



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 10:15 AM EDT

PDB ID : 9OAS / pdb\_00009oas  
Title : Crystal structure of antibody Fab G001-14 from IAVI G001 human trial in complex with a germline-targeting gp120 engineered outer domain eOD-GT8-mingly-N276  
Authors : Lin, X.; Wilson, I.A.  
Deposited on : 2025-04-21  
Resolution : 2.79 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 ⓘ symbol.

The types of validation reports are described at

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

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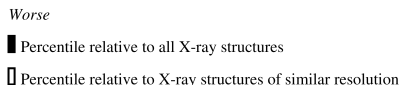
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

**i**

## X-RAY DIFFRACTION

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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain	
1	F	210	<div> <div></div> <div></div> </div> <div>81%18%</div>	•
1	K	210	<div> <div></div> <div></div> </div> <div>86%13%</div>	•
1	L	210	<div> <div></div> <div></div> </div> <div>86%13%</div>	•
1	R	210	<div> <div></div> <div></div> </div> <div>70%29%</div>	•

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Mol	Chain	Length	Quality of chain
2	C	184	<div><div></div><div>77%15%8%</div></div>
2	D	184	<div><div>%</div><div>77%15%8%</div></div>
2	M	184	<div><div>%</div><div>81%10%8%</div></div>
2	P	184	<div><div>3%</div><div>74%17%8%</div></div>
3	E	224	<div><div>2%</div><div>85%13%</div></div>
3	H	224	<div><div>%</div><div>84%13%</div></div>
3	J	224	<div><div>%</div><div>84%13%</div></div>
3	Q	224	<div><div>4%</div><div>82%16%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18474 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 G001-14 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	208	Total	C	N	O	S	0	0	0
			1606	1005	266	330	5			
1	L	208	Total	C	N	O	S	0	0	0
			1606	1005	266	330	5			
1	R	208	Total	C	N	O	S	0	0	0
			1606	1005	266	330	5			
1	F	208	Total	C	N	O	S	0	0	0
			1606	1005	266	330	5			

- Molecule 2 is a protein called Germline-targeting HIV-1 gp120 engineered outer domain eOD-GT8-mingly-N276.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	169	Total	C	N	O	S	0	0	0
			1284	807	225	244	8			
2	C	169	Total	C	N	O	S	0	0	0
			1284	807	225	244	8			
2	D	169	Total	C	N	O	S	0	0	0
			1284	807	225	244	8			
2	P	169	Total	C	N	O	S	0	0	0
			1284	807	225	244	8			

- Molecule 3 is a protein called G001-14 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	219	Total	C	N	O	S	0	0	0
			1653	1046	279	321	7			
3	H	219	Total	C	N	O	S	0	0	0
			1653	1046	279	321	7			
3	Q	219	Total	C	N	O	S	0	0	0
			1653	1046	279	321	7			
3	E	219	Total	C	N	O	S	0	0	0
			1653	1046	279	321	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	1	Total	C	N	O	0	0
			14	8	1	5		
4	M	1	Total	C	N	O	0	0
			14	8	1	5		
4	M	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		

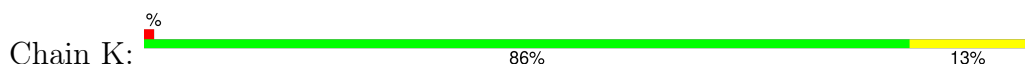
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	8	Total O 8 8	0	0
5	M	6	Total O 6 6	0	0
5	J	13	Total O 13 13	0	0
5	L	17	Total O 17 17	0	0
5	H	14	Total O 14 14	0	0
5	C	13	Total O 13 13	0	0
5	D	15	Total O 15 15	0	0
5	R	2	Total O 2 2	0	0
5	Q	13	Total O 13 13	0	0
5	P	9	Total O 9 9	0	0
5	F	16	Total O 16 16	0	0
5	E	8	Total O 8 8	0	0

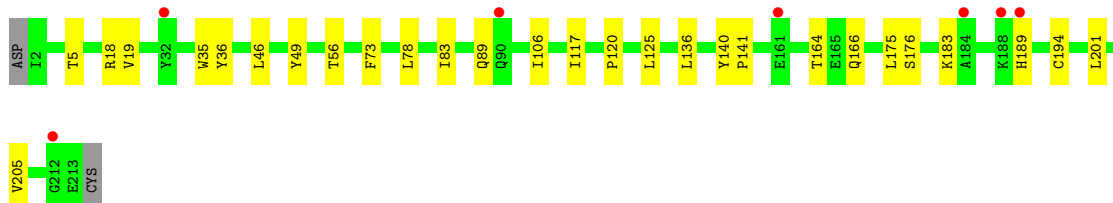
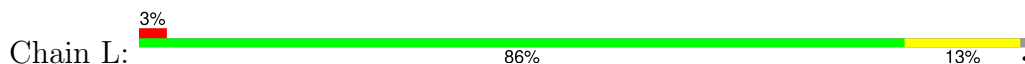
### 3 Residue-property plots [i](#)

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.

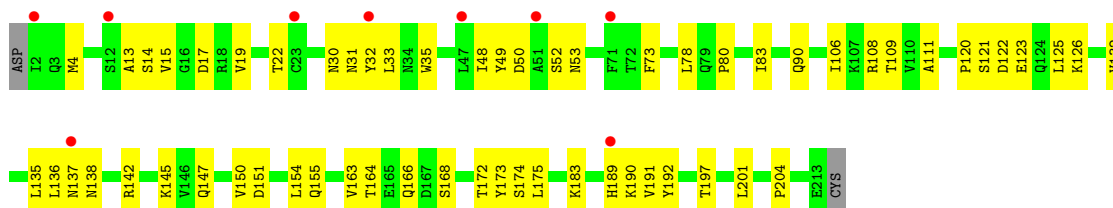
- Molecule 1: G001-14 Fab light chain



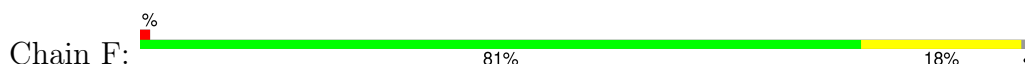
- Molecule 1: G001-14 Fab light chain



- Molecule 1: G001-14 Fab light chain

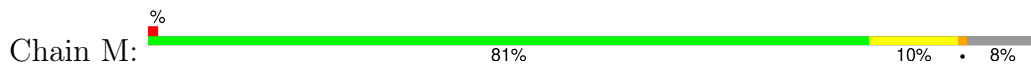


- Molecule 1: G001-14 Fab light chain

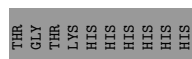




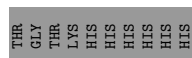
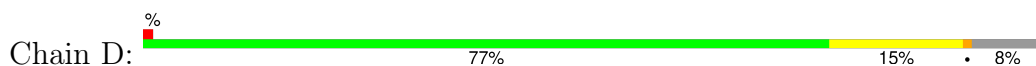
- Molecule 2: Germline-targeting HIV-1 gp120 engineered outer domain eOD-GT8-mingly-N276



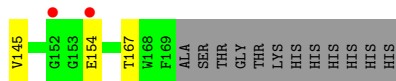
- Molecule 2: Germline-targeting HIV-1 gp120 engineered outer domain eOD-GT8-mingly-N276



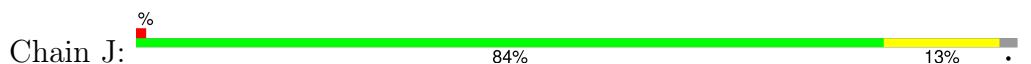
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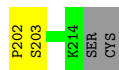
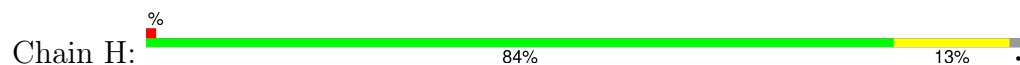
- Molecule 3: G001-14 Fab heavy chain



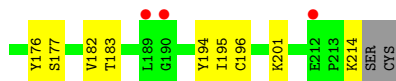
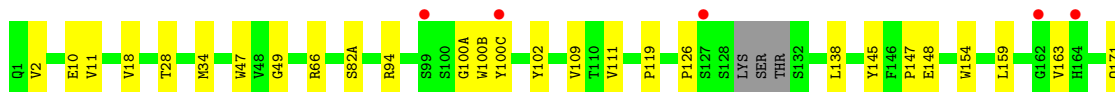
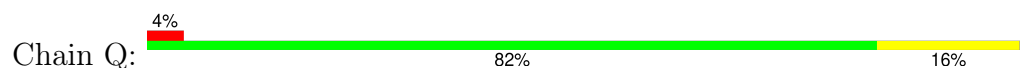




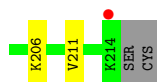
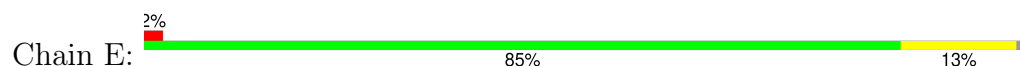
- Molecule 3: G001-14 Fab heavy chain



- Molecule 3: G001-14 Fab heavy chain



- Molecule 3: G001-14 Fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.06Å 75.52Å 158.15Å 90.00° 92.36° 90.00°	Depositor
Resolution (Å)	26.08 – 2.79 26.08 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.6 (26.08-2.79) 97.4 (26.08-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.214 , 0.255 0.214 , 0.255	Depositor DCC
$R_{free}$ test set	3931 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	F	0.18	0/1640	0.41	0/2226
1	K	0.16	0/1640	0.41	0/2226
1	L	0.21	0/1640	0.45	0/2226
1	R	0.16	0/1640	0.43	0/2226
2	C	0.23	0/1314	0.36	0/1787
2	D	0.20	0/1314	0.36	0/1787
2	M	0.18	0/1314	0.28	0/1787
2	P	0.16	0/1314	0.34	0/1787
3	E	0.14	0/1697	0.36	0/2312
3	H	0.18	0/1697	0.38	0/2312
3	J	0.20	0/1697	0.40	0/2312
3	Q	0.14	0/1697	0.37	0/2312
All	All	0.18	0/18604	0.38	0/25300

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	F	1606	0	1544	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1606	0	1544	17	0
1	L	1606	0	1544	17	0
1	R	1606	0	1544	46	0
2	C	1284	0	1241	17	0
2	D	1284	0	1241	16	0
2	M	1284	0	1241	12	0
2	P	1284	0	1241	18	0
3	E	1653	0	1604	14	0
3	H	1653	0	1604	21	0
3	J	1653	0	1604	17	0
3	Q	1653	0	1604	23	0
4	C	42	0	39	0	0
4	D	42	0	39	1	0
4	M	42	0	39	0	0
4	P	42	0	39	1	0
5	C	13	0	0	1	0
5	D	15	0	0	0	0
5	E	8	0	0	0	0
5	F	16	0	0	0	0
5	H	14	0	0	1	0
5	J	13	0	0	0	0
5	K	8	0	0	0	0
5	L	17	0	0	0	0
5	M	6	0	0	0	0
5	P	9	0	0	0	0
5	Q	13	0	0	1	0
5	R	2	0	0	0	0
All	All	18474	0	17712	233	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (233) 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)
1:R:166:GLN:HG2	1:R:173:TYR:HE1	1.44	0.82
2:P:17:SER:HB3	4:P:202:NAG:HN2	1.46	0.80
3:H:11:VAL:HB	3:H:147:PRO:HG3	1.67	0.76
3:E:199:ASN:HD21	3:E:206:LYS:HE2	1.50	0.76
3:H:201:LYS:HG2	3:H:202:PRO:HD3	1.69	0.73
1:L:136:LEU:HB2	1:L:175:LEU:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.22	0.71
2:D:17:SER:HB3	4:D:202:NAG:HN2	1.55	0.71
3:E:11:VAL:HB	3:E:147:PRO:HG3	1.72	0.70
1:R:190:LYS:HG3	1:R:191:VAL:HG23	1.73	0.69
1:R:32:TYR:O	1:R:90:GLN:NE2	2.24	0.69
1:R:166:GLN:HG2	1:R:173:TYR:CE1	2.26	0.69
3:Q:11:VAL:HB	3:Q:147:PRO:HG3	1.73	0.68
1:R:35:TRP:HB2	1:R:48:ILE:HB	1.79	0.65
2:C:50:ARG:NH1	2:C:78:GLU:OE2	2.30	0.64
1:R:49:TYR:HB2	3:Q:100(C):TYR:HE2	1.63	0.63
3:J:193:THR:HG23	3:J:210:LYS:HD2	1.81	0.63
1:R:108:ARG:NH2	1:R:111:ALA:HB2	2.14	0.62
1:K:161:GLU:HG2	1:K:175:LEU:HD21	1.81	0.62
2:P:36:VAL:HG23	2:P:130:LYS:HG2	1.80	0.62
3:J:200:HIS:HD1	3:J:203:SER:HG	1.48	0.62
3:H:201:LYS:NZ	5:H:301:HOH:O	2.32	0.62
3:Q:126:PRO:HG3	3:Q:138:LEU:HB3	1.81	0.62
3:Q:34:MET:HE1	3:Q:94:ARG:HG3	1.82	0.61
1:F:32:TYR:HA	1:F:50:ASP:HA	1.83	0.61
1:F:151:ASP:OD2	1:F:189:HIS:ND1	2.35	0.60
1:K:32:TYR:CE2	1:K:90:GLN:HG2	2.37	0.60
2:P:19:ILE:HD13	2:P:62:LEU:HD13	1.84	0.59
3:H:9:ALA:H	3:H:201:LYS:HE3	1.68	0.58
1:R:19:VAL:HG21	1:R:78:LEU:HD13	1.85	0.58
2:D:133:ILE:HG12	2:D:167:THR:HG23	1.83	0.58
3:J:11:VAL:HG12	3:J:110:THR:HB	1.84	0.58
3:Q:119:PRO:HB3	3:Q:145:TYR:HB3	1.85	0.58
1:K:164:THR:HG22	1:K:174:SER:H	1.69	0.57
1:L:136:LEU:HD13	1:L:175:LEU:HD12	1.86	0.57
1:R:120:PRO:HD3	1:R:132:VAL:HG22	1.85	0.57
2:M:151:CYS:HB3	2:M:156:PHE:HE2	1.70	0.57
1:F:25:ALA:O	1:F:69:THR:OG1	2.23	0.57
2:C:117:LYS:HD2	2:C:168:TRP:CZ3	2.40	0.56
2:P:133:ILE:HG12	2:P:167:THR:HG23	1.87	0.56
1:F:167:ASP:OD2	1:F:169:LYS:HE2	2.05	0.56
1:R:32:TYR:OH	3:Q:100(B):TRP:N	2.35	0.55
2:M:5:LEU:HD11	2:M:107:ILE:HD12	1.88	0.55
2:D:35:THR:HG22	2:D:131:THR:HB	1.89	0.55
1:L:46:LEU:HD11	1:L:49:TYR:HB3	1.88	0.55
2:C:97:ILE:HB	2:C:107:ILE:HD11	1.89	0.55
1:R:108:ARG:HH22	1:R:111:ALA:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:VAL:HG21	1:K:196:VAL:HG21	1.89	0.55
2:C:76:ARG:NH2	5:C:302:HOH:O	2.40	0.55
1:F:197:THR:HG22	1:F:204:PRO:HB3	1.89	0.54
2:C:19:ILE:HD13	2:C:62:LEU:HD13	1.89	0.54
1:R:147:GLN:OE1	1:R:154:LEU:HD21	2.07	0.54
1:R:142:ARG:HB2	1:R:173:TYR:CE2	2.41	0.54
1:K:136:LEU:HD13	1:K:175:LEU:HD12	1.88	0.54
3:H:64:GLN:OE1	2:C:27:GLN:NE2	2.37	0.54
1:F:167:ASP:OD2	1:F:169:LYS:HB2	2.07	0.53
1:R:13:ALA:O	1:R:106:ILE:HA	2.09	0.53
1:F:46:LEU:HD21	1:F:49:TYR:HB3	1.91	0.53
2:P:1:ASP:OD1	2:P:2:THR:N	2.41	0.53
1:R:80:PRO:HA	1:R:106:ILE:HD12	1.91	0.53
1:F:35:TRP:CE2	1:F:73:PHE:HB2	2.44	0.53
1:R:122:ASP:HA	1:R:125:LEU:HD13	1.92	0.52
3:J:19:LYS:HG3	3:J:81:GLU:HB2	1.91	0.52
1:R:49:TYR:HB2	3:Q:100(C):TYR:CE2	2.45	0.52
3:J:119:PRO:HB3	3:J:145:TYR:HB3	1.92	0.52
3:J:12:LYS:HG3	3:J:18:VAL:HB	1.92	0.52
3:Q:18:VAL:HG11	3:Q:109:VAL:HG11	1.91	0.52
1:F:36:TYR:CZ	1:F:46:LEU:HD12	2.45	0.51
1:F:32:TYR:OH	3:E:100(B):TRP:N	2.41	0.51
1:L:19:VAL:HG21	1:L:78:LEU:HD13	1.93	0.51
1:R:142:ARG:HB2	1:R:173:TYR:HE2	1.76	0.51
3:H:170:LEU:HD13	3:H:176:TYR:CZ	2.46	0.50
2:D:99:CYS:HA	2:D:105:CYS:HA	1.94	0.50
3:H:100(C):TYR:C	3:H:100(C):TYR:HD1	2.20	0.50
3:J:186:SER:HA	3:J:189:LEU:HD13	1.94	0.49
1:R:108:ARG:NH1	1:R:109:THR:OG1	2.46	0.49
3:H:143:LYS:NZ	3:H:144:ASP:OD1	2.46	0.49
1:K:136:LEU:HB2	1:K:175:LEU:HB3	1.94	0.49
2:P:18:ASN:HB3	2:P:94:SER:HB2	1.94	0.49
1:F:190:LYS:HG3	1:F:191:VAL:HG12	1.94	0.49
1:L:125:LEU:O	1:L:183:LYS:HD2	2.12	0.49
1:L:164:THR:HG23	3:H:166:PHE:CD1	2.48	0.49
3:J:151:THR:OG1	3:J:199:ASN:HB3	2.13	0.49
3:J:163:VAL:HG12	3:J:182:VAL:HB	1.94	0.49
1:L:18:ARG:O	1:F:7:SER:OG	2.30	0.48
1:R:32:TYR:HA	1:R:50:ASP:HA	1.95	0.48
1:R:197:THR:HG22	1:R:204:PRO:HB3	1.95	0.48
1:R:135:LEU:HD21	1:R:137:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:138:ASN:ND2	1:R:172:THR:OG1	2.45	0.48
3:E:63:PHE:O	3:E:67:VAL:HG12	2.13	0.48
2:M:75:ILE:HD12	2:M:123:LEU:HD23	1.95	0.48
2:C:99:CYS:HA	2:C:105:CYS:HA	1.95	0.48
2:C:133:ILE:HG12	2:C:167:THR:HG23	1.95	0.48
1:F:35:TRP:HB2	1:F:48:ILE:HB	1.96	0.48
3:H:100(C):TYR:C	3:H:100(C):TYR:CD1	2.91	0.48
2:C:59:SER:OG	2:C:62:LEU:O	2.22	0.48
3:Q:154:TRP:CH2	3:Q:196:CYS:HB3	2.47	0.48
1:R:163:VAL:HG22	1:R:175:LEU:HD12	1.96	0.48
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.96	0.47
2:D:74:VAL:HG13	2:D:90:GLN:HB3	1.96	0.47
1:R:53:ASN:OD1	1:R:53:ASN:N	2.47	0.47
1:F:83:ILE:O	1:F:83:ILE:HG13	2.13	0.46
1:F:186:TYR:O	1:F:192:TYR:OH	2.31	0.46
3:E:117:LYS:NZ	3:E:144:ASP:HB3	2.30	0.46
3:H:200:HIS:ND1	3:H:203:SER:OG	2.34	0.46
2:P:75:ILE:HG22	2:P:89:VAL:HG22	1.97	0.46
1:K:149:LYS:HE3	1:K:152:ASN:HA	1.97	0.46
1:L:35:TRP:CE2	1:L:73:PHE:HB2	2.50	0.46
1:L:83:ILE:O	1:L:83:ILE:HG13	2.15	0.46
2:D:50:ARG:HH11	2:D:78:GLU:CD	2.23	0.46
2:P:51:CYS:O	2:P:52:GLN:HG2	2.16	0.46
1:R:137:ASN:ND2	3:Q:183:THR:HG21	2.30	0.46
2:C:74:VAL:HG11	2:C:76:ARG:HH11	1.81	0.46
1:R:151:ASP:CG	1:R:189:HIS:HB3	2.41	0.46
1:K:108:ARG:HD2	1:K:170:ASP:O	2.17	0.45
1:F:140:TYR:CG	1:F:141:PRO:HA	2.51	0.45
1:K:35:TRP:CE2	1:K:73:PHE:HB2	2.52	0.45
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.99	0.45
2:D:6:PRO:HD2	2:D:159:ALA:HB3	1.98	0.45
3:Q:163:VAL:HG12	3:Q:182:VAL:HB	1.99	0.45
2:P:11:PRO:HG2	2:P:105:CYS:SG	2.56	0.45
2:M:75:ILE:HG22	2:M:89:VAL:HG22	1.98	0.45
3:Q:159:LEU:HD21	3:Q:182:VAL:HG21	1.97	0.45
1:K:115:VAL:HA	1:K:135:LEU:O	2.16	0.45
1:L:117:ILE:HD13	1:L:194:CYS:SG	2.57	0.45
2:C:38:PHE:CE1	2:C:123:LEU:HD13	2.51	0.45
3:E:47:TRP:CZ2	3:E:49:GLY:HA2	2.52	0.45
2:M:18:ASN:HB3	2:M:94:SER:HB2	1.98	0.45
1:F:19:VAL:HG21	1:F:78:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:47:TRP:CZ2	3:J:49:GLY:HA2	2.52	0.44
2:D:5:LEU:HD21	2:D:163:LEU:HG	1.99	0.44
3:E:72:ASP:OD1	3:E:74:SER:OG	2.32	0.44
1:L:120:PRO:HB2	1:L:125:LEU:HD21	1.98	0.44
1:L:140:TYR:CG	1:L:141:PRO:HA	2.52	0.44
1:K:105:GLU:OE1	1:K:173:TYR:OH	2.34	0.44
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.51	0.44
3:H:143:LYS:HZ2	3:H:144:ASP:CG	2.25	0.44
1:R:122:ASP:O	1:R:126:LYS:HE2	2.17	0.44
1:F:134:CYS:HB2	1:F:148:TRP:CZ2	2.53	0.44
3:E:154:TRP:CZ3	3:E:196:CYS:HB3	2.52	0.44
3:J:200:HIS:CD2	3:J:202:PRO:HD2	2.53	0.44
2:C:37:ILE:HD13	2:C:135:LYS:NZ	2.32	0.44
2:D:80:TRP:CD2	2:D:126:GLN:HG2	2.52	0.44
3:H:85:ASP:OD1	3:H:85:ASP:N	2.49	0.44
3:J:148:GLU:OE2	3:J:168:ALA:HB3	2.18	0.44
1:L:36:TYR:HE1	1:L:89:GLN:HB3	1.83	0.44
1:K:122:ASP:HA	1:K:125:LEU:HB2	2.00	0.44
3:H:132:SER:HB3	3:H:133:GLY:H	1.53	0.44
3:J:200:HIS:ND1	3:J:203:SER:OG	2.42	0.44
3:H:83:ARG:O	3:H:111:VAL:HG21	2.17	0.44
1:R:145:LYS:HE2	1:R:147:GLN:HE21	1.83	0.44
3:Q:10:GLU:OE1	5:Q:301:HOH:O	2.21	0.44
2:P:38:PHE:CE1	2:P:123:LEU:HD13	2.53	0.44
1:F:69:THR:HG23	1:F:70:ASP:OD1	2.18	0.44
1:F:169:LYS:HE2	1:F:169:LYS:HB2	1.74	0.44
3:E:40:ALA:HB3	3:E:43:GLN:HB2	2.00	0.44
2:M:60:THR:O	2:M:62:LEU:N	2.47	0.43
2:D:12:PRO:HB2	2:D:14:HIS:CD2	2.52	0.43
1:F:124:GLN:O	1:F:127:SER:OG	2.25	0.43
2:C:22:LEU:HD21	2:C:112:TRP:CH2	2.53	0.43
1:R:125:LEU:O	1:R:183:LYS:HD2	2.19	0.43
1:K:4:MET:HE1	1:K:90:GLN:HB3	2.01	0.43
2:M:23:ILE:HG13	2:M:41:SER:HB2	2.01	0.43
1:K:4:MET:CE	1:K:90:GLN:HB3	2.48	0.43
3:Q:148:GLU:HG3	3:Q:176:TYR:CE2	2.54	0.43
2:D:60:THR:O	2:D:62:LEU:N	2.48	0.43
1:R:121:SER:HB2	1:R:123:GLU:OE1	2.18	0.43
3:Q:47:TRP:CZ2	3:Q:49:GLY:HA2	2.53	0.43
1:L:106:ILE:H	1:L:166:GLN:HE22	1.65	0.42
2:P:97:ILE:HD12	2:P:107:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:119:PRO:HB3	3:E:145:TYR:HB3	2.01	0.42
1:K:42:LYS:HD2	1:K:42:LYS:N	2.35	0.42
3:Q:154:TRP:CZ3	3:Q:196:CYS:HB3	2.54	0.42
3:J:85:ASP:OD1	3:J:85:ASP:N	2.51	0.42
2:D:51:CYS:O	2:D:52:GLN:HG2	2.19	0.42
3:J:209:LYS:HA	3:J:209:LYS:HD3	1.93	0.42
2:C:38:PHE:CZ	2:C:123:LEU:HD13	2.54	0.42
2:C:47:ASP:OD2	2:C:86:SER:OG	2.36	0.42
1:F:150:VAL:HG22	1:F:192:TYR:CD2	2.54	0.42
1:L:83:ILE:HG22	1:L:106:ILE:HG13	2.01	0.42
2:D:143:GLU:H	2:D:143:GLU:HG2	1.58	0.42
3:Q:2:VAL:HG23	3:Q:102:TYR:CE1	2.55	0.42
3:Q:171:GLN:NE2	3:Q:177:SER:HB3	2.34	0.42
1:F:36:TYR:HE1	1:F:89:GLN:HB3	1.85	0.42
3:H:63:PHE:O	3:H:67:VAL:HG12	2.19	0.42
1:F:28:ASP:OD1	1:F:68:GLY:HA2	2.19	0.42
1:F:50:ASP:O	1:F:52:SER:N	2.44	0.42
1:K:108:ARG:NE	1:K:109:THR:O	2.45	0.41
2:M:68:LEU:HD23	2:M:68:LEU:HA	1.90	0.41
2:M:99:CYS:HA	2:M:105:CYS:HA	2.01	0.41
1:R:14:SER:N	1:R:17:ASP:OD1	2.53	0.41
2:P:109:ARG:HE	2:P:109:ARG:HB2	1.68	0.41
2:P:142:PRO:HA	2:P:145:VAL:HG12	2.02	0.41
3:E:116:THR:HG22	3:E:203:SER:OG	2.21	0.41
1:K:113:PRO:HD2	1:K:201:LEU:CD1	2.51	0.41
2:C:117:LYS:HD2	2:C:168:TRP:HZ3	1.85	0.41
2:D:11:PRO:HA	2:D:12:PRO:HD3	1.94	0.41
1:R:154:LEU:HD22	1:R:154:LEU:HA	1.88	0.41
3:J:63:PHE:O	3:J:67:VAL:HG12	2.21	0.41
2:D:40:PRO:HG3	2:D:164:PHE:CE2	2.55	0.41
1:R:14:SER:O	1:R:17:ASP:OD1	2.39	0.41
1:R:201:LEU:HD23	1:R:201:LEU:HA	1.87	0.41
3:E:170:LEU:HD13	3:E:176:TYR:CZ	2.56	0.41
1:R:154:LEU:HD13	1:R:155:GLN:N	2.36	0.41
2:P:121:SER:O	2:P:125:GLU:HG3	2.21	0.41
1:R:50:ASP:O	1:R:52:SER:N	2.46	0.41
2:P:60:THR:O	2:P:62:LEU:N	2.50	0.41
2:M:143:GLU:H	2:M:143:GLU:HG3	1.52	0.41
1:R:32:TYR:CZ	3:Q:100(A):GLY:HA3	2.56	0.41
1:R:145:LYS:HE2	1:R:147:GLN:NE2	2.36	0.41
2:P:3:ILE:HD11	2:P:109:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:TYR:CD2	3:E:94:ARG:HG2	2.56	0.41
3:J:82(B):ARG:HD3	3:E:133:GLY:C	2.45	0.41
3:H:18:VAL:HG11	3:H:109:VAL:HG11	2.02	0.41
1:R:4:MET:HE1	1:R:33:LEU:HD11	2.01	0.41
1:R:83:ILE:HD11	1:R:168:SER:HA	2.03	0.41
3:Q:194:TYR:C	3:Q:195:ILE:HD12	2.45	0.41
3:Q:201:LYS:HE2	3:Q:201:LYS:HB3	1.80	0.41
3:Q:214:LYS:HE2	3:Q:214:LYS:HB2	1.84	0.41
1:R:15:VAL:HG22	1:R:80:PRO:HD3	2.03	0.41
2:P:47:ASP:OD2	2:P:86:SER:OG	2.39	0.41
2:P:143:GLU:H	2:P:143:GLU:HG2	1.54	0.41
1:F:190:LYS:HG3	1:F:191:VAL:N	2.36	0.41
2:M:85:LYS:HA	2:M:85:LYS:HD3	1.87	0.40
1:R:136:LEU:O	1:R:174:SER:HA	2.21	0.40
1:R:35:TRP:CE2	1:R:73:PHE:HB2	2.56	0.40
1:R:150:VAL:HG22	1:R:192:TYR:CD2	2.56	0.40
2:M:122:LYS:N	2:M:122:LYS:HD2	2.35	0.40
1:L:176:SER:HB2	3:H:166:PHE:CE2	2.56	0.40
2:C:148:SER:HB3	2:C:155:PHE:CE2	2.55	0.40
2:D:11:PRO:HG2	2:D:105:CYS:SG	2.61	0.40
1:R:30:ASN:HB3	1:R:31:ASN:H	1.77	0.40
3:Q:66:ARG:HB3	3:Q:82(A):SER:O	2.22	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	F	206/210 (98%)	199 (97%)	6 (3%)	1 (0%)	25 56
1	K	206/210 (98%)	199 (97%)	6 (3%)	1 (0%)	25 56
1	L	206/210 (98%)	198 (96%)	7 (3%)	1 (0%)	25 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	206/210 (98%)	198 (96%)	8 (4%)	0	100	100
2	C	167/184 (91%)	159 (95%)	8 (5%)	0	100	100
2	D	167/184 (91%)	159 (95%)	8 (5%)	0	100	100
2	M	167/184 (91%)	158 (95%)	9 (5%)	0	100	100
2	P	167/184 (91%)	160 (96%)	7 (4%)	0	100	100
3	E	215/224 (96%)	210 (98%)	5 (2%)	0	100	100
3	H	215/224 (96%)	211 (98%)	4 (2%)	0	100	100
3	J	215/224 (96%)	211 (98%)	4 (2%)	0	100	100
3	Q	215/224 (96%)	210 (98%)	5 (2%)	0	100	100
All	All	2352/2472 (95%)	2272 (97%)	77 (3%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	189	HIS
1	K	188	LYS
1	F	138	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	F	183/185 (99%)	183 (100%)	0	100	100
1	K	183/185 (99%)	182 (100%)	1 (0%)	86	95
1	L	183/185 (99%)	181 (99%)	2 (1%)	70	90
1	R	183/185 (99%)	181 (99%)	2 (1%)	70	90
2	C	139/151 (92%)	137 (99%)	2 (1%)	62	87
2	D	139/151 (92%)	137 (99%)	2 (1%)	62	87
2	M	139/151 (92%)	137 (99%)	2 (1%)	62	87
2	P	139/151 (92%)	136 (98%)	3 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	183/188 (97%)	180 (98%)	3 (2%)	58	85
3	H	183/188 (97%)	180 (98%)	3 (2%)	58	85
3	J	183/188 (97%)	181 (99%)	2 (1%)	70	90
3	Q	183/188 (97%)	181 (99%)	2 (1%)	70	90
All	All	2020/2096 (96%)	1996 (99%)	24 (1%)	67	89

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	2	ILE
2	M	22	LEU
2	M	143	GLU
3	J	135	THR
3	J	205	THR
1	L	5	THR
1	L	56	THR
3	H	132	SER
3	H	135	THR
3	H	191	THR
2	C	51	CYS
2	C	143	GLU
2	D	51	CYS
2	D	70	GLU
1	R	22	THR
1	R	164	THR
3	Q	28	THR
3	Q	111	VAL
2	P	51	CYS
2	P	81	THR
2	P	154	GLU
3	E	28	THR
3	E	111	VAL
3	E	211	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	152	ASN
2	M	147	HIS
3	J	43	GLN

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Mol	Chain	Res	Type
1	L	24	GLN
1	L	155	GLN
1	L	166	GLN
3	H	43	GLN
3	H	52	ASN
2	C	14	HIS
2	C	162	GLN
1	R	160	GLN
1	R	166	GLN
3	Q	43	GLN
3	Q	97	GLN
3	Q	164	HIS
3	Q	171	GLN
2	P	52	GLN
1	F	90	GLN
3	E	53	ASN
3	E	61	GLN
3	E	199	ASN

### 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](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	P	203	2	14,14,15	0.70	0	17,19,21	0.84	0
4	NAG	D	201	2	14,14,15	0.72	0	17,19,21	1.20	1 (5%)
4	NAG	M	203	2	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
4	NAG	D	202	2	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
4	NAG	P	201	2	14,14,15	0.69	0	17,19,21	1.10	1 (5%)
4	NAG	P	202	2	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
4	NAG	C	202	2	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
4	NAG	C	203	2	14,14,15	0.66	0	17,19,21	0.80	0
4	NAG	D	203	2	14,14,15	0.73	0	17,19,21	0.86	0
4	NAG	M	201	2	14,14,15	0.70	0	17,19,21	1.08	1 (5%)
4	NAG	C	201	2	14,14,15	0.73	0	17,19,21	1.14	1 (5%)
4	NAG	M	202	2	14,14,15	0.71	0	17,19,21	0.98	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	P	203	2	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2	-	2/6/23/26	0/1/1/1
4	NAG	M	203	2	-	0/6/23/26	0/1/1/1
4	NAG	D	202	2	-	0/6/23/26	0/1/1/1
4	NAG	P	201	2	-	2/6/23/26	0/1/1/1
4	NAG	P	202	2	-	2/6/23/26	0/1/1/1
4	NAG	C	202	2	-	0/6/23/26	0/1/1/1
4	NAG	C	203	2	-	0/6/23/26	0/1/1/1
4	NAG	D	203	2	-	0/6/23/26	0/1/1/1
4	NAG	M	201	2	-	2/6/23/26	0/1/1/1
4	NAG	C	201	2	-	2/6/23/26	0/1/1/1
4	NAG	M	202	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	NAG	C2-N2-C7	3.20	127.19	122.90
4	D	201	NAG	C2-N2-C7	3.14	127.11	122.90
4	P	201	NAG	C2-N2-C7	2.98	126.89	122.90
4	M	201	NAG	C2-N2-C7	2.85	126.73	122.90
4	M	202	NAG	C1-O5-C5	2.68	115.78	112.19
4	C	202	NAG	C1-O5-C5	2.42	115.42	112.19
4	D	202	NAG	C1-O5-C5	2.39	115.38	112.19
4	M	203	NAG	C1-O5-C5	2.30	115.27	112.19
4	P	202	NAG	C1-O5-C5	2.24	115.19	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	202	NAG	O5-C5-C6-O6
4	P	202	NAG	C4-C5-C6-O6
4	P	201	NAG	C1-C2-N2-C7
4	M	201	NAG	C3-C2-N2-C7
4	C	201	NAG	C3-C2-N2-C7
4	D	201	NAG	C3-C2-N2-C7
4	P	201	NAG	C3-C2-N2-C7
4	M	201	NAG	C1-C2-N2-C7
4	C	201	NAG	C1-C2-N2-C7
4	D	201	NAG	C1-C2-N2-C7

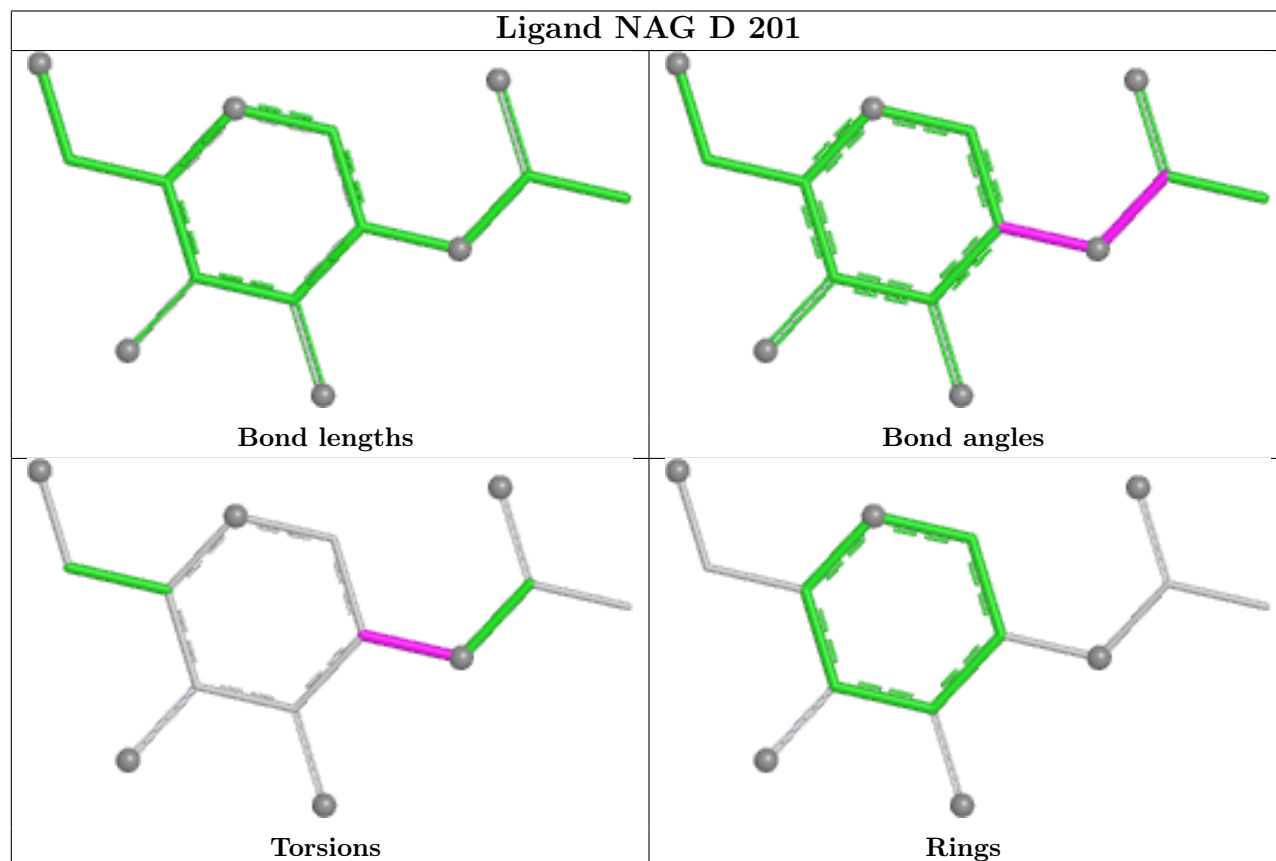
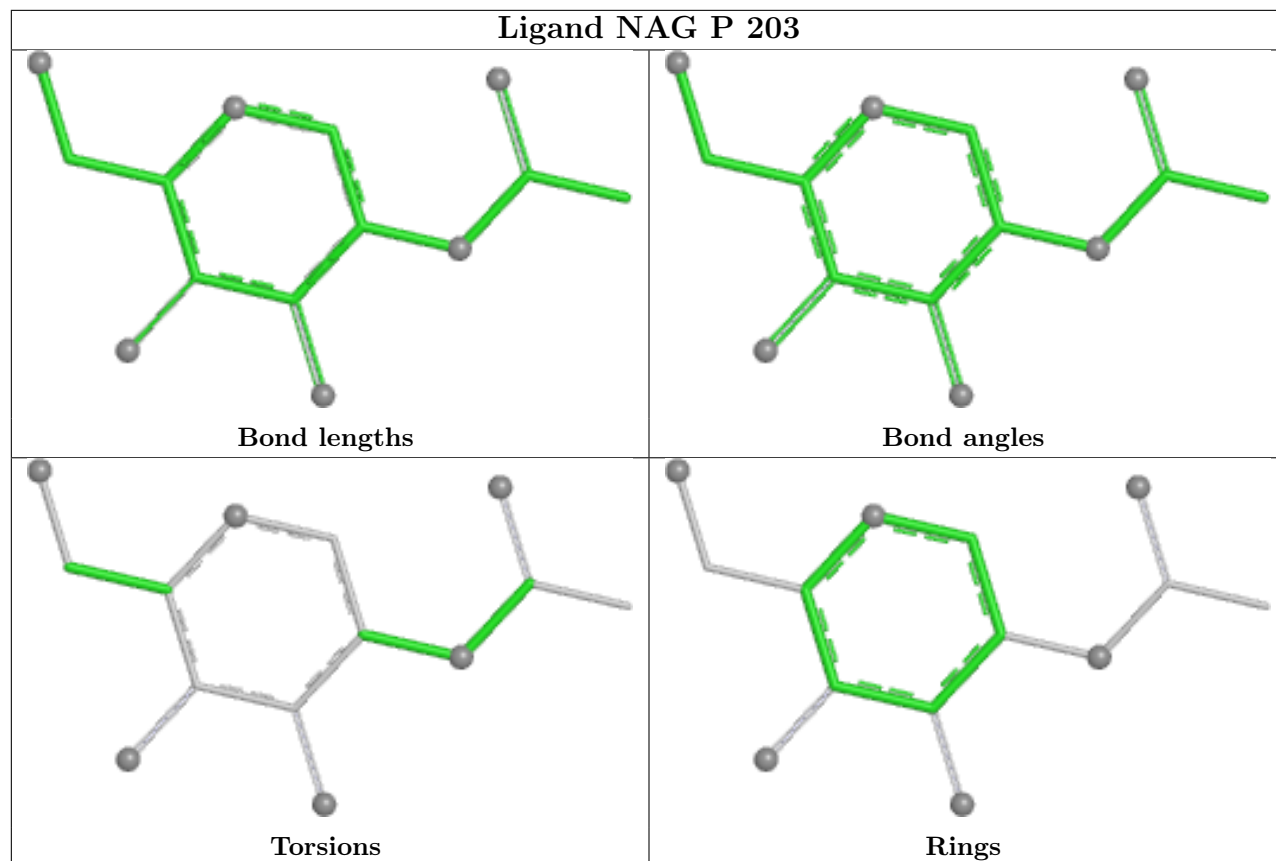
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	202	NAG	1	0
4	P	202	NAG	1	0

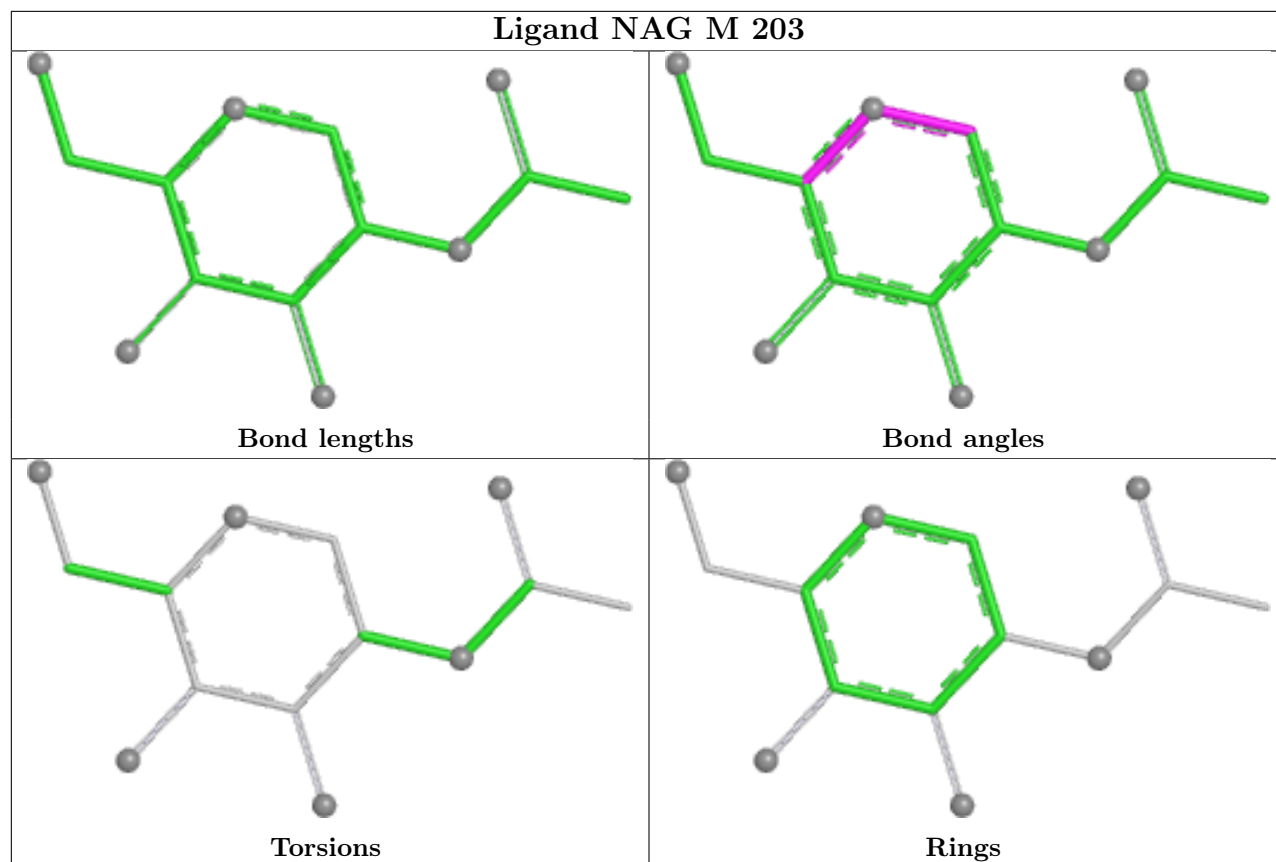
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

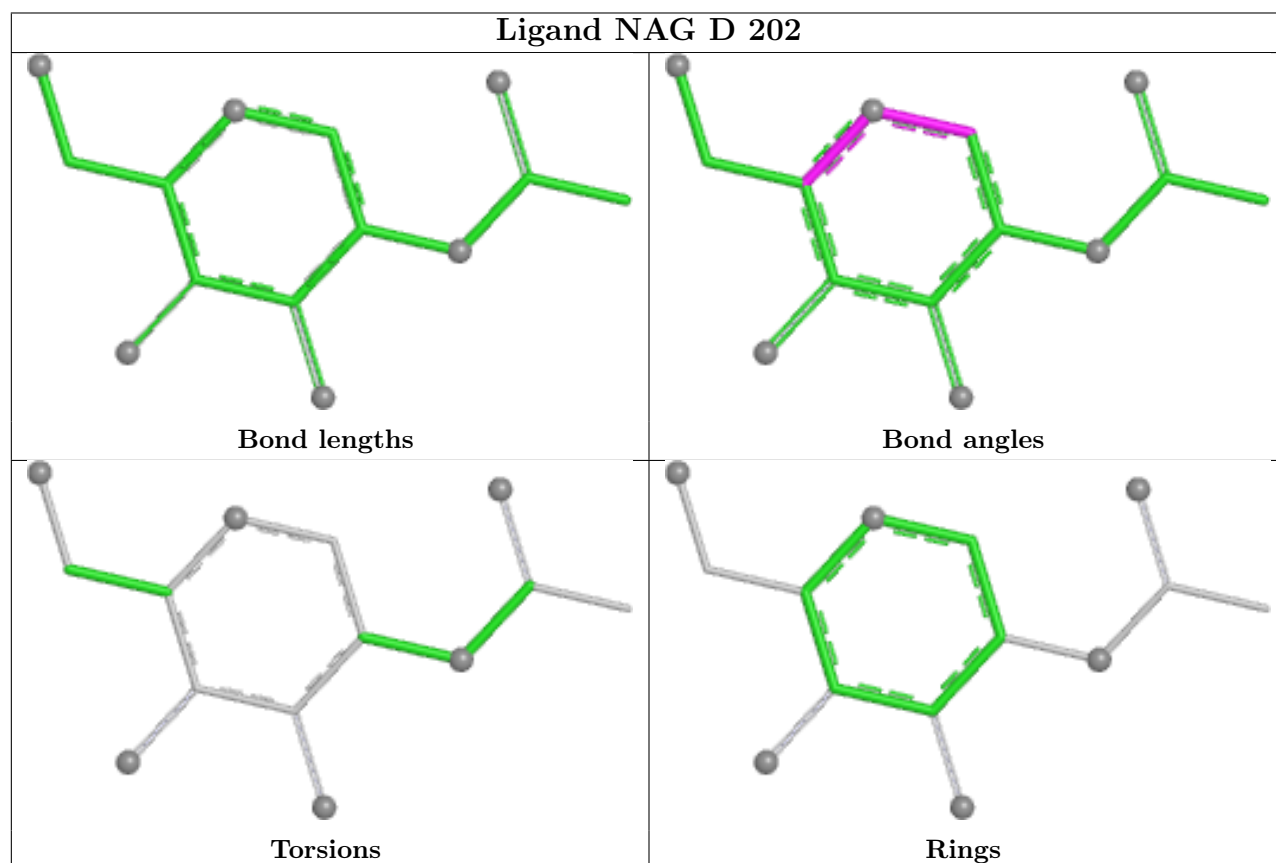


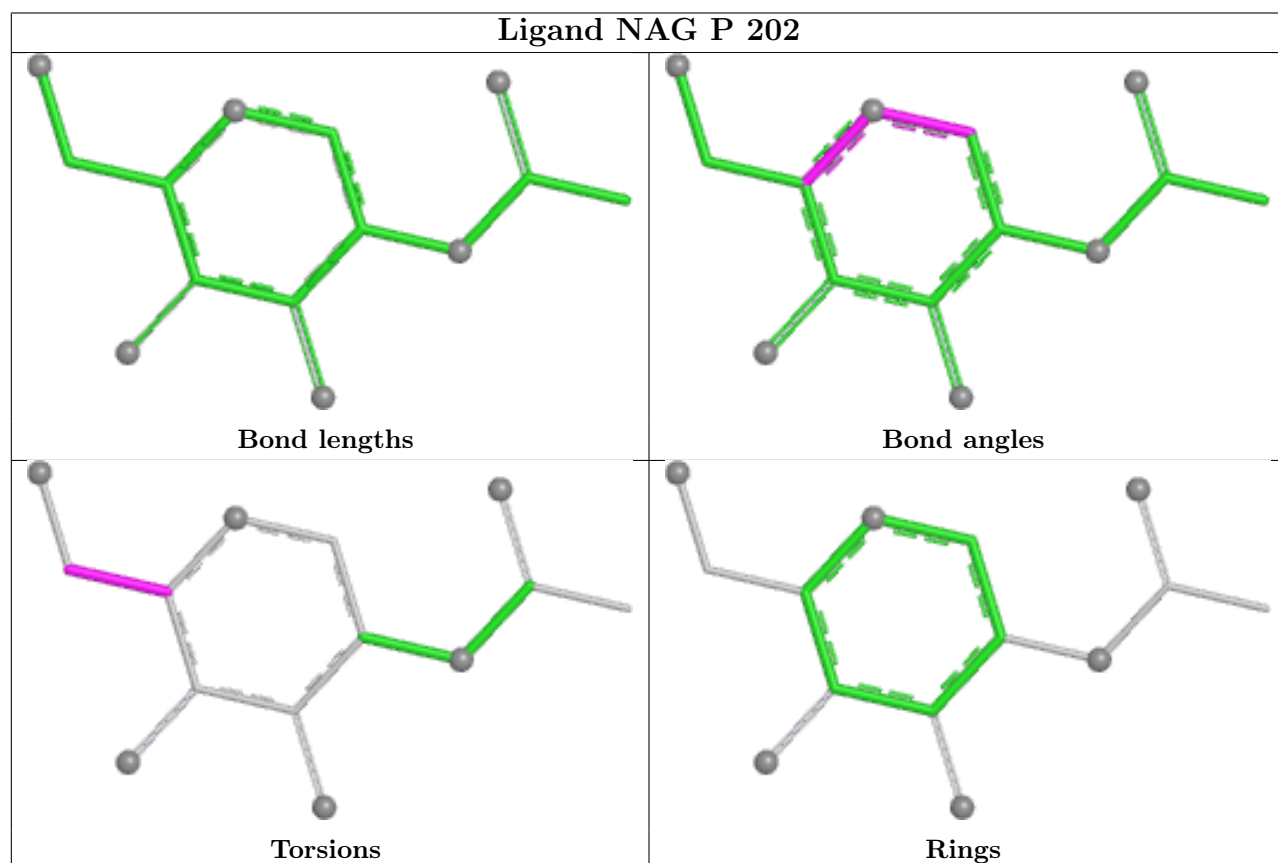
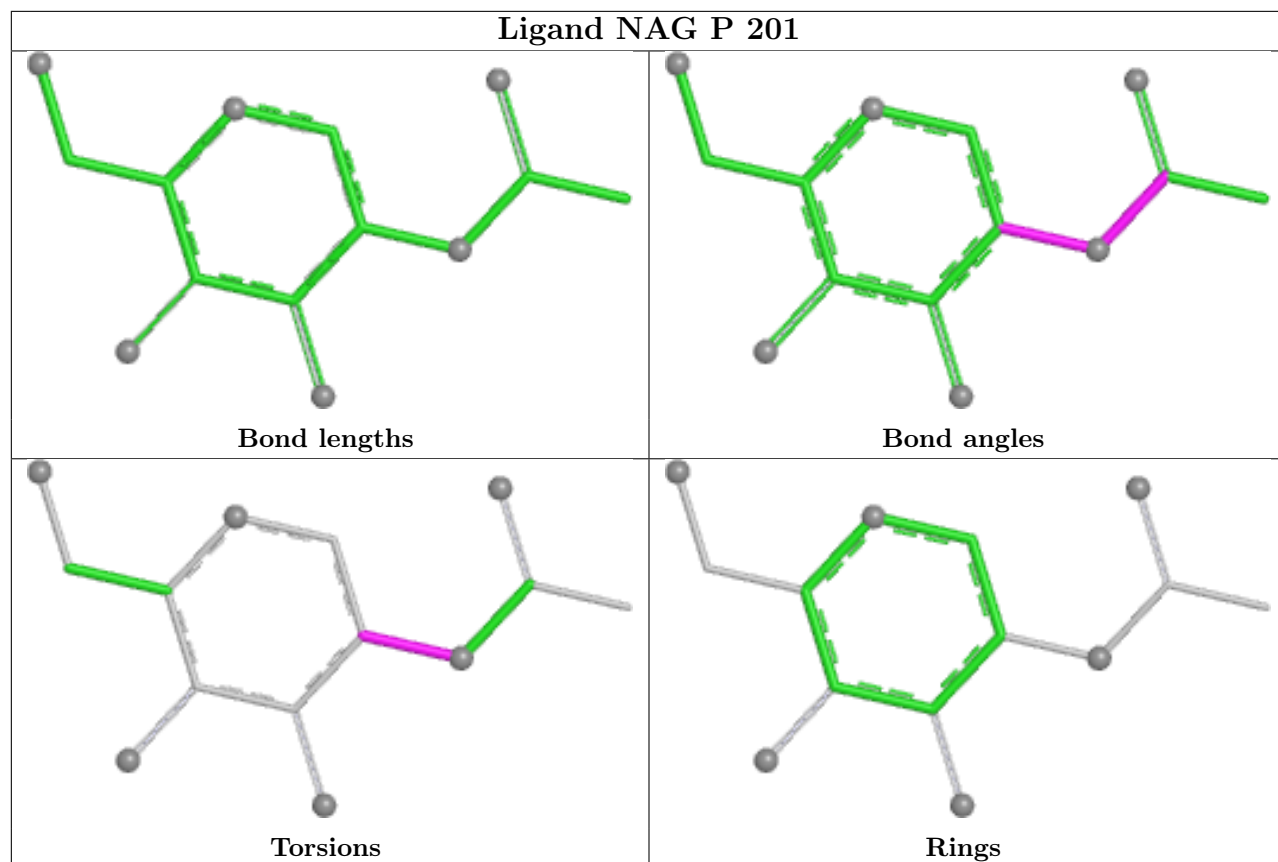


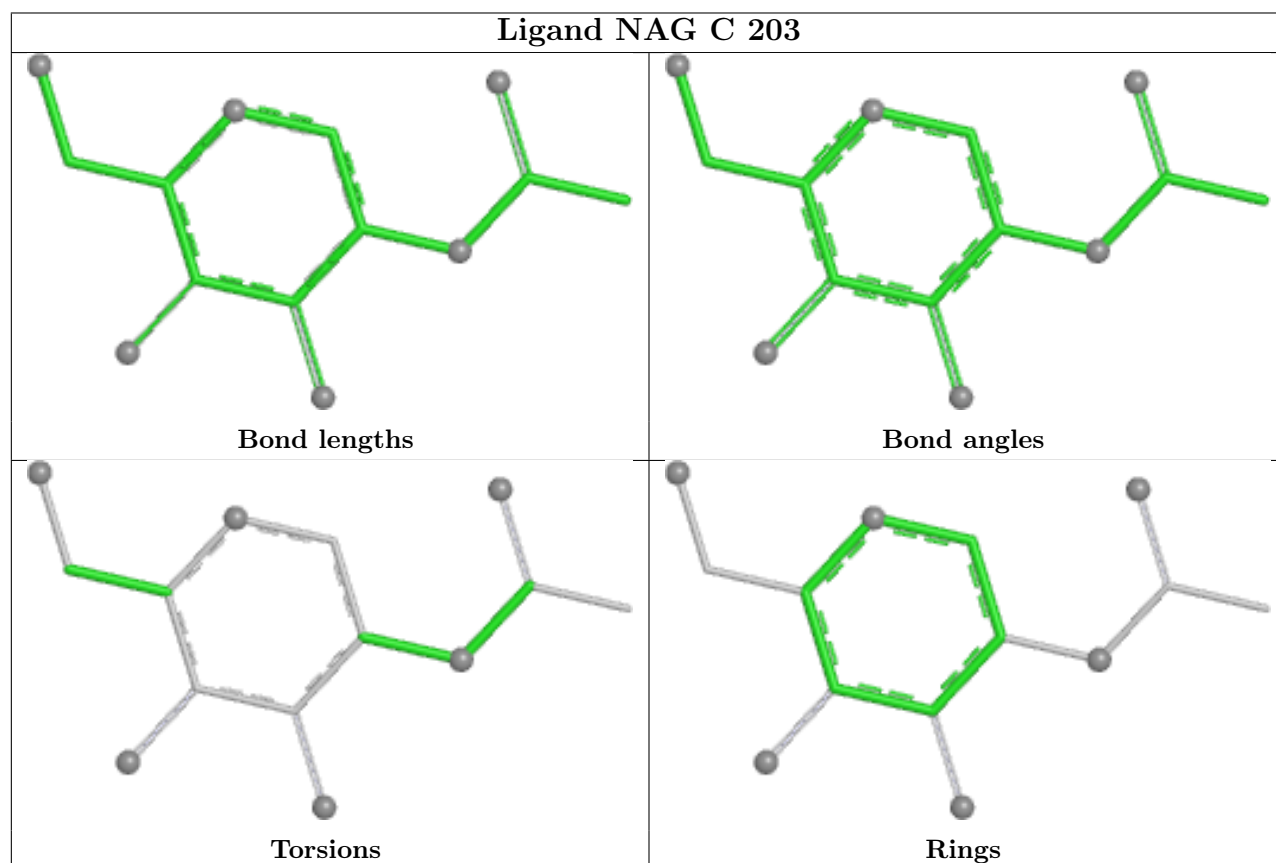
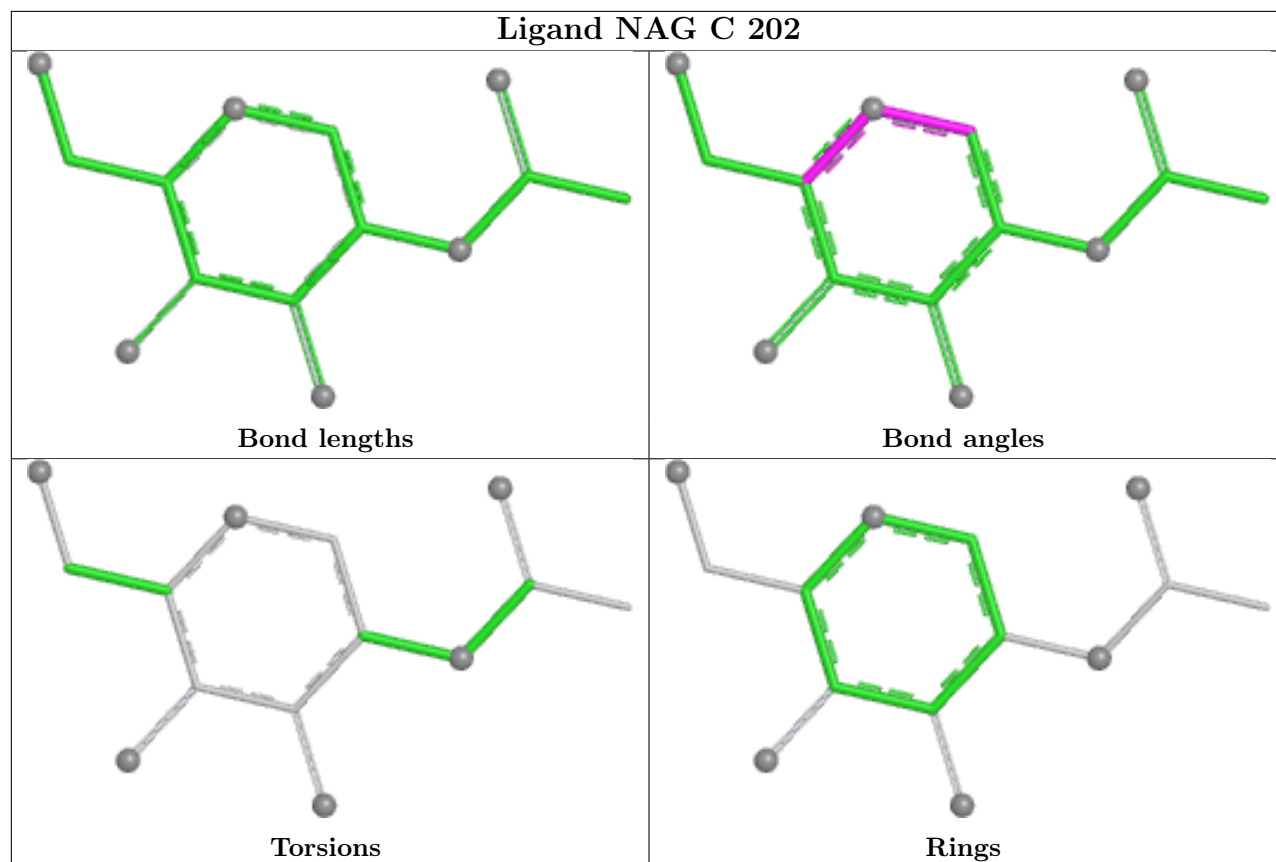
## Ligand NAG M 203

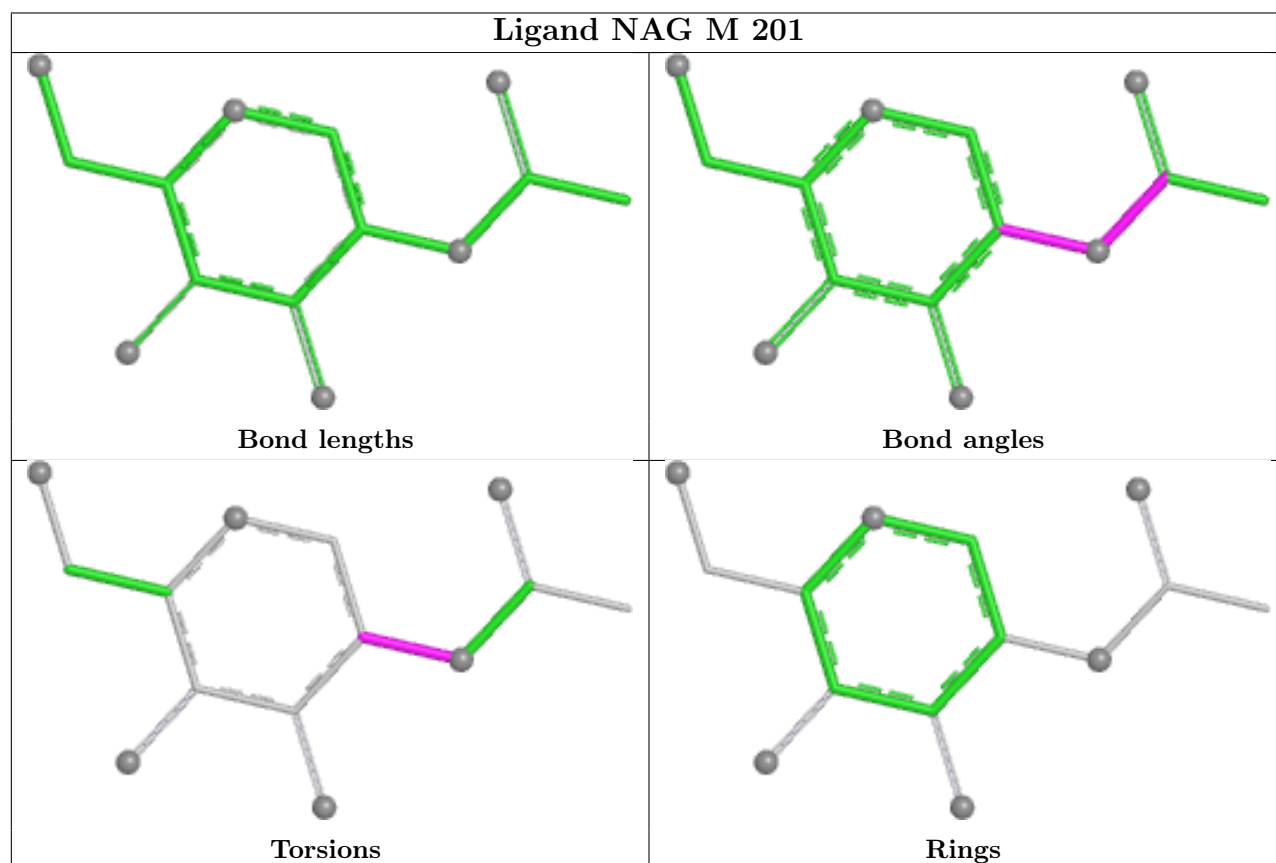
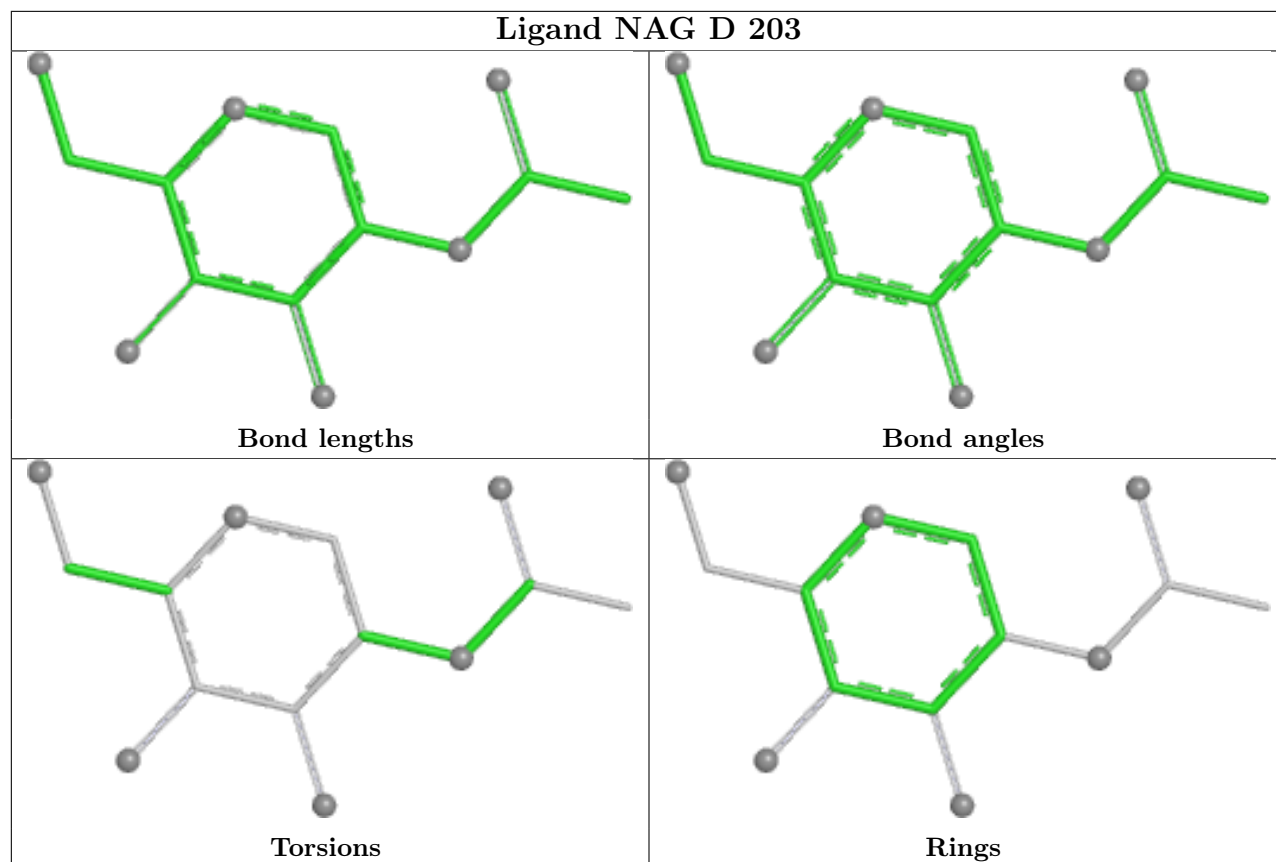


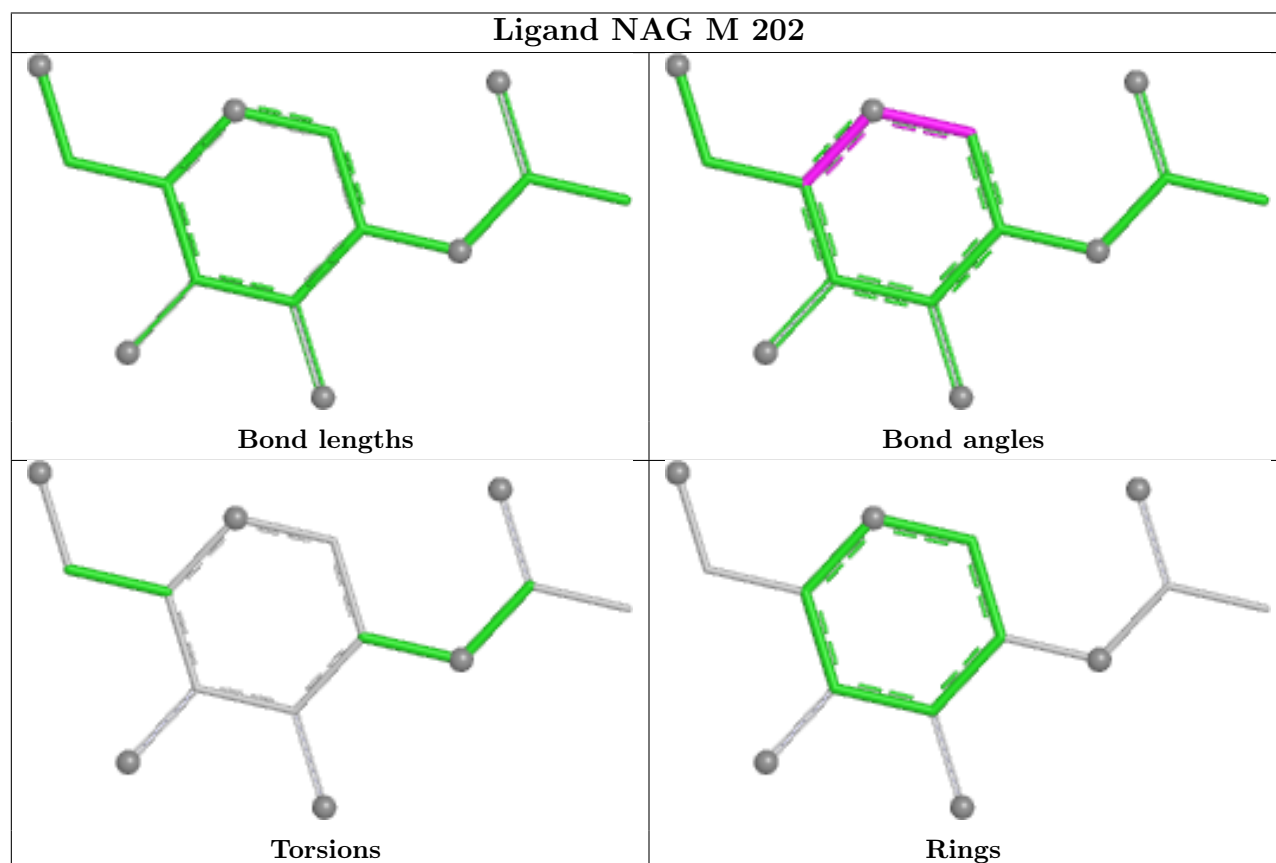
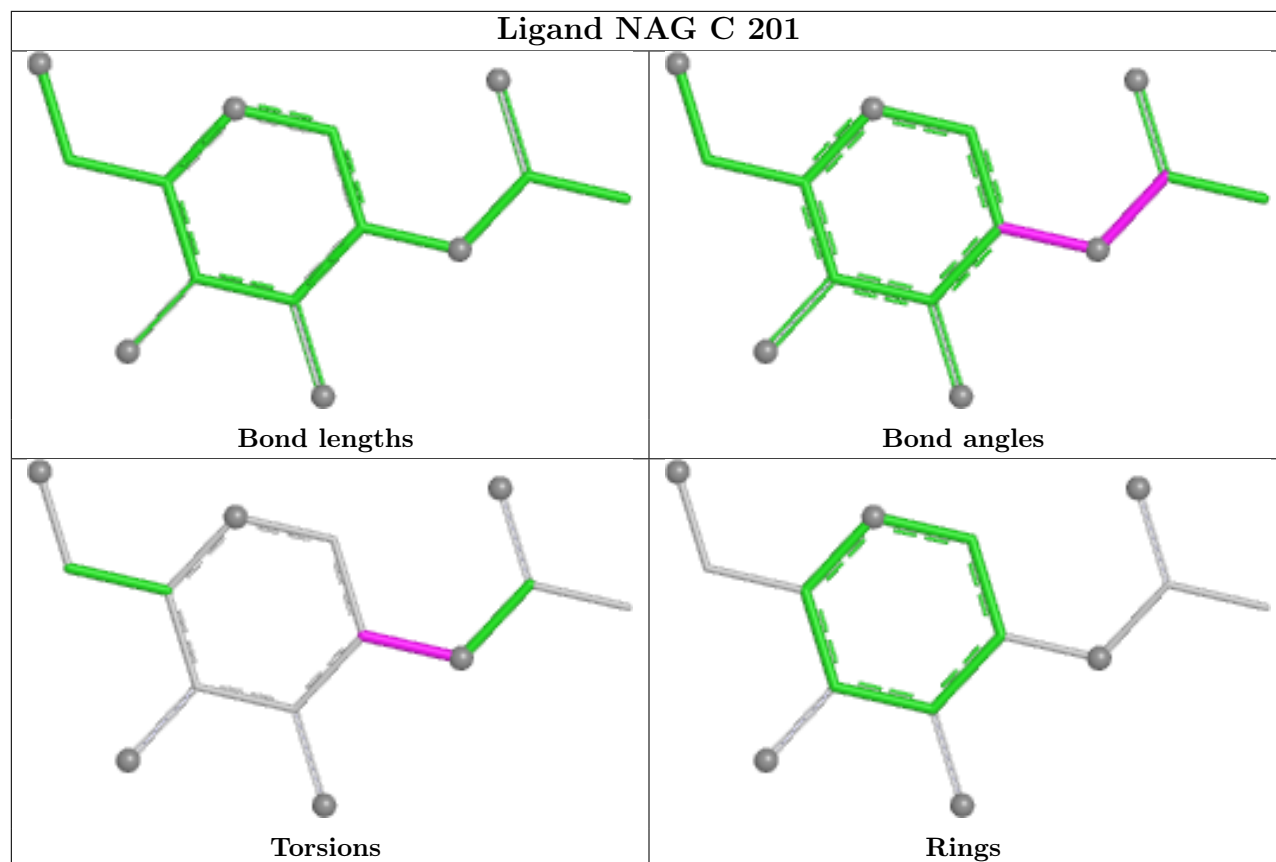
## Ligand NAG D 202











## 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, 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	F	208/210 (99%)	-0.03	2 (0%) 79 73	36, 63, 106, 129	0
1	K	208/210 (99%)	0.08	2 (0%) 79 73	47, 69, 89, 97	0
1	L	208/210 (99%)	0.00	7 (3%) 48 40	35, 62, 107, 142	0
1	R	208/210 (99%)	0.58	9 (4%) 40 32	55, 85, 111, 149	0
2	C	169/184 (91%)	-0.27	0 100 100	38, 54, 84, 124	0
2	D	169/184 (91%)	-0.17	2 (1%) 76 69	35, 54, 82, 120	0
2	M	169/184 (91%)	-0.12	1 (0%) 85 81	41, 61, 87, 116	0
2	P	169/184 (91%)	0.16	5 (2%) 52 44	39, 67, 100, 119	0
3	E	219/224 (97%)	0.04	4 (1%) 67 60	36, 65, 100, 129	0
3	H	219/224 (97%)	-0.17	3 (1%) 73 66	33, 57, 99, 131	0
3	J	219/224 (97%)	-0.31	2 (0%) 81 75	39, 59, 90, 107	0
3	Q	219/224 (97%)	0.17	8 (3%) 45 37	41, 69, 115, 136	0
All	All	2384/2472 (96%)	0.00	45 (1%) 66 58	33, 64, 103, 149	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	2	ILE	3.6
1	R	32	TYR	3.3
1	F	32	TYR	3.3
3	E	146	PHE	3.2
1	L	32	TYR	3.1
1	R	2	ILE	3.0
3	Q	189	LEU	3.0
2	D	169	PHE	3.0
1	K	189	HIS	2.9
1	R	189	HIS	2.9
1	R	51	ALA	2.8

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*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Q	100(C)	TYR	2.8
3	E	30	THR	2.8
2	P	152	GLY	2.8
1	R	137	ASN	2.6
2	P	14	HIS	2.6
3	Q	212	GLU	2.6
3	E	147	PRO	2.6
3	H	140	CYS	2.5
2	P	154	GLU	2.5
1	L	184	ALA	2.5
1	R	12	SER	2.5
1	L	161	GLU	2.4
2	P	143	GLU	2.4
3	Q	190	GLY	2.3
2	P	104	HIS	2.3
3	H	30	THR	2.3
3	E	214	LYS	2.3
3	J	164	HIS	2.3
1	R	47	LEU	2.3
1	R	23	CYS	2.3
1	L	90	GLN	2.3
1	L	212	GLY	2.3
3	Q	164	HIS	2.2
2	M	34	ASN	2.2
1	F	23	CYS	2.2
3	Q	162	GLY	2.1
3	Q	99	SER	2.1
3	Q	127	SER	2.1
1	R	71	PHE	2.1
1	L	189	HIS	2.1
1	L	188	LYS	2.1
2	D	104	HIS	2.0
3	J	30	THR	2.0
3	H	1	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

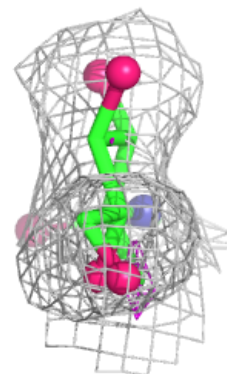
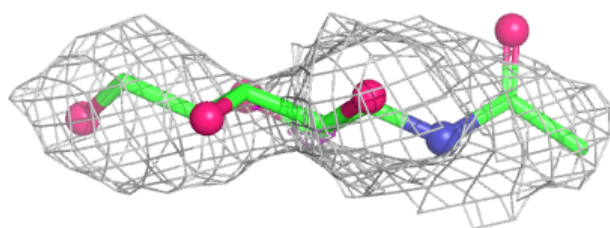
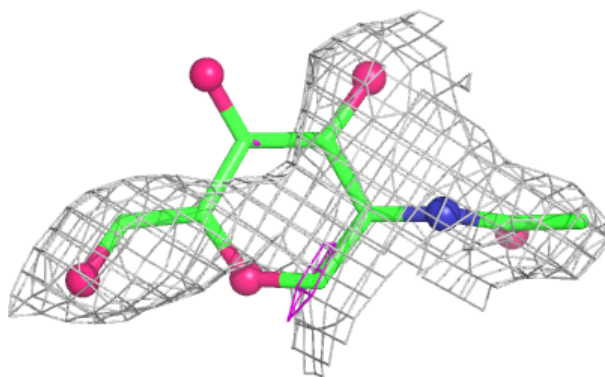
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	P	203	14/15	0.44	0.16	76,102,119,120	0
4	NAG	C	203	14/15	0.50	0.17	82,106,116,117	0
4	NAG	D	203	14/15	0.57	0.17	94,111,121,126	0
4	NAG	D	201	14/15	0.70	0.10	71,93,106,108	0
4	NAG	P	201	14/15	0.74	0.13	80,96,109,114	0
4	NAG	M	203	14/15	0.81	0.10	71,85,91,91	0
4	NAG	M	201	14/15	0.83	0.12	73,96,106,110	0
4	NAG	C	202	14/15	0.87	0.11	58,72,83,93	0
4	NAG	C	201	14/15	0.88	0.09	70,77,92,93	0
4	NAG	P	202	14/15	0.90	0.10	77,81,94,97	0
4	NAG	M	202	14/15	0.91	0.10	55,63,70,78	0
4	NAG	D	202	14/15	0.94	0.07	50,59,65,68	0

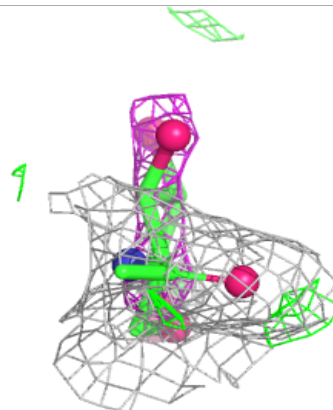
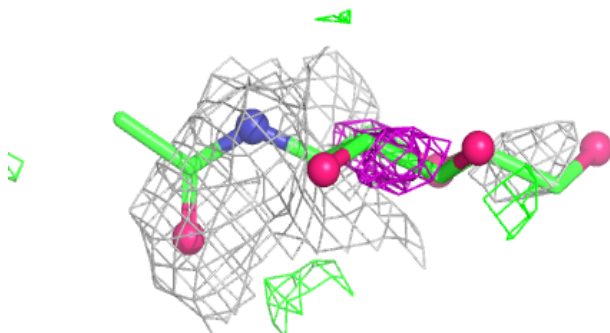
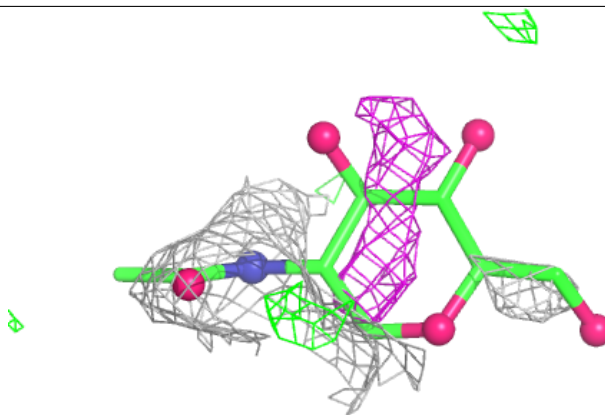
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAG P 203:**

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

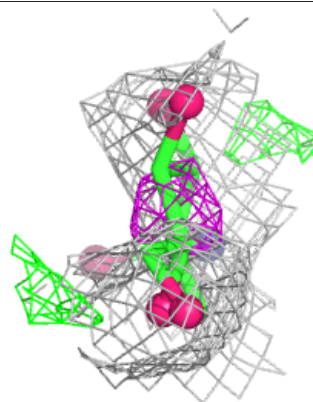
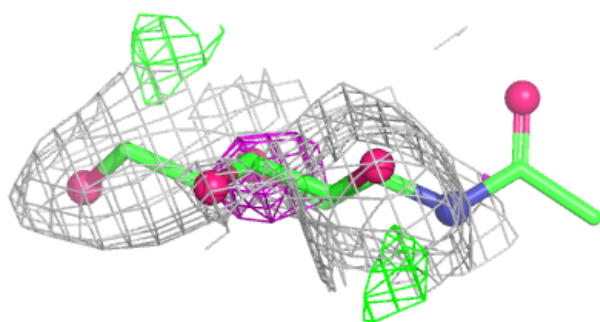
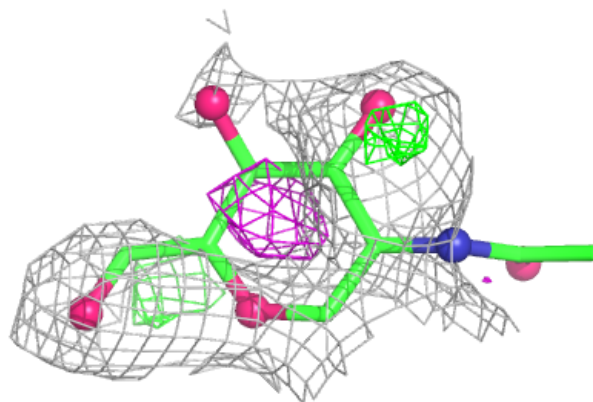
**Electron density around NAG C 203:**

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and green (positive)

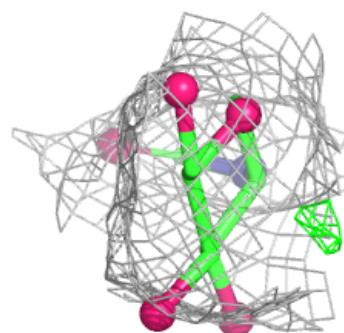
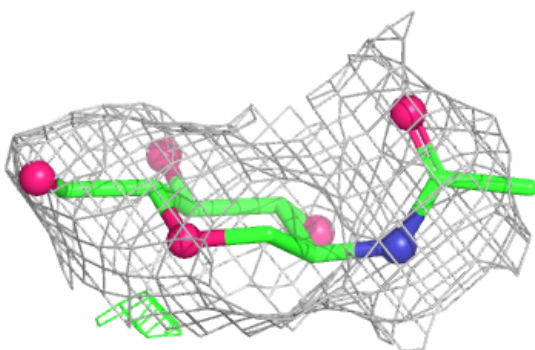
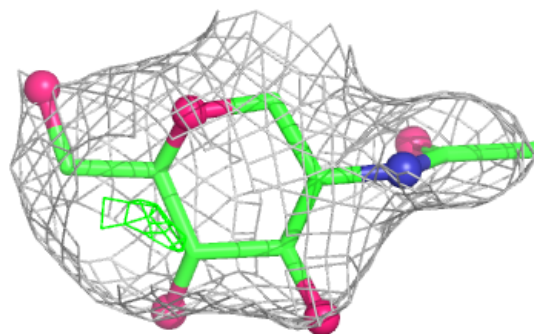


**Electron density around NAG D 203:**

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

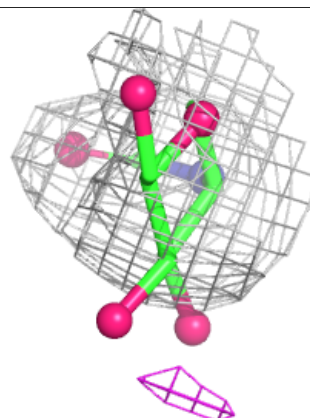
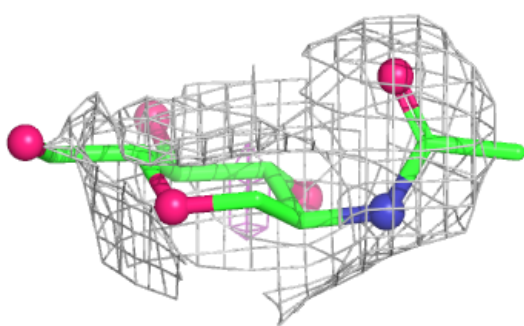
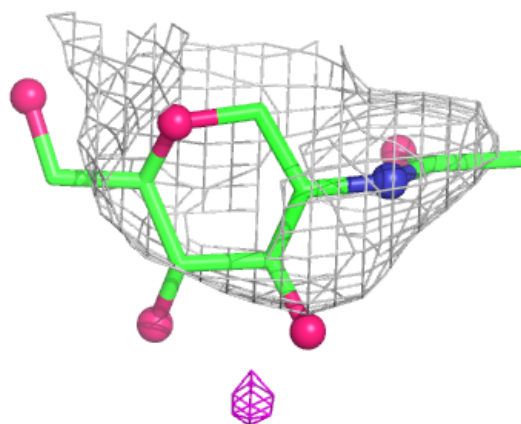
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and green (positive)

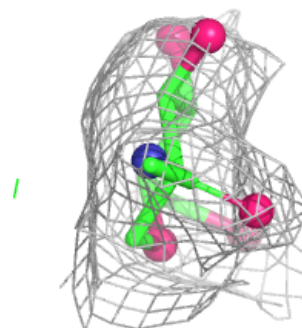
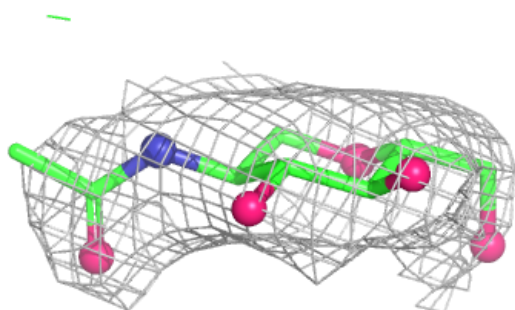
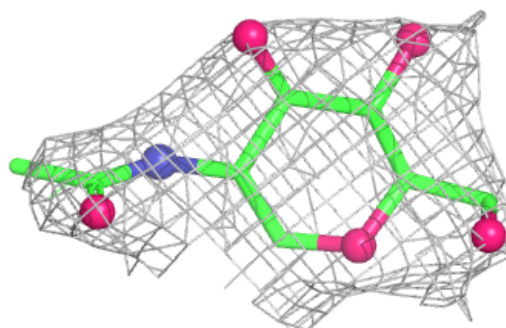


**Electron density around NAG P 201:**

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

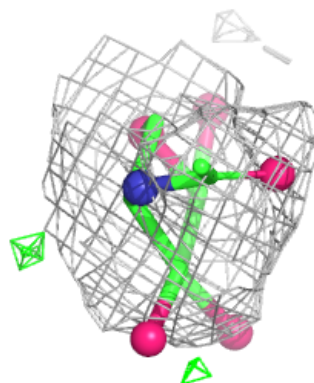
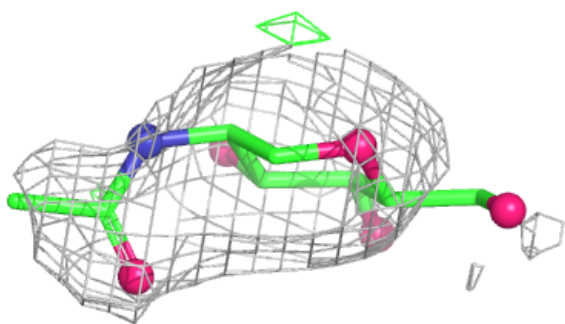
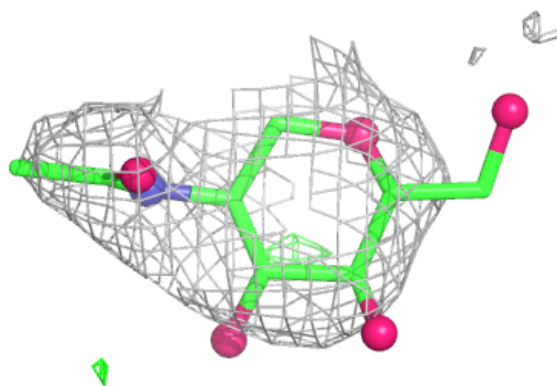
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and green (positive)



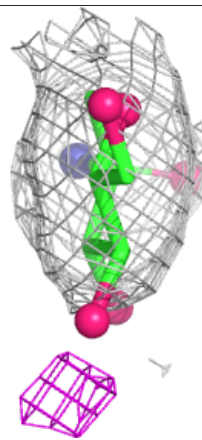
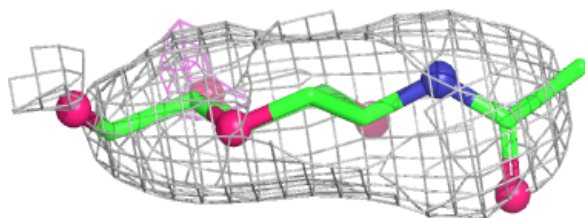
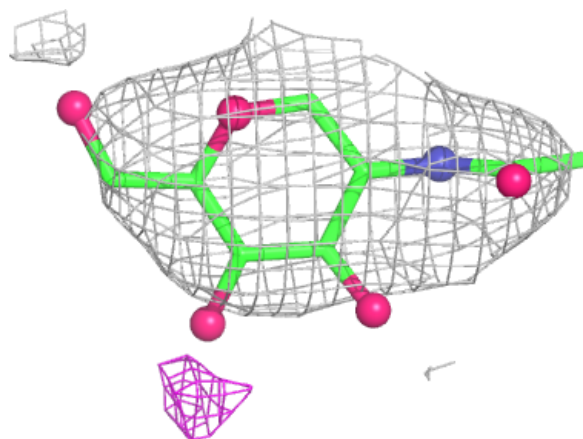
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and green (positive)



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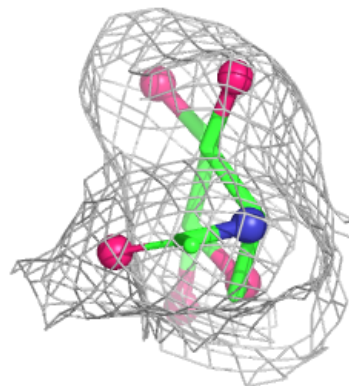
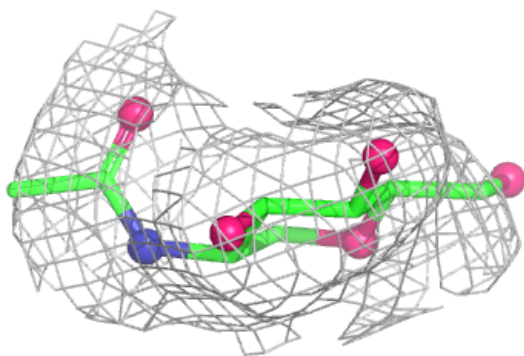
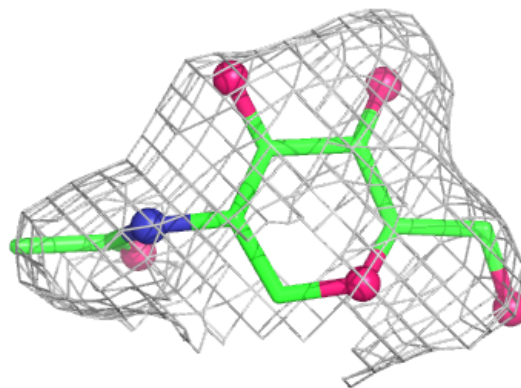
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



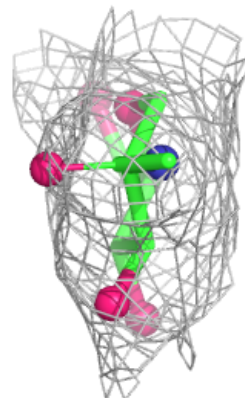
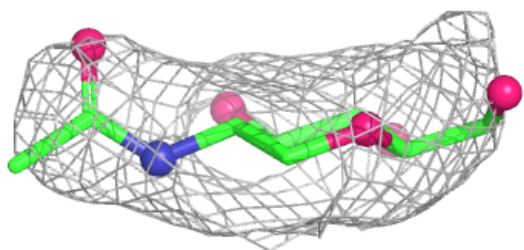
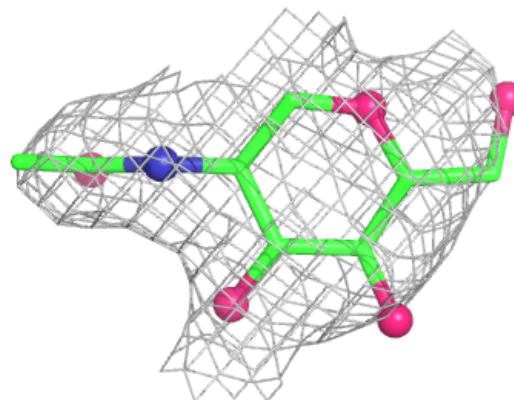


**Electron density around NAG C 201:**

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and green (positive)

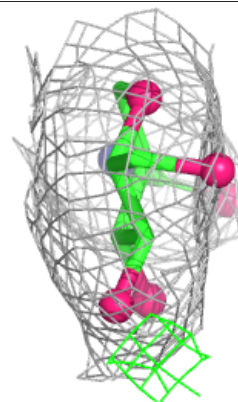
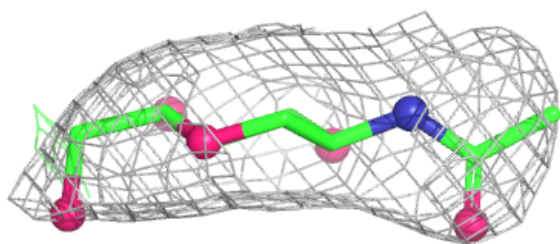
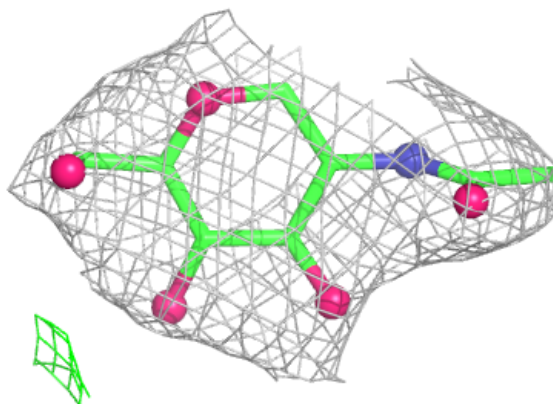
**Electron density around NAG P 202:**

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and green (positive)

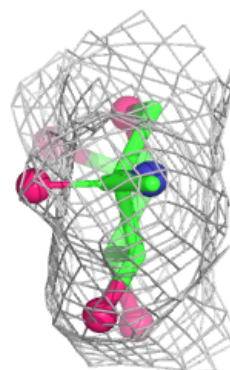
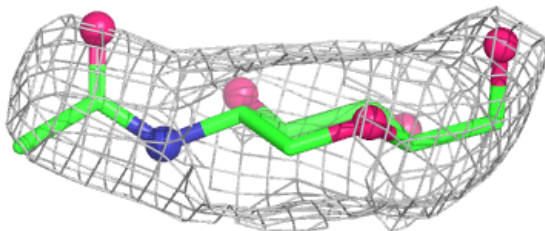
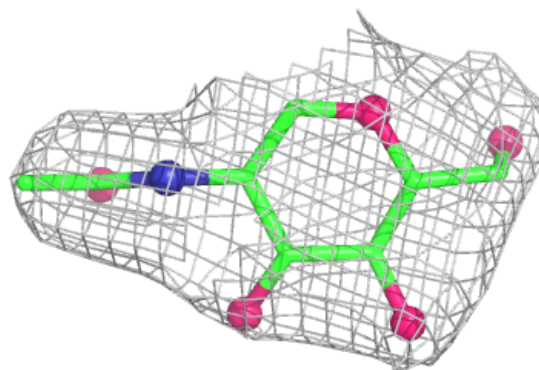


**Electron density around NAG M 202:**

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

**Electron density around NAG D 202:**

$2mF_o-DF_c$  (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.