



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:24 AM UTC

PDB ID : 8WDE / pdb_00008wde
EMDB ID : EMD-37462
Title : CryoEM structure of the spike protein of human CoV 229E in complex with receptor hAPN (composite map)
Authors : Hsu, S.T.D.; Tsai, Y.X.
Deposited on : 2023-09-15
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary 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:

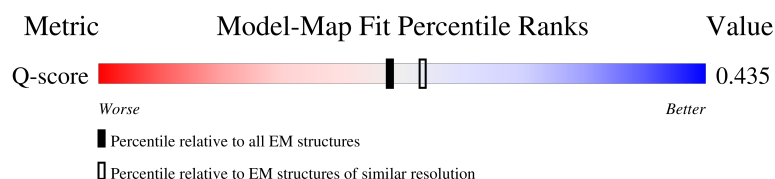
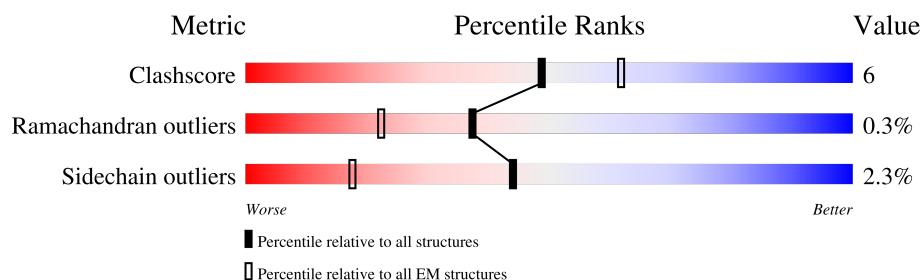
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.60 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	12797 (3.10 - 4.10)

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	1165	
1	B	1165	
1	C	1165	
2	D	943	

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Mol	Chain	Length	Quality of chain
2	E	943	
3	F	3	
3	H	3	
3	J	3	
4	G	2	
4	I	2	
4	K	2	
4	L	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33348 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	864	Total	C	N	O	S	0	0
			6661	4255	1095	1278	33		
1	B	826	Total	C	N	O	S	0	0
			6398	4095	1052	1221	30		
1	C	828	Total	C	N	O	S	0	0
			6410	4101	1054	1225	30		

- Molecule 2 is a protein called Aminopeptidase N.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	883	Total	C	N	O	S	0	0
			7163	4578	1204	1357	24		
2	E	760	Total	C	N	O	S	0	0
			6207	3977	1044	1166	20		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	968	GLN	-	expression tag	UNP P15144
D	969	ASP	-	expression tag	UNP P15144
D	970	ASN	-	expression tag	UNP P15144
D	971	SER	-	expression tag	UNP P15144
D	972	ALA	-	expression tag	UNP P15144
D	973	ASP	-	expression tag	UNP P15144
D	974	ILE	-	expression tag	UNP P15144
D	975	GLN	-	expression tag	UNP P15144
D	976	HIS	-	expression tag	UNP P15144
D	977	SER	-	expression tag	UNP P15144
D	978	GLY	-	expression tag	UNP P15144
D	979	ARG	-	expression tag	UNP P15144
D	980	PRO	-	expression tag	UNP P15144
D	981	LEU	-	expression tag	UNP P15144
D	982	GLU	-	expression tag	UNP P15144

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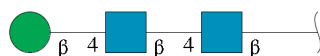
Chain	Residue	Modelled	Actual	Comment	Reference
D	983	SER	-	expression tag	UNP P15144
D	984	ARG	-	expression tag	UNP P15144
D	985	GLY	-	expression tag	UNP P15144
D	986	PRO	-	expression tag	UNP P15144
D	987	PHE	-	expression tag	UNP P15144
D	988	GLU	-	expression tag	UNP P15144
D	989	GLN	-	expression tag	UNP P15144
D	990	LYS	-	expression tag	UNP P15144
D	991	LEU	-	expression tag	UNP P15144
D	992	ILE	-	expression tag	UNP P15144
D	993	SER	-	expression tag	UNP P15144
D	994	GLU	-	expression tag	UNP P15144
D	995	GLU	-	expression tag	UNP P15144
D	996	ASP	-	expression tag	UNP P15144
D	997	LEU	-	expression tag	UNP P15144
D	998	ASN	-	expression tag	UNP P15144
D	999	MET	-	expression tag	UNP P15144
D	1000	HIS	-	expression tag	UNP P15144
D	1001	THR	-	expression tag	UNP P15144
D	1002	GLY	-	expression tag	UNP P15144
D	1003	HIS	-	expression tag	UNP P15144
D	1004	HIS	-	expression tag	UNP P15144
D	1005	HIS	-	expression tag	UNP P15144
D	1006	HIS	-	expression tag	UNP P15144
D	1007	HIS	-	expression tag	UNP P15144
D	1008	HIS	-	expression tag	UNP P15144
E	968	GLN	-	expression tag	UNP P15144
E	969	ASP	-	expression tag	UNP P15144
E	970	ASN	-	expression tag	UNP P15144
E	971	SER	-	expression tag	UNP P15144
E	972	ALA	-	expression tag	UNP P15144
E	973	ASP	-	expression tag	UNP P15144
E	974	ILE	-	expression tag	UNP P15144
E	975	GLN	-	expression tag	UNP P15144
E	976	HIS	-	expression tag	UNP P15144
E	977	SER	-	expression tag	UNP P15144
E	978	GLY	-	expression tag	UNP P15144
E	979	ARG	-	expression tag	UNP P15144
E	980	PRO	-	expression tag	UNP P15144
E	981	LEU	-	expression tag	UNP P15144
E	982	GLU	-	expression tag	UNP P15144
E	983	SER	-	expression tag	UNP P15144

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Chain	Residue	Modelled	Actual	Comment	Reference
E	984	ARG	-	expression tag	UNP P15144
E	985	GLY	-	expression tag	UNP P15144
E	986	PRO	-	expression tag	UNP P15144
E	987	PHE	-	expression tag	UNP P15144
E	988	GLU	-	expression tag	UNP P15144
E	989	GLN	-	expression tag	UNP P15144
E	990	LYS	-	expression tag	UNP P15144
E	991	LEU	-	expression tag	UNP P15144
E	992	ILE	-	expression tag	UNP P15144
E	993	SER	-	expression tag	UNP P15144
E	994	GLU	-	expression tag	UNP P15144
E	995	GLU	-	expression tag	UNP P15144
E	996	ASP	-	expression tag	UNP P15144
E	997	LEU	-	expression tag	UNP P15144
E	998	ASN	-	expression tag	UNP P15144
E	999	MET	-	expression tag	UNP P15144
E	1000	HIS	-	expression tag	UNP P15144
E	1001	THR	-	expression tag	UNP P15144
E	1002	GLY	-	expression tag	UNP P15144
E	1003	HIS	-	expression tag	UNP P15144
E	1004	HIS	-	expression tag	UNP P15144
E	1005	HIS	-	expression tag	UNP P15144
E	1006	HIS	-	expression tag	UNP P15144
E	1007	HIS	-	expression tag	UNP P15144
E	1008	HIS	-	expression tag	UNP P15144

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



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

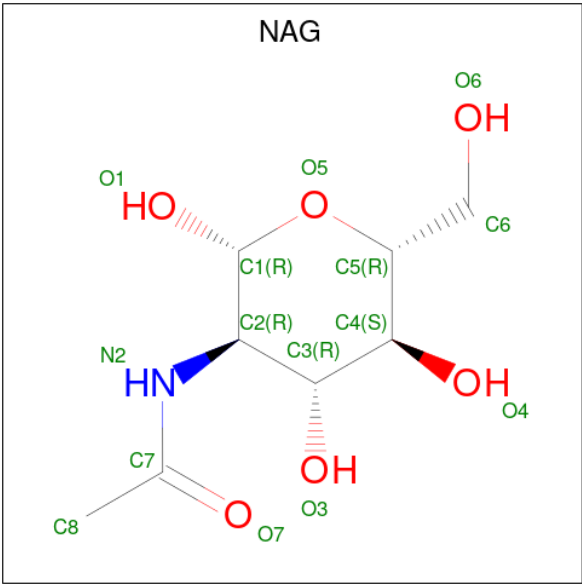
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		

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

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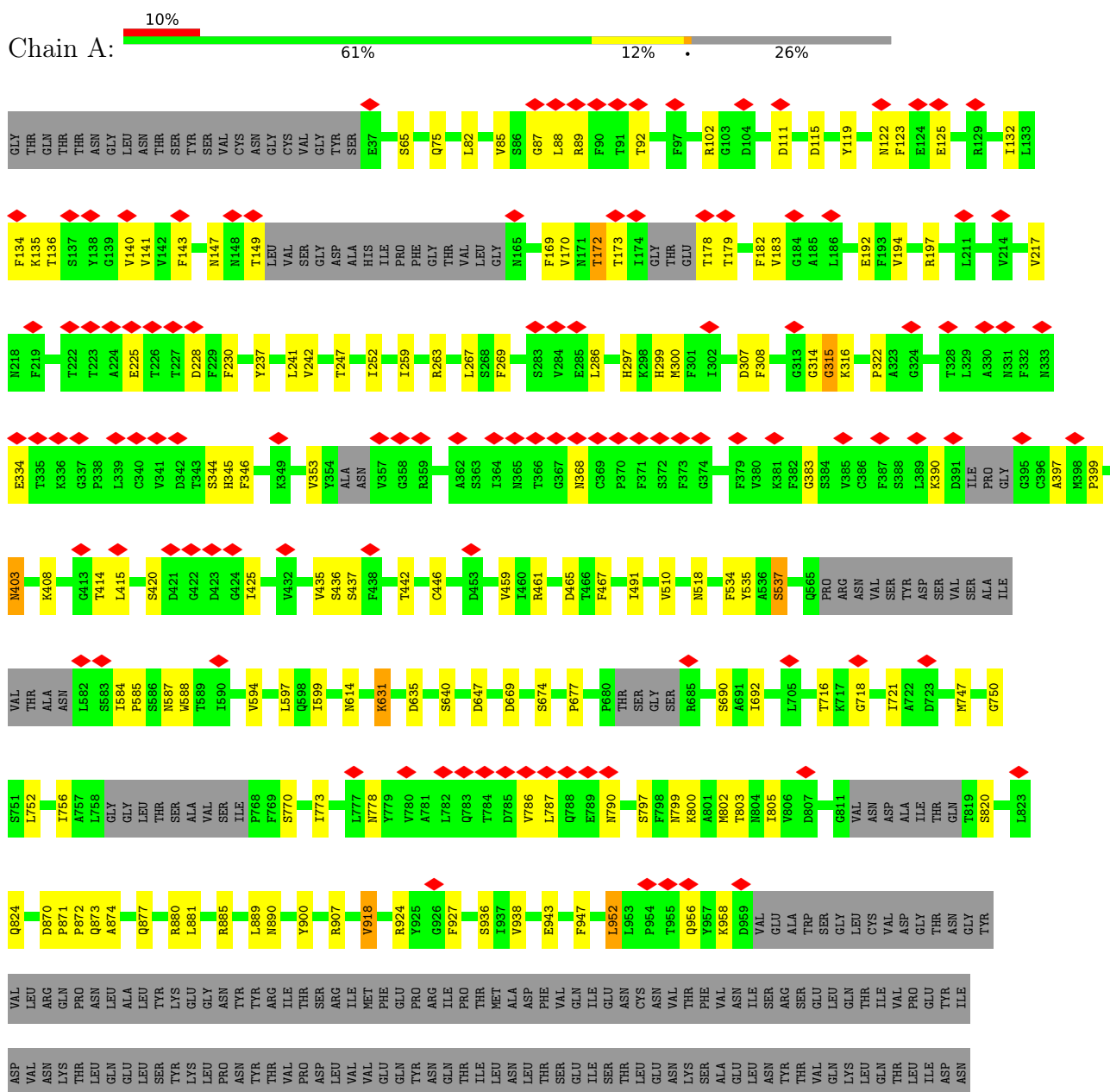
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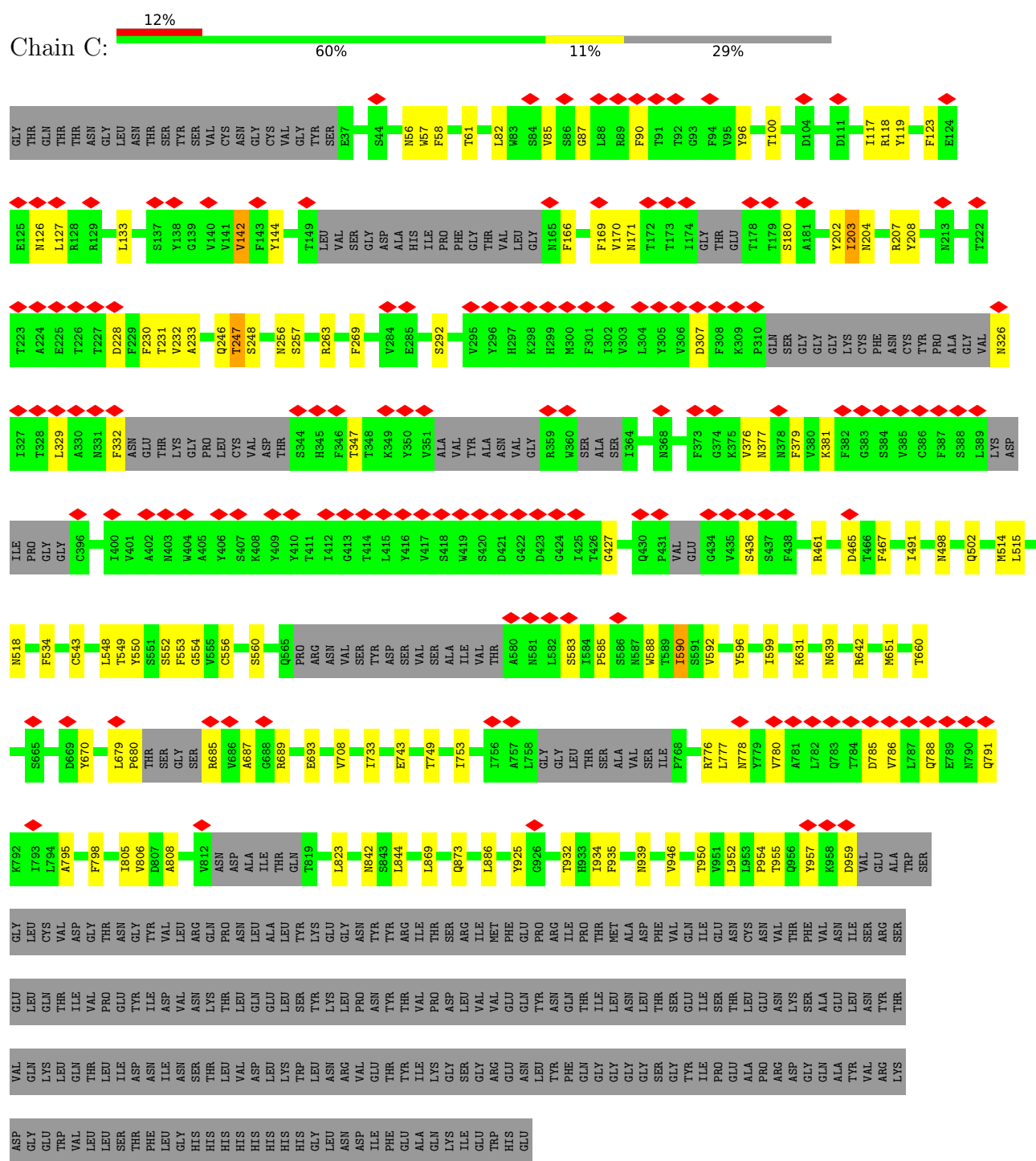
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5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

3 Residue-property plots

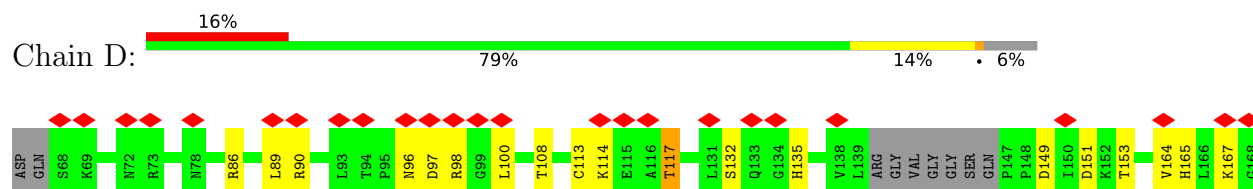
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

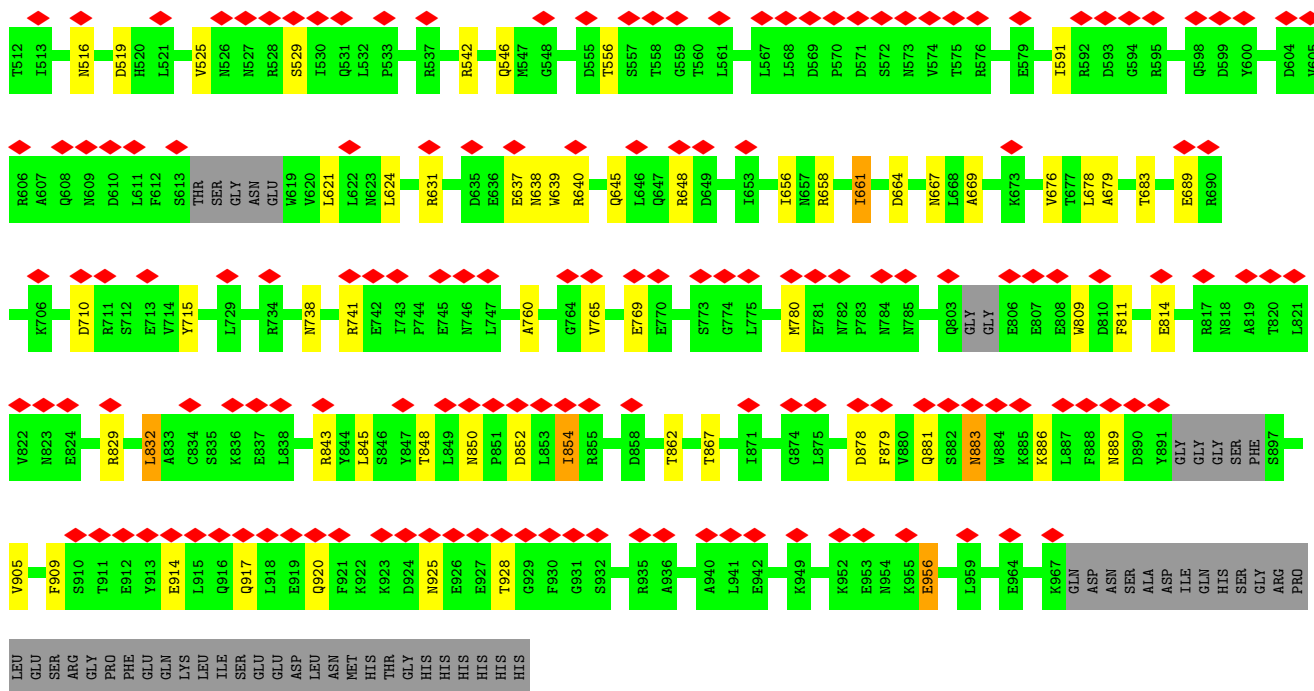




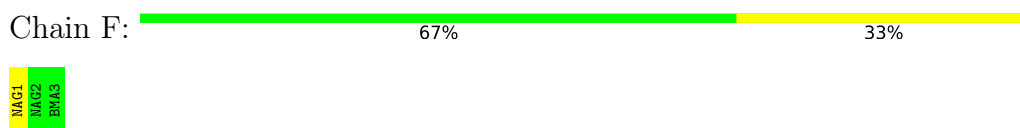
- Molecule 2: Aminopeptidase N



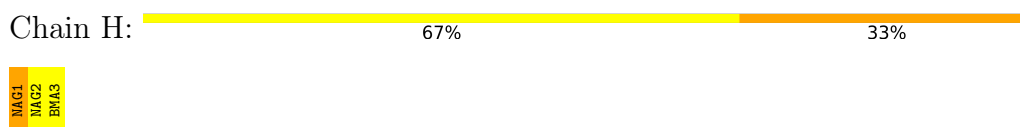




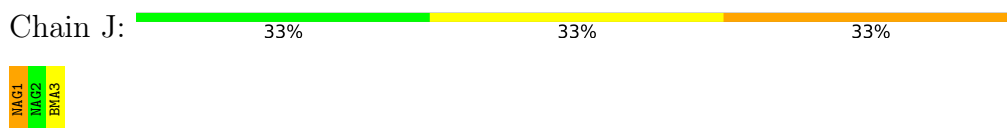
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





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

Chain I:  100%



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

Chain K:  50% 50%



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

Chain L:  50% 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	253164	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	83.063	Depositor
Minimum map value	-34.767	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	0.853	Depositor
Recommended contour level	18	Depositor
Map size (Å)	885.60004, 885.60004, 885.60004	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4760001, 1.4760001, 1.4760001	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, BMA

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	0.40	0/6797	0.53	0/9249
1	B	0.40	0/6523	0.49	0/8869
1	C	0.44	0/6537	0.53	0/8891
2	D	0.41	0/7347	0.49	0/10005
2	E	0.34	0/6361	0.48	0/8654
All	All	0.40	0/33565	0.50	0/45668

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	338	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6661	0	6513	92	0
1	B	6398	0	6268	74	0
1	C	6410	0	6276	71	0
2	D	7163	0	6942	87	0
2	E	6207	0	6016	63	0
3	F	39	0	34	0	0
3	H	39	0	34	2	0
3	J	39	0	34	1	0
4	G	28	0	25	0	0
4	I	28	0	25	1	0
4	K	28	0	25	1	0
4	L	28	0	25	1	0
5	A	70	0	65	0	0
5	B	70	0	65	2	0
5	C	84	0	78	2	0
5	D	42	0	39	1	0
5	E	14	0	13	0	0
All	All	33348	0	32477	380	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 6.

The worst 5 of 380 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:90:ARG:HG2	2:D:238:ILE:HB	1.62	0.80
1:C:556:CYS:SG	1:C:560:SER:OG	2.40	0.78
1:C:585:PRO:HA	1:C:957:TYR:HA	1.69	0.75
1:C:379:PHE:O	1:C:381:LYS:NZ	2.19	0.75
1:B:652:LEU:O	1:B:744:ARG:NH2	2.20	0.73

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	846/1165 (73%)	795 (94%)	46 (5%)	5 (1%)	21	54
1	B	796/1165 (68%)	755 (95%)	40 (5%)	1 (0%)	48	79
1	C	802/1165 (69%)	753 (94%)	46 (6%)	3 (0%)	30	61
2	D	873/943 (93%)	835 (96%)	37 (4%)	1 (0%)	48	79
2	E	736/943 (78%)	699 (95%)	33 (4%)	4 (0%)	24	57
All	All	4053/5381 (75%)	3837 (95%)	202 (5%)	14 (0%)	37	65

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	338	LEU
1	A	943	GLU
1	B	541	TYR
2	E	214	ALA
2	E	339	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	746/1007 (74%)	729 (98%)	17 (2%)	44	64
1	B	718/1007 (71%)	704 (98%)	14 (2%)	50	67
1	C	719/1007 (71%)	703 (98%)	16 (2%)	45	65
2	D	790/837 (94%)	770 (98%)	20 (2%)	42	63
2	E	684/837 (82%)	666 (97%)	18 (3%)	40	62
All	All	3657/4695 (78%)	3572 (98%)	85 (2%)	44	64

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	771	MET

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Mol	Chain	Res	Type
2	E	356	ASN
2	D	785	ASN
2	D	887	LEU
2	E	661	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	75	GLN
2	E	785	ASN
1	C	839	GLN
2	E	720	ASN
1	C	430	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 ⓘ

17 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	F	1	3,1	14,14,15	0.96	1 (7%)	17,19,21	0.84	0
3	NAG	F	2	3	14,14,15	0.58	0	17,19,21	0.39	0
3	BMA	F	3	3	11,11,12	0.65	0	15,15,17	0.71	0
4	NAG	G	1	4,1	14,14,15	0.28	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	0.61	0
3	NAG	H	1	3,1	14,14,15	1.25	1 (7%)	17,19,21	0.73	0
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	0.42	0
3	BMA	H	3	3	11,11,12	0.68	0	15,15,17	1.13	2 (13%)
4	NAG	I	1	4,1	14,14,15	0.60	1 (7%)	17,19,21	0.57	0
4	NAG	I	2	4	14,14,15	0.27	0	17,19,21	0.78	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.59	0	17,19,21	0.80	1 (5%)
3	NAG	J	2	3	14,14,15	0.15	0	17,19,21	0.60	0
3	BMA	J	3	3	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
4	NAG	K	1	4,1	14,14,15	0.49	0	17,19,21	0.73	1 (5%)
4	NAG	K	2	4	14,14,15	0.51	0	17,19,21	0.57	0
4	NAG	L	1	4	14,14,15	1.00	1 (7%)	17,19,21	0.53	0
4	NAG	L	2	4	14,14,15	0.27	0	17,19,21	0.88	1 (5%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-4.56	1.36	1.43
3	F	1	NAG	O5-C1	-3.55	1.37	1.43
4	L	1	NAG	O5-C1	-3.53	1.37	1.43
4	I	1	NAG	O5-C1	-2.06	1.40	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	3.31	116.62	112.19
4	L	2	NAG	C1-O5-C5	3.10	116.33	112.19
4	I	2	NAG	C1-O5-C5	2.93	116.11	112.19
3	J	3	BMA	C1-O5-C5	2.80	115.94	112.19
3	J	1	NAG	C1-O5-C5	2.57	115.62	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

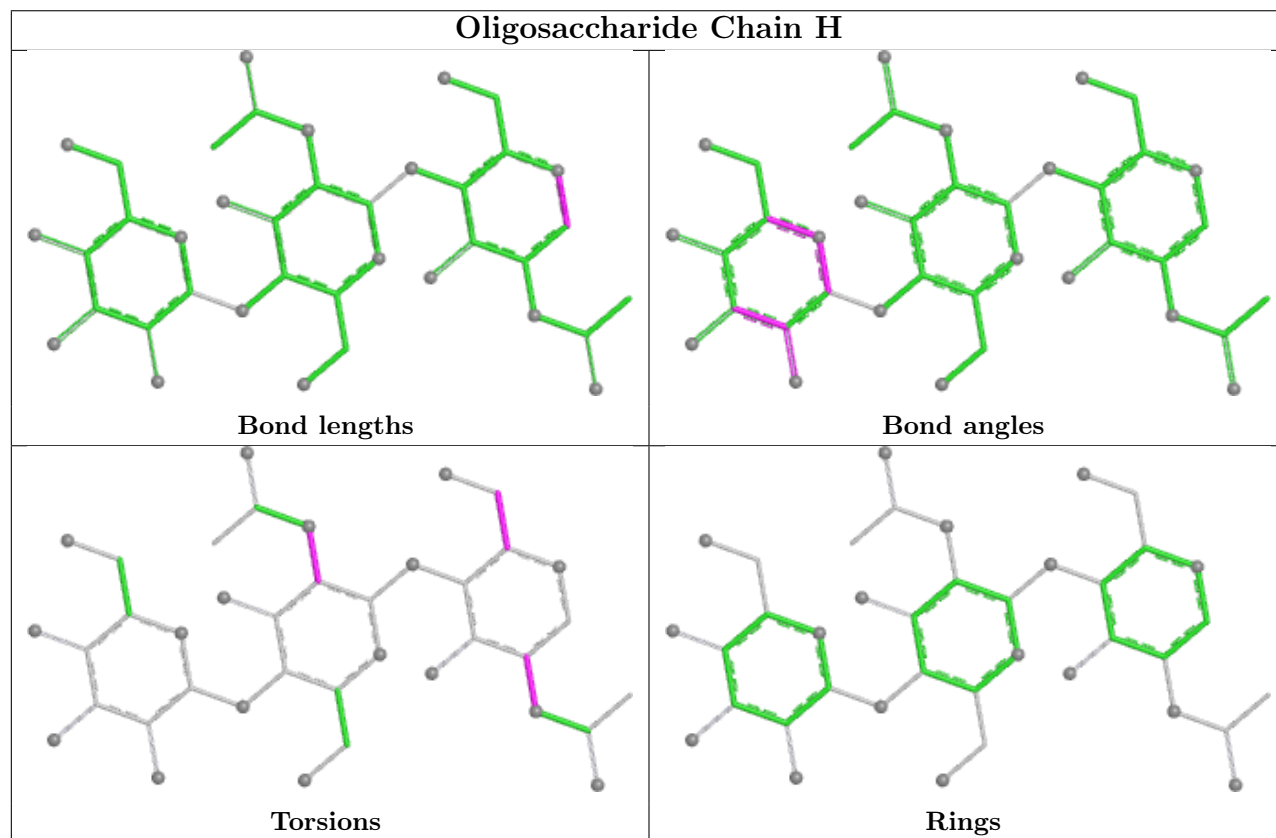
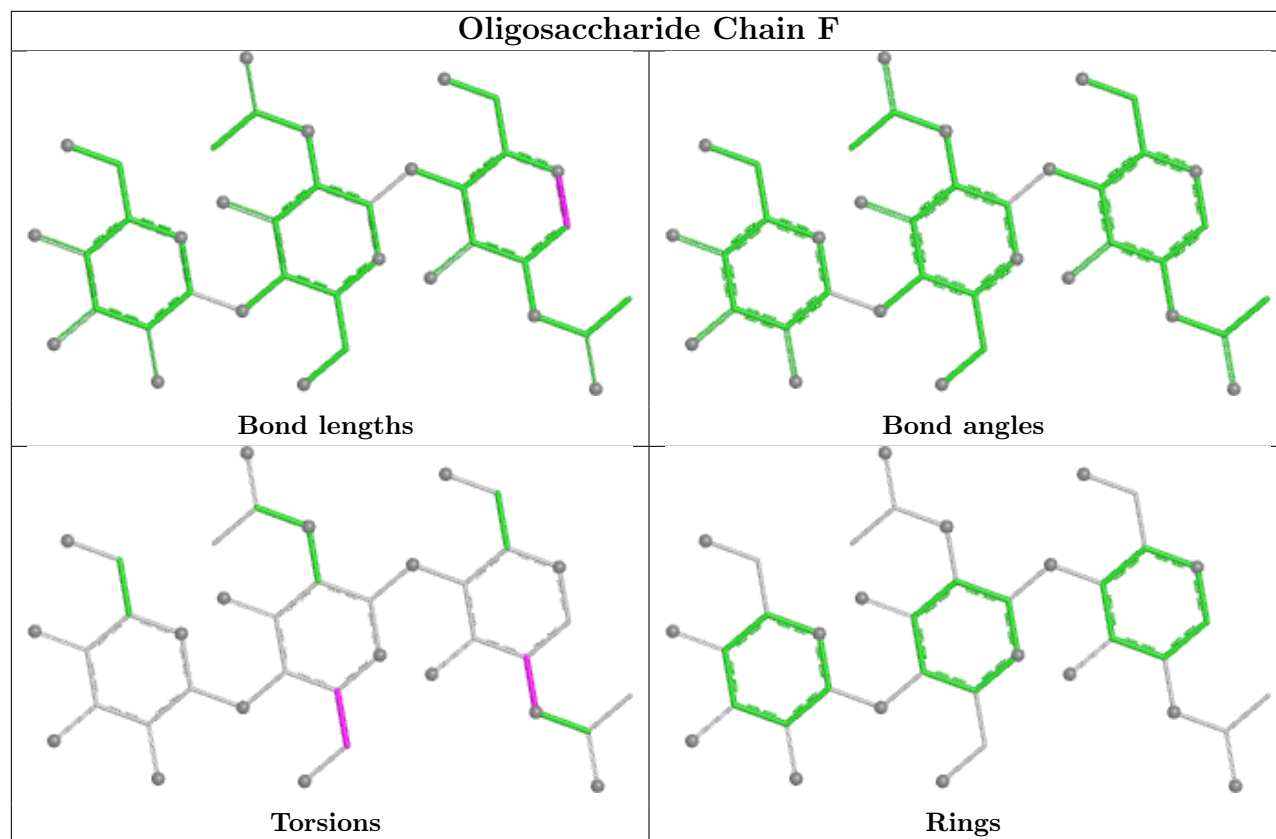
Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6

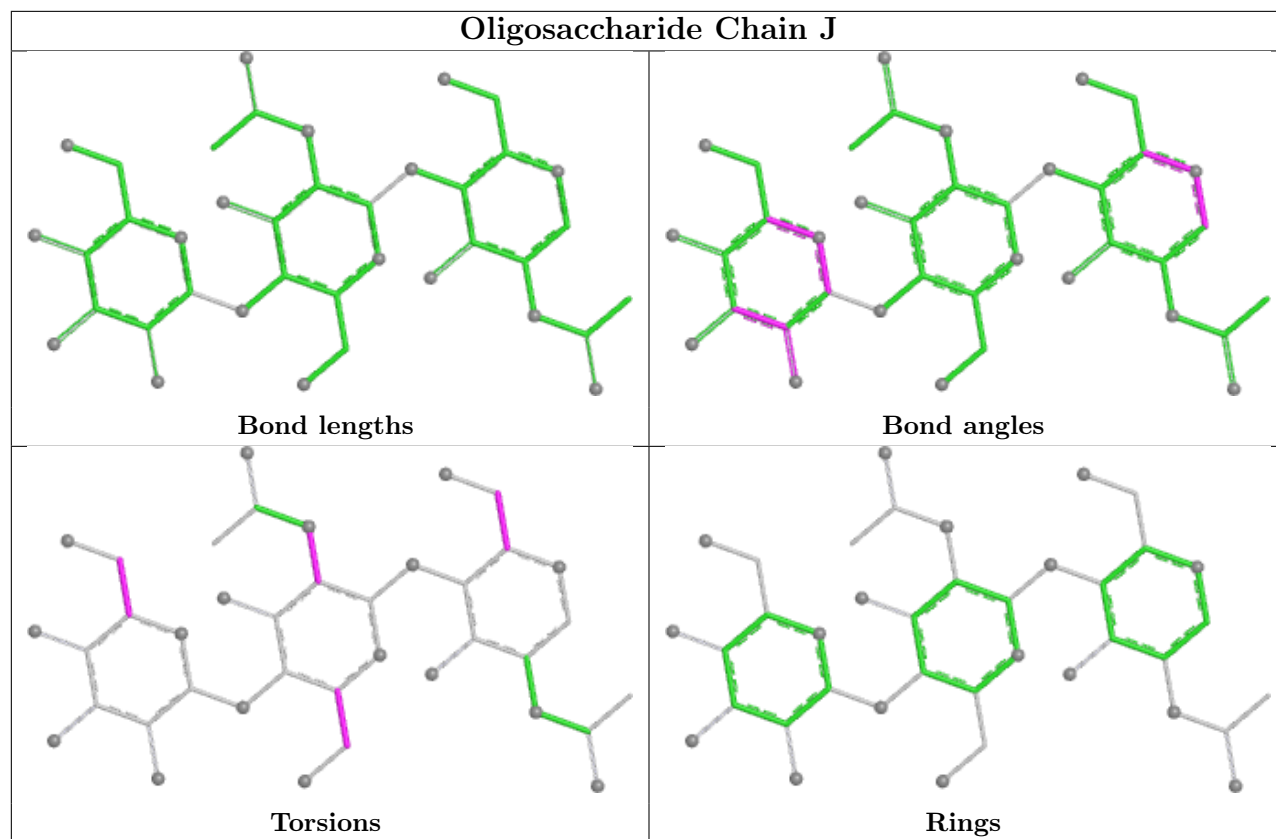
There are no ring outliers.

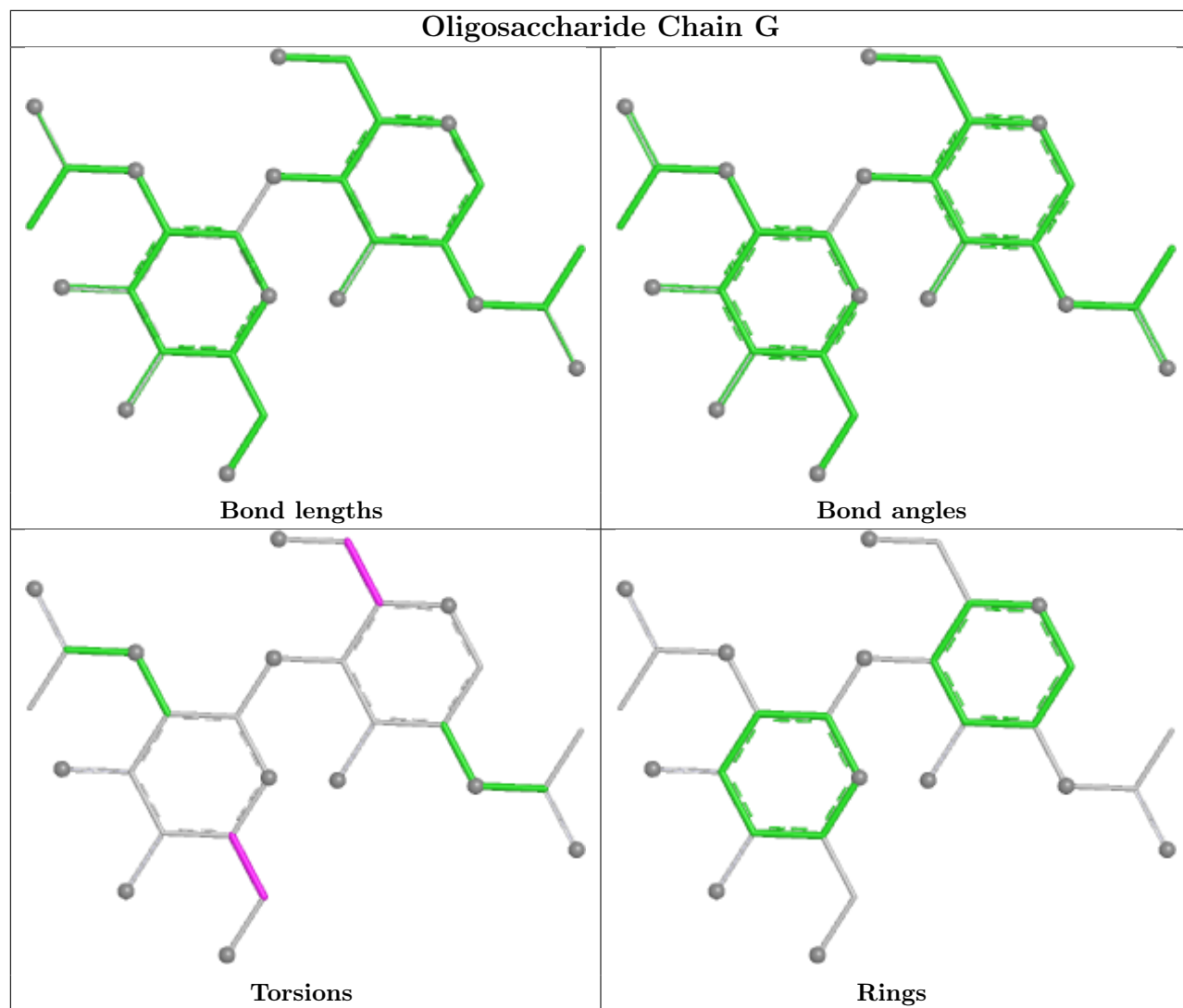
8 monomers are involved in 6 short contacts:

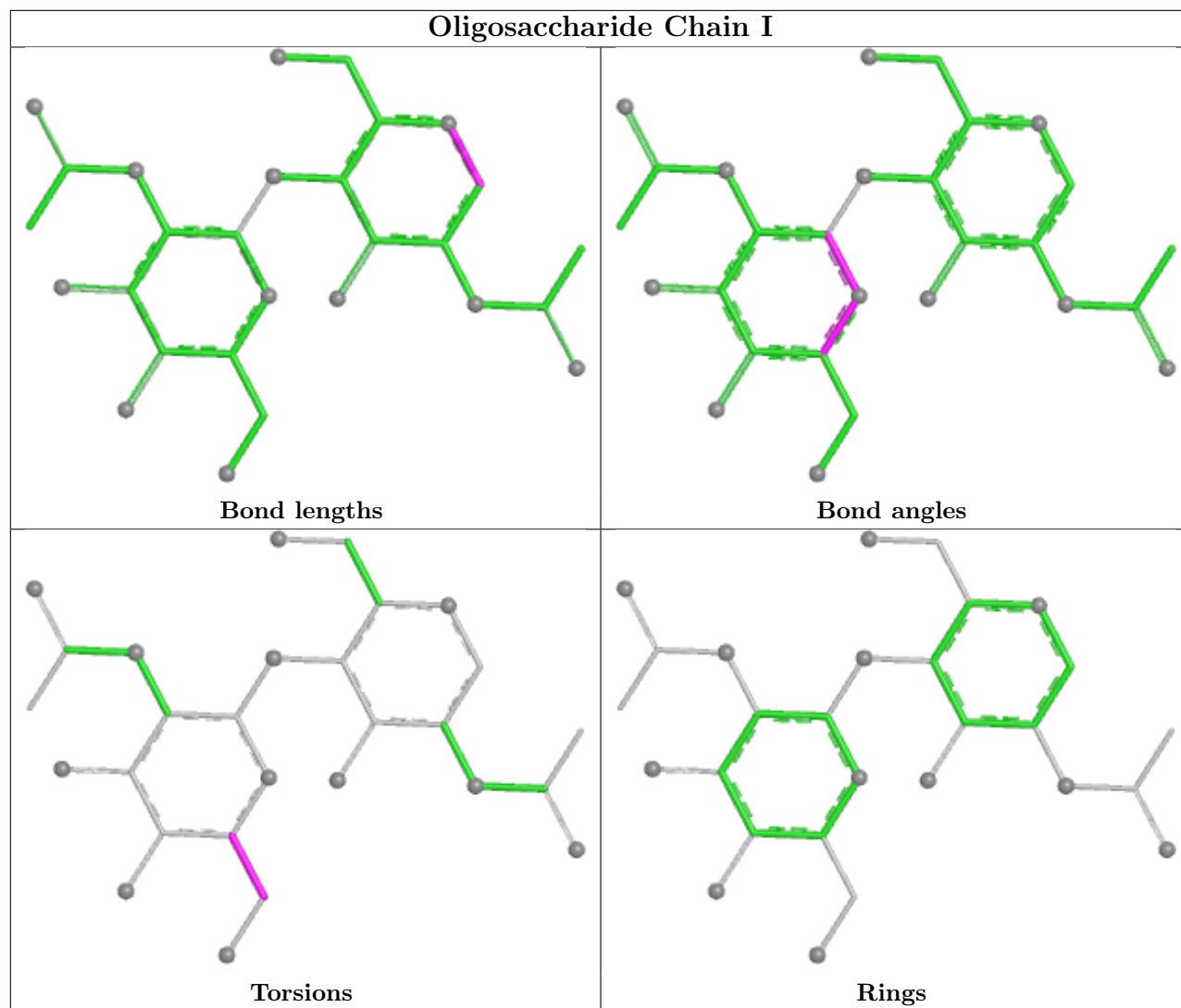
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
4	L	1	NAG	1	0
3	J	1	NAG	1	0
4	I	1	NAG	1	0
4	K	1	NAG	1	0
4	I	2	NAG	1	0
3	H	2	NAG	1	0
4	K	2	NAG	1	0

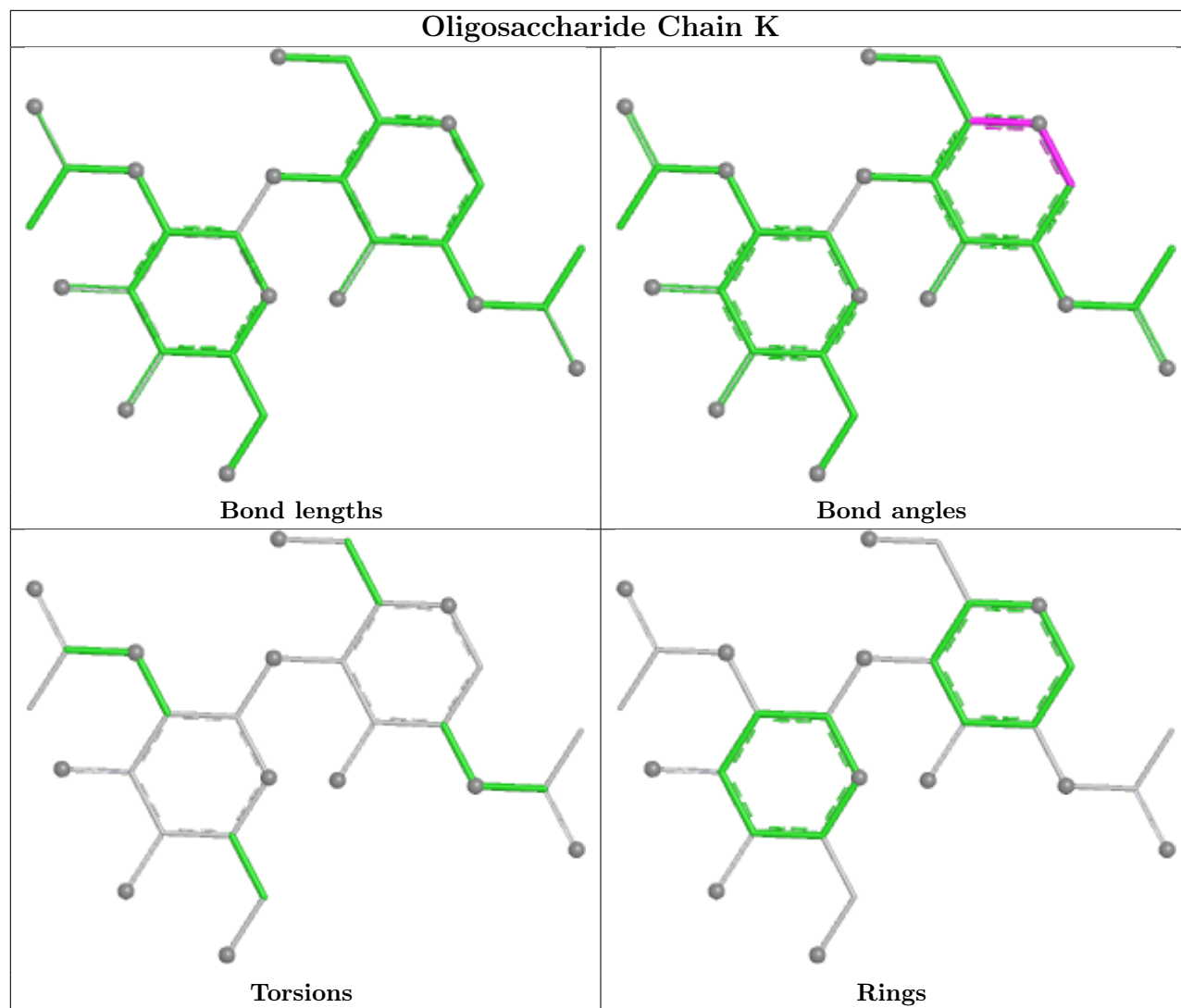
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

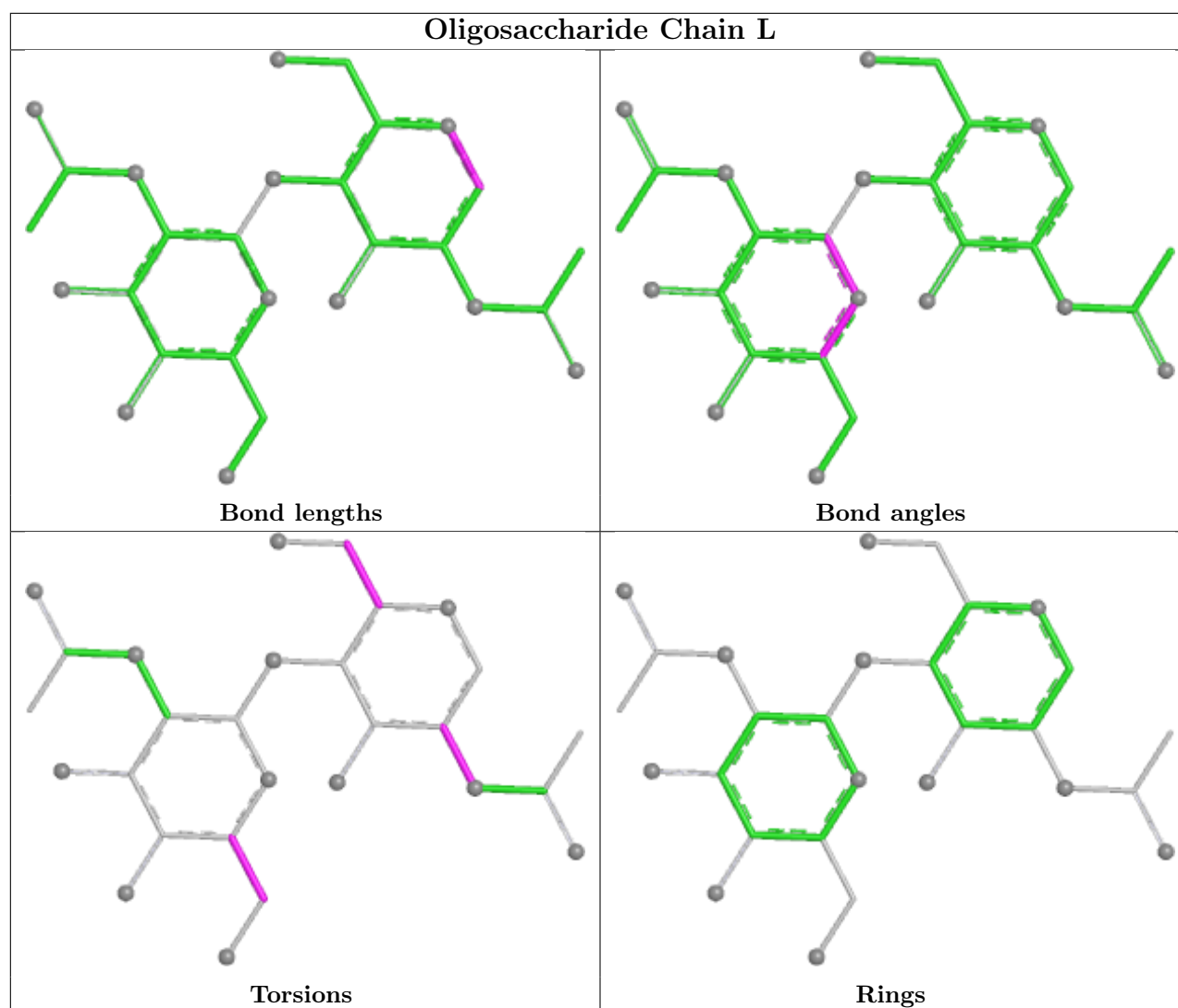












5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1201	1	14,14,15	0.75	1 (7%)	17,19,21	0.68	1 (5%)
5	NAG	C	1203	1	14,14,15	0.43	0	17,19,21	0.64	1 (5%)
5	NAG	C	1201	1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1205	1	14,14,15	0.35	0	17,19,21	0.48	0
5	NAG	A	1202	1	14,14,15	0.18	0	17,19,21	0.90	1 (5%)
5	NAG	D	1103	2	14,14,15	0.26	0	17,19,21	0.77	1 (5%)
5	NAG	C	1206	1	14,14,15	0.33	0	17,19,21	0.62	0
5	NAG	A	1203	1	14,14,15	0.45	0	17,19,21	0.74	1 (5%)
5	NAG	E	1101	2	14,14,15	0.38	0	17,19,21	0.94	1 (5%)
5	NAG	B	1203	1	14,14,15	0.22	0	17,19,21	0.74	1 (5%)
5	NAG	A	1201	1	14,14,15	0.14	0	17,19,21	0.49	0
5	NAG	C	1202	1	14,14,15	0.37	0	17,19,21	0.35	0
5	NAG	C	1204	1	14,14,15	0.22	0	17,19,21	0.78	1 (5%)
5	NAG	B	1202	1	14,14,15	0.21	0	17,19,21	0.49	0
5	NAG	C	1205	1	14,14,15	0.28	0	17,19,21	0.55	0
5	NAG	D	1101	2	14,14,15	0.99	1 (7%)	17,19,21	0.82	0
5	NAG	D	1102	2	14,14,15	0.20	0	17,19,21	0.56	0
5	NAG	B	1205	1	14,14,15	0.37	0	17,19,21	0.62	0
5	NAG	A	1204	1	14,14,15	0.58	1 (7%)	17,19,21	0.40	0
5	NAG	B	1204	1	14,14,15	0.28	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1103	2	-	1/6/23/26	0/1/1/1
5	NAG	C	1206	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1101	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1203	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1204	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1205	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	1101	2	-	1/6/23/26	0/1/1/1
5	NAG	D	1102	2	-	4/6/23/26	0/1/1/1
5	NAG	B	1205	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1204	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1101	NAG	C1-C2	3.32	1.56	1.52
5	B	1201	NAG	C1-C2	2.48	1.55	1.52
5	A	1204	NAG	O5-C1	-2.09	1.40	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1101	NAG	C1-O5-C5	3.64	117.06	112.19
5	A	1202	NAG	C1-O5-C5	3.32	116.64	112.19
5	D	1103	NAG	C1-O5-C5	2.89	116.05	112.19
5	C	1204	NAG	C1-O5-C5	2.55	115.61	112.19
5	B	1201	NAG	C1-O5-C5	2.30	115.27	112.19

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1101	NAG	C1-C2-N2-C7
5	A	1201	NAG	O5-C5-C6-O6
5	A	1205	NAG	C4-C5-C6-O6
5	B	1201	NAG	C4-C5-C6-O6
5	C	1204	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

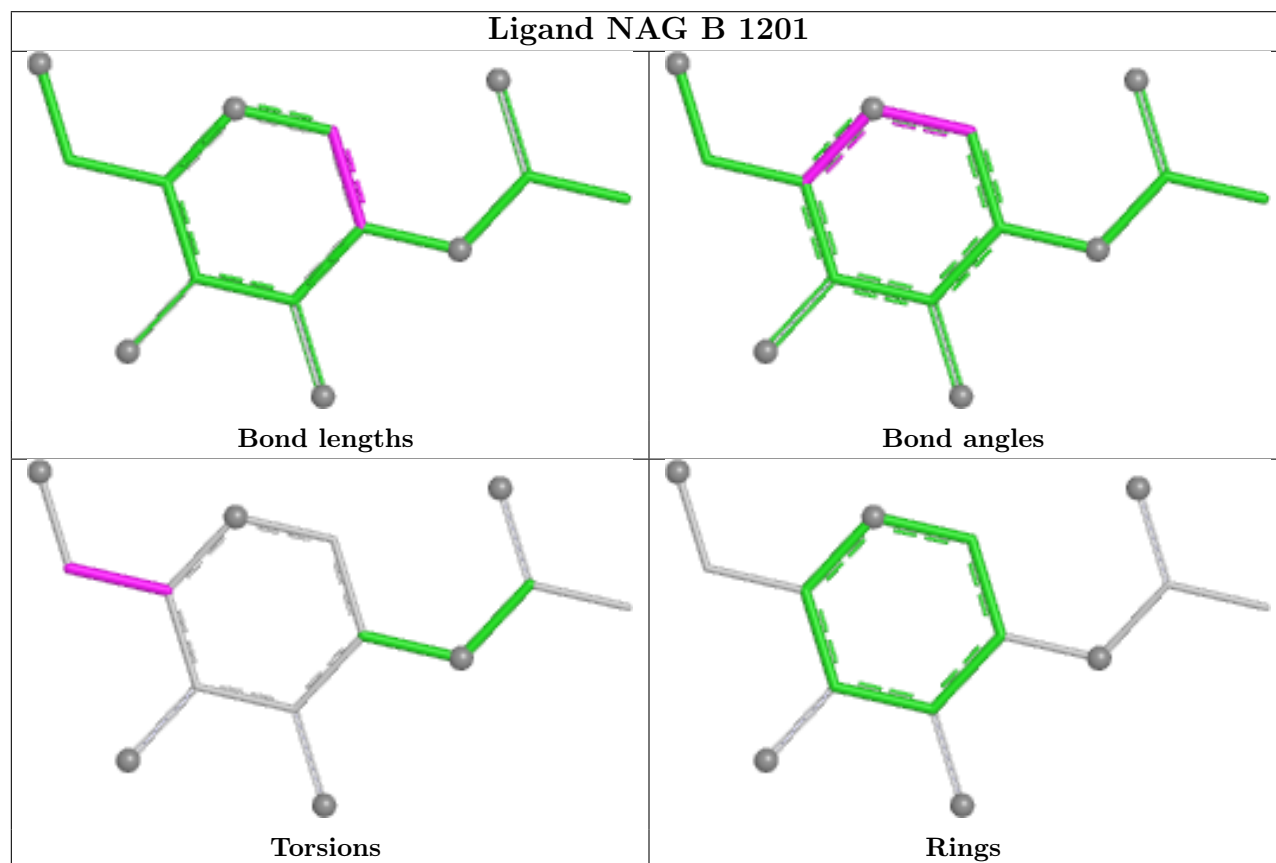
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	NAG	1	0
5	C	1201	NAG	1	0
5	B	1203	NAG	1	0
5	C	1202	NAG	1	0

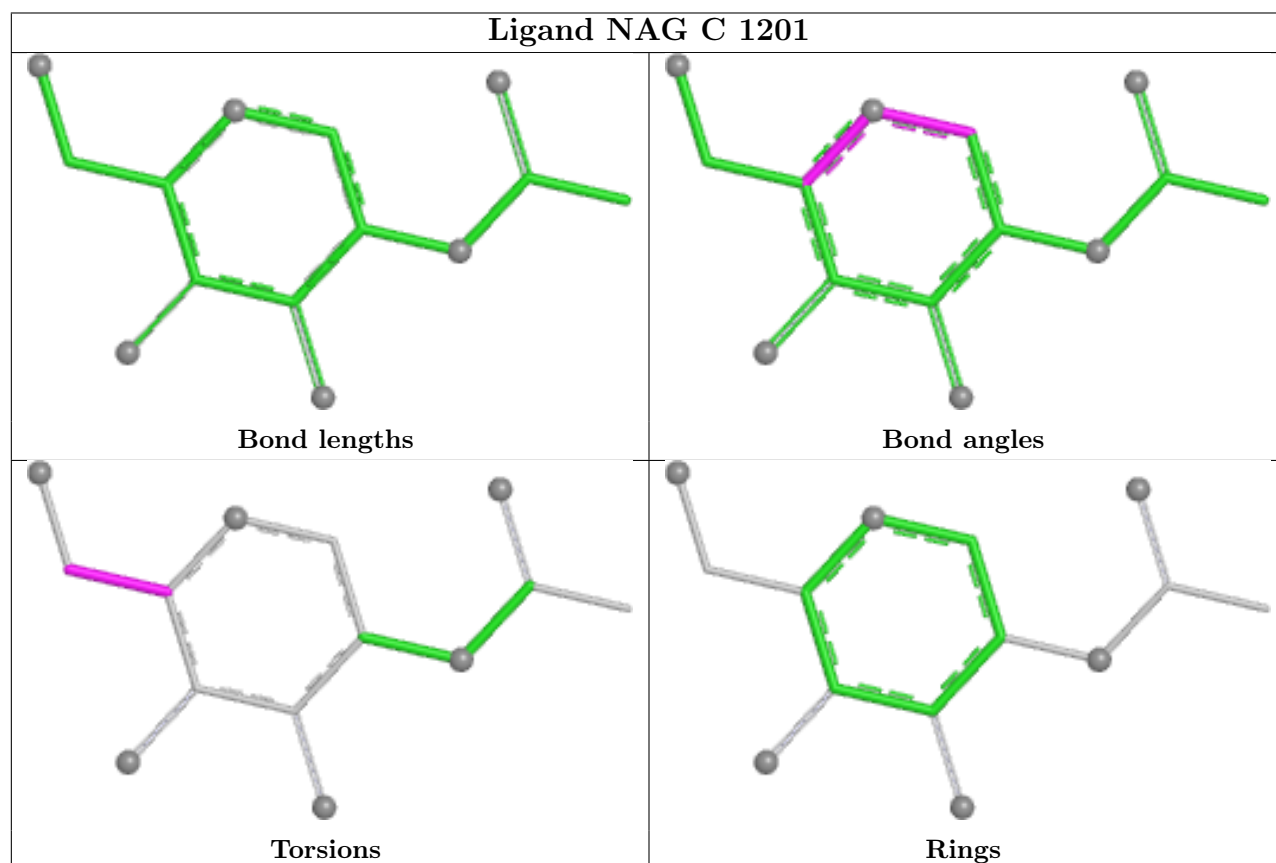
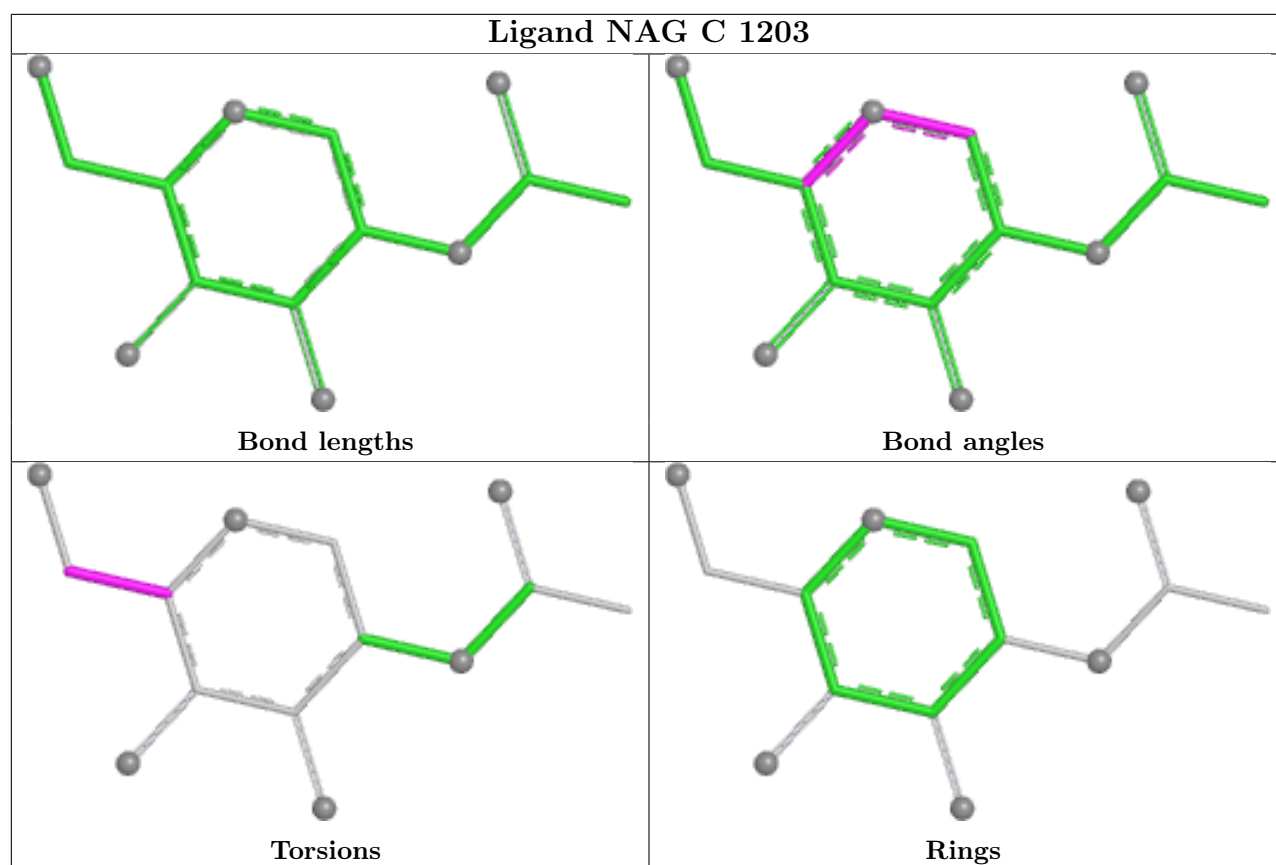
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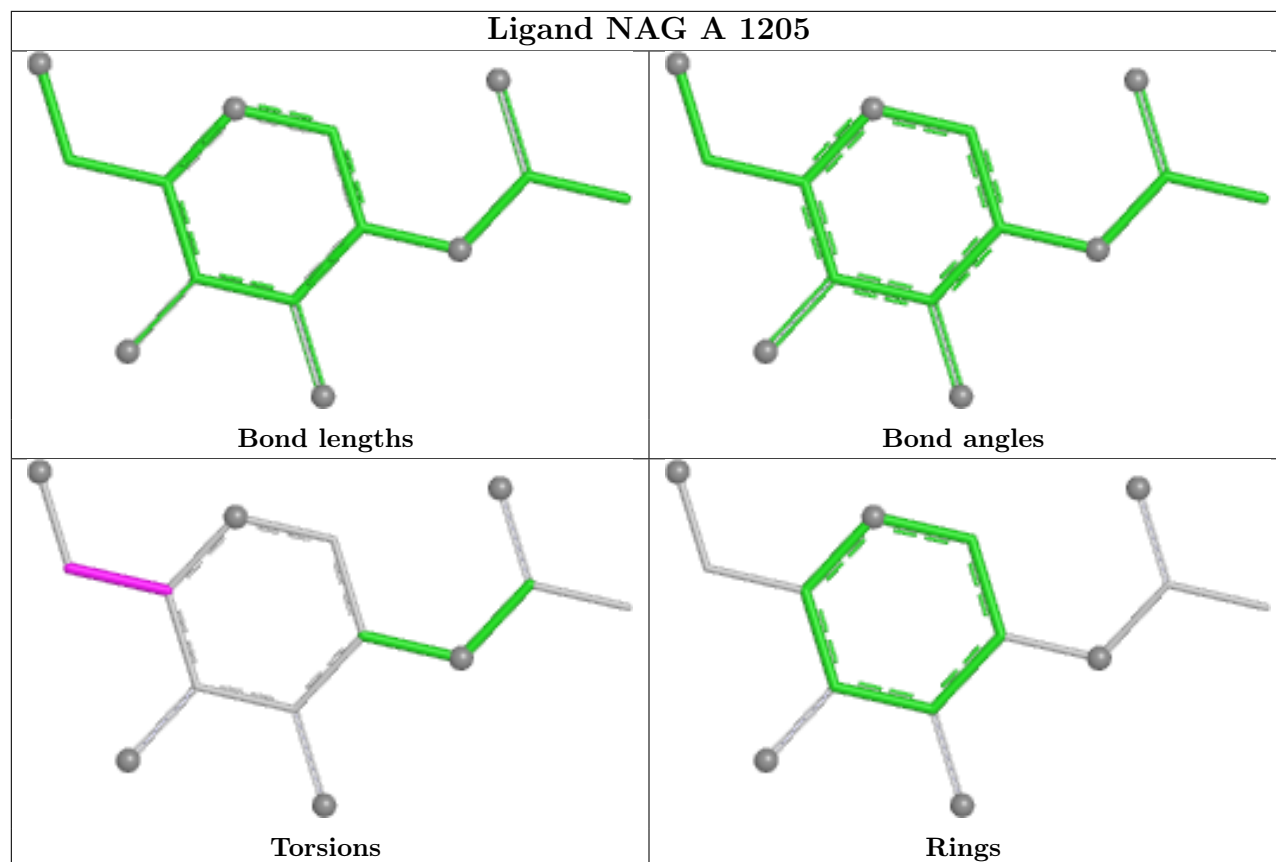
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1101	NAG	1	0

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.

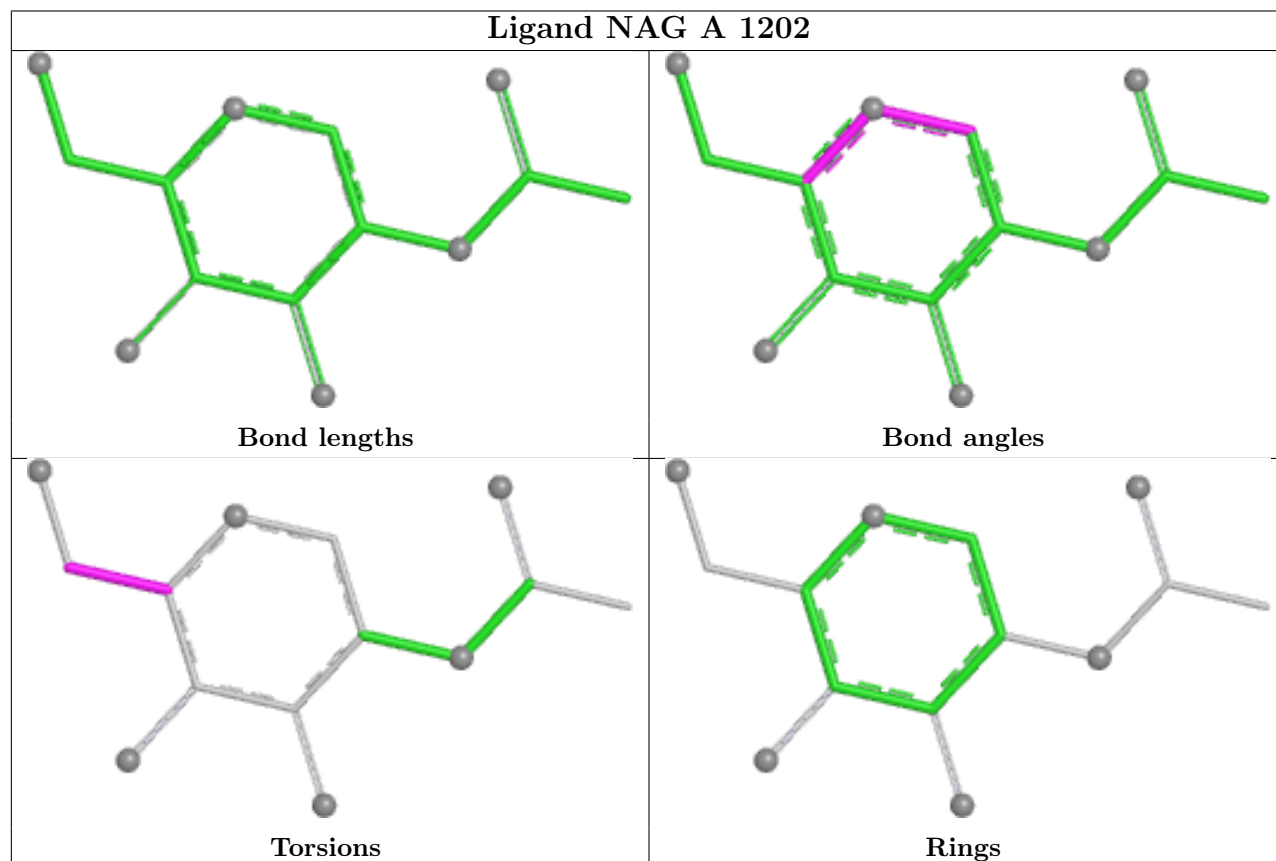




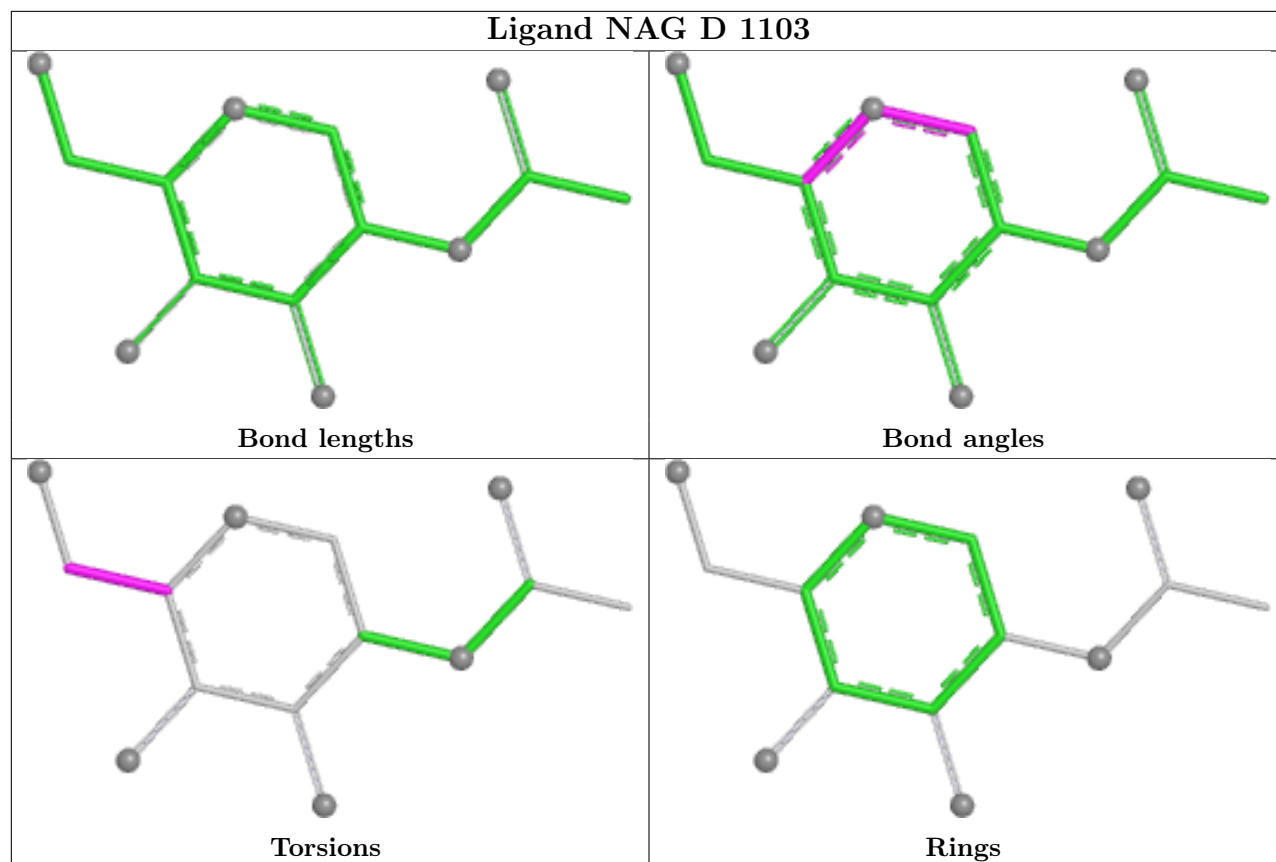
Ligand NAG A 1205



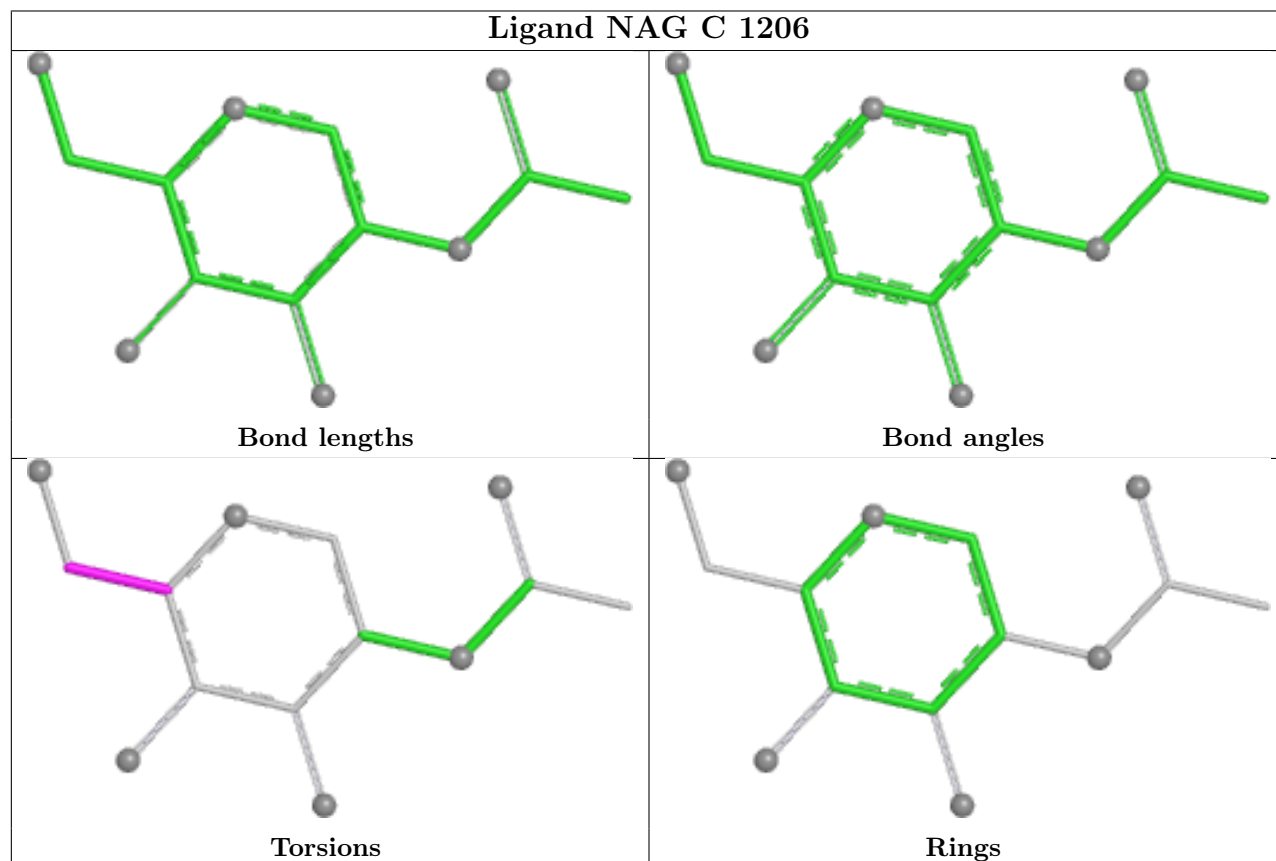
Ligand NAG A 1202



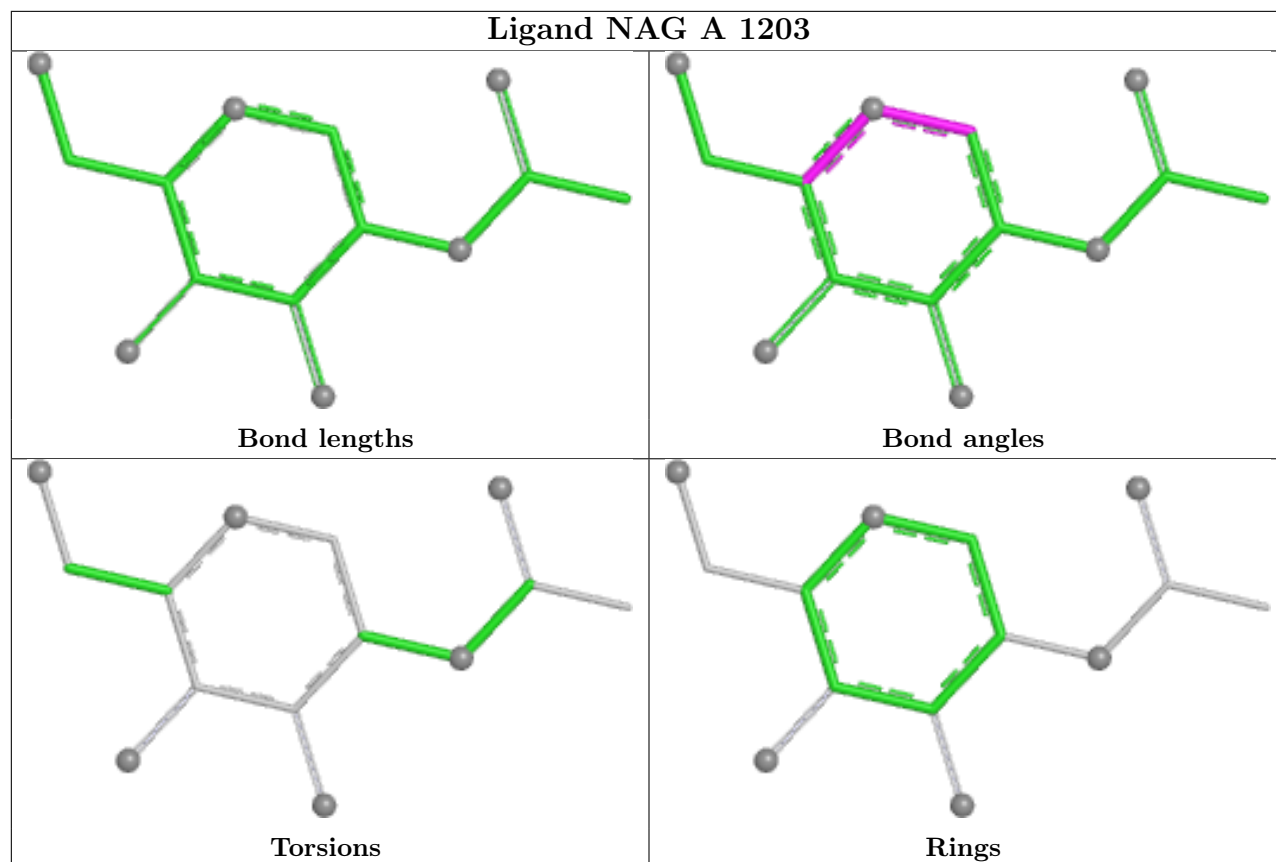
Ligand NAG D 1103



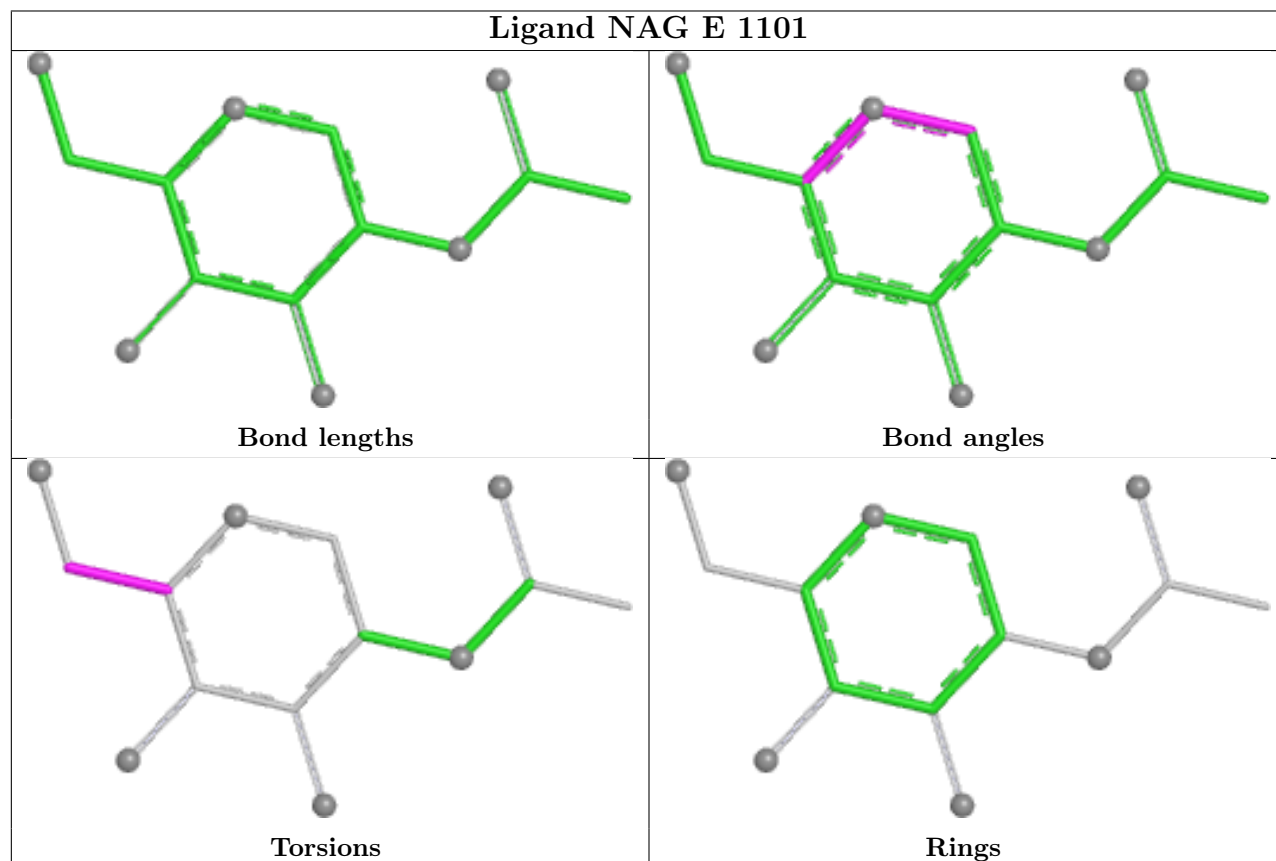
Ligand NAG C 1206



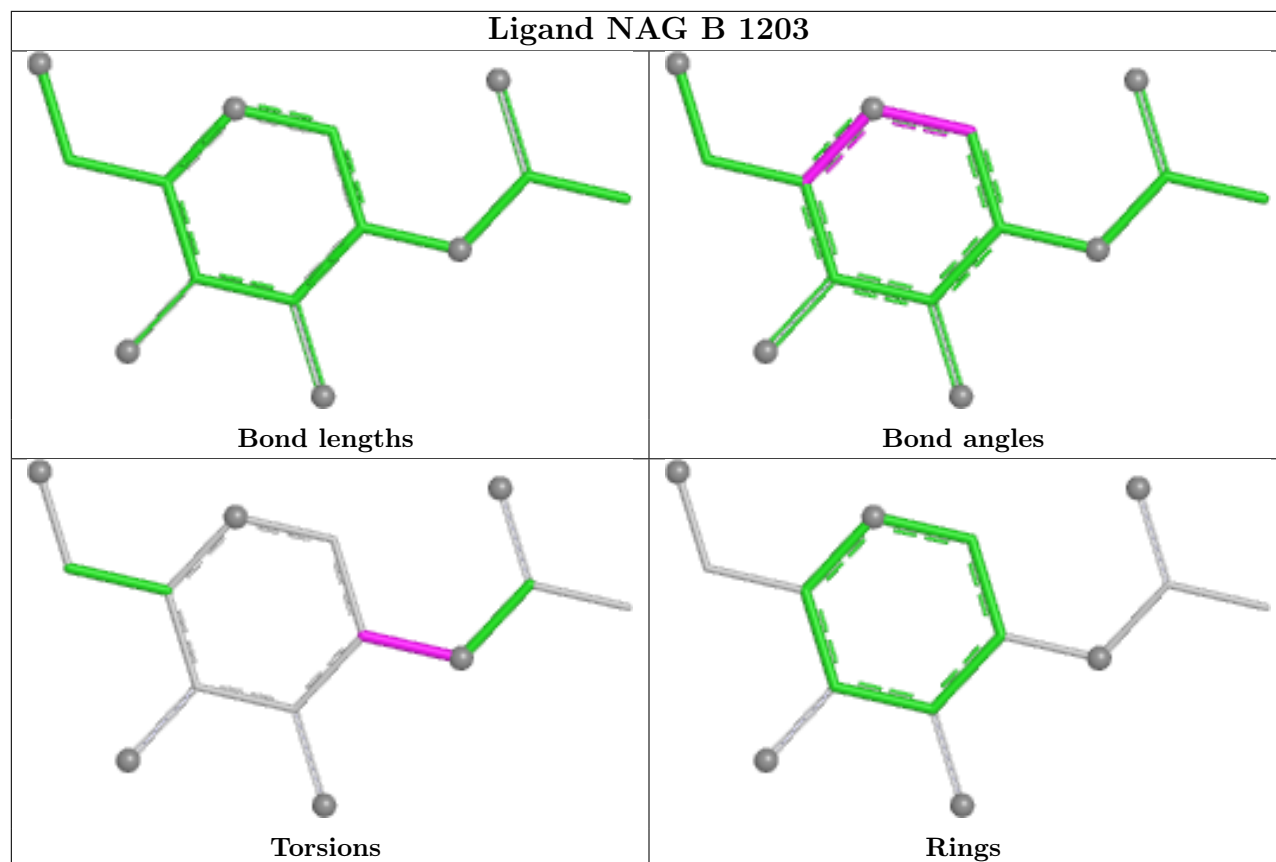
Ligand NAG A 1203



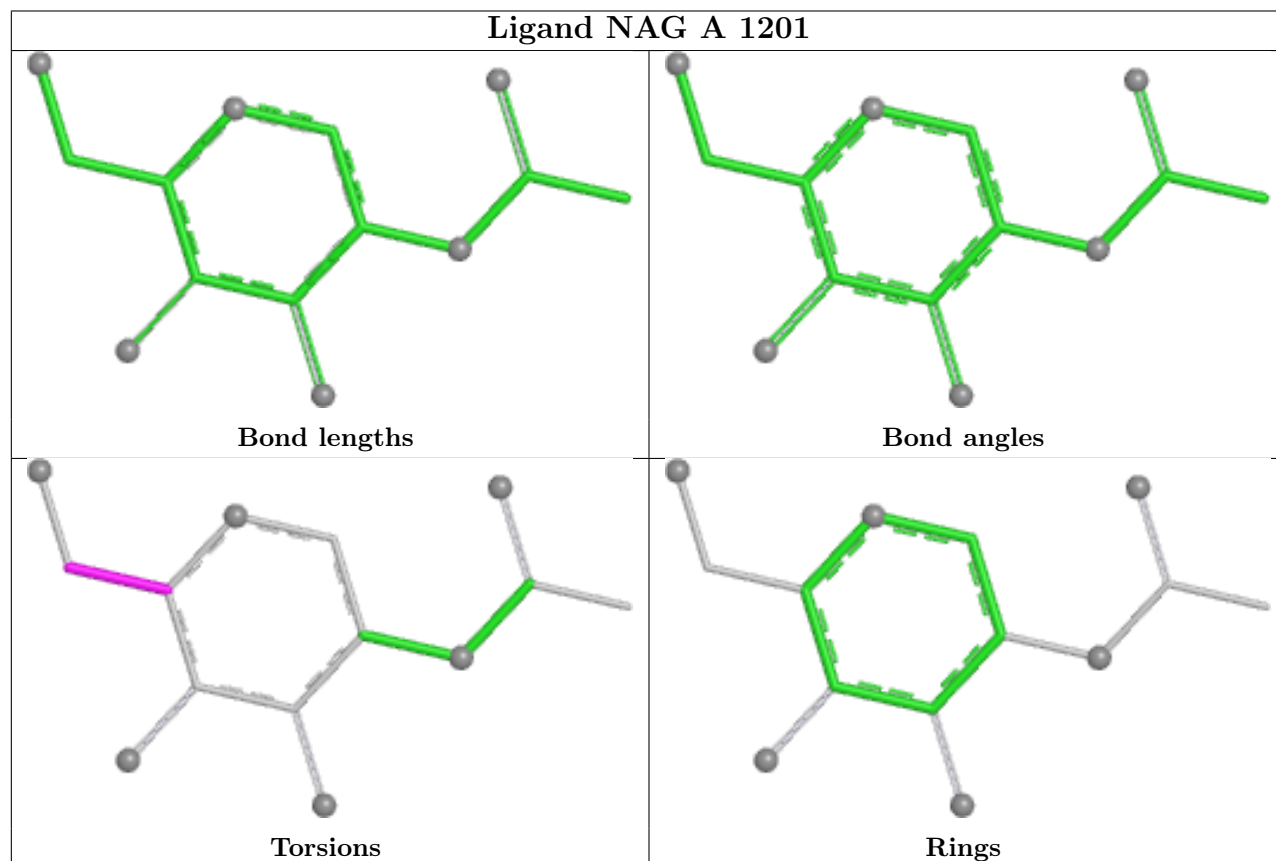
Ligand NAG E 1101



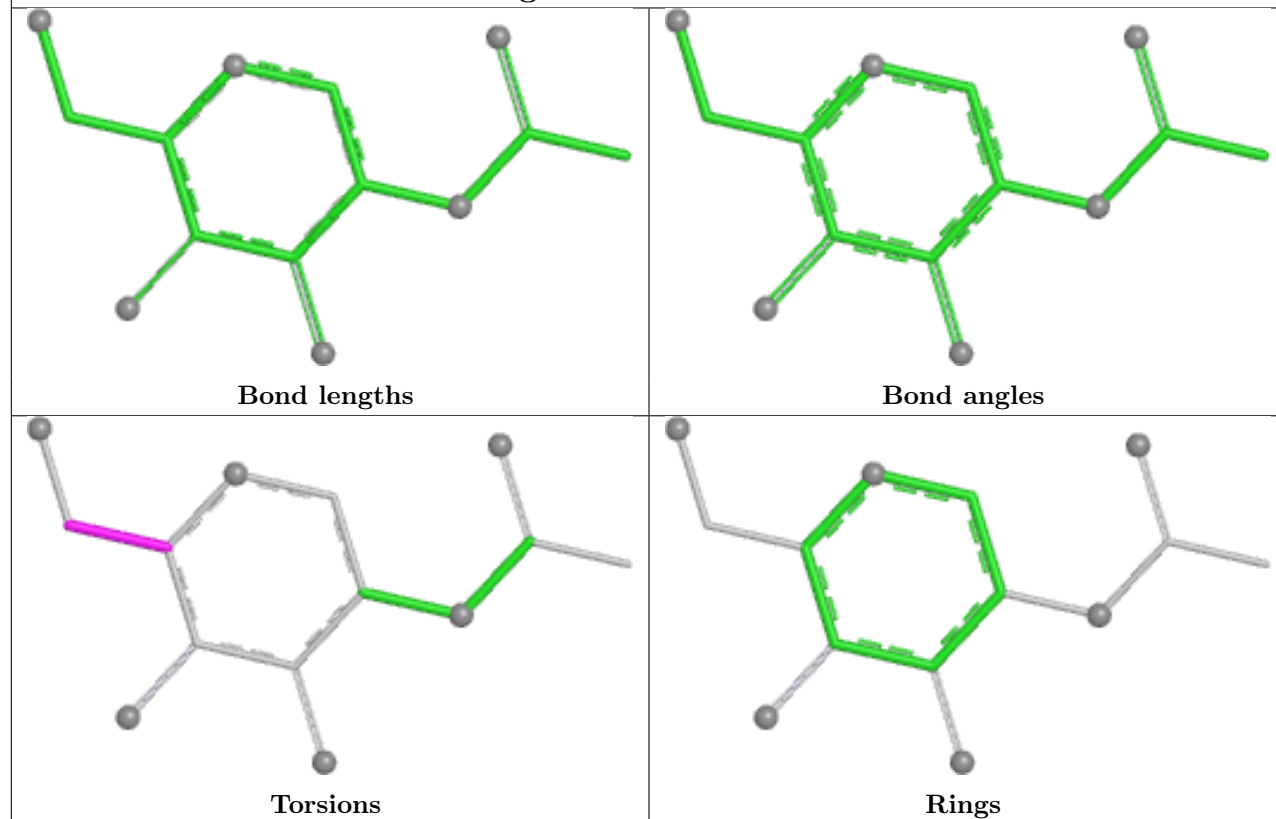
Ligand NAG B 1203



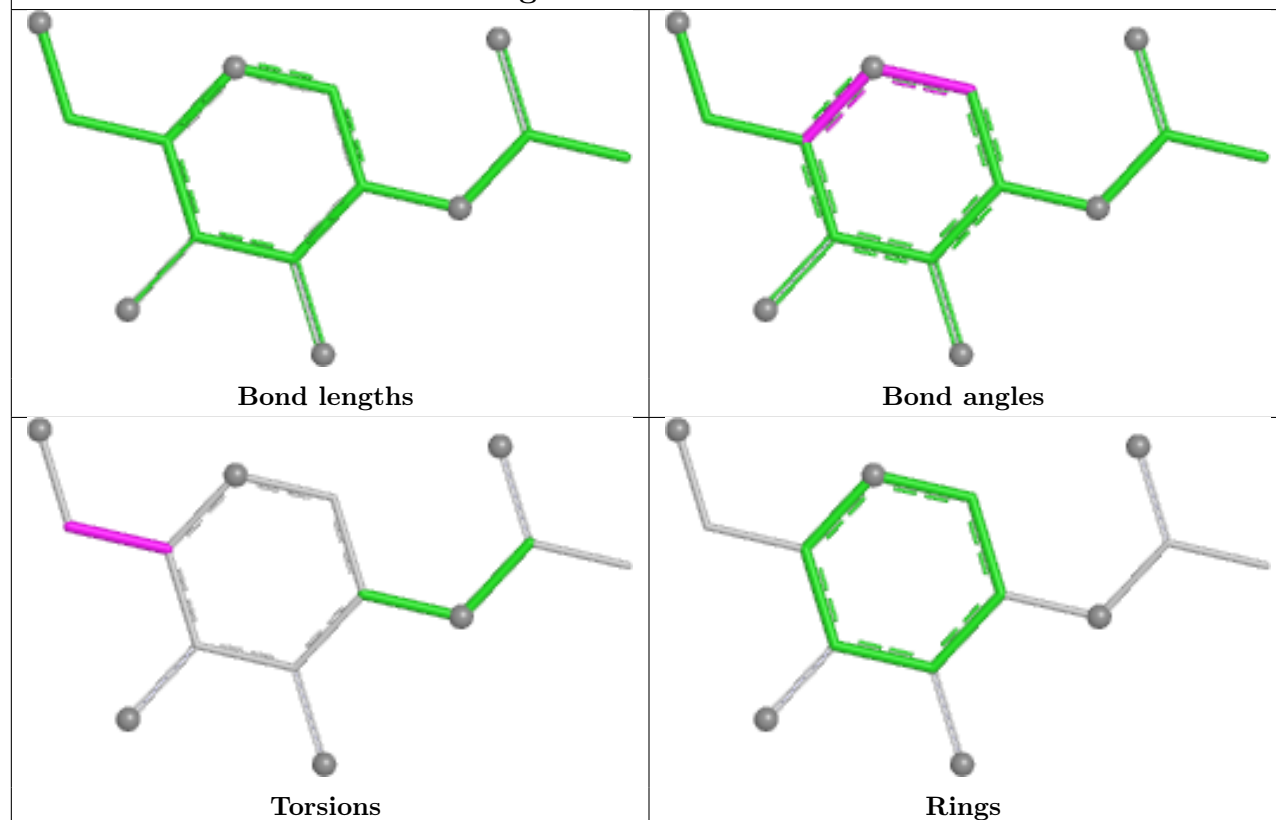
Ligand NAG A 1201



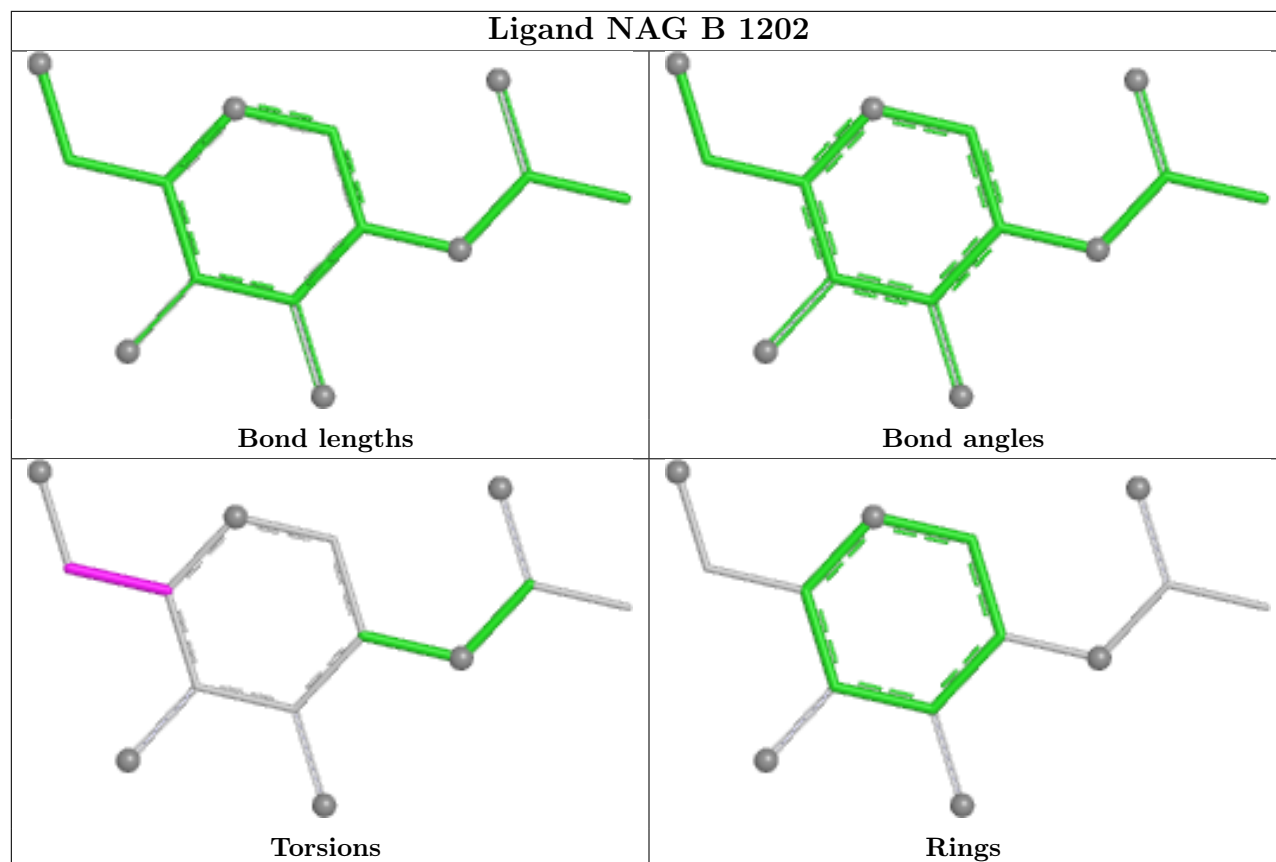
Ligand NAG C 1202



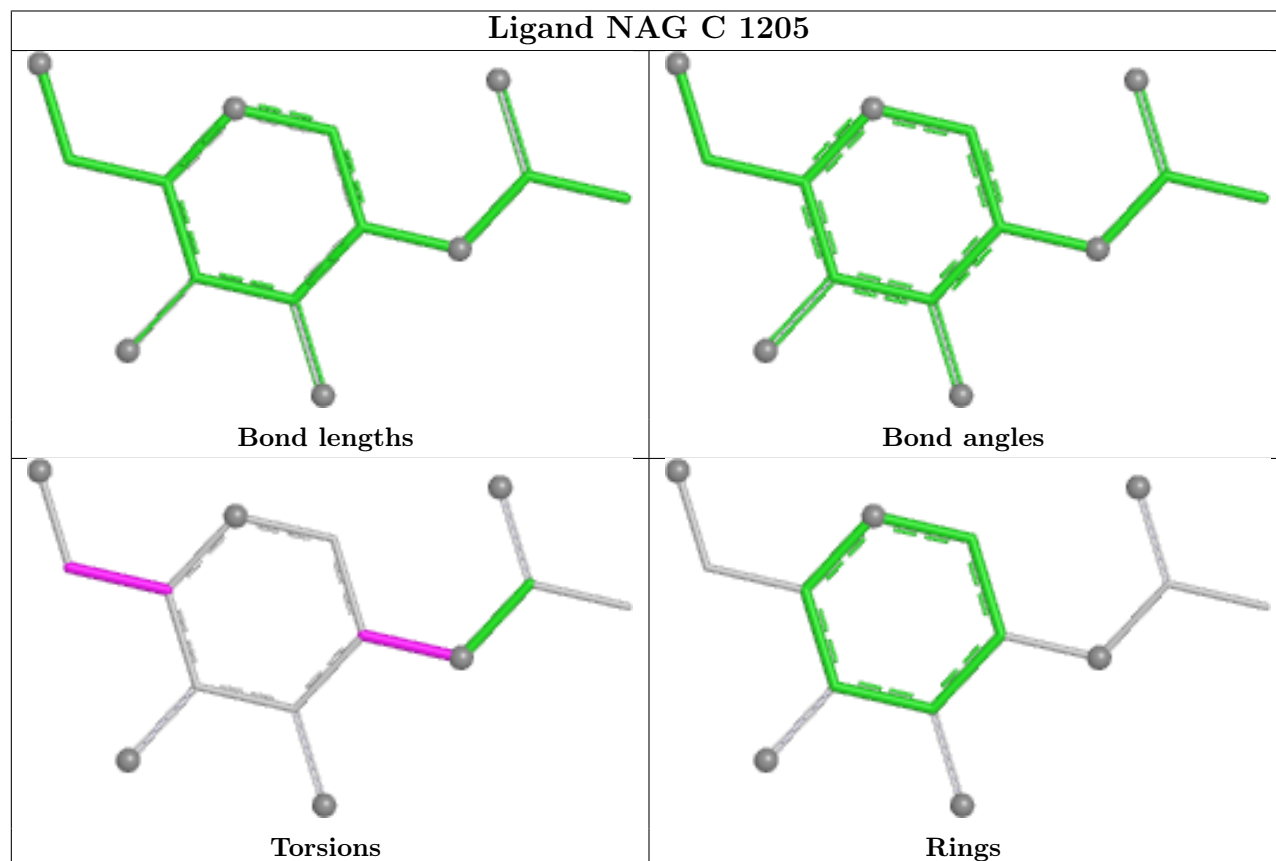
Ligand NAG C 1204



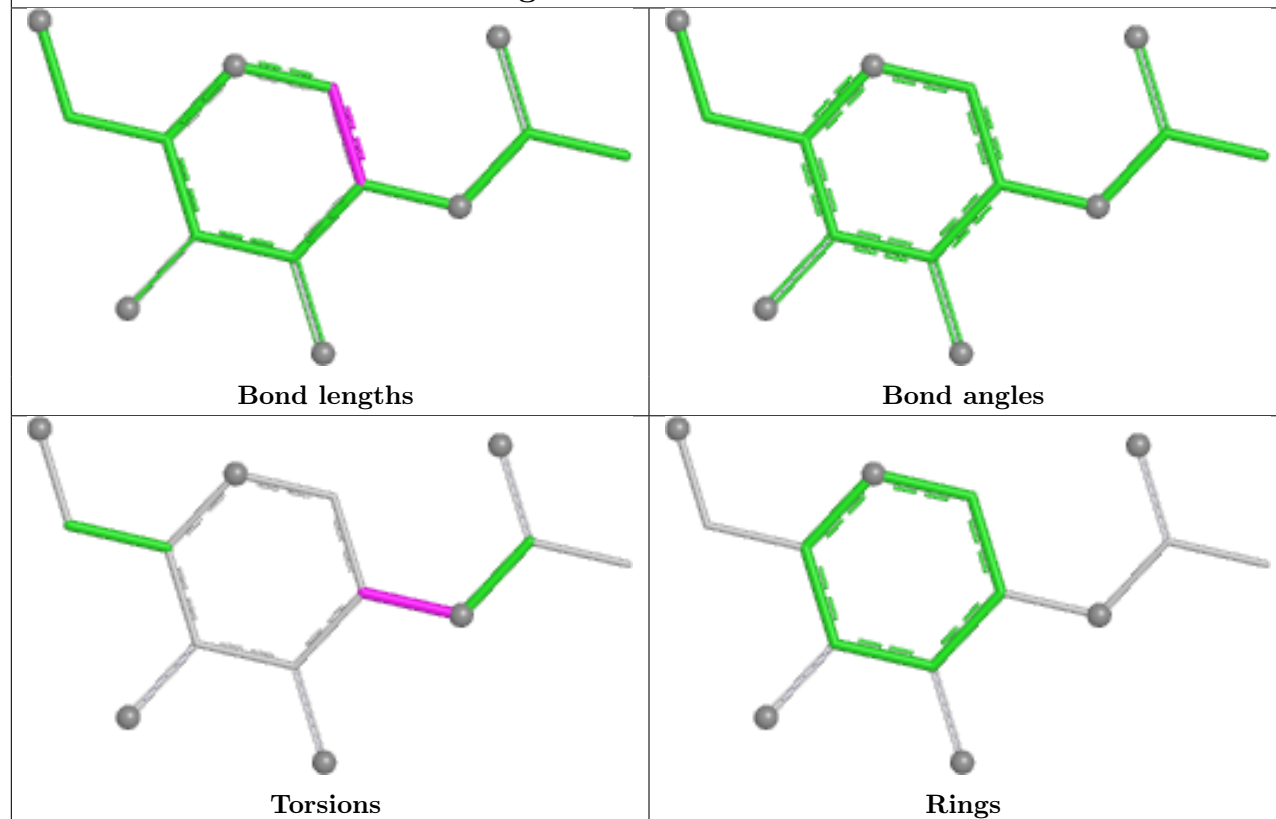
Ligand NAG B 1202



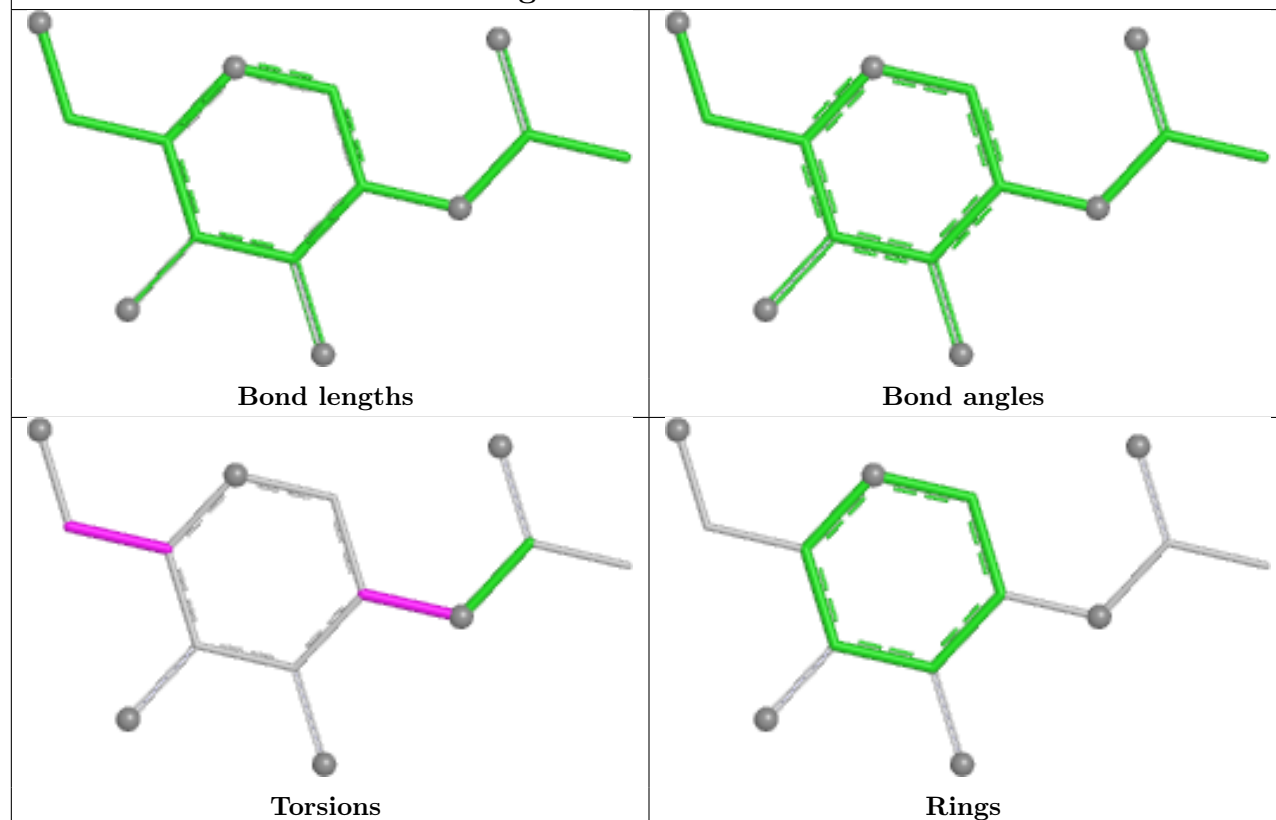
Ligand NAG C 1205



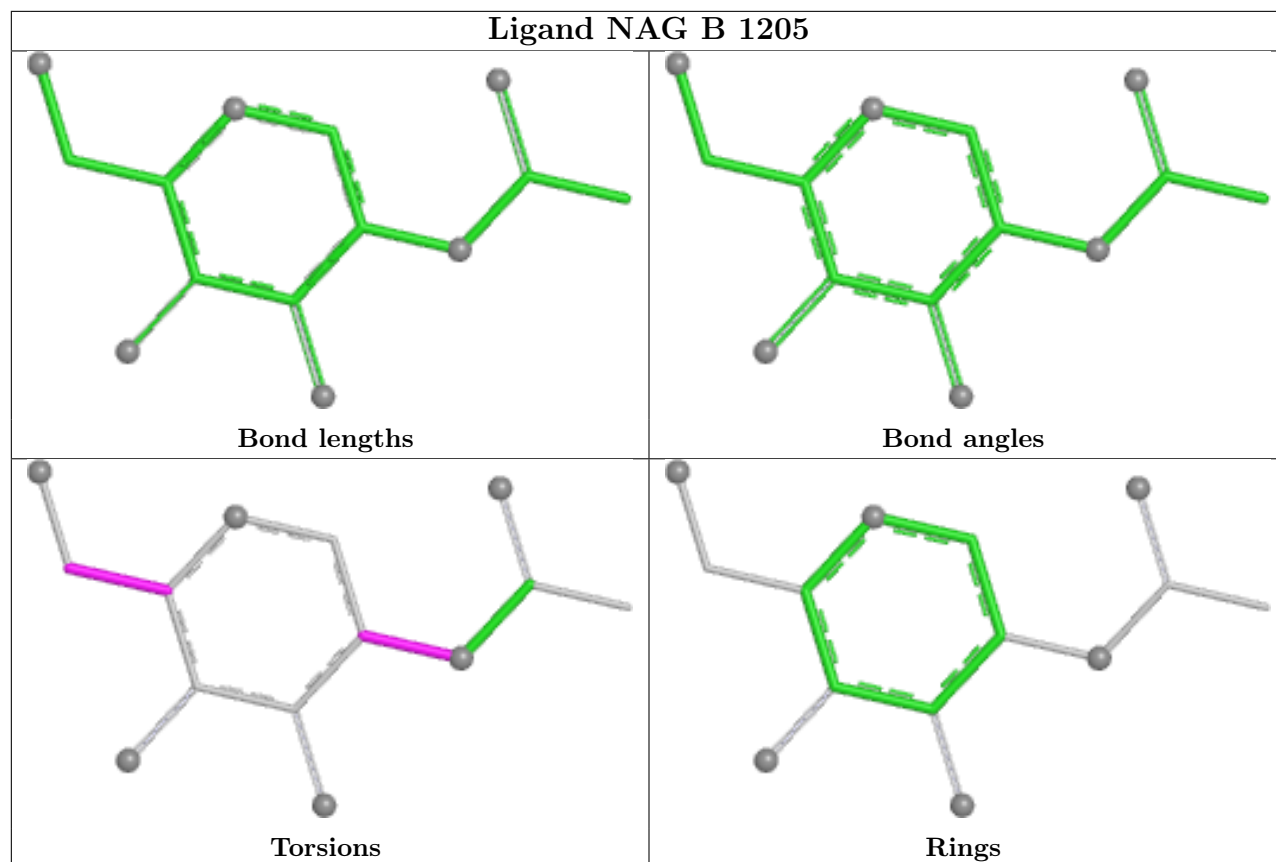
Ligand NAG D 1101



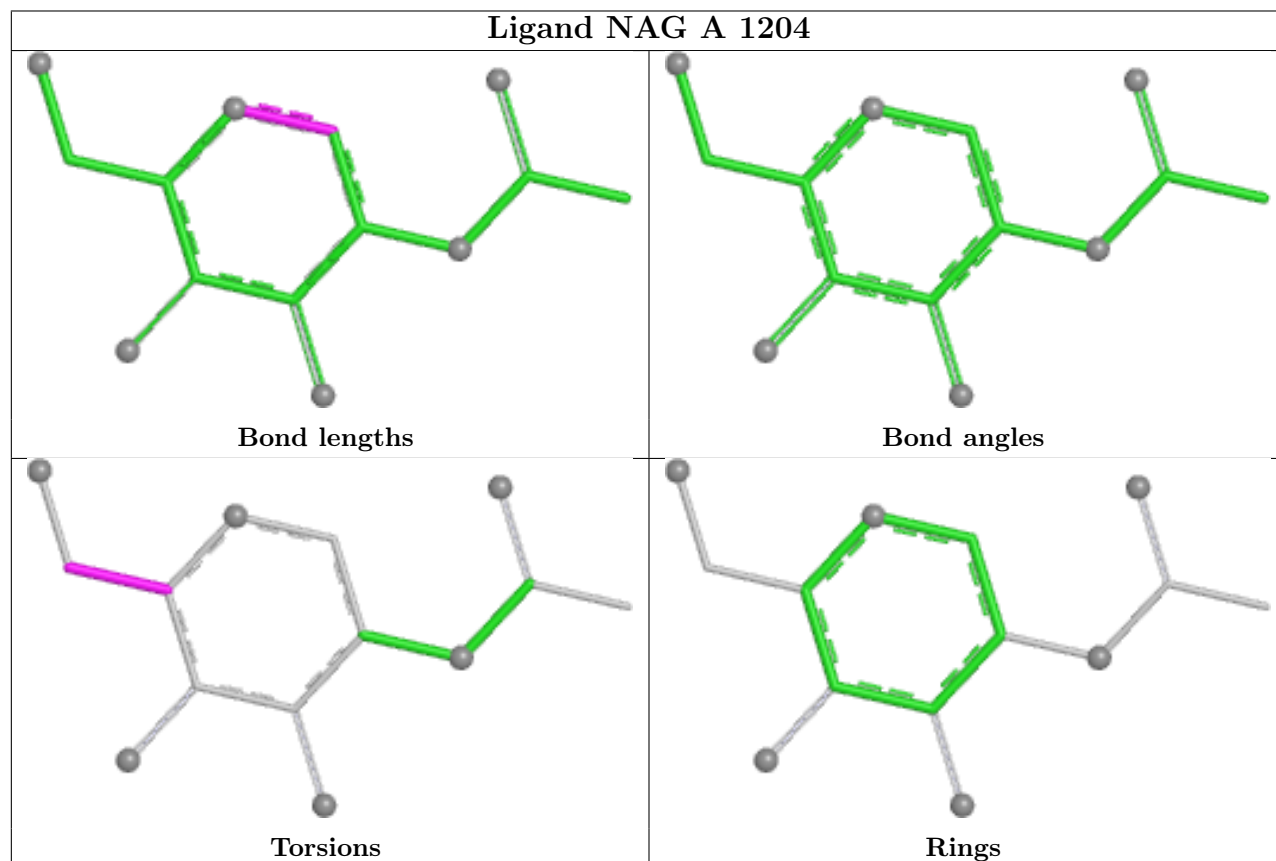
Ligand NAG D 1102

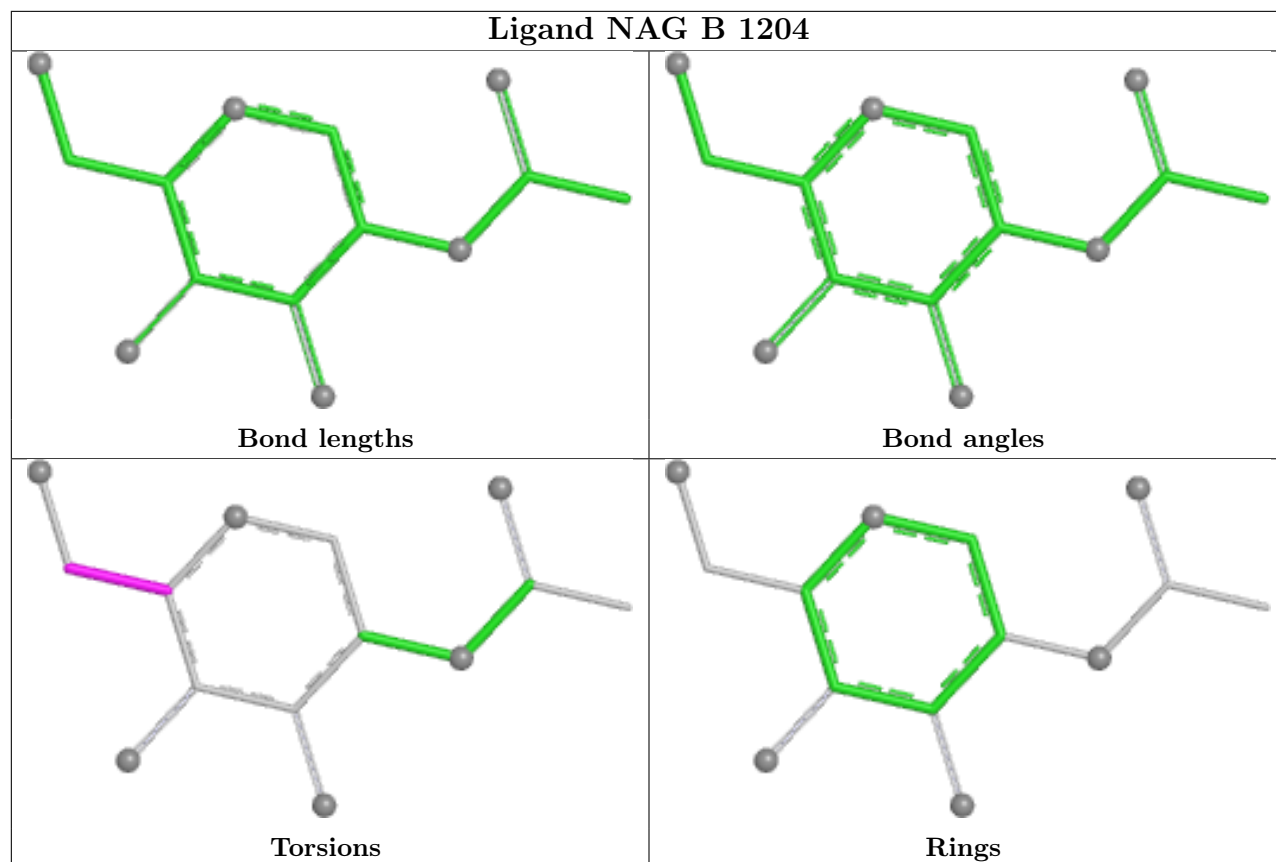


Ligand NAG B 1205



Ligand NAG A 1204





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.

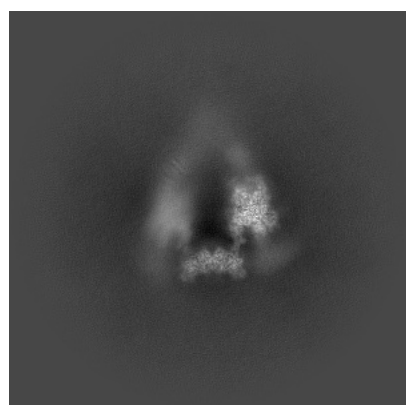
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37462. These allow visual inspection of the internal detail of the map and identification of artifacts.

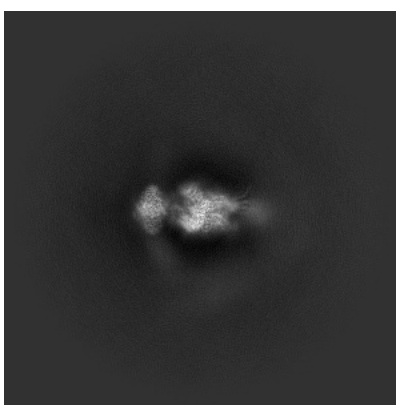
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

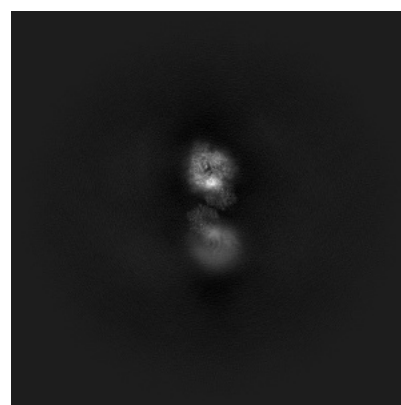
6.1.1 Primary map



X



Y



Z

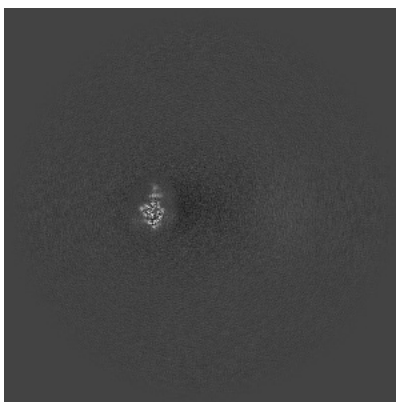
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

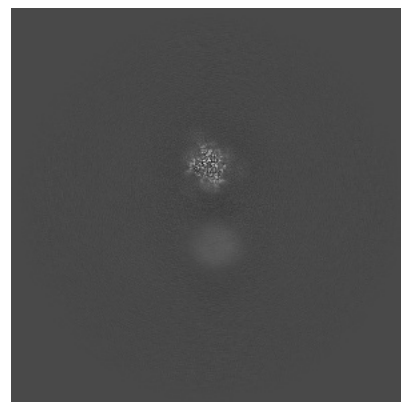
6.2.1 Primary map



X Index: 300



Y Index: 300



Z Index: 300

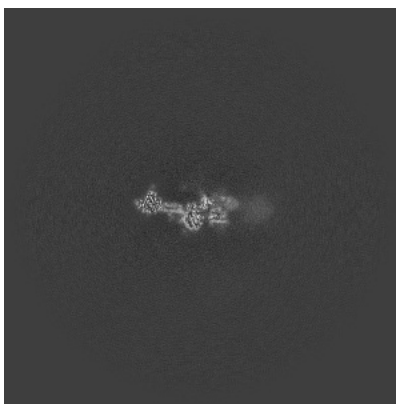
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

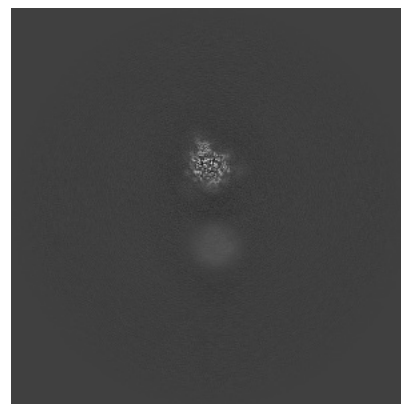
6.3.1 Primary map



X Index: 301



Y Index: 341



Z Index: 297

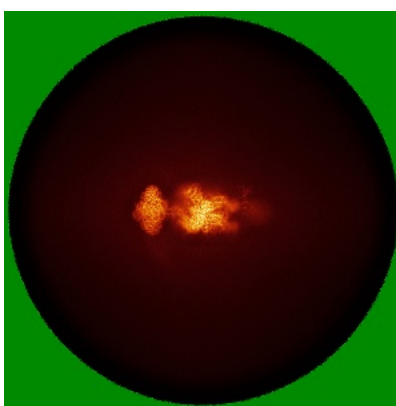
The images above show the largest variance slices of the map in three orthogonal directions.

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

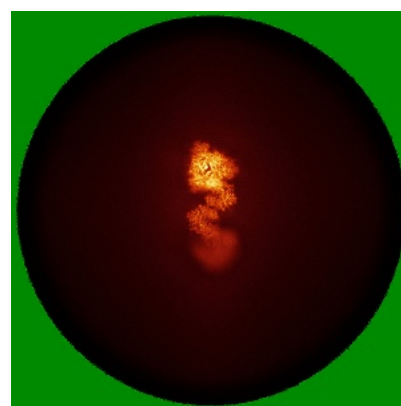
6.4.1 Primary map



X



Y

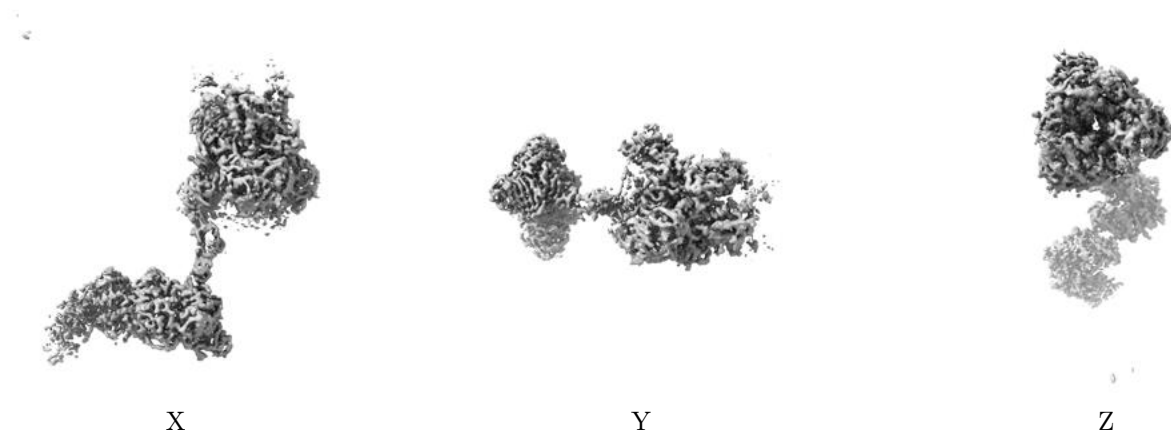


Z

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

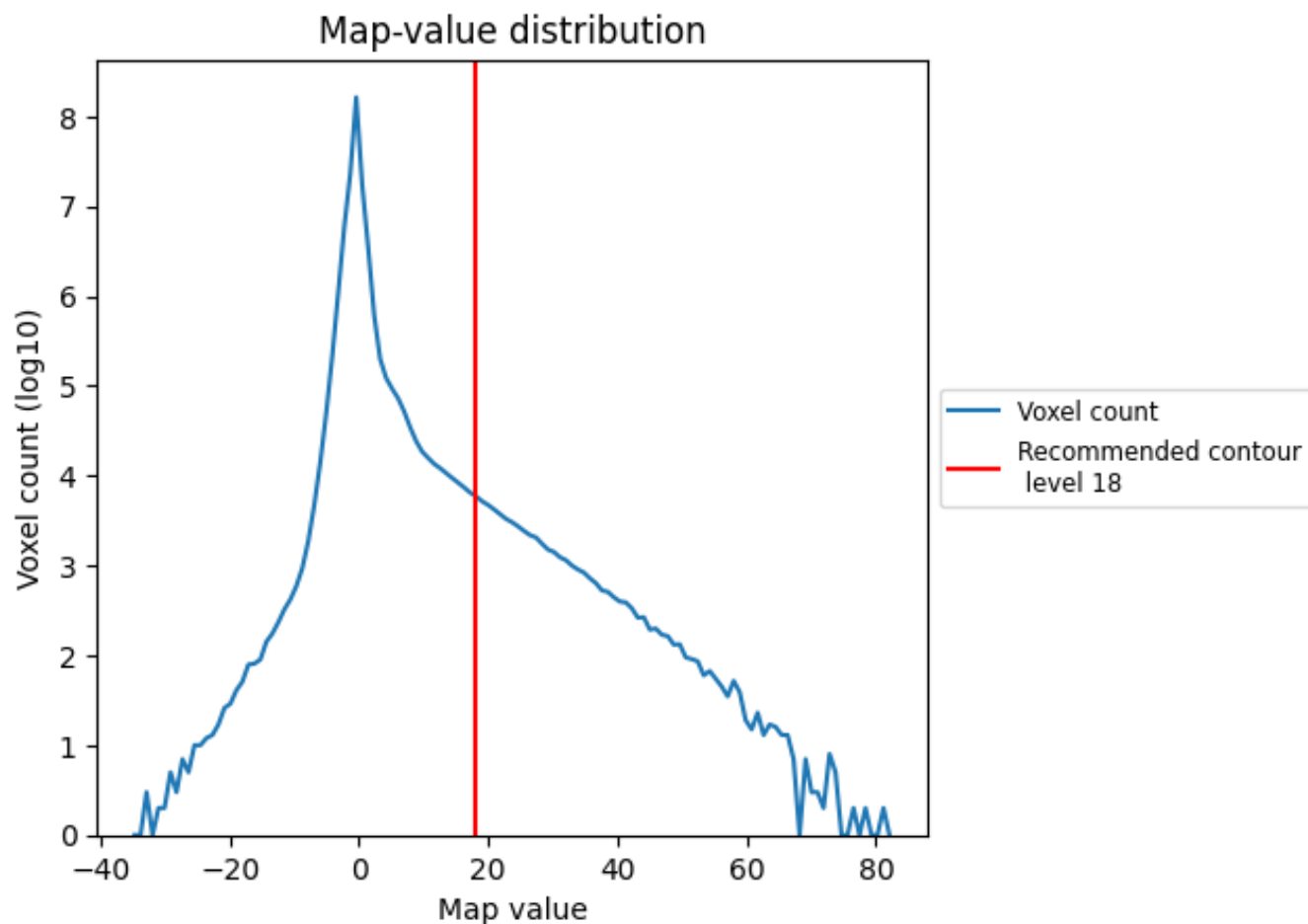
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

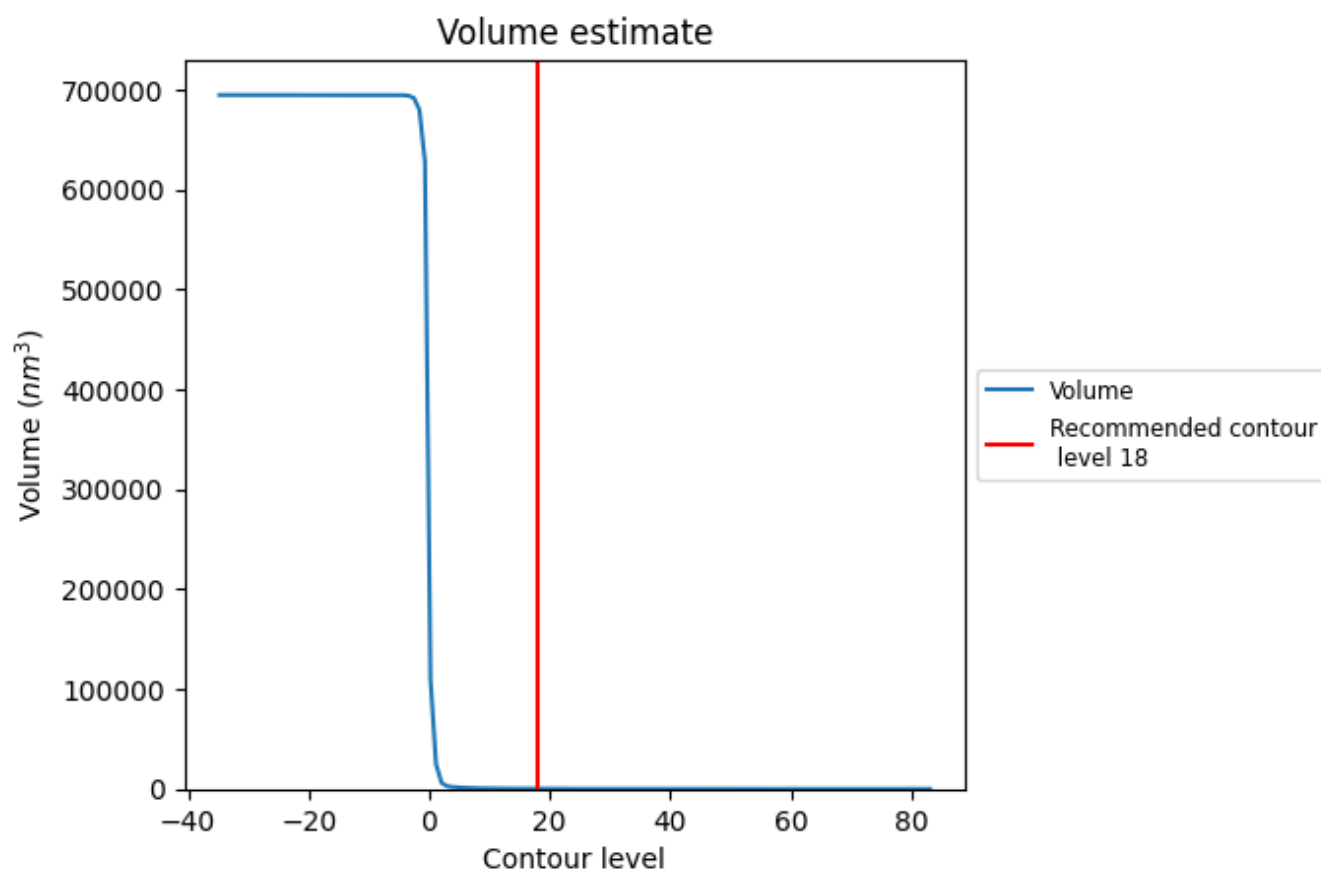
This section contains the results of statistical analysis of the map.

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.

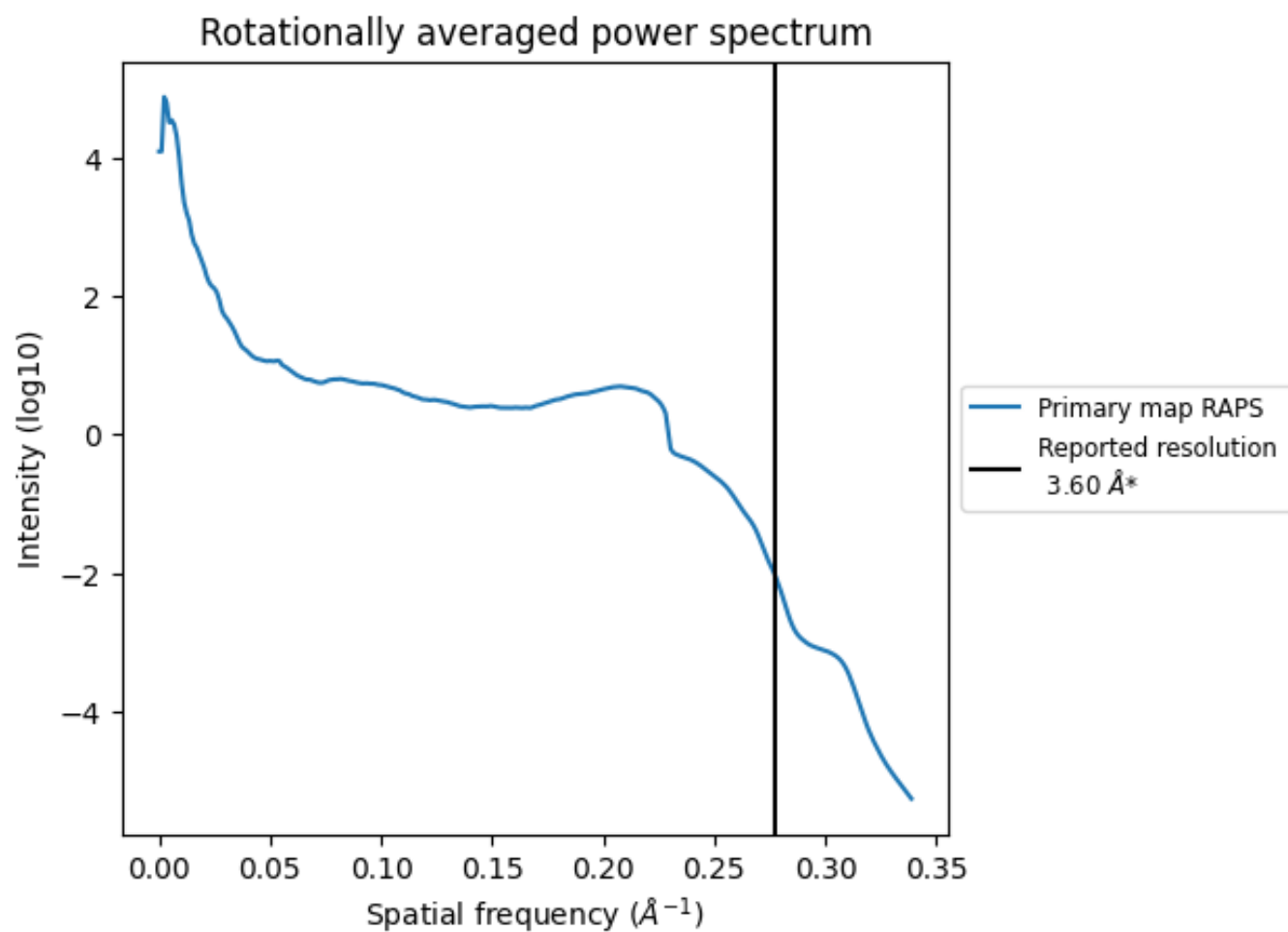
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm^3 ; this corresponds to an approximate mass of 164 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 0.278 Å⁻¹

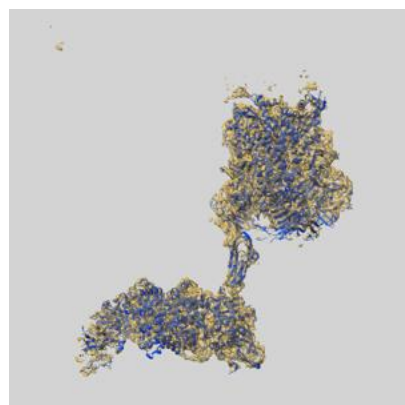
8 Fourier-Shell correlation

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

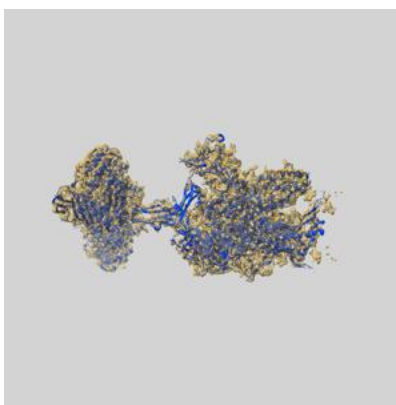
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37462 and PDB model 8WDE. Per-residue inclusion information can be found in section [3](#) on page [9](#).

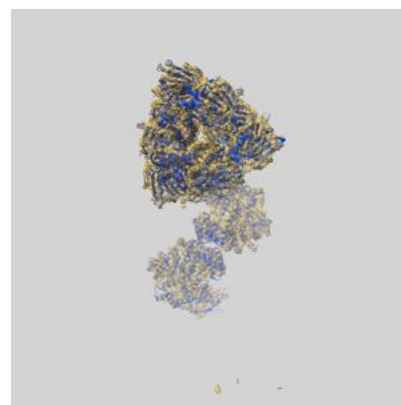
9.1 Map-model overlay [i](#)



X



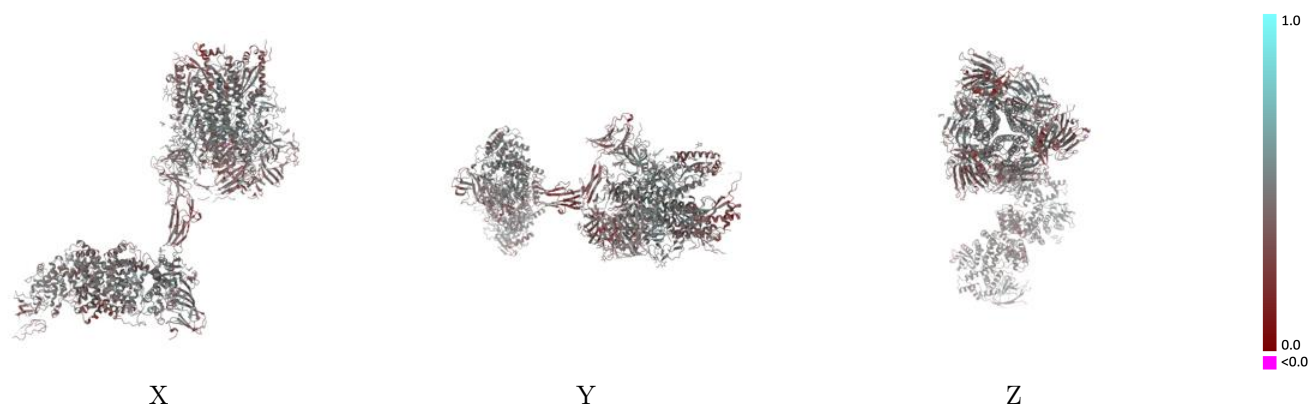
Y



Z

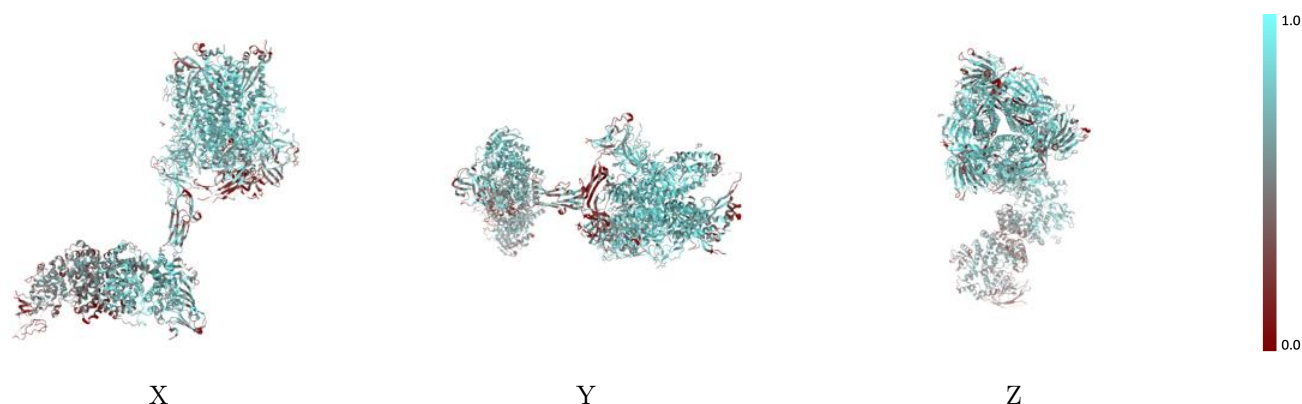
The images above show the 3D surface view of the map at the recommended contour level 18.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



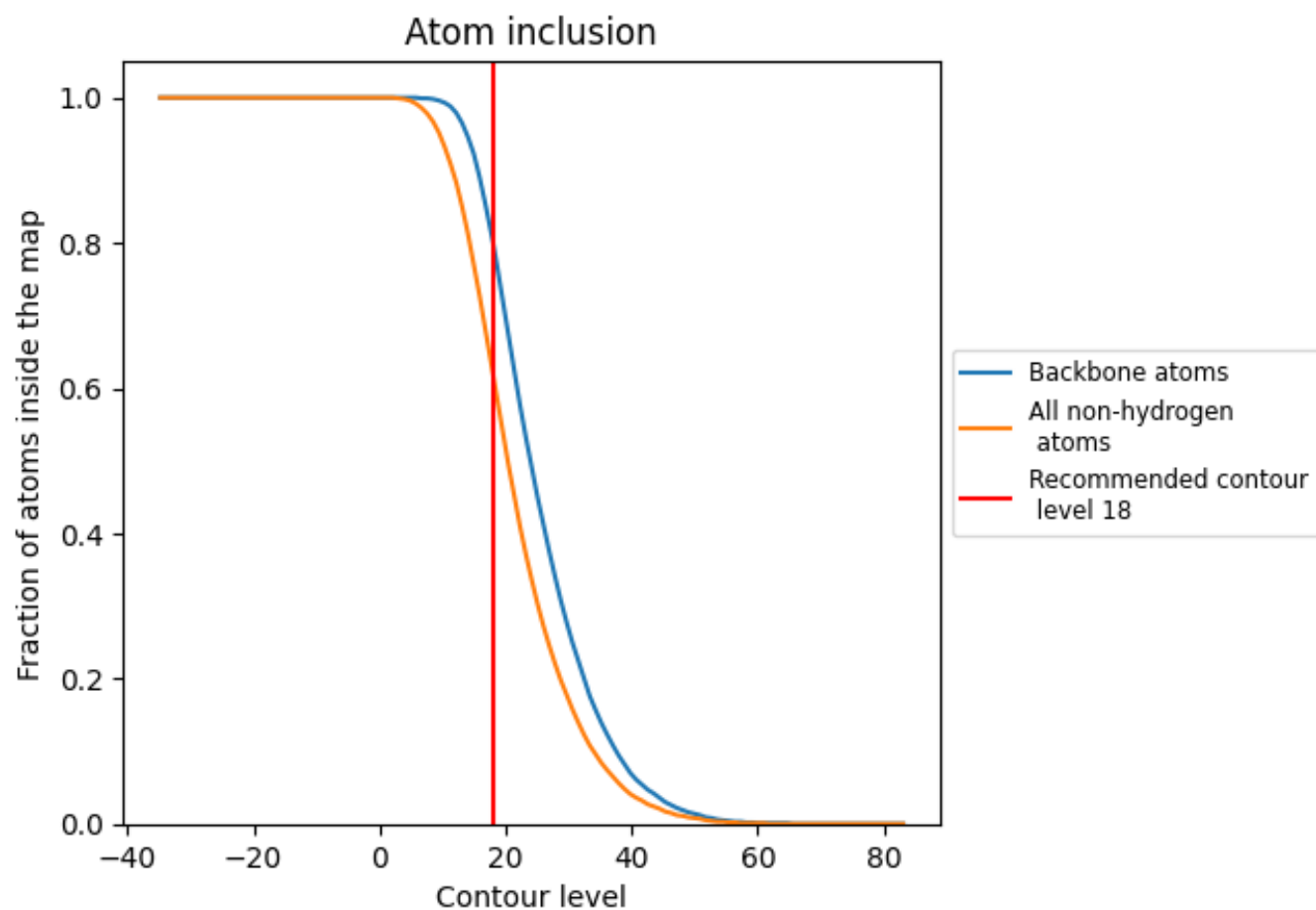
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (18).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 62% 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 (18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.4350
A	0.6820	0.4220
B	0.6740	0.4370
C	0.6560	0.4340
D	0.6210	0.4520
E	0.4560	0.4300
F	0.6150	0.4220
G	0.6430	0.4720
H	0.6670	0.4150
I	0.6070	0.4570
J	0.5380	0.4380
K	0.6790	0.4780
L	0.4640	0.4270

1.0

0.0

<0.0