



# Full wwPDB X-ray Structure Validation Report i

Apr 18, 2024 – 04:42 pm BST

PDB ID : 8S7C  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

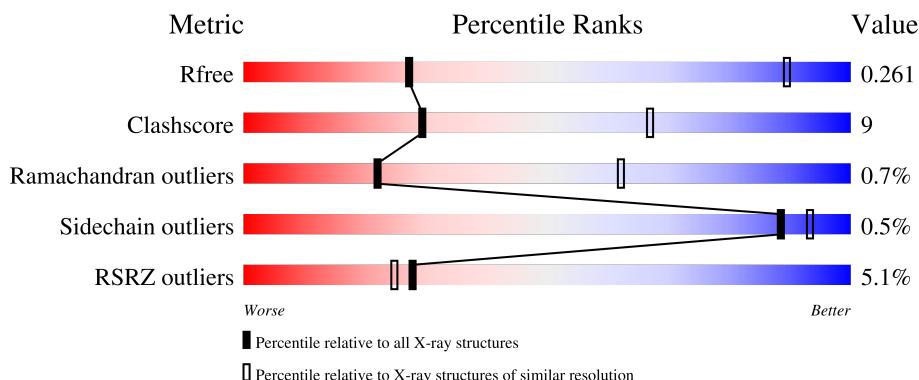
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1085 (5.58-3.80)
Clashscore	141614	1159 (5.60-3.80)
Ramachandran outliers	138981	1094 (5.58-3.80)
Sidechain outliers	138945	1074 (5.58-3.80)
RSRZ outliers	127900	1118 (5.70-3.70)

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  $\geq 3$ , 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.



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## 2 Entry composition (i)

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 8059	N 5068	O 1385	S 1547	59	0	0
1	D	1030	Total	C 8059	N 5068	O 1385	S 1547	59	0	0
1	G	1030	Total	C 8059	N 5068	O 1385	S 1547	59	0	0

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			
			4848	3042	859	922	25	0	0	0
3	F	609	Total	C	N	O	S			
			4848	3042	859	922	25	0	0	0
3	I	609	Total	C	N	O	S			
			4848	3042	859	922	25	0	0	0

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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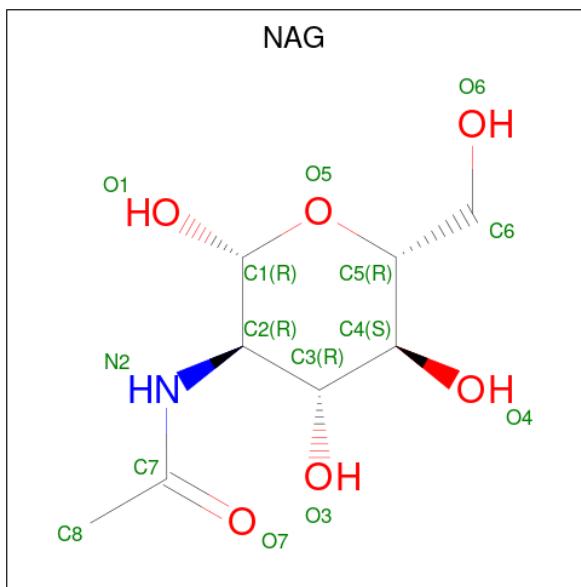
Chain	Residue	Modelled	Actual	Comment	Reference
I	627	THR	-	expression tag	UNP O75581
I	628	GLY	-	expression tag	UNP O75581
I	1245	GLY	-	expression tag	UNP O75581
I	1246	THR	-	expression tag	UNP O75581
I	1247	LYS	-	expression tag	UNP O75581
I	1248	HIS	-	expression tag	UNP O75581
I	1249	HIS	-	expression 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 28 16 2 10	0	0	0
4	K	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (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	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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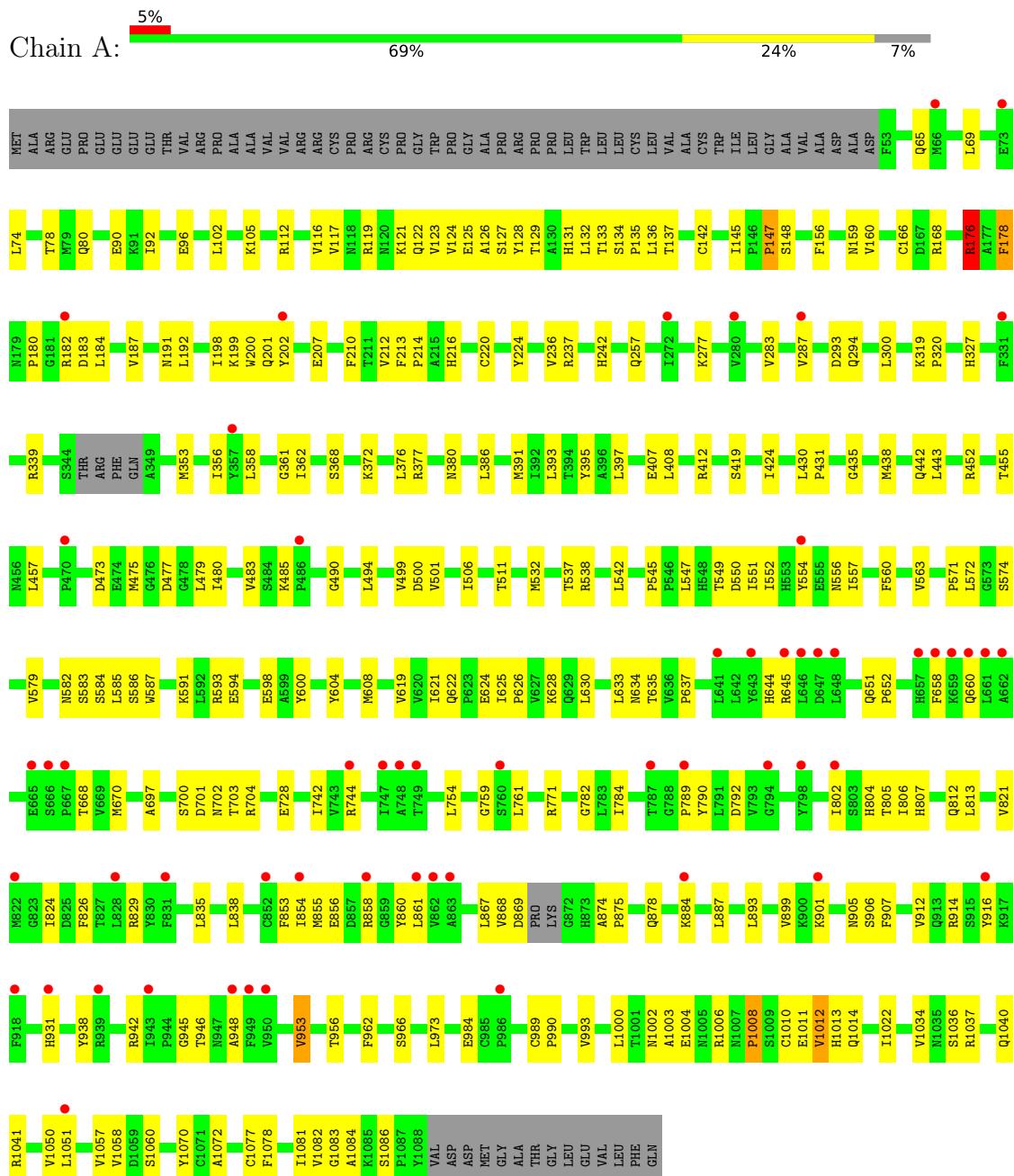
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	H	1	Total C N O 14 8 1 5	0	0
5	I	1	Total C N O 14 8 1 5	0	0
5	I	1	Total C N O 14 8 1 5	0	0
5	I	1	Total C N O 14 8 1 5	0	0

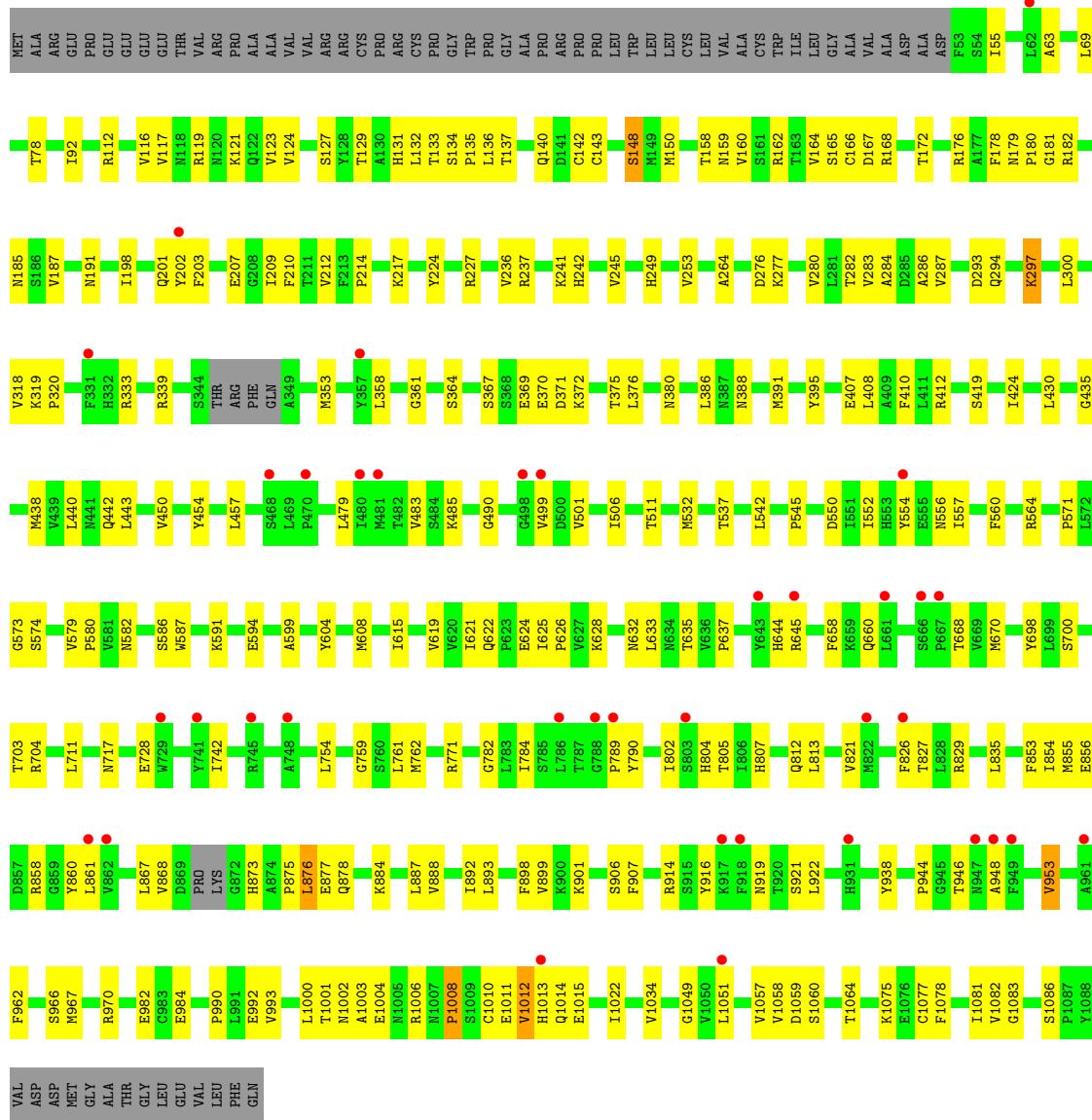
### 3 Residue-property plots

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.

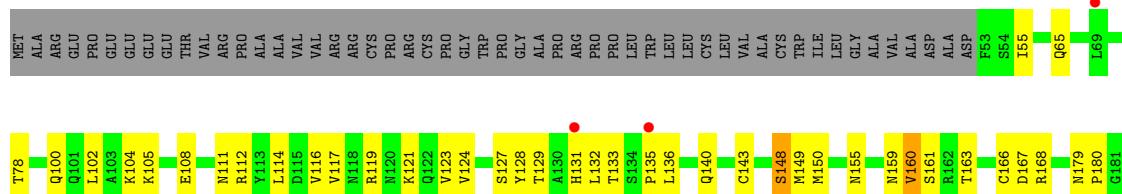
- Molecule 1: VWFA and cache domain-containing protein 1

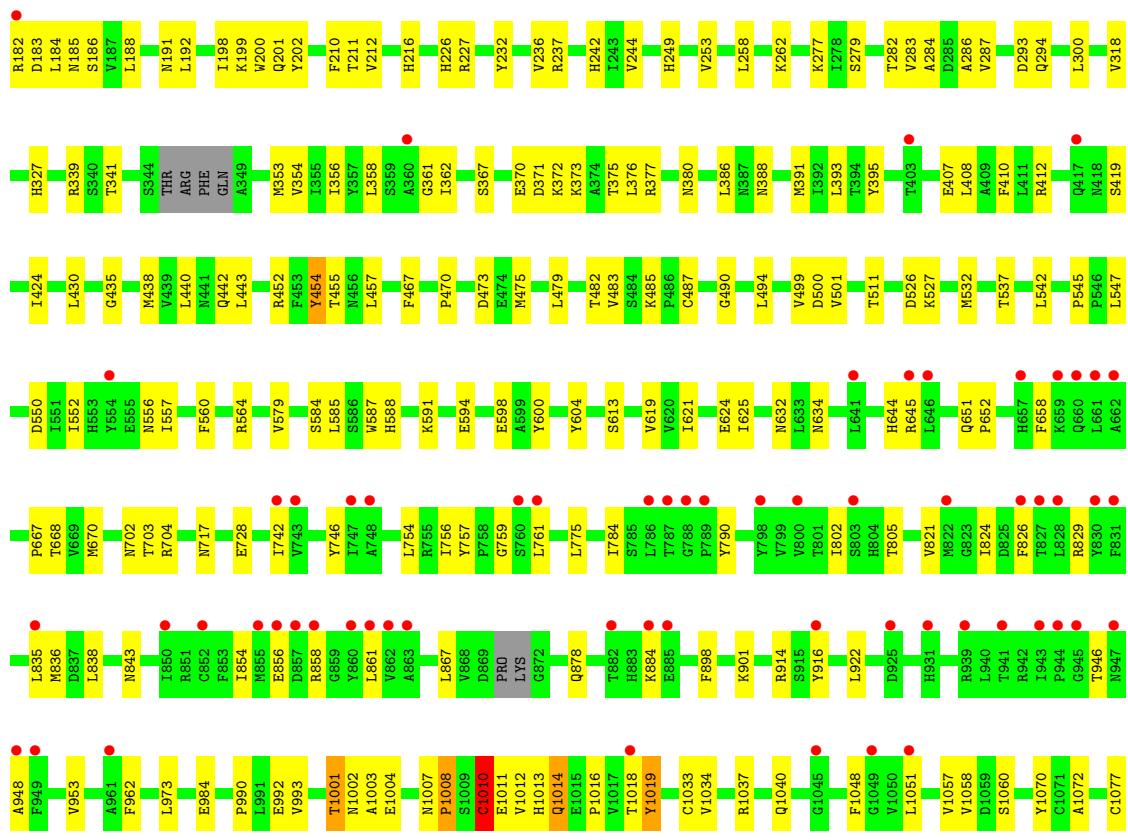


- Molecule 1: VWFA and cache domain-containing protein 1



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

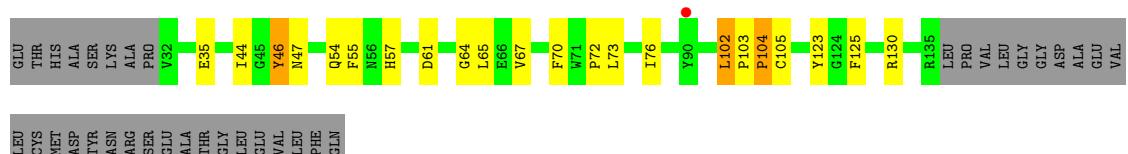




- Molecule 2: Frizzled-5

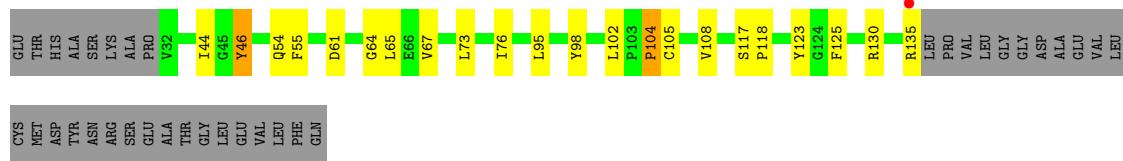


- Molecule 2: Frizzled-5

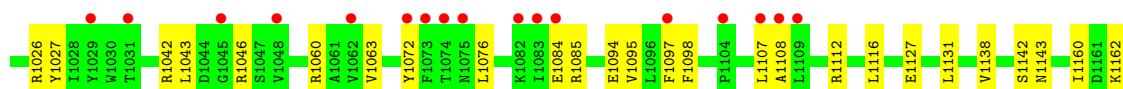


- Molecule 2: Frizzled-5

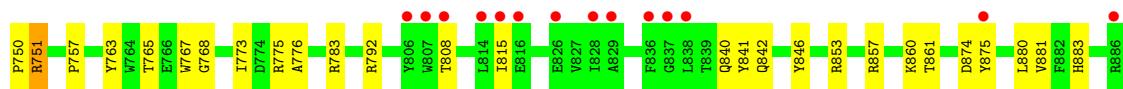




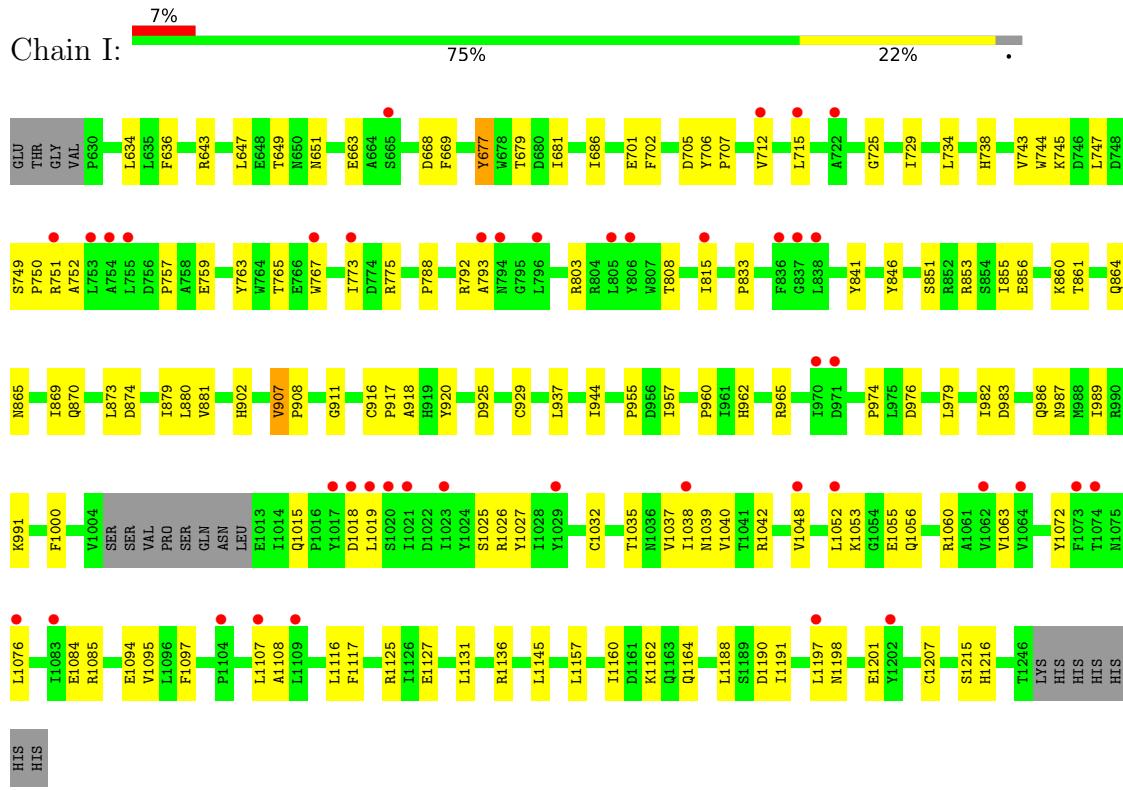
- Molecule 3: Low-density lipoprotein receptor-related protein 6



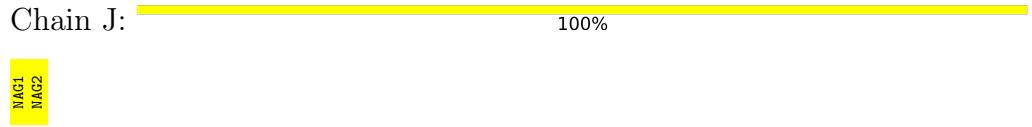
- Molecule 3: Low-density lipoprotein receptor-related protein 6



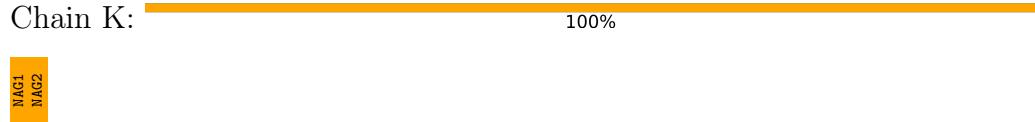
- Molecule 3: Low-density lipoprotein receptor-related protein 6



- 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 i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	283.70 Å    198.24 Å    218.82 Å 90.00°    128.07°    90.00°	Depositor
Resolution (Å)	86.13 – 4.70 172.27 – 4.70	Depositor EDS
% Data completeness (in resolution range)	47.2 (86.13-4.70) 47.3 (172.27-4.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.75 (at 4.66 Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ????)	Depositor
$R$ , $R_{free}$	0.206 , 0.261 0.206 , 0.261	Depositor DCC
$R_{free}$ test set	1188 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	188.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 166.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	41714	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/8224	0.46	0/11169
1	D	0.24	0/8224	0.45	0/11169
1	G	0.24	0/8224	0.44	0/11169
2	B	0.24	0/867	0.42	0/1179
2	E	0.26	0/867	0.45	0/1179
2	H	0.25	0/867	0.45	0/1179
3	C	0.24	0/4950	0.46	0/6716
3	F	0.24	0/4950	0.47	0/6716
3	I	0.25	0/4950	0.48	0/6716
All	All	0.24	0/42123	0.46	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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8059	0	7939	184	0
1	D	8059	0	7940	179	0
1	G	8059	0	7939	155	0
2	B	839	0	790	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	839	0	790	18	0
2	H	839	0	790	15	0
3	C	4848	0	4727	73	0
3	F	4848	0	4726	90	0
3	I	4848	0	4725	91	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	0	0
5	H	14	0	13	0	0
5	I	42	0	39	3	0
All	All	41714	0	40806	780	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 9.

All (780) 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:A:584:SER:HG	1:A:600:TYR:HH	1.46	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
3:I:1162:LYS:NZ	3:I:1188:LEU:O	2.27	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
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
1:A:670:MET:HB3	1:A:754:LEU:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1012:VAL:C	1:A:1014:GLN:H	2.14	0.51
3:C:1107:LEU:HD11	3:C:1116:LEU:HD11	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:992:GLU:HG2	1:G:1004:GLU:CD	2.32	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1012:VAL:C	1:D:1014:GLN:H	2.16	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: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
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:391:MET:HE3	1:A:435:GLY:HA2	1.96	0.48
1:A:829:ARG:NH2	1:A:867:LEU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:452:ARG:HH21	1:G:455:THR:HG21	1.81	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:482:THR:OG1	1:G:500:ASP:OD1	2.25	0.45
3:I:677:TYR:HE2	3:I:734:LEU:HD22	1.80	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
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: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
3:I:908:PRO:HD2	3:I:911:GLY:C	2.36	0.45
1:A:136:LEU:HB3	1:A:180:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:I:1032:CYS:HG	3:I:1035:THR:HG1	1.65	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: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: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:391:MET:HE3	1:D:435:GLY:HA2	2.00	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
1:G:584:SER:OG	1:G:600:TYR:OH	2.35	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:649:THR:C	3:I:651:ASN:H	2.22	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
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: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:284:ALA:C	1:D:286:ALA:H	2.23	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
2:E:103:PRO:O	2:E:104:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
3:I:1084:GLU:HG2	3:I:1095:VAL:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:148:SER:C	1:G:150:MET:H	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
1:G:391:MET:HE3	1:G:435:GLY:HA2	2.03	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:582:ASN:O	1:A:583:SER:OG	2.31	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
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
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:284:ALA:C	1:G:286:ALA:H	2.24	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%)	22 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	1024/1102 (93%)	910 (89%)	104 (10%)	10 (1%)	15 54
1	G	1024/1102 (93%)	915 (89%)	97 (10%)	12 (1%)	13 50
2	B	102/140 (73%)	94 (92%)	7 (7%)	1 (1%)	15 54
2	E	102/140 (73%)	92 (90%)	8 (8%)	2 (2%)	7 40
2	H	102/140 (73%)	93 (91%)	8 (8%)	1 (1%)	15 54
3	C	605/628 (96%)	551 (91%)	53 (9%)	1 (0%)	47 81
3	F	605/628 (96%)	551 (91%)	52 (9%)	2 (0%)	41 76
3	I	605/628 (96%)	553 (91%)	50 (8%)	2 (0%)	41 76
All	All	5193/5610 (93%)	4676 (90%)	479 (9%)	38 (1%)	22 62

All (38) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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 [\(i\)](#)

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%)	918 (100%)	3 (0%)	92 95
1	D	921/979 (94%)	918 (100%)	3 (0%)	92 95
1	G	921/979 (94%)	911 (99%)	10 (1%)	73 85
2	B	95/124 (77%)	95 (100%)	0	100 100
2	E	95/124 (77%)	94 (99%)	1 (1%)	73 85
2	H	95/124 (77%)	94 (99%)	1 (1%)	73 85
3	C	530/548 (97%)	527 (99%)	3 (1%)	86 92
3	F	530/548 (97%)	529 (100%)	1 (0%)	93 96
3	I	530/548 (97%)	529 (100%)	1 (0%)	93 96
All	All	4638/4953 (94%)	4615 (100%)	23 (0%)	88 93

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	178	PHE

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Mol	Chain	Res	Type
1	A	953	VAL
3	C	935	PHE
3	C	1097	PHE
3	C	1098	PHE
1	D	297	LYS
1	D	582	ASN
1	D	953	VAL
2	E	46	TYR
3	F	751	ARG
1	G	149	MET
1	G	160	VAL
1	G	166	CYS
1	G	454	TYR
1	G	527	LYS
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	380	ASN
1	A	812	GLN
1	A	878	GLN
1	D	120	ASN
1	D	159	ASN
1	D	201	GLN
1	D	380	ASN
1	D	660	GLN
1	D	812	GLN
1	D	878	GLN
1	G	201	GLN
1	G	380	ASN
1	G	931	HIS

### 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	1.65	1 (7%)	17,19,21	1.35	2 (11%)
4	NAG	J	2	4	14,14,15	0.87	1 (7%)	17,19,21	1.49	2 (11%)
4	NAG	K	1	3,4	14,14,15	0.75	1 (7%)	17,19,21	2.14	5 (29%)
4	NAG	K	2	4	14,14,15	0.59	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	-	5/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-5.72	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	-2.49	1.39	1.43
4	K	1	NAG	O5-C1	-2.34	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C3-C4-C5	4.86	118.92	110.24
4	K	2	NAG	C3-C4-C5	4.78	118.77	110.24
4	K	1	NAG	C2-N2-C7	4.51	129.32	122.90
4	J	1	NAG	C3-C4-C5	4.48	118.23	110.24
4	K	1	NAG	C1-C2-N2	4.11	117.51	110.49
4	K	1	NAG	C3-C4-C5	3.22	115.99	110.24
4	K	1	NAG	C1-O5-C5	3.17	116.49	112.19
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 (9) torsion outliers are listed below:

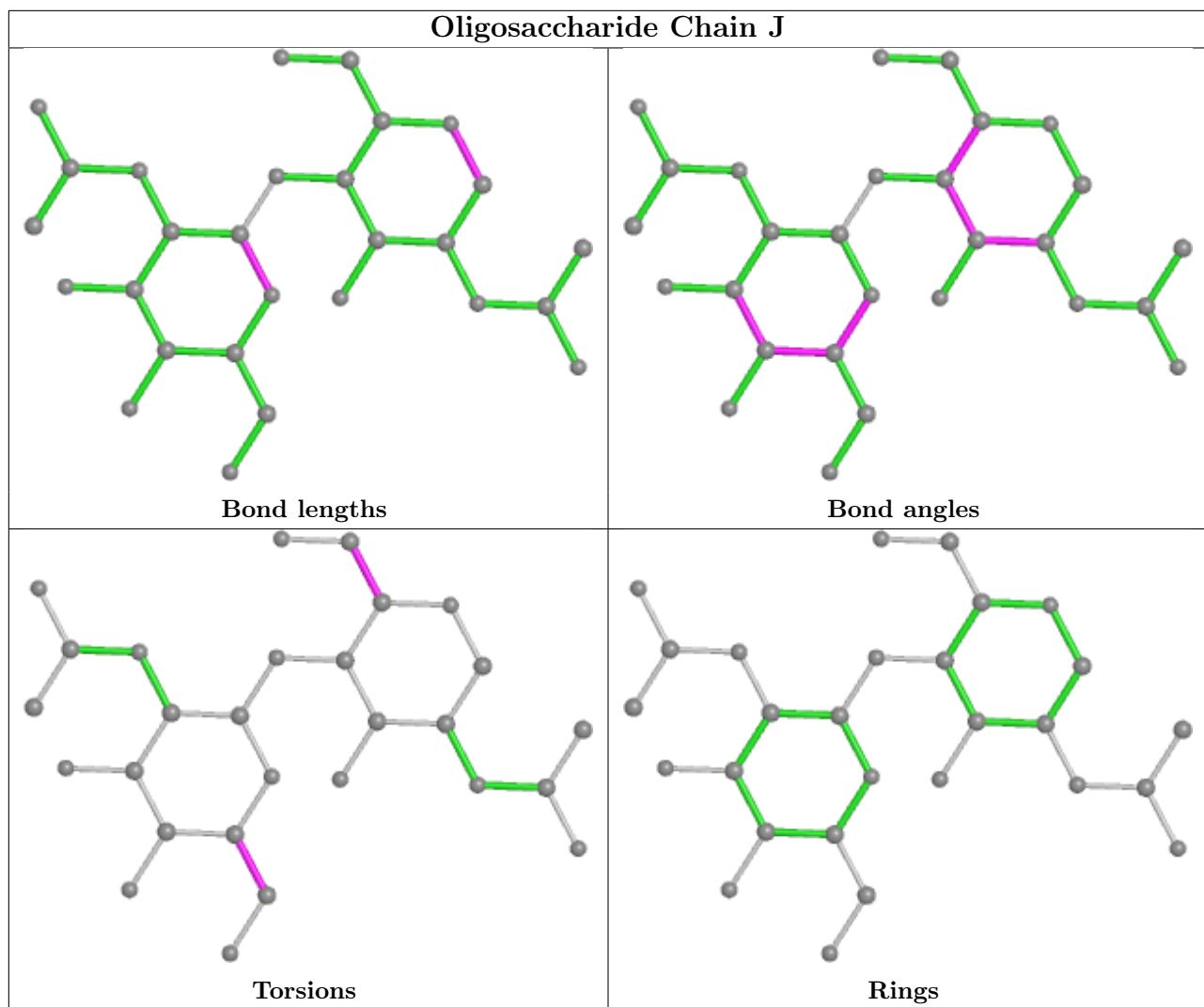
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	K	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C3-C2-N2-C7

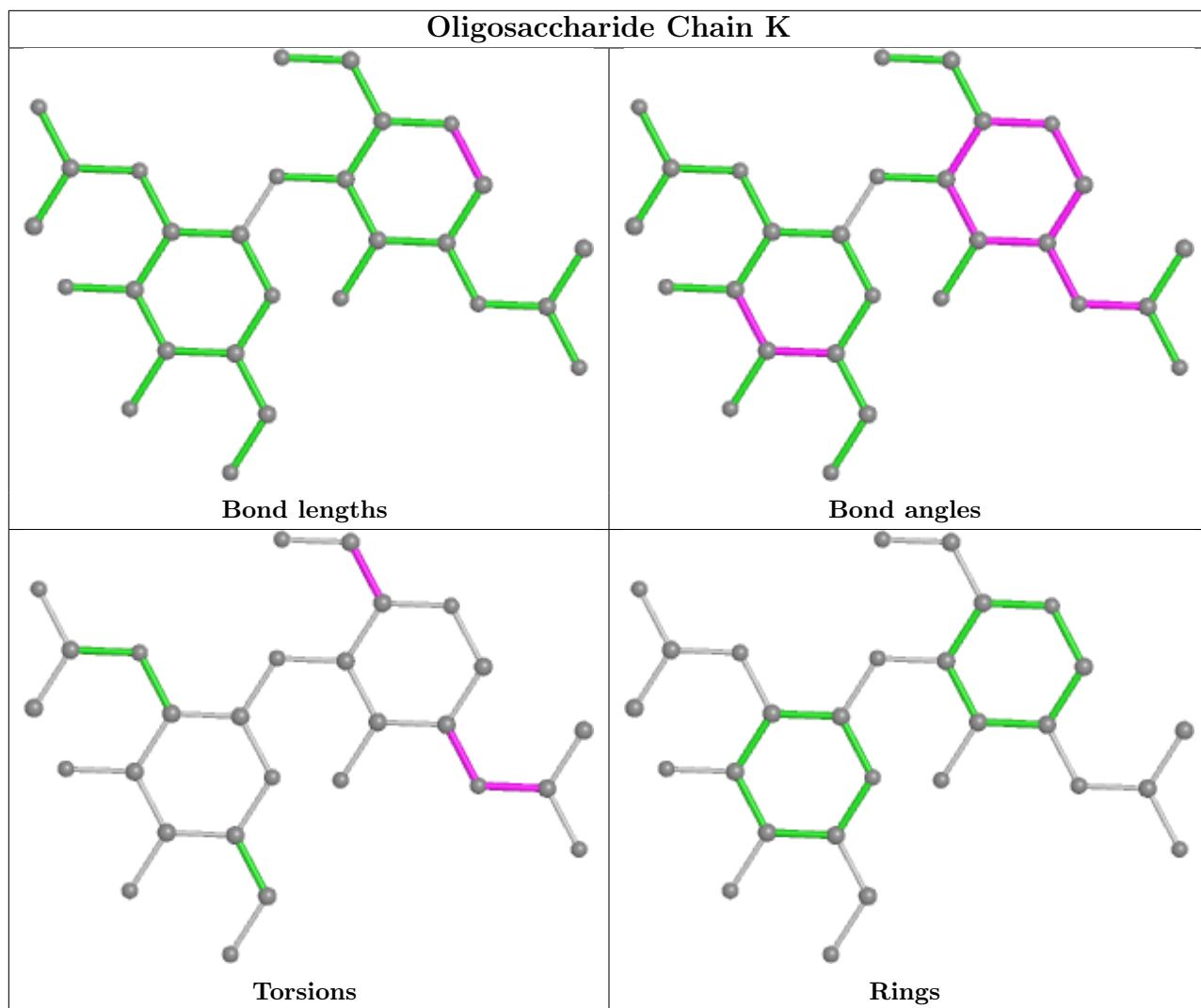
There are no ring outliers.

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	G	1205	1	14,14,15	0.17	0	17,19,21	0.38	0
5	NAG	D	1203	-	14,14,15	0.35	0	17,19,21	0.37	0
5	NAG	G	1203	1	14,14,15	0.43	0	17,19,21	0.57	0
5	NAG	D	1204	1	14,14,15	0.17	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	G	1204	1	14,14,15	0.23	0	17,19,21	0.34	0
5	NAG	A	1201	1	14,14,15	0.35	0	17,19,21	0.50	0
5	NAG	C	1301	3	14,14,15	0.26	0	17,19,21	0.53	0
5	NAG	C	1302	3	14,14,15	0.52	0	17,19,21	0.37	0
5	NAG	F	1303	3	14,14,15	0.58	0	17,19,21	0.47	0
5	NAG	D	1201	1	14,14,15	0.35	0	17,19,21	0.49	0
5	NAG	C	1303	3	14,14,15	1.70	2 (14%)	17,19,21	1.28	1 (5%)
5	NAG	C	1304	-	14,14,15	0.86	1 (7%)	17,19,21	0.53	0
5	NAG	A	1205	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	G	1202	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	D	1202	1	14,14,15	0.50	0	17,19,21	0.56	0
5	NAG	I	1302	3	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	D	1205	1	14,14,15	1.01	1 (7%)	17,19,21	2.08	1 (5%)
5	NAG	I	1303	3	14,14,15	0.54	0	17,19,21	0.48	0
5	NAG	A	1203	1	14,14,15	0.18	0	17,19,21	0.38	0
5	NAG	F	1305	-	14,14,15	1.27	1 (7%)	17,19,21	1.13	1 (5%)
5	NAG	E	200	-	14,14,15	0.20	0	17,19,21	0.49	0
5	NAG	G	1206	1	14,14,15	0.50	0	17,19,21	0.39	0
5	NAG	G	1201	-	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
5	NAG	A	1204	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	I	1301	3	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	F	1304	-	14,14,15	0.23	0	17,19,21	0.64	0
5	NAG	A	1202	1	14,14,15	0.48	0	17,19,21	0.64	1 (5%)
5	NAG	F	1302	3	14,14,15	0.33	0	17,19,21	0.49	0
5	NAG	H	200	-	14,14,15	0.17	0	17,19,21	0.42	0
5	NAG	F	1301	3	14,14,15	0.33	0	17,19,21	0.41	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	G	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1203	-	-	1/6/23/26	0/1/1/1
5	NAG	G	1203	1	-	4/6/23/26	0/1/1/1
5	NAG	D	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	A	1201	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1301	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1302	3	-	4/6/23/26	0/1/1/1
5	NAG	F	1303	3	-	2/6/23/26	0/1/1/1
5	NAG	D	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	G	1202	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1202	1	-	1/6/23/26	0/1/1/1
5	NAG	I	1302	3	-	2/6/23/26	0/1/1/1
5	NAG	D	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1303	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1305	-	-	2/6/23/26	0/1/1/1
5	NAG	E	200	-	-	2/6/23/26	0/1/1/1
5	NAG	G	1206	1	-	3/6/23/26	0/1/1/1
5	NAG	G	1201	-	-	4/6/23/26	0/1/1/1
5	NAG	A	1204	1	-	4/6/23/26	0/1/1/1
5	NAG	I	1301	3	-	0/6/23/26	0/1/1/1
5	NAG	F	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1302	3	-	2/6/23/26	0/1/1/1
5	NAG	H	200	-	-	2/6/23/26	0/1/1/1
5	NAG	F	1301	3	-	0/6/23/26	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	5.09	1.51	1.43
5	F	1305	NAG	O5-C1	-4.16	1.37	1.43
5	D	1205	NAG	O5-C1	3.66	1.49	1.43
5	C	1303	NAG	C1-C2	3.63	1.57	1.52
5	C	1304	NAG	O5-C1	-3.11	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	8.07	123.12	112.19
5	C	1303	NAG	C1-O5-C5	4.72	118.58	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1305	NAG	C3-C4-C5	3.83	117.07	110.24
5	G	1201	NAG	C1-O5-C5	2.71	115.86	112.19
5	A	1202	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

All (64) 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	A	1203	NAG	C4-C5-C6-O6
5	G	1203	NAG	C4-C5-C6-O6
5	D	1205	NAG	C4-C5-C6-O6
5	G	1203	NAG	O5-C5-C6-O6
5	F	1305	NAG	C4-C5-C6-O6
5	F	1303	NAG	C1-C2-N2-C7
5	G	1202	NAG	O5-C5-C6-O6
5	F	1304	NAG	O5-C5-C6-O6
5	A	1204	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
5	G	1201	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
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	D	1201	NAG	C4-C5-C6-O6
5	G	1201	NAG	O5-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	F	1302	NAG	C4-C5-C6-O6
5	I	1303	NAG	C1-C2-N2-C7
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	C	1302	NAG	C1-C2-N2-C7
5	D	1201	NAG	O5-C5-C6-O6
5	F	1302	NAG	O5-C5-C6-O6
5	E	200	NAG	C4-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	1203	NAG	C4-C5-C6-O6
5	C	1302	NAG	C3-C2-N2-C7
5	I	1303	NAG	C3-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 12 short contacts:

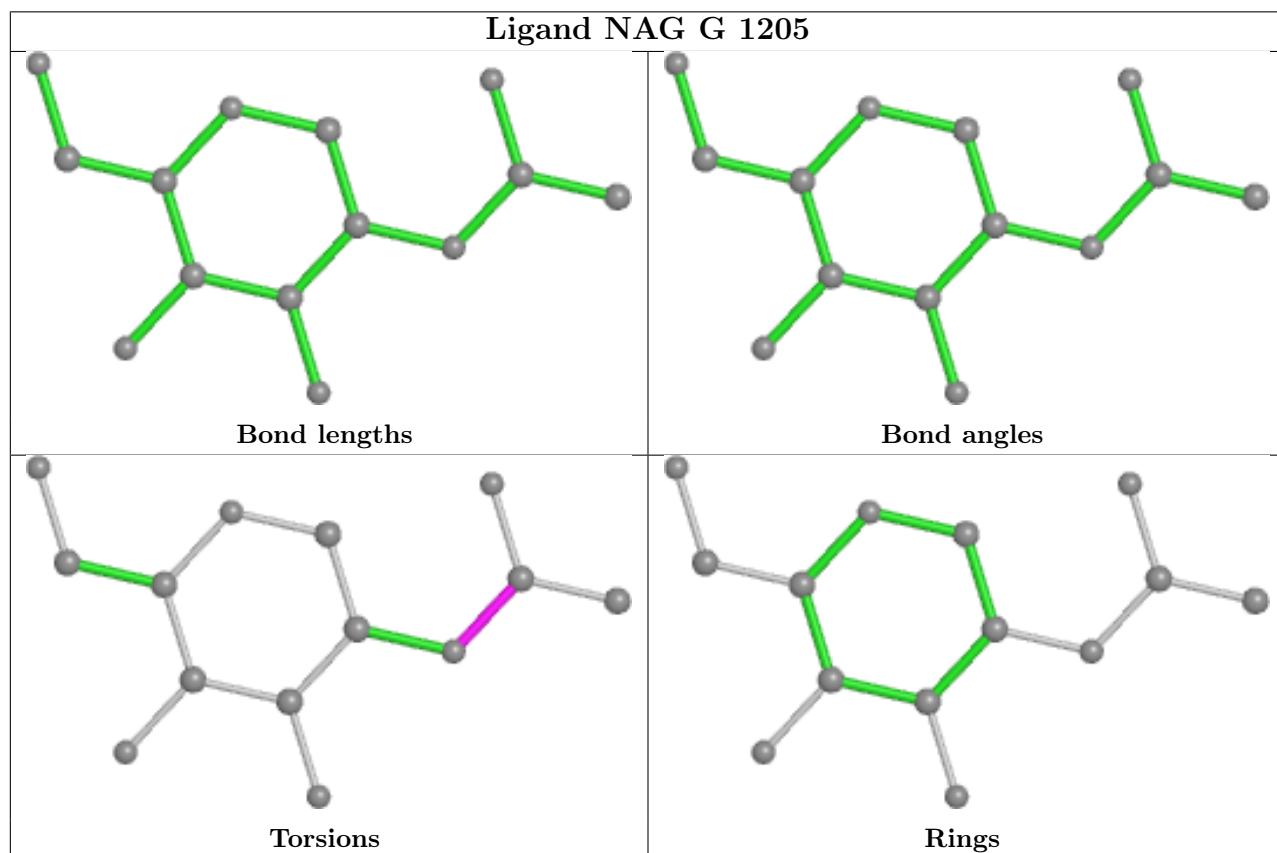
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1203	NAG	2	0
5	C	1302	NAG	1	0
5	F	1303	NAG	1	0
5	C	1303	NAG	1	0
5	C	1304	NAG	2	0
5	I	1302	NAG	1	0
5	I	1303	NAG	2	0

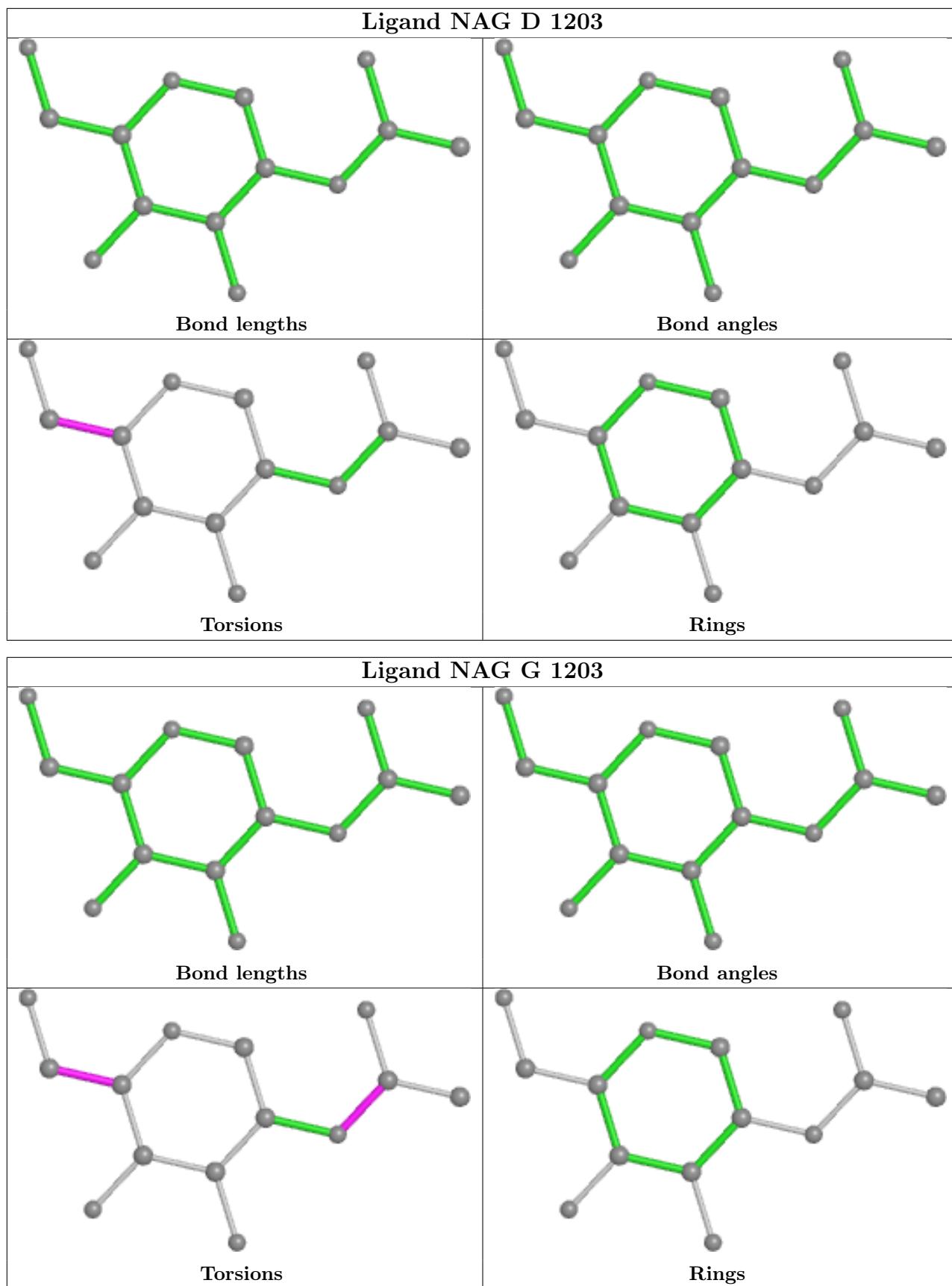
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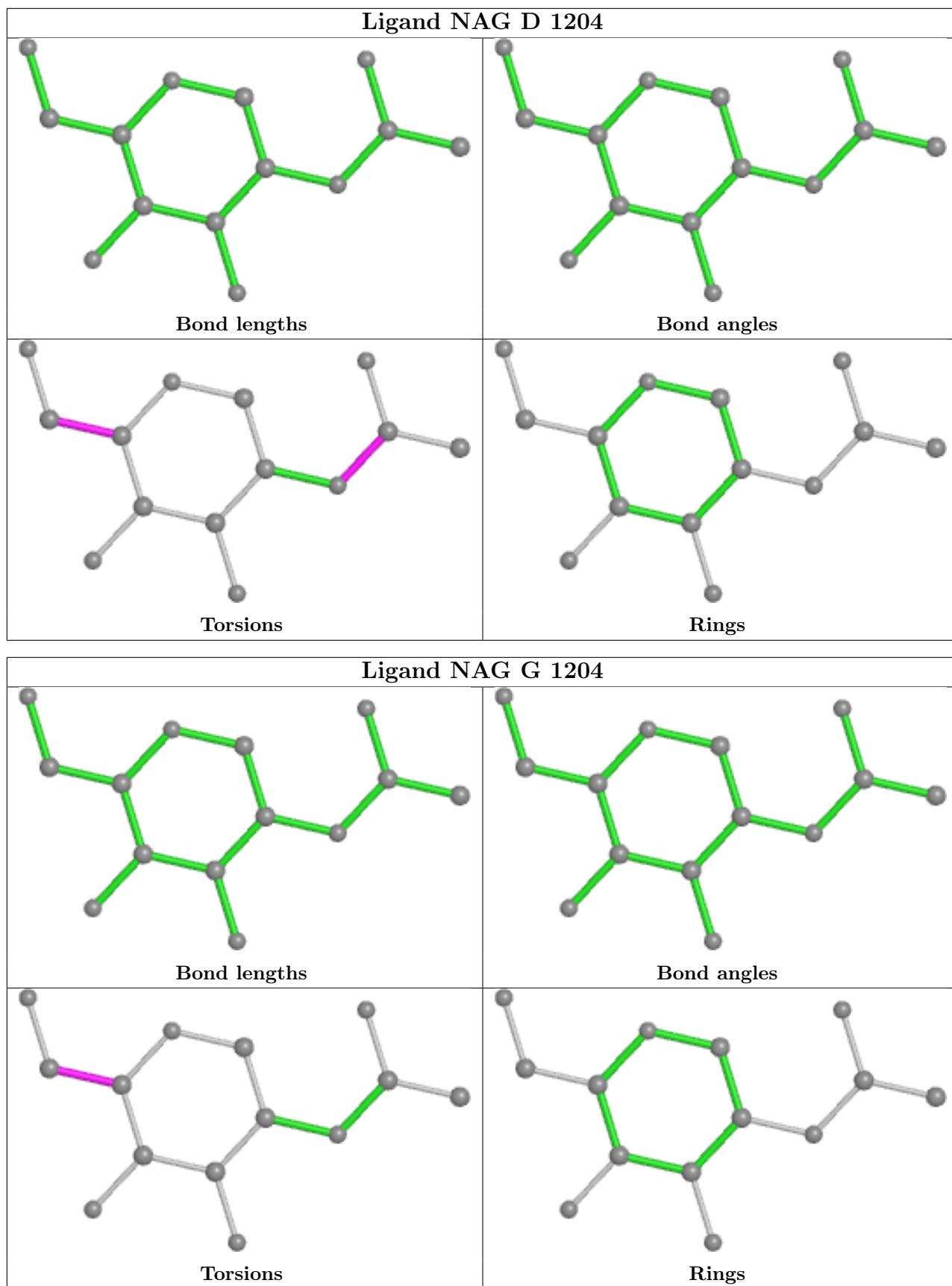
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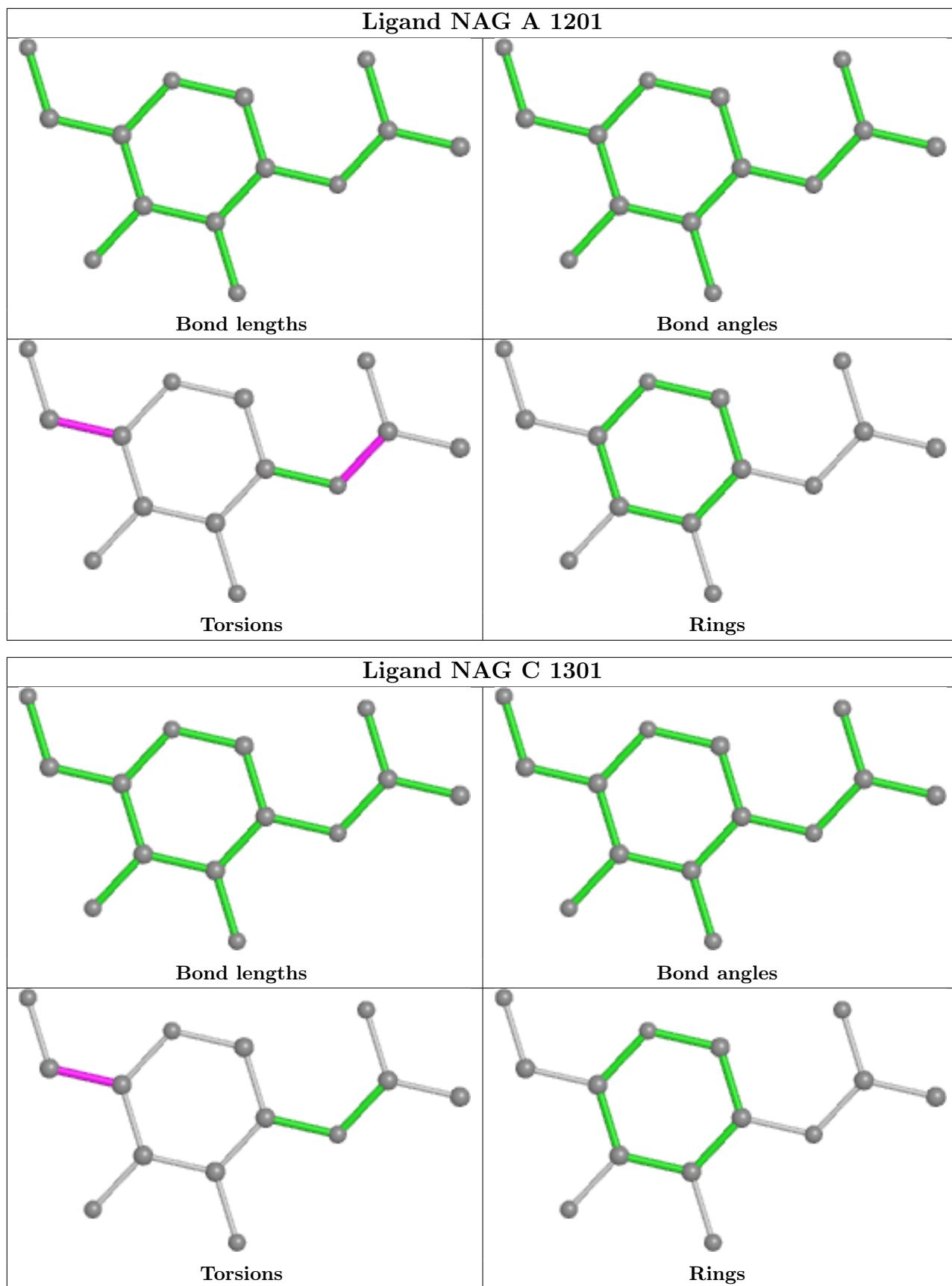
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1305	NAG	1	0
5	A	1204	NAG	1	0
5	F	1304	NAG	2	0

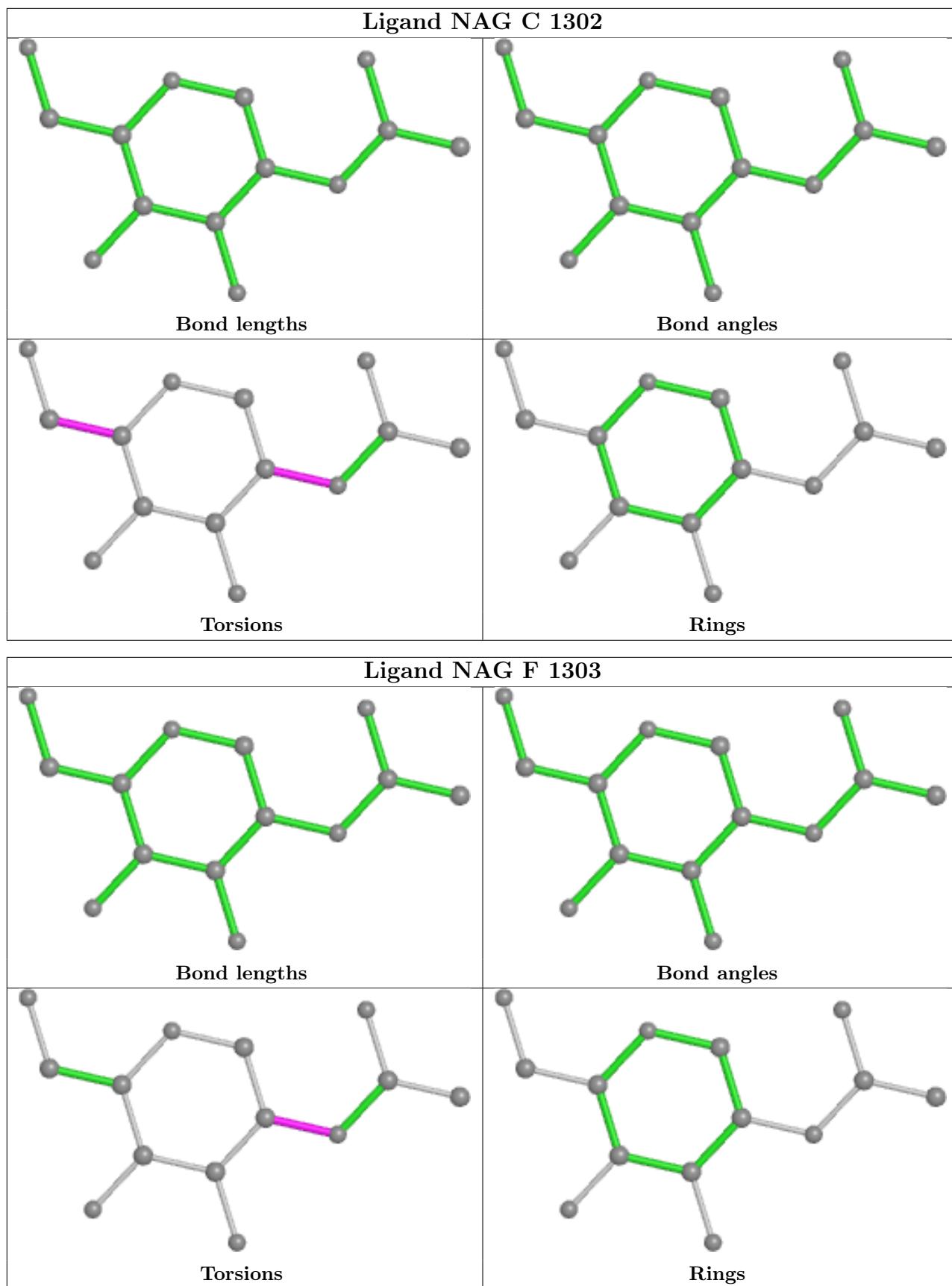
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

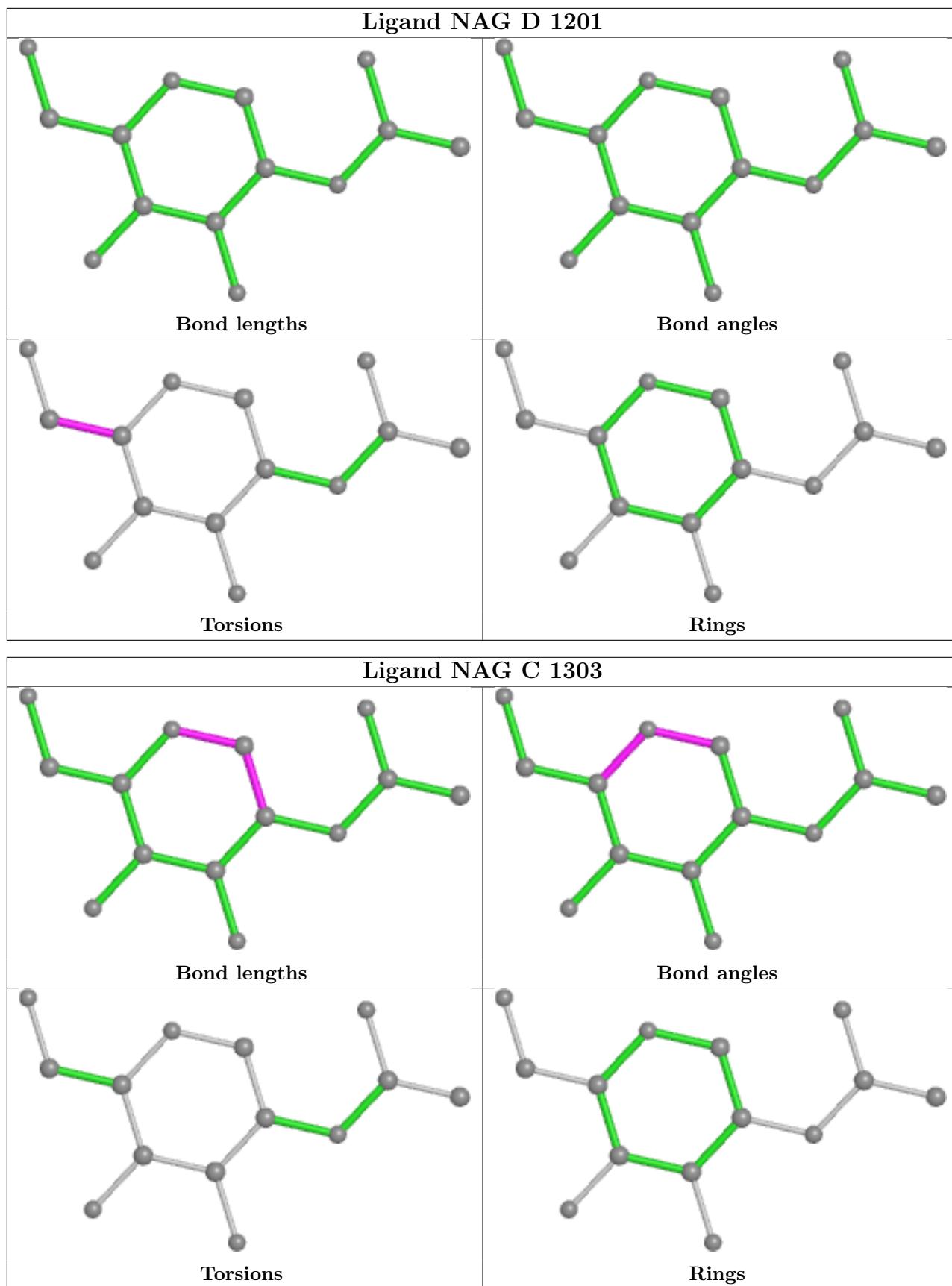


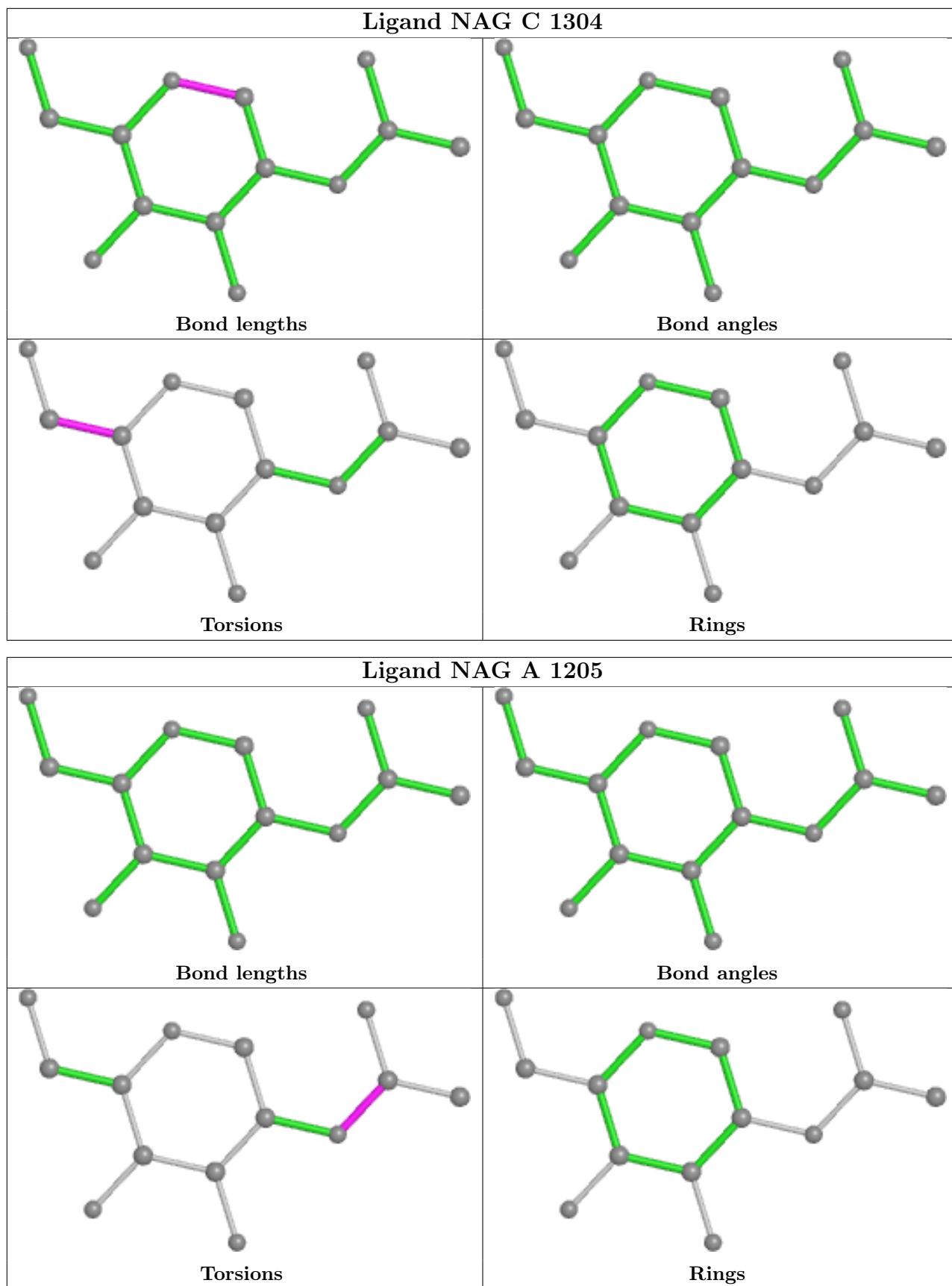


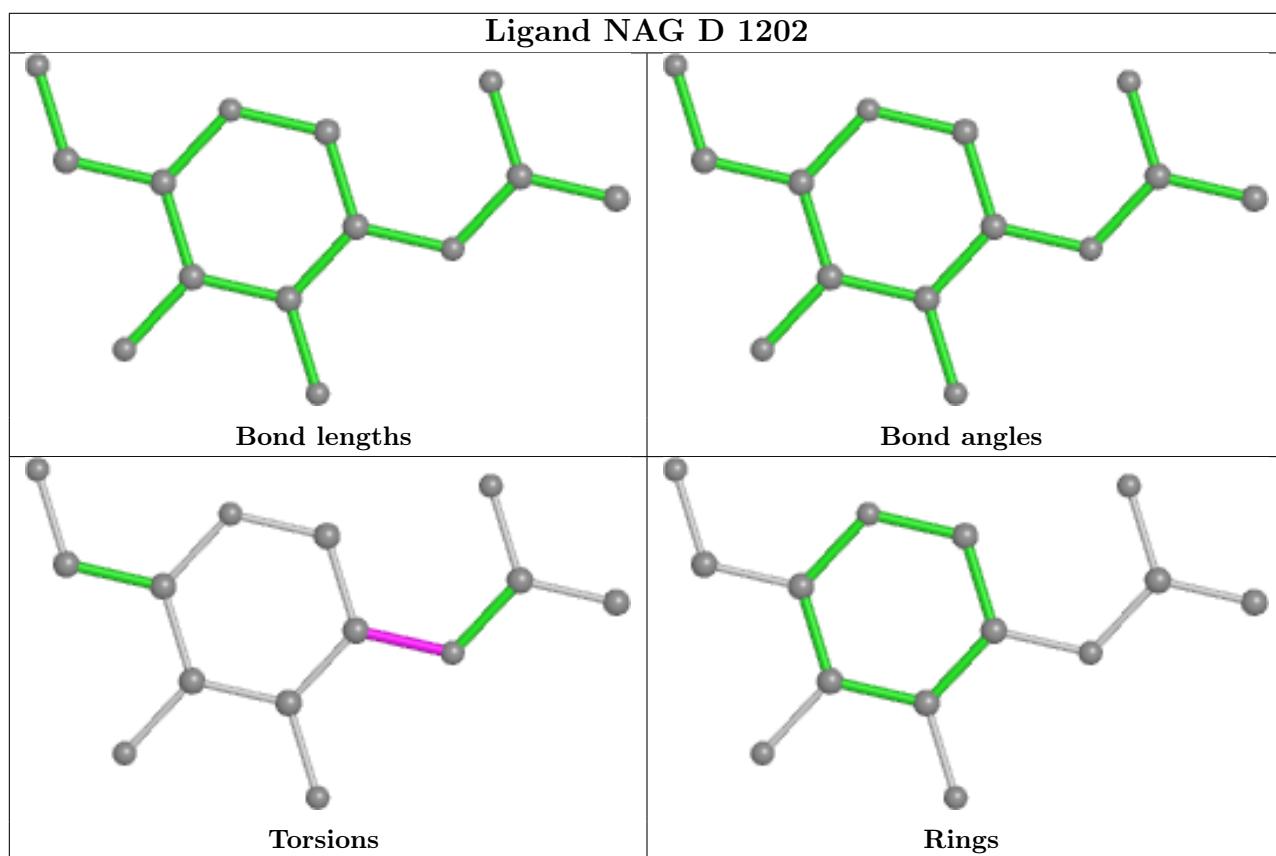
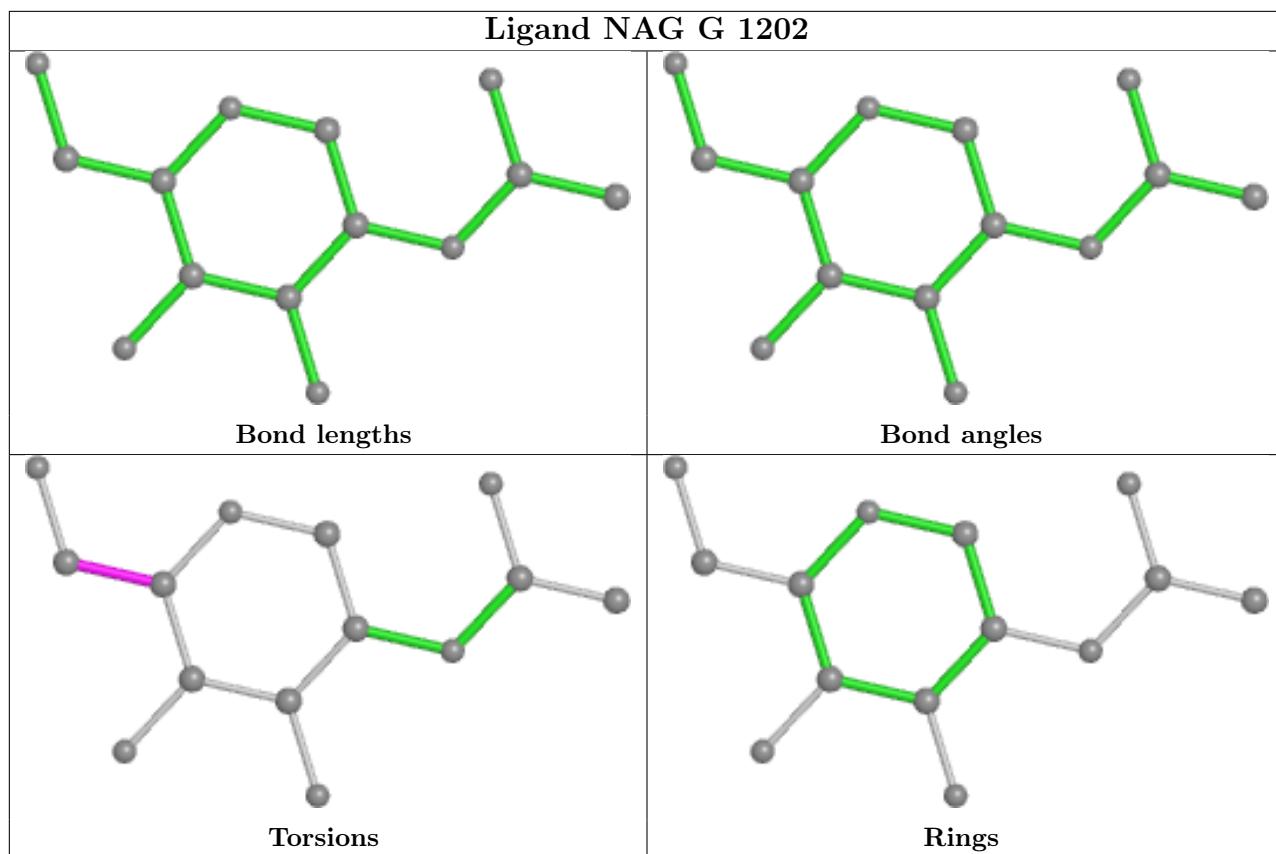


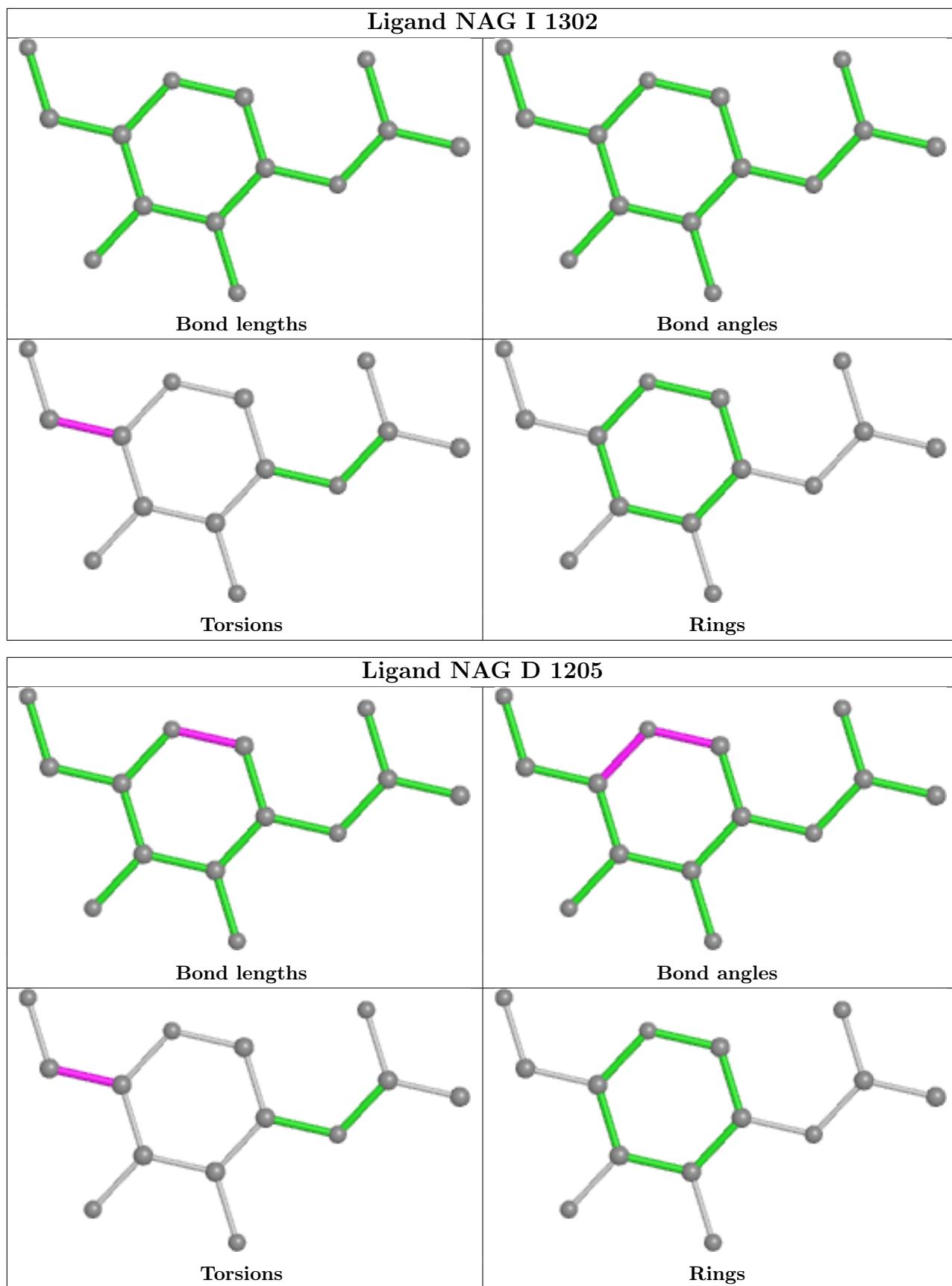


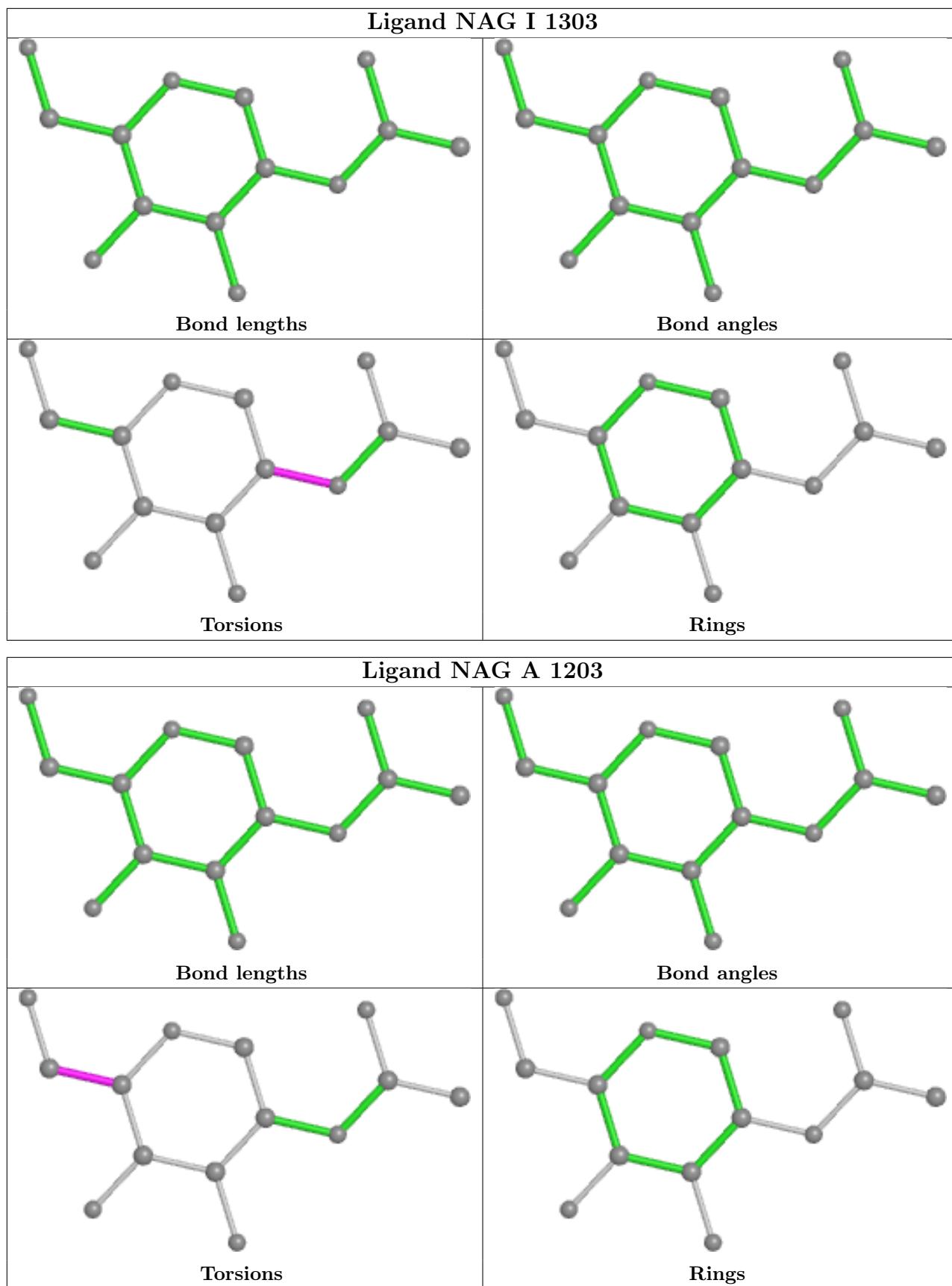


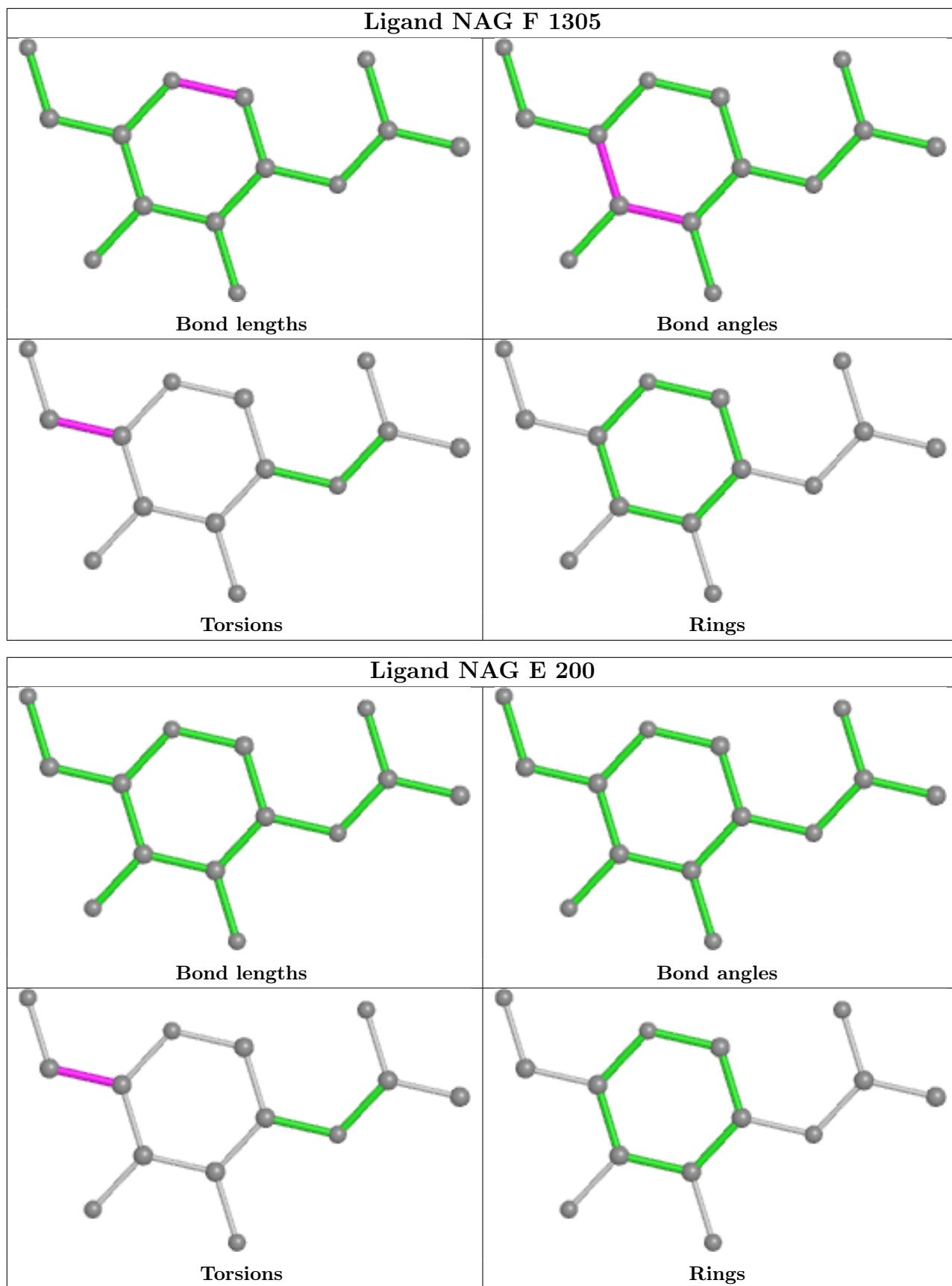


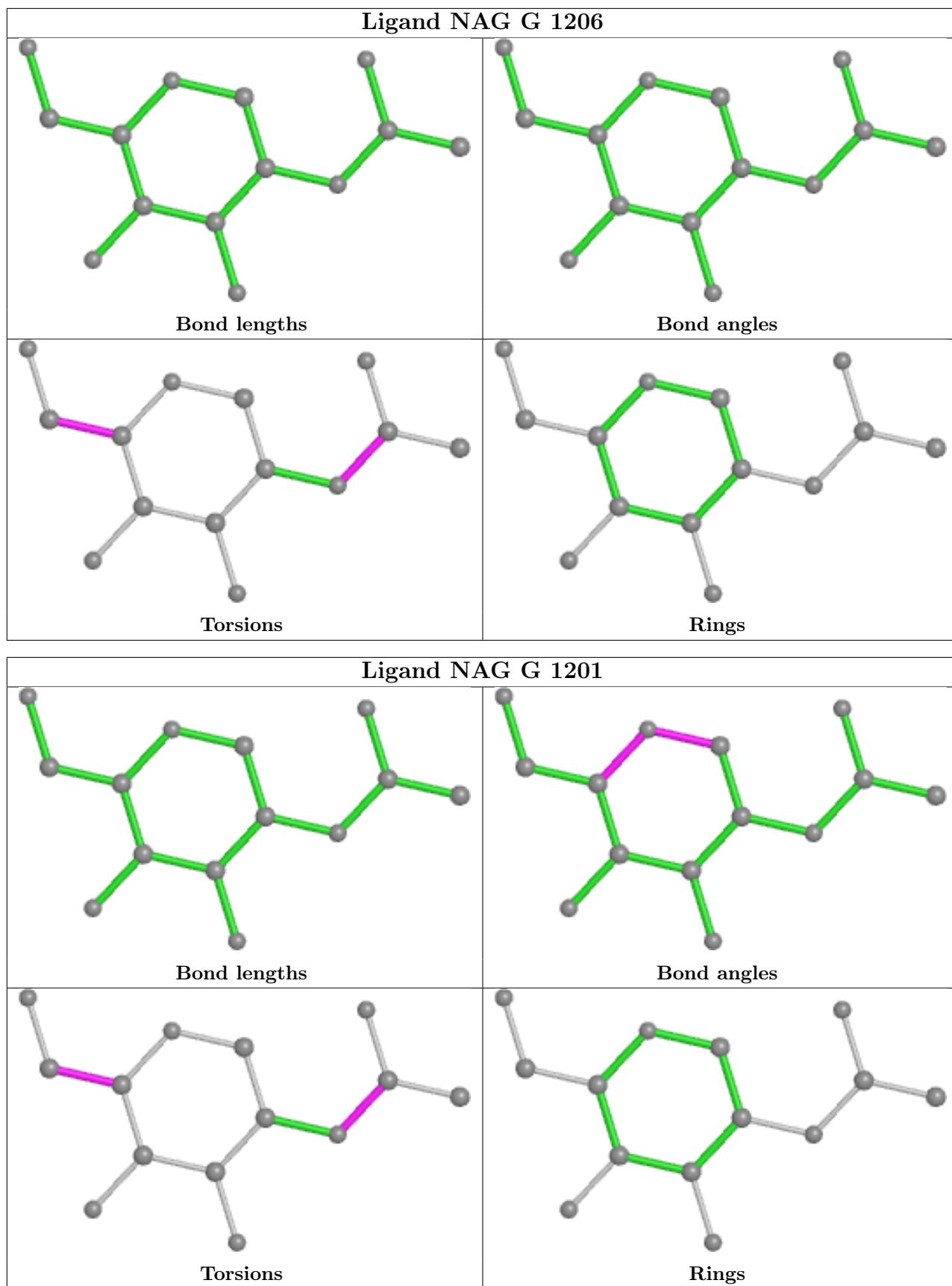


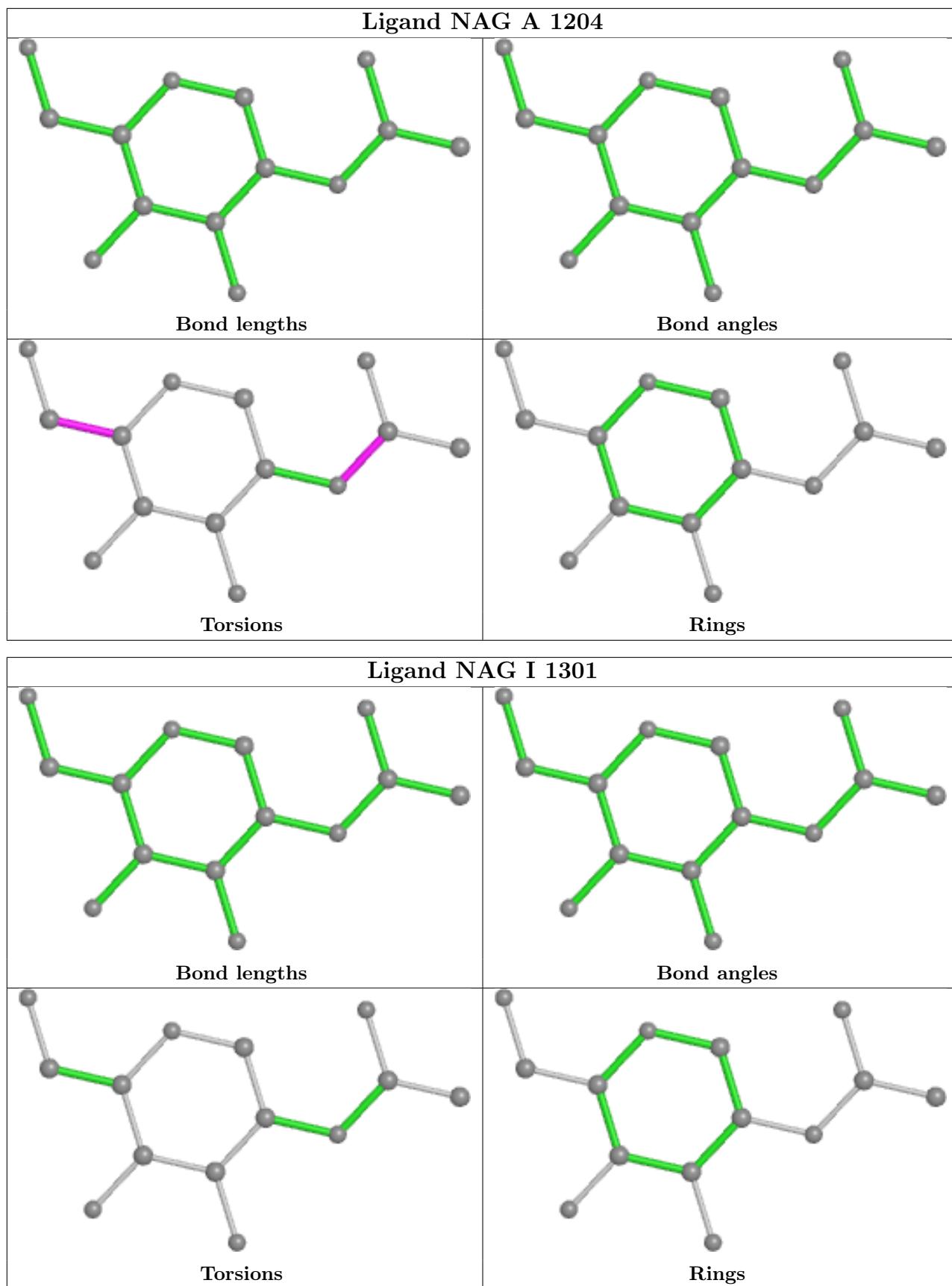


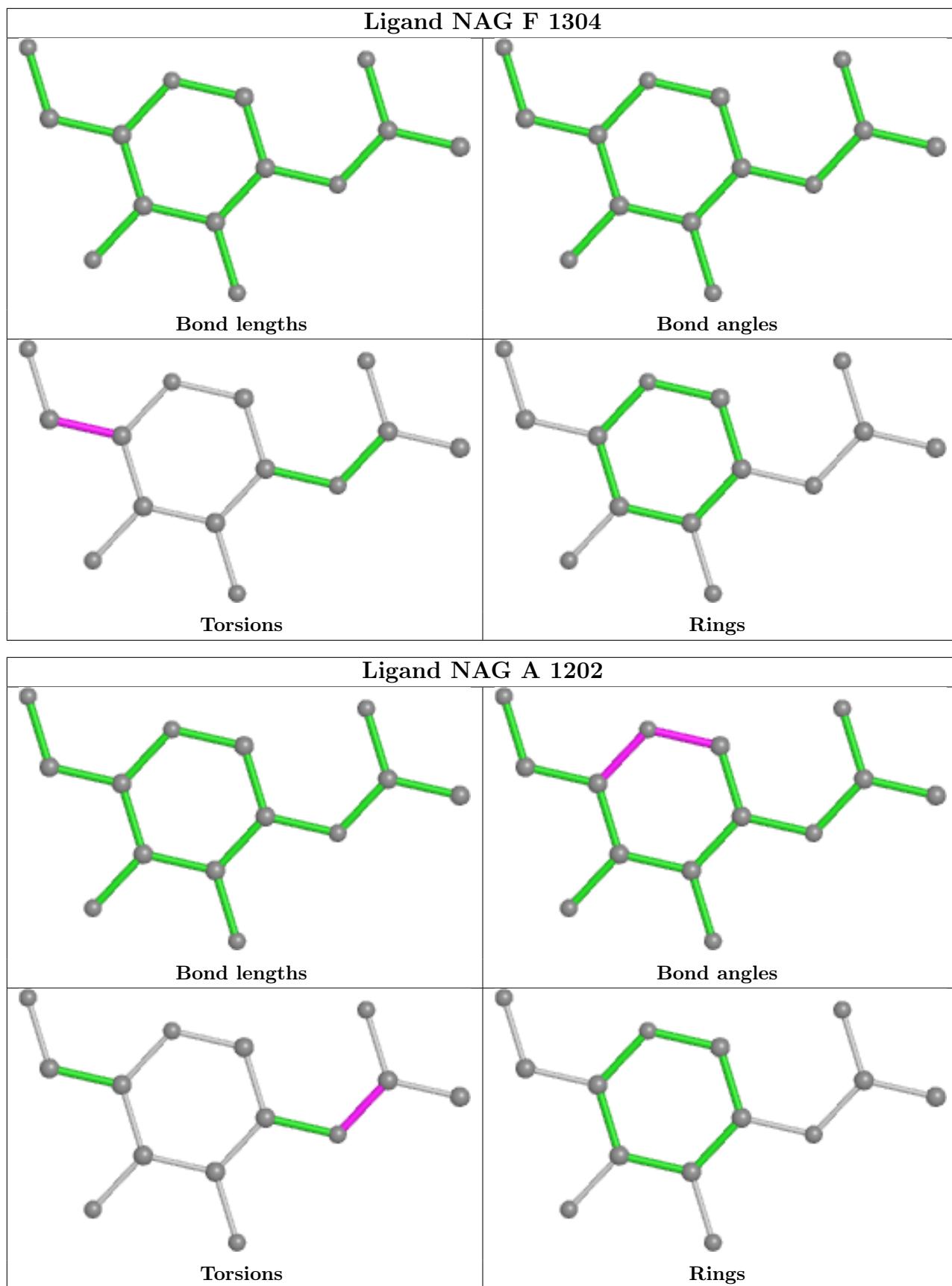


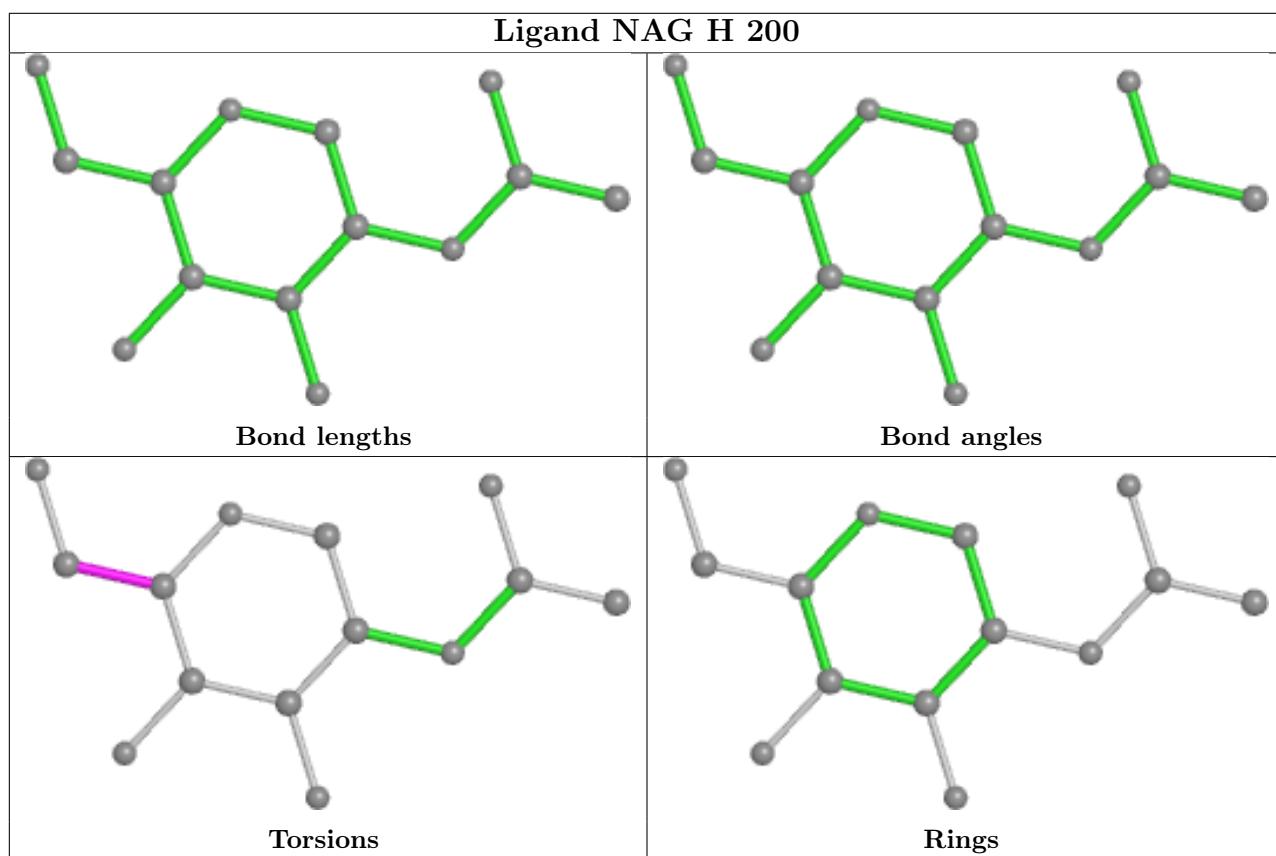
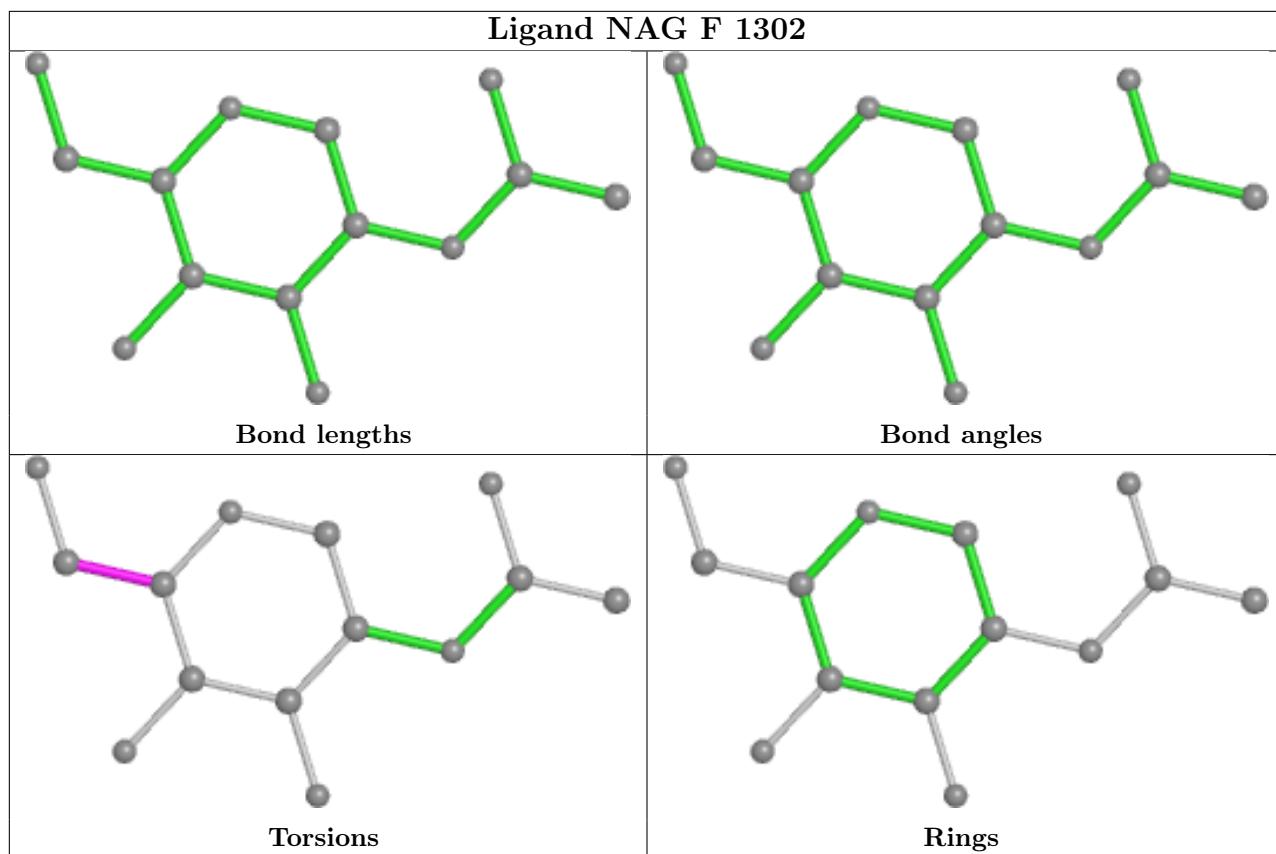


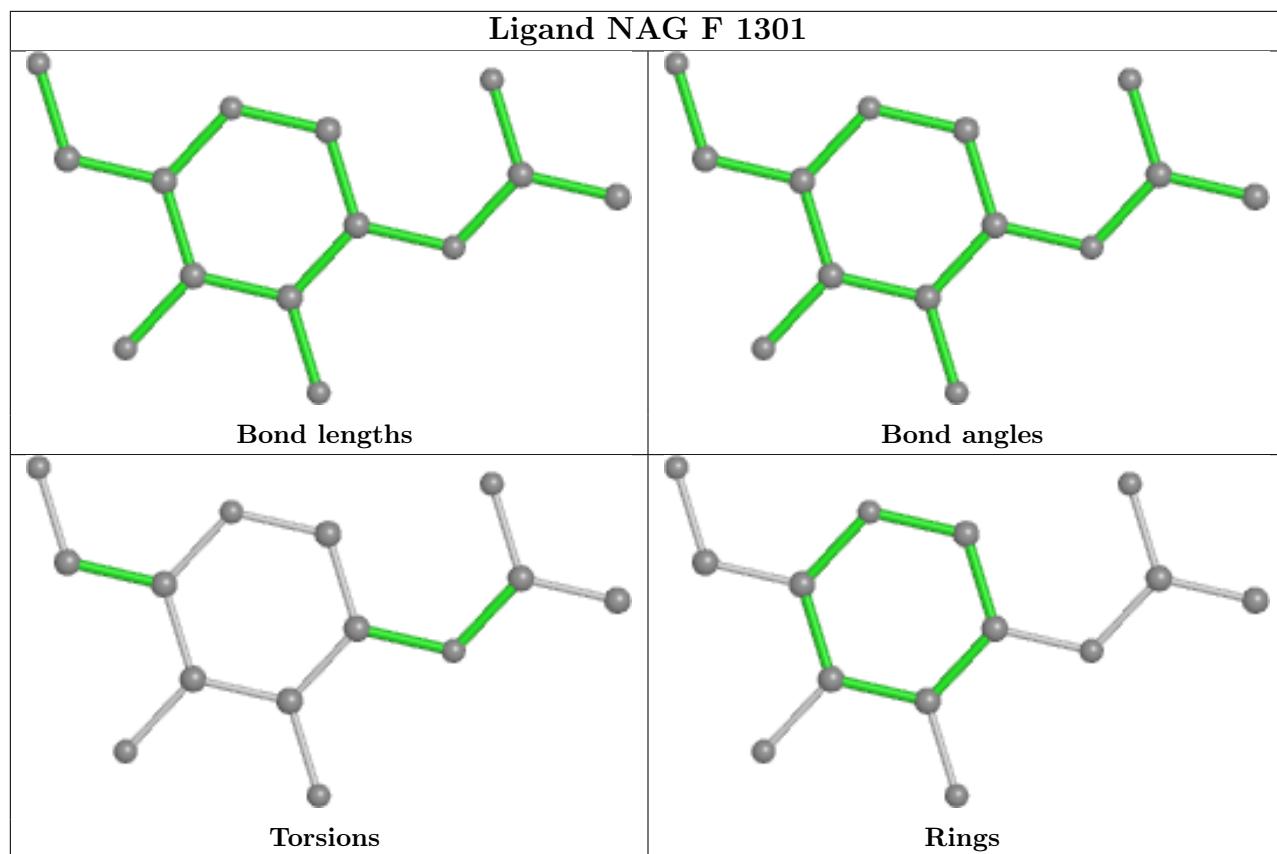












## 5.7 Other polymers (i)

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 i

### 6.1 Protein, DNA and RNA chains i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1030/1102 (93%)	0.23	58 (5%) 24 21	126, 218, 281, 373	0
1	D	1030/1102 (93%)	0.12	37 (3%) 42 35	123, 211, 286, 349	0
1	G	1030/1102 (93%)	0.24	65 (6%) 20 16	137, 212, 300, 366	0
2	B	104/140 (74%)	-0.18	1 (0%) 82 74	195, 283, 337, 366	0
2	E	104/140 (74%)	-0.25	1 (0%) 82 74	196, 266, 311, 324	0
2	H	104/140 (74%)	-0.18	1 (0%) 82 74	188, 256, 313, 341	0
3	C	609/628 (96%)	0.32	42 (6%) 16 14	139, 203, 260, 302	0
3	F	609/628 (96%)	0.16	21 (3%) 45 37	132, 178, 218, 252	0
3	I	609/628 (96%)	0.28	42 (6%) 16 14	136, 205, 262, 331	0
All	All	5229/5610 (93%)	0.19	268 (5%) 28 25	123, 209, 287, 373	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	862	VAL	6.4
1	G	947	ASN	5.6
1	A	862	VAL	5.5
3	C	1073	PHE	5.3
1	D	862	VAL	5.2
1	G	831	PHE	5.0
1	G	931	HIS	4.8
3	C	1082	LYS	4.6
1	G	760	SER	4.3
1	A	661	LEU	4.3
1	G	661	LEU	4.2
1	D	947	ASN	4.1
1	A	660	GLN	4.1
3	F	808	THR	4.1
1	G	916	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	748	ALA	4.0
3	I	751	ARG	4.0
1	D	1051	LEU	4.0
3	F	815	ILE	4.0
3	C	1084	GLU	4.0
1	G	1051	LEU	3.9
1	A	748	ALA	3.9
1	G	944	PRO	3.8
1	G	852	CYS	3.8
3	I	1064	VAL	3.8
1	G	789	PRO	3.8
3	C	1083	ILE	3.8
1	A	645	ARG	3.8
1	A	986	PRO	3.7
1	D	667	PRO	3.7
1	A	641	LEU	3.7
3	I	1019	LEU	3.7
1	G	826	PHE	3.6
3	F	807	TRP	3.6
1	A	666	SER	3.6
1	G	856	GLU	3.6
3	I	971	ASP	3.6
1	G	660	GLN	3.5
3	C	1107	LEU	3.5
1	D	661	LEU	3.5
3	I	1029	TYR	3.5
1	D	918	PHE	3.4
1	D	748	ALA	3.4
3	I	767	TRP	3.4
1	A	949	PHE	3.4
3	F	828	ILE	3.3
1	D	357	TYR	3.3
1	G	827	THR	3.3
3	I	1021	ILE	3.3
3	I	1073	PHE	3.3
3	I	1083	ILE	3.3
1	G	761	LEU	3.3
1	G	742	ILE	3.3
1	A	916	TYR	3.2
1	A	884	LYS	3.2
1	A	760	SER	3.2
3	C	1019	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	751	ARG	3.2
1	G	800	VAL	3.1
1	D	861	LEU	3.1
3	F	681	ILE	3.1
1	G	855	MET	3.1
1	G	885	GLU	3.1
3	F	816	GLU	3.1
3	C	875	TYR	3.1
1	G	857	ASP	3.0
1	D	745	ARG	3.0
3	F	837	GLY	3.0
1	G	135	PRO	3.0
1	G	961	ALA	3.0
3	F	875	TYR	3.0
1	G	657	HIS	3.0
1	A	901	LYS	3.0
1	A	744	ARG	3.0
1	G	788	GLY	3.0
1	D	822	MET	3.0
1	D	789	PRO	3.0
1	G	830	TYR	3.0
1	A	667	PRO	2.9
1	G	803	SER	2.9
1	A	554	TYR	2.9
1	G	949	PHE	2.9
3	I	970	ILE	2.9
3	I	1048	VAL	2.9
1	D	481	MET	2.9
3	I	755	LEU	2.9
1	D	470	PRO	2.9
3	C	836	PHE	2.9
3	I	815	ILE	2.9
3	I	793	ALA	2.9
1	G	939	ARG	2.9
1	G	863	ALA	2.8
1	G	861	LEU	2.8
2	B	131	MET	2.8
3	F	836	PHE	2.8
3	C	806	TYR	2.8
1	D	786	LEU	2.8
3	F	838	LEU	2.8
3	I	754	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	I	1109	LEU	2.8
3	C	1072	TYR	2.8
3	I	712	VAL	2.8
3	C	1021	ILE	2.8
1	A	939	ARG	2.8
1	A	787	THR	2.8
1	G	858	ARG	2.7
1	D	666	SER	2.7
3	C	1097	PHE	2.7
3	C	1075	ASN	2.7
3	I	794	ASN	2.7
3	I	1038	ILE	2.7
1	A	852	CYS	2.7
1	G	948	ALA	2.7
3	I	806	TYR	2.7
1	G	925	ASP	2.7
1	A	486	PRO	2.7
1	G	662	ALA	2.7
3	F	806	TYR	2.7
1	A	822	MET	2.7
1	A	854	ILE	2.7
3	F	1107	LEU	2.7
3	C	1104	PRO	2.7
3	I	837	GLY	2.7
1	G	747	ILE	2.7
1	G	835	LEU	2.7
3	C	1029	TYR	2.6
3	I	1023	ILE	2.6
3	F	644	ARG	2.6
1	G	403	THR	2.6
1	D	803	SER	2.6
1	G	786	LEU	2.6
3	I	805	LEU	2.6
1	A	831	PHE	2.6
1	A	646	LEU	2.6
1	A	858	ARG	2.6
3	I	838	LEU	2.6
3	C	733	LYS	2.5
1	G	828	LEU	2.5
3	I	1020	SER	2.5
1	D	499	VAL	2.5
3	C	850	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	287	VAL	2.5
1	D	498	GLY	2.5
1	A	662	ALA	2.5
1	G	69	LEU	2.5
1	A	470	PRO	2.5
1	D	949	PHE	2.5
1	A	665	GLU	2.5
3	C	712	VAL	2.5
1	A	657	HIS	2.5
1	A	643	TYR	2.5
1	D	788	GLY	2.5
3	C	1109	LEU	2.5
1	A	66	MET	2.5
3	F	886	ARG	2.5
1	G	646	LEU	2.5
3	I	836	PHE	2.5
3	C	750	PRO	2.5
1	G	659	LYS	2.5
1	D	331	PHE	2.5
3	I	1062	VAL	2.5
1	D	643	TYR	2.4
3	I	715	LEU	2.4
1	A	747	ILE	2.4
3	I	1076	LEU	2.4
3	C	755	LEU	2.4
1	A	931	HIS	2.4
1	G	884	LYS	2.4
1	A	280	VAL	2.4
1	D	554	TYR	2.4
3	I	773	ILE	2.4
1	D	468	SER	2.4
1	A	863	ALA	2.4
1	D	729	TRP	2.4
1	G	945	GLY	2.4
2	E	90	TYR	2.4
3	F	829	ALA	2.4
1	D	931	HIS	2.4
3	I	1052	LEU	2.3
1	A	182	ARG	2.3
1	G	641	LEU	2.3
1	G	850	ILE	2.3
3	F	892	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	882	THR	2.3
1	A	798	TYR	2.3
1	G	798	TYR	2.3
3	C	838	LEU	2.3
1	A	659	LYS	2.3
1	A	948	ALA	2.3
3	C	1062	VAL	2.3
1	G	645	ARG	2.3
1	A	331	PHE	2.3
1	G	941	THR	2.3
3	F	1203	ARG	2.3
3	C	886	ARG	2.3
1	A	648	LEU	2.3
1	D	1013	HIS	2.3
1	G	787	THR	2.3
1	A	658	PHE	2.3
3	I	1017	TYR	2.3
1	D	961	ALA	2.3
3	C	753	LEU	2.3
3	I	1104	PRO	2.3
3	I	1018	ASP	2.3
3	C	881	VAL	2.3
1	D	62	LEU	2.3
3	C	837	GLY	2.2
1	A	202	TYR	2.2
1	G	943	ILE	2.2
1	A	789	PRO	2.2
1	A	647	ASP	2.2
3	C	946	ARG	2.2
1	G	417	GLN	2.2
3	C	1074	THR	2.2
1	A	749	THR	2.2
1	G	182	ARG	2.2
3	I	796	LEU	2.2
1	D	480	ILE	2.2
1	D	826	PHE	2.2
1	G	822	MET	2.2
3	I	1107	LEU	2.2
1	A	794	GLY	2.2
3	I	1074	THR	2.2
3	C	1048	VAL	2.2
1	A	357	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	918	PHE	2.2
3	F	826	GLU	2.2
3	I	722	ALA	2.2
1	D	645	ARG	2.2
3	C	1108	ALA	2.2
1	A	950	VAL	2.2
1	D	202	TYR	2.2
3	C	732	SER	2.2
3	I	665	SER	2.2
1	A	828	LEU	2.1
3	C	1031	THR	2.1
1	G	360	ALA	2.1
1	D	948	ALA	2.1
3	C	829	ALA	2.1
1	G	743	VAL	2.1
1	D	741	TYR	2.1
3	F	814	LEU	2.1
3	C	757	PRO	2.1
1	A	861	LEU	2.1
1	D	917	LYS	2.1
3	C	667	LEU	2.1
3	I	753	LEU	2.1
1	A	943	ILE	2.1
1	G	1049	GLY	2.1
3	I	1197	LEU	2.1
3	I	1202	TYR	2.1
1	A	1051	LEU	2.1
1	A	73	GLU	2.1
1	G	131	HIS	2.1
1	G	554	TYR	2.1
2	H	135	ARG	2.1
3	C	720	TYR	2.1
3	F	1112	ARG	2.1
3	C	994	GLU	2.1
1	A	272	ILE	2.1
3	F	938	PHE	2.0
3	C	876	VAL	2.0
1	G	860	TYR	2.0
1	G	1045	GLY	2.0
1	G	1018	THR	2.0
3	C	967	VAL	2.0
1	A	802	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	1045	GLY	2.0

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

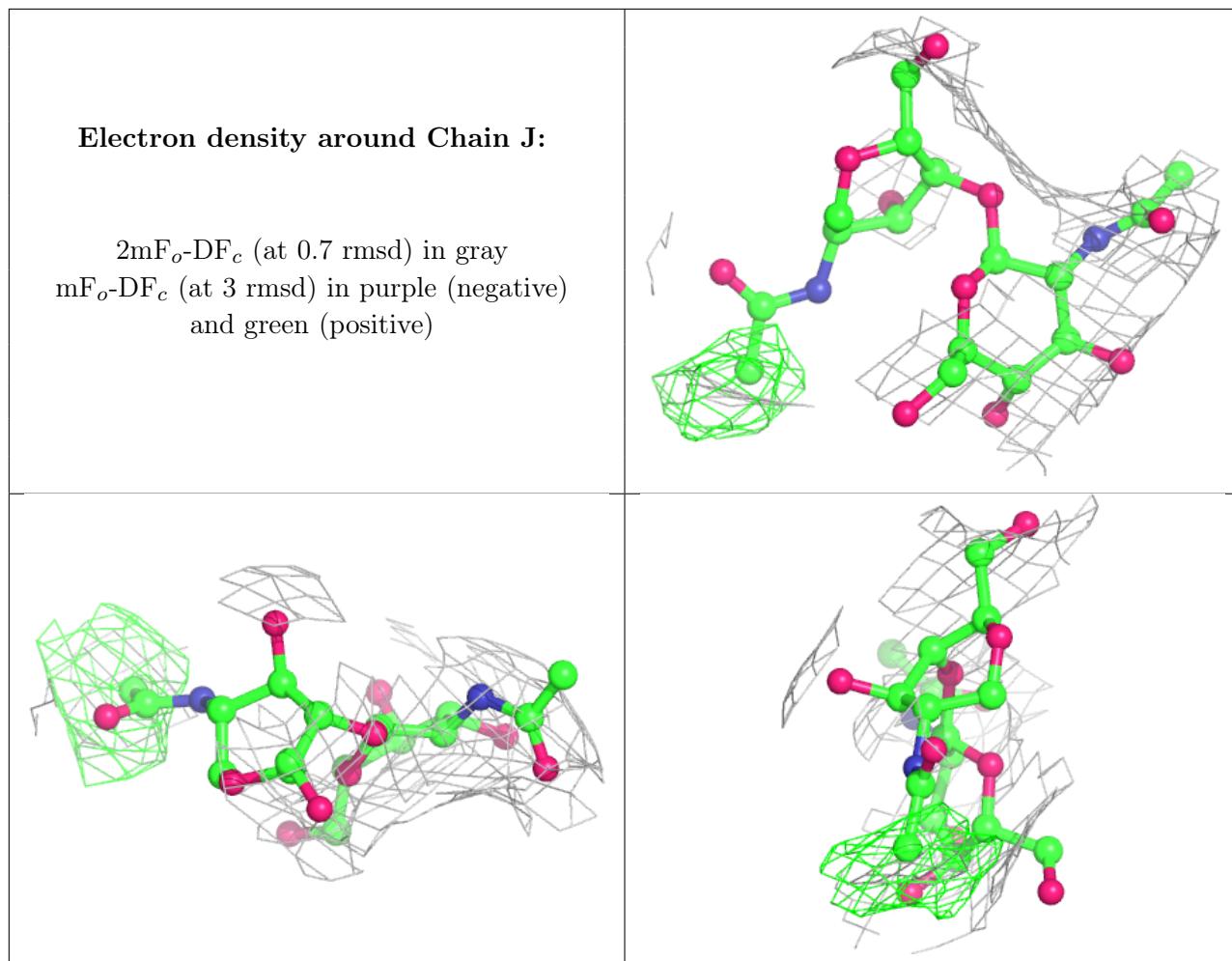
There are no non-standard protein/DNA/RNA residues in this entry.

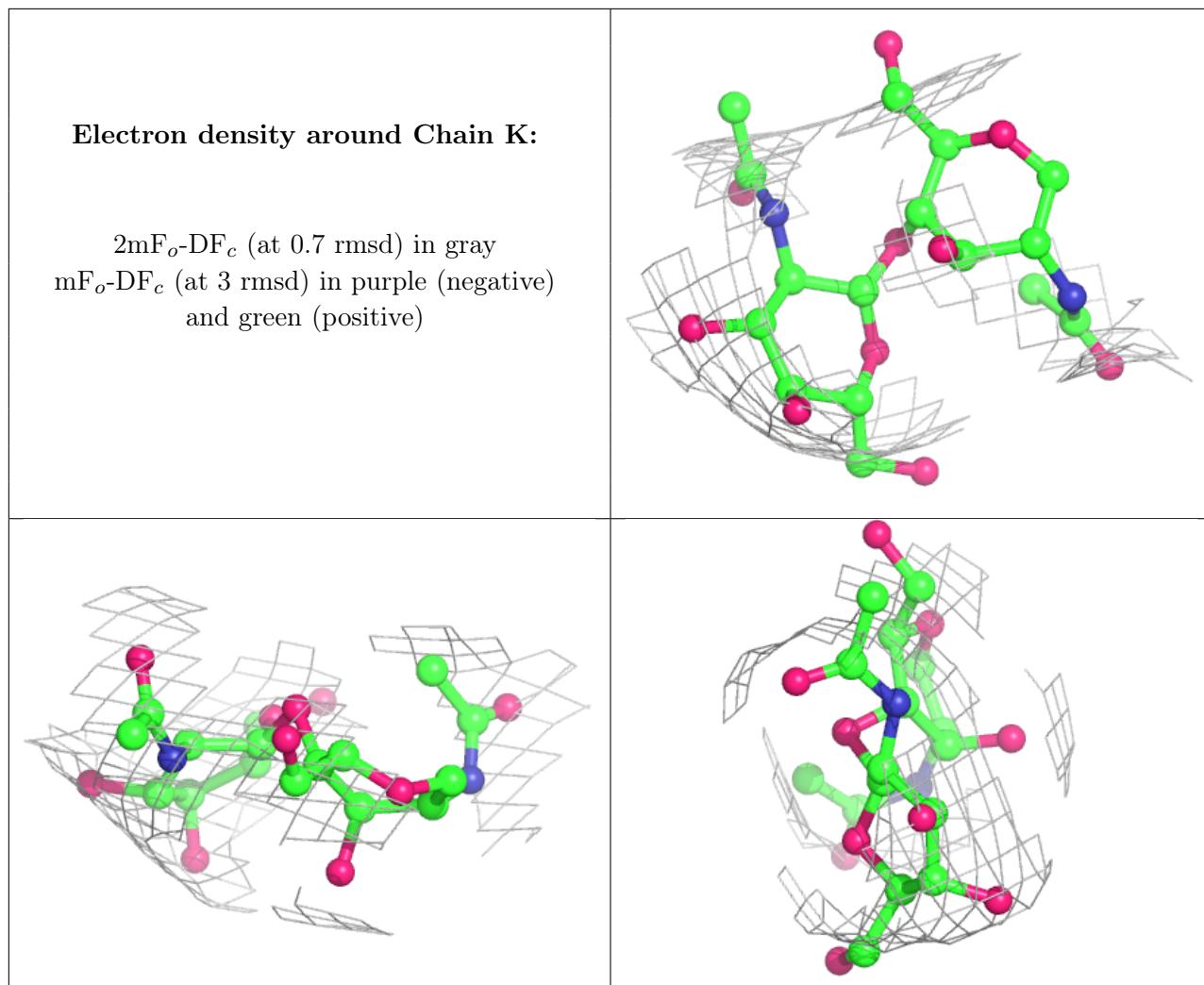
## 6.3 Carbohydrates [\(i\)](#)

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	NAG	J	2	14/15	0.79	0.28	195,245,293,301	0
4	NAG	K	1	14/15	0.83	0.29	205,222,228,234	0
4	NAG	J	1	14/15	0.85	0.25	177,211,249,290	0
4	NAG	K	2	14/15	0.90	0.26	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.





## 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, 95<sup>th</sup> 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.

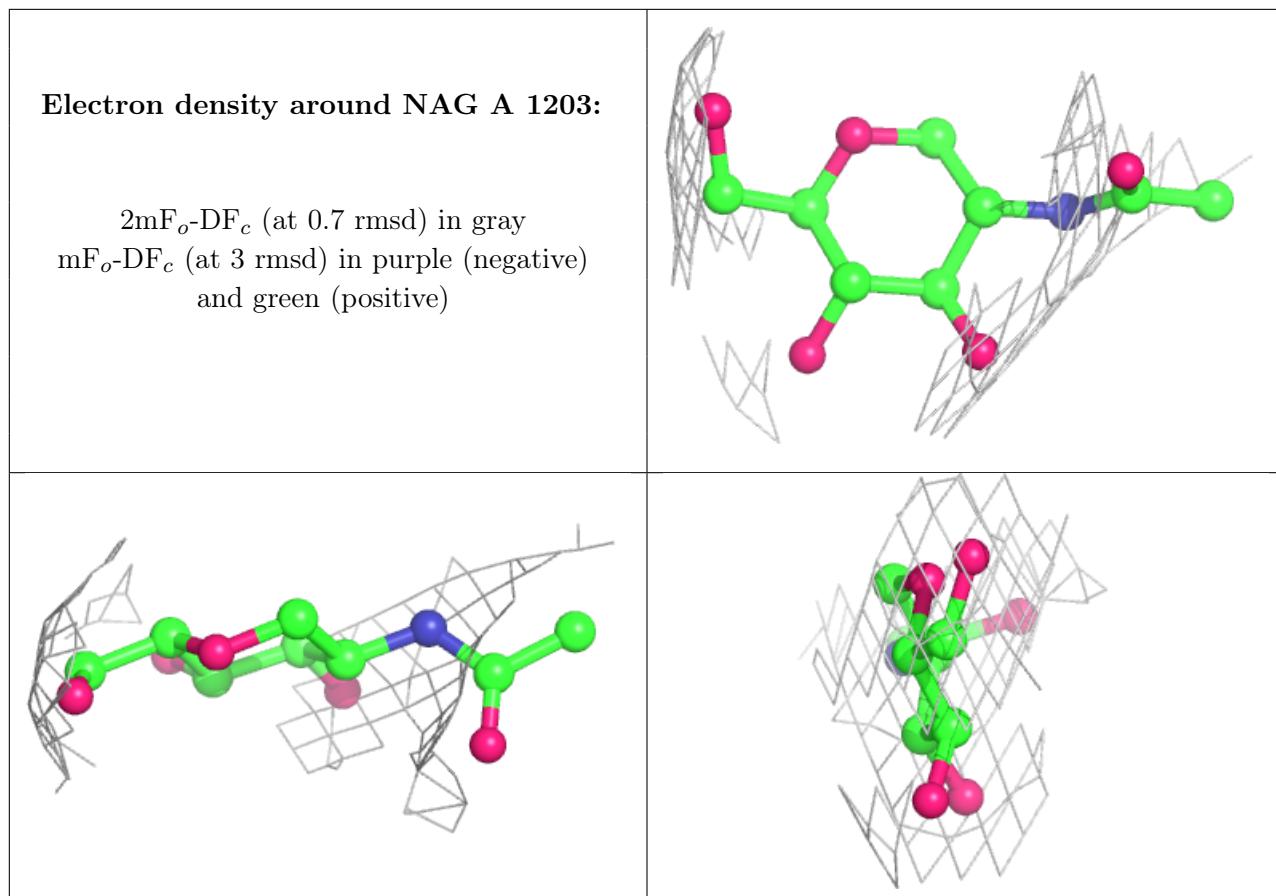
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	NAG	A	1203	14/15	0.75	0.26	233,259,276,278	0
5	NAG	C	1301	14/15	0.78	0.34	183,199,227,240	0
5	NAG	F	1302	14/15	0.80	0.32	213,231,247,250	0
5	NAG	G	1206	14/15	0.80	0.31	219,254,306,326	0
5	NAG	D	1202	14/15	0.82	0.31	175,195,206,208	0
5	NAG	D	1204	14/15	0.82	0.23	235,250,271,300	0
5	NAG	C	1304	14/15	0.82	0.31	189,197,228,231	0
5	NAG	G	1204	14/15	0.82	0.25	225,255,282,288	0
5	NAG	D	1201	14/15	0.82	0.29	194,272,278,292	0

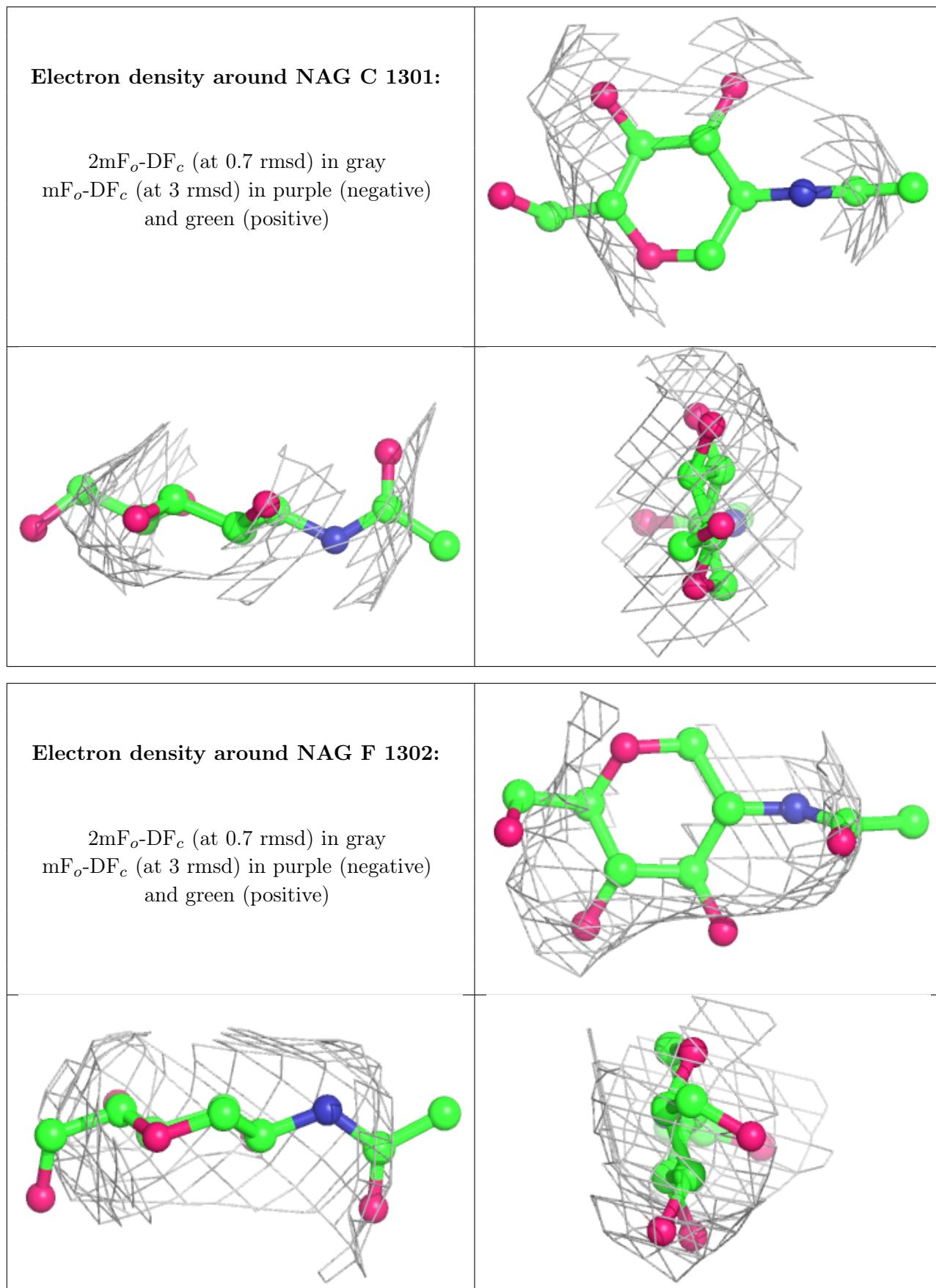
*Continued on next page...*

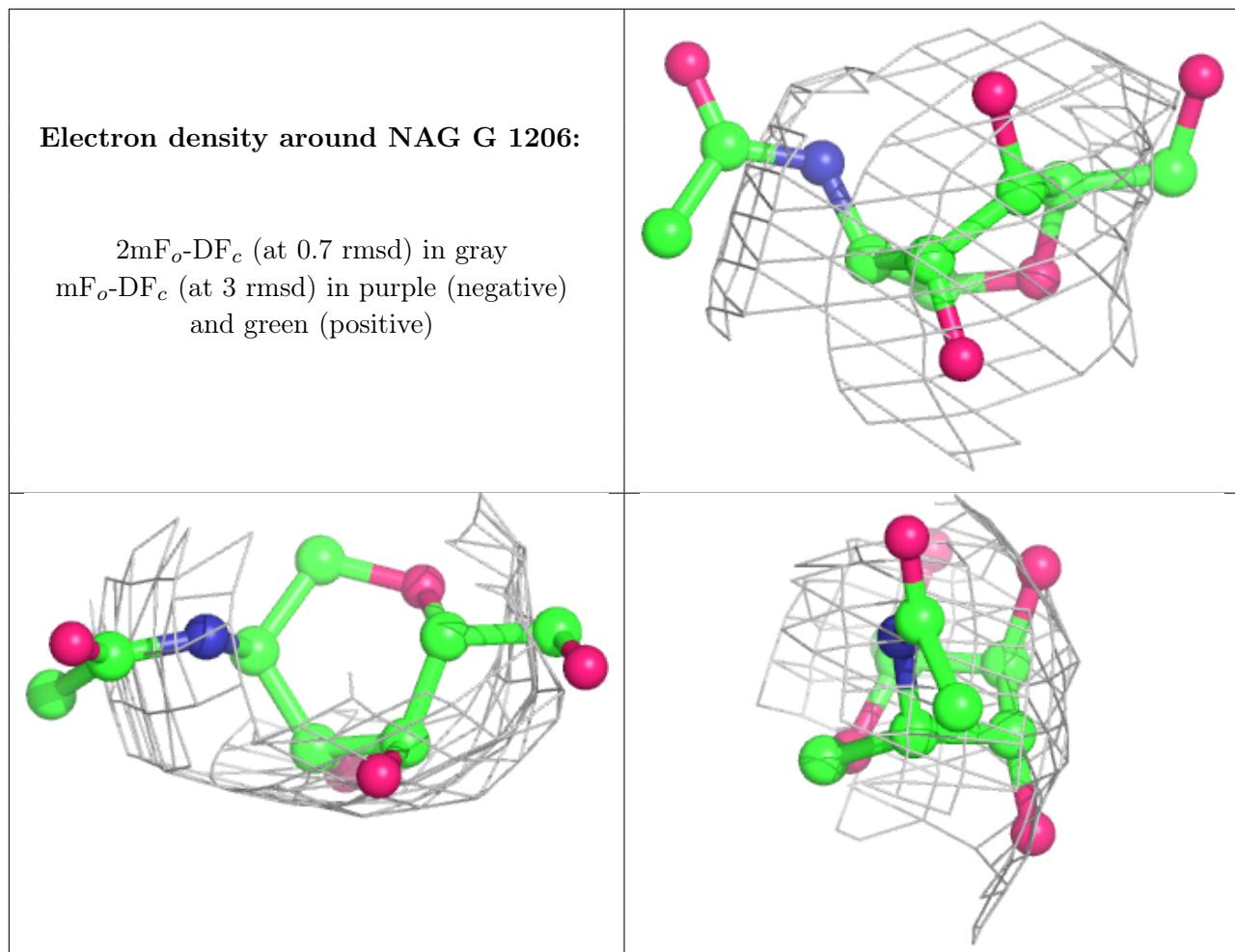
*Continued from previous page...*

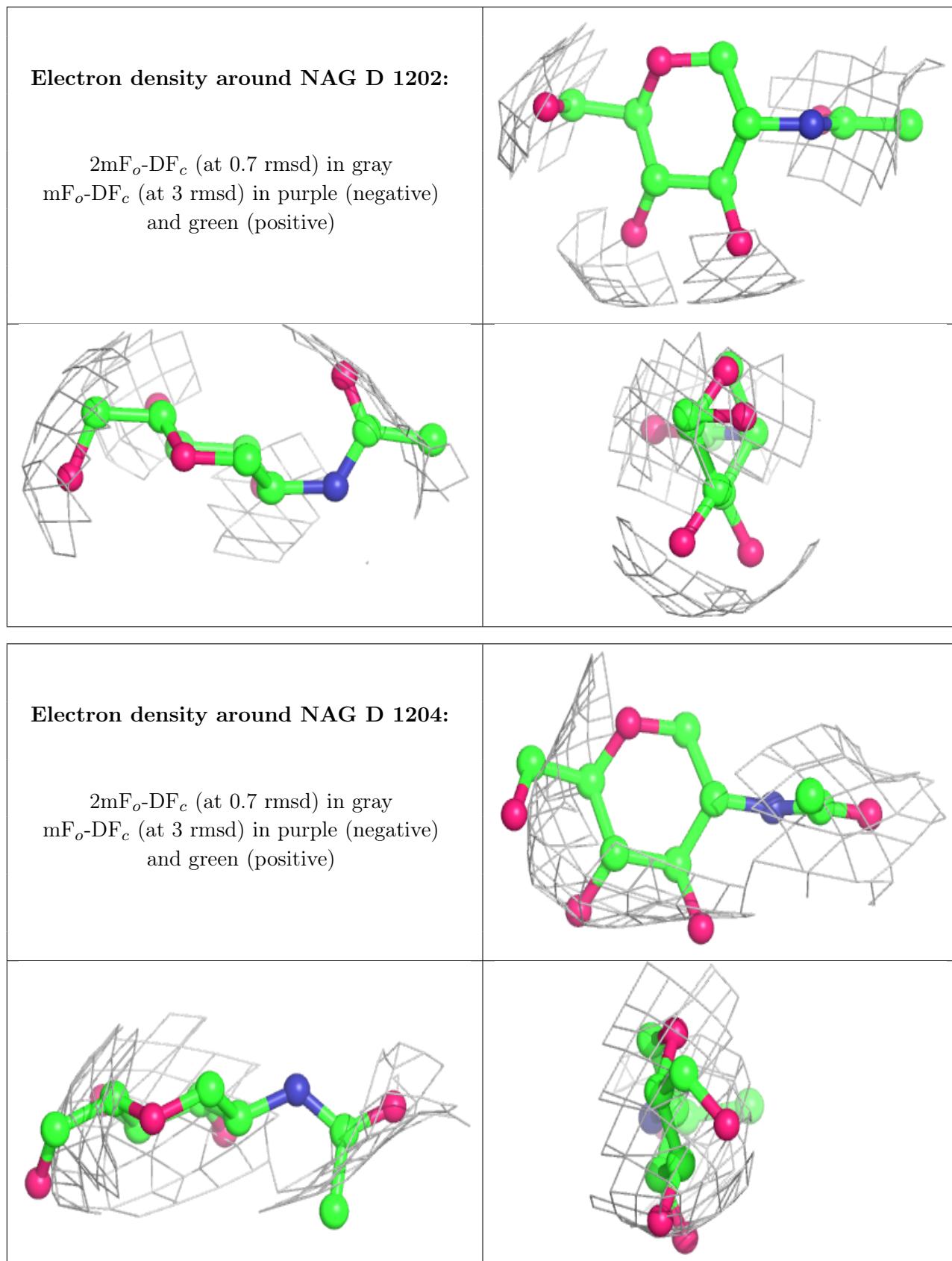
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	G	1205	14/15	0.83	0.34	181,219,248,272	0
5	NAG	G	1201	14/15	0.83	0.24	223,278,310,322	0
5	NAG	D	1205	14/15	0.84	0.28	197,239,256,261	0
5	NAG	I	1302	14/15	0.84	0.27	174,219,231,237	0
5	NAG	I	1301	14/15	0.86	0.28	192,215,236,249	0
5	NAG	F	1305	14/15	0.86	0.33	120,179,195,218	0
5	NAG	E	200	14/15	0.88	0.26	198,216,229,232	0
5	NAG	H	200	14/15	0.88	0.27	225,230,243,251	0
5	NAG	C	1303	14/15	0.88	0.41	180,203,249,252	0
5	NAG	A	1204	14/15	0.88	0.19	223,252,272,278	0
5	NAG	A	1201	14/15	0.89	0.28	219,239,264,288	0
5	NAG	F	1303	14/15	0.89	0.26	165,224,239,255	0
5	NAG	D	1203	14/15	0.90	0.25	221,233,266,270	0
5	NAG	G	1202	14/15	0.90	0.27	149,235,303,323	0
5	NAG	F	1301	14/15	0.91	0.28	173,192,197,201	0
5	NAG	F	1304	14/15	0.92	0.42	143,175,209,212	0
5	NAG	I	1303	14/15	0.92	0.20	185,201,215,223	0
5	NAG	A	1202	14/15	0.93	0.19	172,196,209,218	0
5	NAG	C	1302	14/15	0.93	0.29	168,190,208,225	0
5	NAG	A	1205	14/15	0.93	0.23	182,198,216,226	0
5	NAG	G	1203	14/15	0.94	0.21	148,188,196,207	0

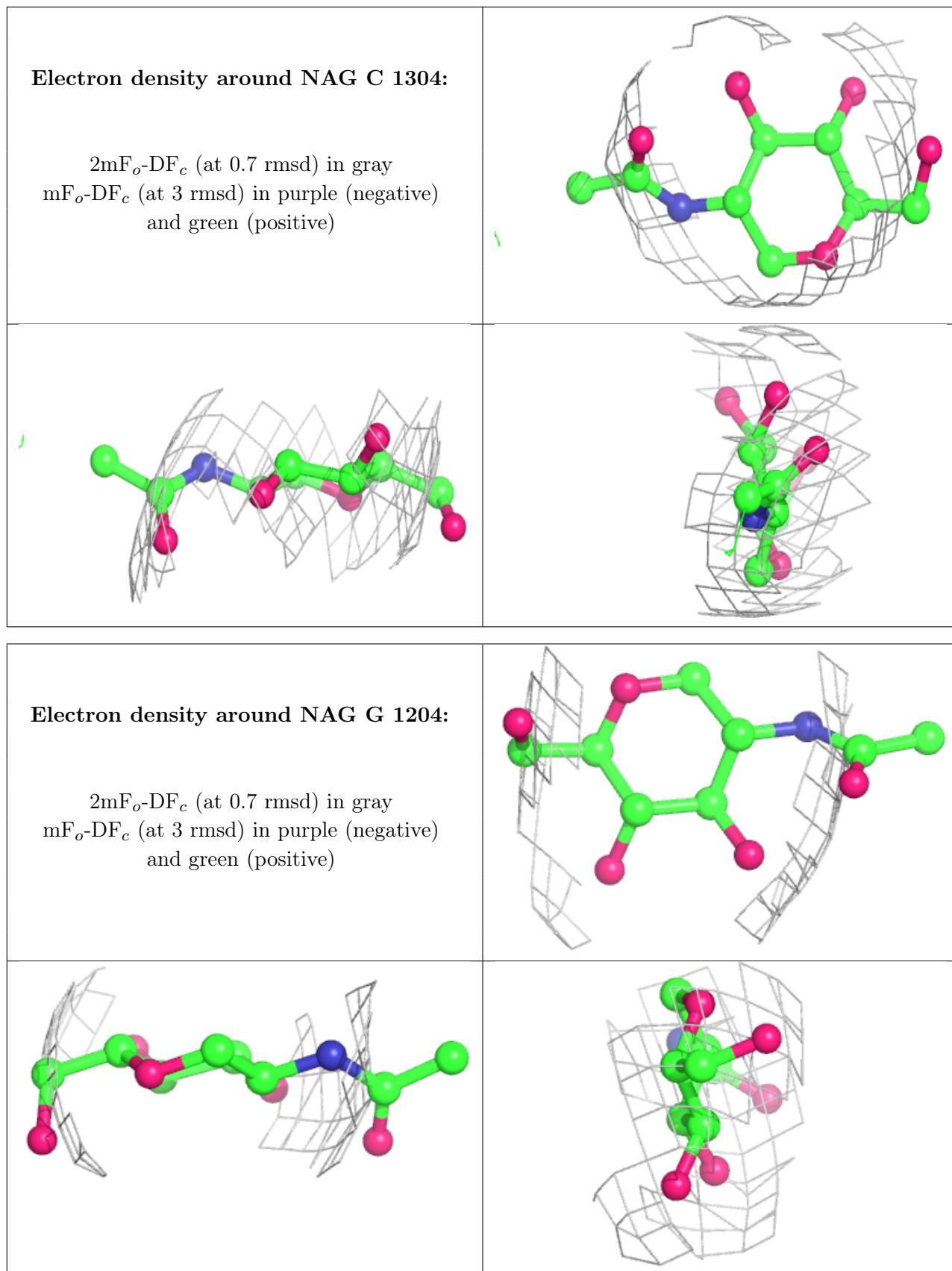
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

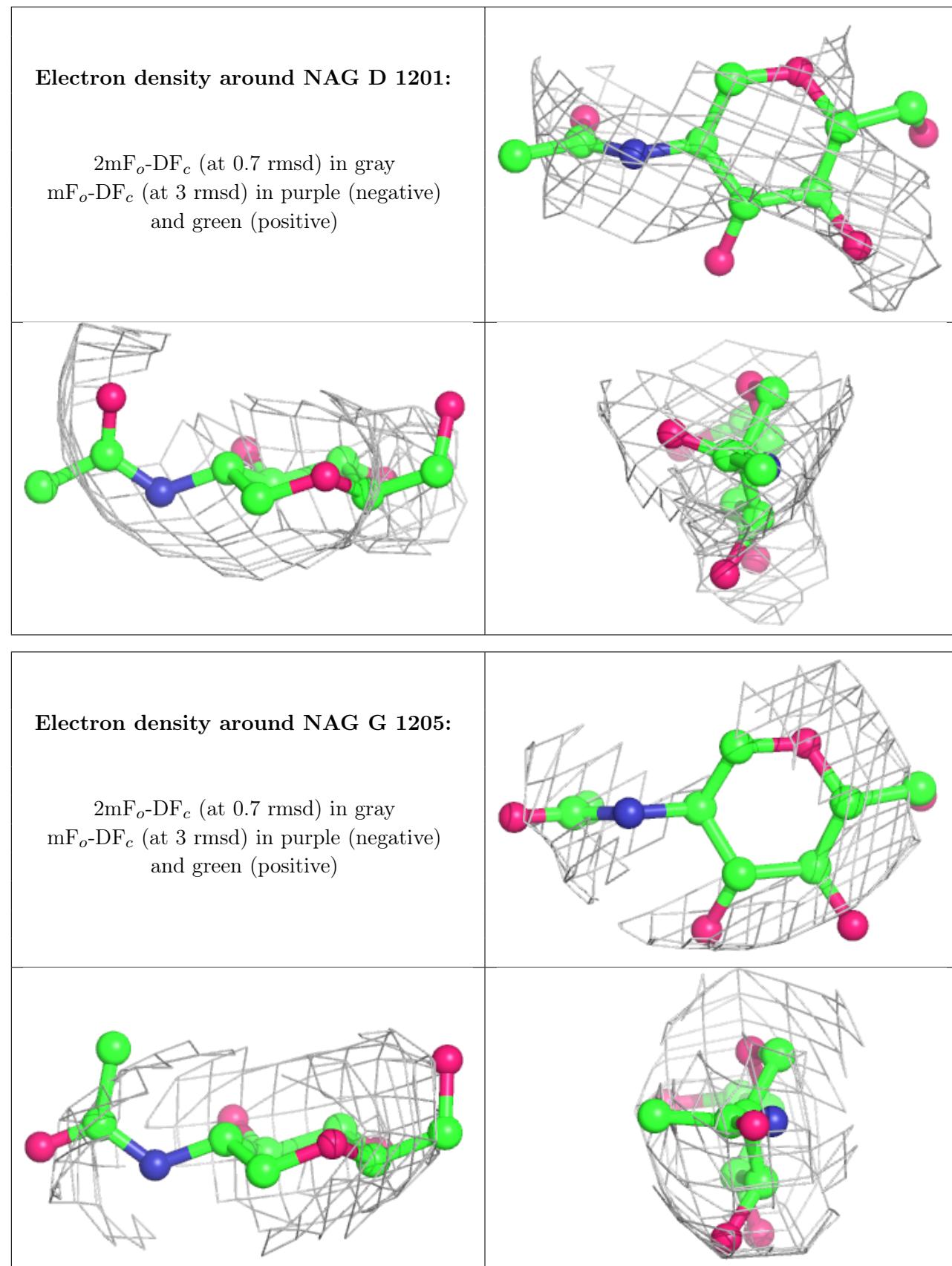


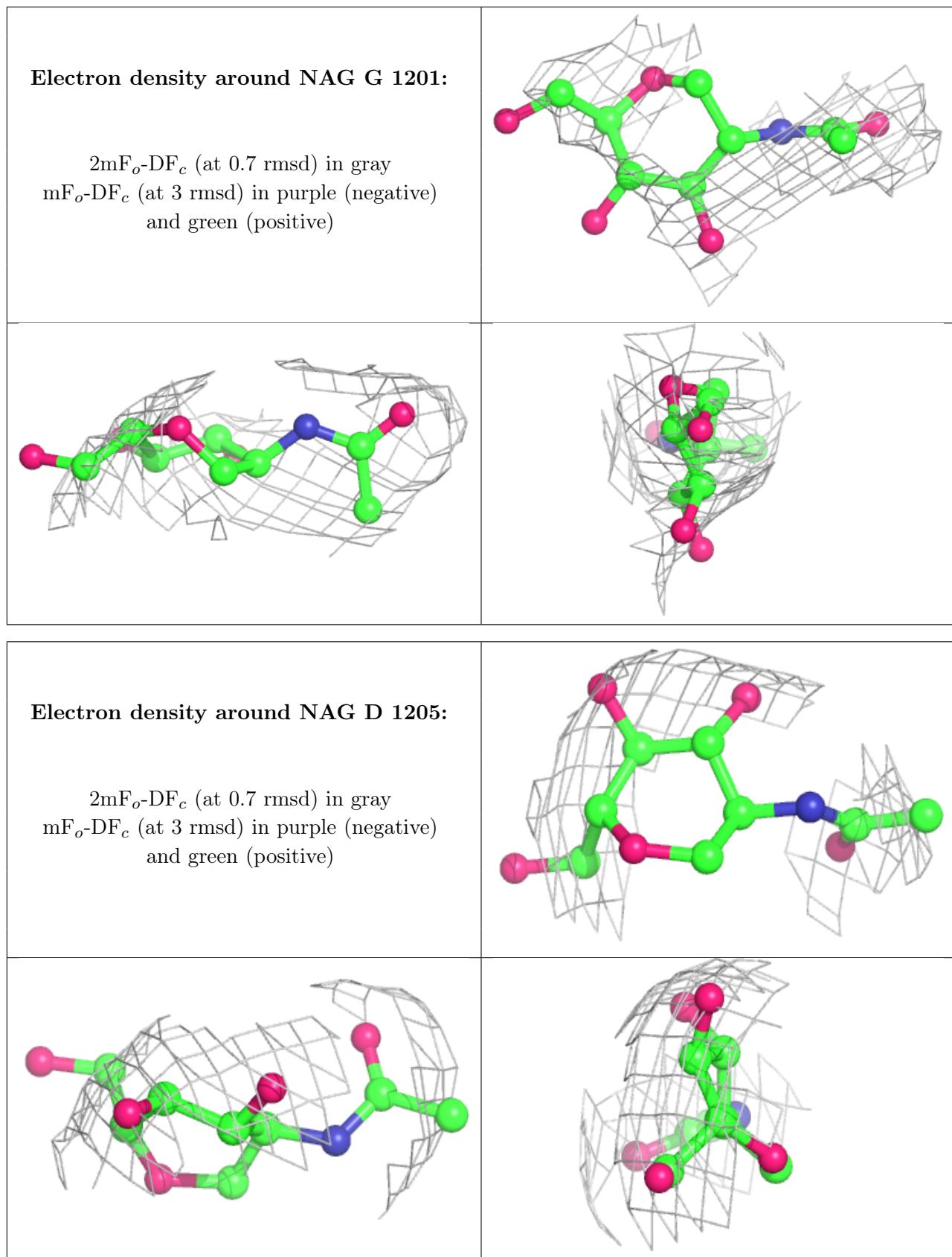


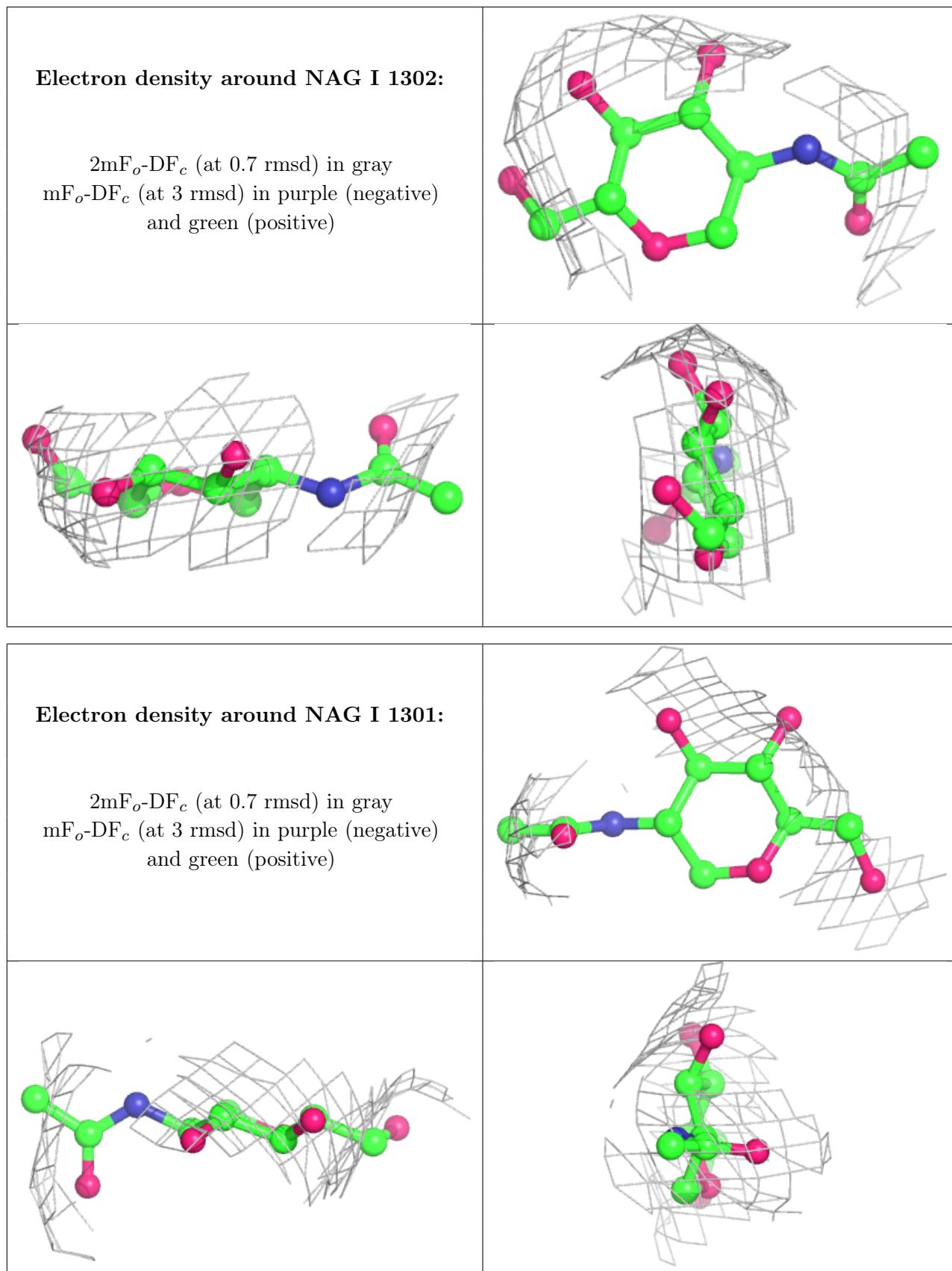


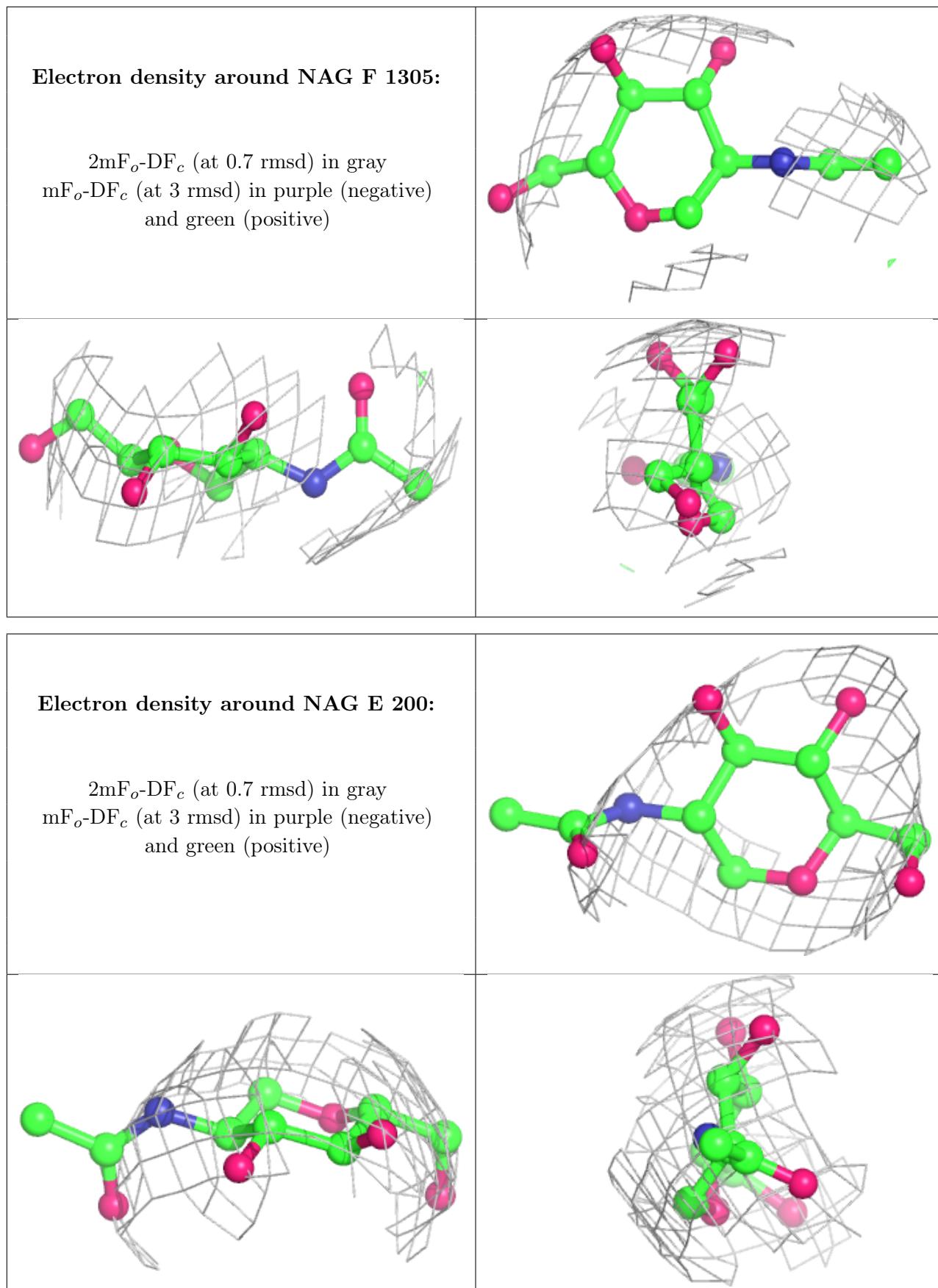


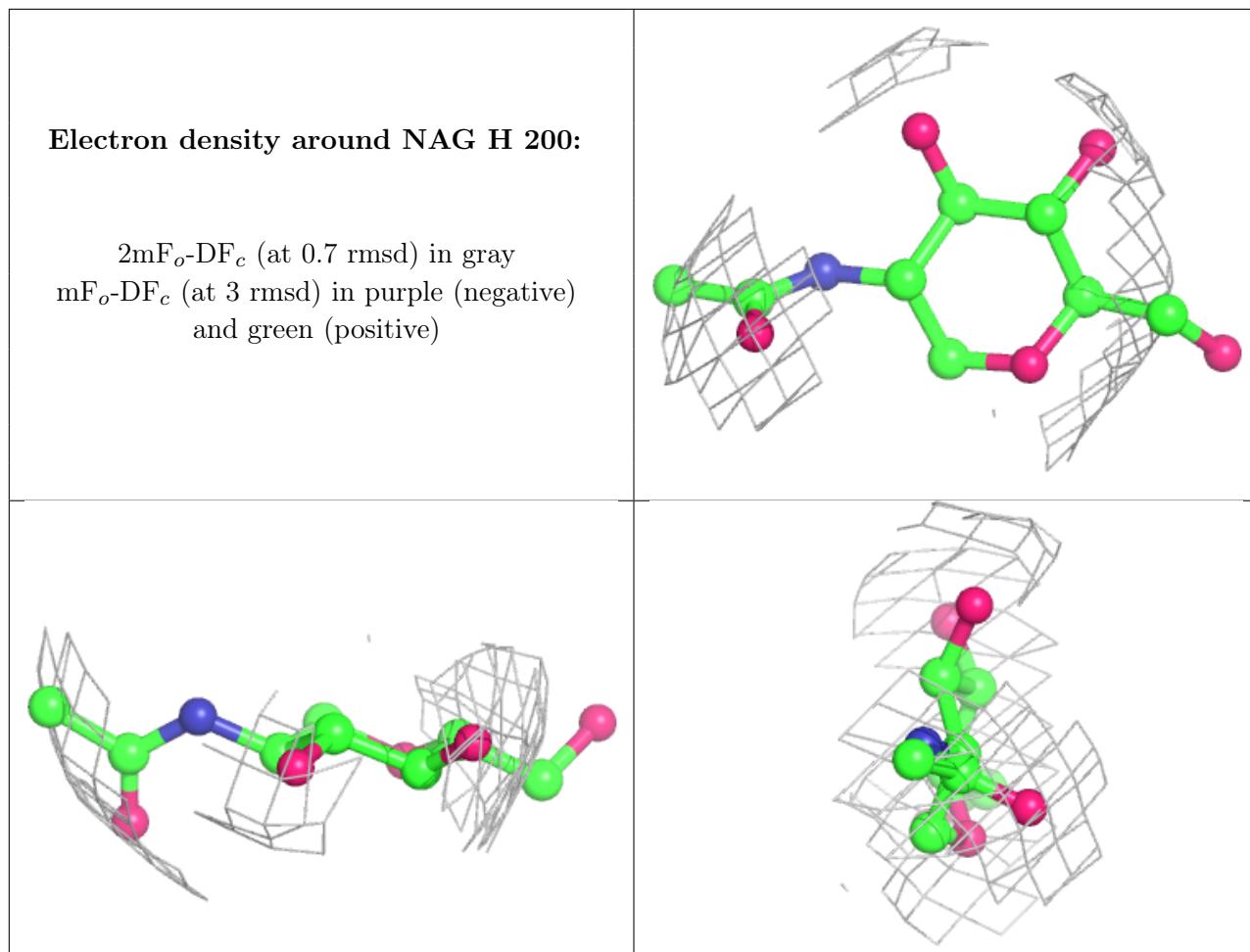


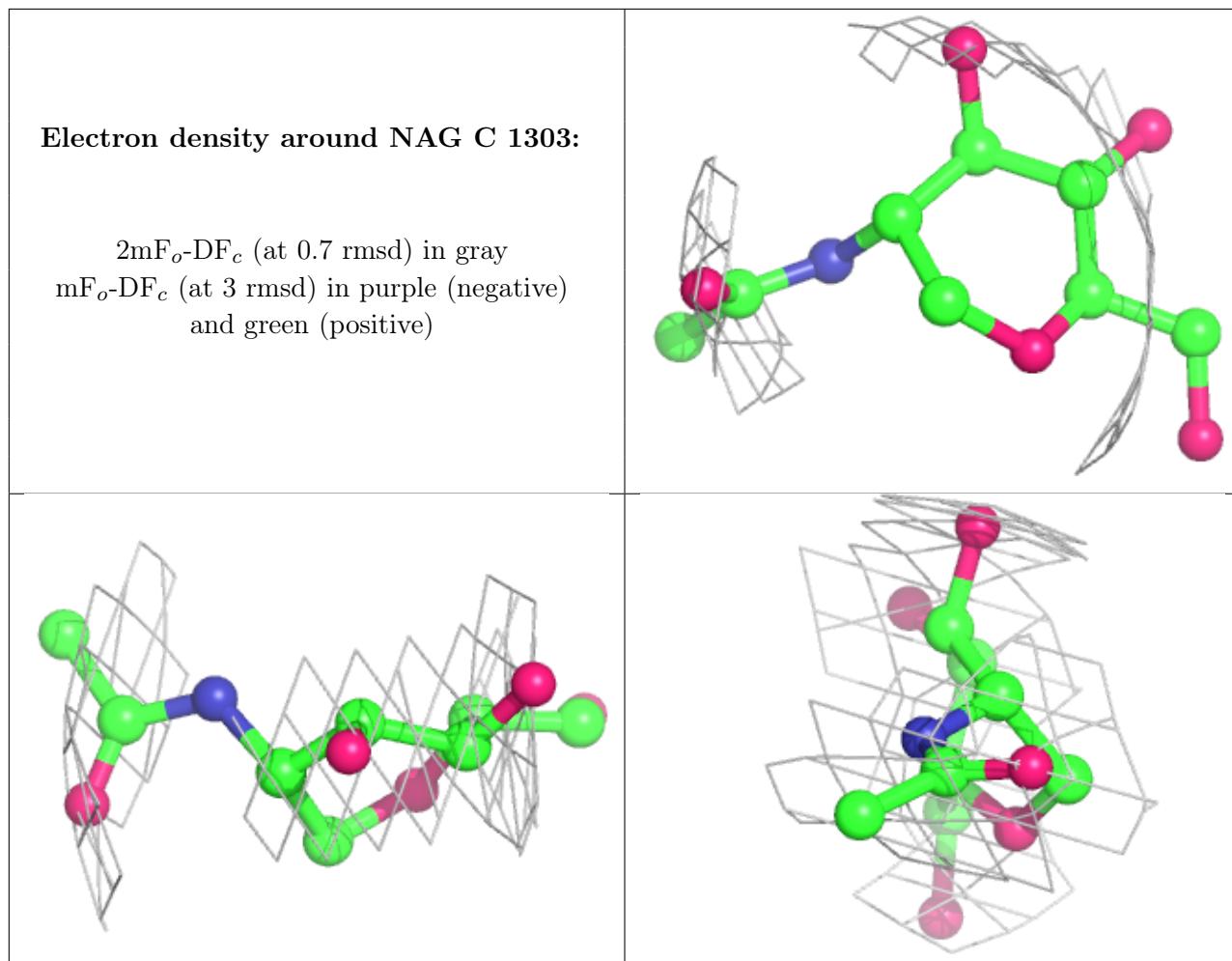


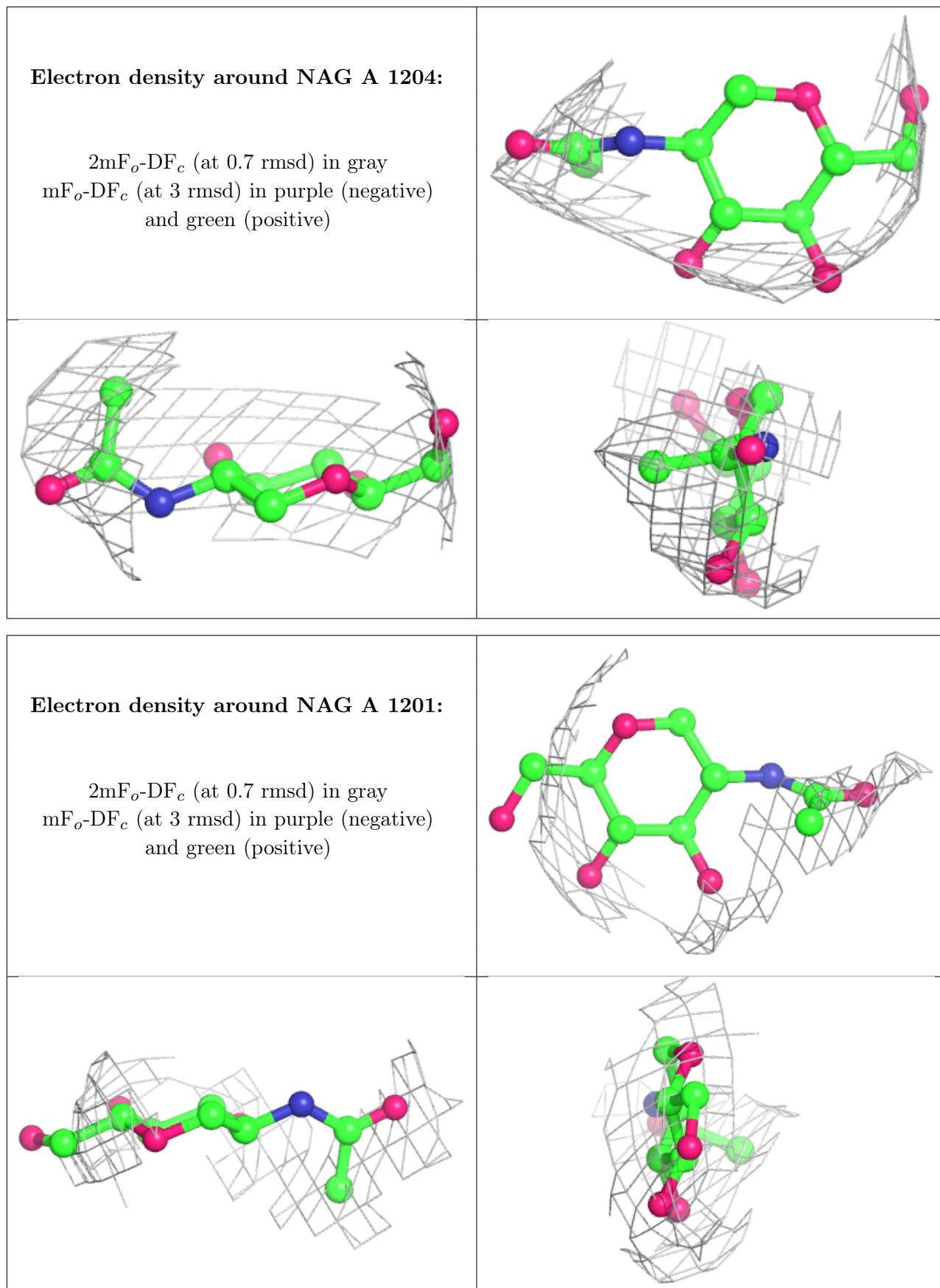


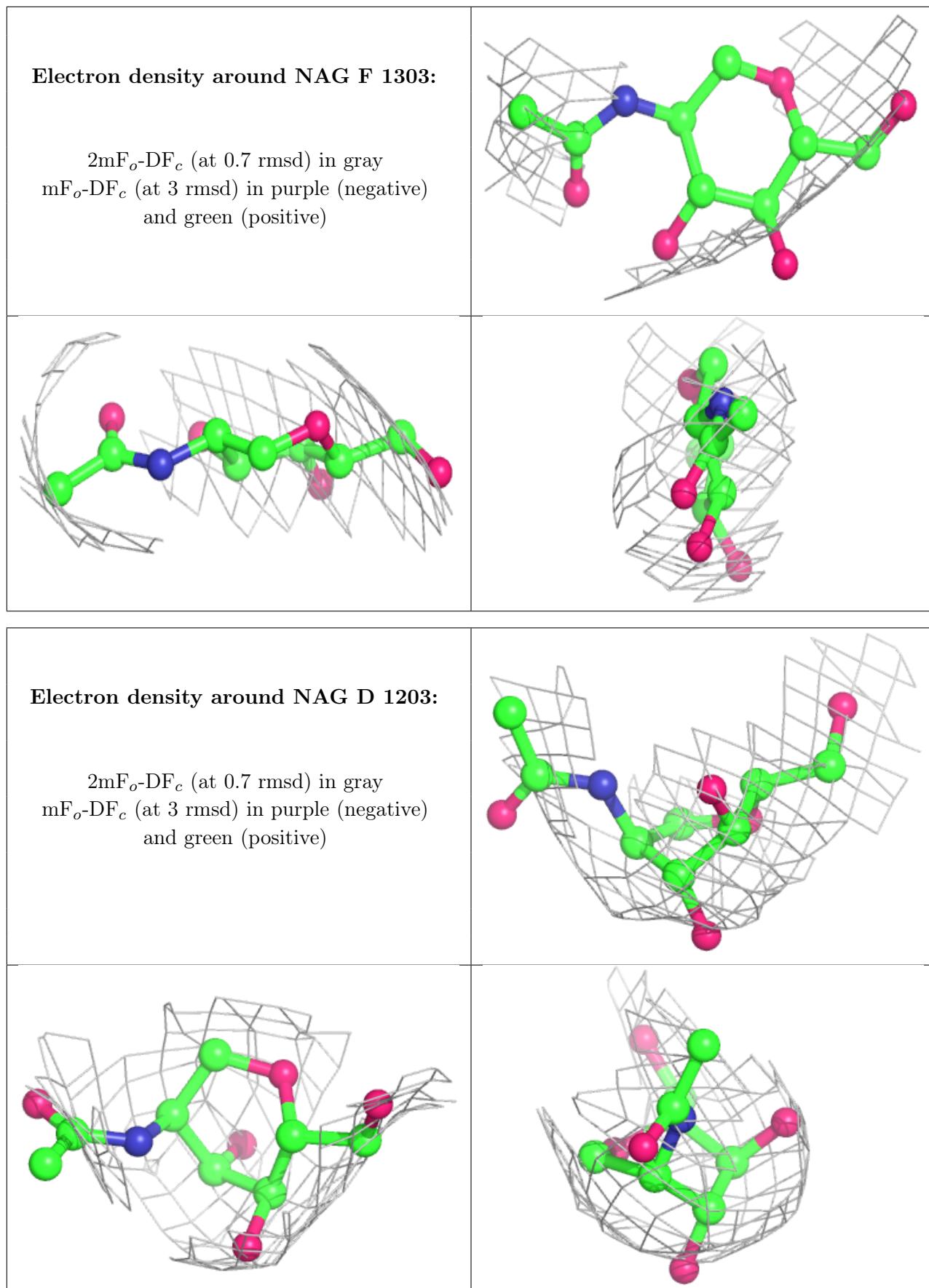


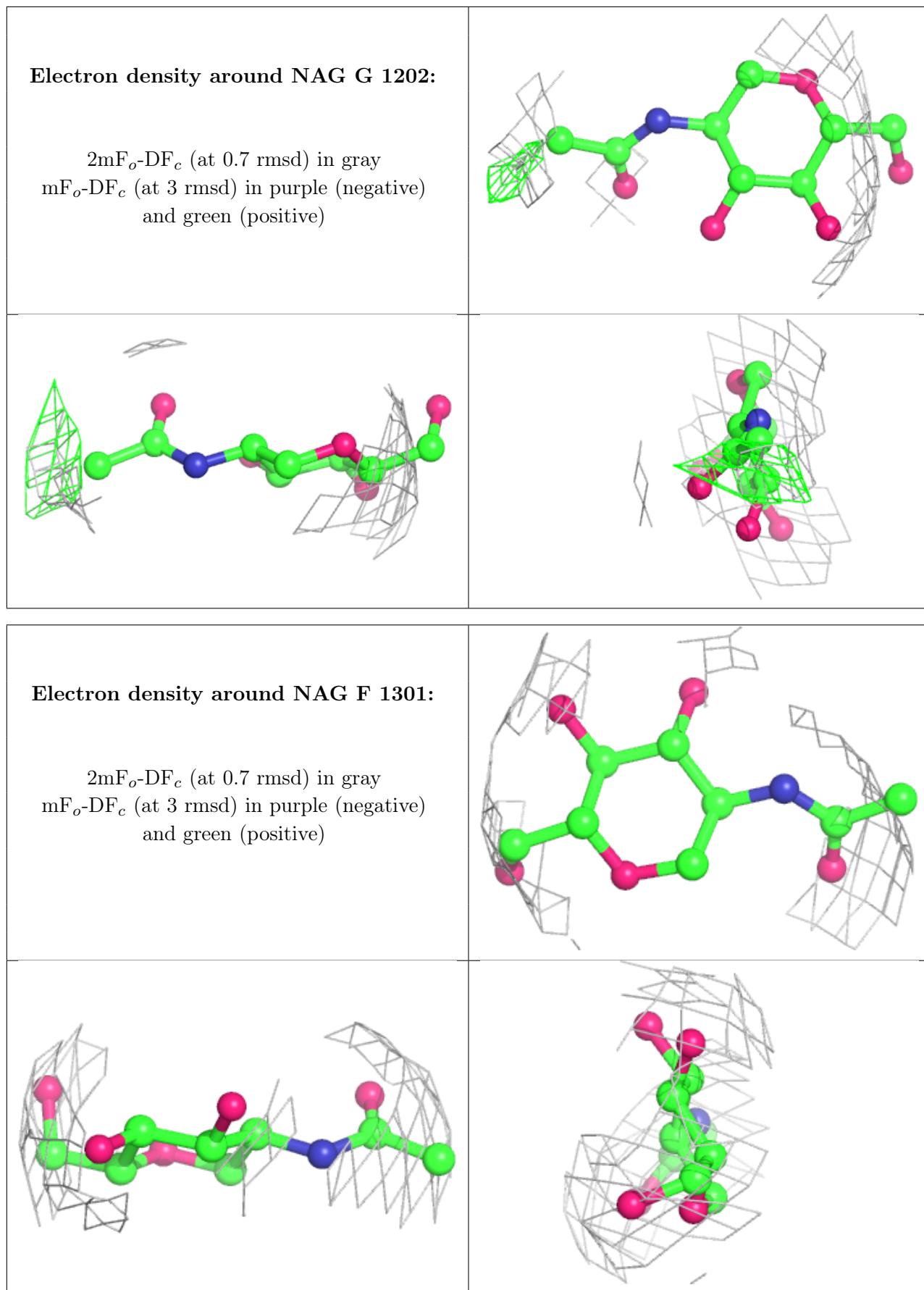


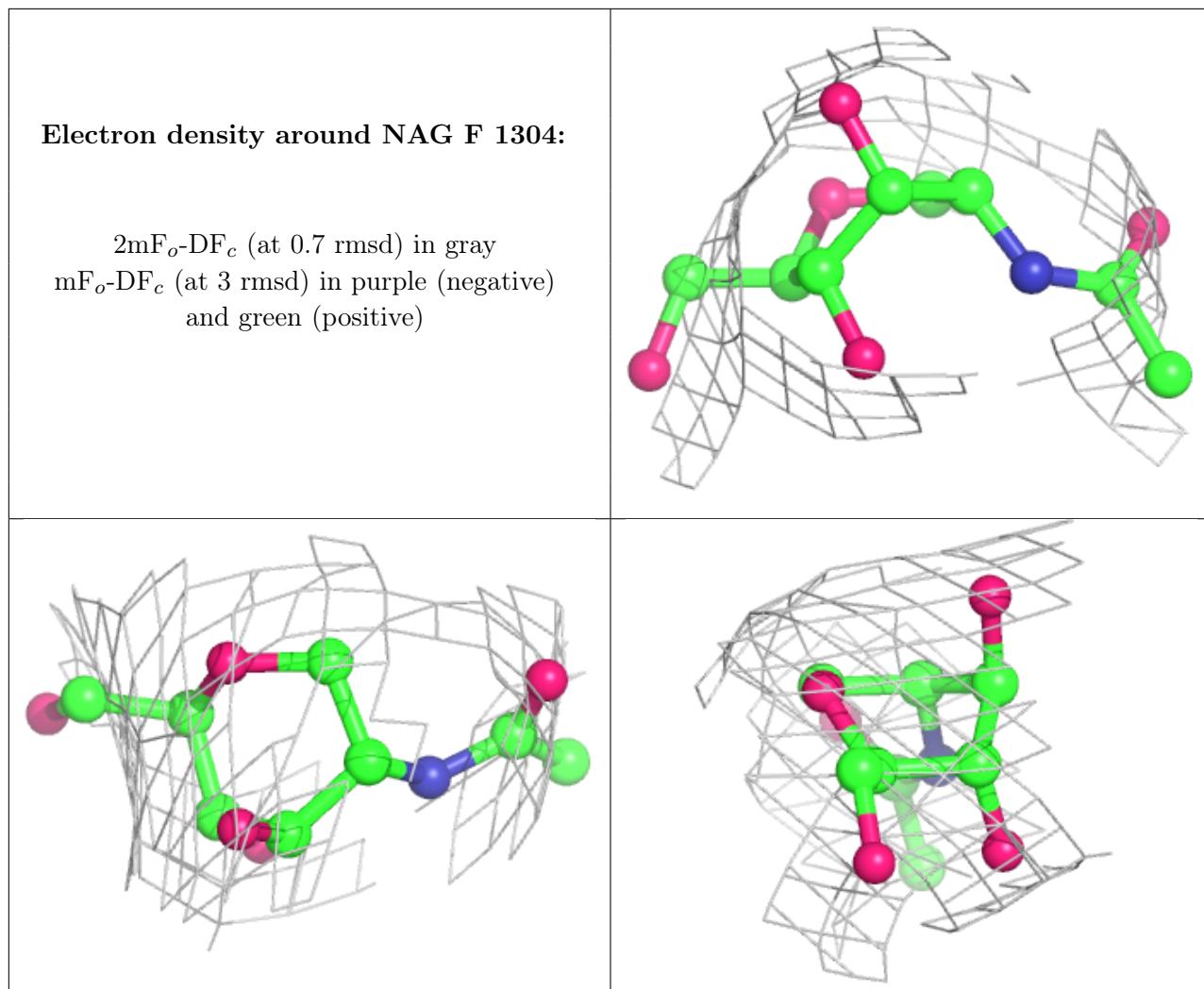


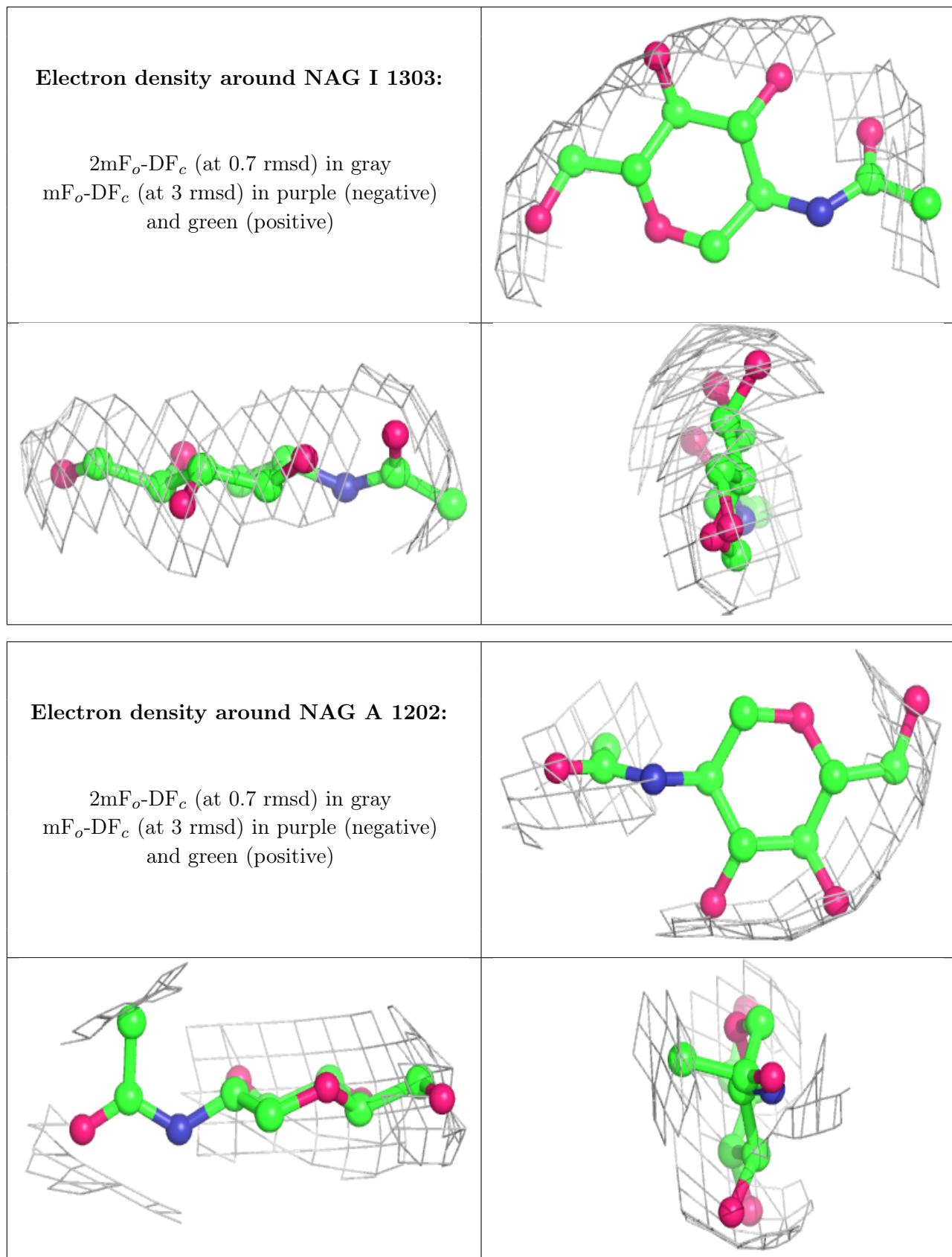


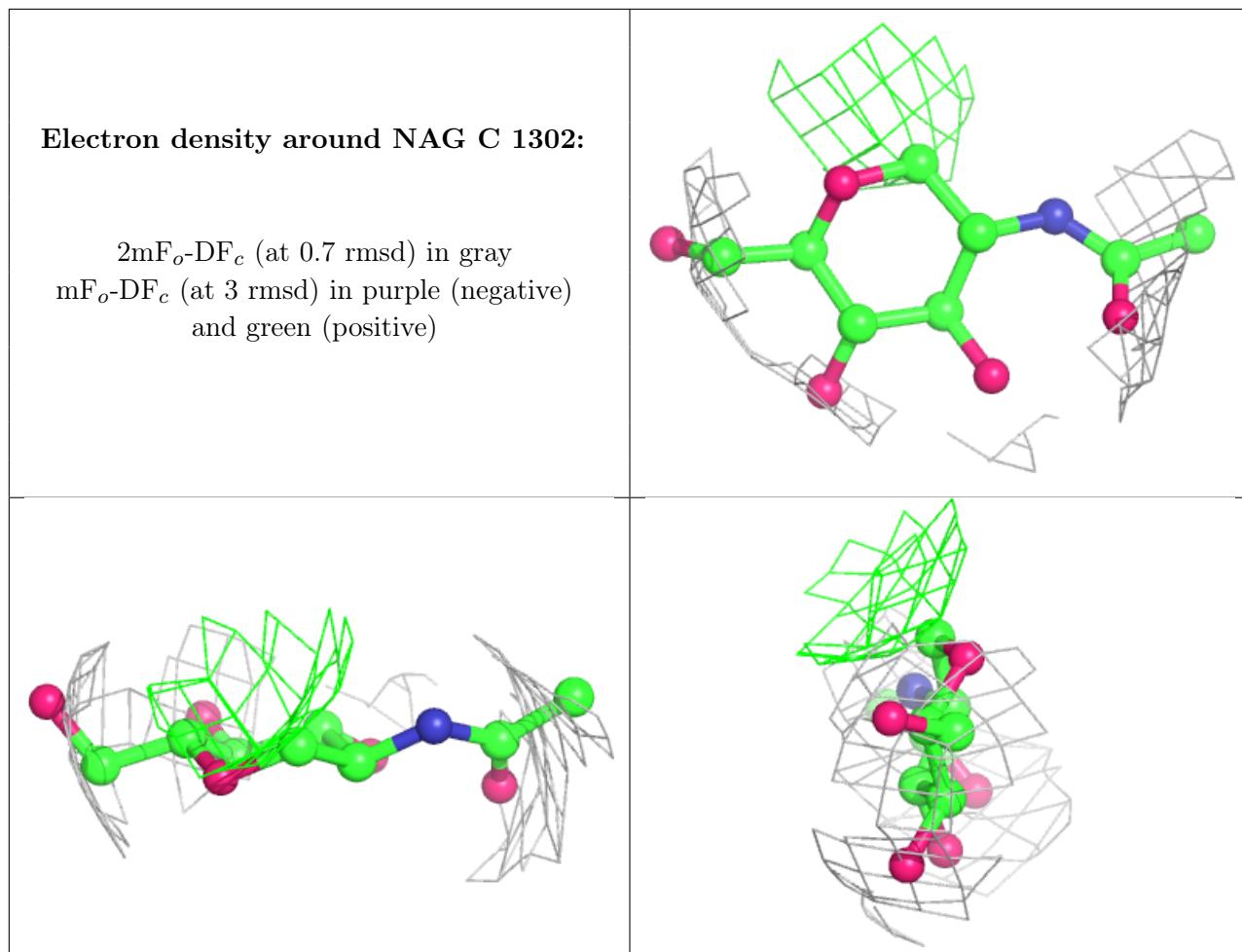


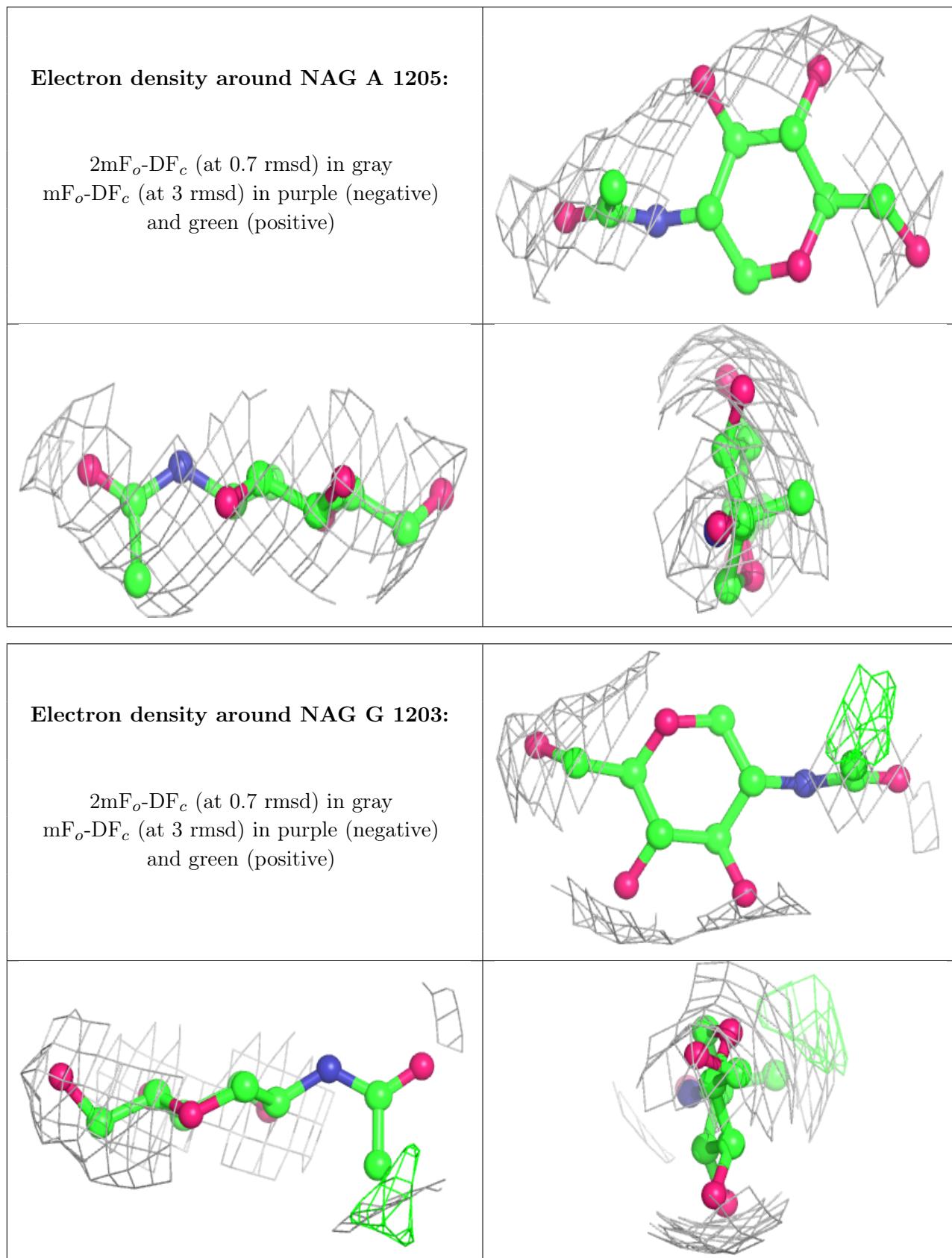












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.