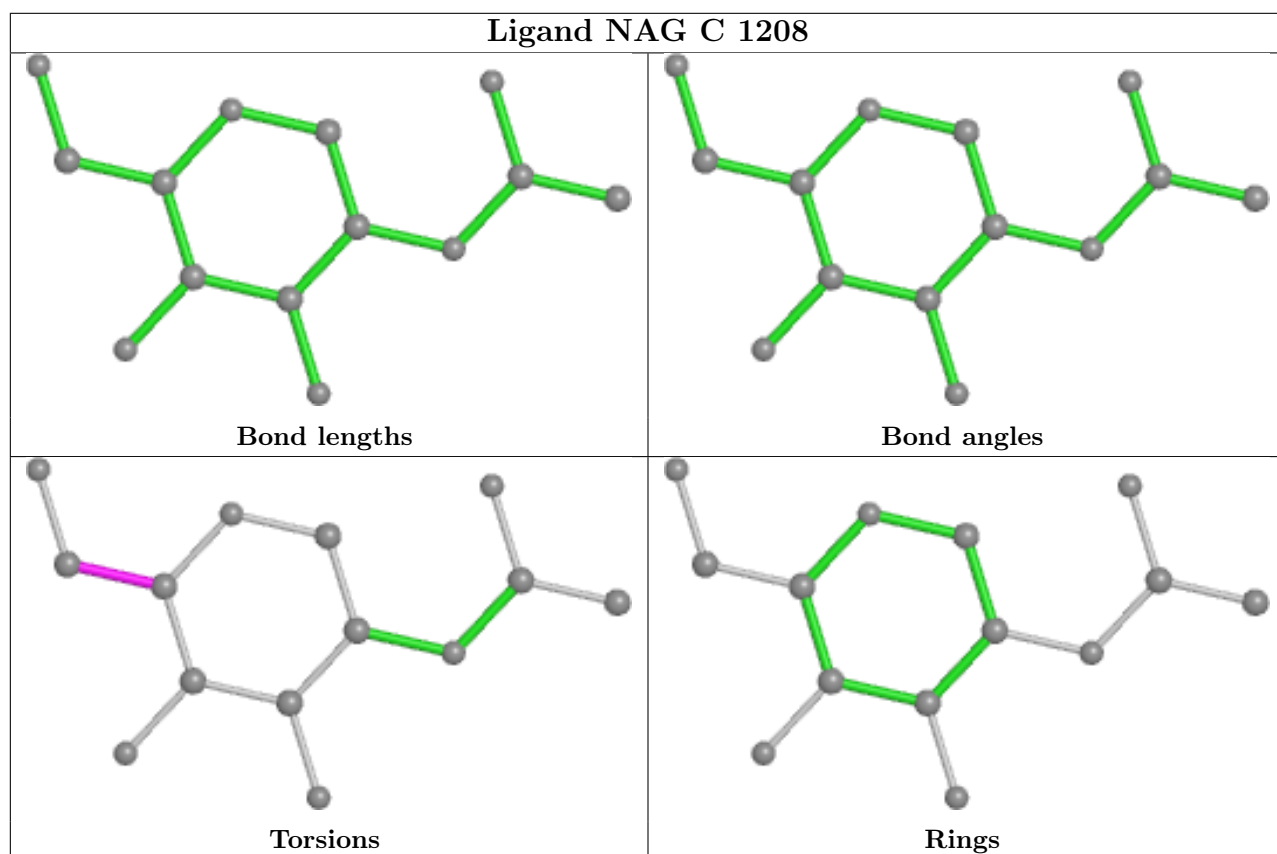
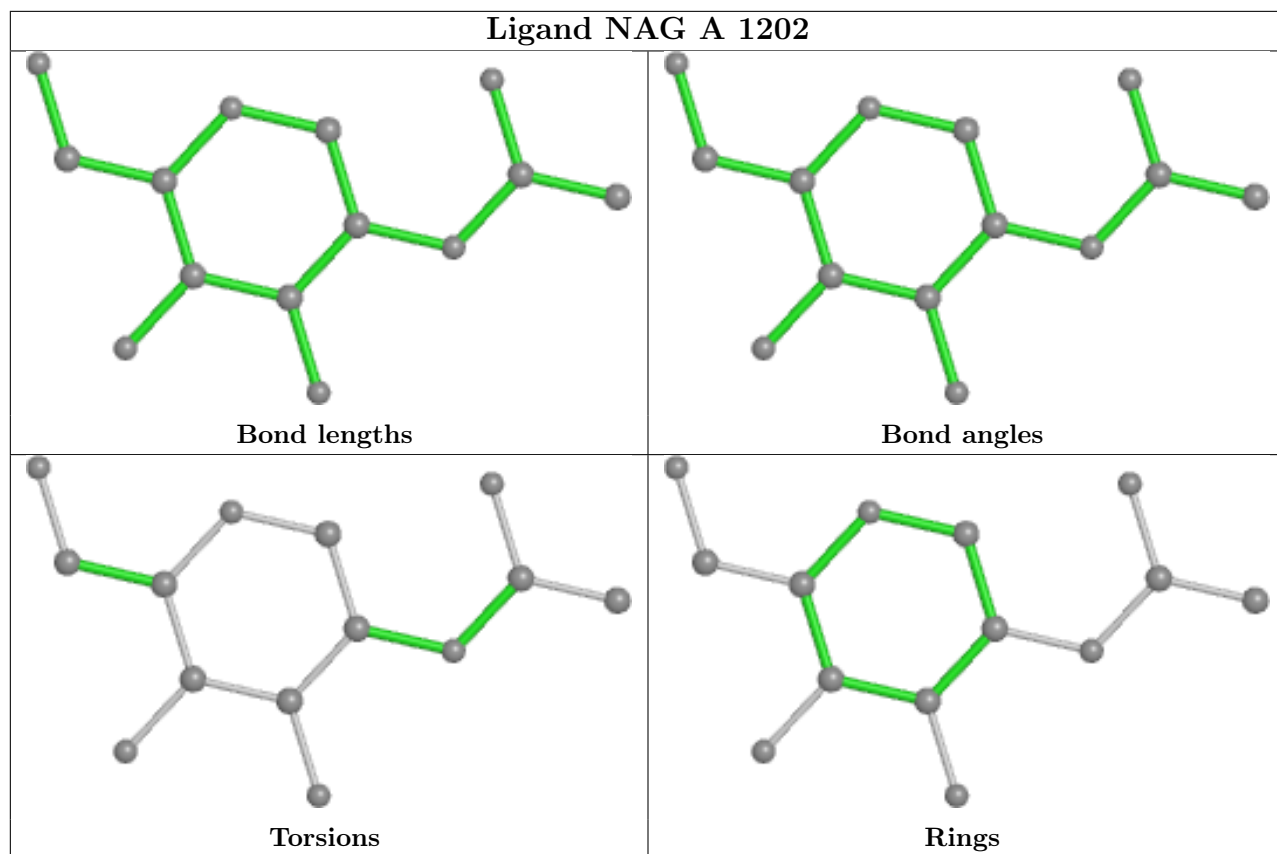


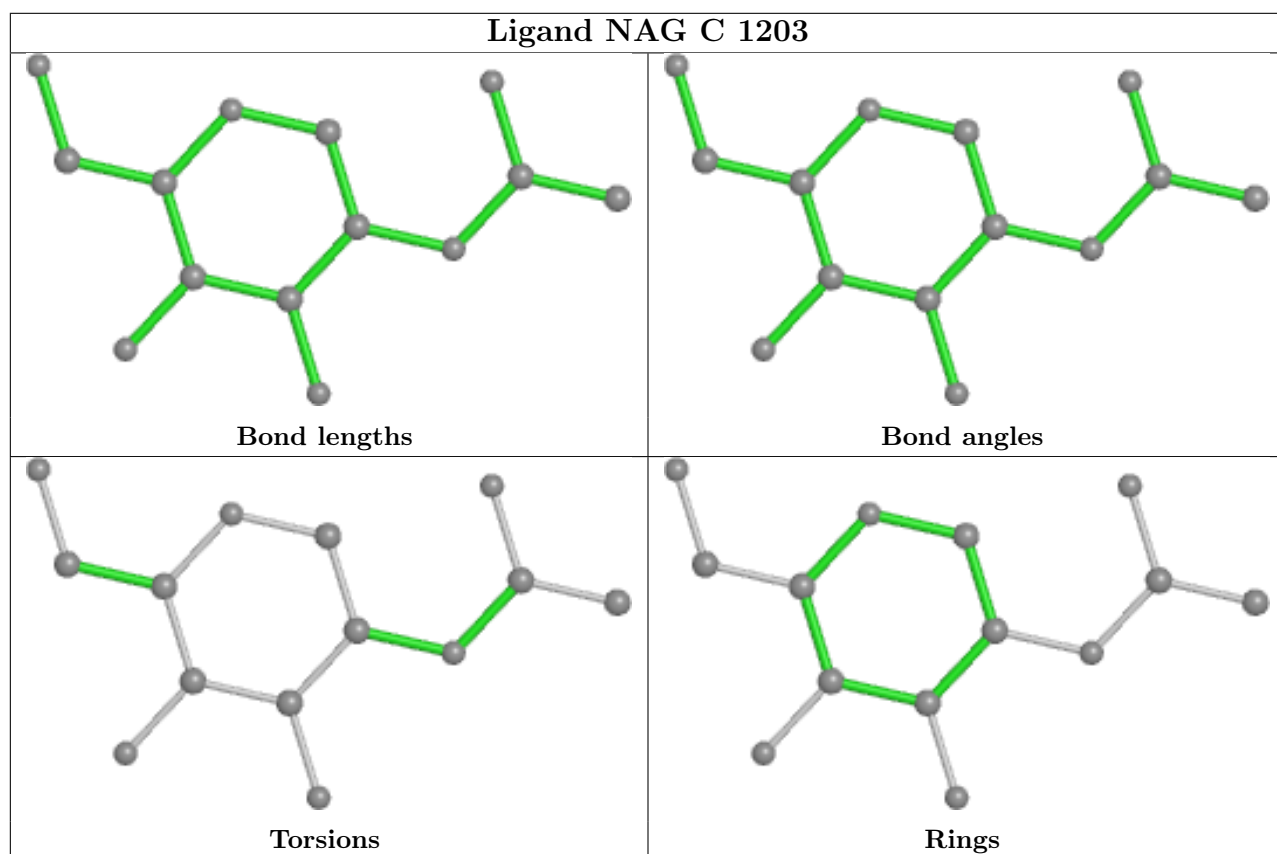
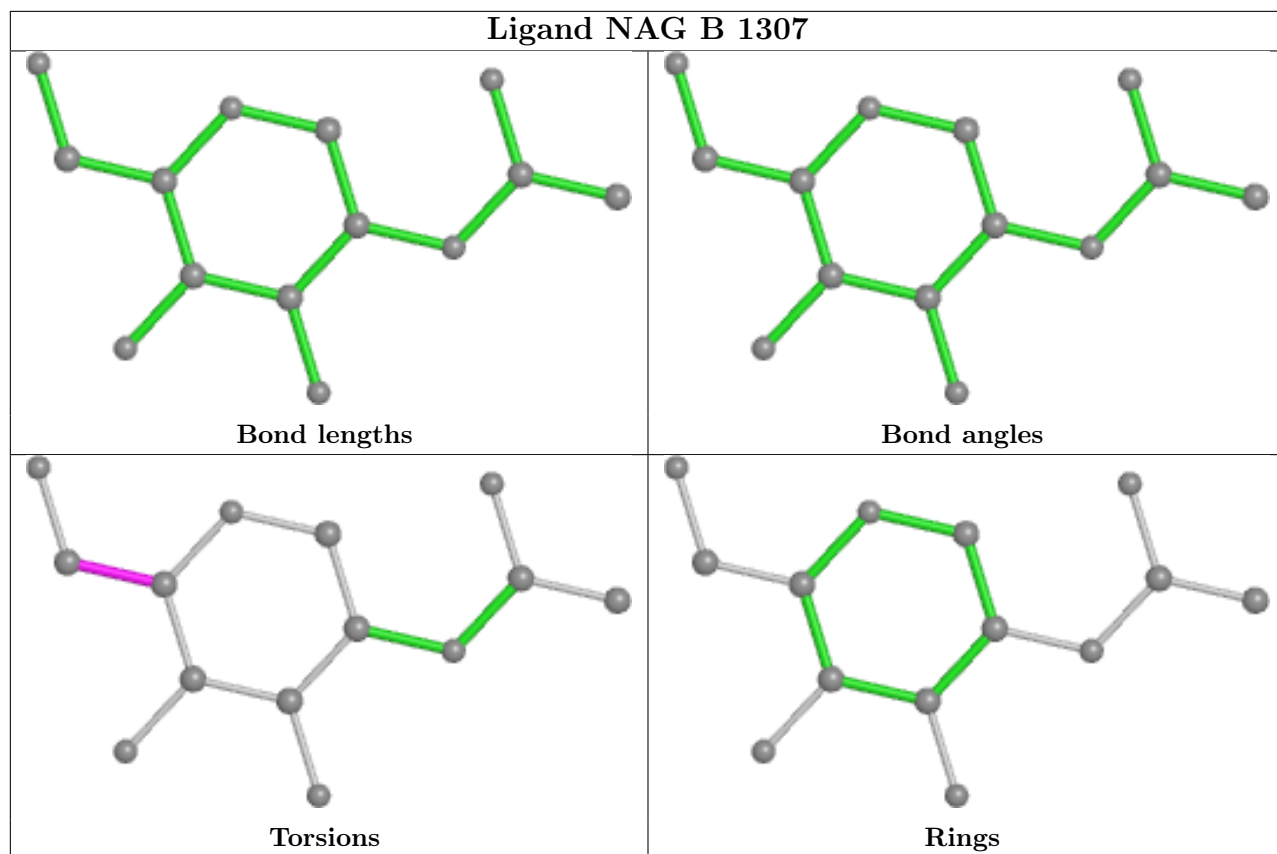


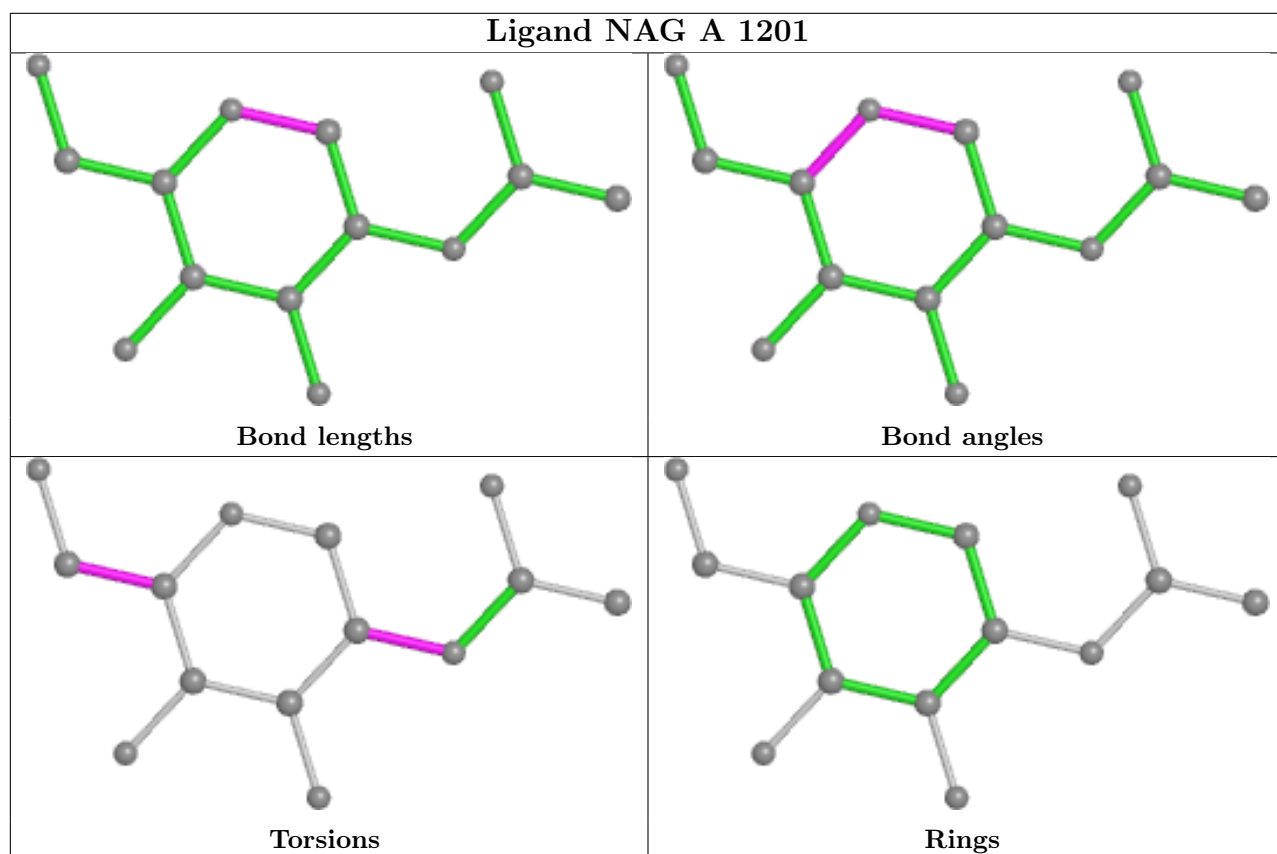
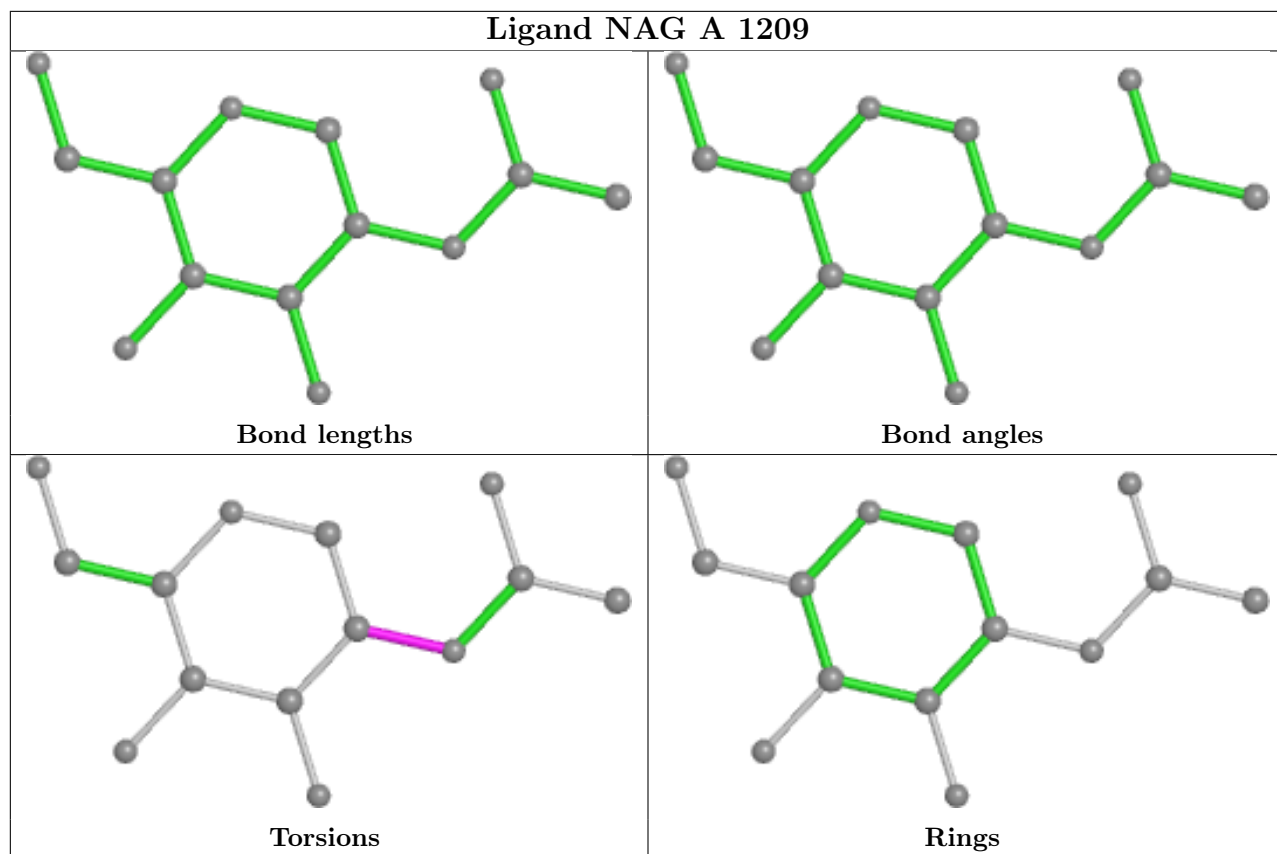


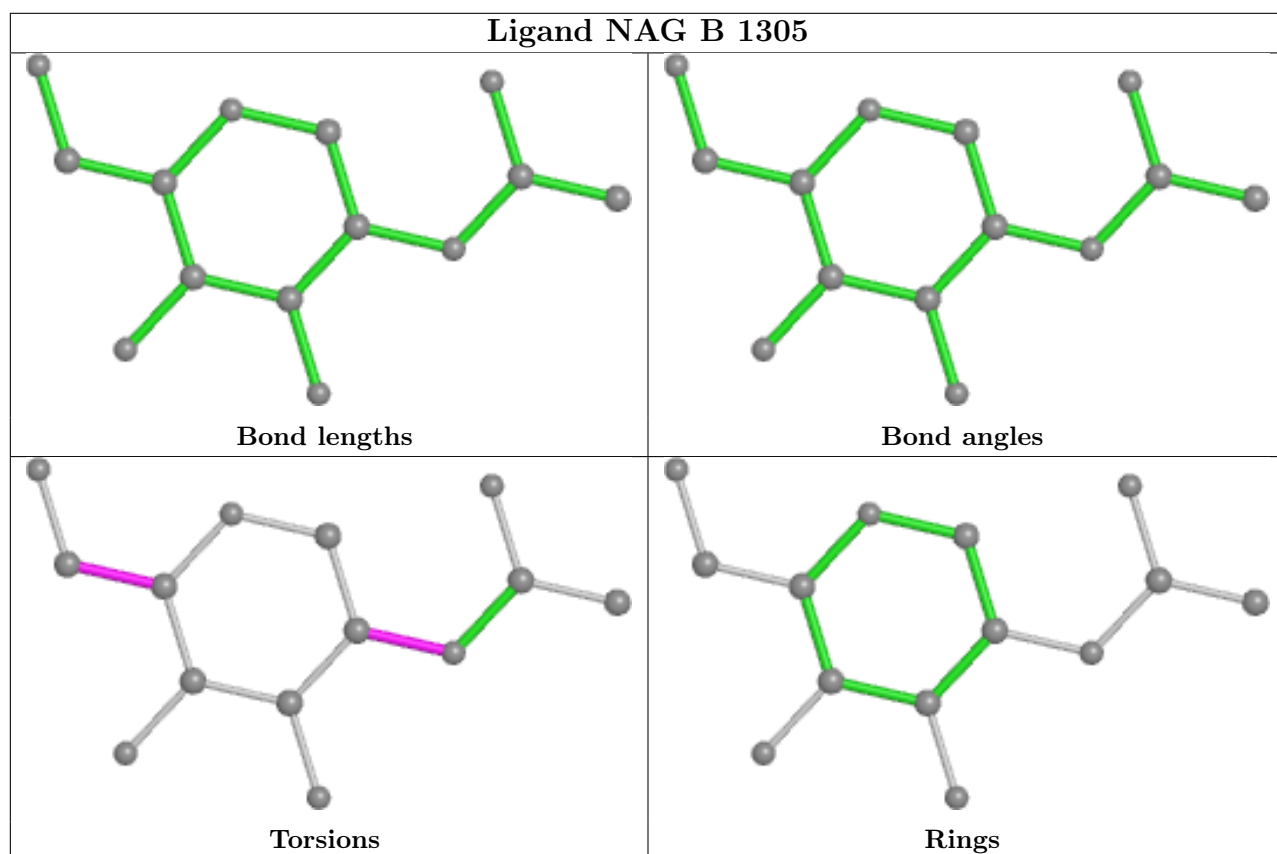
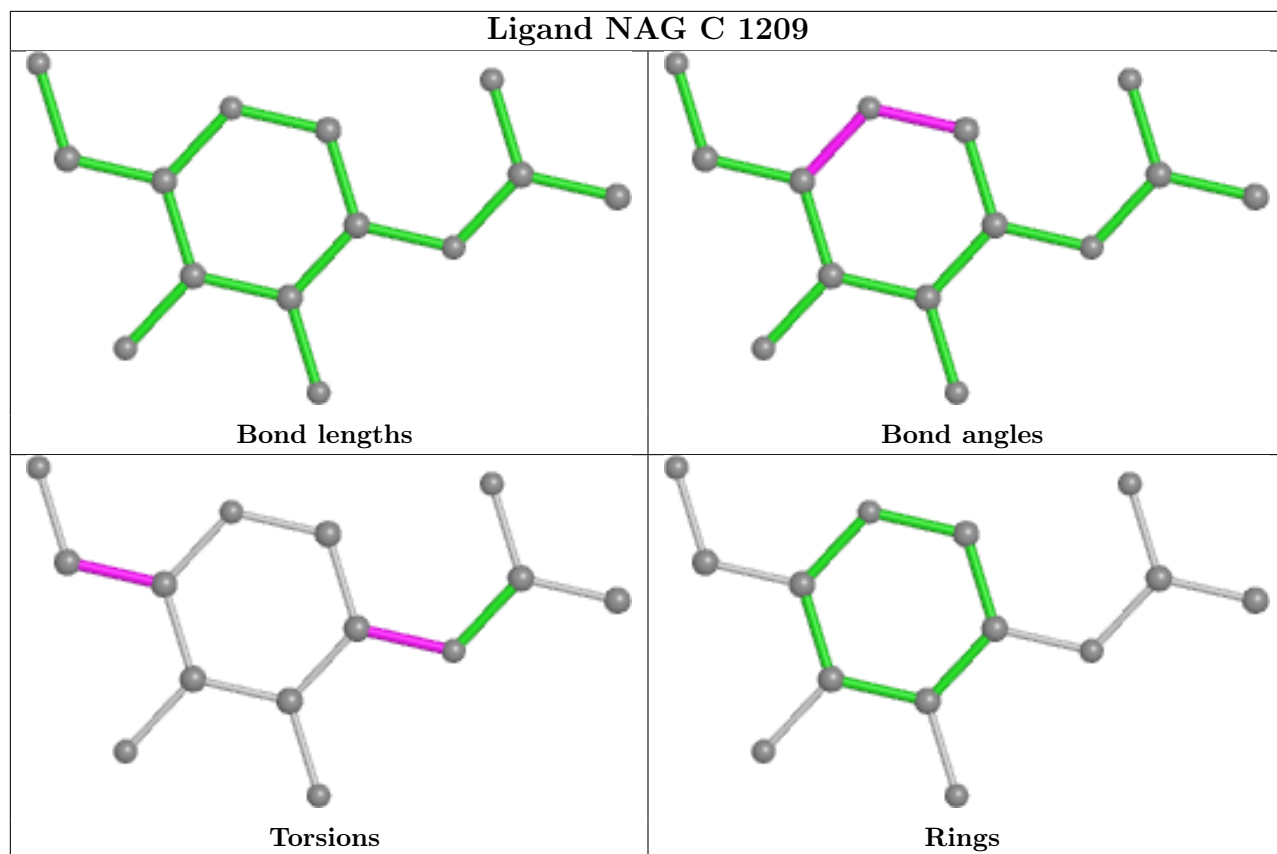


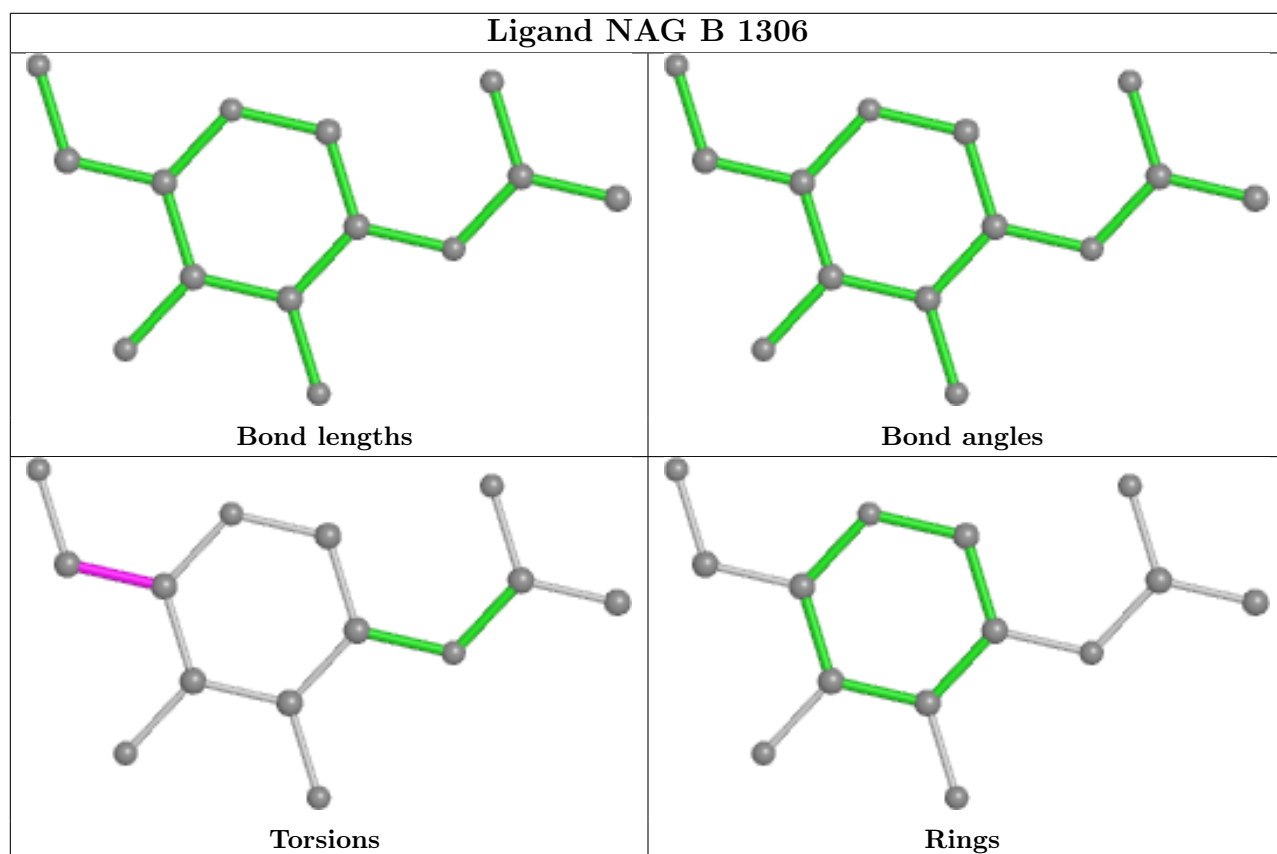
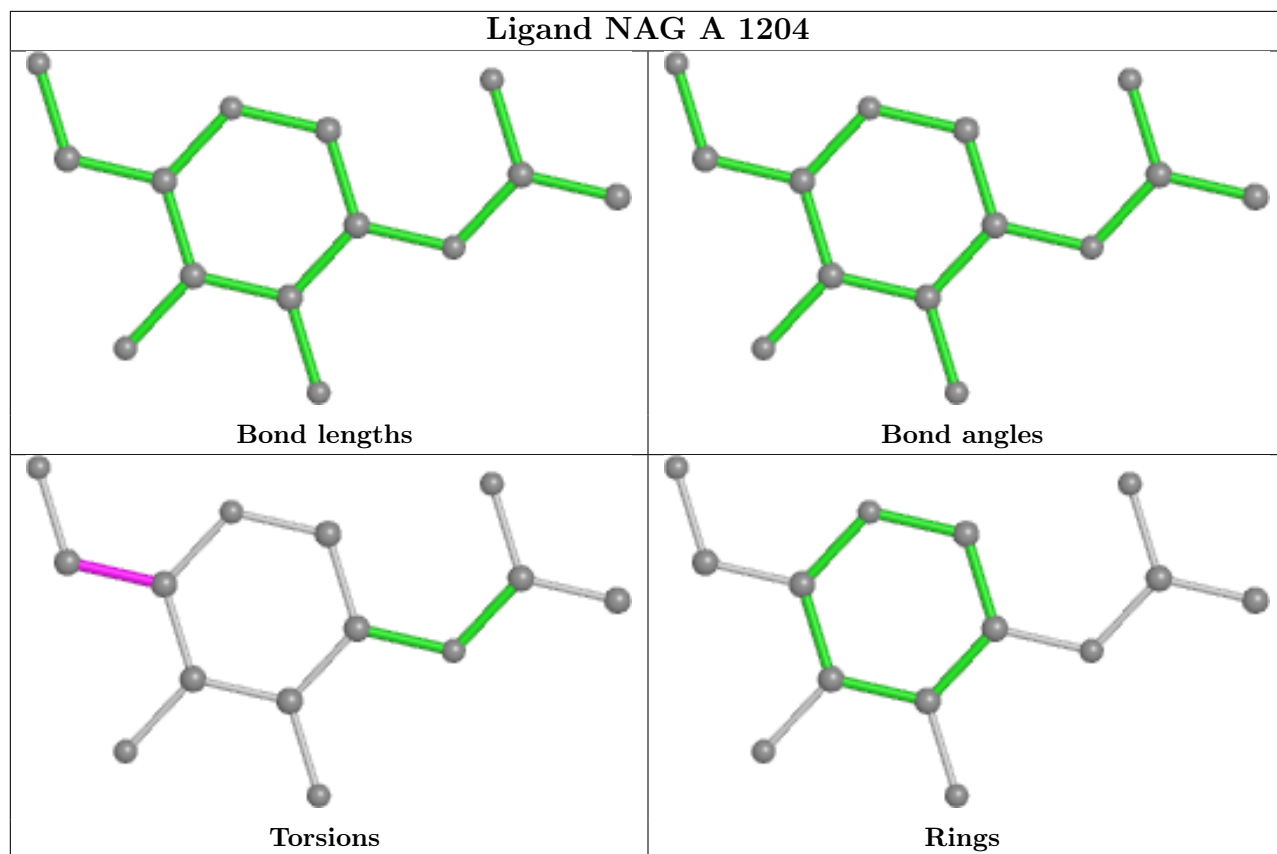


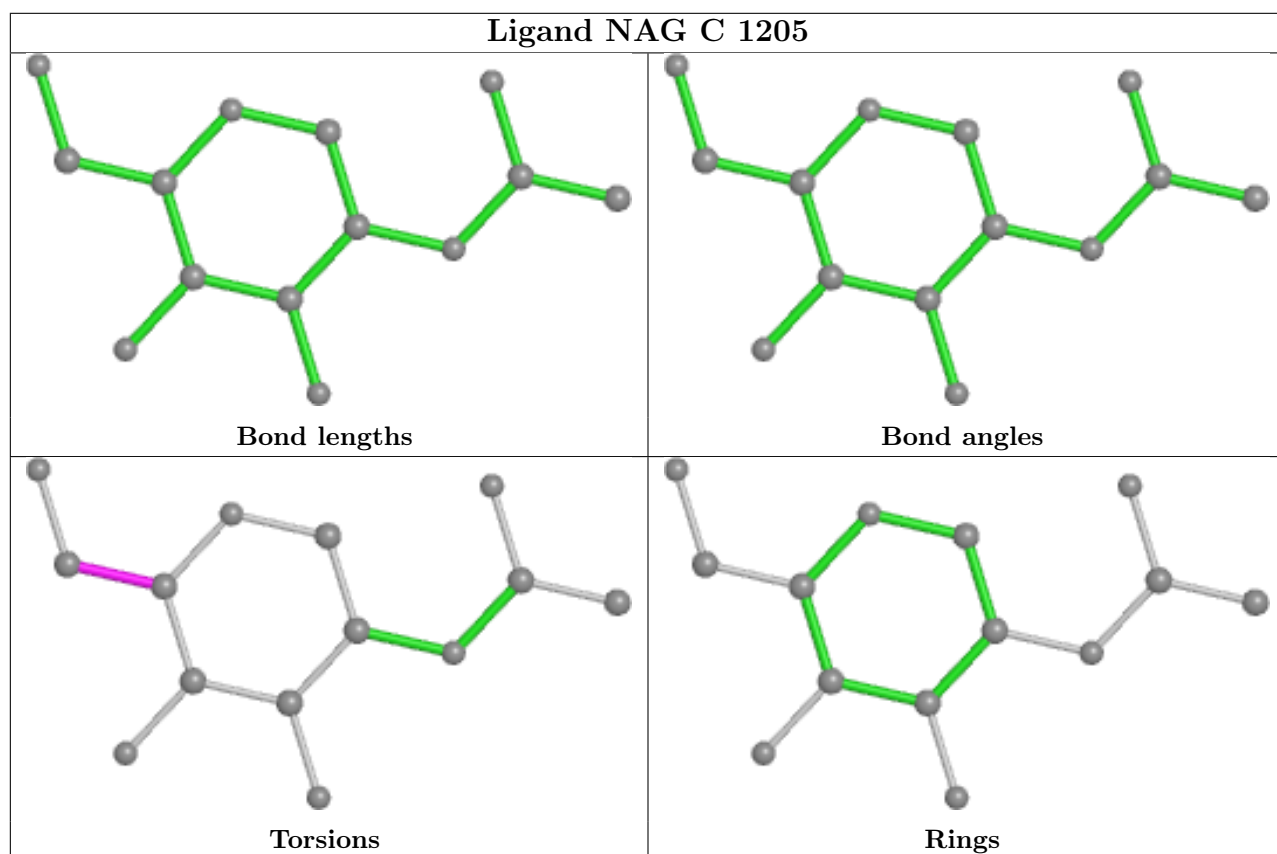
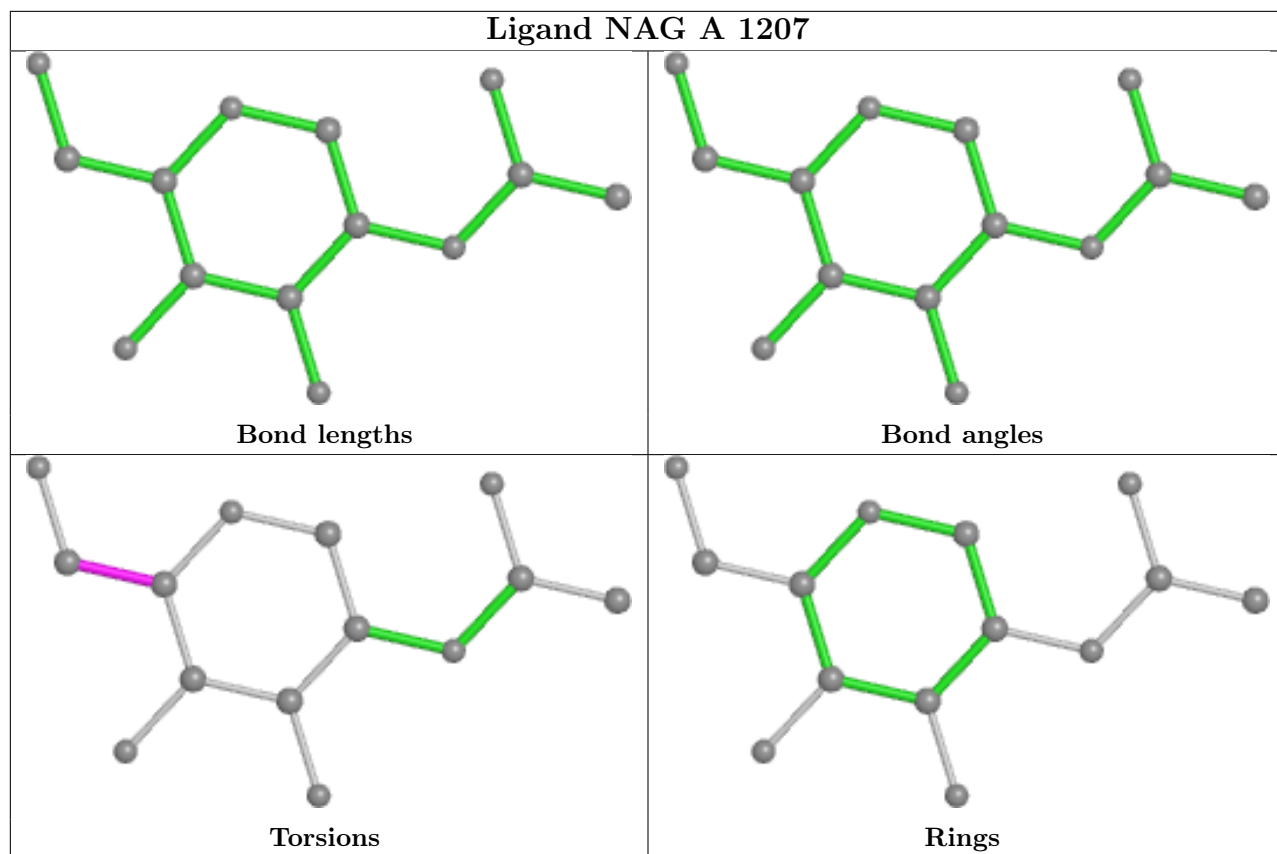


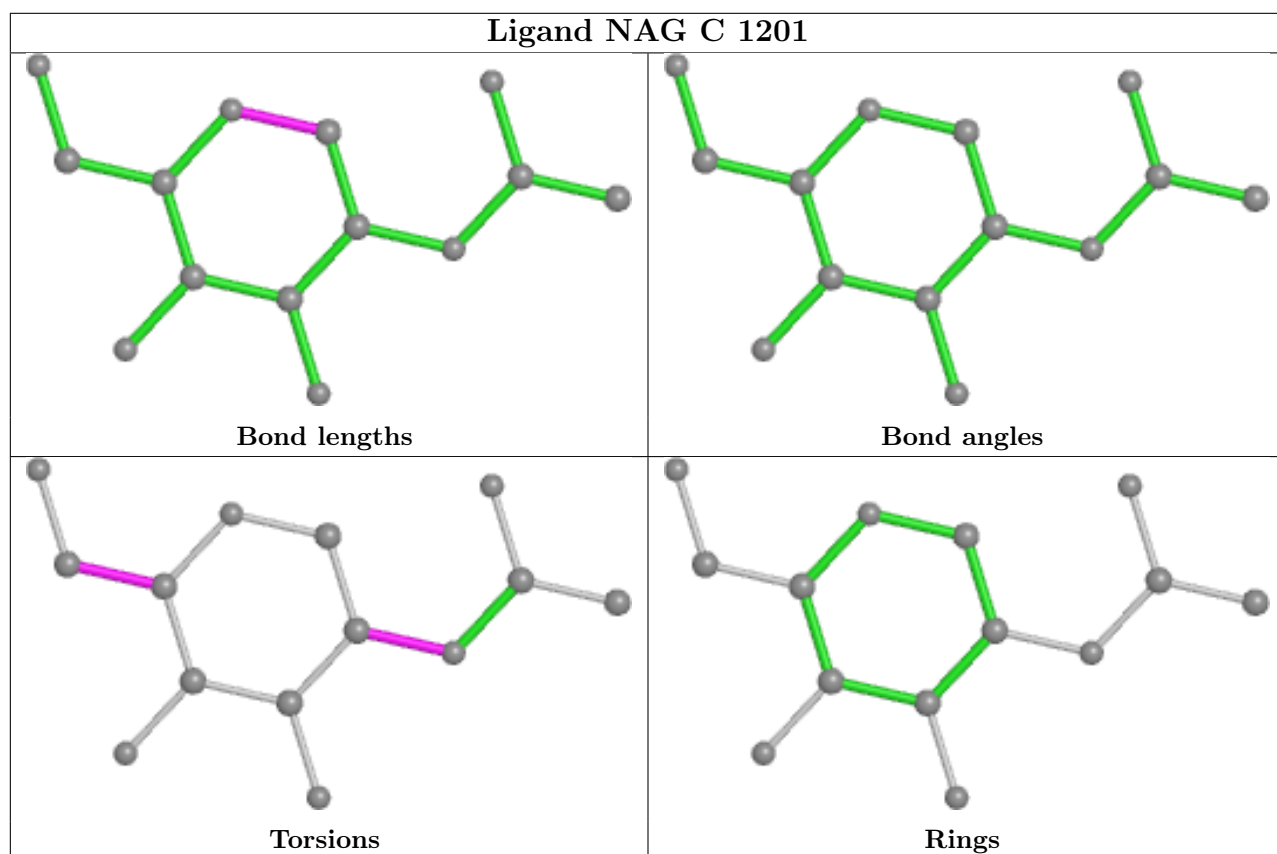
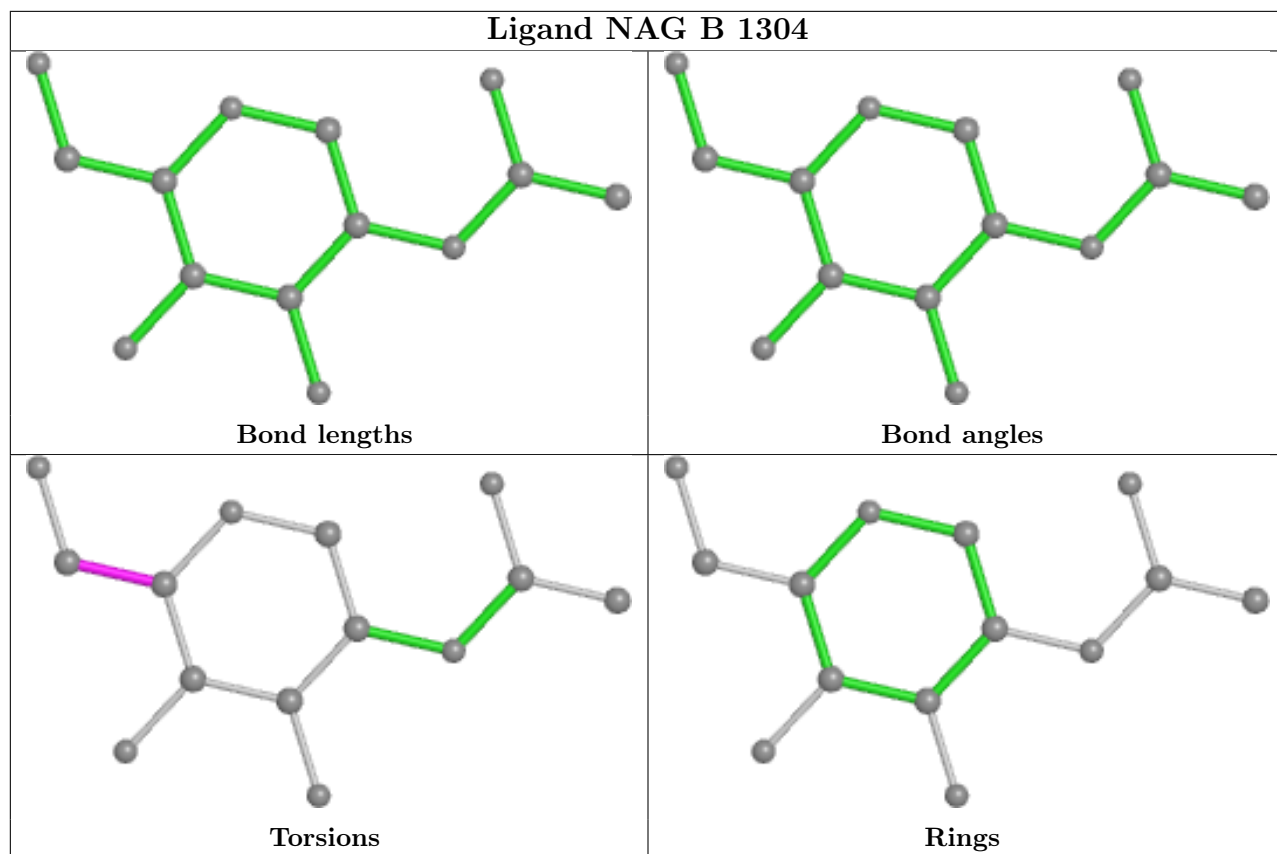












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

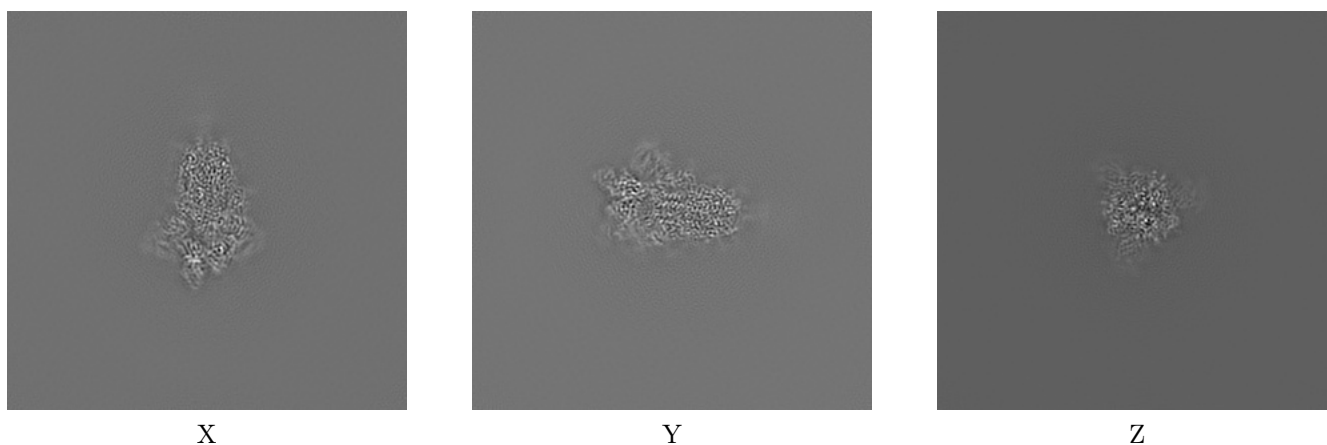
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28856. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

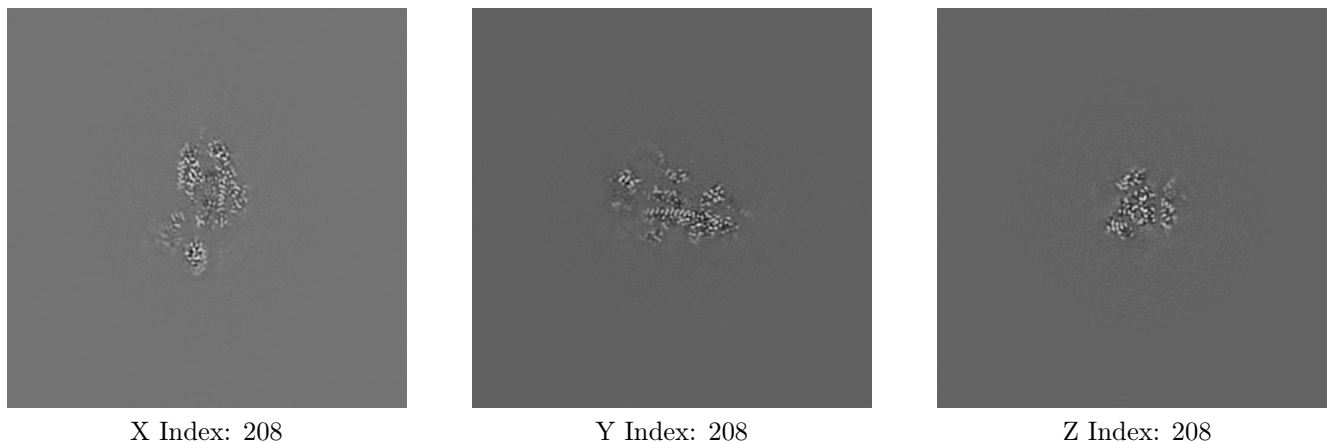
6.1.1 Primary map



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

6.2 Central slices [i](#)

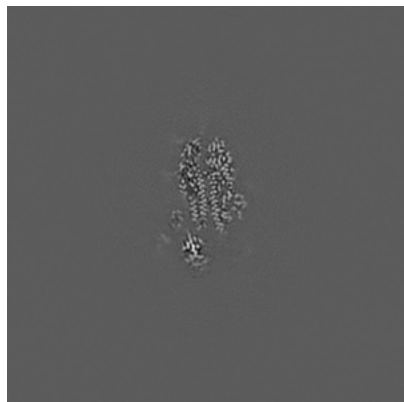
6.2.1 Primary map



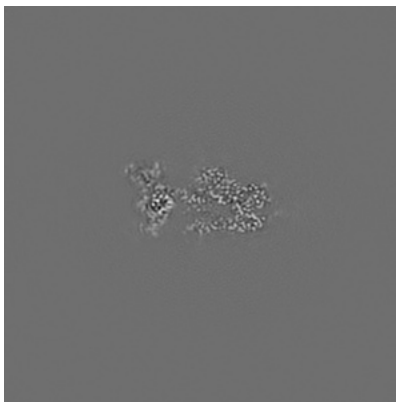
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

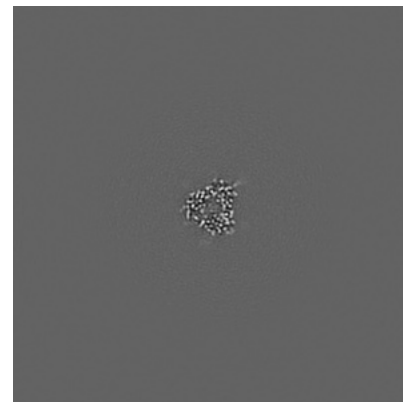
6.3.1 Primary map



X Index: 214



Y Index: 196

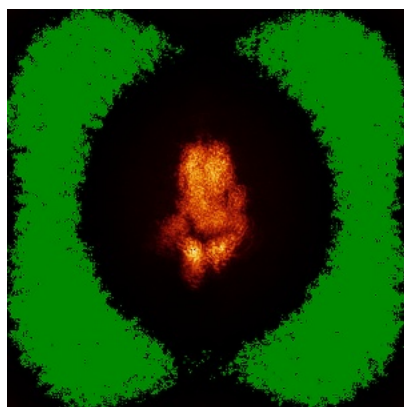


Z Index: 248

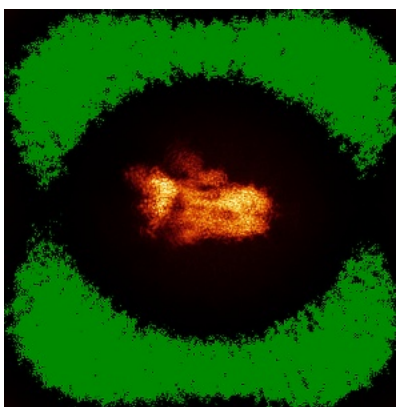
The images above show the largest variance slices of the map in three orthogonal directions.

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

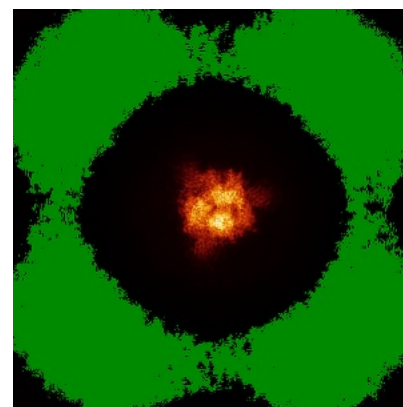
6.4.1 Primary map



X



Y

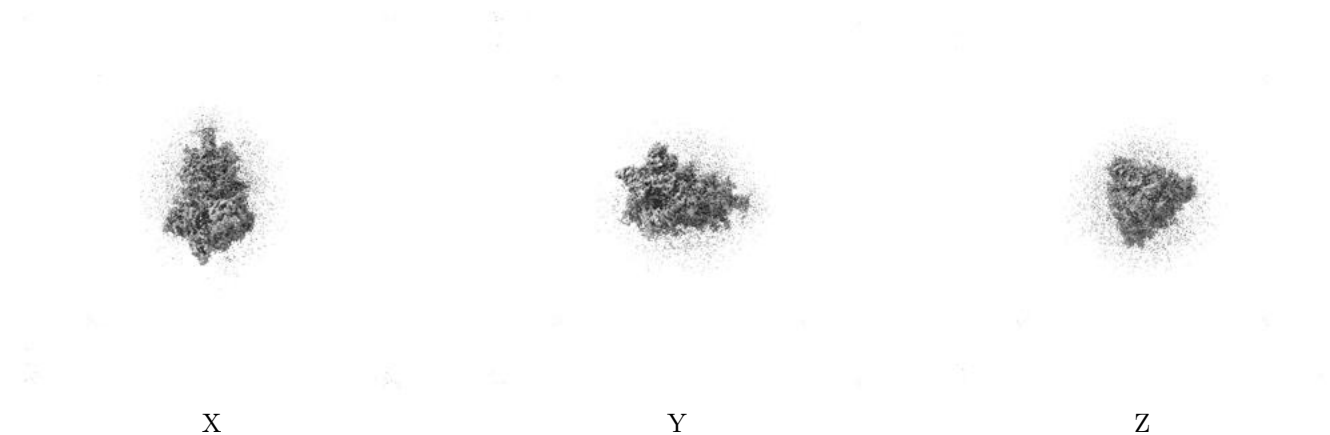


Z

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 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

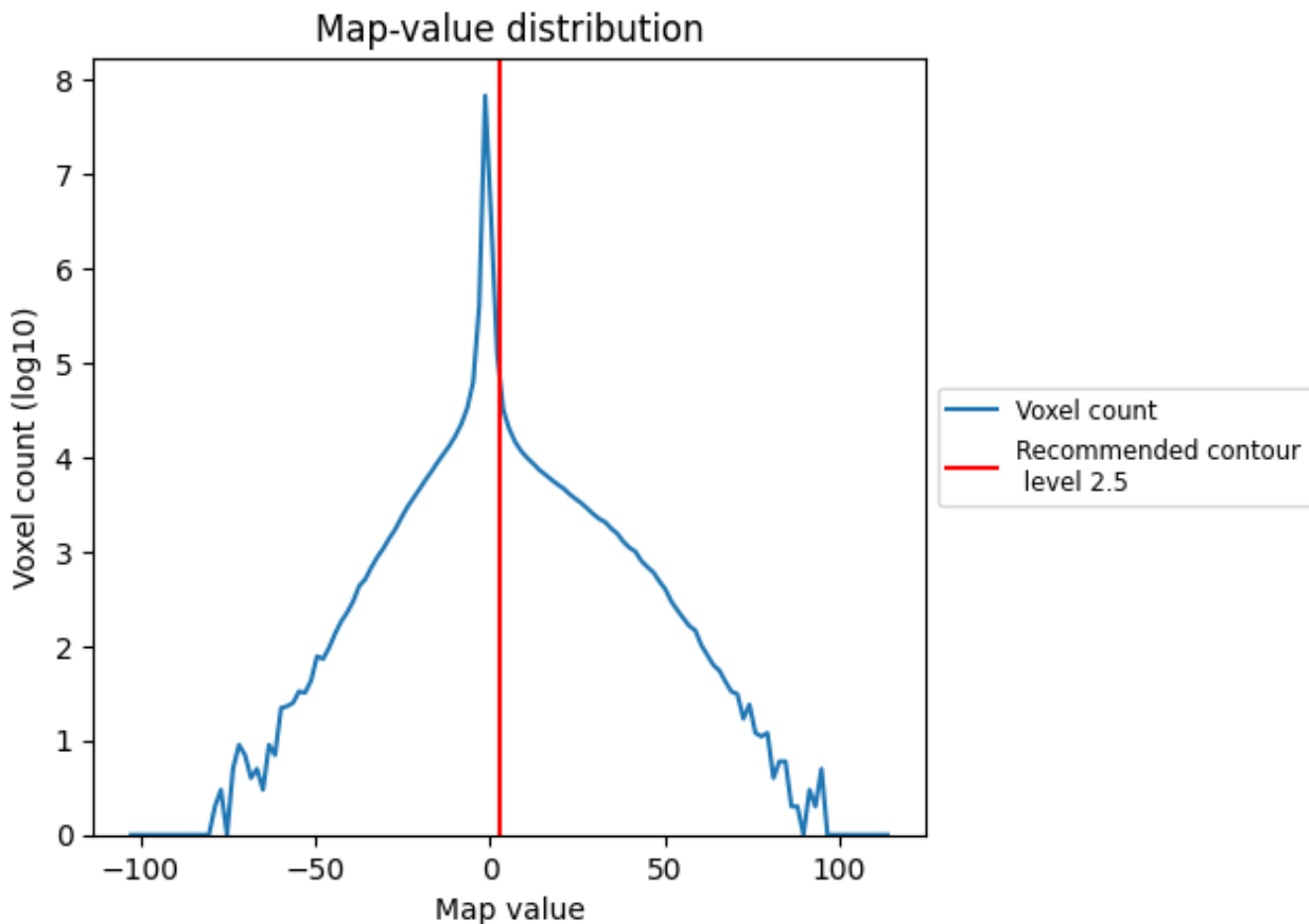
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

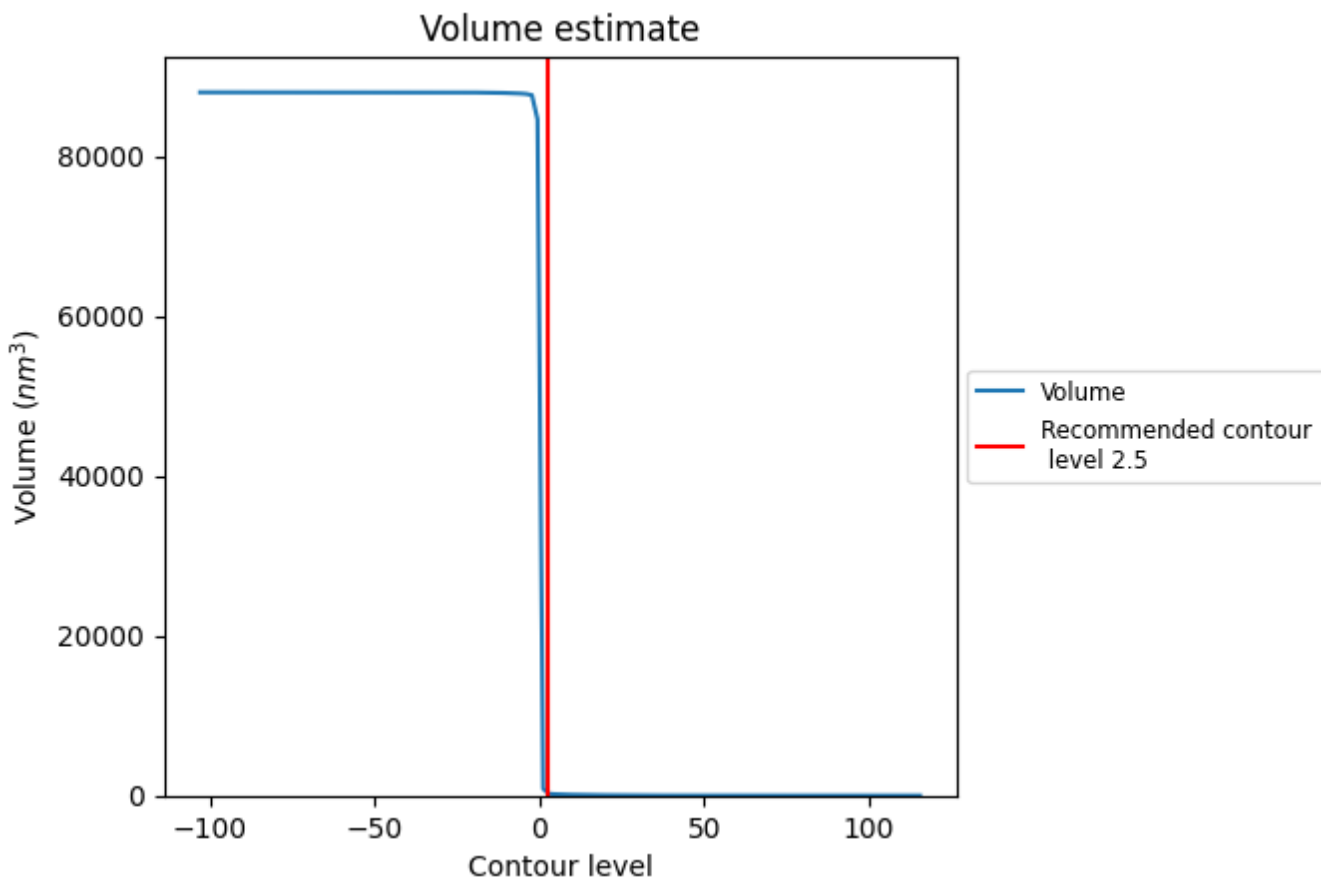
This section contains the results of statistical analysis of the map.

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.

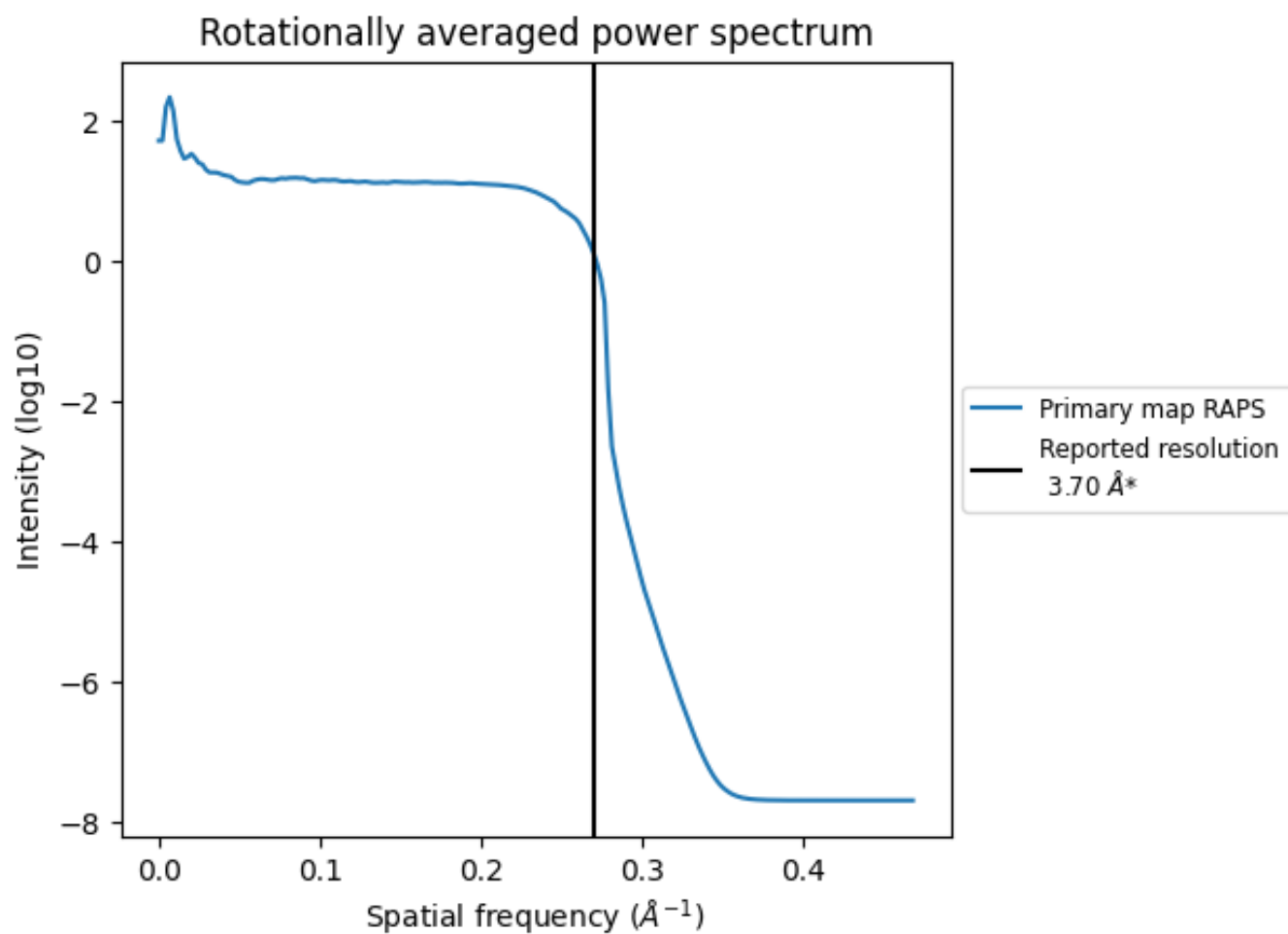
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

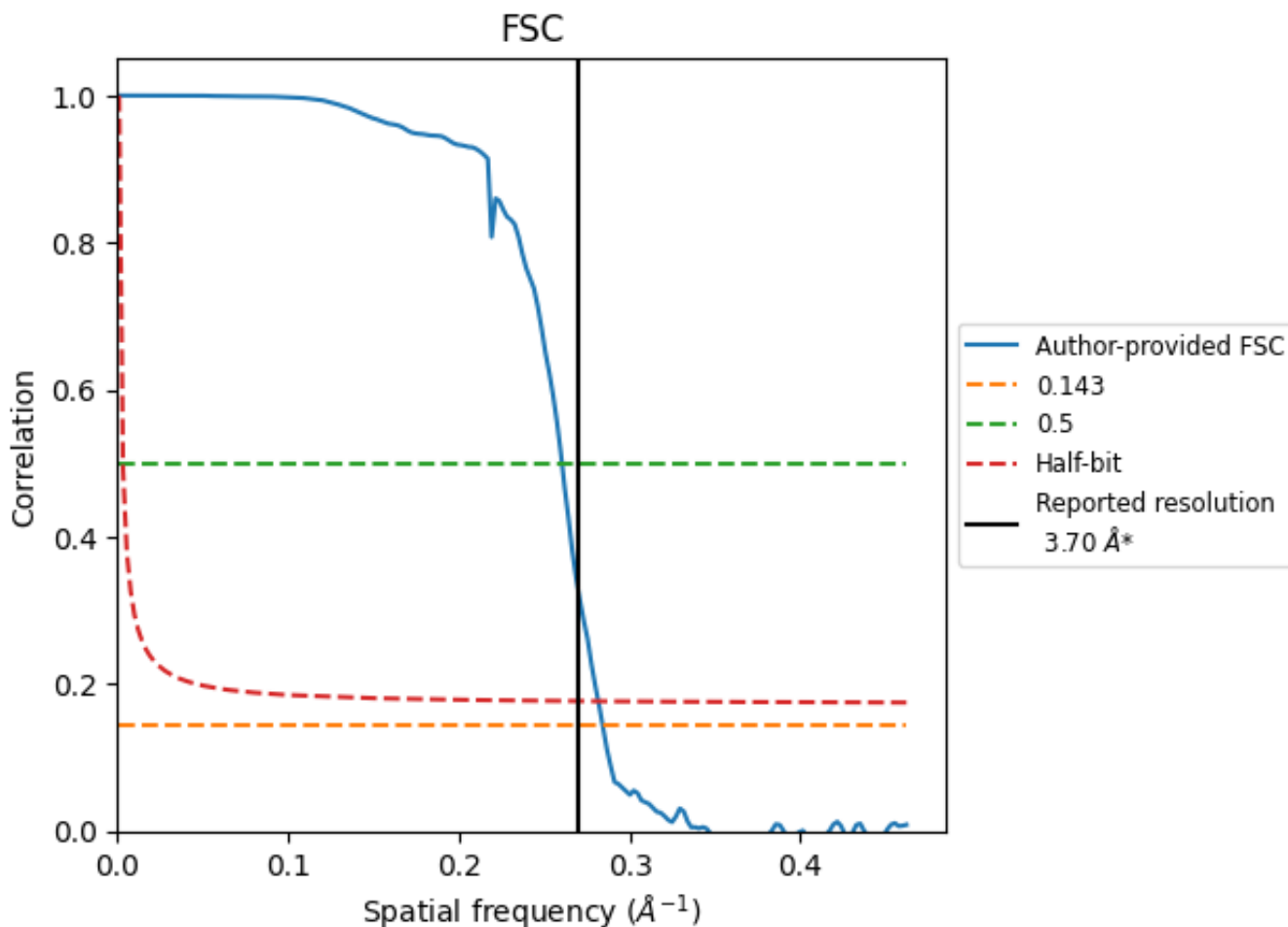


*Reported resolution corresponds to spatial frequency of 0.270\AA^{-1}

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

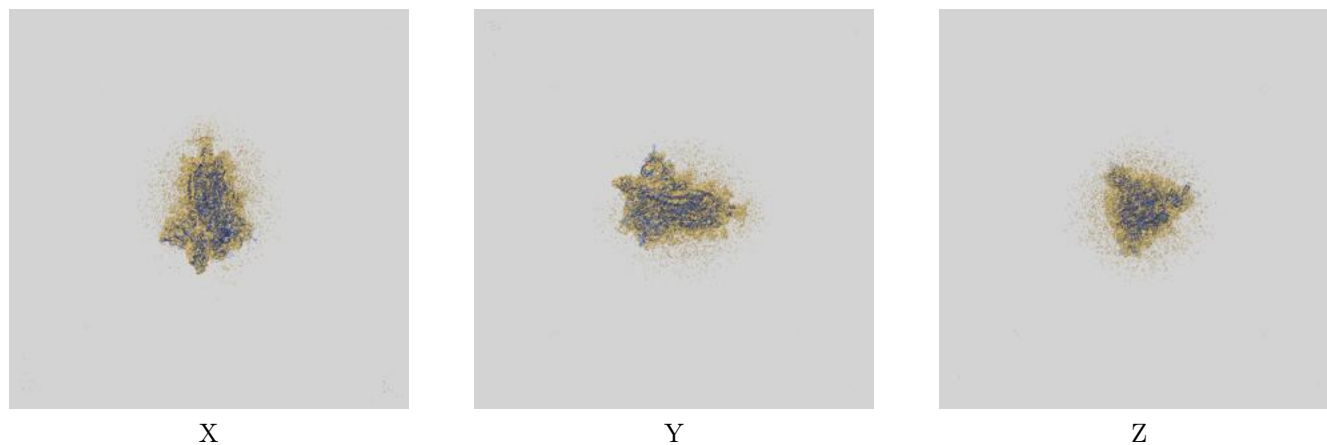
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.70	-
Author-provided FSC curve	3.52	3.84	3.55
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

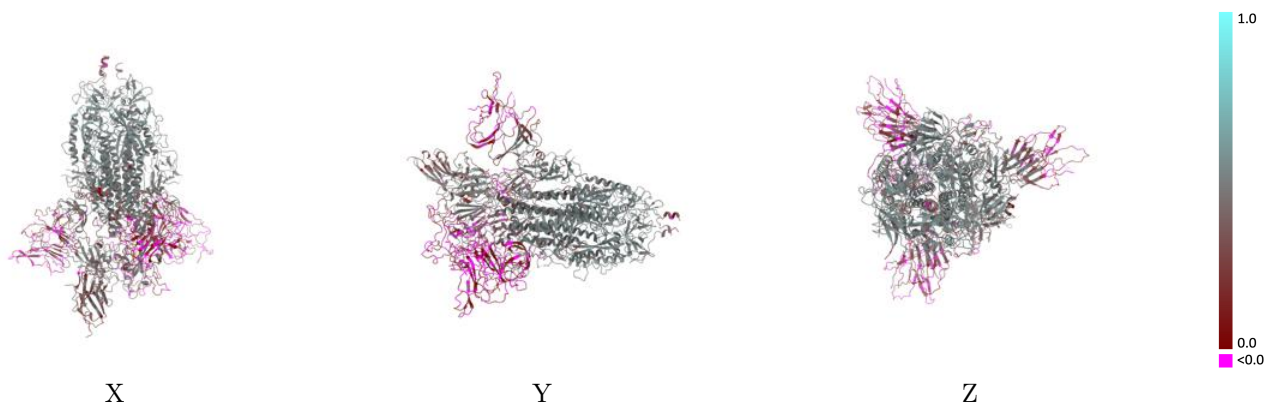
This section contains information regarding the fit between EMDB map EMD-28856 and PDB model 8F4P. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



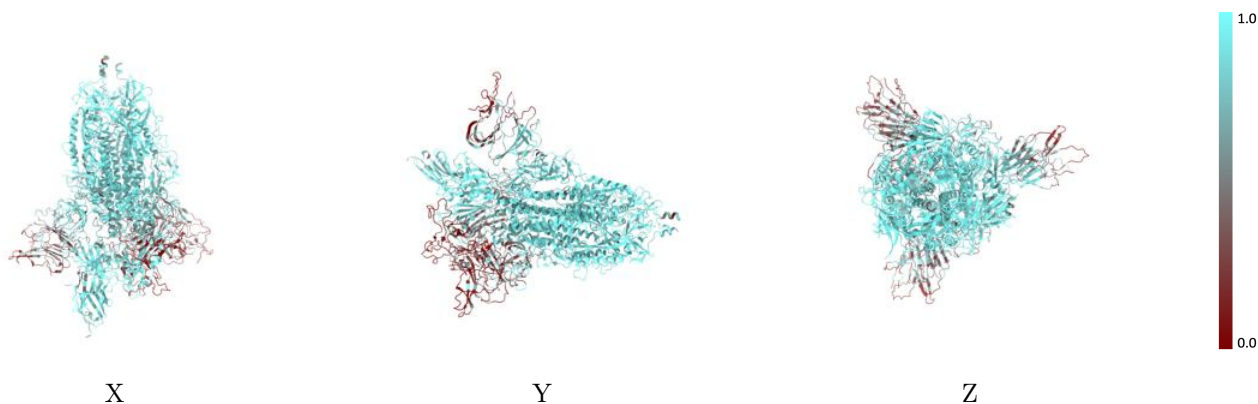
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



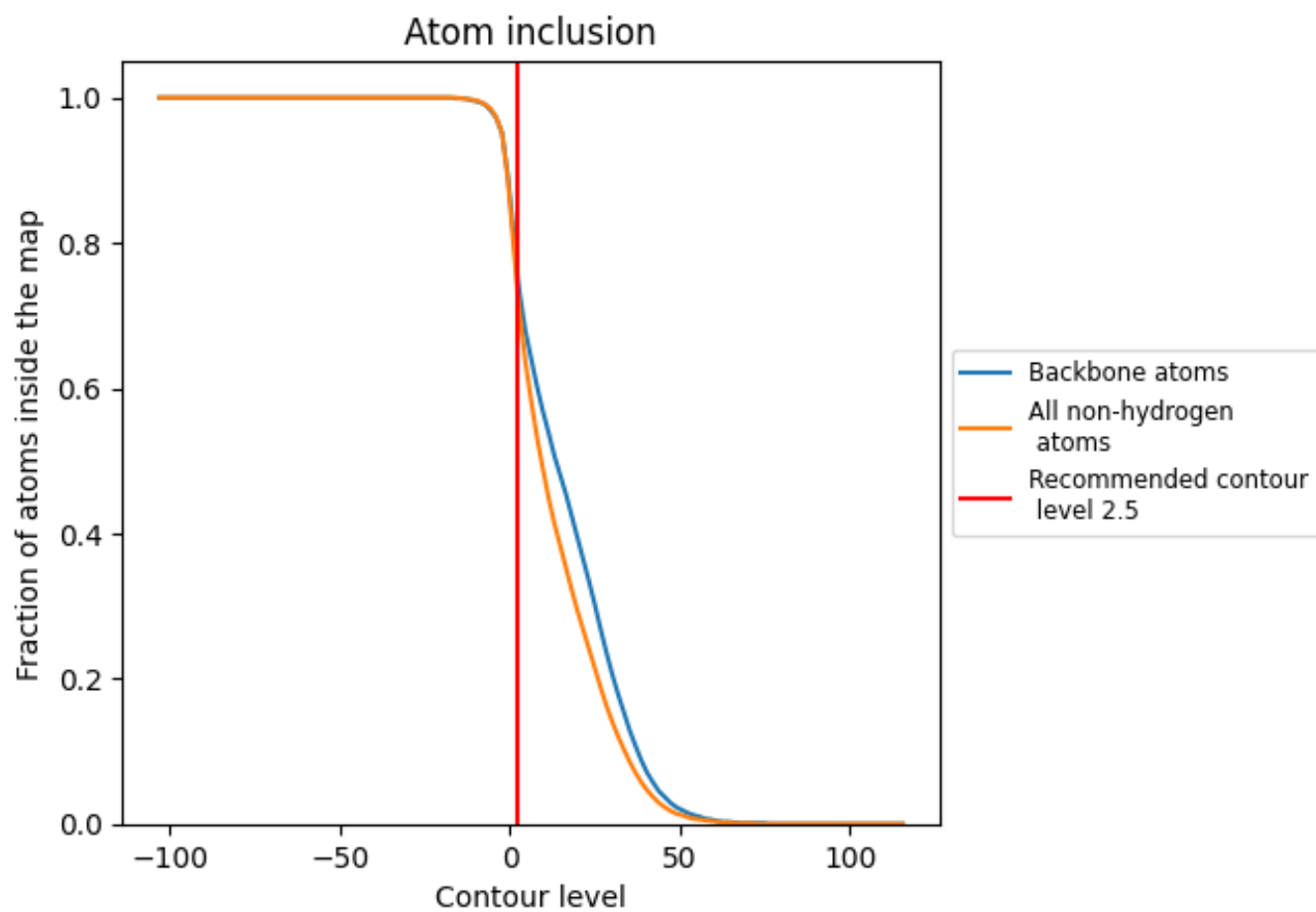
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).























9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7230	 0.3460
A	 0.7480	 0.3590
B	 0.7910	 0.3890
C	 0.6210	 0.2910
D	 0.8090	 0.3440
E	 0.7140	 0.2510
F	 0.8570	 0.4110
G	 0.8570	 0.2560
H	 0.9640	 0.4530
I	 0.8570	 0.4000
J	 0.3210	 0.0730

