



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:44 AM UTC

PDB ID : 8S7C / pdb_00008s7c
Title : Ternary Complex of Cachd1, FZD5 and LRP6
Authors : Zhao, Y.; Ren, J.; Jones, E.Y.
Deposited on : 2024-02-29
Resolution : 4.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

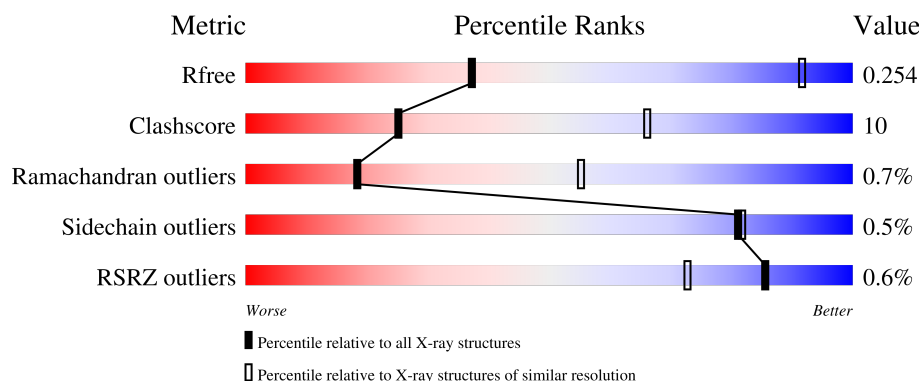
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1020 (5.48-3.92)
Clashscore	190562	1005 (5.40-3.96)
Ramachandran outliers	187476	1095 (5.50-3.90)
Sidechain outliers	187428	1077 (5.50-3.90)
RSRZ outliers	180081	1015 (5.48-3.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1102	
1	D	1102	
1	G	1102	
2	B	140	
2	E	140	

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Mol	Chain	Length	Quality of chain
2	H	140	57%16%26%
3	C	628	80%17%
3	F	628	%76%20%
3	I	628	%75%22%
4	J	2	100%
4	K	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41714 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 VWFA and cache domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1030	Total	C	N	O	S	0	0	0
			8059	5068	1385	1547	59			
1	D	1030	Total	C	N	O	S	0	0	0
			8059	5068	1385	1547	59			
1	G	1030	Total	C	N	O	S	0	0	0
			8059	5068	1385	1547	59			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1095	THR	-	expression tag	UNP Q6PDJ1
A	1096	GLY	-	expression tag	UNP Q6PDJ1
A	1097	LEU	-	expression tag	UNP Q6PDJ1
A	1098	GLU	-	expression tag	UNP Q6PDJ1
A	1099	VAL	-	expression tag	UNP Q6PDJ1
A	1100	LEU	-	expression tag	UNP Q6PDJ1
A	1101	PHE	-	expression tag	UNP Q6PDJ1
A	1102	GLN	-	expression tag	UNP Q6PDJ1
D	1095	THR	-	expression tag	UNP Q6PDJ1
D	1096	GLY	-	expression tag	UNP Q6PDJ1
D	1097	LEU	-	expression tag	UNP Q6PDJ1
D	1098	GLU	-	expression tag	UNP Q6PDJ1
D	1099	VAL	-	expression tag	UNP Q6PDJ1
D	1100	LEU	-	expression tag	UNP Q6PDJ1
D	1101	PHE	-	expression tag	UNP Q6PDJ1
D	1102	GLN	-	expression tag	UNP Q6PDJ1
G	1095	THR	-	expression tag	UNP Q6PDJ1
G	1096	GLY	-	expression tag	UNP Q6PDJ1
G	1097	LEU	-	expression tag	UNP Q6PDJ1
G	1098	GLU	-	expression tag	UNP Q6PDJ1
G	1099	VAL	-	expression tag	UNP Q6PDJ1
G	1100	LEU	-	expression tag	UNP Q6PDJ1
G	1101	PHE	-	expression tag	UNP Q6PDJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1102	GLN	-	expression tag	UNP Q6PDJ1

- Molecule 2 is a protein called Frizzled-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			839	531	147	147	14			
2	E	104	Total	C	N	O	S	0	0	0
			839	531	147	147	14			
2	H	104	Total	C	N	O	S	0	0	0
			839	531	147	147	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	GLU	-	expression tag	UNP Q9EQD0
B	25	THR	-	expression tag	UNP Q9EQD0
B	26	HIS	-	expression tag	UNP Q9EQD0
B	157	GLY	-	expression tag	UNP Q9EQD0
B	158	LEU	-	expression tag	UNP Q9EQD0
B	159	GLU	-	expression tag	UNP Q9EQD0
B	160	VAL	-	expression tag	UNP Q9EQD0
B	161	LEU	-	expression tag	UNP Q9EQD0
B	162	PHE	-	expression tag	UNP Q9EQD0
B	163	GLN	-	expression tag	UNP Q9EQD0
E	24	GLU	-	expression tag	UNP Q9EQD0
E	25	THR	-	expression tag	UNP Q9EQD0
E	26	HIS	-	expression tag	UNP Q9EQD0
E	157	GLY	-	expression tag	UNP Q9EQD0
E	158	LEU	-	expression tag	UNP Q9EQD0
E	159	GLU	-	expression tag	UNP Q9EQD0
E	160	VAL	-	expression tag	UNP Q9EQD0
E	161	LEU	-	expression tag	UNP Q9EQD0
E	162	PHE	-	expression tag	UNP Q9EQD0
E	163	GLN	-	expression tag	UNP Q9EQD0
H	24	GLU	-	expression tag	UNP Q9EQD0
H	25	THR	-	expression tag	UNP Q9EQD0
H	26	HIS	-	expression tag	UNP Q9EQD0
H	157	GLY	-	expression tag	UNP Q9EQD0
H	158	LEU	-	expression tag	UNP Q9EQD0
H	159	GLU	-	expression tag	UNP Q9EQD0
H	160	VAL	-	expression tag	UNP Q9EQD0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	161	LEU	-	expression tag	UNP Q9EQD0
H	162	PHE	-	expression tag	UNP Q9EQD0
H	163	GLN	-	expression tag	UNP Q9EQD0

- Molecule 3 is a protein called Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	609	Total	C	N	O	S	0	0	0
			4848	3042	859	922	25			
3	F	609	Total	C	N	O	S	0	0	0
			4848	3042	859	922	25			
3	I	609	Total	C	N	O	S	0	0	0
			4848	3042	859	922	25			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	626	GLU	-	expression tag	UNP O75581
C	627	THR	-	expression tag	UNP O75581
C	628	GLY	-	expression tag	UNP O75581
C	1245	GLY	-	expression tag	UNP O75581
C	1246	THR	-	expression tag	UNP O75581
C	1247	LYS	-	expression tag	UNP O75581
C	1248	HIS	-	expression tag	UNP O75581
C	1249	HIS	-	expression tag	UNP O75581
C	1250	HIS	-	expression tag	UNP O75581
C	1251	HIS	-	expression tag	UNP O75581
C	1252	HIS	-	expression tag	UNP O75581
C	1253	HIS	-	expression tag	UNP O75581
F	626	GLU	-	expression tag	UNP O75581
F	627	THR	-	expression tag	UNP O75581
F	628	GLY	-	expression tag	UNP O75581
F	1245	GLY	-	expression tag	UNP O75581
F	1246	THR	-	expression tag	UNP O75581
F	1247	LYS	-	expression tag	UNP O75581
F	1248	HIS	-	expression tag	UNP O75581
F	1249	HIS	-	expression tag	UNP O75581
F	1250	HIS	-	expression tag	UNP O75581
F	1251	HIS	-	expression tag	UNP O75581
F	1252	HIS	-	expression tag	UNP O75581
F	1253	HIS	-	expression tag	UNP O75581
I	626	GLU	-	expression tag	UNP O75581

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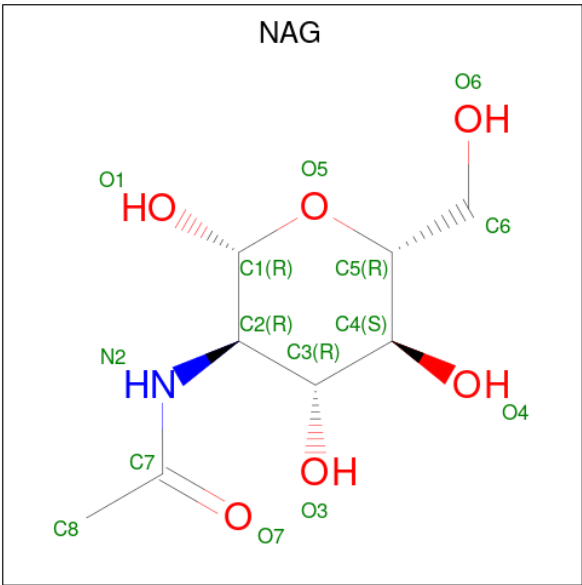
Chain	Residue	Modelled	Actual	Comment	Reference
I	627	THR	-	expression tag	UNP O75581
I	628	GLY	-	expression tag	UNP O75581
I	1245	GLY	-	expression tag	UNP O75581
I	1246	THR	-	expression tag	UNP O75581
I	1247	LYS	-	expression tag	UNP O75581
I	1248	HIS	-	expression tag	UNP O75581
I	1249	HIS	-	expression tag	UNP O75581
I	1250	HIS	-	expression tag	UNP O75581
I	1251	HIS	-	expression tag	UNP O75581
I	1252	HIS	-	expression tag	UNP O75581
I	1253	HIS	-	expression tag	UNP O75581

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	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				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

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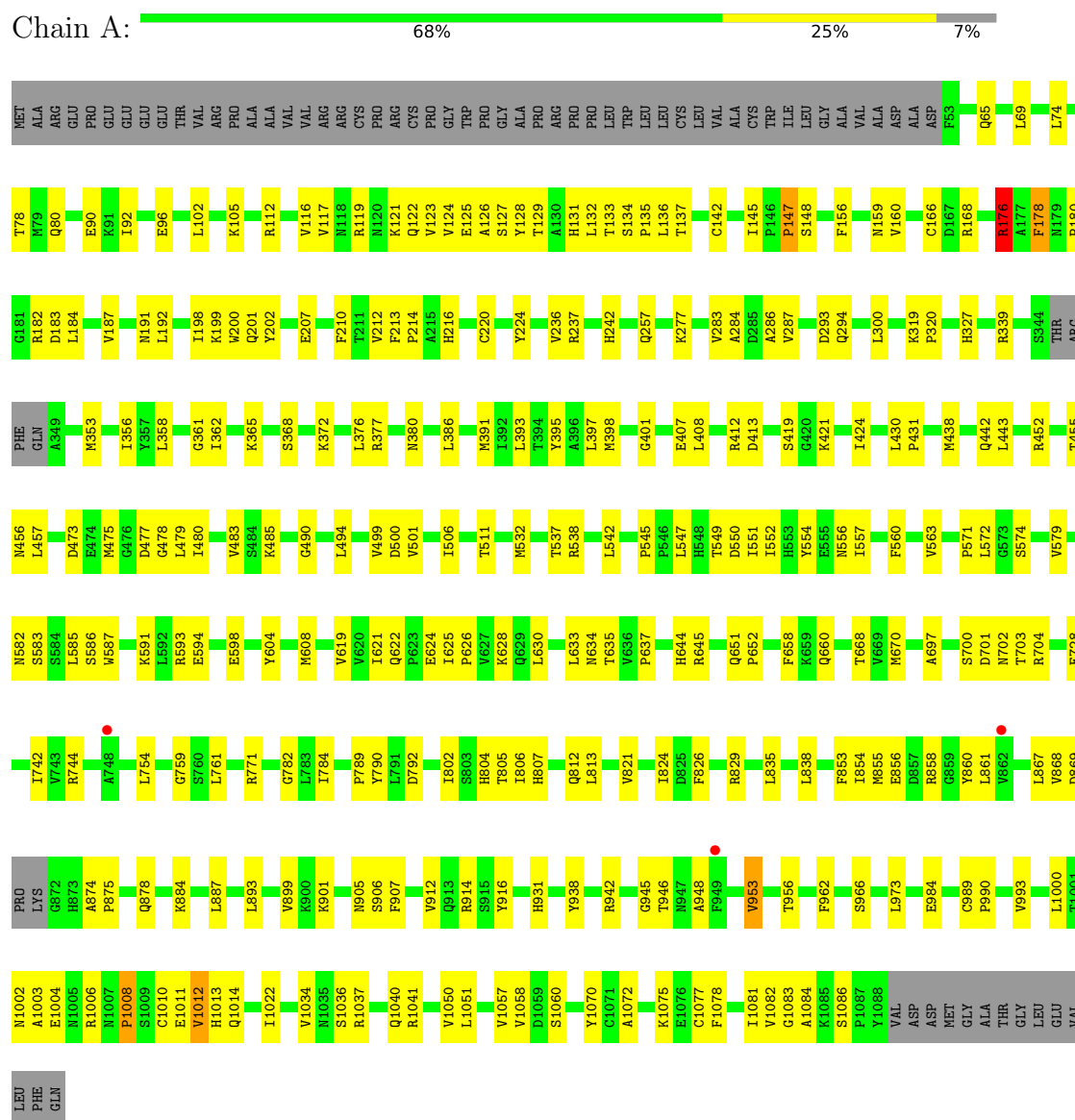
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		

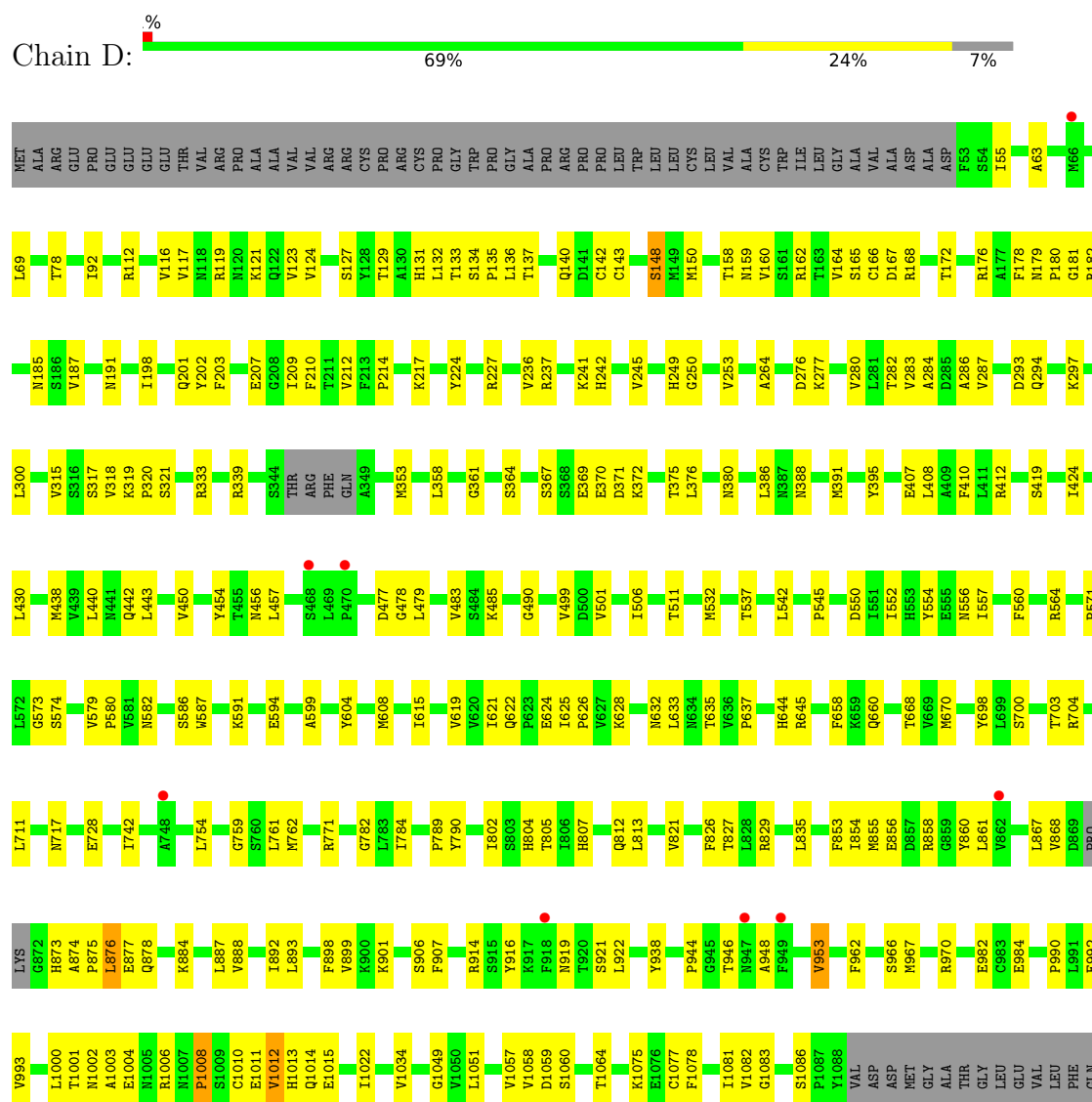
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

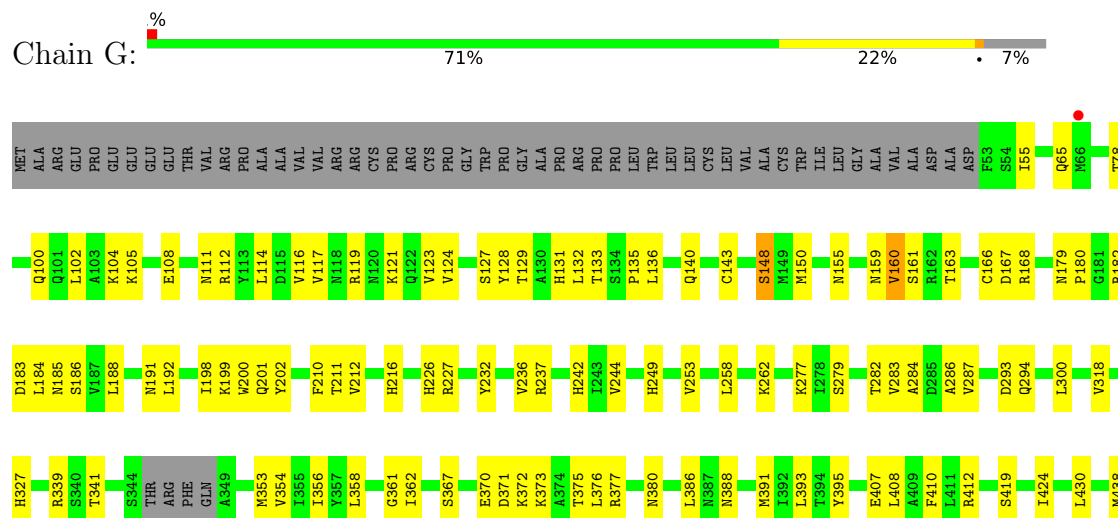
- Molecule 1: VWFA and cache domain-containing protein 1

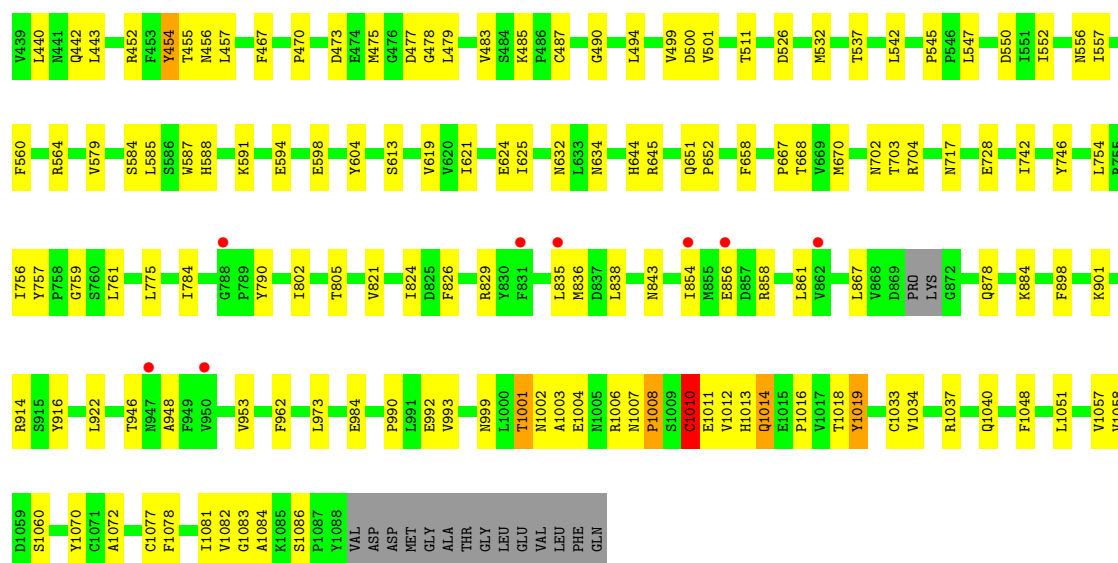


- Molecule 1: VWFA and cache domain-containing protein 1

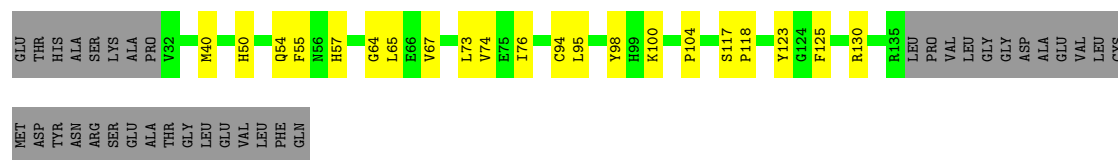


- Molecule 1: VWFA and cache domain-containing protein 1

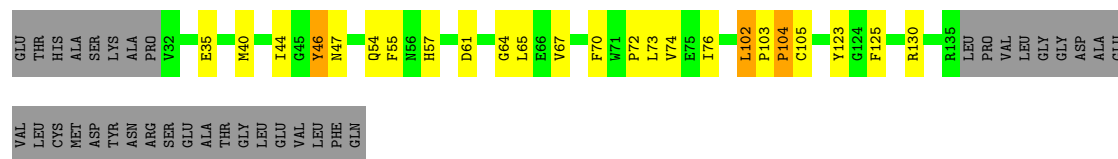




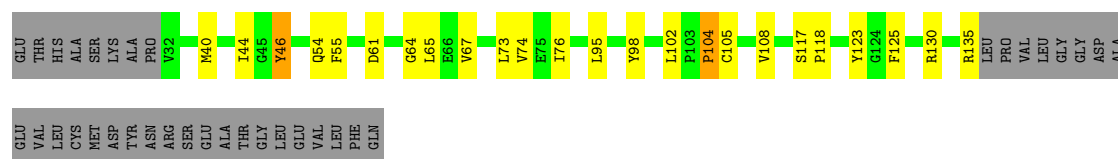
- Molecule 2: Frizzled-5



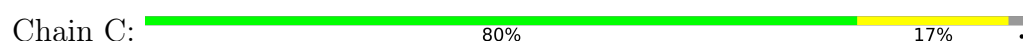
- Molecule 2: Frizzled-5

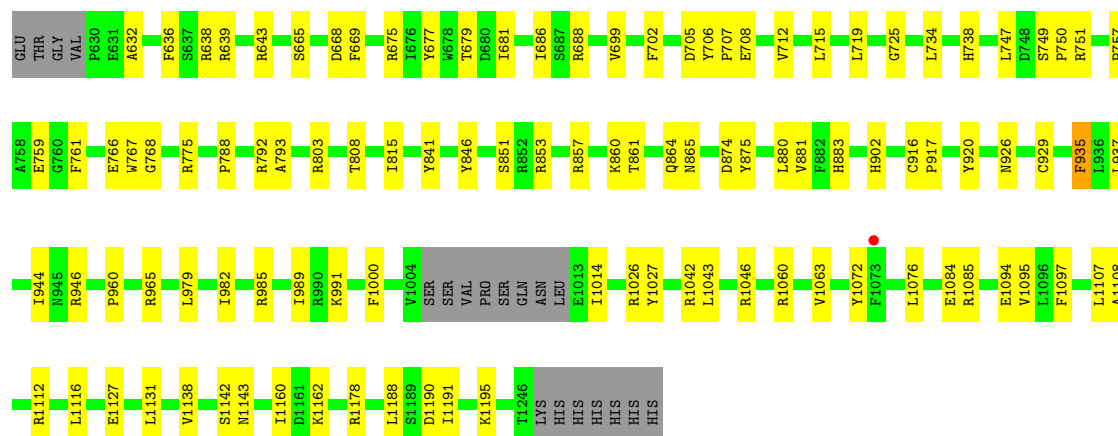


- Molecule 2: Frizzled-5

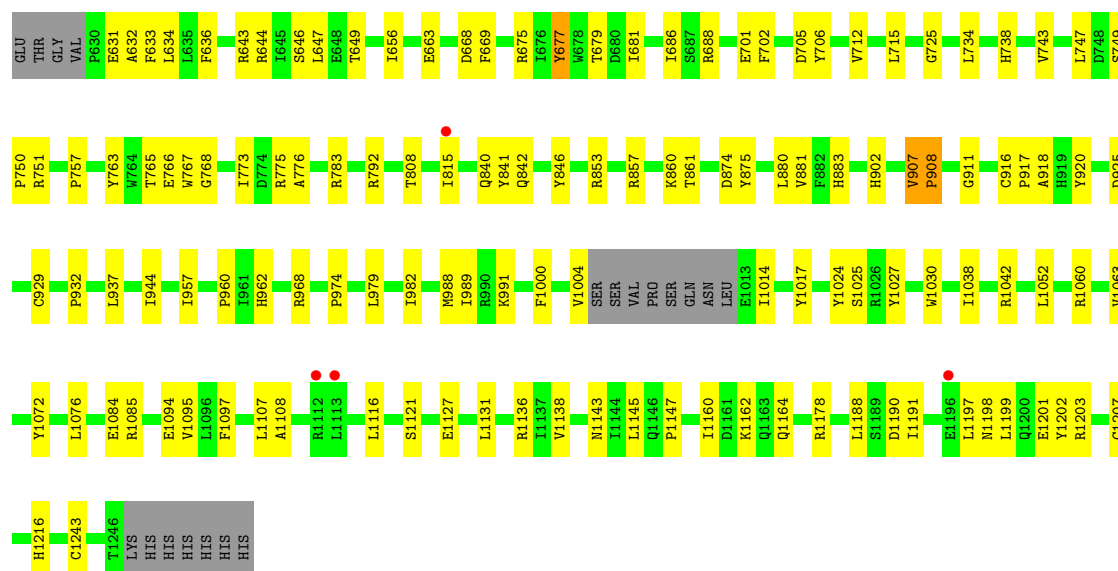
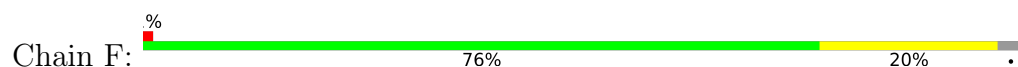


- Molecule 3: Low-density lipoprotein receptor-related protein 6

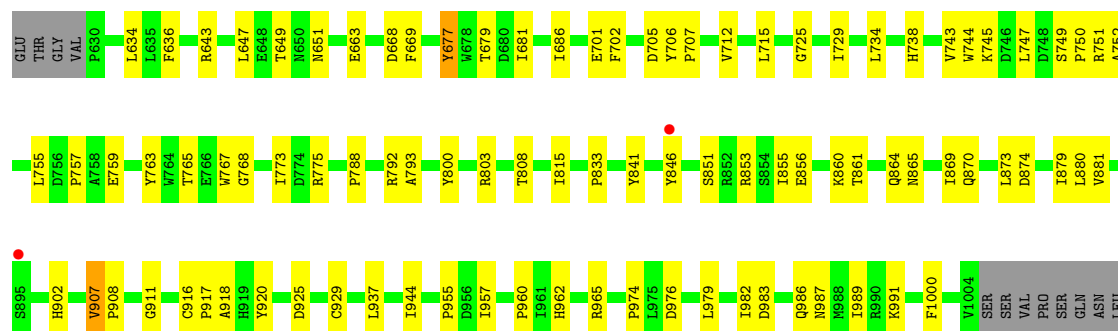
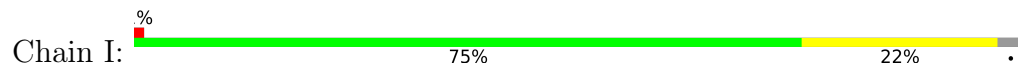


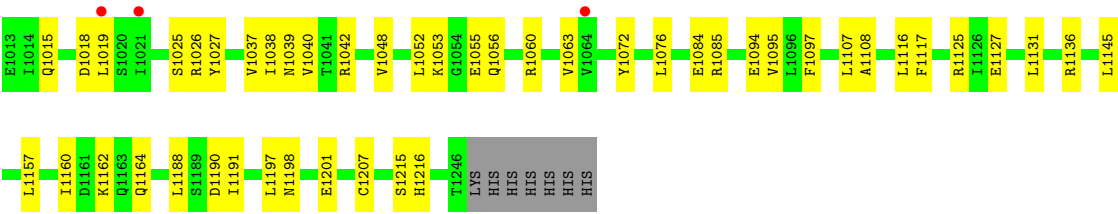


• Molecule 3: Low-density lipoprotein receptor-related protein 6



• Molecule 3: Low-density lipoprotein receptor-related protein 6





● 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	283.70Å 198.24Å 218.82Å 90.00° 128.07° 90.00°	Depositor
Resolution (Å)	86.13 – 4.70 86.13 – 4.70	Depositor EDS
% Data completeness (in resolution range)	47.2 (86.13-4.70) 47.3 (86.13-4.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 4.66Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.206 , 0.261 0.207 , 0.254	Depositor DCC
R_{free} test set	1188 reflections (2.39%)	wwPDB-VP
Wilson B-factor (Å ²)	188.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 251.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	41714	wwPDB-VP
Average B, all atoms (Å ²)	214.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.11	0/8224	0.36	0/11169
1	D	0.11	0/8224	0.34	0/11169
1	G	0.11	0/8224	0.33	0/11169
2	B	0.12	0/867	0.35	0/1179
2	E	0.15	0/867	0.40	0/1179
2	H	0.12	0/867	0.37	0/1179
3	C	0.11	0/4950	0.32	0/6716
3	F	0.11	0/4950	0.34	0/6716
3	I	0.11	0/4950	0.35	0/6716
All	All	0.11	0/42123	0.34	0/57192

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

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	8059	0	7939	192	0
1	D	8059	0	7940	186	0
1	G	8059	0	7939	157	0
2	B	839	0	790	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	839	0	790	19	0
2	H	839	0	790	16	0
3	C	4848	0	4727	73	0
3	F	4848	0	4726	92	0
3	I	4848	0	4725	92	0
4	J	28	0	25	0	0
4	K	28	0	25	1	0
5	A	70	0	65	1	0
5	C	56	0	52	3	0
5	D	70	0	65	2	0
5	E	14	0	13	0	0
5	F	70	0	65	3	0
5	G	84	0	78	1	0
5	H	14	0	13	0	0
5	I	42	0	39	3	0
All	All	41714	0	40806	803	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 10.

All (803) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:675:ARG:HD3	3:F:688:ARG:HD3	1.60	0.84
3:I:846:TYR:HE1	3:I:855:ILE:HG23	1.44	0.83
1:D:914:ARG:NH1	1:D:984:GLU:OE2	2.14	0.81
3:I:855:ILE:HG22	3:I:869:ILE:HB	1.64	0.79
3:F:907:VAL:HB	3:F:908:PRO:HD3	1.63	0.79
3:C:1085:ARG:NE	3:C:1094:GLU:OE2	2.16	0.78
3:I:846:TYR:CE1	3:I:855:ILE:HG23	2.17	0.78
1:A:135:PRO:HD2	3:C:751:ARG:HH22	1.49	0.78
1:G:132:LEU:HD11	3:I:681:ILE:HD12	1.65	0.78
1:D:875:PRO:HB3	1:D:967:MET:HG2	1.64	0.77
1:A:124:VAL:HA	1:A:127:SER:HB2	1.65	0.76
1:A:132:LEU:HD11	3:C:681:ILE:HD12	1.67	0.76
1:D:282:THR:HG21	1:D:318:VAL:HG11	1.68	0.73
1:G:339:ARG:HG2	1:G:386:LEU:HD21	1.71	0.73
3:I:1085:ARG:NE	3:I:1094:GLU:OE2	2.22	0.72
1:D:875:PRO:HG2	1:D:878:GLN:HB3	1.71	0.72
1:D:124:VAL:HA	1:D:127:SER:HB2	1.71	0.72
3:F:925:ASP:HA	5:F:1303:NAG:H82	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:1304:NAG:H3	5:F:1305:NAG:H5	1.71	0.71
3:I:765:THR:HG22	3:I:773:ILE:HG12	1.72	0.71
1:A:176:ARG:HG3	1:A:207:GLU:HG2	1.73	0.71
1:D:339:ARG:HG2	1:D:386:LEU:HD21	1.72	0.70
3:I:944:ILE:HG21	3:I:979:LEU:HD21	1.74	0.70
1:A:376:LEU:O	1:A:380:ASN:ND2	2.24	0.70
1:G:183:ASP:HB3	3:I:792:ARG:HH22	1.57	0.70
1:A:339:ARG:HG2	1:A:386:LEU:HD21	1.73	0.70
1:A:956:THR:HG21	5:A:1204:NAG:H83	1.73	0.69
1:G:1014:GLN:O	1:G:1014:GLN:NE2	2.24	0.69
1:A:134:SER:HA	3:C:751:ARG:HH12	1.58	0.69
1:A:198:ILE:HA	1:A:501:VAL:HG12	1.74	0.69
1:G:380:ASN:HD21	1:G:419:SER:HB2	1.58	0.69
1:D:380:ASN:HD21	1:D:419:SER:HB2	1.57	0.69
3:F:1162:LYS:NZ	3:F:1188:LEU:O	2.23	0.68
1:G:282:THR:HG21	1:G:318:VAL:HG11	1.74	0.68
3:I:1060:ARG:HG3	3:I:1076:LEU:HD12	1.74	0.68
3:I:907:VAL:HB	3:I:908:PRO:HD3	1.76	0.68
1:A:637:PRO:HG3	1:A:700:SER:HB2	1.75	0.68
1:A:658:PHE:HZ	1:A:1051:LEU:HB2	1.59	0.68
1:D:367:SER:HA	1:D:370:GLU:HB3	1.75	0.68
1:G:914:ARG:NH1	1:G:984:GLU:OE2	2.26	0.67
3:I:983:ASP:OD2	3:I:986:GLN:NE2	2.27	0.67
1:D:129:THR:HB	3:F:663:GLU:OE2	1.95	0.67
1:D:131:HIS:HA	1:D:134:SER:HB3	1.77	0.67
1:A:117:VAL:HG11	1:A:483:VAL:HG13	1.77	0.67
1:D:637:PRO:HG3	1:D:700:SER:HB2	1.76	0.67
1:A:658:PHE:CZ	1:A:1051:LEU:HB2	2.30	0.67
1:G:550:ASP:OD2	1:G:564:ARG:NH2	2.28	0.67
3:I:738:HIS:HB3	3:I:917:PRO:HG3	1.77	0.66
1:D:376:LEU:O	1:D:380:ASN:ND2	2.28	0.66
1:D:168:ARG:HG2	1:D:224:TYR:HB3	1.77	0.66
1:A:914:ARG:NH1	1:A:984:GLU:OE2	2.28	0.65
1:D:143:CYS:HA	1:D:217:LYS:HG2	1.77	0.65
1:D:148:SER:HB3	1:D:158:THR:HB	1.78	0.65
1:G:361:GLY:HA3	1:G:407:GLU:HB3	1.76	0.65
1:G:102:LEU:HD12	1:G:105:LYS:HD2	1.78	0.65
1:D:1057:VAL:HG23	1:D:1058:VAL:HG23	1.77	0.65
3:F:1085:ARG:NE	3:F:1094:GLU:OE2	2.29	0.65
1:G:1057:VAL:HG23	1:G:1058:VAL:HG23	1.77	0.65
2:E:102:LEU:H	2:E:103:PRO:HD2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:944:ILE:HG21	3:C:979:LEU:HD21	1.79	0.65
3:F:1060:ARG:HG3	3:F:1076:LEU:HD12	1.78	0.65
3:I:669:PHE:HD1	3:I:880:LEU:HD21	1.61	0.65
1:A:277:LYS:HB3	1:A:300:LEU:HB3	1.79	0.64
3:F:944:ILE:HG21	3:F:979:LEU:HD21	1.79	0.64
3:C:1060:ARG:HG3	3:C:1076:LEU:HD12	1.79	0.64
1:D:117:VAL:HG11	1:D:483:VAL:HG13	1.79	0.64
1:D:132:LEU:HD13	3:F:706:TYR:HB3	1.79	0.64
1:D:159:ASN:HD21	1:D:214:PRO:HG2	1.62	0.64
3:C:1160:ILE:HB	3:C:1188:LEU:HD13	1.78	0.64
3:F:853:ARG:HE	3:F:874:ASP:HB3	1.63	0.64
1:A:242:HIS:HB2	1:A:353:MET:HG2	1.80	0.64
1:A:557:ILE:HD11	1:A:579:VAL:HG11	1.79	0.64
1:D:571:PRO:HB3	1:D:608:MET:HE2	1.78	0.64
1:A:586:SER:OG	1:A:1011:GLU:OE2	2.16	0.64
3:C:688:ARG:HD2	3:C:699:VAL:HG11	1.80	0.64
3:I:702:PHE:CD2	3:I:960:PRO:HA	2.33	0.64
1:A:119:ARG:HG3	3:C:853:ARG:HH21	1.63	0.63
1:D:165:SER:OG	1:D:185:ASN:OD1	2.12	0.63
1:G:65:GLN:HE21	1:G:838:LEU:HD21	1.63	0.63
1:G:117:VAL:HG11	1:G:483:VAL:HG13	1.80	0.63
1:A:574:SER:HB3	1:D:571:PRO:HG2	1.79	0.63
1:A:1057:VAL:HG23	1:A:1058:VAL:HG23	1.78	0.63
1:A:361:GLY:HA3	1:A:407:GLU:HB3	1.81	0.63
3:F:669:PHE:HD1	3:F:880:LEU:HD21	1.63	0.63
1:G:163:THR:HG22	1:G:185:ASN:HB3	1.81	0.63
2:E:35:GLU:HG3	2:E:47:ASN:HB3	1.81	0.63
1:D:242:HIS:HB2	1:D:353:MET:HG2	1.81	0.63
3:F:749:SER:HB3	3:F:751:ARG:HH21	1.63	0.63
3:C:669:PHE:HD1	3:C:880:LEU:HD21	1.64	0.62
1:G:790:TYR:OH	1:G:858:ARG:NH2	2.31	0.62
1:D:660:GLN:NE2	1:D:761:LEU:O	2.32	0.62
1:D:135:PRO:HD3	3:F:751:ARG:HH22	1.65	0.62
1:D:297:LYS:HG2	1:D:333:ARG:HH22	1.64	0.62
1:A:1081:ILE:HB	1:A:1084:ALA:HB2	1.82	0.62
3:C:738:HIS:HB3	3:C:917:PRO:HG3	1.82	0.61
1:G:1010:CYS:HB2	1:G:1013:HIS:CE1	2.35	0.61
3:I:1039:ASN:OD1	3:I:1040:VAL:N	2.32	0.61
1:A:571:PRO:HB3	1:A:608:MET:HE2	1.82	0.61
1:D:369:GLU:HG3	1:D:372:LYS:HD2	1.82	0.61
1:D:789:PRO:HD2	1:D:860:TYR:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:ILE:HA	1:G:501:VAL:HG12	1.82	0.61
1:A:380:ASN:HD21	1:A:419:SER:HB2	1.64	0.61
1:G:148:SER:HA	1:G:160:VAL:HG22	1.83	0.60
1:D:992:GLU:OE2	1:D:1001:THR:HB	2.00	0.60
1:G:557:ILE:HD11	1:G:579:VAL:HG11	1.83	0.60
3:C:1014:ILE:HD11	5:C:1304:NAG:H83	1.84	0.60
1:G:129:THR:HB	3:I:663:GLU:OE2	2.01	0.60
1:D:658:PHE:CZ	1:D:1051:LEU:HB2	2.37	0.60
1:A:835:LEU:HD11	1:A:854:ILE:HG13	1.83	0.60
1:D:283:VAL:HG22	1:D:287:VAL:HG12	1.83	0.60
2:H:95:LEU:HB2	2:H:98:TYR:HB2	1.82	0.59
3:F:860:LYS:HG3	3:F:861:THR:HG23	1.82	0.59
3:I:1160:ILE:HB	3:I:1188:LEU:HD13	1.82	0.59
1:G:186:SER:OG	3:I:851:SER:HB3	2.03	0.59
1:A:789:PRO:HD2	1:A:860:TYR:HB3	1.83	0.59
3:F:677:TYR:HE2	3:F:734:LEU:HD22	1.68	0.59
1:G:237:ARG:NH1	1:G:454:TYR:O	2.36	0.59
1:G:1081:ILE:HG22	1:G:1083:GLY:H	1.68	0.59
1:A:452:ARG:HH21	1:A:455:THR:HG21	1.68	0.58
1:D:557:ILE:HD11	1:D:579:VAL:HG11	1.85	0.58
1:G:277:LYS:HB3	1:G:300:LEU:HB3	1.85	0.58
1:A:571:PRO:HG2	1:D:574:SER:HB3	1.84	0.58
3:C:860:LYS:HG3	3:C:861:THR:HG23	1.84	0.58
1:D:277:LYS:HB3	1:D:300:LEU:HB3	1.85	0.58
1:G:670:MET:HB3	1:G:754:LEU:HB3	1.85	0.58
1:A:142:CYS:HA	1:A:166:CYS:HB2	1.85	0.58
1:D:982:GLU:HG3	2:E:72:PRO:HG3	1.84	0.58
1:A:537:THR:HB	1:A:542:LEU:HD21	1.84	0.58
3:F:634:LEU:HB2	3:F:647:LEU:HD21	1.86	0.58
1:A:1060:SER:HB3	1:A:1082:VAL:HG23	1.86	0.58
3:I:1063:VAL:HG21	3:I:1108:ALA:HA	1.86	0.58
1:D:771:ARG:NH2	1:D:790:TYR:HE2	2.02	0.57
3:I:1162:LYS:NZ	3:I:1188:LEU:O	2.27	0.57
1:A:96:GLU:OE2	1:D:571:PRO:HB2	2.04	0.57
1:A:121:LYS:HD2	1:A:485:LYS:HD2	1.85	0.57
1:G:594:GLU:HG3	1:G:625:ILE:HG12	1.87	0.57
3:I:729:ILE:HB	3:I:743:VAL:HB	1.87	0.57
1:A:168:ARG:HG2	1:A:224:TYR:HB3	1.86	0.57
1:D:550:ASP:OD2	1:D:564:ARG:NH2	2.37	0.57
3:F:1038:ILE:HD12	3:F:1052:LEU:HD13	1.86	0.57
1:A:131:HIS:ND1	1:A:134:SER:O	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:MET:HB3	1:A:754:LEU:HB3	1.85	0.57
1:D:388:ASN:HB2	1:D:430:LEU:HD22	1.87	0.57
1:G:376:LEU:O	1:G:380:ASN:ND2	2.38	0.57
1:D:537:THR:HB	1:D:542:LEU:HD21	1.86	0.57
1:D:142:CYS:HA	1:D:166:CYS:HB2	1.87	0.57
1:G:651:GLN:HG3	1:G:652:PRO:HD3	1.87	0.57
1:G:946:THR:HG23	1:G:948:ALA:H	1.70	0.57
1:D:703:THR:HG22	1:D:704:ARG:H	1.70	0.57
3:F:644:ARG:HD3	3:F:656:ILE:HD11	1.86	0.57
1:G:179:ASN:HD22	1:G:211:THR:HG21	1.70	0.56
1:A:1081:ILE:HG22	1:A:1083:GLY:H	1.70	0.56
3:C:864:GLN:HG2	3:C:865:ASN:H	1.69	0.56
1:G:835:LEU:HD11	1:G:854:ILE:HG13	1.86	0.56
1:A:771:ARG:NH2	1:A:790:TYR:HE2	2.03	0.56
3:F:763:TYR:CE1	3:F:775:ARG:HG3	2.41	0.56
1:G:283:VAL:HG22	1:G:287:VAL:HG12	1.86	0.56
3:I:679:THR:HG22	3:I:686:ILE:HG12	1.86	0.56
2:E:102:LEU:H	2:E:103:PRO:CD	2.19	0.56
1:G:962:PHE:HB3	2:H:125:PHE:CE1	2.41	0.56
1:A:102:LEU:HD12	1:A:105:LYS:HD2	1.86	0.56
1:D:249:HIS:HE1	1:D:282:THR:HB	1.71	0.56
3:F:705:ASP:OD2	3:F:725:GLY:HA3	2.05	0.56
1:A:1012:VAL:C	1:A:1014:GLN:H	2.14	0.56
3:F:701:GLU:OE2	3:F:962:HIS:NE2	2.37	0.56
1:G:131:HIS:CD2	1:G:180:PRO:HG3	2.41	0.56
1:D:670:MET:HB3	1:D:754:LEU:HB3	1.88	0.56
3:C:1042:ARG:HD2	3:C:1046:ARG:HB3	1.87	0.56
1:D:624:GLU:HG2	1:D:625:ILE:HD12	1.88	0.56
1:A:380:ASN:ND2	1:A:424:ILE:HG21	2.21	0.55
1:D:591:LYS:HD2	1:D:621:ILE:HD13	1.87	0.55
1:G:124:VAL:HA	1:G:127:SER:HB2	1.88	0.55
2:E:54:GLN:HG2	2:E:130:ARG:HD3	1.88	0.55
3:F:808:THR:HG22	3:F:815:ILE:HG12	1.87	0.55
1:A:257:GLN:NE2	1:A:397:LEU:O	2.34	0.55
5:C:1303:NAG:H3	5:C:1304:NAG:H3	1.87	0.55
1:D:1060:SER:HB3	1:D:1082:VAL:HG23	1.87	0.55
3:F:738:HIS:HB3	3:F:917:PRO:HG3	1.89	0.55
1:G:358:LEU:HD23	1:G:395:TYR:HB2	1.89	0.55
1:D:594:GLU:HG3	1:D:625:ILE:HG12	1.89	0.55
3:I:1072:TYR:HD2	3:I:1116:LEU:HD13	1.72	0.55
1:D:121:LYS:HD2	1:D:485:LYS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1027:TYR:HB3	3:F:1042:ARG:HG2	1.87	0.55
3:I:705:ASP:OD2	3:I:725:GLY:HA3	2.07	0.55
1:D:119:ARG:HH21	1:D:187:VAL:HG13	1.72	0.55
1:D:861:LEU:HD12	1:D:884:LYS:HD2	1.89	0.55
1:D:946:THR:HG23	1:D:948:ALA:H	1.72	0.55
3:F:765:THR:HG22	3:F:773:ILE:HG12	1.87	0.55
3:F:1127:GLU:HG2	3:F:1138:VAL:HG22	1.88	0.55
1:A:660:GLN:NE2	1:A:761:LEU:O	2.39	0.55
1:D:868:VAL:HG23	1:D:878:GLN:HE22	1.71	0.55
1:G:1060:SER:HB3	1:G:1082:VAL:HG23	1.88	0.55
3:I:860:LYS:HG3	3:I:861:THR:HG23	1.88	0.55
1:A:511:THR:O	1:A:538:ARG:NH1	2.40	0.54
1:G:1019:TYR:CD1	1:G:1019:TYR:N	2.74	0.54
3:I:701:GLU:OE2	3:I:962:HIS:NE2	2.31	0.54
3:I:925:ASP:HA	5:I:1303:NAG:H82	1.88	0.54
1:A:116:VAL:HG12	1:A:499:VAL:HG21	1.89	0.54
1:A:119:ARG:HG3	3:C:853:ARG:NH2	2.22	0.54
1:D:132:LEU:HD11	3:F:681:ILE:HD12	1.88	0.54
3:F:679:THR:HG22	3:F:686:ILE:HG12	1.90	0.54
1:G:140:GLN:HB2	1:G:167:ASP:OD2	2.07	0.54
1:G:992:GLU:HG2	1:G:1004:GLU:CD	2.32	0.54
3:I:864:GLN:HG2	3:I:865:ASN:H	1.72	0.54
1:D:380:ASN:ND2	1:D:424:ILE:HG21	2.22	0.54
3:F:846:TYR:HE1	3:F:857:ARG:HG3	1.72	0.54
1:G:537:THR:HB	1:G:542:LEU:HD21	1.89	0.54
1:G:658:PHE:HZ	1:G:1051:LEU:HB2	1.71	0.54
1:A:283:VAL:HG22	1:A:287:VAL:HG12	1.88	0.54
1:D:198:ILE:HD12	1:D:201:GLN:HE21	1.72	0.54
3:I:1145:LEU:HD12	3:I:1164:GLN:HG3	1.90	0.54
3:F:747:LEU:HD21	3:F:750:PRO:HG3	1.88	0.54
3:F:1072:TYR:HD2	3:F:1116:LEU:HD13	1.73	0.54
1:D:1012:VAL:HG12	1:D:1015:GLU:H	1.72	0.54
3:I:808:THR:HG22	3:I:815:ILE:HG12	1.90	0.54
1:D:198:ILE:HA	1:D:501:VAL:HG12	1.89	0.54
3:F:1038:ILE:HB	3:F:1052:LEU:HB3	1.90	0.54
3:F:1063:VAL:HG21	3:F:1108:ALA:HA	1.89	0.54
3:I:763:TYR:CE1	3:I:775:ARG:HG3	2.43	0.54
2:B:98:TYR:CE2	2:B:100:LYS:HB2	2.42	0.54
3:C:688:ARG:NH1	3:C:734:LEU:O	2.41	0.54
3:F:1160:ILE:HB	3:F:1188:LEU:HD13	1.90	0.54
1:G:227:ARG:HA	1:G:232:TYR:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:742:ILE:HG12	1:G:826:PHE:CE1	2.43	0.54
3:I:1107:LEU:HD11	3:I:1116:LEU:HD11	1.90	0.53
3:I:1160:ILE:HD12	3:I:1188:LEU:HB3	1.89	0.53
1:A:131:HIS:CE1	1:A:180:PRO:HG3	2.42	0.53
1:A:624:GLU:HG2	1:A:625:ILE:HD12	1.89	0.53
1:D:876:LEU:HD22	1:D:970:ARG:HG2	1.90	0.53
3:F:763:TYR:HE1	3:F:775:ARG:HG3	1.72	0.53
1:G:1019:TYR:N	1:G:1019:TYR:HD1	2.07	0.53
2:B:54:GLN:HG2	2:B:130:ARG:HD3	1.90	0.53
3:F:916:CYS:HB3	3:F:920:TYR:HB2	1.91	0.53
3:C:749:SER:HB3	3:C:751:ARG:HH21	1.72	0.53
1:D:1012:VAL:C	1:D:1014:GLN:H	2.16	0.53
3:F:743:VAL:HG22	3:F:783:ARG:HD3	1.90	0.53
1:A:861:LEU:HD12	1:A:884:LYS:HD2	1.90	0.53
1:A:1070:TYR:CE2	1:A:1072:ALA:HB2	2.44	0.53
1:A:145:ILE:HG13	1:A:147:PRO:HD2	1.89	0.53
1:A:198:ILE:HD12	1:A:201:GLN:HE21	1.73	0.53
3:C:1162:LYS:NZ	3:C:1188:LEU:O	2.27	0.53
1:D:249:HIS:CE1	1:D:282:THR:HB	2.44	0.53
1:D:608:MET:HG2	1:D:615:ILE:HG12	1.90	0.53
3:F:968:ARG:HH21	3:F:1017:TYR:HE1	1.57	0.53
1:G:132:LEU:HD13	3:I:706:TYR:CG	2.44	0.53
3:I:1038:ILE:HB	3:I:1052:LEU:HB3	1.91	0.53
1:A:92:ILE:HD11	1:A:626:PRO:HG3	1.91	0.53
1:A:703:THR:HG22	1:A:704:ARG:H	1.73	0.53
3:C:747:LEU:HD21	3:C:750:PRO:HG3	1.90	0.53
1:D:906:SER:HB3	1:D:1010:CYS:HB2	1.90	0.53
3:I:634:LEU:HB2	3:I:647:LEU:HD21	1.91	0.53
3:C:705:ASP:OD2	3:C:725:GLY:HA3	2.09	0.52
1:D:236:VAL:HG23	1:D:237:ARG:HG2	1.91	0.52
1:A:946:THR:HG23	1:A:948:ALA:H	1.75	0.52
3:C:702:PHE:CD2	3:C:960:PRO:HA	2.43	0.52
3:C:1127:GLU:HG2	3:C:1138:VAL:HG22	1.91	0.52
1:G:78:THR:HG21	1:G:728:GLU:OE2	2.08	0.52
3:I:715:LEU:HD12	3:I:757:PRO:HB2	1.91	0.52
1:A:168:ARG:NH1	1:A:220:CYS:SG	2.83	0.52
1:A:377:ARG:HD3	1:A:424:ILE:HD12	1.92	0.52
1:A:398:MET:HE3	1:A:401:GLY:HA2	1.91	0.52
1:D:361:GLY:HA3	1:D:407:GLU:HB3	1.90	0.52
1:D:919:ASN:OD1	5:D:1203:NAG:O6	2.27	0.52
3:F:1107:LEU:HD11	3:F:1116:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD13	1:A:545:PRO:HB3	1.92	0.52
2:H:54:GLN:HG2	2:H:130:ARG:HD3	1.90	0.52
1:A:1034:VAL:HG21	1:A:1051:LEU:HD21	1.90	0.52
1:D:168:ARG:N	1:D:210:PHE:O	2.41	0.52
1:G:1018:THR:OG1	1:G:1019:TYR:N	2.42	0.52
1:A:869:ASP:H	1:A:878:GLN:HE22	1.58	0.52
1:D:604:TYR:HE1	1:D:619:VAL:HG13	1.74	0.52
1:A:126:ALA:HA	1:A:129:THR:HG22	1.92	0.52
2:B:40:MET:HE3	2:B:74:VAL:HG21	1.92	0.52
1:D:1078:PHE:CE2	1:D:1086:SER:HA	2.44	0.52
3:C:1026:ARG:O	3:C:1043:LEU:HG	2.09	0.52
1:D:1075:LYS:HA	1:D:1078:PHE:HE1	1.75	0.52
3:F:907:VAL:HB	3:F:908:PRO:CD	2.39	0.52
1:A:571:PRO:HA	1:A:608:MET:HG3	1.93	0.51
1:A:868:VAL:HA	1:A:878:GLN:NE2	2.24	0.51
1:D:479:LEU:HD21	1:D:545:PRO:HD3	1.91	0.51
1:A:962:PHE:HB3	2:B:125:PHE:CE1	2.45	0.51
1:D:165:SER:HB2	1:D:182:ARG:HD2	1.91	0.51
1:A:931:HIS:CD2	2:B:65:LEU:HB3	2.45	0.51
3:C:1107:LEU:HD11	3:C:1116:LEU:HD11	1.92	0.51
1:D:391:MET:HE1	1:D:456:ASN:HB3	1.91	0.51
3:F:1145:LEU:HD12	3:F:1164:GLN:HG3	1.91	0.51
3:I:987:ASN:ND2	3:I:1015:GLN:OE1	2.43	0.51
1:A:136:LEU:HD23	1:A:137:THR:H	1.75	0.51
1:A:479:LEU:HD21	1:A:545:PRO:HD3	1.91	0.51
3:F:631:GLU:OE2	3:F:633:PHE:CZ	2.63	0.51
1:A:901:LYS:HE3	1:A:916:TYR:HE1	1.74	0.51
1:G:168:ARG:HB3	1:G:210:PHE:HB3	1.93	0.51
1:D:131:HIS:CE1	1:D:180:PRO:HG2	2.45	0.51
1:D:658:PHE:HZ	1:D:1051:LEU:HB2	1.74	0.51
3:F:937:LEU:HD13	3:F:979:LEU:HD13	1.93	0.51
3:I:902:HIS:CE1	3:I:929:CYS:HB2	2.46	0.51
1:A:236:VAL:HG23	1:A:237:ARG:HG2	1.93	0.51
1:D:835:LEU:HD11	1:D:854:ILE:HG13	1.92	0.51
1:G:1034:VAL:HG21	1:G:1051:LEU:HD21	1.92	0.51
3:I:1038:ILE:HD12	3:I:1052:LEU:HD13	1.92	0.51
1:A:380:ASN:HD22	1:A:424:ILE:HG21	1.75	0.51
1:A:178:PHE:N	1:A:178:PHE:CD1	2.78	0.50
3:I:865:ASN:ND2	5:I:1302:NAG:O7	2.45	0.50
1:A:645:ARG:HA	1:A:761:LEU:HD13	1.93	0.50
1:D:380:ASN:HD22	1:D:424:ILE:HG21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD12	1:A:431:PRO:HD2	1.93	0.50
3:C:1072:TYR:HD2	3:C:1116:LEU:HD13	1.76	0.50
1:D:962:PHE:HB3	2:E:125:PHE:CE1	2.47	0.50
3:F:1072:TYR:OH	3:F:1131:LEU:O	2.29	0.50
3:I:982:ILE:HG12	3:I:989:ILE:HG12	1.94	0.50
1:A:192:LEU:HA	1:A:198:ILE:HD11	1.94	0.50
1:A:742:ILE:HD13	1:A:824:ILE:HD11	1.94	0.50
3:C:935:PHE:CD2	3:C:946:ARG:HD2	2.47	0.50
1:D:442:GLN:HG2	1:D:443:LEU:HD22	1.92	0.50
3:F:767:TRP:CE3	3:F:792:ARG:HD2	2.45	0.50
1:A:237:ARG:NH1	1:A:457:LEU:O	2.45	0.50
1:D:237:ARG:NH1	1:D:457:LEU:O	2.44	0.50
1:D:901:LYS:HE3	1:D:916:TYR:HE1	1.77	0.50
1:G:244:VAL:HG12	1:G:279:SER:HB2	1.92	0.50
1:G:300:LEU:HB2	1:G:341:THR:HG21	1.94	0.50
1:D:92:ILE:HD11	1:D:626:PRO:HG3	1.92	0.50
1:D:182:ARG:HG3	1:D:185:ASN:HD21	1.77	0.50
1:D:586:SER:OG	1:D:1011:GLU:OE2	2.29	0.50
1:G:132:LEU:HD12	1:G:133:THR:HG22	1.93	0.50
1:A:973:LEU:HB2	2:B:123:TYR:HE2	1.76	0.49
1:G:128:TYR:HB2	1:G:494:LEU:HD21	1.94	0.49
1:A:69:LEU:HD13	1:A:826:PHE:HE2	1.75	0.49
3:F:1143:ASN:HB2	3:F:1178:ARG:HH12	1.77	0.49
1:G:179:ASN:ND2	1:G:211:THR:HG21	2.27	0.49
1:G:227:ARG:HA	1:G:232:TYR:CD2	2.46	0.49
1:G:388:ASN:HB2	1:G:430:LEU:HD22	1.93	0.49
1:G:634:ASN:ND2	1:G:702:ASN:O	2.43	0.49
3:F:632:ALA:HB2	3:F:883:HIS:CD2	2.47	0.49
3:I:908:PRO:HD2	3:I:911:GLY:C	2.36	0.49
1:A:391:MET:HE1	1:A:456:ASN:HB3	1.94	0.49
1:A:557:ILE:HG22	1:A:560:PHE:HB2	1.94	0.49
1:D:1081:ILE:HG22	1:D:1083:GLY:H	1.76	0.49
1:G:861:LEU:HD12	1:G:884:LYS:HD2	1.94	0.49
1:A:473:ASP:OD2	1:A:475:MET:HB2	2.12	0.49
3:C:808:THR:HG22	3:C:815:ILE:HG12	1.95	0.49
3:C:1072:TYR:OH	3:C:1131:LEU:O	2.30	0.49
1:G:703:THR:HG22	1:G:704:ARG:H	1.77	0.49
1:A:74:LEU:HD13	1:A:824:ILE:HB	1.93	0.49
1:A:191:ASN:HB2	1:A:201:GLN:HE22	1.77	0.49
1:A:1077:CYS:HB3	1:A:1082:VAL:HG12	1.94	0.49
1:D:408:LEU:O	1:D:412:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASN:HB3	1:D:1008:PRO:HD3	1.93	0.49
3:I:855:ILE:HD12	3:I:873:LEU:HD12	1.93	0.49
1:A:327:HIS:NE2	1:A:362:ILE:HB	2.28	0.49
1:G:236:VAL:HG23	1:G:237:ARG:HG2	1.94	0.49
1:G:973:LEU:HB2	2:H:123:TYR:HE2	1.77	0.49
1:A:187:VAL:HG22	3:C:851:SER:HA	1.93	0.49
1:D:633:LEU:HD13	1:D:635:THR:HG23	1.94	0.49
2:E:44:ILE:HD11	2:E:46:TYR:CE1	2.48	0.49
3:F:767:TRP:CD2	3:F:792:ARG:HB3	2.48	0.49
3:F:902:HIS:CE1	3:F:929:CYS:HB2	2.47	0.49
3:F:1025:SER:HB2	3:F:1027:TYR:CE1	2.47	0.49
3:I:965:ARG:HB3	3:I:983:ASP:OD2	2.13	0.49
1:A:993:VAL:HG12	1:A:1000:LEU:HD23	1.95	0.49
1:D:202:TYR:HB3	1:D:212:VAL:HG23	1.95	0.49
1:D:829:ARG:NH2	1:D:867:LEU:HB2	2.27	0.49
1:G:380:ASN:ND2	1:G:424:ILE:HG21	2.28	0.49
1:A:856:GLU:HG3	1:A:858:ARG:H	1.78	0.49
1:D:119:ARG:O	1:D:123:VAL:HG23	2.12	0.49
3:F:1025:SER:HB2	3:F:1027:TYR:HE1	1.78	0.49
1:G:191:ASN:HB2	1:G:201:GLN:HE22	1.78	0.49
1:G:198:ILE:HD12	1:G:201:GLN:HE21	1.77	0.49
3:I:634:LEU:HD21	3:I:846:TYR:CZ	2.48	0.49
3:I:747:LEU:HD21	3:I:750:PRO:HG3	1.94	0.49
1:A:358:LEU:HD23	1:A:395:TYR:HB2	1.95	0.48
1:A:633:LEU:HD13	1:A:635:THR:HG23	1.95	0.48
1:A:805:THR:HG22	1:A:821:VAL:HG12	1.94	0.48
1:D:1034:VAL:HG21	1:D:1051:LEU:HD21	1.95	0.48
3:F:840:GLN:NE2	3:F:842:GLN:O	2.46	0.48
3:F:841:TYR:HB2	3:F:881:VAL:HG21	1.94	0.48
1:G:114:LEU:HD21	1:G:467:PHE:HZ	1.77	0.48
1:A:90:GLU:HG2	1:A:628:LYS:HG2	1.95	0.48
1:A:905:ASN:HD22	1:A:912:VAL:HG22	1.78	0.48
1:D:136:LEU:HA	1:D:180:PRO:HA	1.94	0.48
1:D:993:VAL:HG12	1:D:1000:LEU:HD23	1.94	0.48
1:G:391:MET:HE1	1:G:456:ASN:HB3	1.95	0.48
1:G:526:ASP:OD2	1:G:613:SER:HB2	2.13	0.48
3:I:763:TYR:HE1	3:I:775:ARG:HG3	1.78	0.48
1:D:172:THR:OG1	1:D:227:ARG:NH2	2.46	0.48
1:D:1002:ASN:OD1	1:D:1003:ALA:N	2.46	0.48
1:G:121:LYS:HD2	1:G:485:LYS:HD2	1.95	0.48
1:D:191:ASN:HB2	1:D:201:GLN:HE22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:ARG:HA	1:D:761:LEU:HD13	1.94	0.48
1:D:875:PRO:O	1:D:877:GLU:N	2.46	0.48
3:F:1121:SER:HA	3:F:1147:PRO:HD2	1.94	0.48
1:G:371:ASP:O	1:G:375:THR:HG23	2.14	0.48
1:A:168:ARG:HB3	1:A:210:PHE:HB3	1.94	0.48
1:A:829:ARG:NH2	1:A:867:LEU:HB2	2.28	0.48
3:F:974:PRO:HB2	3:F:1197:LEU:HB2	1.96	0.48
1:D:160:VAL:HG12	1:D:162:ARG:HG3	1.94	0.48
3:C:1084:GLU:HG2	3:C:1095:VAL:HA	1.96	0.48
3:F:1024:TYR:HA	3:F:1202:TYR:CE1	2.49	0.48
1:G:442:GLN:HG2	1:G:443:LEU:HD22	1.96	0.48
1:A:1078:PHE:CE2	1:A:1086:SER:HA	2.49	0.48
3:C:632:ALA:HB2	3:C:883:HIS:CD2	2.49	0.48
1:D:371:ASP:O	1:D:375:THR:HG23	2.14	0.48
1:G:249:HIS:HA	1:G:253:VAL:HG11	1.94	0.48
1:G:557:ILE:HG22	1:G:560:PHE:HB2	1.95	0.48
1:D:856:GLU:HG3	1:D:858:ARG:H	1.79	0.48
1:D:1060:SER:HB2	1:D:1083:GLY:HA3	1.96	0.48
1:G:511:THR:HG22	1:G:532:MET:HG2	1.96	0.48
1:D:116:VAL:HG12	1:D:499:VAL:HG21	1.96	0.47
1:G:116:VAL:HG12	1:G:499:VAL:HG21	1.96	0.47
1:A:180:PRO:HG2	1:A:183:ASP:HB3	1.96	0.47
1:D:660:GLN:NE2	1:D:762:MET:SD	2.87	0.47
1:G:836:MET:O	1:G:843:ASN:ND2	2.45	0.47
3:I:649:THR:C	3:I:651:ASN:H	2.22	0.47
1:A:1002:ASN:OD1	1:A:1003:ALA:N	2.47	0.47
3:C:982:ILE:HG12	3:C:989:ILE:HG12	1.97	0.47
1:D:148:SER:HA	1:D:160:VAL:HG22	1.96	0.47
1:G:1002:ASN:OD1	1:G:1003:ALA:N	2.48	0.47
1:A:356:ILE:HG13	1:A:393:LEU:HB2	1.96	0.47
1:A:591:LYS:HD2	1:A:621:ILE:HD13	1.96	0.47
1:D:571:PRO:HA	1:D:608:MET:HG3	1.96	0.47
1:D:784:ILE:HG23	1:D:802:ILE:HG23	1.97	0.47
3:C:688:ARG:HH12	3:C:734:LEU:HD22	1.79	0.47
1:D:284:ALA:C	1:D:286:ALA:H	2.23	0.47
1:D:876:LEU:CD2	1:D:970:ARG:HG2	2.45	0.47
3:F:982:ILE:HG12	3:F:989:ILE:HG12	1.96	0.47
1:A:319:LYS:HB3	1:A:320:PRO:HD2	1.95	0.47
1:A:875:PRO:HB3	1:A:966:SER:O	2.14	0.47
1:D:557:ILE:HG22	1:D:560:PHE:HB2	1.95	0.47
1:D:632:ASN:HA	1:D:717:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:PRO:O	2:E:104:PRO:C	2.58	0.47
3:F:749:SER:CB	3:F:751:ARG:HH21	2.27	0.47
1:G:192:LEU:HA	1:G:198:ILE:HD11	1.95	0.47
1:G:470:PRO:HD2	1:G:547:LEU:HG	1.97	0.47
3:I:991:LYS:HE2	3:I:1000:PHE:CD2	2.50	0.47
3:C:1042:ARG:HG3	3:C:1046:ARG:O	2.14	0.47
3:F:636:PHE:CZ	3:F:643:ARG:HB3	2.50	0.47
1:G:591:LYS:HD2	1:G:621:ILE:HD13	1.97	0.47
1:G:1070:TYR:CE2	1:G:1072:ALA:HB2	2.50	0.47
1:A:604:TYR:HE1	1:A:619:VAL:HG13	1.80	0.47
3:C:1160:ILE:HD12	3:C:1188:LEU:HB3	1.96	0.47
1:D:179:ASN:O	1:D:181:GLY:N	2.48	0.47
2:H:44:ILE:HD11	2:H:46:TYR:CE1	2.50	0.47
1:A:784:ILE:HG23	1:A:802:ILE:HG23	1.97	0.47
1:D:179:ASN:HD21	1:D:203:PHE:HD2	1.62	0.47
1:G:293:ASP:OD1	1:G:294:GLN:N	2.47	0.47
1:D:176:ARG:HD2	1:D:207:GLU:CG	2.45	0.46
1:D:358:LEU:HD23	1:D:395:TYR:HB2	1.97	0.46
3:F:738:HIS:ND1	3:F:902:HIS:HD2	2.13	0.46
1:G:645:ARG:HA	1:G:761:LEU:HD13	1.97	0.46
1:G:901:LYS:HE3	1:G:916:TYR:HE1	1.79	0.46
2:H:64:GLY:HA2	2:H:67:VAL:HG12	1.96	0.46
2:H:130:ARG:HA	2:H:135:ARG:NH1	2.30	0.46
1:G:155:ASN:HB3	1:G:159:ASN:ND2	2.29	0.46
1:G:200:TRP:HB2	1:G:500:ASP:HB2	1.97	0.46
1:A:634:ASN:ND2	1:A:702:ASN:O	2.45	0.46
1:A:887:LEU:HD22	1:A:938:TYR:HE2	1.81	0.46
1:A:912:VAL:N	1:A:989:CYS:O	2.43	0.46
3:C:747:LEU:HD12	3:C:766:GLU:OE2	2.15	0.46
1:D:1059:ASP:HB3	1:D:1064:THR:HB	1.97	0.46
3:I:841:TYR:HB2	3:I:881:VAL:HG21	1.97	0.46
1:A:112:ARG:O	1:A:116:VAL:HG23	2.15	0.46
3:C:665:SER:HB3	3:C:708:GLU:HG2	1.97	0.46
1:D:511:THR:HG22	1:D:532:MET:HG2	1.95	0.46
1:G:237:ARG:NH1	1:G:457:LEU:O	2.49	0.46
1:A:906:SER:HB3	1:A:1010:CYS:HB2	1.97	0.46
1:D:69:LEU:HD13	1:D:826:PHE:HE2	1.80	0.46
3:F:767:TRP:CE2	3:F:792:ARG:HB3	2.50	0.46
1:A:119:ARG:O	1:A:123:VAL:HG23	2.16	0.46
1:G:148:SER:C	1:G:150:MET:H	2.23	0.46
1:G:452:ARG:HH21	1:G:455:THR:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:542:LEU:HD13	1:G:545:PRO:HB3	1.97	0.46
1:A:216:HIS:NE2	1:A:475:MET:HB3	2.30	0.46
1:A:563:VAL:HG11	1:A:604:TYR:HD2	1.81	0.46
3:F:668:ASP:HB3	3:F:712:VAL:HG23	1.96	0.46
2:H:102:LEU:O	2:H:104:PRO:HD3	2.16	0.46
1:A:962:PHE:HB3	2:B:125:PHE:CD1	2.51	0.46
3:C:688:ARG:HH21	3:C:719:LEU:HD22	1.81	0.46
1:D:132:LEU:HD21	3:F:681:ILE:HD12	1.98	0.46
1:G:604:TYR:HE1	1:G:619:VAL:HG13	1.80	0.46
3:I:853:ARG:HG3	3:I:874:ASP:HB3	1.98	0.46
1:D:78:THR:HG21	1:D:728:GLU:OE2	2.15	0.46
1:G:552:ILE:HD12	1:G:560:PHE:HD2	1.81	0.46
1:G:670:MET:N	1:G:754:LEU:O	2.48	0.46
1:G:784:ILE:HG23	1:G:802:ILE:HG23	1.97	0.46
3:C:846:TYR:HE1	3:C:857:ARG:HG3	1.81	0.46
1:D:245:VAL:HB	1:D:280:VAL:HG22	1.98	0.46
1:D:264:ALA:HB1	1:D:450:VAL:HG11	1.97	0.46
1:A:132:LEU:HD13	3:C:706:TYR:CD1	2.51	0.45
1:A:869:ASP:H	1:A:878:GLN:NE2	2.14	0.45
1:G:584:SER:N	1:G:1007:ASN:HD22	2.14	0.45
1:G:775:LEU:HD13	1:G:1011:GLU:HG3	1.96	0.45
1:A:552:ILE:HD12	1:A:560:PHE:HD2	1.80	0.45
1:A:594:GLU:HG3	1:A:625:ILE:HG12	1.98	0.45
3:C:759:GLU:HG3	3:C:803:ARG:HH22	1.80	0.45
1:D:136:LEU:HD12	1:D:181:GLY:H	1.80	0.45
1:D:1077:CYS:HB3	1:D:1082:VAL:HG12	1.98	0.45
3:F:633:PHE:CD1	3:F:646:SER:HA	2.51	0.45
3:I:677:TYR:HE2	3:I:734:LEU:HD22	1.80	0.45
3:I:767:TRP:CD1	3:I:768:GLY:H	2.34	0.45
1:A:78:THR:HG21	1:A:728:GLU:OE2	2.16	0.45
1:A:156:PHE:HB2	1:A:477:ASP:OD1	2.16	0.45
3:F:715:LEU:HD12	3:F:757:PRO:HB2	1.96	0.45
3:I:634:LEU:HD11	3:I:846:TYR:CE2	2.51	0.45
3:I:751:ARG:HD2	3:I:793:ALA:O	2.16	0.45
1:D:782:GLY:O	1:D:804:HIS:NE2	2.47	0.45
1:D:898:PHE:CE1	1:D:922:LEU:HD22	2.51	0.45
3:F:1084:GLU:HG2	3:F:1095:VAL:HG22	1.98	0.45
3:I:846:TYR:CD2	3:I:879:ILE:HD12	2.51	0.45
3:I:1198:ASN:HB3	3:I:1201:GLU:HB2	1.99	0.45
1:A:202:TYR:HB3	1:A:212:VAL:HG23	1.98	0.45
1:A:744:ARG:NH1	1:A:792:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:993:VAL:O	1:G:1001:THR:OG1	2.34	0.45
1:D:131:HIS:ND1	1:D:180:PRO:HG2	2.32	0.45
1:D:181:GLY:O	1:D:182:ARG:HG2	2.17	0.45
1:G:999:ASN:OD1	5:G:1206:NAG:O3	2.26	0.45
1:A:123:VAL:HG22	3:C:875:TYR:OH	2.17	0.45
1:A:628:LYS:NZ	1:A:812:GLN:HE22	2.14	0.45
1:A:893:LEU:HD23	1:A:899:VAL:HG11	1.99	0.45
1:D:395:TYR:HB3	1:D:440:LEU:HD13	1.99	0.45
3:F:846:TYR:CE1	3:F:857:ARG:HG3	2.51	0.45
1:A:136:LEU:HB3	1:A:180:PRO:HA	1.98	0.45
1:A:511:THR:HG22	1:A:532:MET:HG2	1.97	0.45
1:A:556:ASN:HB3	1:A:1008:PRO:HD3	1.99	0.45
1:G:182:ARG:NE	1:G:188:LEU:HD11	2.32	0.45
1:G:284:ALA:C	1:G:286:ALA:H	2.24	0.45
1:G:742:ILE:HD13	1:G:824:ILE:HD11	1.99	0.45
3:F:991:LYS:HE2	3:F:1000:PHE:CD2	2.52	0.45
1:A:200:TRP:HB2	1:A:500:ASP:HB2	1.98	0.44
1:A:782:GLY:O	1:A:804:HIS:NE2	2.50	0.44
2:B:95:LEU:HB2	2:B:98:TYR:HB3	1.99	0.44
1:D:853:PHE:HE1	1:D:953:VAL:HG12	1.82	0.44
3:F:1198:ASN:HB3	3:F:1201:GLU:HB3	1.99	0.44
1:D:123:VAL:HG22	3:F:875:TYR:OH	2.17	0.44
1:D:554:TYR:CZ	1:D:907:PHE:HD2	2.35	0.44
3:I:855:ILE:HB	3:I:870:GLN:O	2.17	0.44
3:I:1042:ARG:NH2	3:I:1215:SER:O	2.51	0.44
1:A:598:GLU:OE1	1:A:598:GLU:N	2.49	0.44
1:D:552:ILE:HD12	1:D:560:PHE:HD2	1.81	0.44
1:D:962:PHE:CD2	2:E:70:PHE:HE1	2.35	0.44
1:G:119:ARG:O	1:G:123:VAL:HG23	2.17	0.44
2:H:40:MET:HE3	2:H:74:VAL:HG21	1.99	0.44
1:D:887:LEU:HD22	1:D:938:TYR:HE2	1.81	0.44
3:F:646:SER:HB3	3:F:649:THR:O	2.17	0.44
1:G:658:PHE:CZ	1:G:1051:LEU:HB2	2.51	0.44
1:A:148:SER:OG	1:A:160:VAL:HG23	2.17	0.44
1:A:395:TYR:CD1	1:A:438:MET:HB2	2.52	0.44
1:A:853:PHE:HE1	1:A:953:VAL:HG12	1.83	0.44
3:C:1112:ARG:CZ	3:C:1195:LYS:HE3	2.47	0.44
1:A:128:TYR:HB2	1:A:494:LEU:HD21	2.00	0.44
1:A:128:TYR:O	1:A:132:LEU:HG	2.17	0.44
2:B:64:GLY:HA2	2:B:67:VAL:HG12	1.99	0.44
3:C:681:ILE:HG22	3:C:707:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:937:LEU:HD13	3:I:979:LEU:HD13	1.99	0.44
1:A:1078:PHE:CD2	1:A:1086:SER:HA	2.53	0.44
3:C:902:HIS:CE1	3:C:929:CYS:HB2	2.53	0.44
1:D:249:HIS:HA	1:D:253:VAL:HG11	1.99	0.44
1:G:159:ASN:OD1	1:G:216:HIS:HB3	2.18	0.44
1:G:327:HIS:NE2	1:G:362:ILE:HB	2.33	0.44
1:G:1012:VAL:O	1:G:1014:GLN:N	2.44	0.44
1:A:942:ARG:HH12	1:A:945:GLY:H	1.66	0.44
3:C:636:PHE:CZ	3:C:643:ARG:HB3	2.52	0.44
1:A:1004:GLU:C	1:A:1006:ARG:H	2.25	0.44
1:D:191:ASN:CB	1:D:201:GLN:HE22	2.31	0.44
1:D:966:SER:HA	2:E:123:TYR:CD1	2.53	0.44
2:E:103:PRO:O	2:E:105:CYS:N	2.50	0.44
1:G:487:CYS:HB2	1:G:494:LEU:HB2	2.00	0.44
1:A:587:TRP:HE1	1:A:1011:GLU:HG2	1.83	0.43
1:A:644:HIS:CD2	1:A:670:MET:HG3	2.53	0.43
1:D:164:VAL:HG13	1:D:182:ARG:HH21	1.83	0.43
1:D:698:TYR:CE2	1:D:711:LEU:HD12	2.53	0.43
1:G:632:ASN:OD1	1:G:717:ASN:ND2	2.44	0.43
1:G:1004:GLU:C	1:G:1006:ARG:H	2.26	0.43
1:A:572:LEU:HD12	1:D:573:GLY:HA2	2.00	0.43
3:C:841:TYR:HB2	3:C:881:VAL:HG11	1.99	0.43
3:C:937:LEU:HD13	3:C:979:LEU:HD13	1.99	0.43
3:F:776:ALA:HB2	3:F:783:ARG:HG2	2.00	0.43
1:G:202:TYR:HB3	1:G:212:VAL:HG23	1.99	0.43
1:A:132:LEU:HD13	3:C:706:TYR:HB3	1.99	0.43
1:A:574:SER:O	1:D:571:PRO:HD2	2.18	0.43
1:D:580:PRO:HA	1:D:599:ALA:HA	1.99	0.43
3:C:767:TRP:CE3	3:C:792:ARG:HD2	2.53	0.43
2:H:55:PHE:CE1	2:H:130:ARG:HD2	2.54	0.43
3:I:1025:SER:OG	3:I:1207:CYS:HB3	2.19	0.43
1:A:368:SER:O	1:A:372:LYS:HG3	2.19	0.43
1:A:413:ASP:OD2	1:A:421:LYS:NZ	2.38	0.43
1:G:805:THR:HG22	1:G:821:VAL:HG12	2.00	0.43
2:H:61:ASP:O	2:H:65:LEU:HG	2.18	0.43
3:I:1037:VAL:HG12	3:I:1053:LYS:HG3	2.01	0.43
1:A:78:THR:HG21	1:A:728:GLU:CD	2.43	0.43
1:A:442:GLN:HG2	1:A:443:LEU:HD22	1.99	0.43
1:D:112:ARG:O	1:D:116:VAL:HG23	2.19	0.43
1:D:628:LYS:NZ	1:D:812:GLN:HE22	2.16	0.43
3:F:1216:HIS:ND1	3:F:1243:CYS:SG	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:856:GLU:HG3	1:G:858:ARG:H	1.83	0.43
1:G:1077:CYS:HB3	1:G:1082:VAL:HG12	2.01	0.43
2:H:104:PRO:HB2	2:H:105:CYS:H	1.65	0.43
3:I:1025:SER:HB2	3:I:1027:TYR:CE1	2.54	0.43
1:D:178:PHE:CE1	1:D:207:GLU:OE2	2.72	0.43
1:G:829:ARG:NH2	1:G:867:LEU:HB2	2.32	0.43
3:I:738:HIS:ND1	3:I:902:HIS:HD2	2.17	0.43
3:I:751:ARG:HG3	3:I:752:ALA:H	1.84	0.43
1:A:145:ILE:C	1:A:147:PRO:HD2	2.43	0.43
1:A:585:LEU:HD12	1:A:587:TRP:HD1	1.84	0.43
2:B:55:PHE:HB2	2:B:57:HIS:CD2	2.54	0.43
1:D:587:TRP:HE1	1:D:1011:GLU:HG2	1.83	0.43
1:D:807:HIS:CE1	1:D:813:LEU:HG	2.53	0.43
3:I:668:ASP:HB3	3:I:712:VAL:HG23	2.00	0.43
1:A:1012:VAL:C	1:A:1014:GLN:N	2.77	0.43
2:B:50:HIS:HB2	2:B:94:CYS:SG	2.59	0.43
2:B:73:LEU:O	2:B:76:ILE:HG22	2.19	0.43
3:C:965:ARG:HG3	3:C:985:ARG:HD3	2.00	0.43
1:D:63:ALA:HB2	1:D:944:PRO:HD2	2.01	0.43
1:G:746:TYR:HB3	1:G:756:ILE:HG22	2.01	0.43
1:D:644:HIS:CD2	1:D:670:MET:HG3	2.54	0.43
1:D:901:LYS:HG2	1:D:916:TYR:CE1	2.54	0.43
3:I:1055:GLU:OE2	3:I:1056:GLN:HG2	2.19	0.43
1:A:199:LYS:HD3	1:A:480:ILE:HD11	2.00	0.42
1:D:372:LYS:HG2	1:D:410:PHE:CE1	2.54	0.42
1:D:1078:PHE:HE2	1:D:1086:SER:HA	1.84	0.42
3:F:908:PRO:HD2	3:F:911:GLY:HA3	2.01	0.42
3:F:1025:SER:OG	3:F:1207:CYS:HB3	2.19	0.42
1:G:108:GLU:HA	1:G:111:ASN:HB2	2.01	0.42
1:G:327:HIS:HB2	1:G:375:THR:HG21	2.00	0.42
1:G:742:ILE:HG12	1:G:826:PHE:HE1	1.83	0.42
3:C:679:THR:HG22	3:C:686:ILE:HG12	1.99	0.42
3:C:738:HIS:ND1	3:C:902:HIS:HD2	2.17	0.42
3:C:991:LYS:HE2	3:C:1000:PHE:CD2	2.54	0.42
1:D:137:THR:HG21	3:F:768:GLY:HA2	2.01	0.42
1:D:668:THR:HG23	1:D:759:GLY:HA3	2.00	0.42
1:D:1004:GLU:HA	1:D:1006:ARG:HD2	2.00	0.42
1:G:1011:GLU:HB3	1:G:1012:VAL:H	1.58	0.42
3:I:1018:ASP:OD1	3:I:1019:LEU:N	2.51	0.42
1:A:501:VAL:HG21	1:A:506:ILE:HD11	2.01	0.42
1:A:1011:GLU:O	1:A:1013:HIS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ARG:O	1:G:116:VAL:HG23	2.20	0.42
1:G:372:LYS:HG2	1:G:410:PHE:CE1	2.54	0.42
1:G:585:LEU:HD12	1:G:587:TRP:HD1	1.83	0.42
3:I:974:PRO:HB2	3:I:1197:LEU:HB2	2.00	0.42
3:I:1190:ASP:OD1	3:I:1191:ILE:N	2.52	0.42
1:A:69:LEU:HD13	1:A:826:PHE:CE2	2.53	0.42
1:A:284:ALA:C	1:A:286:ALA:H	2.26	0.42
1:A:293:ASP:OD1	1:A:294:GLN:N	2.48	0.42
3:C:1190:ASP:OD1	3:C:1191:ILE:N	2.53	0.42
1:D:1004:GLU:C	1:D:1006:ARG:H	2.28	0.42
1:G:898:PHE:CE1	1:G:922:LEU:HD22	2.55	0.42
3:I:916:CYS:HB3	3:I:920:TYR:HB2	2.00	0.42
1:A:122:GLN:HB3	3:C:639:ARG:NH2	2.34	0.42
1:A:962:PHE:CD1	2:B:125:PHE:HA	2.54	0.42
1:G:136:LEU:HD22	3:I:792:ARG:HD3	2.01	0.42
1:G:242:HIS:HB2	1:G:353:MET:HG2	2.02	0.42
1:A:1037:ARG:O	1:A:1040:GLN:HG2	2.19	0.42
3:C:761:PHE:CD1	3:C:775:ARG:HD3	2.55	0.42
1:D:176:ARG:HH11	1:D:207:GLU:HG3	1.84	0.42
3:I:976:ASP:OD2	3:I:1026:ARG:NH2	2.53	0.42
1:A:582:ASN:O	1:A:583:SER:OG	2.31	0.42
1:A:668:THR:HG23	1:A:759:GLY:HA3	2.01	0.42
3:C:1143:ASN:HB2	3:C:1178:ARG:NH1	2.35	0.42
1:D:133:THR:O	3:F:751:ARG:NH1	2.52	0.42
1:D:209:ILE:O	1:D:209:ILE:HG13	2.19	0.42
1:D:893:LEU:HD23	1:D:899:VAL:HG11	2.00	0.42
1:G:667:PRO:HB3	1:G:757:TYR:HB2	2.00	0.42
1:G:1037:ARG:O	1:G:1040:GLN:HG2	2.18	0.42
1:A:547:LEU:O	1:A:549:THR:N	2.52	0.42
1:D:250:GLY:HA2	1:D:321:SER:C	2.44	0.42
1:D:501:VAL:HG21	1:D:506:ILE:HD11	2.01	0.42
1:D:742:ILE:HG12	1:D:826:PHE:HE1	1.83	0.42
2:E:64:GLY:HA2	2:E:67:VAL:HG12	2.01	0.42
3:F:702:PHE:CD2	3:F:960:PRO:HA	2.55	0.42
3:F:1190:ASP:OD1	3:F:1191:ILE:N	2.52	0.42
1:G:556:ASN:HB3	1:G:1008:PRO:HD3	2.02	0.42
3:I:744:TRP:CD1	3:I:745:LYS:HG3	2.54	0.42
1:A:132:LEU:HD12	1:A:133:THR:HG22	2.02	0.42
1:A:622:GLN:HB3	1:A:625:ILE:HD13	2.01	0.42
1:D:241:LYS:HE2	1:D:276:ASP:OD2	2.20	0.42
1:D:293:ASP:OD1	1:D:294:GLN:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:827:THR:OG1	1:D:1049:GLY:HA2	2.20	0.42
3:F:918:ALA:HB3	3:F:957:ILE:HD13	2.02	0.42
1:G:354:VAL:HG22	1:G:391:MET:HB3	2.00	0.42
1:G:473:ASP:OD2	1:G:475:MET:HB2	2.19	0.42
1:A:630:LEU:HD11	1:A:633:LEU:HD23	2.02	0.42
1:A:670:MET:N	1:A:754:LEU:O	2.50	0.42
1:A:868:VAL:HA	1:A:878:GLN:HE22	1.84	0.42
2:B:55:PHE:CE1	2:B:130:ARG:HD2	2.54	0.42
1:D:805:THR:HG22	1:D:821:VAL:HG12	2.02	0.42
2:E:55:PHE:HB2	2:E:57:HIS:HD2	1.84	0.42
3:I:846:TYR:HD1	3:I:856:GLU:O	2.02	0.42
1:A:1004:GLU:HA	1:A:1006:ARG:HD2	2.01	0.41
1:G:199:LYS:HE2	1:G:200:TRP:NE1	2.35	0.41
1:G:199:LYS:HZ1	1:G:477:ASP:CG	2.27	0.41
3:I:1084:GLU:HG2	3:I:1095:VAL:HA	2.02	0.41
1:A:477:ASP:CG	1:A:478:GLY:H	2.28	0.41
1:A:554:TYR:CZ	1:A:907:PHE:HD2	2.38	0.41
3:C:668:ASP:HB3	3:C:712:VAL:HG23	2.00	0.41
1:D:364:SER:HB2	1:D:367:SER:HB2	2.02	0.41
3:F:747:LEU:HD11	3:F:750:PRO:HB3	2.02	0.41
3:F:1014:ILE:HD12	3:F:1030:TRP:CH2	2.55	0.41
2:H:95:LEU:O	2:H:98:TYR:HB2	2.21	0.41
1:A:159:ASN:HD21	1:A:214:PRO:CG	2.33	0.41
1:A:1041:ARG:HH12	1:A:1050:VAL:HG11	1.85	0.41
3:C:767:TRP:NE1	3:C:793:ALA:O	2.45	0.41
1:D:395:TYR:CD1	1:D:438:MET:HB2	2.55	0.41
3:I:1072:TYR:OH	3:I:1131:LEU:O	2.39	0.41
1:D:176:ARG:NH1	1:D:207:GLU:HG3	2.35	0.41
1:G:167:ASP:OD1	1:G:167:ASP:N	2.51	0.41
1:G:184:LEU:HD22	1:G:184:LEU:H	1.85	0.41
3:I:755:LEU:O	3:I:800:TYR:OH	2.31	0.41
3:I:918:ALA:HB3	3:I:957:ILE:HD13	2.02	0.41
1:D:237:ARG:NH1	1:D:454:TYR:O	2.53	0.41
1:D:319:LYS:HB3	1:D:320:PRO:HD2	2.02	0.41
1:D:477:ASP:CG	1:D:478:GLY:H	2.29	0.41
1:G:668:THR:HG23	1:G:759:GLY:HA3	2.01	0.41
3:I:1048:VAL:HG13	3:I:1216:HIS:HD2	1.85	0.41
1:A:184:LEU:H	1:A:184:LEU:HD22	1.85	0.41
3:C:638:ARG:NH2	3:C:874:ASP:OD1	2.48	0.41
1:D:140:GLN:HG2	1:D:167:ASP:HB3	2.03	0.41
3:F:1199:LEU:O	3:F:1203:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:LEU:HG	1:G:262:LYS:HE3	2.02	0.41
2:H:105:CYS:O	2:H:108:VAL:HG12	2.21	0.41
3:I:636:PHE:CZ	3:I:643:ARG:HB3	2.55	0.41
3:I:1117:PHE:HD2	3:I:1157:LEU:HD13	1.86	0.41
4:K:1:NAG:H62	4:K:2:NAG:H82	2.03	0.41
1:A:122:GLN:HA	1:A:125:GLU:HB2	2.01	0.41
1:A:327:HIS:CE1	1:A:362:ILE:HB	2.54	0.41
1:A:697:ALA:O	1:A:701:ASP:HB2	2.20	0.41
3:C:1027:TYR:CD1	3:C:1042:ARG:HG2	2.55	0.41
3:F:920:TYR:CD1	3:F:932:PRO:HD3	2.55	0.41
3:F:1097:PHE:CE1	3:F:1136:ARG:HD2	2.55	0.41
1:G:356:ILE:HG13	1:G:393:LEU:HB2	2.02	0.41
1:G:395:TYR:HB3	1:G:440:LEU:HD13	2.03	0.41
1:G:479:LEU:HD21	1:G:545:PRO:HD3	2.03	0.41
1:G:1078:PHE:CE2	1:G:1086:SER:HA	2.55	0.41
2:H:73:LEU:O	2:H:76:ILE:HG22	2.20	0.41
3:I:1125:ARG:NE	3:I:1127:GLU:OE2	2.53	0.41
2:B:55:PHE:HB2	2:B:57:HIS:HD2	1.86	0.41
3:C:675:ARG:HB3	3:C:677:TYR:CE1	2.55	0.41
3:C:1063:VAL:HG21	3:C:1108:ALA:HA	2.02	0.41
1:D:150:MET:HB3	1:D:159:ASN:O	2.21	0.41
1:D:921:SER:HB3	5:D:1203:NAG:O6	2.21	0.41
2:E:55:PHE:CE1	2:E:130:ARG:HD2	2.56	0.41
3:F:988:MET:HE2	3:F:1004:VAL:HG23	2.02	0.41
1:G:136:LEU:HB3	1:G:180:PRO:HA	2.03	0.41
1:G:182:ARG:HG3	1:G:184:LEU:HD23	2.03	0.41
1:G:183:ASP:HB3	3:I:792:ARG:NH2	2.29	0.41
3:I:1097:PHE:CE1	3:I:1136:ARG:HD2	2.56	0.41
1:A:408:LEU:O	1:A:412:ARG:HG3	2.21	0.41
1:A:550:ASP:OD1	1:A:551:ILE:N	2.54	0.41
2:B:117:SER:N	2:B:118:PRO:HD2	2.36	0.41
3:C:916:CYS:HB3	3:C:920:TYR:HB2	2.03	0.41
3:C:935:PHE:N	3:C:935:PHE:CD1	2.88	0.41
1:D:622:GLN:HB3	1:D:625:ILE:HD13	2.03	0.41
2:E:40:MET:HE3	2:E:74:VAL:HG21	2.02	0.41
2:E:55:PHE:HB2	2:E:57:HIS:CD2	2.56	0.41
2:E:73:LEU:O	2:E:76:ILE:HG22	2.20	0.41
3:F:841:TYR:HB2	3:F:881:VAL:HG11	2.03	0.41
1:G:624:GLU:HG2	1:G:625:ILE:HD12	2.03	0.41
1:G:644:HIS:CD2	1:G:670:MET:HG3	2.56	0.41
3:I:744:TRP:CE2	3:I:955:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:749:SER:HB3	3:I:767:TRP:CZ2	2.56	0.41
3:I:1025:SER:HB2	3:I:1027:TYR:HE1	1.85	0.41
5:I:1303:NAG:O7	5:I:1303:NAG:O3	2.37	0.41
1:A:65:GLN:HE21	1:A:838:LEU:HD21	1.85	0.41
1:A:213:PHE:CD1	1:A:214:PRO:HA	2.56	0.41
1:D:165:SER:C	1:D:182:ARG:HE	2.28	0.41
1:D:315:VAL:C	1:D:317:SER:H	2.29	0.41
3:F:677:TYR:CE2	3:F:734:LEU:HD22	2.53	0.41
1:G:186:SER:OG	3:I:833:PRO:HB2	2.21	0.41
2:H:117:SER:N	2:H:118:PRO:HD2	2.36	0.41
1:A:651:GLN:HG3	1:A:652:PRO:HD3	2.03	0.40
3:C:688:ARG:NH2	3:C:719:LEU:HB2	2.35	0.40
3:C:715:LEU:HD12	3:C:757:PRO:HB2	2.04	0.40
1:D:874:ALA:C	1:D:876:LEU:H	2.29	0.40
1:D:888:VAL:O	1:D:892:ILE:HG12	2.21	0.40
2:E:61:ASP:O	2:E:65:LEU:HG	2.20	0.40
3:F:766:GLU:C	3:F:767:TRP:HD1	2.29	0.40
1:G:226:HIS:CE1	1:G:232:TYR:HB2	2.56	0.40
1:G:367:SER:HB2	1:G:370:GLU:HB3	2.03	0.40
3:I:759:GLU:HG3	3:I:803:ARG:NH2	2.36	0.40
1:A:855:MET:HG2	1:A:856:GLU:O	2.22	0.40
1:A:874:ALA:HB1	1:A:875:PRO:HA	2.02	0.40
3:C:965:ARG:CG	3:C:985:ARG:HD3	2.51	0.40
3:C:1142:SER:O	3:C:1178:ARG:NH1	2.50	0.40
1:D:159:ASN:HD21	1:D:214:PRO:CG	2.32	0.40
1:D:180:PRO:HB3	3:F:792:ARG:HH12	1.86	0.40
1:D:855:MET:HG2	1:D:856:GLU:O	2.21	0.40
2:E:46:TYR:HD1	2:E:46:TYR:O	2.05	0.40
3:F:1030:TRP:HZ2	5:F:1304:NAG:H61	1.86	0.40
1:G:373:LYS:O	1:G:377:ARG:N	2.54	0.40
1:G:829:ARG:HG2	1:G:1048:PHE:CD1	2.56	0.40
1:G:1081:ILE:HB	1:G:1084:ALA:HB2	2.02	0.40
1:A:80:GLN:HA	1:A:806:ILE:HG23	2.02	0.40
1:A:807:HIS:CE1	1:A:813:LEU:HG	2.56	0.40
1:A:1034:VAL:O	1:A:1036:SER:N	2.46	0.40
3:C:926:ASN:HB2	5:C:1302:NAG:H2	2.03	0.40
1:G:395:TYR:CD1	1:G:438:MET:HB2	2.57	0.40
1:G:477:ASP:CG	1:G:478:GLY:H	2.30	0.40
3:I:681:ILE:HG22	3:I:707:PRO:HD2	2.04	0.40
1:A:182:ARG:HD2	1:A:184:LEU:HD23	2.03	0.40
1:G:100:GLN:O	1:G:104:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:598:GLU:N	1:G:598:GLU:OE1	2.54	0.40
1:A:137:THR:HG21	3:C:768:GLY:HA2	2.03	0.40
1:A:593:ARG:NH2	1:A:622:GLN:O	2.55	0.40
3:F:1143:ASN:HB2	3:F:1178:ARG:NH1	2.36	0.40
1:G:408:LEU:O	1:G:412:ARG:HG3	2.21	0.40
1:G:588:HIS:HA	1:G:621:ILE:HG12	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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	1024/1102 (93%)	917 (90%)	100 (10%)	7 (1%)	18	55
1	D	1024/1102 (93%)	910 (89%)	104 (10%)	10 (1%)	12	47
1	G	1024/1102 (93%)	915 (89%)	97 (10%)	12 (1%)	10	43
2	B	102/140 (73%)	94 (92%)	7 (7%)	1 (1%)	12	47
2	E	102/140 (73%)	92 (90%)	8 (8%)	2 (2%)	6	31
2	H	102/140 (73%)	93 (91%)	8 (8%)	1 (1%)	12	47
3	C	605/628 (96%)	551 (91%)	53 (9%)	1 (0%)	43	78
3	F	605/628 (96%)	551 (91%)	52 (9%)	2 (0%)	36	72
3	I	605/628 (96%)	553 (91%)	50 (8%)	2 (0%)	36	72
All	All	5193/5610 (93%)	4676 (90%)	479 (9%)	38 (1%)	18	55

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	990	PRO
1	A	1008	PRO

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Mol	Chain	Res	Type
2	B	104	PRO
1	D	1008	PRO
2	E	104	PRO
1	A	147	PRO
1	A	176	ARG
1	A	1012	VAL
1	D	990	PRO
3	F	907	VAL
1	G	990	PRO
1	G	1008	PRO
2	H	104	PRO
1	A	490	GLY
1	D	876	LEU
1	D	1012	VAL
2	E	102	LEU
3	F	908	PRO
1	G	135	PRO
1	G	148	SER
3	I	907	VAL
1	D	148	SER
1	G	143	CYS
1	G	490	GLY
1	G	1001	THR
1	G	1033	CYS
1	D	1022	ILE
1	G	161	SER
1	G	1010	CYS
1	G	1016	PRO
1	D	873	HIS
1	D	1013	HIS
1	A	1022	ILE
1	D	490	GLY
3	C	788	PRO
1	G	55	ILE
1	D	55	ILE
3	I	788	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 X-ray entries followed by that with respect to entries of similar resolution.

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	921/979 (94%)	916 (100%)	5 (0%)	81	82
1	D	921/979 (94%)	919 (100%)	2 (0%)	87	86
1	G	921/979 (94%)	913 (99%)	8 (1%)	70	77
2	B	95/124 (77%)	95 (100%)	0	100	100
2	E	95/124 (77%)	94 (99%)	1 (1%)	65	74
2	H	95/124 (77%)	94 (99%)	1 (1%)	65	74
3	C	530/548 (97%)	528 (100%)	2 (0%)	84	83
3	F	530/548 (97%)	529 (100%)	1 (0%)	87	86
3	I	530/548 (97%)	529 (100%)	1 (0%)	87	86
All	All	4638/4953 (94%)	4617 (100%)	21 (0%)	81	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	178	PHE
1	A	365	LYS
1	A	953	VAL
1	A	1075	LYS
3	C	935	PHE
3	C	1097	PHE
1	D	582	ASN
1	D	953	VAL
2	E	46	TYR
3	F	677	TYR
1	G	160	VAL
1	G	166	CYS
1	G	454	TYR
1	G	878	GLN
1	G	953	VAL
1	G	1010	CYS
1	G	1014	GLN
1	G	1019	TYR
2	H	46	TYR
3	I	677	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	174	ASN
1	A	185	ASN
1	A	201	GLN
1	A	226	HIS
1	A	332	HIS
1	A	380	ASN
1	A	456	ASN
1	A	685	GLN
1	A	724	HIS
1	A	812	GLN
1	A	878	GLN
2	B	50	HIS
3	C	840	GLN
3	C	902	HIS
3	C	1211	ASN
3	C	1233	HIS
1	D	65	GLN
1	D	120	ASN
1	D	122	GLN
1	D	159	ASN
1	D	195	ASN
1	D	201	GLN
1	D	257	GLN
1	D	380	ASN
1	D	514	GLN
1	D	660	GLN
1	D	685	GLN
1	D	812	GLN
1	D	878	GLN
1	D	931	HIS
1	D	1065	HIS
2	E	50	HIS
2	E	99	HIS
3	F	902	HIS
3	F	952	GLN
3	F	1065	ASN
3	F	1192	HIS
1	G	65	GLN
1	G	120	ASN
1	G	140	GLN
1	G	201	GLN

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Mol	Chain	Res	Type
1	G	275	HIS
1	G	380	ASN
1	G	445	ASN
1	G	514	GLN
1	G	739	ASN
1	G	905	ASN
1	G	931	HIS
1	G	1040	GLN
2	H	50	HIS
3	I	813	ASN
3	I	870	GLN
3	I	902	HIS
3	I	940	GLN
3	I	987	ASN
3	I	1015	GLN
3	I	1146	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](#)

4 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	$\# Z > 2$
4	NAG	J	1	4	14,14,15	1.60	2 (14%)	17,19,21	1.34	2 (11%)
4	NAG	J	2	4	14,14,15	0.87	1 (7%)	17,19,21	1.49	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	K	1	3,4	14,14,15	0.73	1 (7%)	17,19,21	2.21	5 (29%)
4	NAG	K	2	4	14,14,15	0.57	0	17,19,21	1.48	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	1	4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	3,4	-	6/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-5.43	1.34	1.43
4	J	2	NAG	O5-C1	-2.35	1.39	1.43
4	K	1	NAG	O5-C1	-2.21	1.40	1.43
4	J	1	NAG	C1-C2	-2.16	1.49	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C3-C4-C5	4.79	118.92	110.23
4	K	1	NAG	C2-N2-C7	4.79	129.32	122.90
4	K	2	NAG	C3-C4-C5	4.71	118.77	110.23
4	K	1	NAG	C1-C2-N2	4.49	117.51	110.43
4	J	1	NAG	C3-C4-C5	4.41	118.23	110.23
4	K	1	NAG	C1-O5-C5	3.21	116.49	112.19
4	K	1	NAG	C3-C4-C5	3.17	115.99	110.23
4	K	1	NAG	C4-C3-C2	2.86	115.22	111.02
4	J	1	NAG	C4-C3-C2	2.19	114.23	111.02
4	J	2	NAG	O5-C5-C4	2.03	115.77	110.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

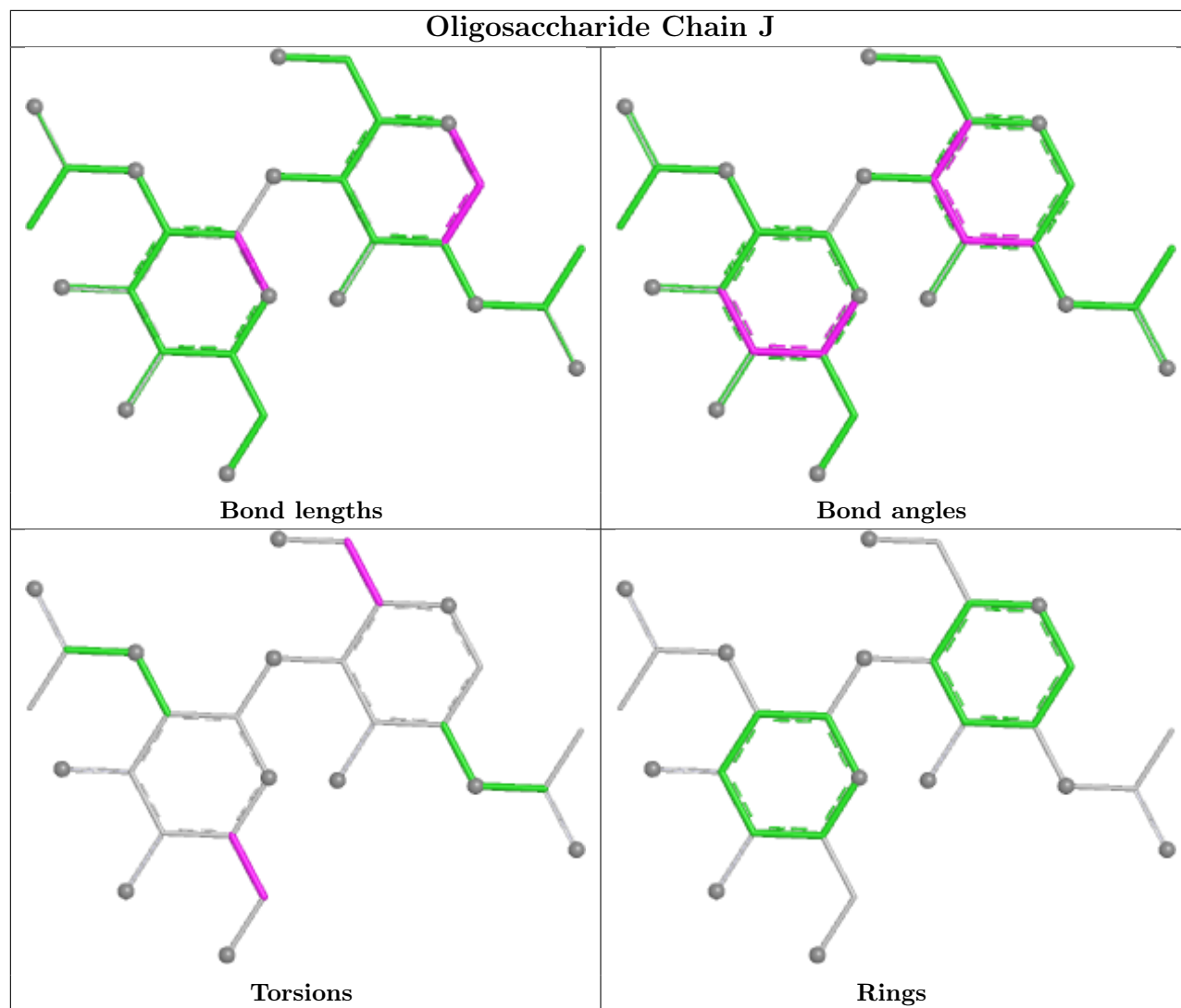
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C1-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7

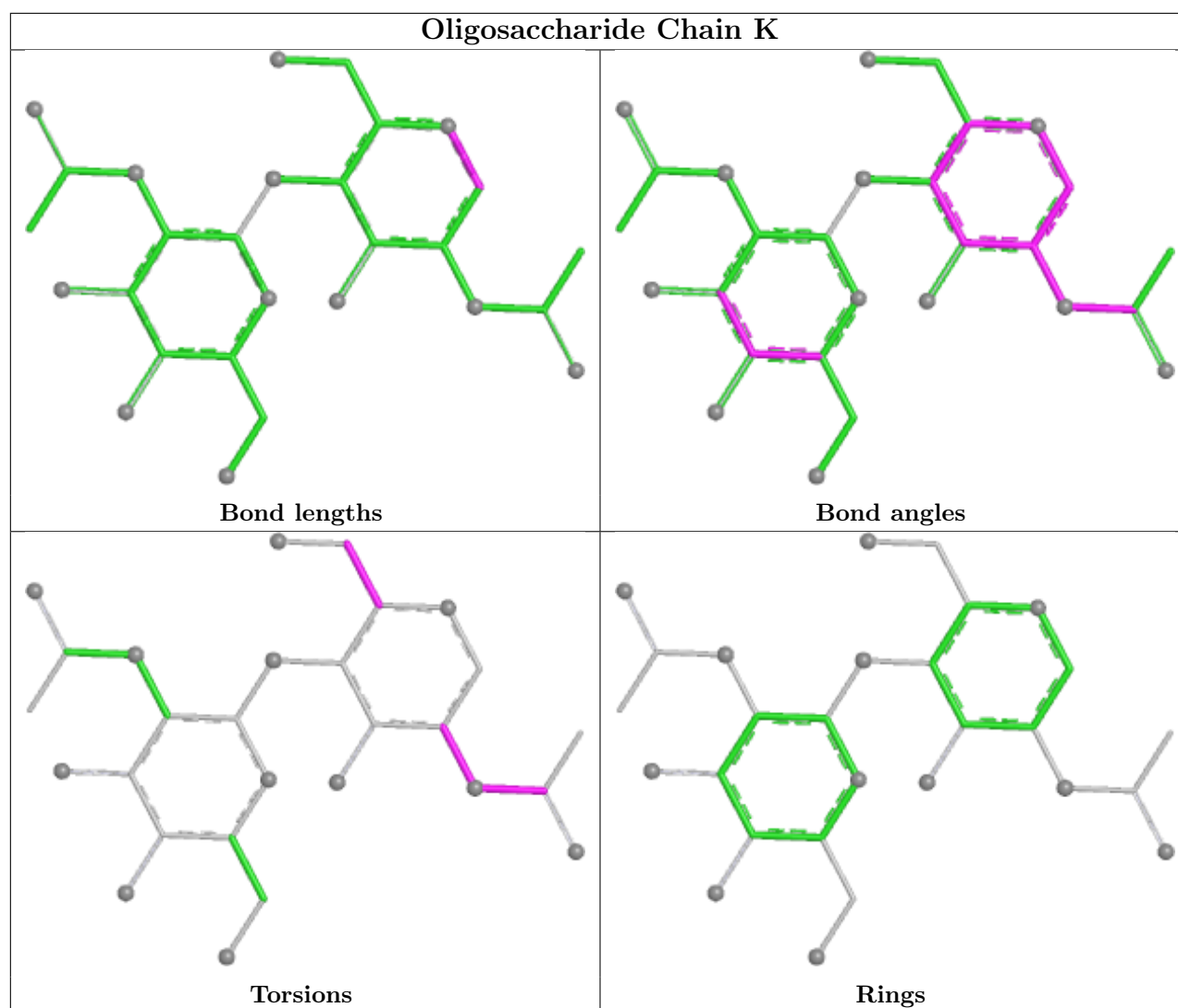
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	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](#)

30 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	D	1201	1	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	G	1203	1	14,14,15	0.46	0	17,19,21	0.58	0
5	NAG	F	1304	-	14,14,15	0.23	0	17,19,21	0.66	0

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	0.21	0	17,19,21	0.51	0
5	NAG	F	1303	3	14,14,15	0.59	0	17,19,21	0.49	0
5	NAG	C	1302	3	14,14,15	0.56	0	17,19,21	0.38	0
5	NAG	I	1301	3	14,14,15	0.33	0	17,19,21	0.50	0
5	NAG	I	1302	3	14,14,15	0.39	0	17,19,21	0.54	0
5	NAG	F	1305	-	14,14,15	1.24	1 (7%)	17,19,21	1.13	1 (5%)
5	NAG	D	1205	1	14,14,15	0.97	1 (7%)	17,19,21	2.10	1 (5%)
5	NAG	F	1301	3	14,14,15	0.35	0	17,19,21	0.43	0
5	NAG	I	1303	3	14,14,15	0.55	0	17,19,21	0.50	0
5	NAG	H	200	-	14,14,15	0.17	0	17,19,21	0.44	0
5	NAG	C	1304	-	14,14,15	0.82	1 (7%)	17,19,21	0.54	0
5	NAG	A	1203	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	F	1302	3	14,14,15	0.35	0	17,19,21	0.51	0
5	NAG	G	1206	1	14,14,15	0.54	0	17,19,21	0.41	0
5	NAG	A	1201	1	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	G	1202	1	14,14,15	0.25	0	17,19,21	0.48	0
5	NAG	E	200	-	14,14,15	0.19	0	17,19,21	0.51	0
5	NAG	A	1202	1	14,14,15	0.52	0	17,19,21	0.65	1 (5%)
5	NAG	A	1204	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	G	1204	1	14,14,15	0.24	0	17,19,21	0.36	0
5	NAG	D	1204	1	14,14,15	0.17	0	17,19,21	0.42	0
5	NAG	G	1205	1	14,14,15	0.18	0	17,19,21	0.40	0
5	NAG	D	1202	1	14,14,15	0.54	0	17,19,21	0.58	0
5	NAG	C	1303	3	14,14,15	1.71	2 (14%)	17,19,21	1.30	1 (5%)
5	NAG	D	1203	-	14,14,15	0.37	0	17,19,21	0.38	0
5	NAG	G	1201	-	14,14,15	0.44	0	17,19,21	0.75	1 (5%)
5	NAG	C	1301	3	14,14,15	0.27	0	17,19,21	0.54	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	D	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	G	1203	1	-	4/6/23/26	0/1/1/1
5	NAG	F	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1303	3	-	1/6/23/26	0/1/1/1
5	NAG	C	1302	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1301	3	-	0/6/23/26	0/1/1/1
5	NAG	I	1302	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1305	-	-	2/6/23/26	0/1/1/1
5	NAG	D	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1301	3	-	0/6/23/26	0/1/1/1
5	NAG	I	1303	3	-	1/6/23/26	0/1/1/1
5	NAG	H	200	-	-	3/6/23/26	0/1/1/1
5	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1302	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1206	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	3/6/23/26	0/1/1/1
5	NAG	G	1202	1	-	2/6/23/26	0/1/1/1
5	NAG	E	200	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1204	1	-	4/6/23/26	0/1/1/1
5	NAG	G	1204	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1204	1	-	4/6/23/26	0/1/1/1
5	NAG	G	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1202	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	3	-	0/6/23/26	0/1/1/1
5	NAG	D	1203	-	-	1/6/23/26	0/1/1/1
5	NAG	G	1201	-	-	4/6/23/26	0/1/1/1
5	NAG	C	1301	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1303	NAG	O5-C1	4.85	1.51	1.43
5	C	1303	NAG	C1-C2	3.98	1.57	1.52
5	F	1305	NAG	O5-C1	-3.94	1.37	1.43
5	D	1205	NAG	O5-C1	3.49	1.49	1.43
5	C	1304	NAG	O5-C1	-2.94	1.38	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1205	NAG	C1-O5-C5	8.16	123.12	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1303	NAG	C1-O5-C5	4.77	118.58	112.19
5	F	1305	NAG	C3-C4-C5	3.77	117.07	110.23
5	G	1201	NAG	C1-O5-C5	2.74	115.86	112.19
5	A	1202	NAG	C1-O5-C5	2.09	114.99	112.19

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1302	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	D	1204	NAG	C4-C5-C6-O6
5	I	1302	NAG	O5-C5-C6-O6
5	A	1203	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	D	1205	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	D	1204	NAG	O5-C5-C6-O6
5	G	1202	NAG	C4-C5-C6-O6
5	A	1204	NAG	O5-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	G	1203	NAG	C4-C5-C6-O6
5	A	1203	NAG	C4-C5-C6-O6
5	D	1205	NAG	C4-C5-C6-O6
5	G	1203	NAG	O5-C5-C6-O6
5	G	1202	NAG	O5-C5-C6-O6
5	F	1305	NAG	C4-C5-C6-O6
5	A	1204	NAG	C4-C5-C6-O6
5	F	1304	NAG	O5-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	A	1201	NAG	C8-C7-N2-C2
5	A	1201	NAG	O7-C7-N2-C2
5	A	1202	NAG	C8-C7-N2-C2
5	A	1202	NAG	O7-C7-N2-C2
5	A	1204	NAG	C8-C7-N2-C2
5	A	1204	NAG	O7-C7-N2-C2
5	A	1205	NAG	C8-C7-N2-C2
5	A	1205	NAG	O7-C7-N2-C2
5	D	1204	NAG	C8-C7-N2-C2
5	D	1204	NAG	O7-C7-N2-C2
5	G	1201	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	G	1201	NAG	O7-C7-N2-C2
5	G	1203	NAG	C8-C7-N2-C2
5	G	1203	NAG	O7-C7-N2-C2
5	G	1205	NAG	C8-C7-N2-C2
5	G	1205	NAG	O7-C7-N2-C2
5	G	1206	NAG	C8-C7-N2-C2
5	G	1206	NAG	O7-C7-N2-C2
5	H	200	NAG	C4-C5-C6-O6
5	G	1201	NAG	O5-C5-C6-O6
5	D	1201	NAG	C4-C5-C6-O6
5	F	1302	NAG	C4-C5-C6-O6
5	F	1305	NAG	O5-C5-C6-O6
5	H	200	NAG	O5-C5-C6-O6
5	A	1201	NAG	O5-C5-C6-O6
5	D	1201	NAG	O5-C5-C6-O6
5	E	200	NAG	C4-C5-C6-O6
5	F	1302	NAG	O5-C5-C6-O6
5	G	1204	NAG	C4-C5-C6-O6
5	G	1206	NAG	O5-C5-C6-O6
5	F	1304	NAG	C4-C5-C6-O6
5	E	200	NAG	O5-C5-C6-O6
5	G	1204	NAG	O5-C5-C6-O6
5	G	1201	NAG	C4-C5-C6-O6
5	D	1202	NAG	C3-C2-N2-C7
5	F	1303	NAG	C3-C2-N2-C7
5	D	1202	NAG	C1-C2-N2-C7
5	H	200	NAG	C1-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7
5	I	1303	NAG	C3-C2-N2-C7
5	D	1203	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 13 short contacts:

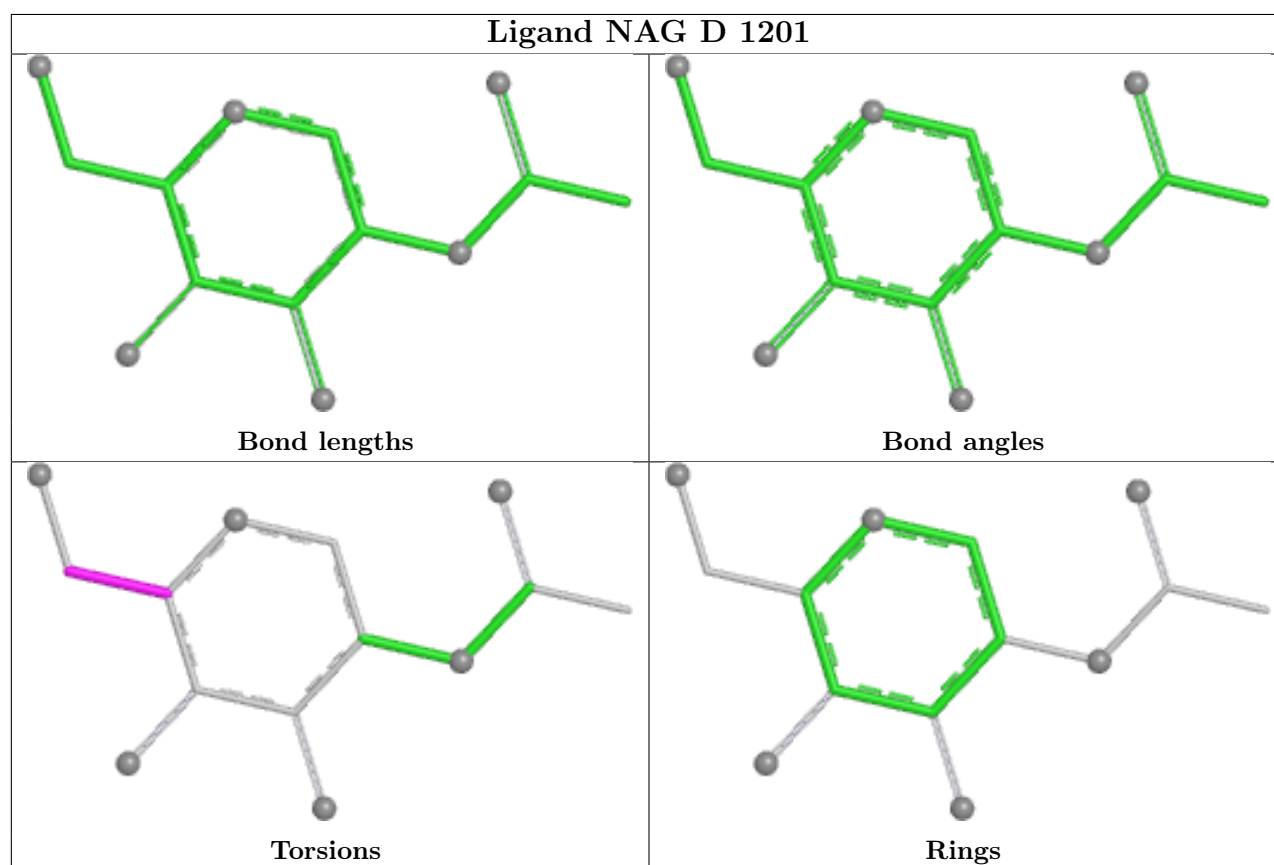
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1304	NAG	2	0
5	F	1303	NAG	1	0
5	C	1302	NAG	1	0
5	I	1302	NAG	1	0
5	F	1305	NAG	1	0
5	I	1303	NAG	2	0
5	C	1304	NAG	2	0

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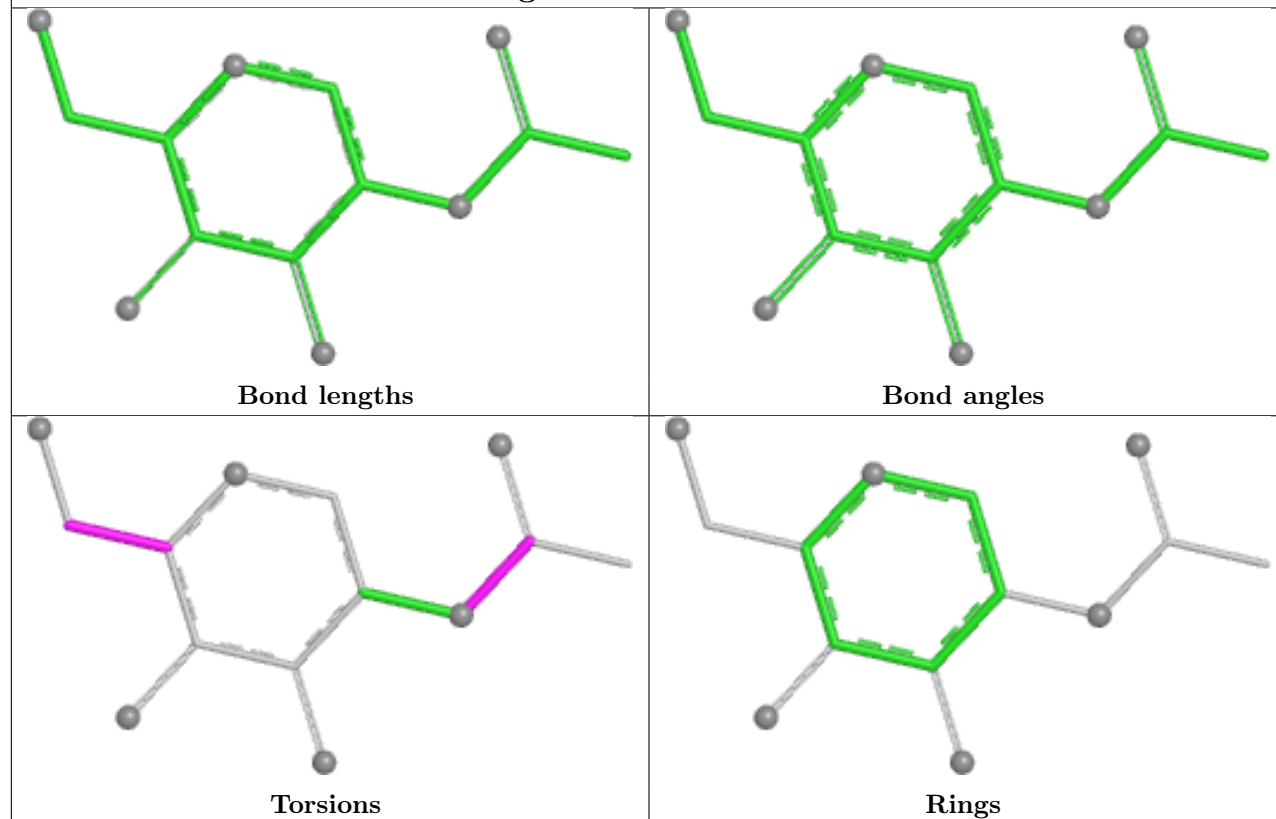
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1206	NAG	1	0
5	A	1204	NAG	1	0
5	C	1303	NAG	1	0
5	D	1203	NAG	2	0

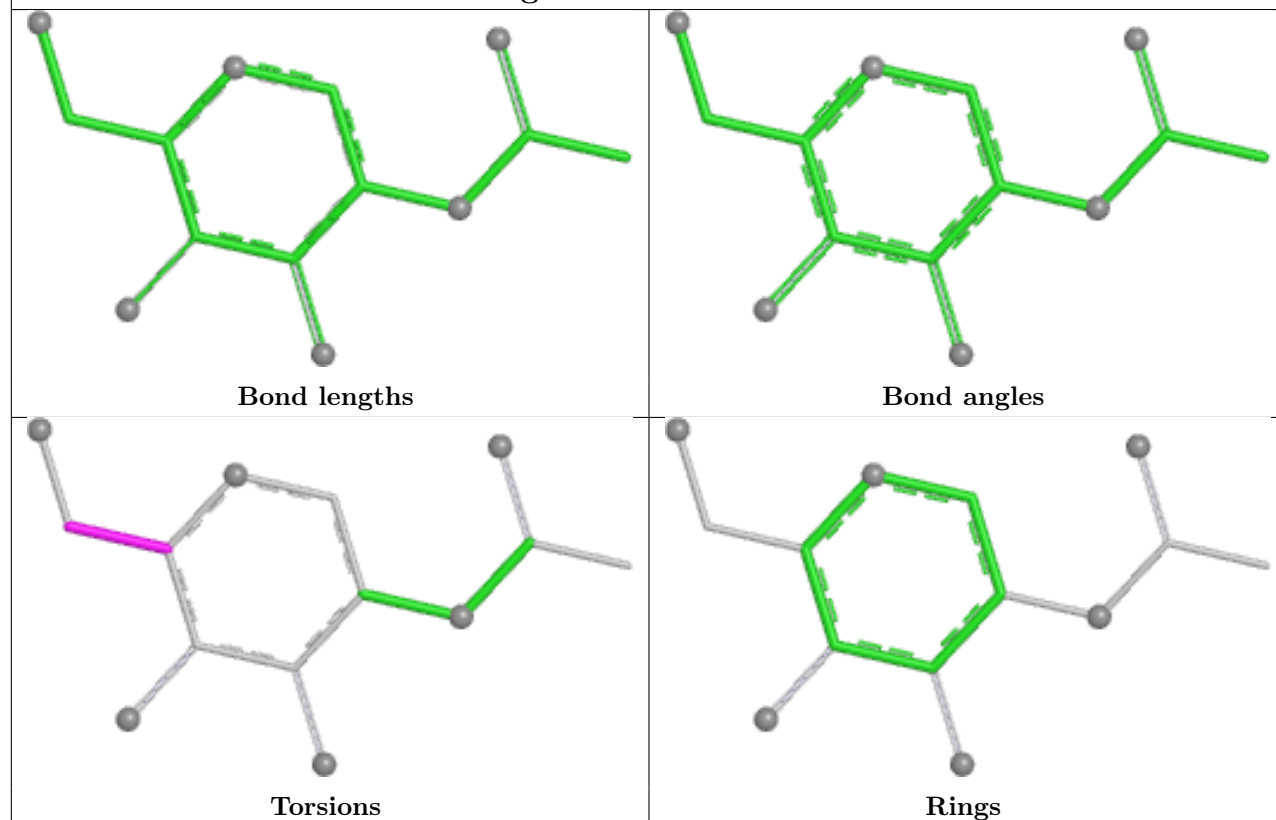
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



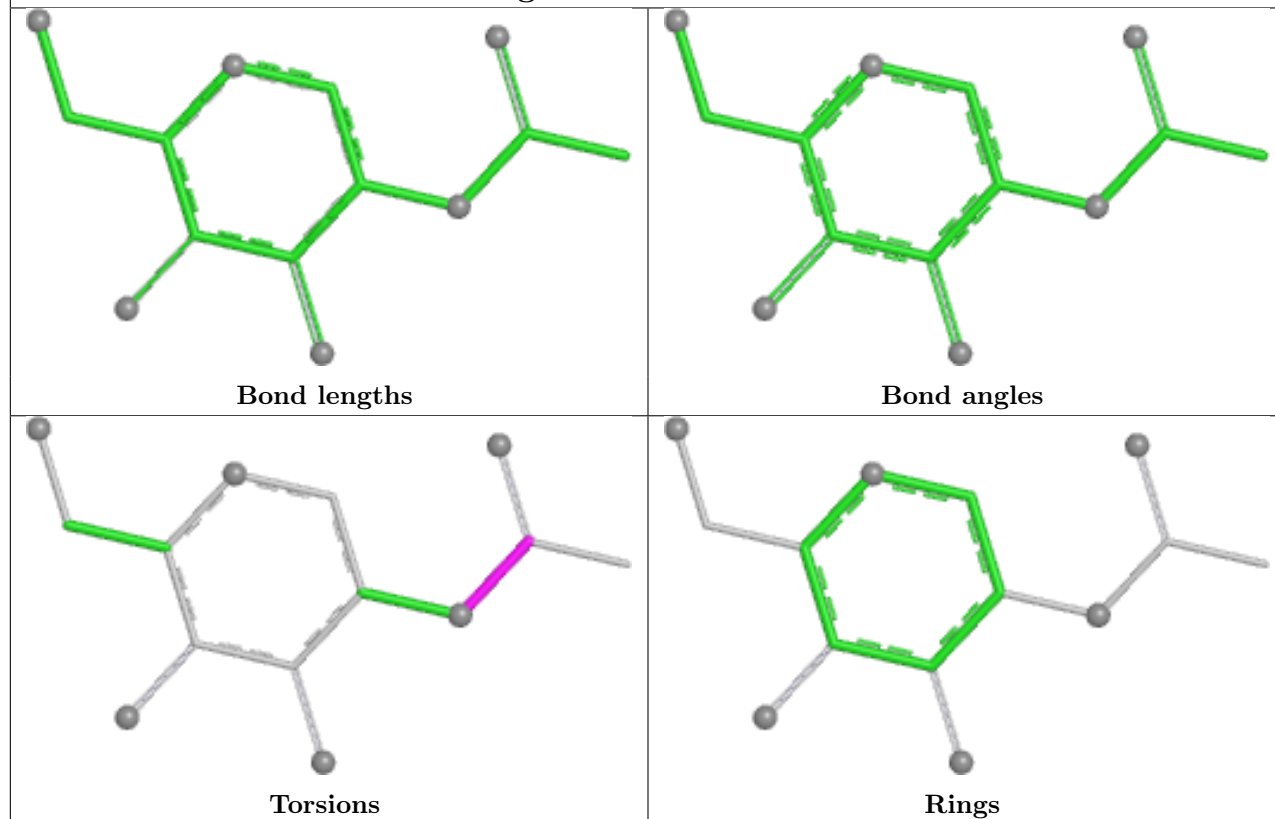
Ligand NAG G 1203



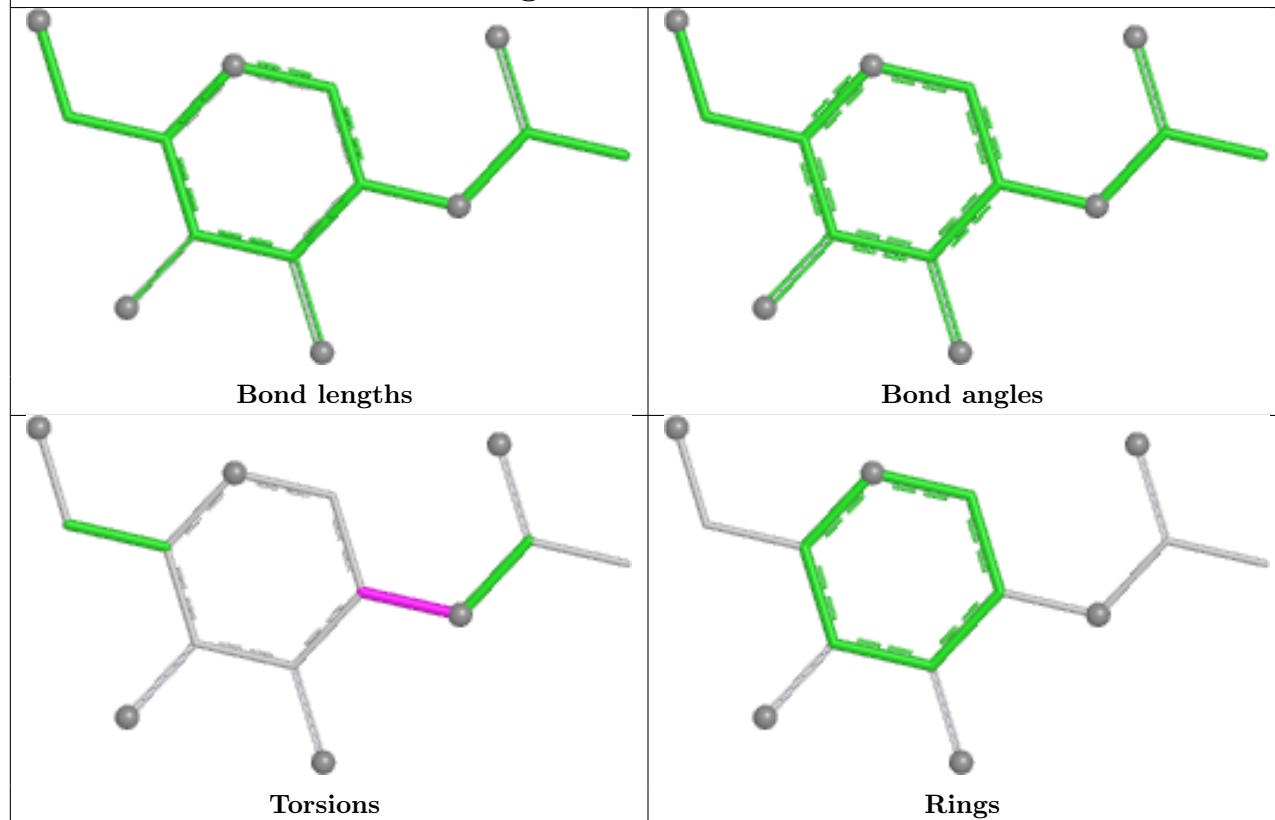
Ligand NAG F 1304



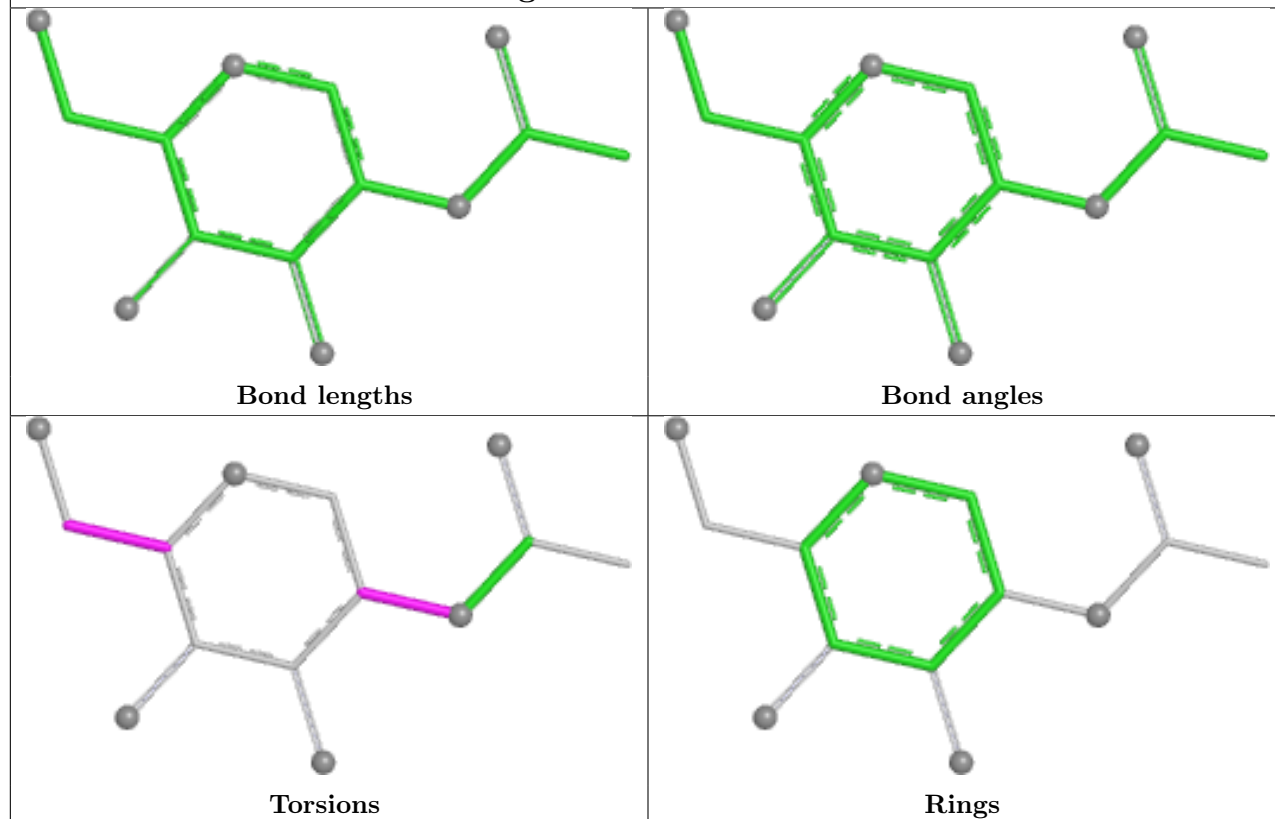
Ligand NAG A 1205



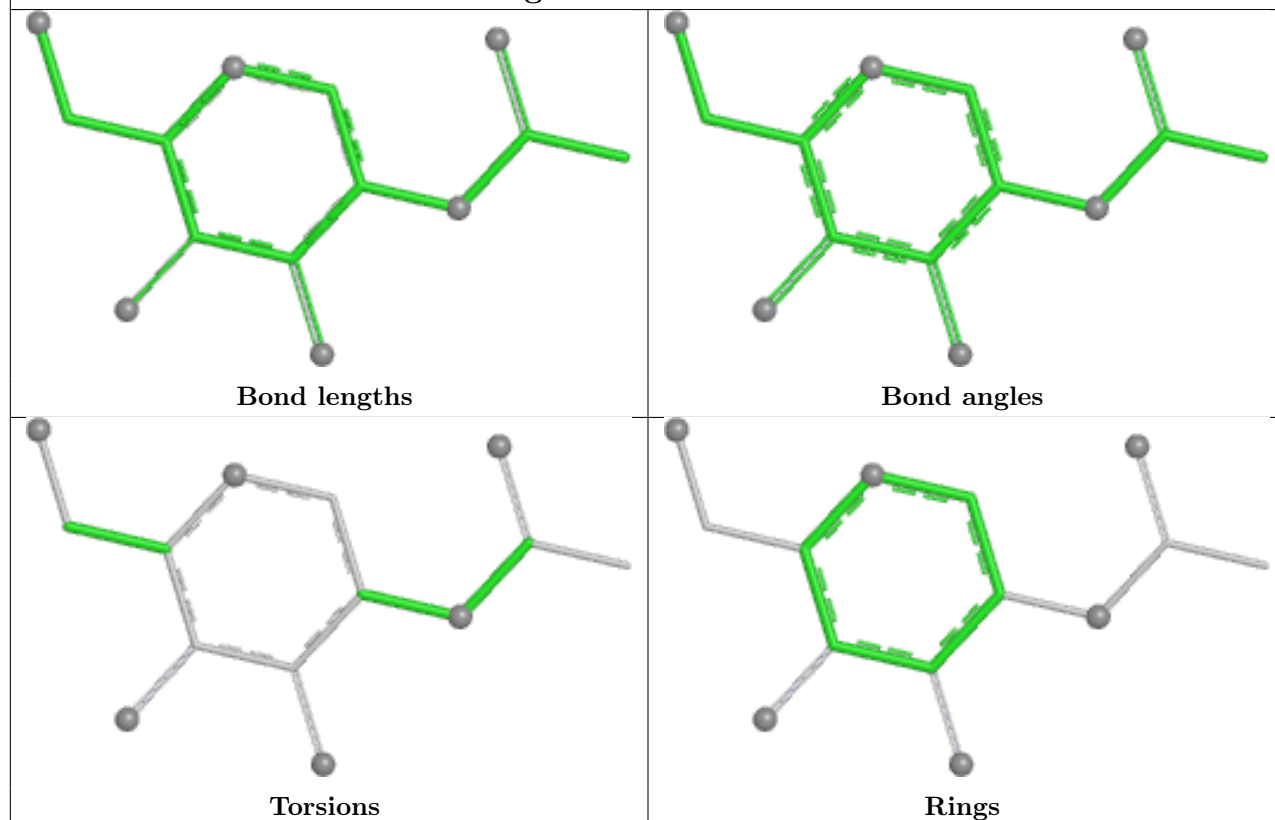
Ligand NAG F 1303



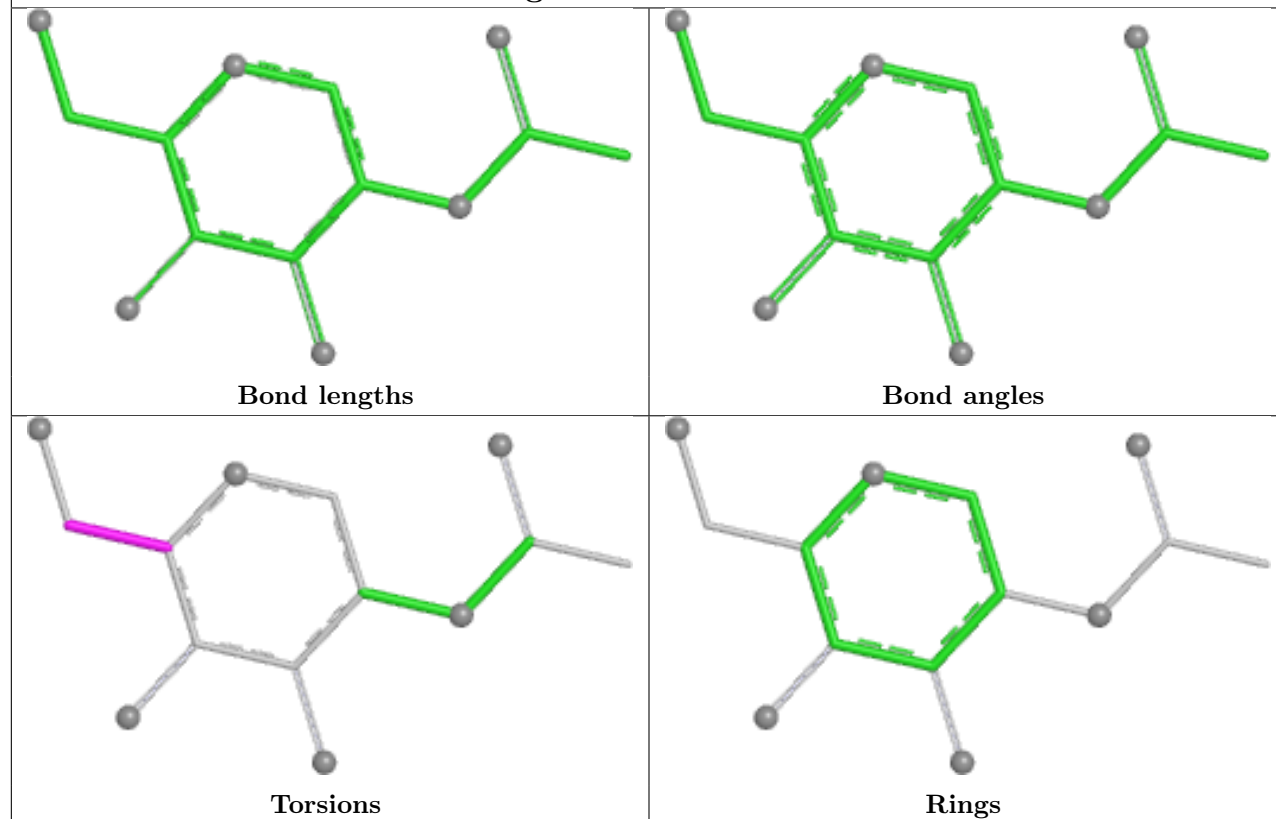
Ligand NAG C 1302



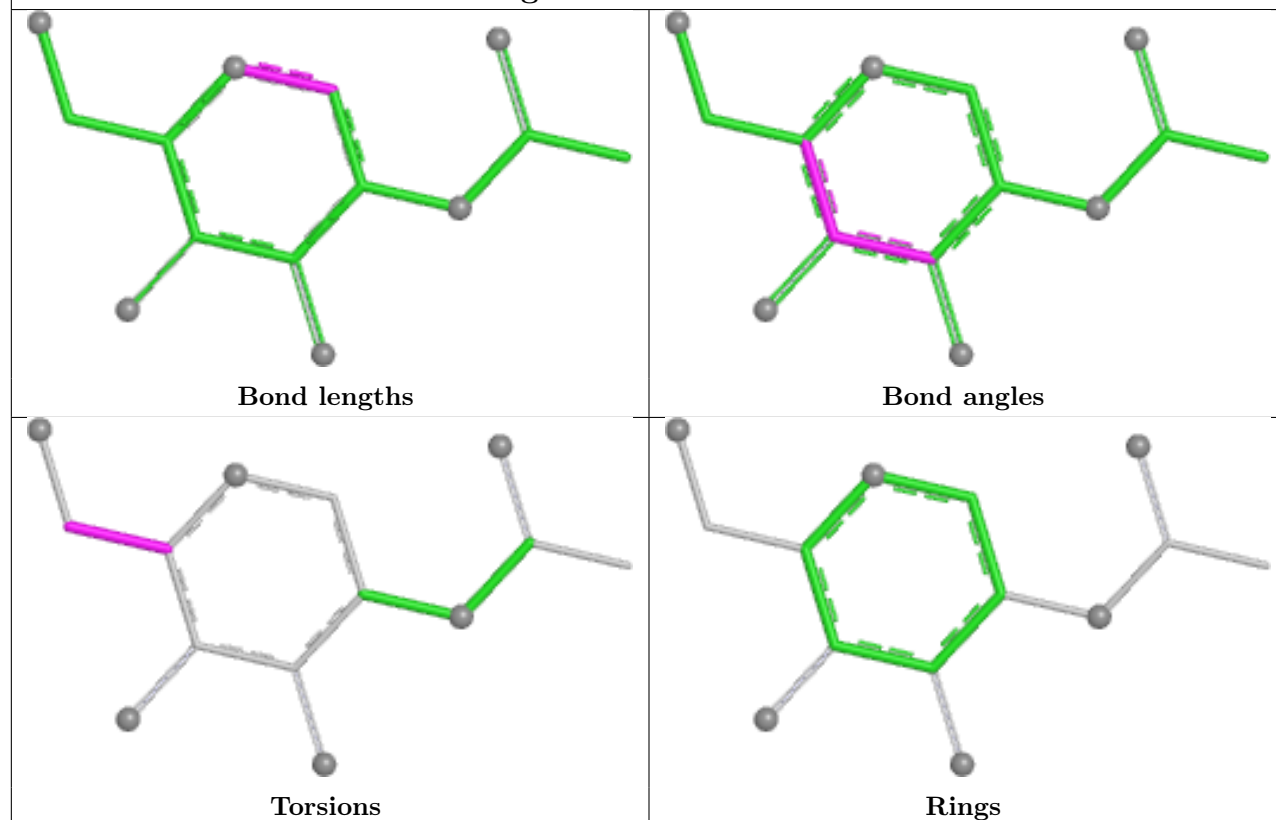
Ligand NAG I 1301



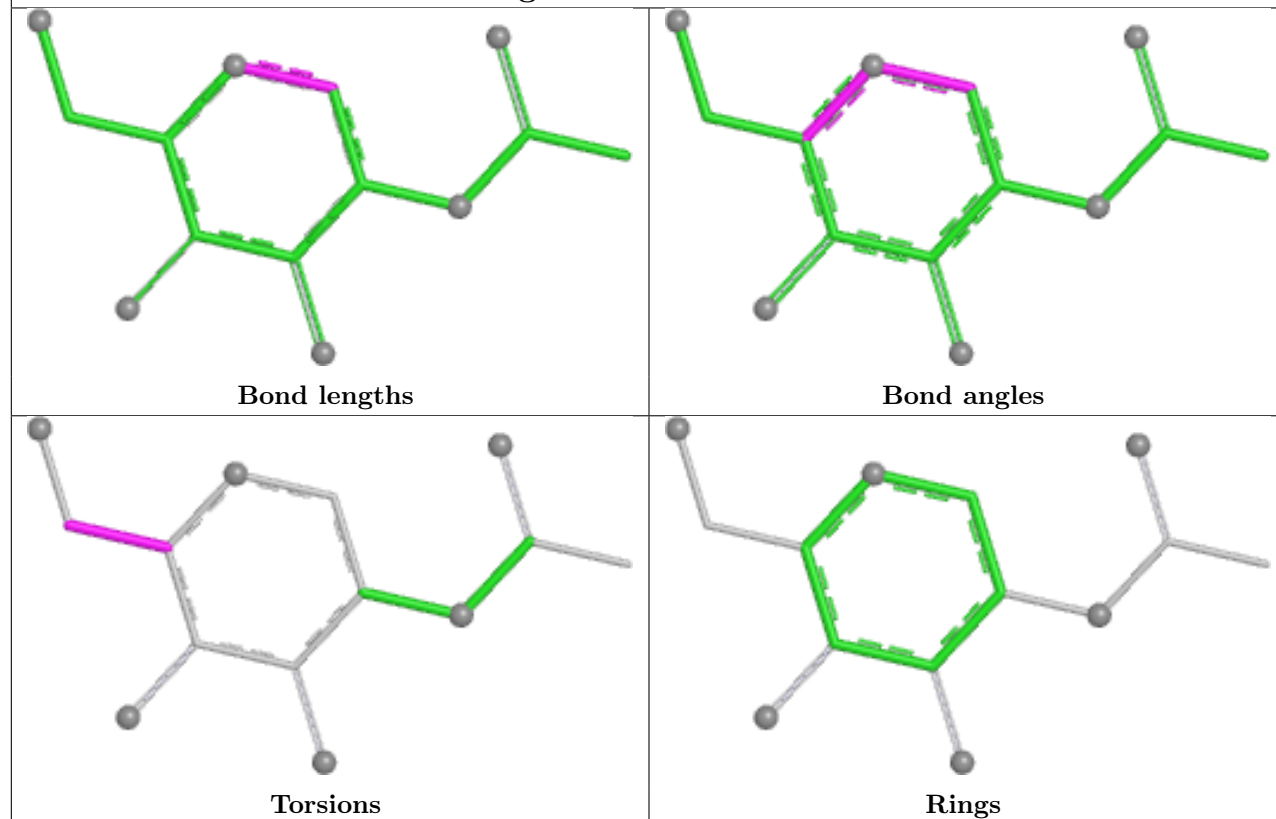
Ligand NAG I 1302



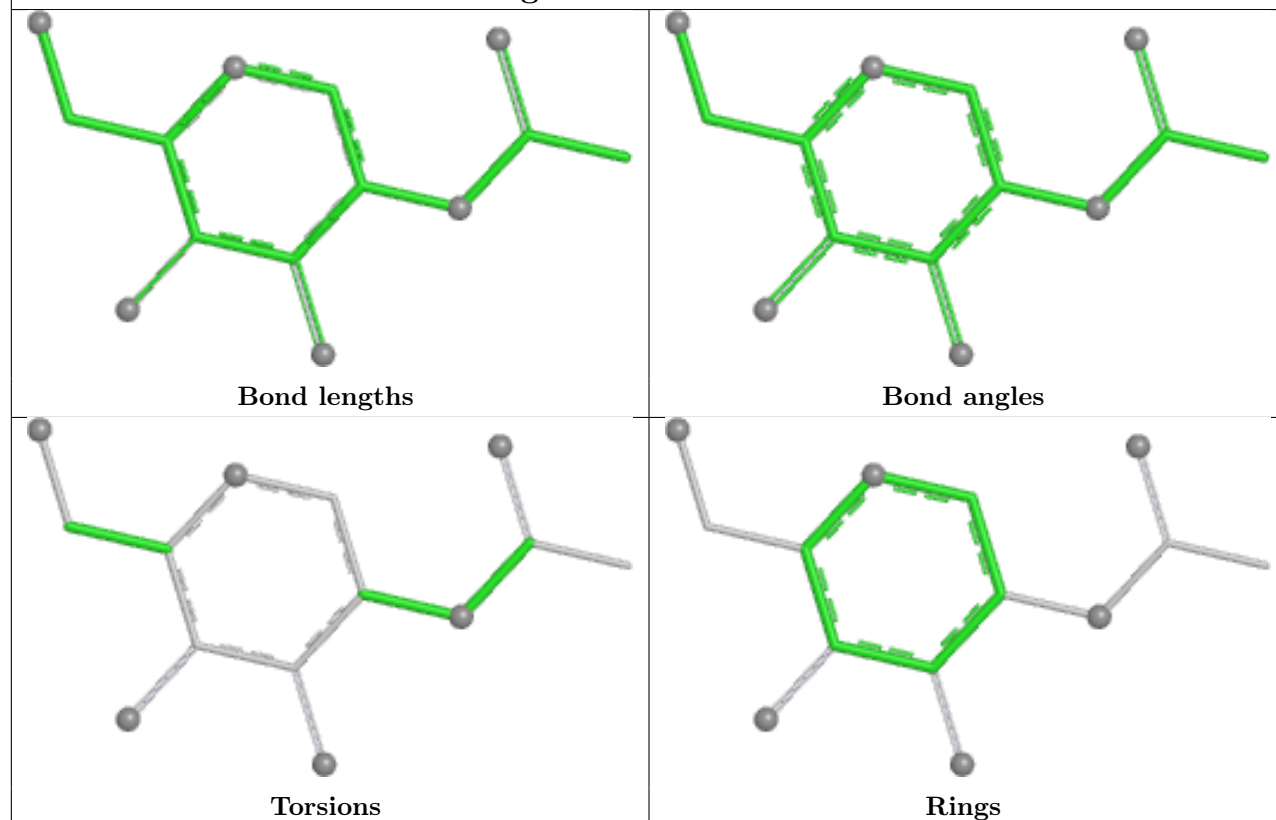
Ligand NAG F 1305

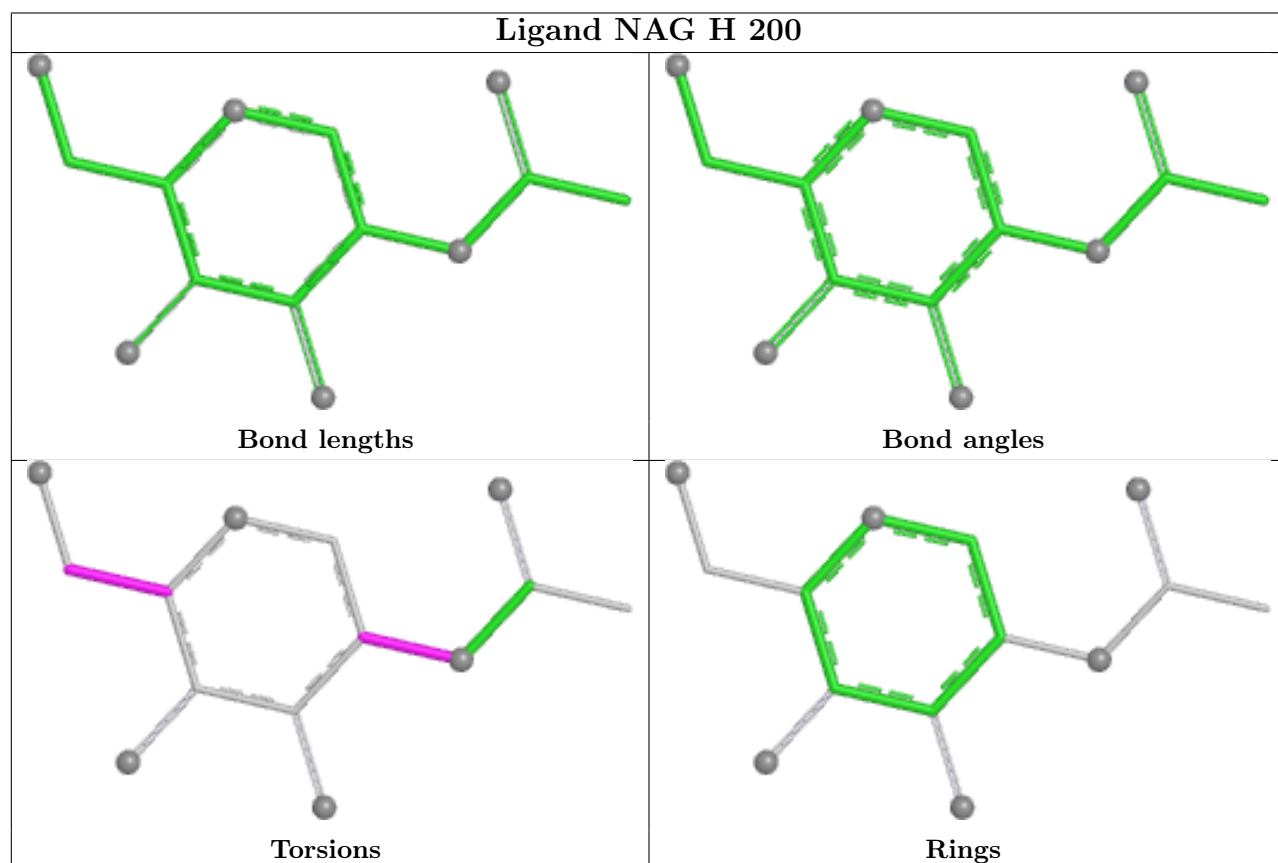
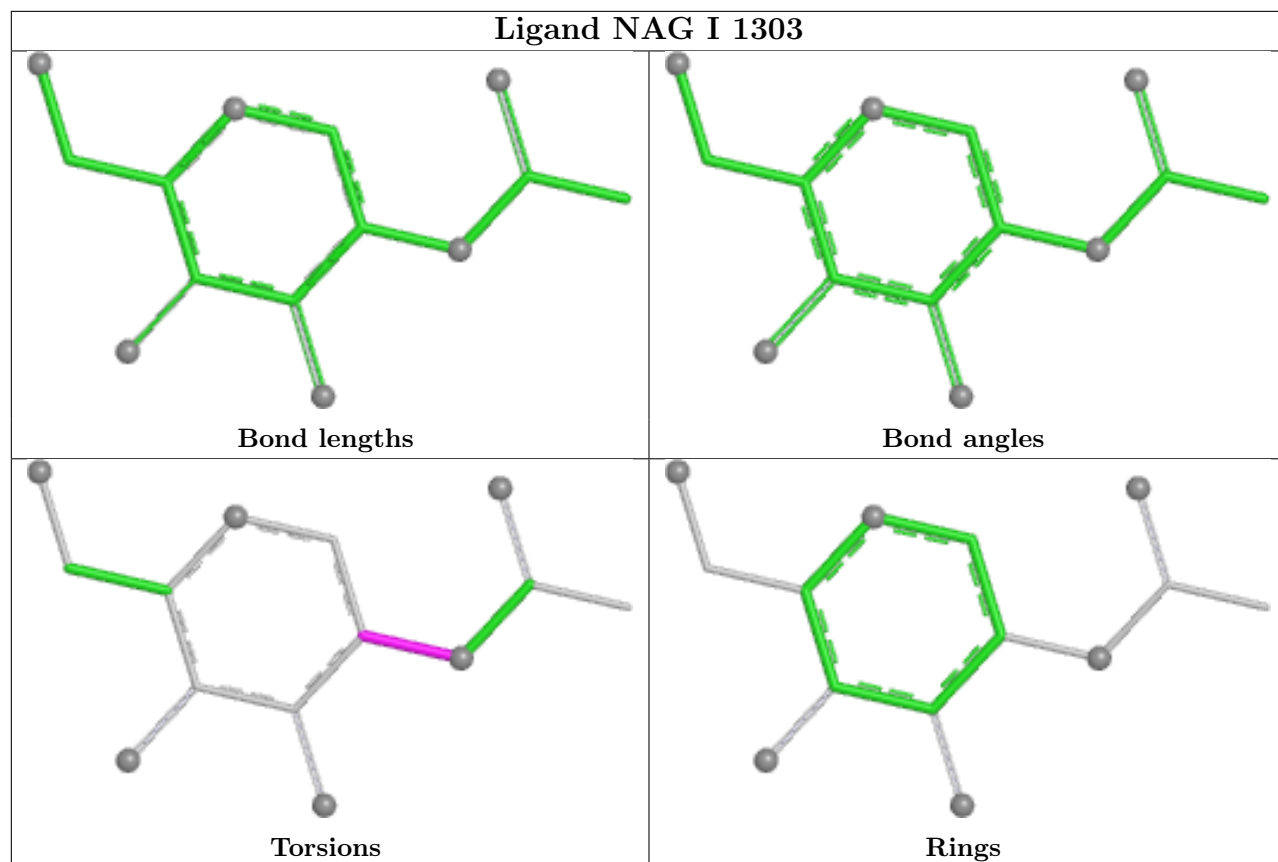


Ligand NAG D 1205

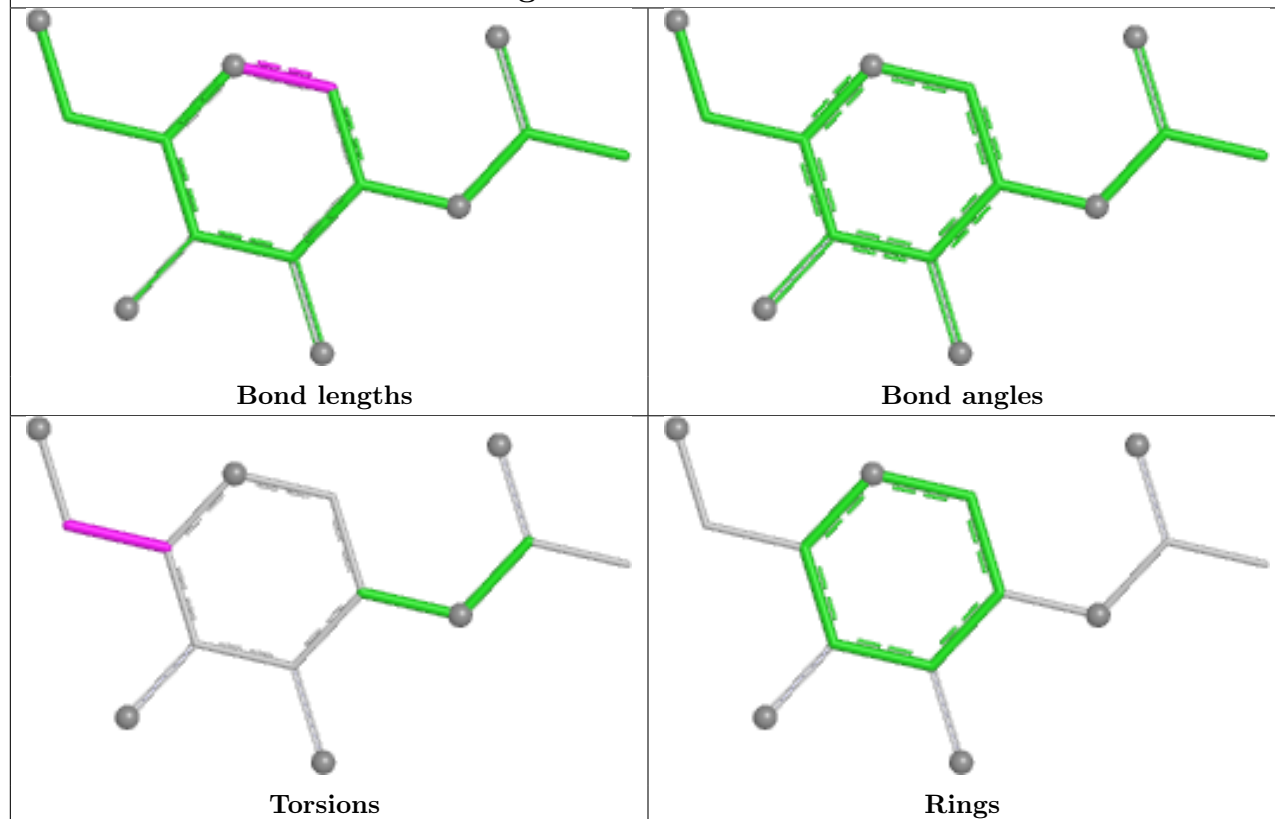


Ligand NAG F 1301

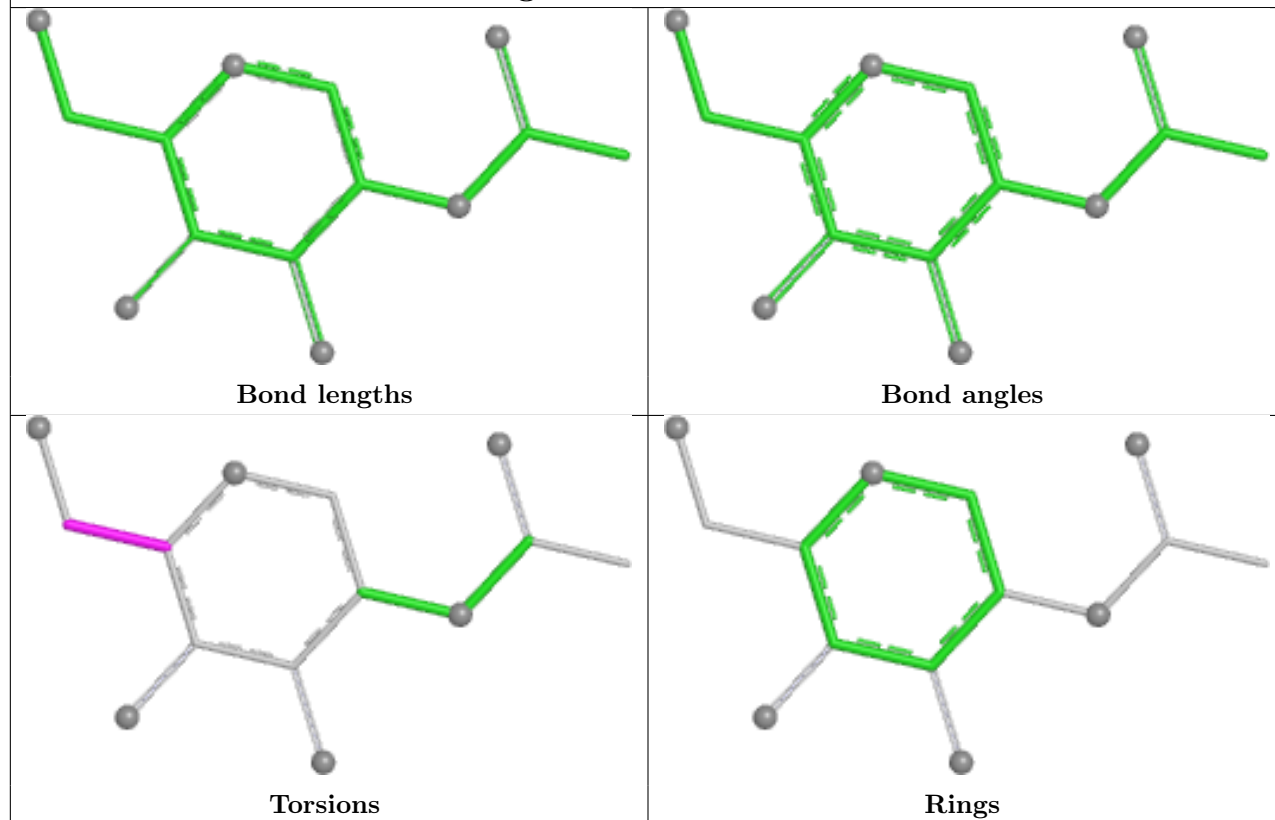




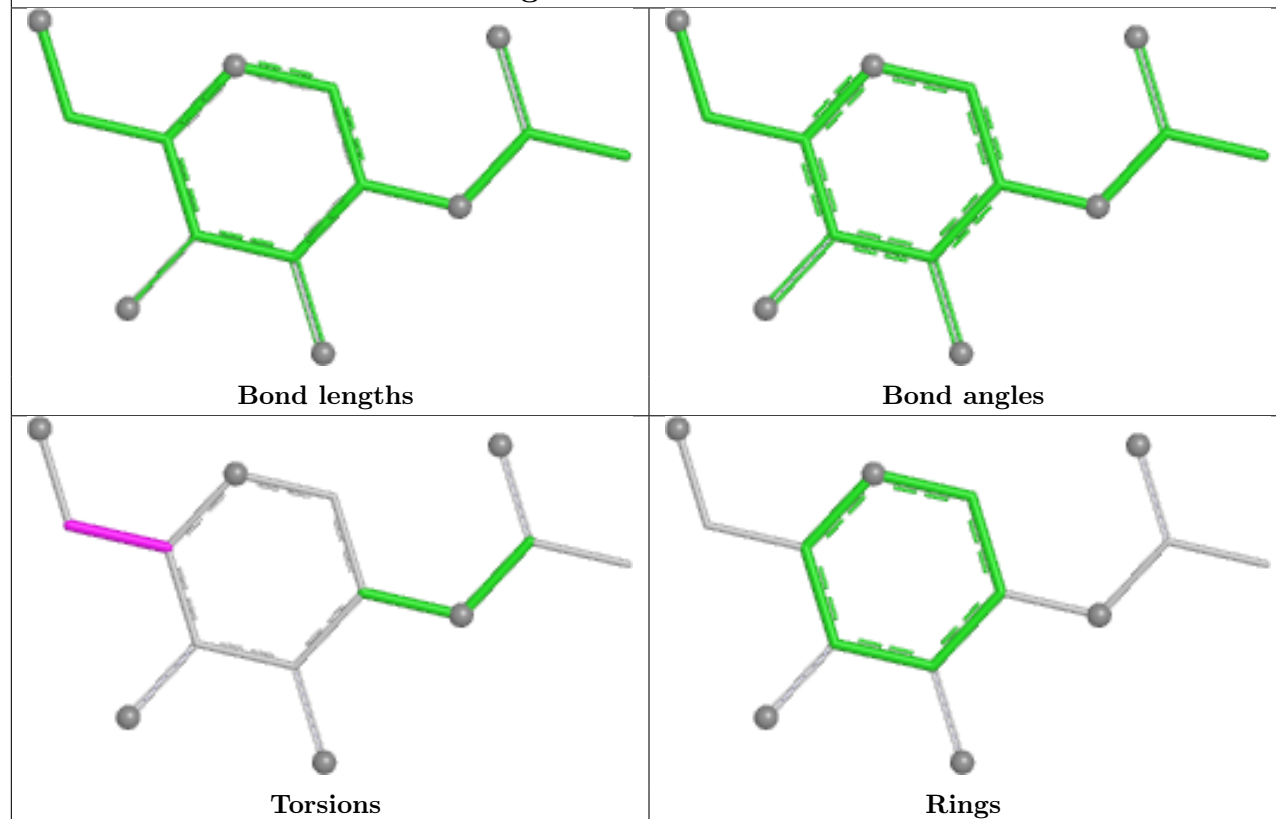
Ligand NAG C 1304



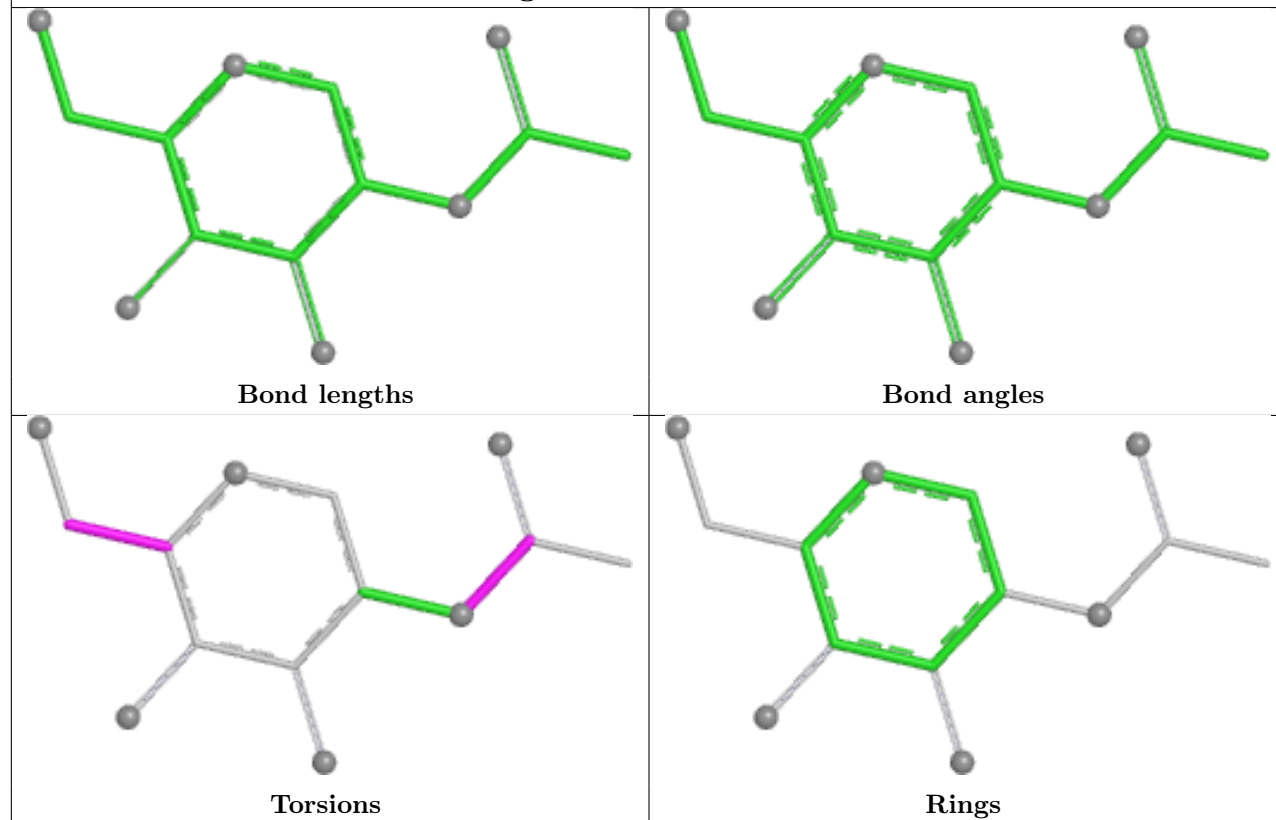
Ligand NAG A 1203



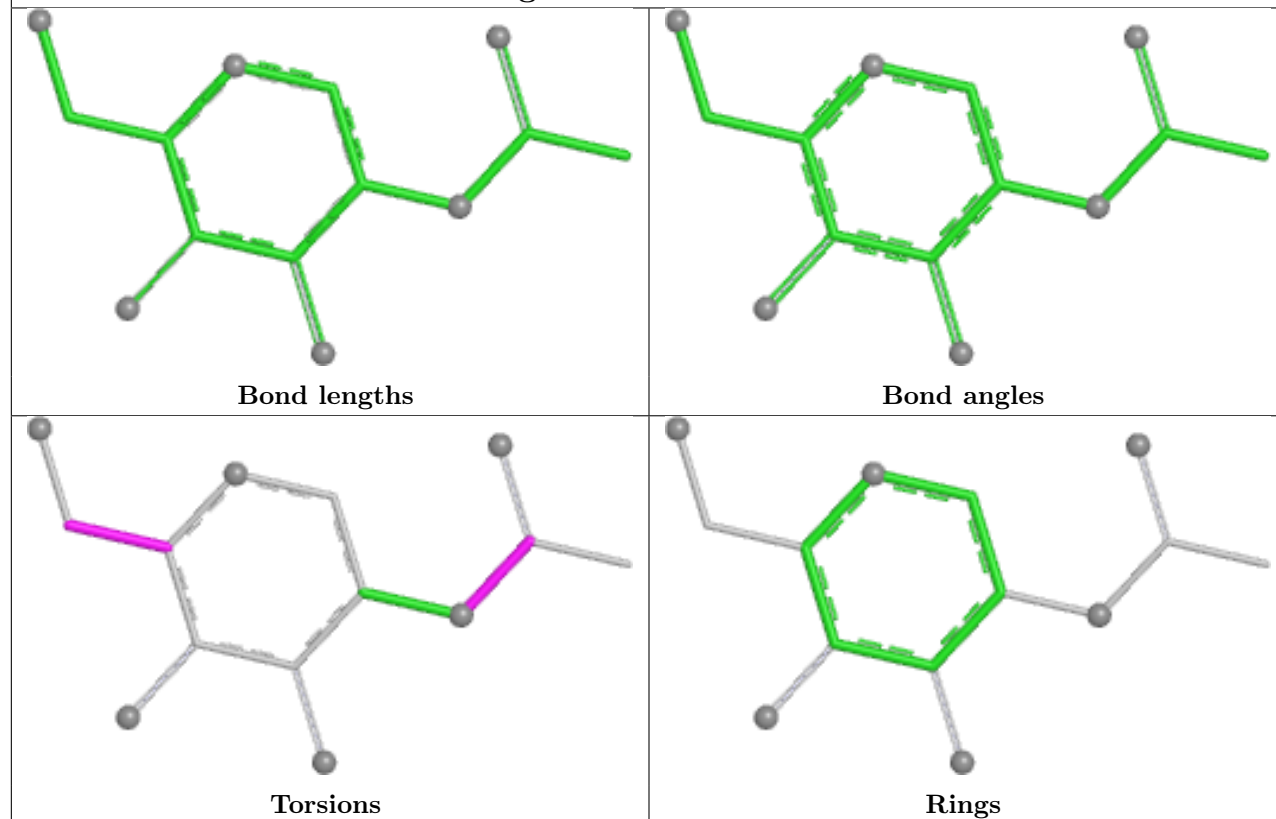
Ligand NAG F 1302



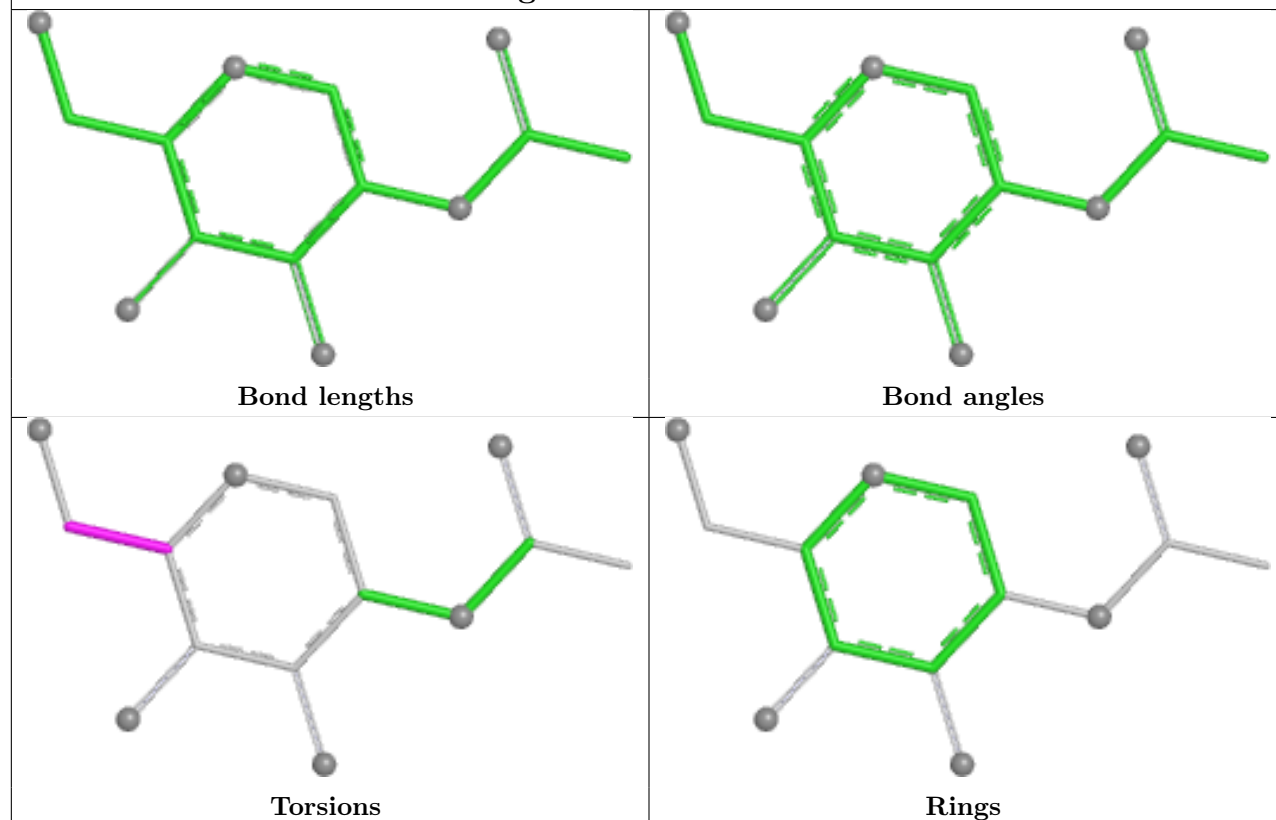
Ligand NAG G 1206

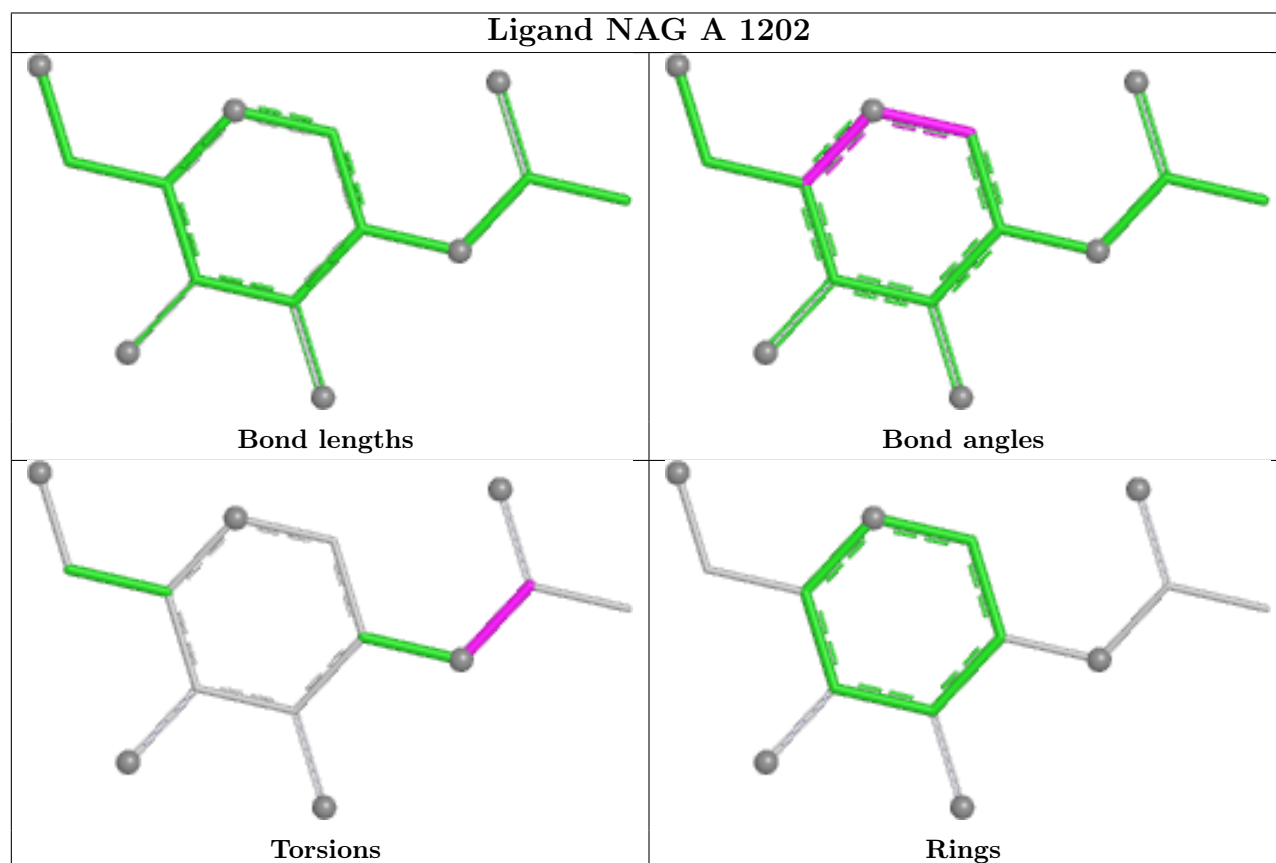
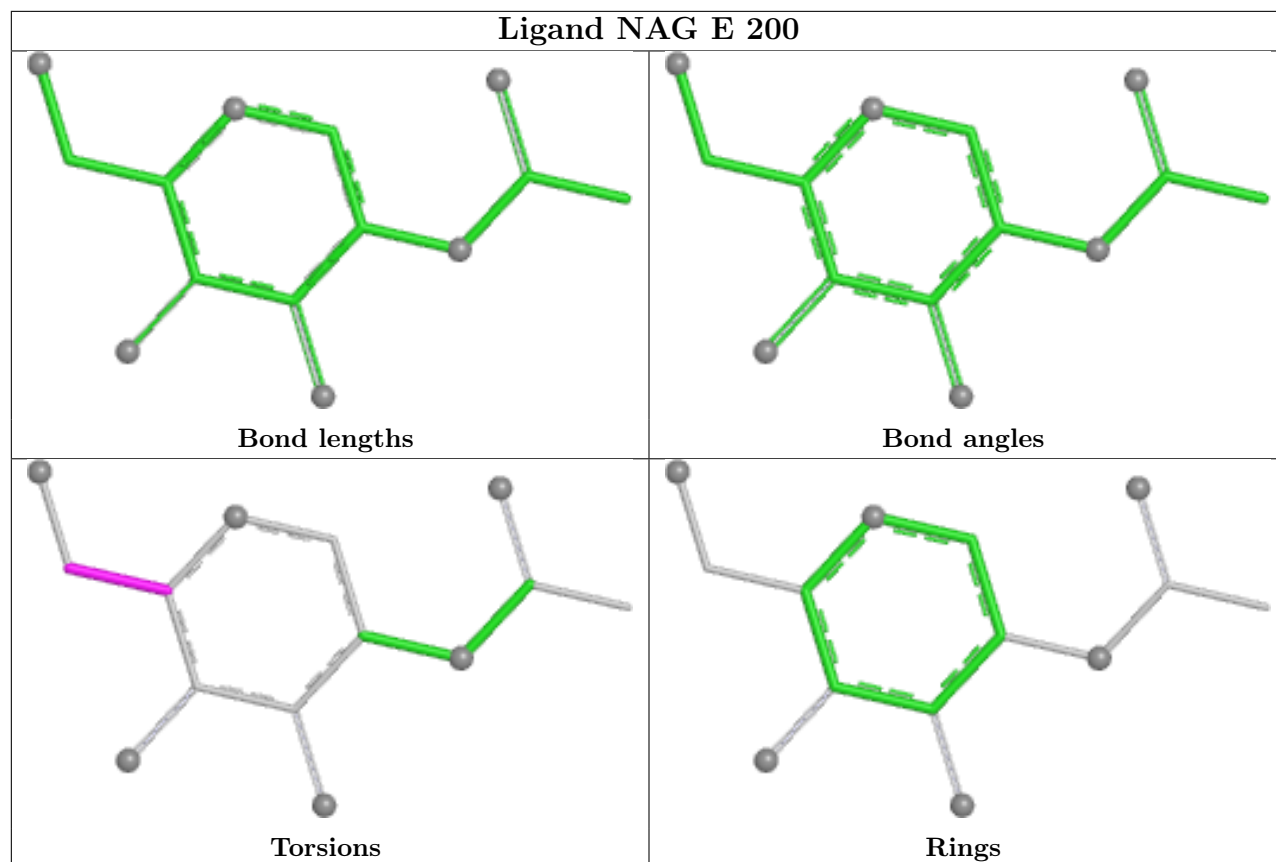


Ligand NAG A 1201

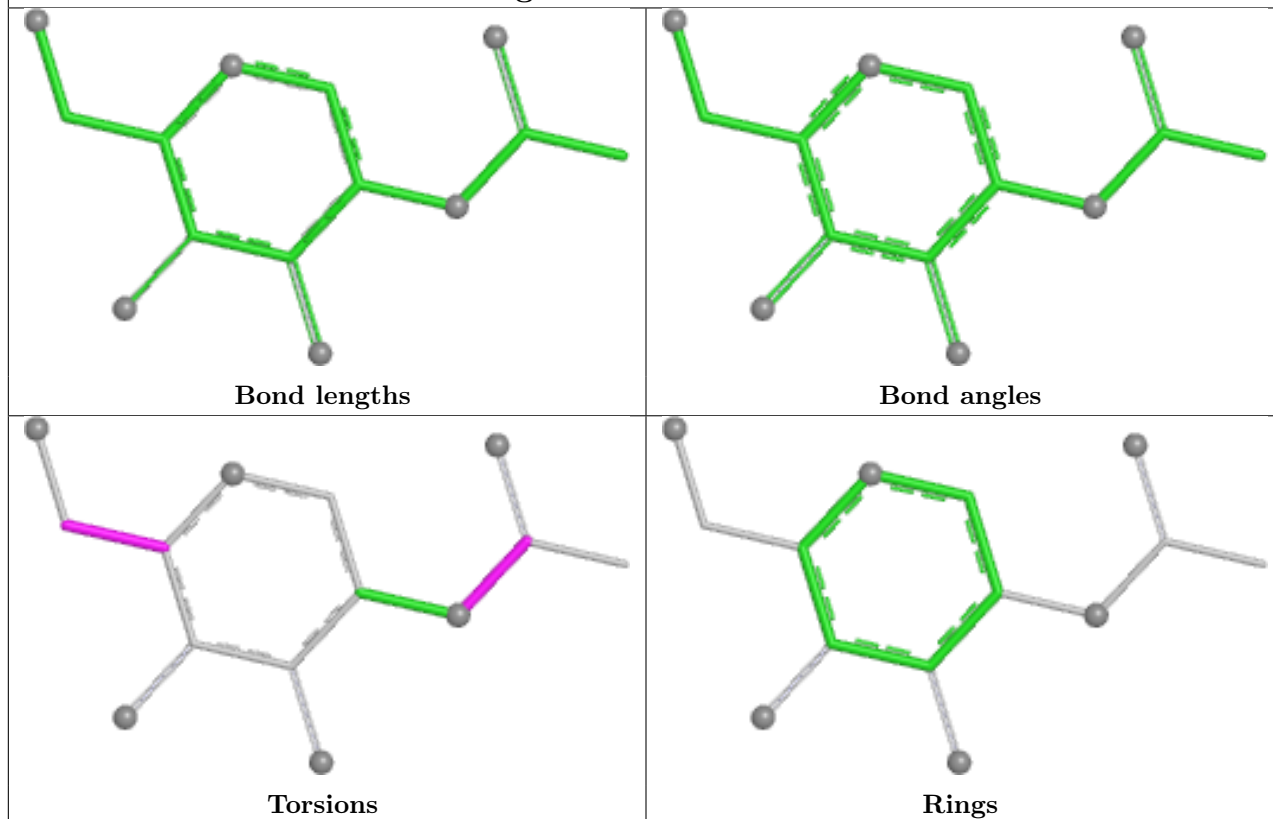


Ligand NAG G 1202

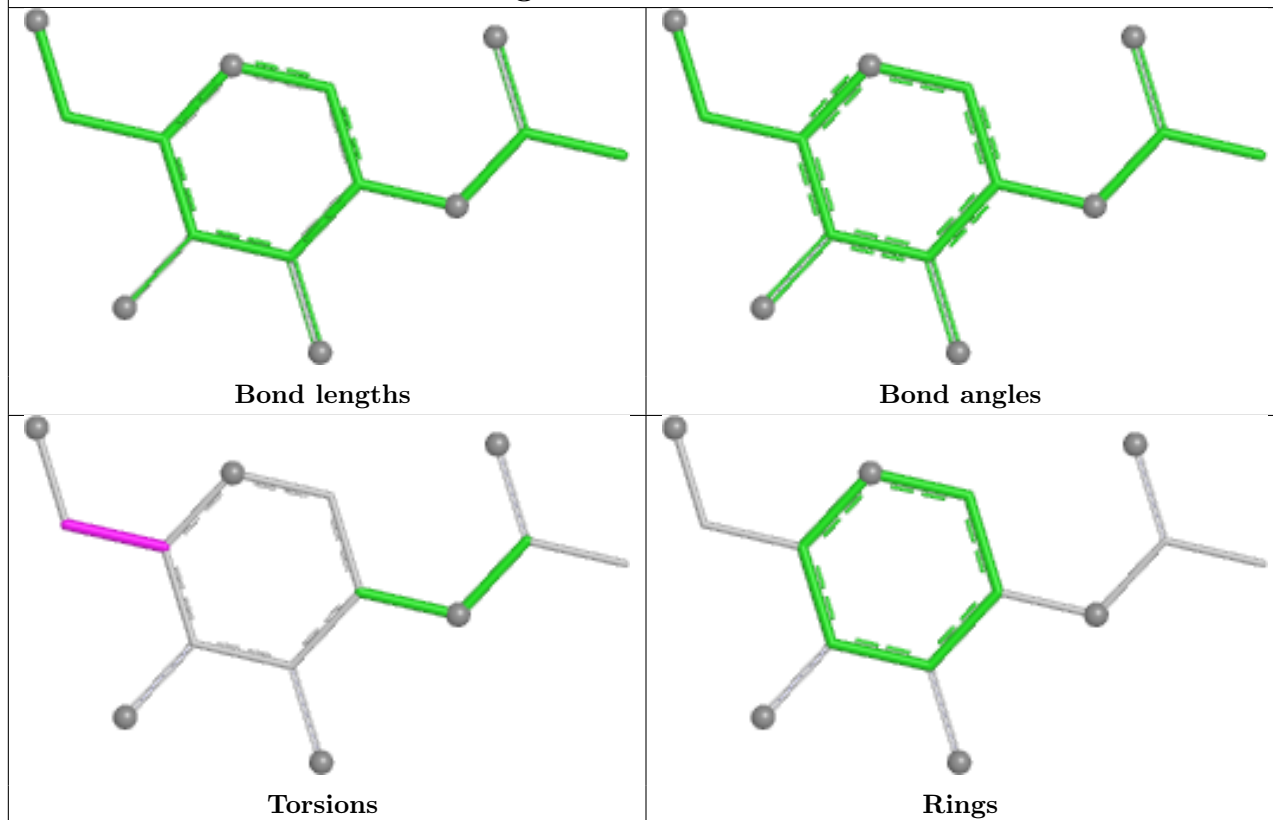




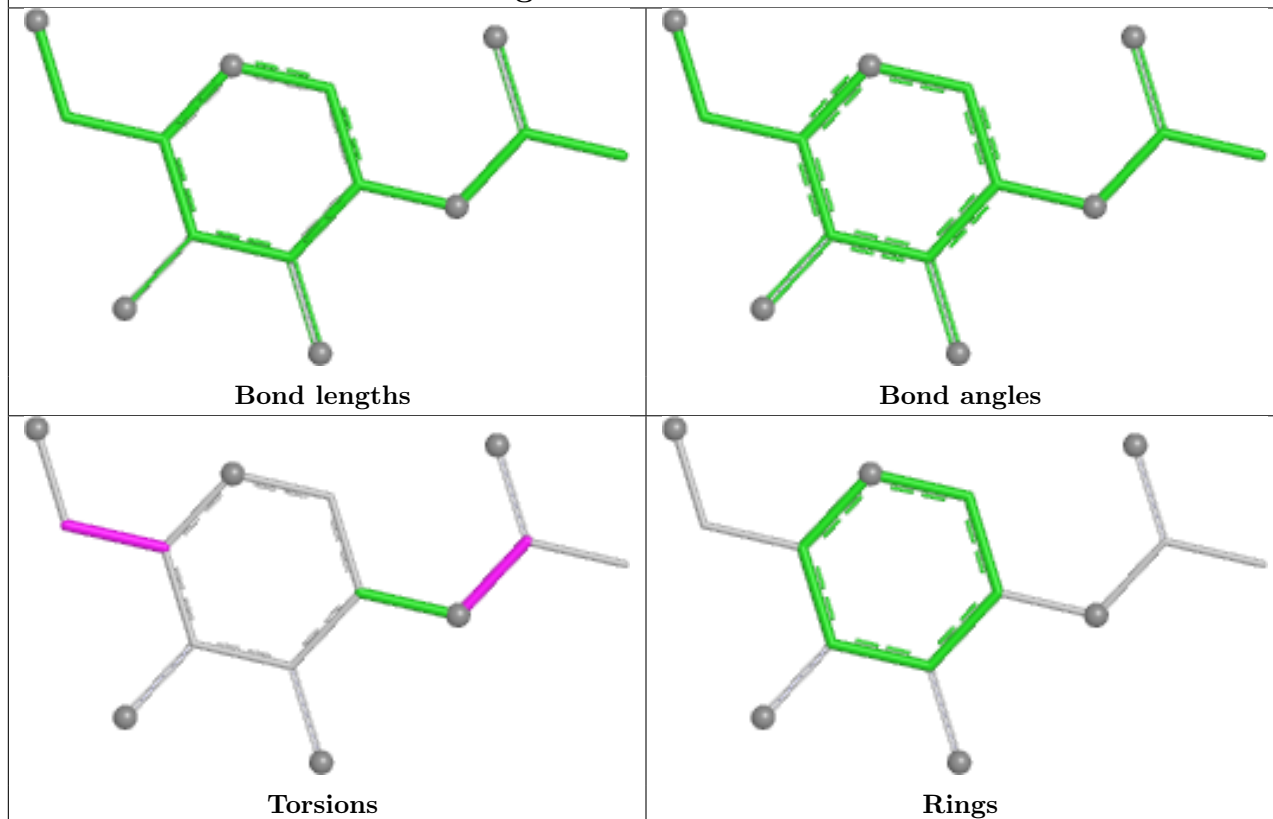
Ligand NAG A 1204



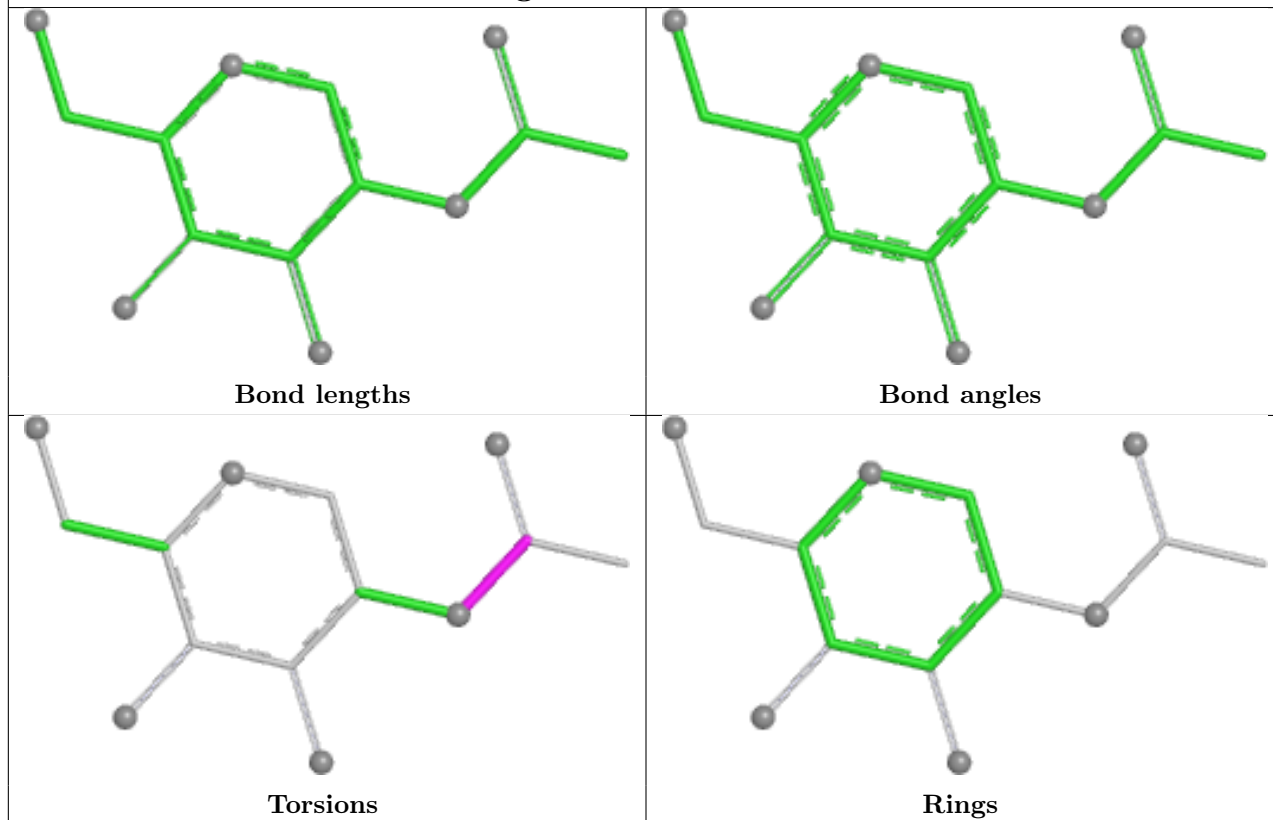
Ligand NAG G 1204



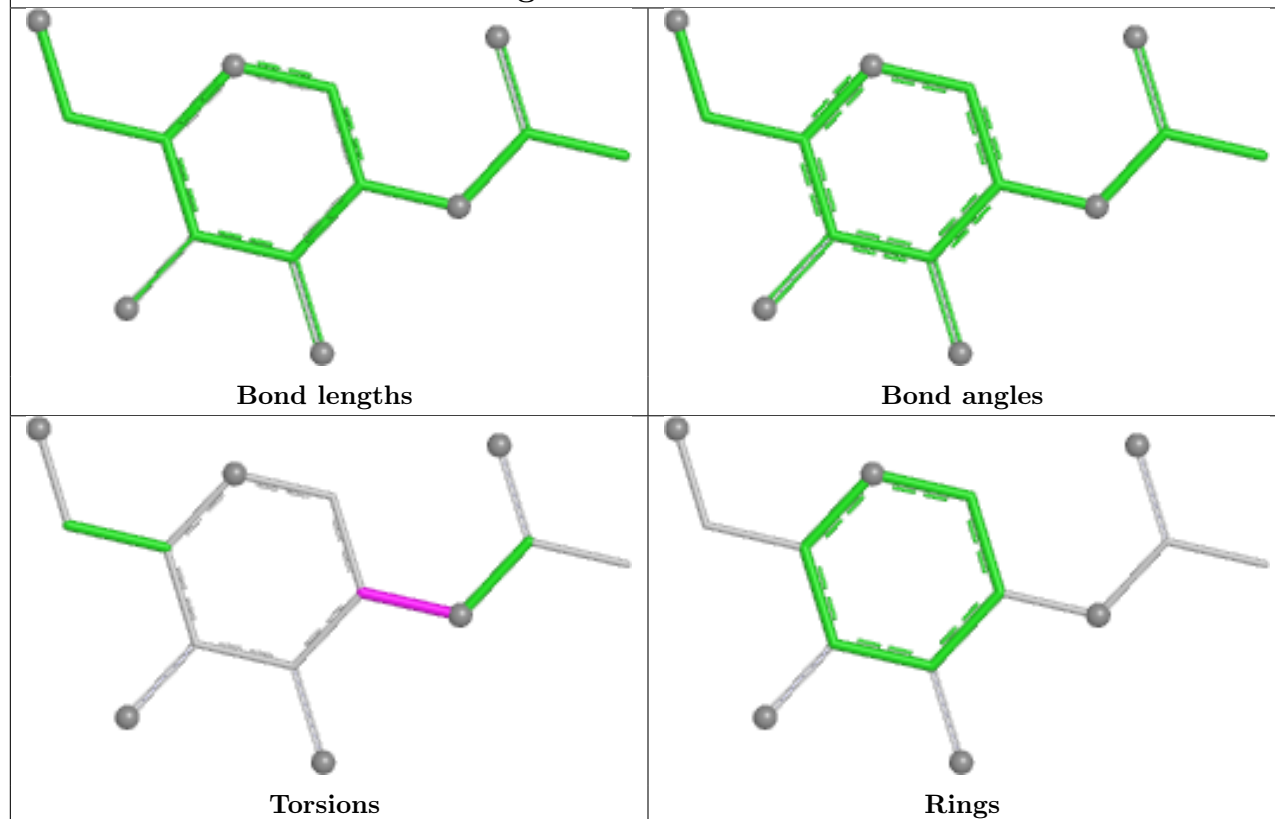
Ligand NAG D 1204



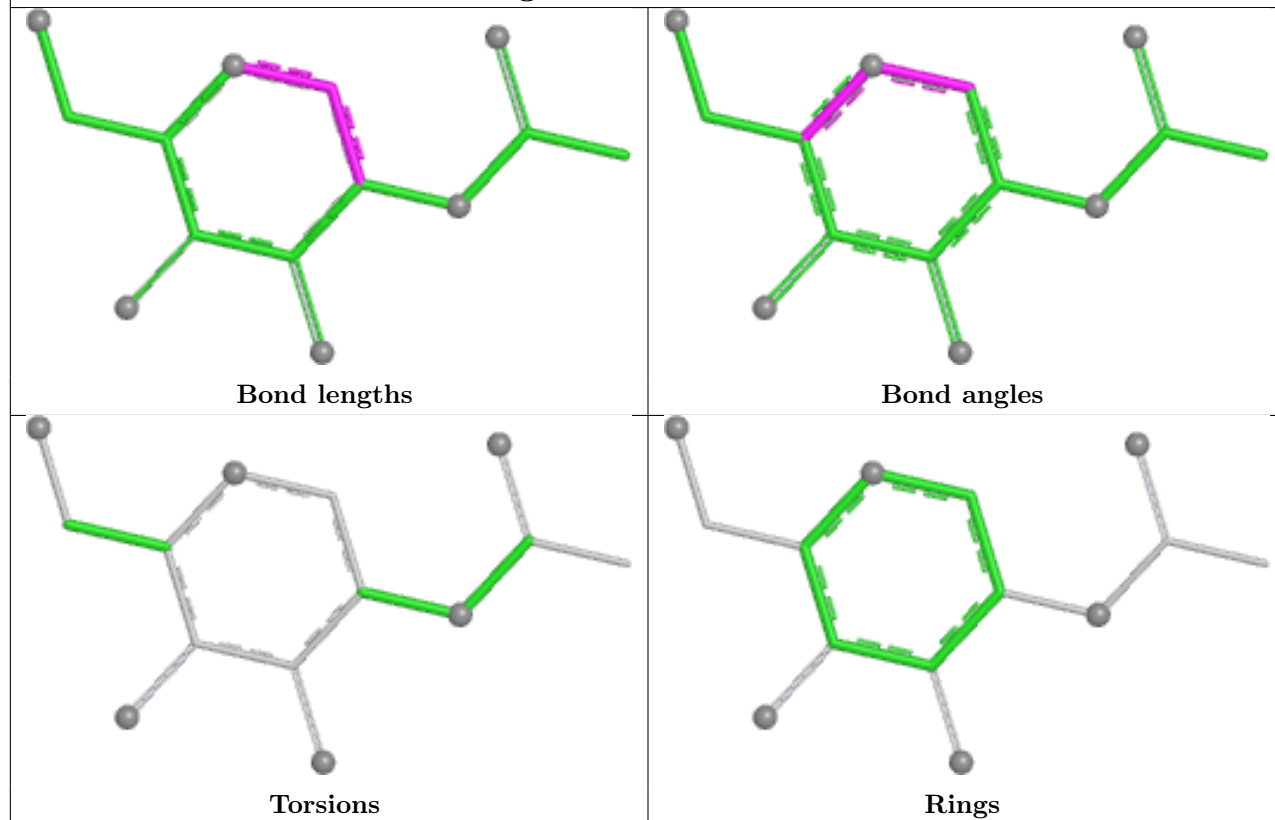
Ligand NAG G 1205



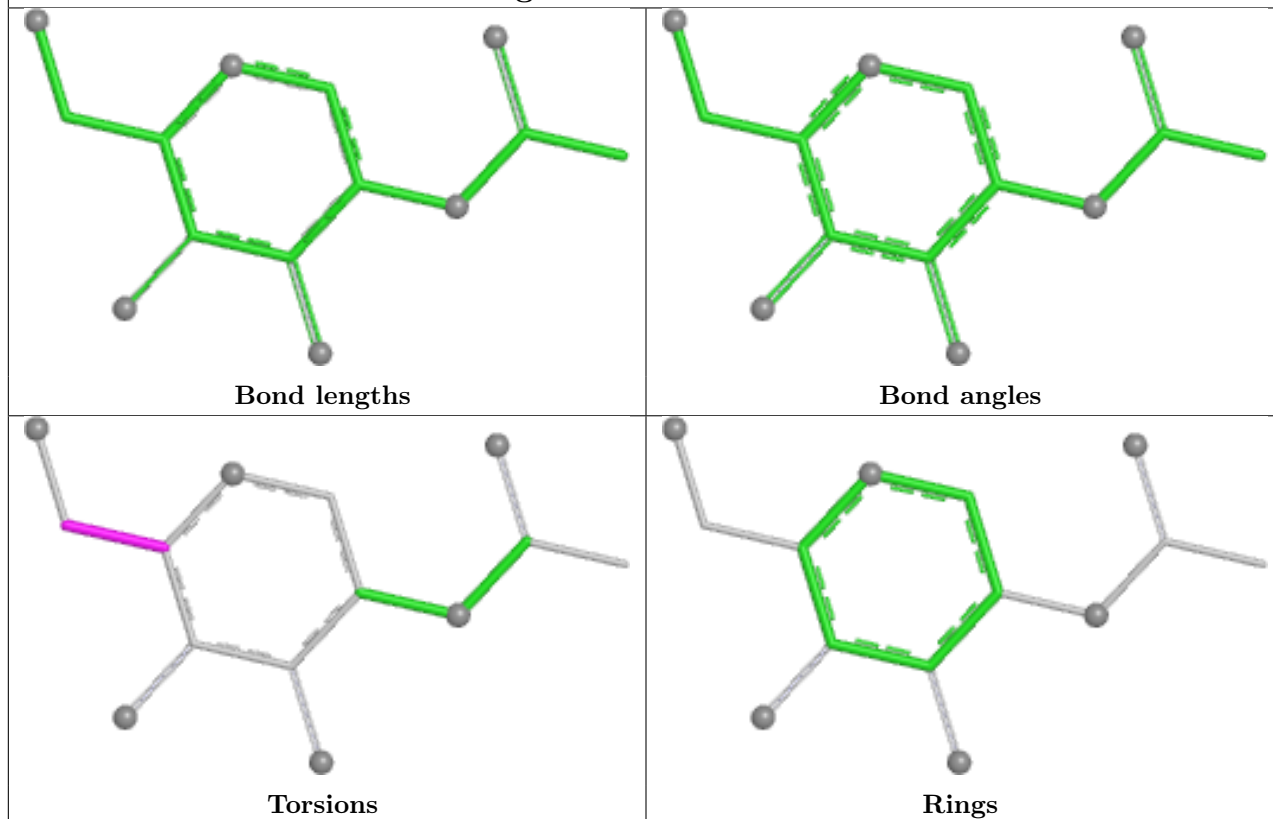
Ligand NAG D 1202



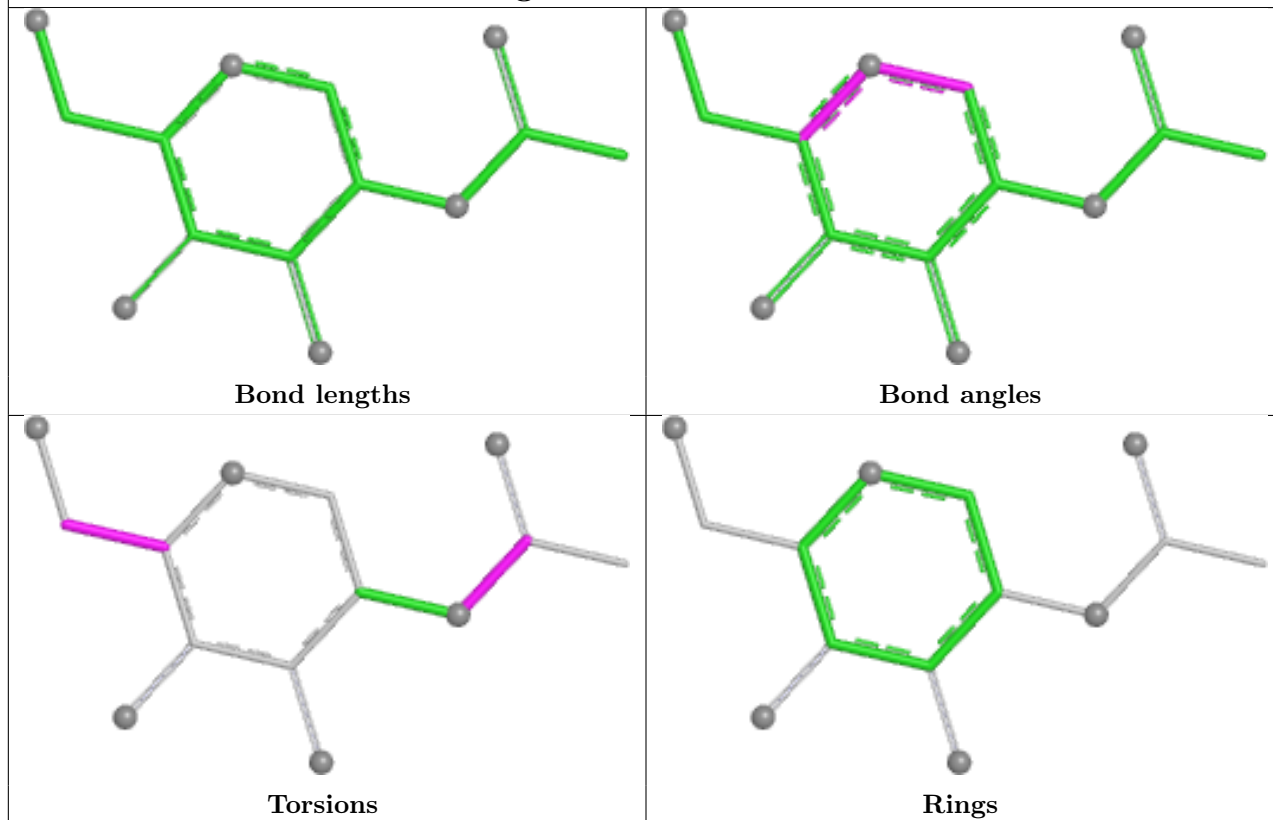
Ligand NAG C 1303

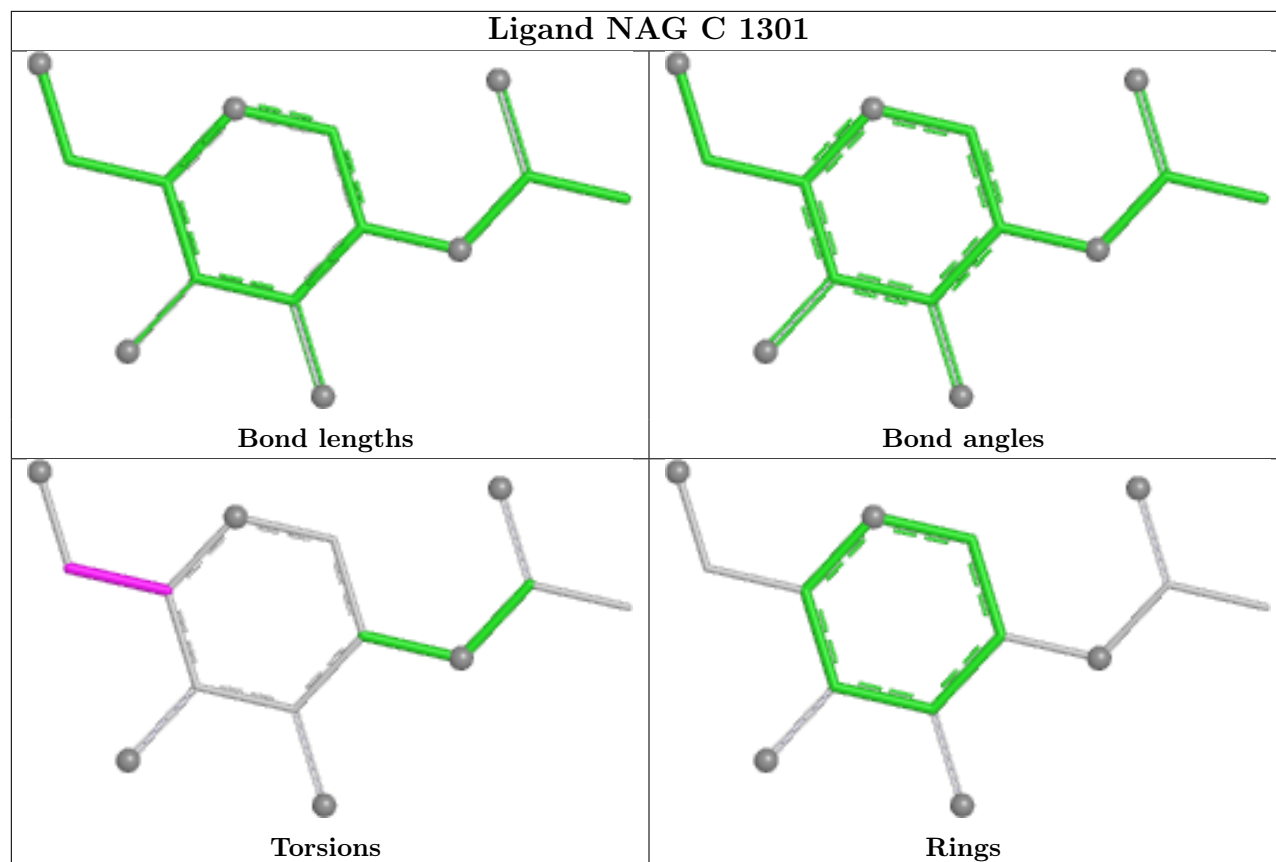


Ligand NAG D 1203



Ligand NAG G 1201





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1030/1102 (93%)	-0.59	3 (0%) 90 80	126, 218, 281, 373	0
1	D	1030/1102 (93%)	-0.55	8 (0%) 82 68	123, 211, 286, 349	0
1	G	1030/1102 (93%)	-0.54	9 (0%) 81 66	137, 212, 300, 366	0
2	B	104/140 (74%)	-0.61	0 100 100	195, 283, 337, 366	0
2	E	104/140 (74%)	-0.60	0 100 100	196, 266, 311, 324	0
2	H	104/140 (74%)	-0.57	0 100 100	188, 256, 313, 341	0
3	C	609/628 (96%)	-0.61	1 (0%) 91 82	139, 203, 260, 302	0
3	F	609/628 (96%)	-0.52	4 (0%) 84 70	132, 178, 218, 252	0
3	I	609/628 (96%)	-0.59	5 (0%) 82 68	136, 205, 262, 331	0
All	All	5229/5610 (93%)	-0.57	30 (0%) 85 73	123, 209, 287, 373	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	862	VAL	4.8
1	G	831	PHE	4.5
3	F	815	ILE	3.5
1	D	66	MET	2.9
1	D	862	VAL	2.9
1	G	835	LEU	2.8
3	I	1019	LEU	2.7
3	I	895	SER	2.6
1	G	856	GLU	2.6
3	F	1196	GLU	2.6
1	A	949	PHE	2.5
1	D	918	PHE	2.5
1	G	950	VAL	2.5
1	D	748	ALA	2.5
1	G	66	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	468	SER	2.4
1	D	947	ASN	2.4
3	F	1112	ARG	2.4
1	G	854	ILE	2.3
1	G	947	ASN	2.3
1	A	862	VAL	2.3
1	A	748	ALA	2.2
1	G	788	GLY	2.2
1	D	949	PHE	2.2
3	I	846	TYR	2.2
1	D	470	PRO	2.2
3	F	1113	LEU	2.1
3	I	1064	VAL	2.1
3	C	1073	PHE	2.1
3	I	1021	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

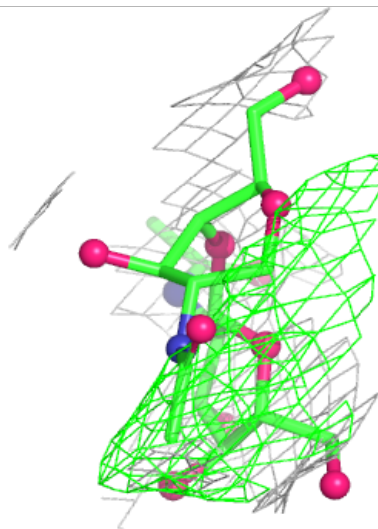
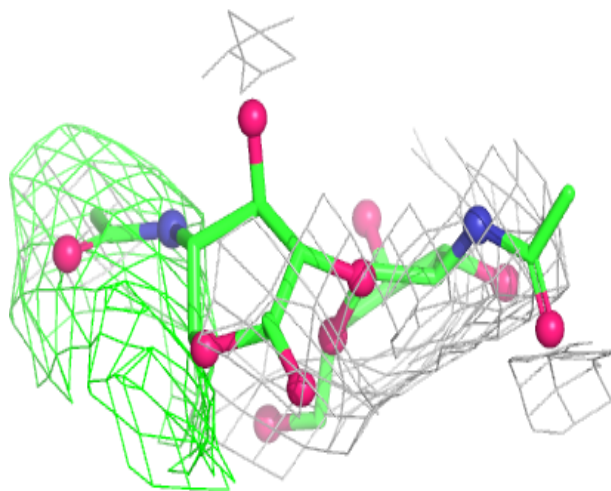
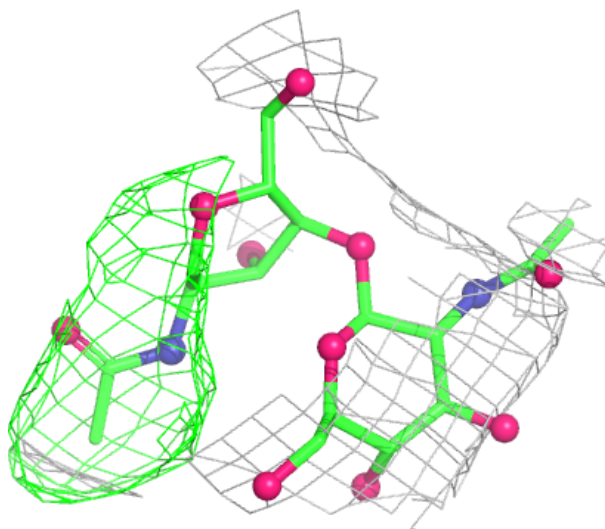
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

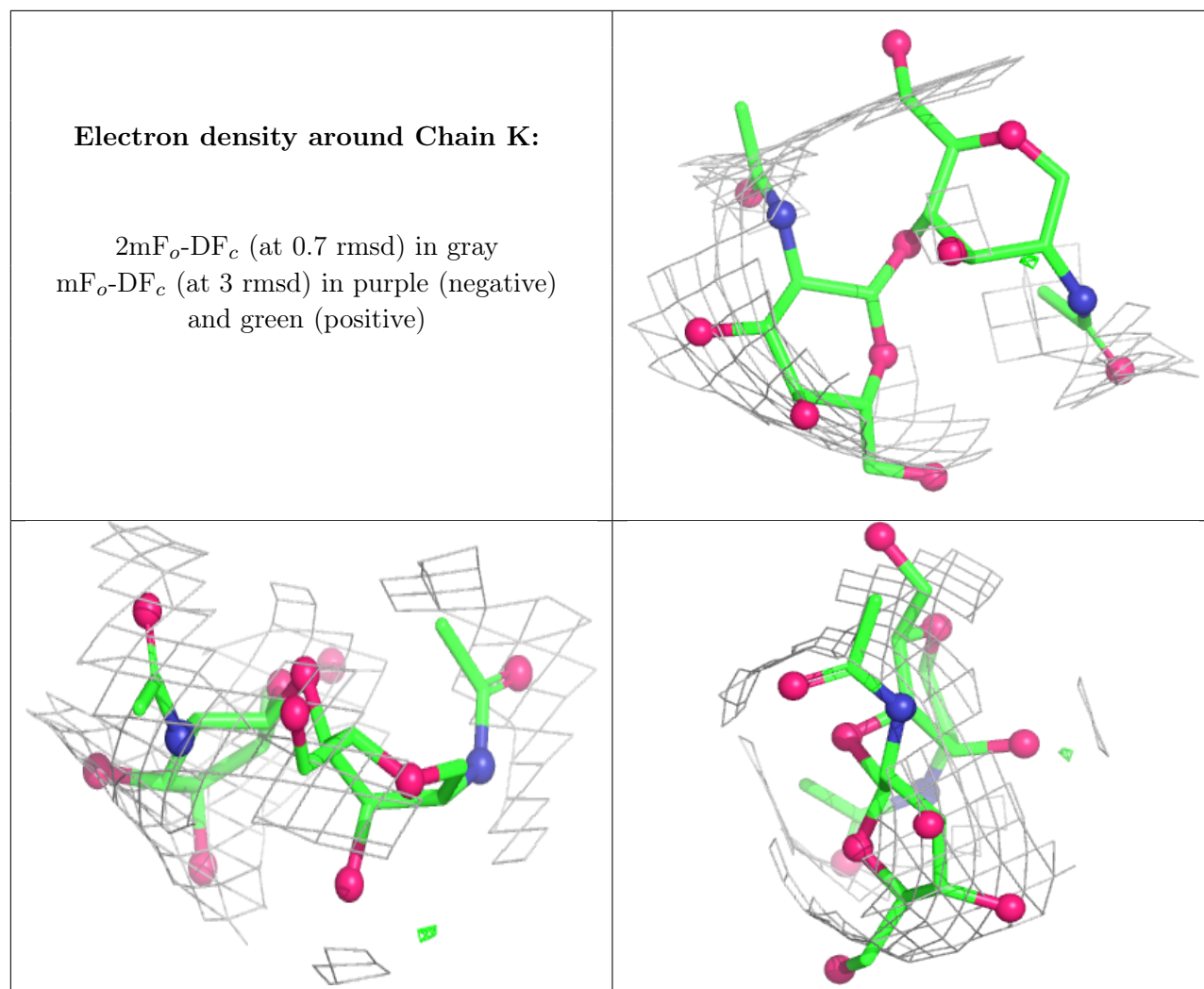
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	J	1	14/15	0.67	0.09	177,211,249,290	0
4	NAG	J	2	14/15	0.78	0.09	195,245,293,301	0
4	NAG	K	1	14/15	0.84	0.08	205,222,228,234	0
4	NAG	K	2	14/15	0.86	0.06	198,246,258,281	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	1206	14/15	0.35	0.09	219,254,306,326	0
5	NAG	G	1201	14/15	0.46	0.08	223,278,310,322	0
5	NAG	E	200	14/15	0.59	0.07	198,216,229,232	0
5	NAG	F	1302	14/15	0.67	0.07	213,231,247,250	0
5	NAG	D	1204	14/15	0.68	0.08	235,250,271,300	0
5	NAG	G	1202	14/15	0.69	0.05	149,235,303,323	0
5	NAG	A	1201	14/15	0.72	0.07	219,239,264,288	0
5	NAG	A	1202	14/15	0.74	0.07	172,196,209,218	0
5	NAG	G	1205	14/15	0.74	0.07	181,219,248,272	0

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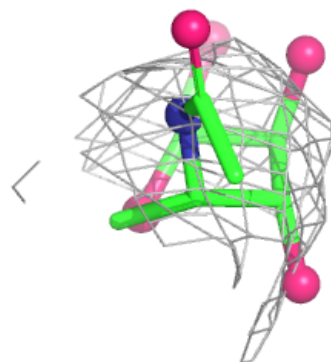
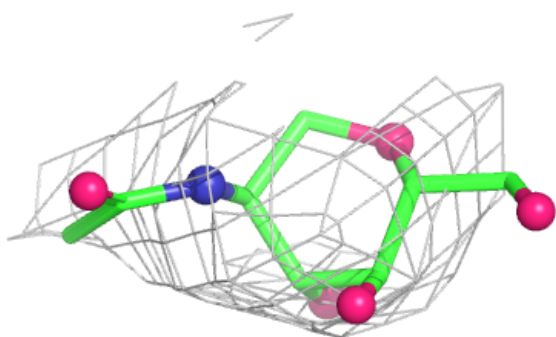
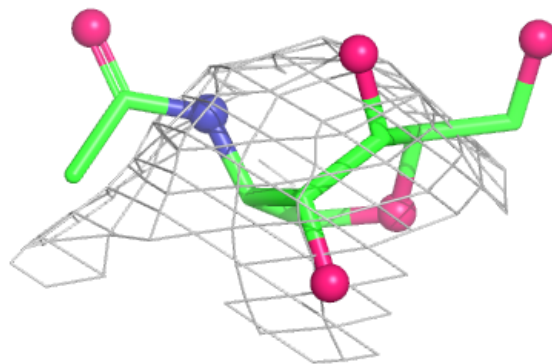
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	1205	14/15	0.74	0.06	182,198,216,226	0
5	NAG	C	1304	14/15	0.76	0.08	189,197,228,231	0
5	NAG	G	1203	14/15	0.76	0.08	148,188,196,207	0
5	NAG	D	1201	14/15	0.77	0.06	194,272,278,292	0
5	NAG	D	1203	14/15	0.77	0.05	221,233,266,270	0
5	NAG	F	1305	14/15	0.78	0.10	120,179,195,218	0
5	NAG	F	1303	14/15	0.78	0.09	165,224,239,255	0
5	NAG	D	1205	14/15	0.81	0.05	197,239,256,261	0
5	NAG	A	1204	14/15	0.84	0.06	223,252,272,278	0
5	NAG	H	200	14/15	0.85	0.07	225,230,243,251	0
5	NAG	A	1203	14/15	0.86	0.06	233,259,276,278	0
5	NAG	I	1302	14/15	0.86	0.05	174,219,231,237	0
5	NAG	F	1301	14/15	0.87	0.06	173,192,197,201	0
5	NAG	D	1202	14/15	0.89	0.06	175,195,206,208	0
5	NAG	I	1301	14/15	0.90	0.06	192,215,236,249	0
5	NAG	C	1303	14/15	0.90	0.07	180,203,249,252	0
5	NAG	I	1303	14/15	0.91	0.04	185,201,215,223	0
5	NAG	G	1204	14/15	0.92	0.04	225,255,282,288	0
5	NAG	C	1301	14/15	0.95	0.05	183,199,227,240	0
5	NAG	C	1302	14/15	0.95	0.05	168,190,208,225	0
5	NAG	F	1304	14/15	0.97	0.06	143,175,209,212	0

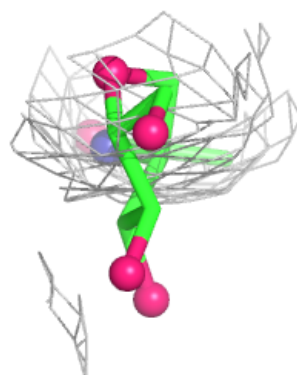
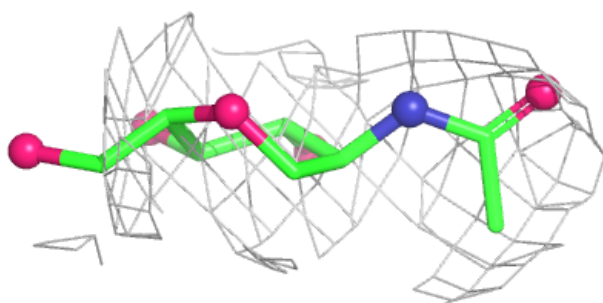
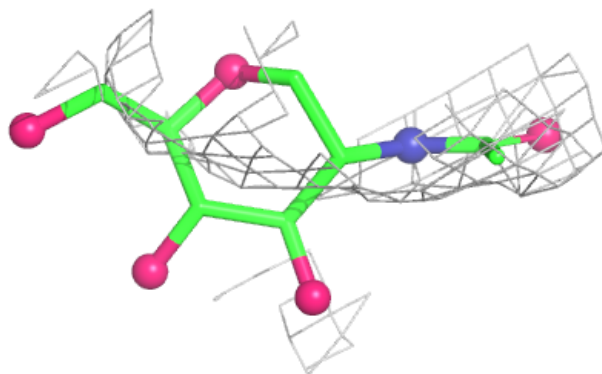
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG G 1206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

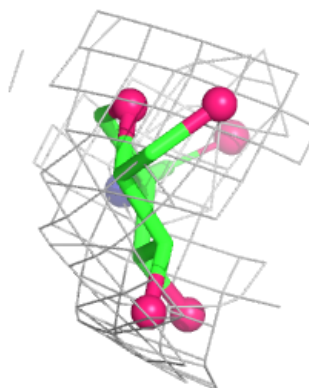
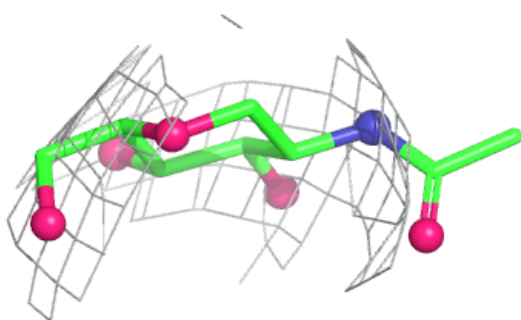
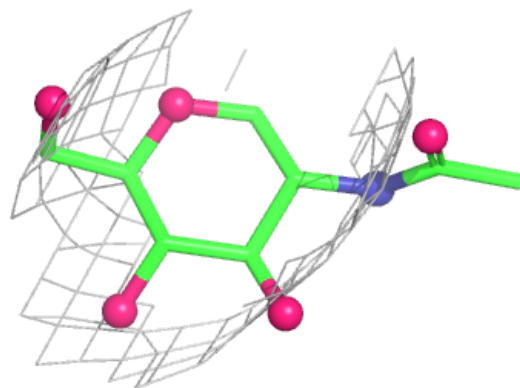
**Electron density around NAG G 1201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

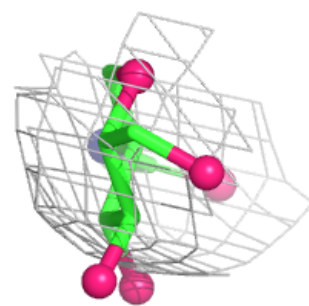
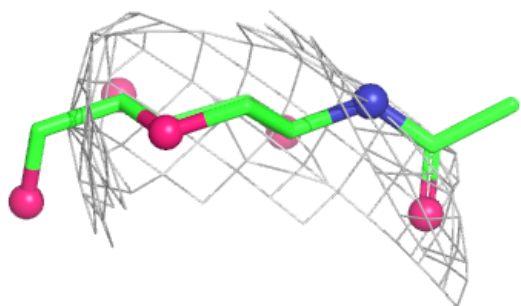
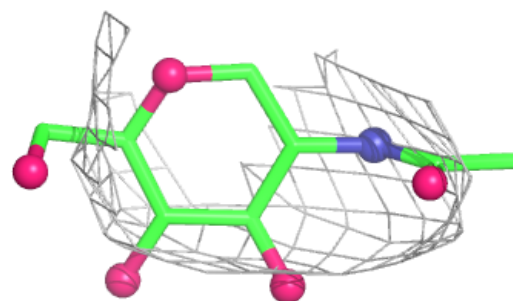


Electron density around NAG E 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

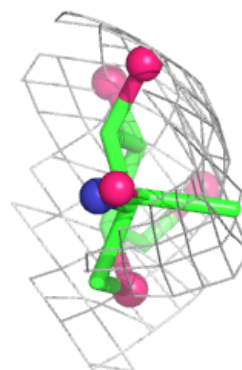
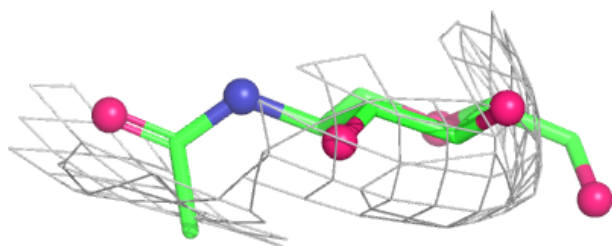
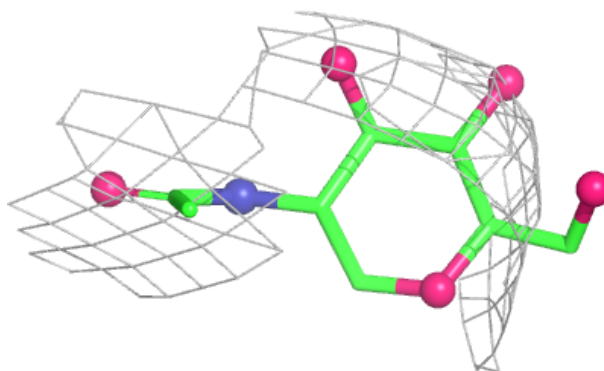
**Electron density around NAG F 1302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

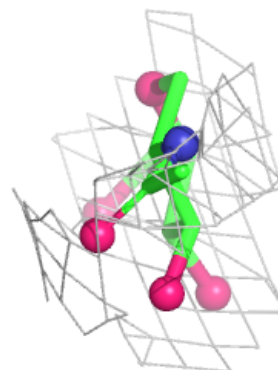
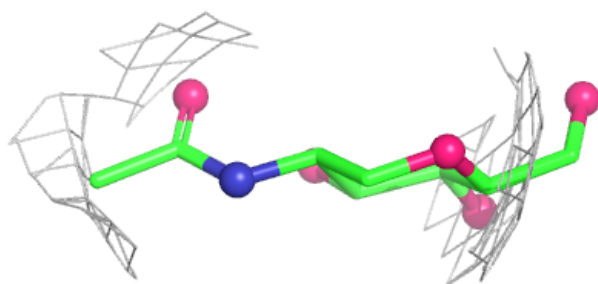
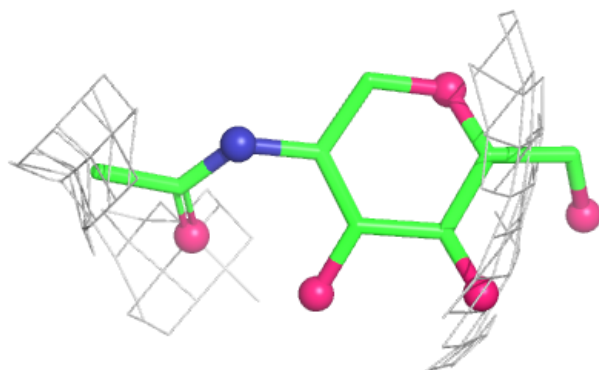


Electron density around NAG D 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

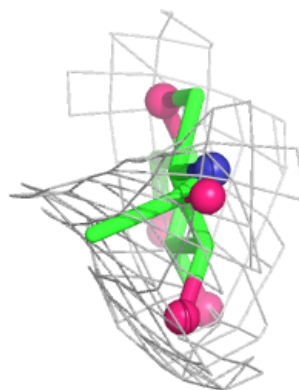
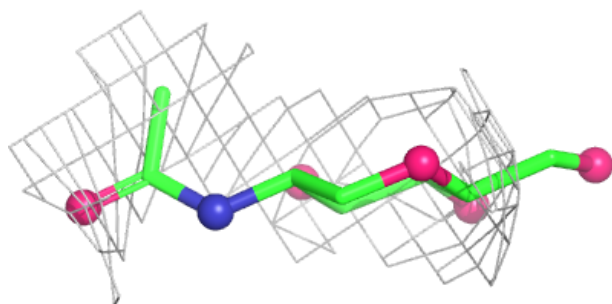
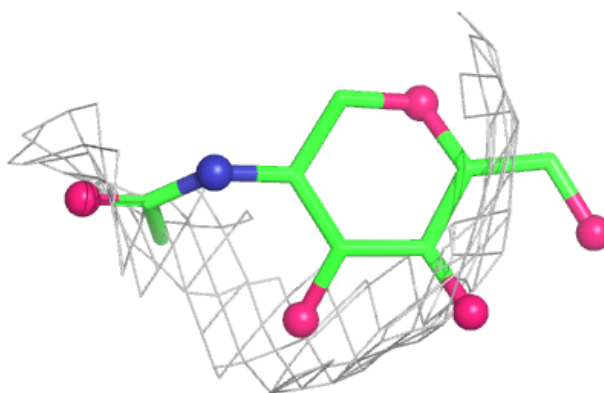
**Electron density around NAG G 1202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

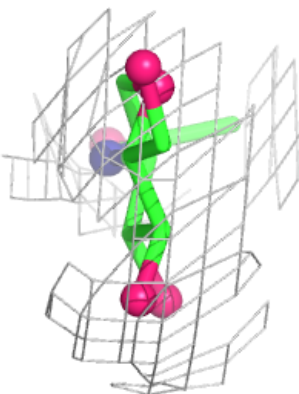
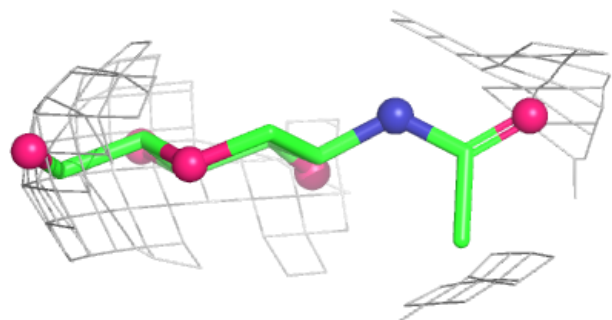
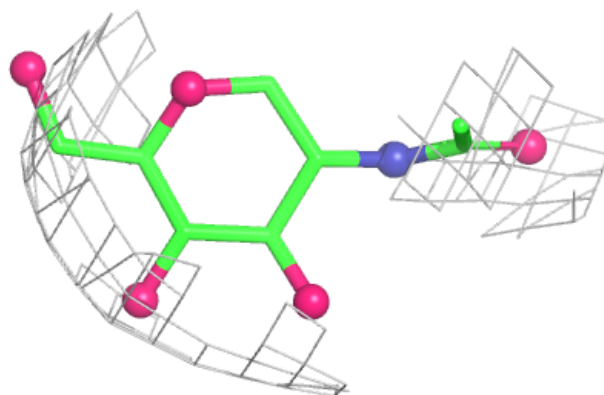


Electron density around NAG A 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

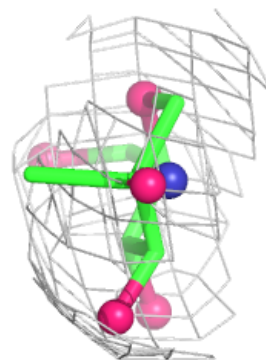
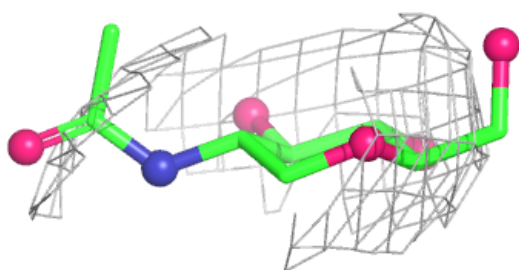
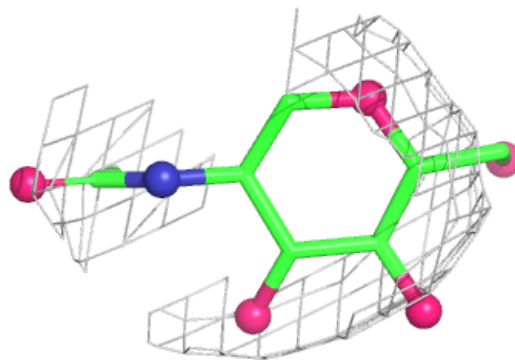
**Electron density around NAG A 1202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

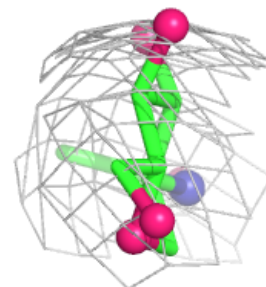
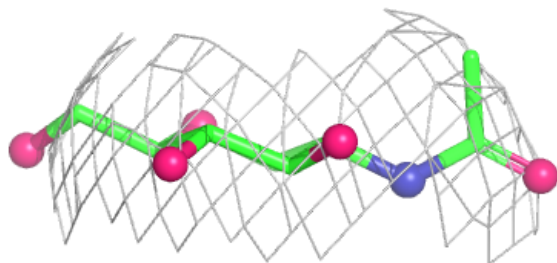
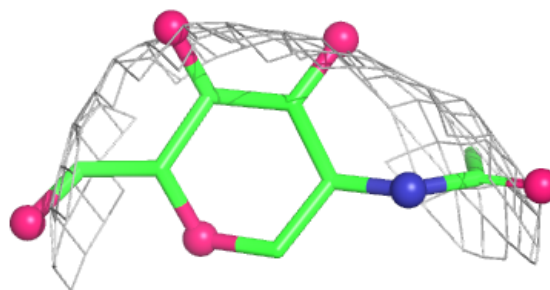


Electron density around NAG G 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

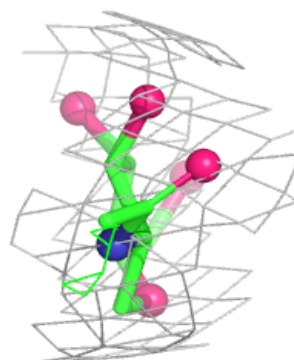
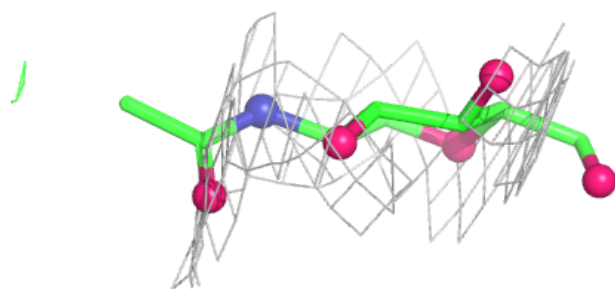
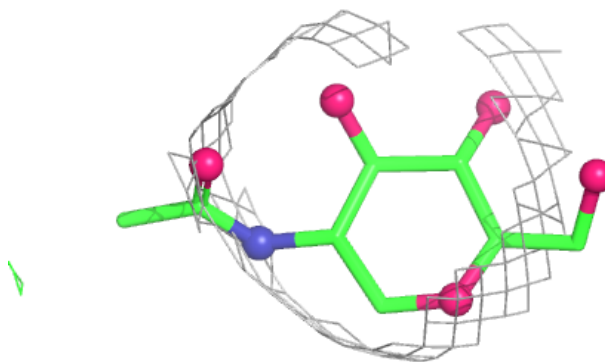
**Electron density around NAG A 1205:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

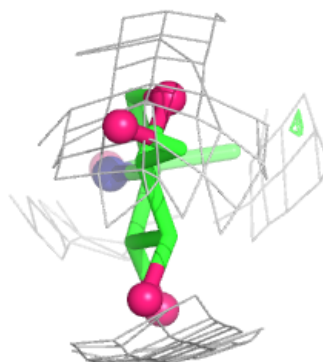
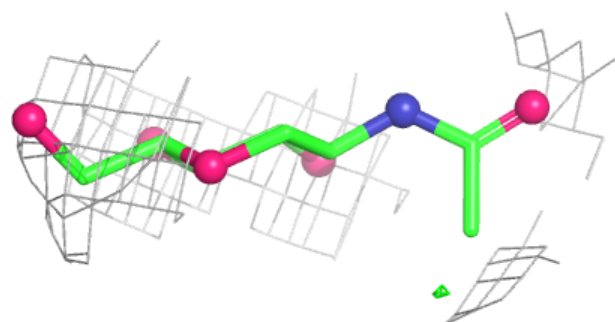
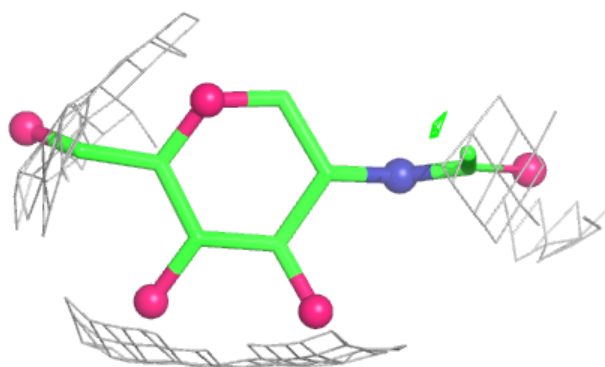


Electron density around NAG C 1304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

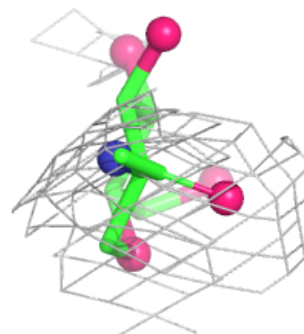
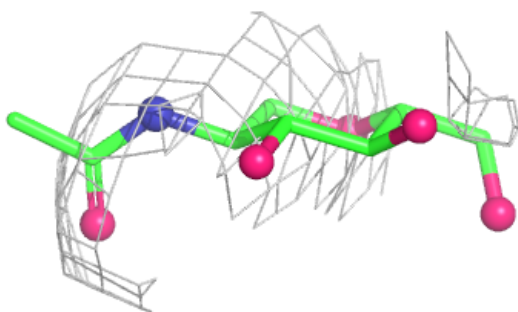
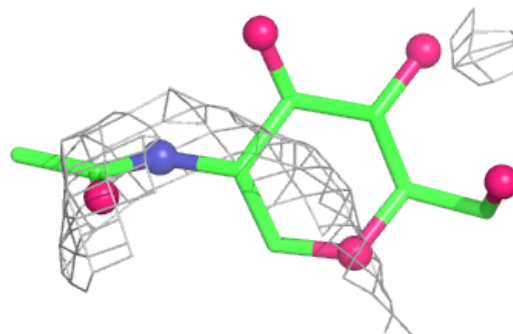
**Electron density around NAG G 1203:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

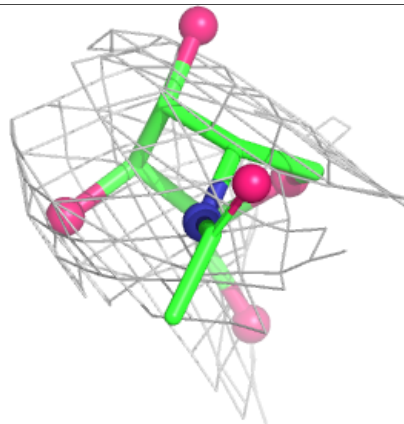
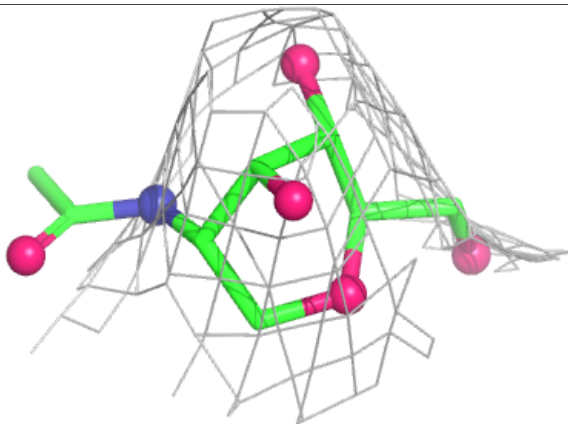
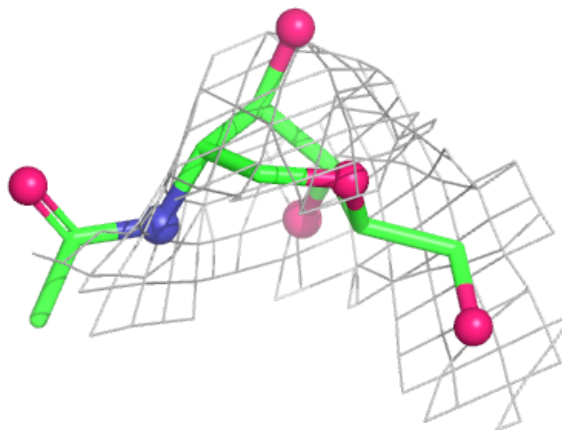


Electron density around NAG D 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

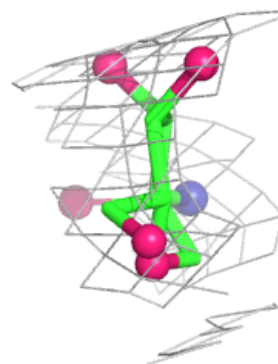
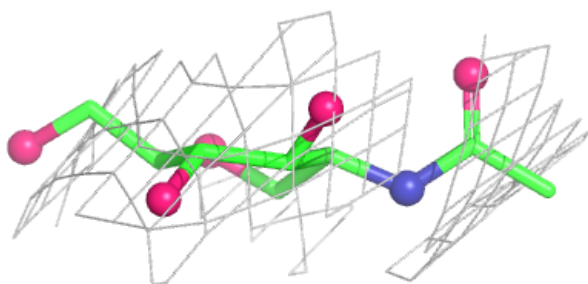
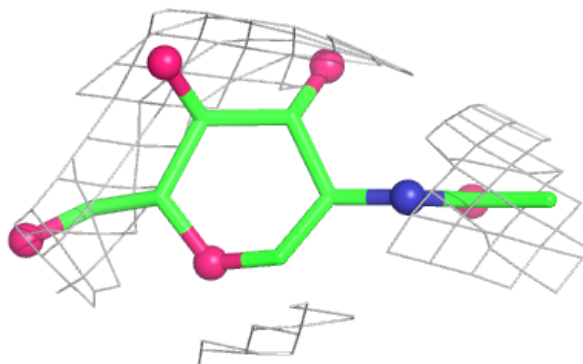
**Electron density around NAG D 1203:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

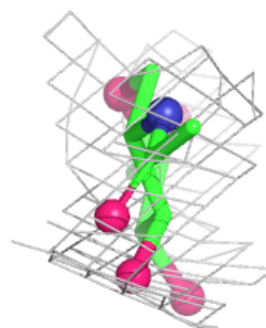
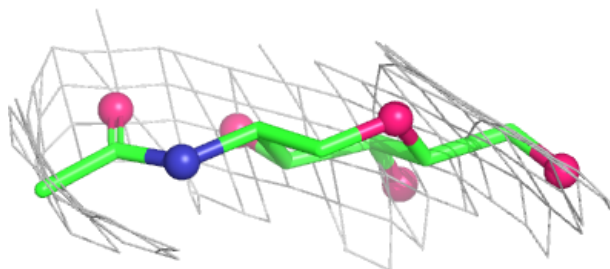
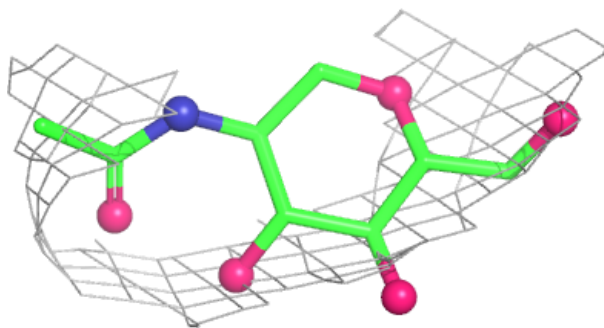


Electron density around NAG F 1305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

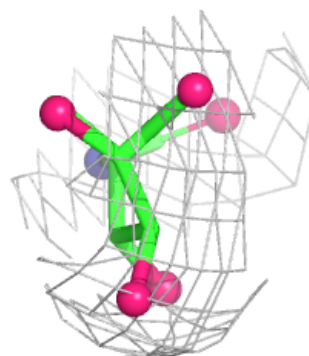
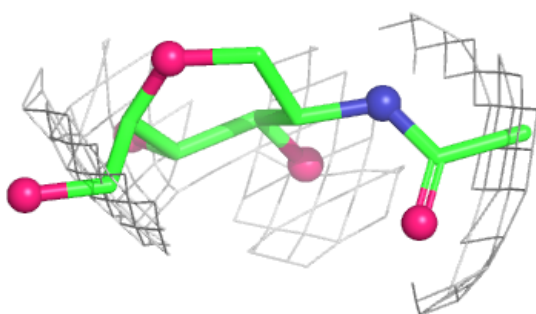
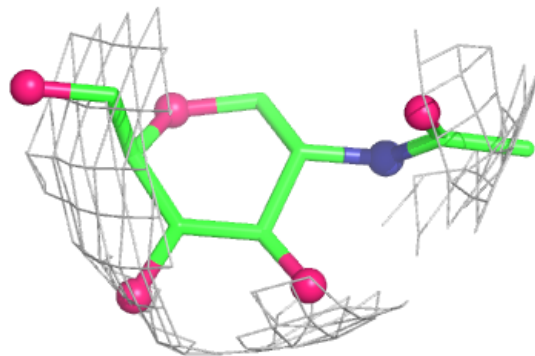
**Electron density around NAG F 1303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

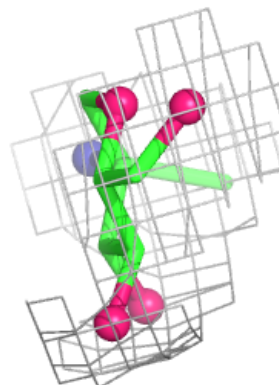
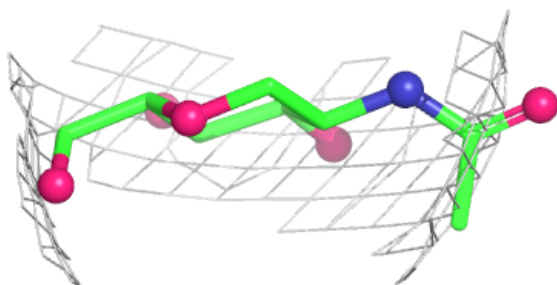
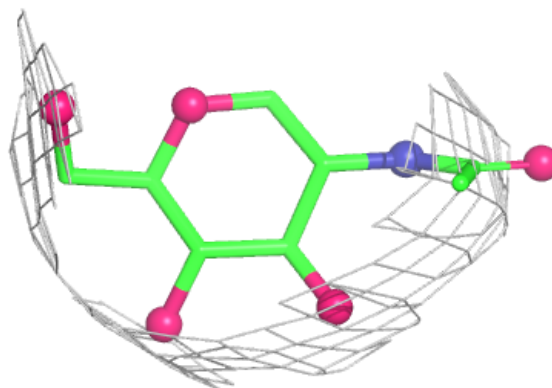


Electron density around NAG D 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

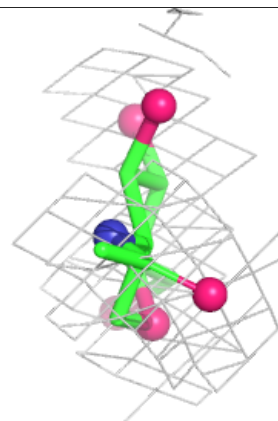
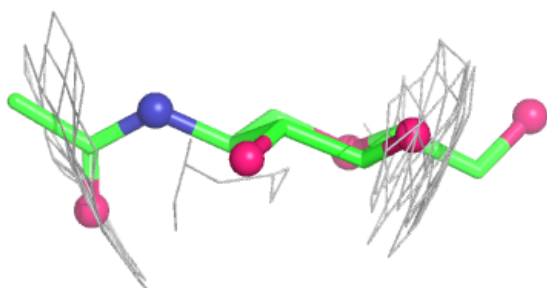
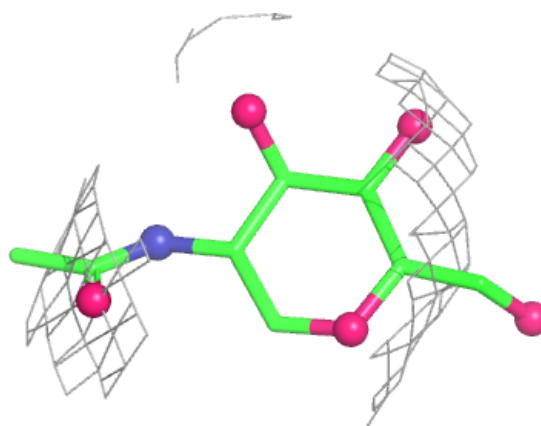
**Electron density around NAG A 1204:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

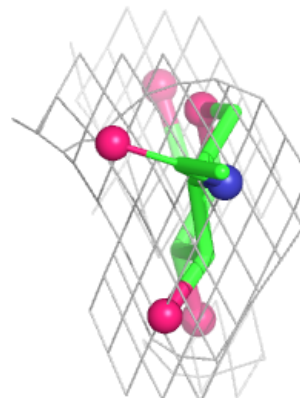
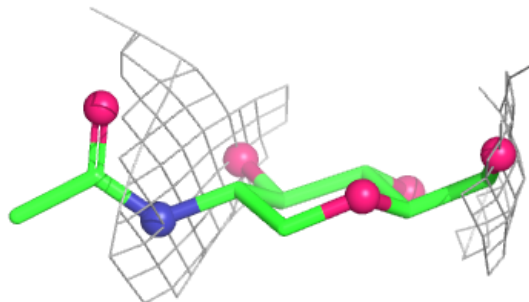
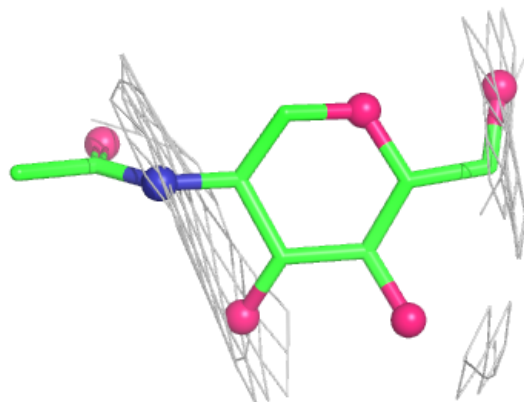


Electron density around NAG H 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

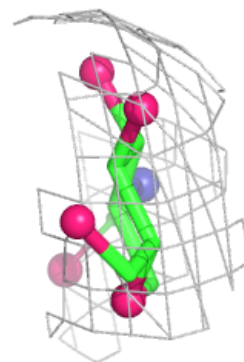
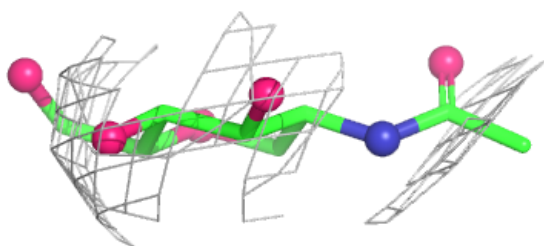
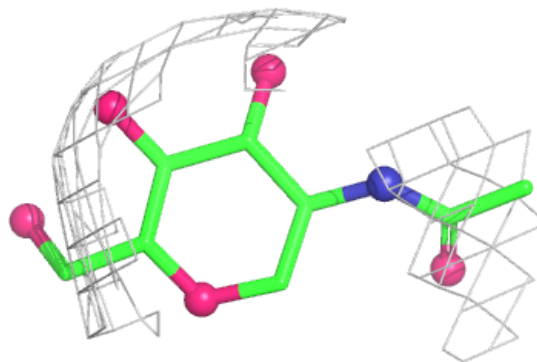
**Electron density around NAG A 1203:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

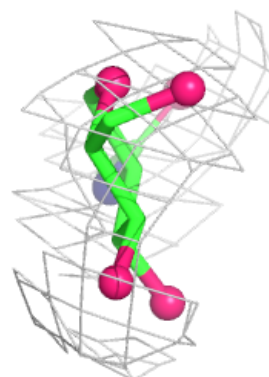
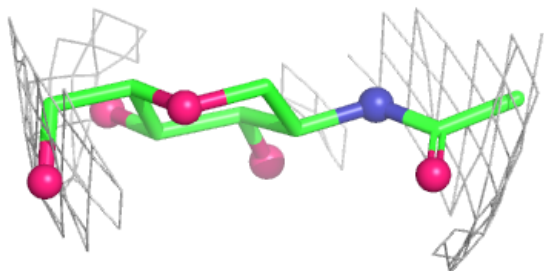
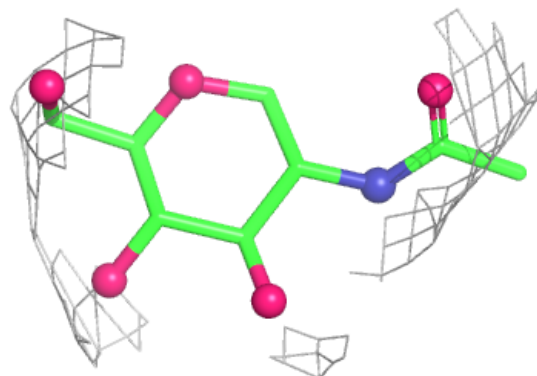


Electron density around NAG I 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

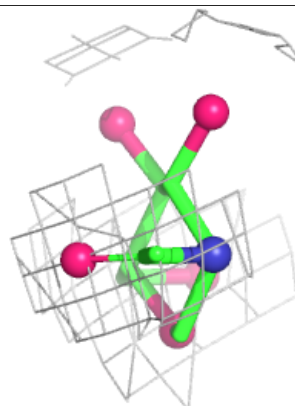
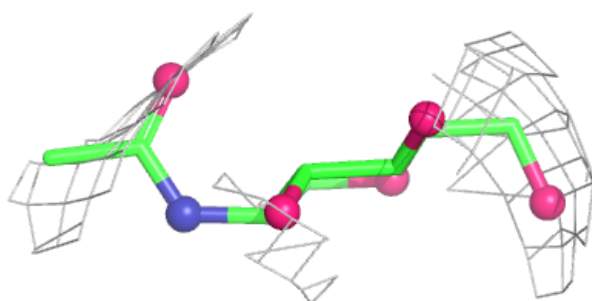
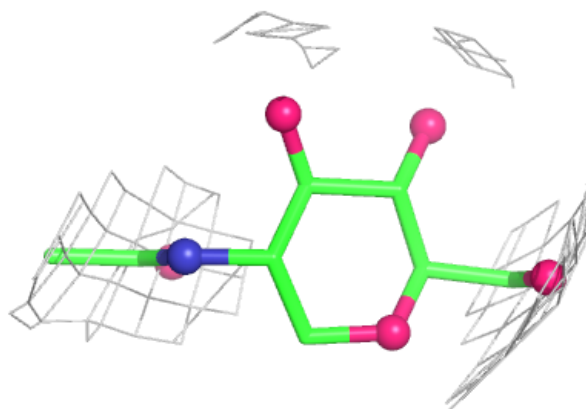
**Electron density around NAG F 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

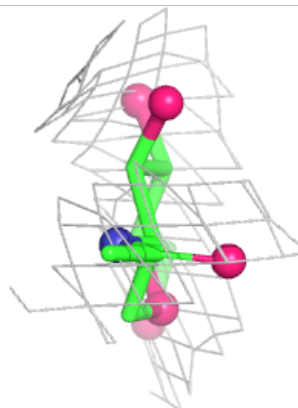
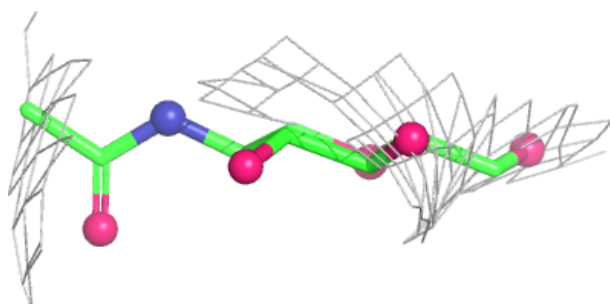
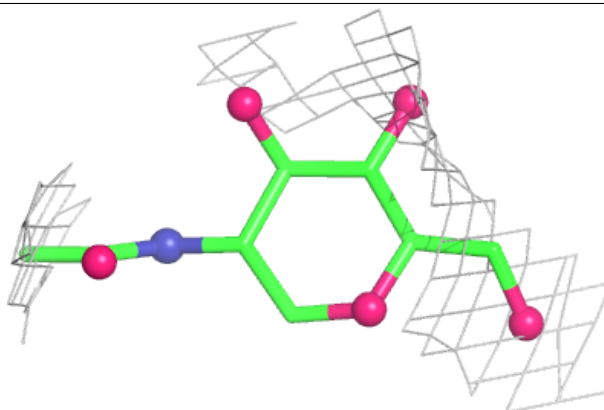


Electron density around NAG D 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

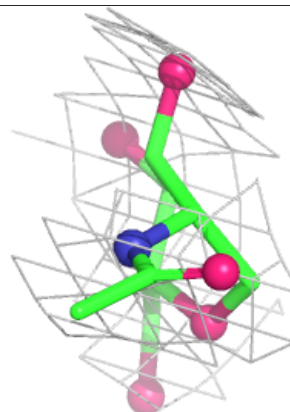
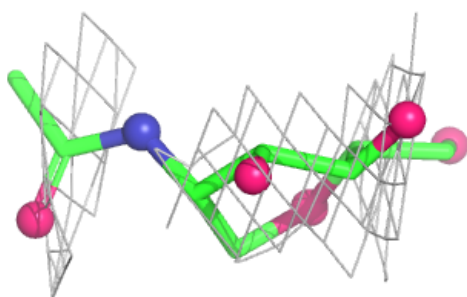
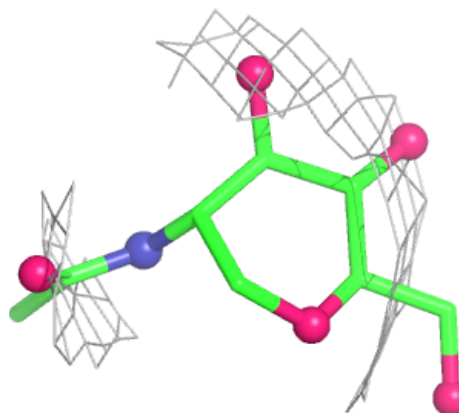
**Electron density around NAG I 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

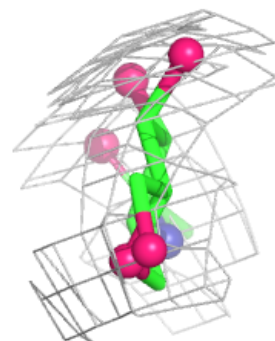
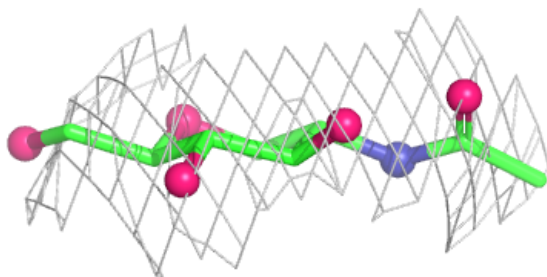
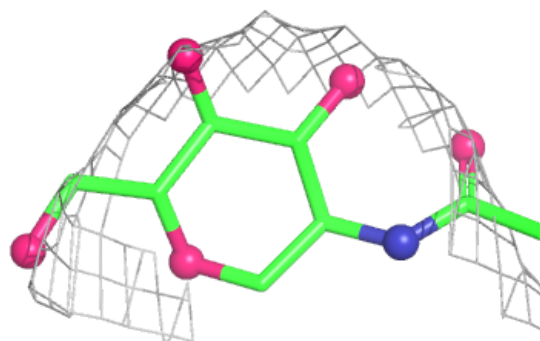


Electron density around NAG C 1303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

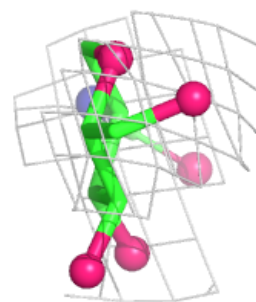
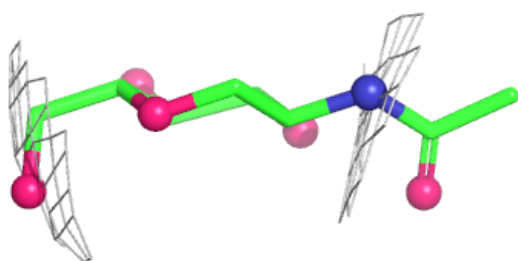
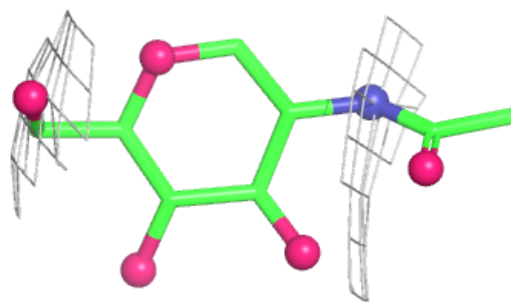
**Electron density around NAG I 1303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

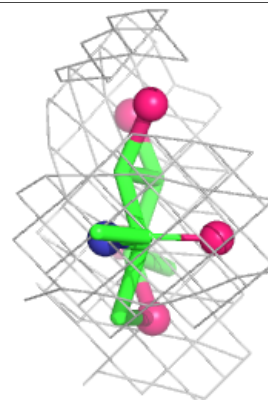
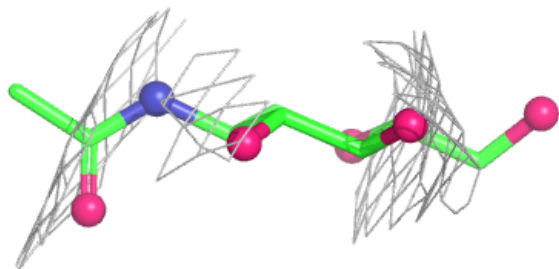
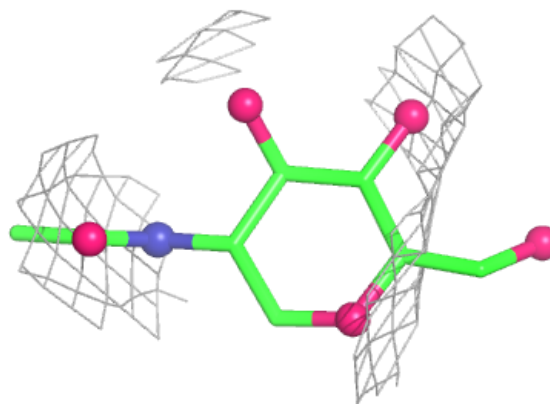


Electron density around NAG G 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

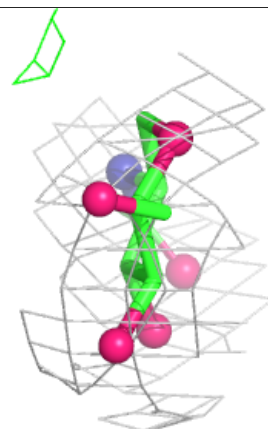
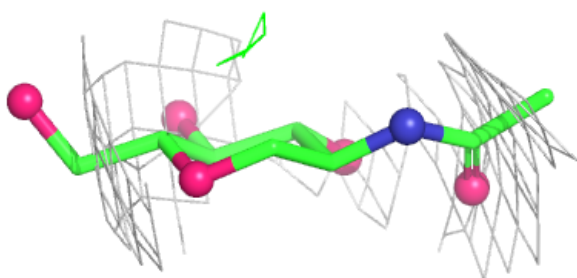
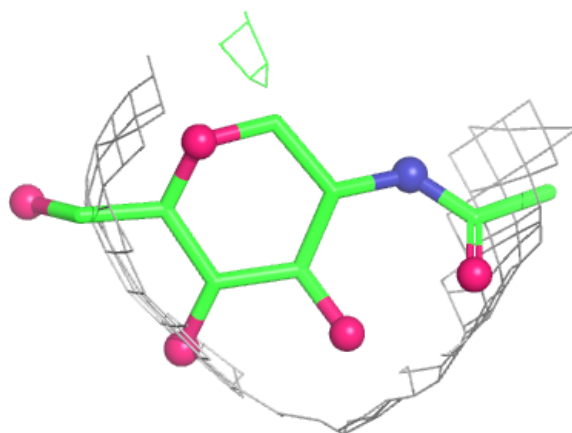
**Electron density around NAG C 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



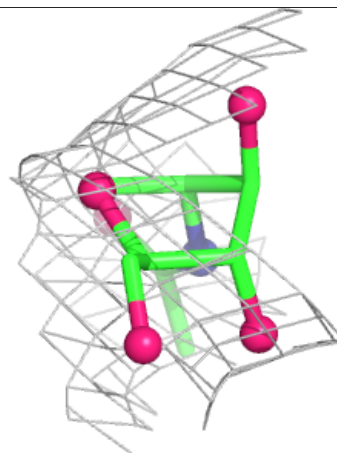
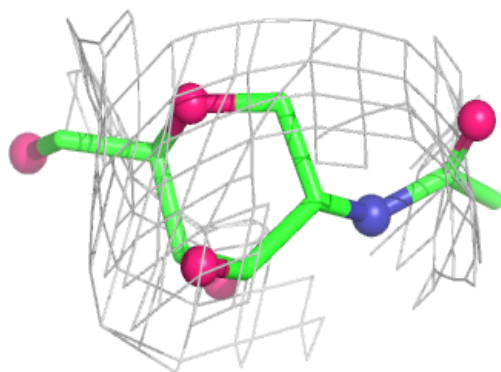
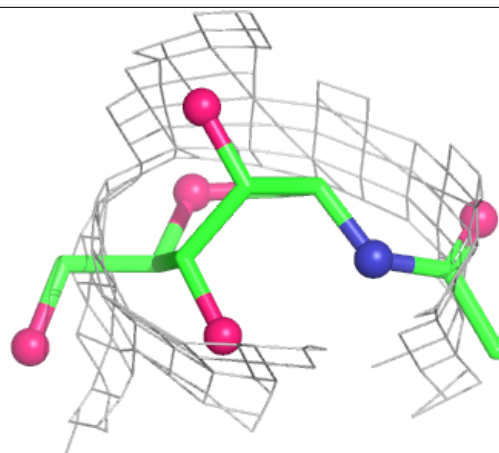
Electron density around NAG C 1302:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAG F 1304:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.