



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2021 – 05:14 PM JST

PDB ID : 7CGW
Title : Complex structure of PD-1 and tislelizumab Fab
Authors : Hong, Y.; Feng, Y.C.; Liu, Y.
Deposited on : 2020-07-02
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

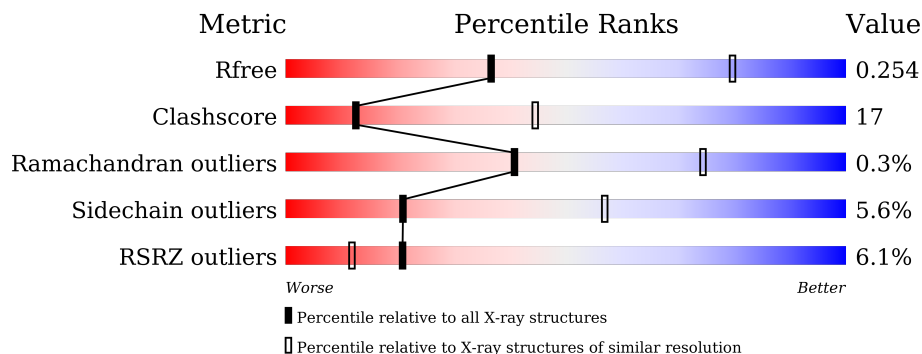
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	228	
1	H	228	
2	B	214	
2	L	214	
3	C	151	
3	P	151	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	203	-	-	X	-
4	NAG	P	202	-	-	X	-
4	NAG	P	204	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8450 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 Heavy chain of tislelizumab Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	Total 1632	C 1030	N 270	O 327	S 5	0	0	0
1	H	218	Total 1632	C 1030	N 270	O 327	S 5	0	0	0

- Molecule 2 is a protein called Light chain of tislelizumab Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	Total 1656	C 1039	N 276	O 335	S 6	0	0	0
2	L	213	Total 1648	C 1035	N 275	O 332	S 6	0	0	0

- Molecule 3 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	114	Total 892	C 552	N 162	O 173	S 5	0	0	0
3	P	114	Total 892	C 552	N 162	O 173	S 5	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

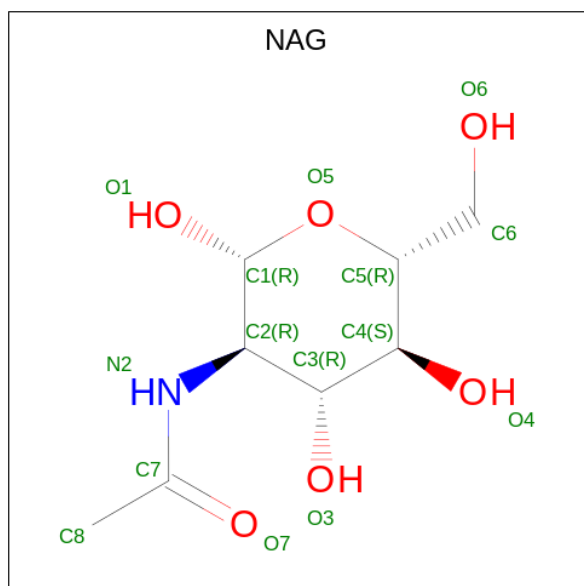
Chain	Residue	Modelled	Actual	Comment	Reference
C	170	GLU	-	expression tag	UNP Q15116
C	171	ASN	-	expression tag	UNP Q15116
C	172	LEU	-	expression tag	UNP Q15116
C	173	TYR	-	expression tag	UNP Q15116
C	174	PHE	-	expression tag	UNP Q15116
C	175	GLN	-	expression tag	UNP Q15116
P	170	GLU	-	expression tag	UNP Q15116
P	171	ASN	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
P	172	LEU	-	expression tag	UNP Q15116
P	173	TYR	-	expression tag	UNP Q15116
P	174	PHE	-	expression tag	UNP Q15116
P	175	GLN	-	expression tag	UNP Q15116

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

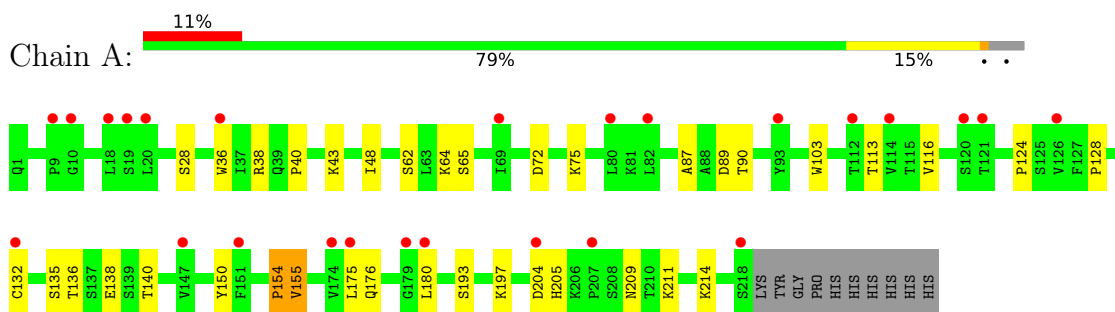


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		

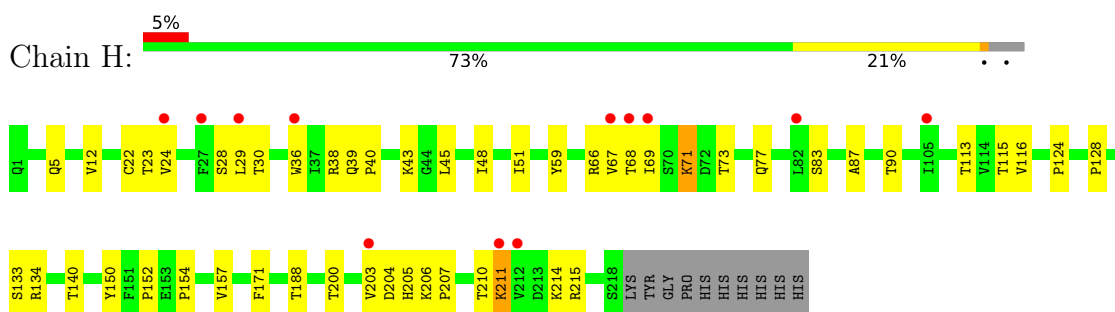
3 Residue-property plots [i](#)

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.

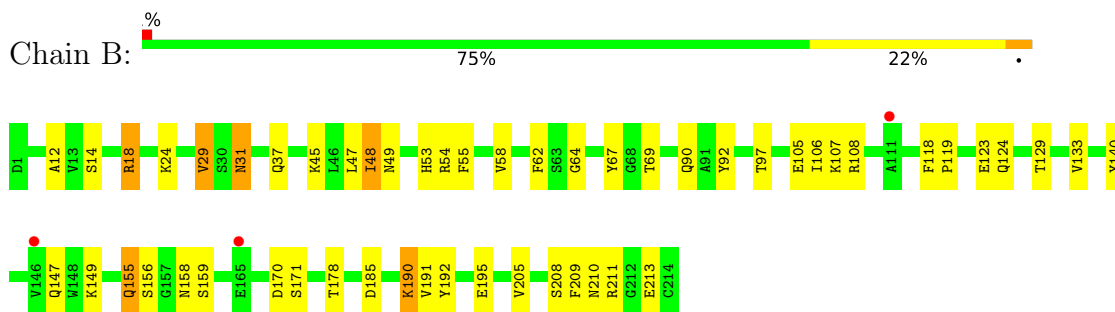
- Molecule 1: Heavy chain of tislelizumab Fab



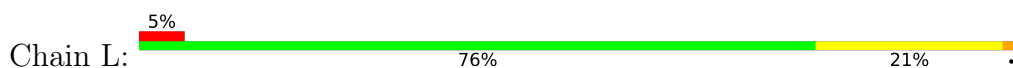
- Molecule 1: Heavy chain of tislelizumab Fab

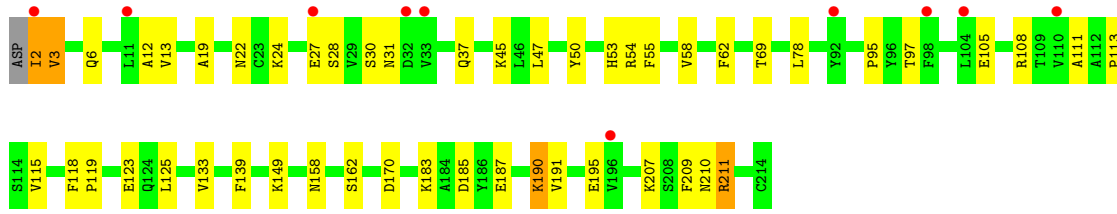


- Molecule 2: Light chain of tislelizumab Fab

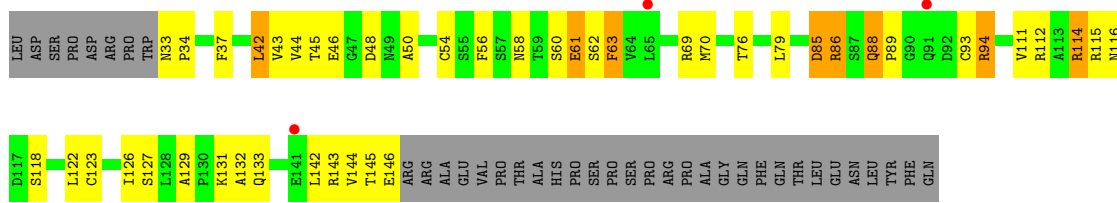


- Molecule 2: Light chain of tislelizumab Fab

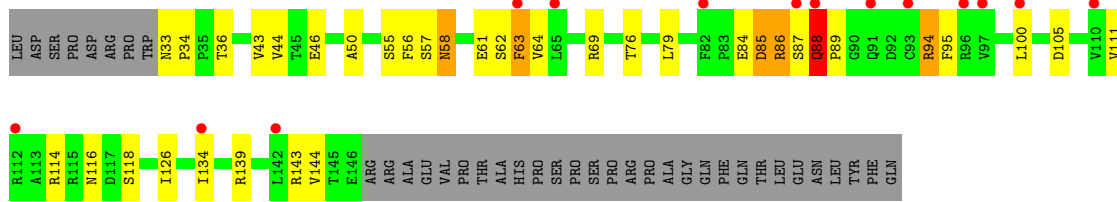




● Molecule 3: Programmed cell death protein 1



● Molecule 3: Programmed cell death protein 1



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	142.64Å 145.57Å 175.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.88 – 3.20 101.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (101.88-3.20) 96.1 (101.88-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.218 , 0.254 0.217 , 0.254	Depositor DCC
R_{free} test set	2005 reflections (6.59%)	wwPDB-VP
Wilson B-factor (Å ²)	98.2	Xtrriage
Anisotropy	0.029	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	8450	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.34	0/1672	0.58	0/2288
1	H	0.32	0/1672	0.56	0/2288
2	B	0.33	0/1694	0.56	0/2302
2	L	0.32	0/1686	0.56	0/2291
3	C	0.43	0/911	0.69	0/1236
3	P	0.44	0/911	0.73	0/1236
All	All	0.36	0/8546	0.60	0/11641

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	1632	0	1607	26	0
1	H	1632	0	1607	36	0
2	B	1656	0	1592	46	0
2	L	1648	0	1585	34	0
3	C	892	0	859	81	0
3	P	892	0	858	62	0
4	C	42	0	39	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	56	0	52	24	0
All	All	8450	0	8199	280	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 17.

All (280) 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:P:88:GLN:HB3	3:P:89:PRO:CD	1.64	1.23
3:P:88:GLN:HB3	3:P:89:PRO:HD3	1.18	1.13
3:C:114:ARG:HD2	4:C:203:NAG:H83	1.20	1.12
3:C:88:GLN:HB3	3:C:89:PRO:CD	1.80	1.11
3:C:88:GLN:HB3	3:C:89:PRO:HD2	1.09	1.04
3:P:139:ARG:HH21	4:P:203:NAG:H61	1.21	0.98
2:B:29:VAL:HG22	2:B:92:TYR:HB2	1.46	0.97
3:P:86:ARG:HD3	3:P:89:PRO:HD2	1.46	0.96
1:A:103:TRP:HE1	3:C:89:PRO:HB3	1.31	0.96
3:C:122:LEU:CD2	3:C:123:CYS:O	2.14	0.95
3:C:122:LEU:HD23	3:C:123:CYS:N	1.80	0.94
3:P:94:ARG:HH22	3:P:114:ARG:NH1	1.64	0.94
2:L:53:HIS:CE1	3:P:76:THR:CG2	2.53	0.92
2:B:29:VAL:CG2	2:B:92:TYR:CB	2.50	0.90
3:C:88:GLN:CB	3:C:89:PRO:HD2	2.00	0.90
2:L:53:HIS:CE1	3:P:76:THR:HG21	2.05	0.90
3:P:88:GLN:CB	3:P:89:PRO:CD	2.47	0.88
3:C:56:PHE:CD1	3:C:63:PHE:HE2	1.90	0.88
3:C:88:GLN:CB	3:C:89:PRO:CD	2.51	0.88
3:C:114:ARG:CD	4:C:203:NAG:H83	2.03	0.88
3:P:94:ARG:HH22	3:P:114:ARG:HH12	1.22	0.88
3:C:118:SER:HB3	3:C:144:VAL:HG22	1.54	0.87
2:B:29:VAL:CG2	2:B:92:TYR:HB2	2.02	0.87
3:P:86:ARG:HD2	3:P:86:ARG:O	1.76	0.85
3:P:114:ARG:HG3	3:P:114:ARG:HH11	1.43	0.84
3:C:114:ARG:HD2	4:C:203:NAG:C8	2.07	0.83
3:C:122:LEU:HD23	3:C:123:CYS:O	1.77	0.82
3:C:63:PHE:HB2	3:C:126:ILE:O	1.79	0.81
3:C:122:LEU:HD21	3:C:123:CYS:O	1.77	0.81
3:C:85:ASP:OD1	3:C:85:ASP:N	2.15	0.79
3:P:139:ARG:HH21	4:P:203:NAG:C6	1.96	0.79
2:B:49:ASN:OD1	2:B:53:HIS:HB3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TRP:HE1	3:C:89:PRO:CB	1.96	0.77
3:P:88:GLN:HB3	3:P:89:PRO:HD2	1.67	0.77
2:B:29:VAL:HG22	2:B:92:TYR:CB	2.15	0.76
2:L:53:HIS:CE1	3:P:76:THR:HG23	2.20	0.75
3:P:58:ASN:OD1	4:P:202:NAG:H2	1.86	0.74
4:P:202:NAG:O7	4:P:202:NAG:O4	2.05	0.74
3:C:43:VAL:HG22	3:C:143:ARG:HB2	1.70	0.74
3:P:85:ASP:OD2	3:P:85:ASP:N	2.16	0.73
2:L:2:ILE:HD13	2:L:27:GLU:HB2	1.70	0.73
3:P:58:ASN:HB3	4:P:202:NAG:O3	1.90	0.72
4:P:201:NAG:O7	4:P:201:NAG:O3	2.05	0.72
2:L:53:HIS:HE1	3:P:76:THR:HG23	1.54	0.72
3:P:116:ASN:HD22	4:P:204:NAG:H61	1.54	0.72
4:C:202:NAG:O7	4:C:202:NAG:H3	1.90	0.71
3:C:45:THR:HG21	3:C:146:GLU:OE2	1.90	0.71
3:C:42:LEU:HD12	3:C:42:LEU:C	2.11	0.70
3:P:94:ARG:NH2	3:P:114:ARG:HH12	1.89	0.70
3:P:58:ASN:ND2	4:P:202:NAG:O3	2.23	0.70
3:P:139:ARG:NH2	4:P:203:NAG:H61	2.03	0.69
3:C:56:PHE:CD1	3:C:63:PHE:CE2	2.79	0.69
3:C:122:LEU:HD23	3:C:123:CYS:C	2.14	0.68
2:B:149:LYS:NZ	2:B:195:GLU:OE1	2.27	0.68
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.77	0.67
1:H:152:PRO:HD2	1:H:207:PRO:HG2	1.77	0.67
3:C:114:ARG:CG	4:C:203:NAG:N2	2.58	0.66
3:C:122:LEU:HD23	3:C:122:LEU:C	2.15	0.66
3:P:86:ARG:HD2	3:P:86:ARG:C	2.14	0.66
1:H:211:LYS:HB3	1:H:211:LYS:HZ3	1.59	0.66
3:C:45:THR:HB	3:C:146:GLU:HB3	1.79	0.65
2:B:29:VAL:HG23	2:B:92:TYR:CB	2.26	0.64
3:C:56:PHE:HD1	3:C:63:PHE:HE2	1.43	0.64
3:P:116:ASN:ND2	4:P:204:NAG:O3	2.28	0.64
1:H:124:PRO:HB3	1:H:150:TYR:HB3	1.79	0.64
3:C:88:GLN:HG2	3:C:89:PRO:HD3	1.80	0.64
3:C:114:ARG:HG3	4:C:203:NAG:N2	2.13	0.64
3:P:88:GLN:CB	3:P:89:PRO:HD2	2.25	0.63
3:P:114:ARG:HH11	3:P:114:ARG:CG	2.12	0.63
2:B:54:ARG:NH1	2:B:62:PHE:O	2.31	0.62
2:L:149:LYS:NZ	2:L:195:GLU:OE1	2.31	0.62
3:P:43:VAL:HG22	3:P:143:ARG:HB2	1.81	0.62
1:A:90:THR:HB	1:A:116:VAL:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ILE:HD12	2:B:64:GLY:N	2.16	0.61
3:C:44:VAL:HG22	3:C:144:VAL:HG12	1.82	0.61
3:C:62:SER:O	3:C:62:SER:OG	2.19	0.61
1:A:103:TRP:NE1	3:C:89:PRO:CB	2.63	0.60
1:H:90:THR:HB	1:H:116:VAL:H	1.66	0.60
3:P:139:ARG:NH2	4:P:203:NAG:C5	2.64	0.60
2:L:37:GLN:HB3	2:L:47:LEU:HD11	1.83	0.60
4:P:204:NAG:O4	4:P:204:NAG:N2	2.35	0.60
3:C:45:THR:HA	3:C:145:THR:O	2.03	0.59
4:P:201:NAG:HO3	4:P:201:NAG:C7	2.09	0.59
3:C:70:MET:SD	3:C:76:THR:HG22	2.43	0.59
3:P:62:SER:OG	3:P:62:SER:O	2.19	0.57
1:H:59:TYR:HB3	1:H:67:VAL:HG11	1.84	0.57
3:C:86:ARG:HG2	3:C:88:GLN:H	1.69	0.57
3:C:114:ARG:HG2	4:C:203:NAG:HN2	1.69	0.57
1:A:155:VAL:HG23	1:A:205:HIS:CD2	2.40	0.57
3:P:95:PHE:N	3:P:95:PHE:CD1	2.72	0.57
3:P:44:VAL:HG21	3:P:50:ALA:HB2	1.85	0.57
2:B:24:LYS:HA	2:B:69:THR:O	2.05	0.56
2:B:29:VAL:CG2	2:B:92:TYR:HB3	2.33	0.56
3:C:122:LEU:HD23	3:C:123:CYS:CA	2.36	0.56
3:P:94:ARG:HH22	3:P:114:ARG:CZ	2.17	0.56
1:H:128:PRO:HD3	1:H:214:LYS:HE3	1.87	0.56
3:C:86:ARG:CZ	3:C:86:ARG:HB3	2.35	0.56
2:L:13:VAL:HG23	2:L:78:LEU:HD22	1.87	0.56
3:C:69:ARG:HB2	3:C:79:LEU:HD11	1.87	0.56
1:H:66:ARG:HD2	1:H:83:SER:O	2.06	0.55
3:C:114:ARG:HG2	4:C:203:NAG:N2	2.21	0.55
2:L:54:ARG:NH1	2:L:62:PHE:O	2.34	0.55
3:P:69:ARG:HB2	3:P:79:LEU:HD11	1.88	0.55
2:B:37:GLN:HB3	2:B:47:LEU:HD11	1.88	0.55
1:H:157:VAL:HG22	1:H:203:VAL:HG22	1.89	0.55
4:P:204:NAG:O3	4:P:204:NAG:H62	2.06	0.55
3:C:56:PHE:CE1	3:C:63:PHE:CE2	2.95	0.54
3:P:116:ASN:ND2	4:P:204:NAG:H61	2.22	0.54
2:L:123:GLU:OE1	2:L:123:GLU:N	2.38	0.54
3:P:58:ASN:CB	4:P:202:NAG:O3	2.55	0.54
3:P:64:VAL:O	3:P:126:ILE:HG12	2.07	0.54
3:C:46:GLU:O	3:C:46:GLU:HG3	2.06	0.53
2:B:29:VAL:HG23	2:B:92:TYR:HB3	1.89	0.53
2:B:106:ILE:HD11	2:B:171:SER:OG	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:ASN:ND2	4:C:203:NAG:C6	2.70	0.53
1:H:206:LYS:HB3	1:H:207:PRO:HD3	1.89	0.53
3:P:61:GLU:OE2	3:P:61:GLU:HA	2.08	0.53
2:B:18:ARG:HB2	2:B:18:ARG:NH1	2.23	0.53
2:B:31:ASN:HB3	2:B:67:TYR:CD2	2.44	0.53
3:P:139:ARG:NH2	4:P:203:NAG:C6	2.68	0.53
3:C:44:VAL:O	3:C:144:VAL:HA	2.09	0.53
3:P:58:ASN:CG	4:P:202:NAG:O3	2.46	0.53
2:B:18:ARG:HH11	2:B:18:ARG:CB	2.22	0.52
3:C:48:ASP:O	3:C:112:ARG:HA	2.08	0.52
1:H:36:TRP:CD1	1:H:69:ILE:HD13	2.44	0.52
1:A:103:TRP:CD1	3:C:89:PRO:HB2	2.44	0.52
2:B:18:ARG:HH11	2:B:18:ARG:HB3	1.74	0.52
3:C:115:ARG:HA	3:C:144:VAL:HG21	1.91	0.52
1:H:51:ILE:HD13	1:H:71:LYS:HB3	1.90	0.52
1:H:211:LYS:HB3	1:H:211:LYS:NZ	2.24	0.52
2:B:18:ARG:NH1	2:B:18:ARG:CB	2.72	0.52
3:P:116:ASN:ND2	4:P:204:NAG:C6	2.70	0.52
1:A:38:ARG:HB2	1:A:48:ILE:HD11	1.91	0.52
2:B:12:ALA:HA	2:B:105:GLU:O	2.10	0.52
2:B:48:ILE:CD1	2:B:64:GLY:N	2.72	0.52
2:L:115:VAL:O	2:L:207:LYS:HD2	2.09	0.52
2:L:190:LYS:O	2:L:211:ARG:N	2.42	0.52
2:L:28:SER:O	2:L:28:SER:OG	2.21	0.52
3:C:116:ASN:ND2	4:C:203:NAG:O6	2.42	0.51
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.92	0.51
1:H:211:LYS:NZ	1:H:211:LYS:CB	2.73	0.51
1:A:132:CYS:HB2	2:B:119:PRO:HG3	1.92	0.51
2:B:155:GLN:HG3	2:B:158:ASN:HD21	1.74	0.51
3:P:114:ARG:HD2	3:P:116:ASN:HB2	1.92	0.51
3:C:61:GLU:O	3:C:61:GLU:HG3	2.10	0.51
1:A:103:TRP:NE1	3:C:89:PRO:HB2	2.26	0.51
2:L:187:GLU:OE1	2:L:211:ARG:NH1	2.45	0.50
3:C:48:ASP:O	3:C:112:ARG:N	2.45	0.50
3:P:94:ARG:NH2	3:P:114:ARG:NH1	2.45	0.50
2:B:31:ASN:HB3	2:B:67:TYR:CE2	2.46	0.50
2:B:48:ILE:HD12	2:B:64:GLY:CA	2.41	0.50
3:P:118:SER:HB3	3:P:144:VAL:HG22	1.94	0.50
2:B:190:LYS:O	2:B:211:ARG:N	2.41	0.50
1:H:133:SER:OG	1:H:134:ARG:N	2.45	0.50
3:C:46:GLU:OE2	3:C:115:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:ARG:HG3	4:C:203:NAG:C7	2.42	0.49
1:A:40:PRO:HB2	1:A:43:LYS:HB2	1.94	0.49
2:B:123:GLU:OE1	2:B:123:GLU:N	2.42	0.49
3:C:129:ALA:O	3:C:132:ALA:N	2.45	0.49
1:H:71:LYS:O	1:H:71:LYS:HG2	2.12	0.49
2:B:170:ASP:OD1	2:B:170:ASP:N	2.44	0.49
1:H:36:TRP:HD1	1:H:69:ILE:HD13	1.76	0.49
2:B:29:VAL:CG2	2:B:92:TYR:CG	2.96	0.49
3:C:46:GLU:OE2	3:C:115:ARG:CG	2.61	0.48
3:C:114:ARG:CG	4:C:203:NAG:HN2	2.24	0.48
3:P:86:ARG:HG2	3:P:88:GLN:HE21	1.79	0.48
1:H:24:VAL:HG21	1:H:29:LEU:HD21	1.95	0.48
2:L:158:ASN:OD1	2:L:158:ASN:N	2.47	0.48
1:A:135:SER:OG	1:A:138:GLU:HB2	2.14	0.48
1:A:72:ASP:OD1	1:A:75:LYS:NZ	2.30	0.48
3:P:139:ARG:NH2	4:P:203:NAG:H5	2.27	0.48
1:H:38:ARG:HB2	1:H:48:ILE:HD11	1.94	0.48
2:L:108:ARG:HH21	2:L:111:ALA:HB2	1.79	0.48
3:P:86:ARG:CG	3:P:88:GLN:HB2	2.44	0.48
3:C:56:PHE:HD1	3:C:63:PHE:CE2	2.29	0.47
3:C:94:ARG:HA	3:C:111:VAL:HG22	1.96	0.47
3:C:127:SER:O	3:C:132:ALA:HA	2.14	0.47
1:A:128:PRO:HD3	1:A:214:LYS:HE3	1.96	0.47
3:C:86:ARG:O	3:C:86:ARG:NE	2.48	0.47
1:A:197:LYS:HD2	1:A:197:LYS:HA	1.63	0.47
3:C:63:PHE:HD1	3:C:63:PHE:H	1.61	0.47
3:C:114:ARG:HA	3:C:114:ARG:HD3	1.56	0.47
3:C:58:ASN:OD1	3:C:61:GLU:HA	2.15	0.47
2:B:118:PHE:HB2	2:B:133:VAL:HG13	1.97	0.47
1:H:23:THR:HG22	1:H:77:GLN:HG2	1.96	0.46
3:P:114:ARG:NH1	3:P:114:ARG:HG3	2.22	0.46
3:C:63:PHE:CD1	3:C:63:PHE:N	2.83	0.46
3:C:86:ARG:C	3:C:86:ARG:CD	2.83	0.46
2:L:24:LYS:HA	2:L:69:THR:O	2.15	0.46
2:B:48:ILE:HD12	2:B:64:GLY:HA3	1.97	0.46
3:C:37:PHE:CD1	3:C:123:CYS:HB2	2.50	0.46
1:H:211:LYS:HZ3	1:H:211:LYS:CB	2.27	0.46
3:C:63:PHE:CD1	3:C:63:PHE:C	2.85	0.46
3:P:126:ILE:HG22	3:P:134:ILE:HA	1.98	0.46
3:C:122:LEU:CD2	3:C:122:LEU:C	2.84	0.46
1:H:12:VAL:HG23	1:H:116:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:VAL:HG23	2:B:92:TYR:CG	2.50	0.46
3:C:45:THR:CA	3:C:145:THR:O	2.65	0.45
3:C:86:ARG:HD3	3:C:89:PRO:HG2	1.98	0.45
3:P:63:PHE:CD1	3:P:63:PHE:C	2.89	0.45
3:P:44:VAL:O	3:P:144:VAL:HG12	2.16	0.45
2:L:119:PRO:HB3	2:L:209:PHE:CE1	2.52	0.45
3:C:37:PHE:CD1	3:C:54:CYS:HB2	2.52	0.45
1:H:90:THR:OG1	1:H:115:THR:HA	2.17	0.45
4:P:202:NAG:N2	4:P:202:NAG:H5	2.32	0.45
3:C:88:GLN:HG2	3:C:89:PRO:CD	2.46	0.45
3:C:88:GLN:CG	3:C:89:PRO:CD	2.95	0.45
2:B:90:GLN:HE21	2:B:97:THR:H	1.63	0.45
3:P:63:PHE:CD1	3:P:63:PHE:O	2.70	0.45
3:C:44:VAL:HG11	3:C:50:ALA:HB2	1.99	0.44
1:A:113:THR:HG21	1:A:154:PRO:HG3	2.00	0.44
2:L:13:VAL:HG21	2:L:19:ALA:HB2	1.98	0.44
2:L:170:ASP:N	2:L:170:ASP:OD1	2.50	0.44
3:P:57:SER:O	3:P:57:SER:OG	2.28	0.44
1:A:38:ARG:NH2	1:A:89:ASP:OD1	2.51	0.44
1:A:113:THR:CG2	1:A:154:PRO:HG3	2.48	0.44
1:A:155:VAL:HG23	1:A:205:HIS:HD2	1.79	0.44
2:L:31:ASN:O	2:L:50:TYR:HA	2.17	0.44
2:L:55:PHE:O	2:L:58:VAL:HG12	2.17	0.44
4:P:204:NAG:C1	4:P:204:NAG:H83	2.48	0.44
2:B:119:PRO:HB3	2:B:209:PHE:CE1	2.53	0.44
3:C:61:GLU:HB2	4:C:202:NAG:C1	2.48	0.44
1:H:29:LEU:HB3	1:H:71:LYS:HE3	1.99	0.44
1:H:30:THR:HG23	1:H:73:THR:HG21	2.00	0.44
2:B:192:TYR:O	2:B:208:SER:HA	2.18	0.44
1:H:87:ALA:O	1:H:90:THR:HG22	2.18	0.43
2:B:190:LYS:O	2:B:210:ASN:HA	2.17	0.43
3:P:36:THR:OG1	3:P:55:SER:OG	2.22	0.43
3:P:114:ARG:NH1	3:P:114:ARG:CG	2.73	0.43
2:B:210:ASN:HB2	2:B:213:GLU:HG3	2.00	0.43
3:C:63:PHE:HD1	3:C:63:PHE:N	2.15	0.43
2:B:55:PHE:O	2:B:58:VAL:HG12	2.19	0.43
3:P:33:ASN:N	3:P:34:PRO:HD3	2.33	0.43
3:C:42:LEU:HD11	3:C:142:LEU:HD13	2.00	0.43
2:L:12:ALA:HA	2:L:105:GLU:O	2.18	0.43
1:A:87:ALA:O	1:A:90:THR:HG22	2.18	0.43
2:B:195:GLU:HA	2:B:205:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:114:ARG:HD3	4:P:204:NAG:H62	2.01	0.43
1:H:5:GLN:O	1:H:22:CYS:HA	2.18	0.43
2:L:108:ARG:NH2	2:L:111:ALA:HB2	2.33	0.43
2:B:105:GLU:H	2:B:105:GLU:HG2	1.65	0.43
1:H:40:PRO:HB2	1:H:43:LYS:HB2	2.01	0.43
1:H:59:TYR:HE1	1:H:69:ILE:HG13	1.84	0.43
2:L:6:GLN:HA	2:L:22:ASN:O	2.19	0.43
1:H:140:THR:HG22	1:H:188:THR:HG22	2.02	0.42
3:C:48:ASP:O	3:C:112:ARG:CA	2.67	0.42
2:B:124:GLN:HG2	2:B:129:THR:O	2.19	0.42
2:L:13:VAL:CG2	2:L:78:LEU:HD22	2.49	0.42
3:P:86:ARG:HG2	3:P:88:GLN:H	1.84	0.42
3:P:139:ARG:H	3:P:139:ARG:HG2	1.72	0.42
2:B:159:SER:HA	2:B:178:THR:O	2.19	0.42
2:L:118:PHE:HB2	2:L:133:VAL:HG13	2.02	0.42
1:A:175:LEU:HD21	2:L:108:ARG:C	2.40	0.42
1:A:204:ASP:HB2	1:A:211:LYS:HD2	2.02	0.42
1:H:59:TYR:CE1	1:H:69:ILE:HG13	2.55	0.42
2:L:95:PRO:O	2:L:97:THR:HG23	2.20	0.42
3:P:100:LEU:HD12	3:P:105:ASP:OD1	2.20	0.41
2:L:191:VAL:HG22	2:L:210:ASN:OD1	2.20	0.41
3:P:86:ARG:HG2	3:P:88:GLN:HB2	2.02	0.41
1:H:36:TRP:O	1:H:48:ILE:HB	2.21	0.41
1:A:193:SER:O	1:A:193:SER:OG	2.37	0.41
3:C:33:ASN:N	3:C:34:PRO:HD3	2.35	0.41
2:B:118:PHE:HB2	2:B:133:VAL:CG1	2.51	0.41
2:L:3:VAL:HG12	2:L:3:VAL:O	2.20	0.41
1:H:200:THR:HG22	1:H:215:ARG:HE	1.86	0.41
2:L:125:LEU:HB3	2:L:183:LYS:HE3	2.03	0.41
2:B:29:VAL:HG22	2:B:92:TYR:CG	2.55	0.41
1:H:113:THR:CG2	1:H:154:PRO:HD3	2.51	0.41
2:B:92:TYR:HA	3:C:86:ARG:HH22	1.85	0.41
3:P:114:ARG:HD3	4:P:204:NAG:C6	2.51	0.41
3:C:131:LYS:HG3	3:C:133:GLN:HG2	2.03	0.41
1:H:171:PHE:HB3	2:L:162:SER:OG	2.21	0.41
3:P:114:ARG:HD2	3:P:116:ASN:H	1.86	0.41
1:A:176:GLN:HG3	1:A:180:LEU:O	2.22	0.40
1:A:36:TRP:O	1:A:48:ILE:HB	2.22	0.40
2:B:107:LYS:HA	2:B:140:TYR:OH	2.21	0.40
1:H:205:HIS:HB3	1:H:210:THR:HB	2.02	0.40
1:A:211:LYS:HE3	1:A:211:LYS:HB3	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:C	3:C:42:LEU:CD1	2.84	0.40
2:L:113:PRO:HB3	2:L:139:PHE:HB3	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	216/228 (95%)	206 (95%)	9 (4%)	1 (0%)	29	67
1	H	216/228 (95%)	204 (94%)	12 (6%)	0	100	100
2	B	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
2	L	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
3	C	112/151 (74%)	104 (93%)	7 (6%)	1 (1%)	17	56
3	P	112/151 (74%)	106 (95%)	5 (4%)	1 (1%)	17	56
All	All	1079/1186 (91%)	1020 (94%)	56 (5%)	3 (0%)	41	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	88	GLN
3	P	88	GLN
1	A	154	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	189/198 (96%)	181 (96%)	8 (4%)	30	65
1	H	189/198 (96%)	184 (97%)	5 (3%)	46	76
2	B	188/188 (100%)	175 (93%)	13 (7%)	15	49
2	L	187/188 (100%)	180 (96%)	7 (4%)	34	68
3	C	100/133 (75%)	91 (91%)	9 (9%)	9	34
3	P	100/133 (75%)	89 (89%)	11 (11%)	6	26
All	All	953/1038 (92%)	900 (94%)	53 (6%)	21	57

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	62	SER
1	A	64	LYS
1	A	65	SER
1	A	136	THR
1	A	140	THR
1	A	155	VAL
1	A	209	ASN
2	B	14	SER
2	B	18	ARG
2	B	29	VAL
2	B	31	ASN
2	B	45	LYS
2	B	48	ILE
2	B	108	ARG
2	B	147	GLN
2	B	155	GLN
2	B	156	SER
2	B	185	ASP
2	B	190	LYS
2	B	191	VAL
3	C	42	LEU
3	C	60	SER
3	C	61	GLU
3	C	63	PHE
3	C	85	ASP
3	C	86	ARG
3	C	93	CYS

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Mol	Chain	Res	Type
3	C	94	ARG
3	C	114	ARG
1	H	28	SER
1	H	68	THR
1	H	71	LYS
1	H	204	ASP
1	H	211	LYS
2	L	2	ILE
2	L	3	VAL
2	L	30	SER
2	L	45	LYS
2	L	185	ASP
2	L	190	LYS
2	L	211	ARG
3	P	46	GLU
3	P	56	PHE
3	P	58	ASN
3	P	63	PHE
3	P	84	GLU
3	P	85	ASP
3	P	86	ARG
3	P	87	SER
3	P	88	GLN
3	P	94	ARG
3	P	111	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
2	B	31	ASN
3	C	66	ASN
1	H	160	ASN
2	L	53	HIS
3	P	88	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	C	202	3	14,14,15	0.49	0	17,19,21	1.49	1 (5%)
4	NAG	P	202	3	14,14,15	0.45	0	17,19,21	1.24	2 (11%)
4	NAG	P	204	3	14,14,15	0.26	0	17,19,21	1.23	3 (17%)
4	NAG	C	203	3	14,14,15	0.41	0	17,19,21	1.53	4 (23%)
4	NAG	C	201	3	14,14,15	0.59	0	17,19,21	2.90	6 (35%)
4	NAG	P	201	3	14,14,15	0.72	0	17,19,21	0.92	0
4	NAG	P	203	3	14,14,15	0.31	0	17,19,21	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	202	3	-	4/6/23/26	0/1/1/1
4	NAG	P	202	3	-	3/6/23/26	0/1/1/1
4	NAG	P	204	3	-	5/6/23/26	0/1/1/1
4	NAG	C	203	3	-	3/6/23/26	0/1/1/1
4	NAG	C	201	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	P	201	3	-	4/6/23/26	0/1/1/1
4	NAG	P	203	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	NAG	C4-C3-C2	-6.43	101.60	111.02
4	C	201	NAG	C1-O5-C5	6.17	120.56	112.19
4	C	201	NAG	O5-C1-C2	-6.09	101.68	111.29
4	C	202	NAG	C1-O5-C5	5.06	119.05	112.19
4	P	204	NAG	C1-O5-C5	3.08	116.37	112.19
4	C	201	NAG	C1-C2-N2	3.03	115.66	110.49
4	C	201	NAG	O5-C5-C4	2.88	117.84	110.83
4	C	203	NAG	C2-N2-C7	2.83	126.94	122.90
4	C	203	NAG	O5-C5-C6	2.79	111.58	107.20
4	C	203	NAG	C4-C3-C2	-2.68	107.10	111.02
4	C	203	NAG	C1-C2-N2	2.58	114.90	110.49
4	P	202	NAG	C1-O5-C5	2.51	115.59	112.19
4	P	202	NAG	O5-C5-C6	2.36	110.90	107.20
4	P	204	NAG	C4-C3-C2	-2.22	107.77	111.02
4	C	201	NAG	C6-C5-C4	-2.21	107.84	113.00
4	P	204	NAG	O5-C5-C6	2.16	110.58	107.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	202	NAG	C3-C2-N2-C7
4	C	203	NAG	C1-C2-N2-C7
4	P	201	NAG	C3-C2-N2-C7
4	P	202	NAG	C3-C2-N2-C7
4	C	203	NAG	O5-C5-C6-O6
4	P	204	NAG	O5-C5-C6-O6
4	P	201	NAG	C8-C7-N2-C2
4	P	204	NAG	C4-C5-C6-O6
4	P	201	NAG	O7-C7-N2-C2
4	P	204	NAG	C8-C7-N2-C2
4	P	204	NAG	O7-C7-N2-C2
4	P	203	NAG	O5-C5-C6-O6
4	C	203	NAG	C4-C5-C6-O6

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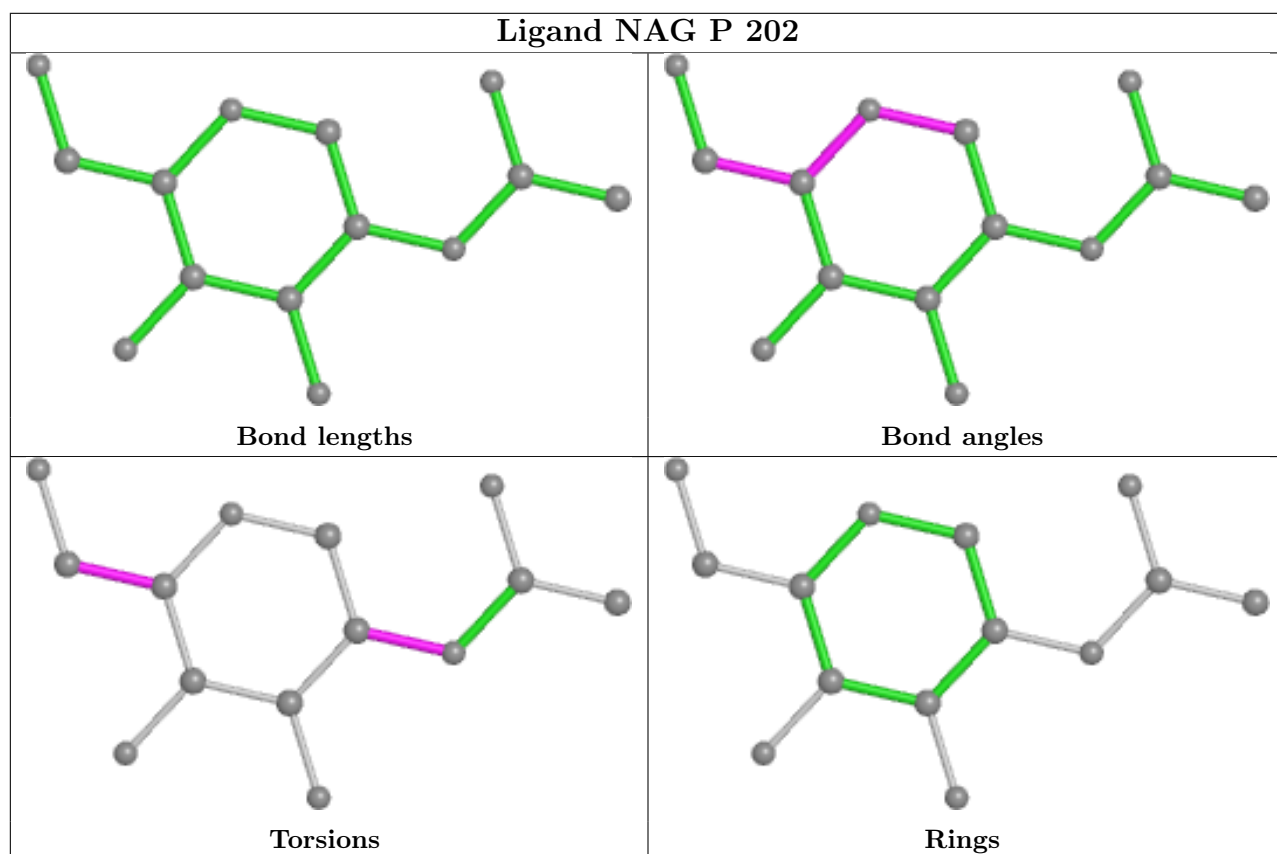
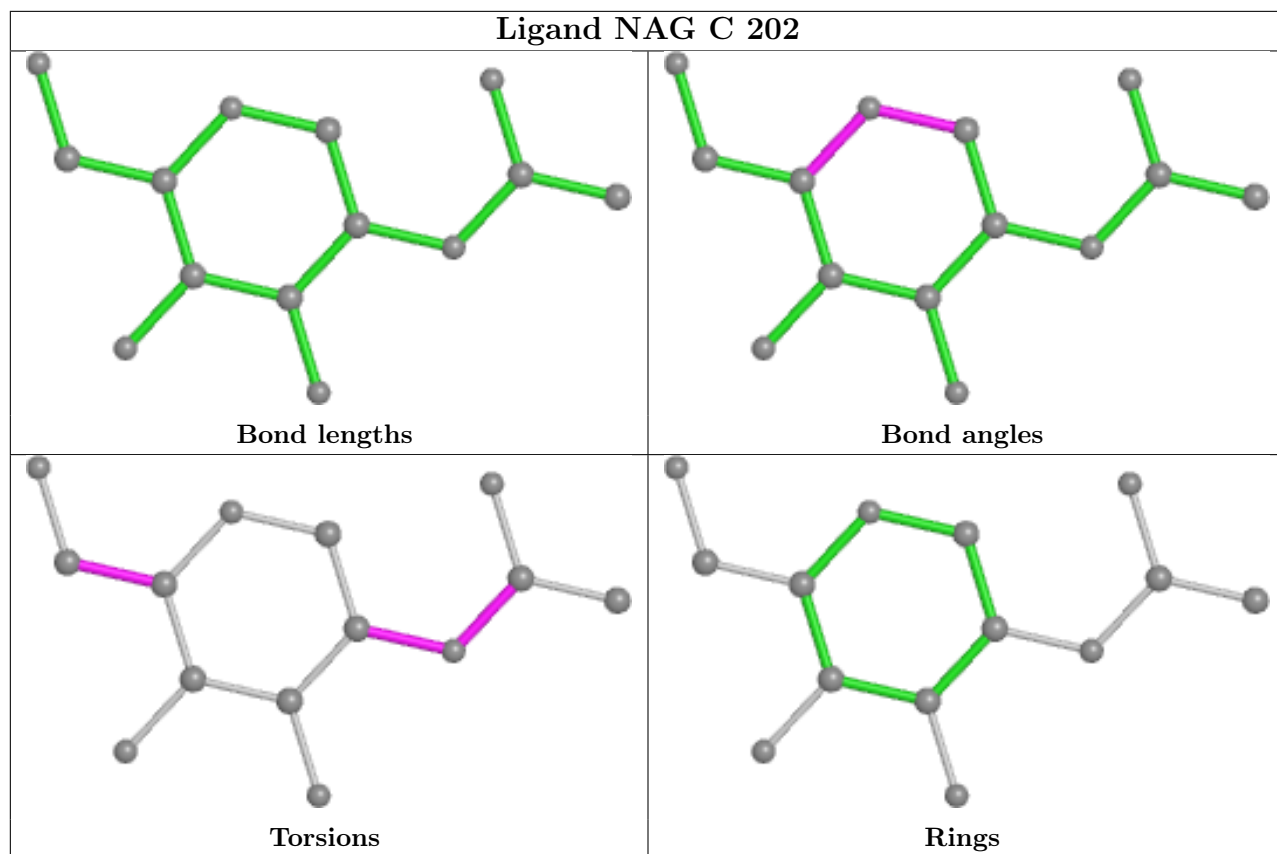
Mol	Chain	Res	Type	Atoms
4	C	201	NAG	C4-C5-C6-O6
4	C	201	NAG	O5-C5-C6-O6
4	P	202	NAG	O5-C5-C6-O6
4	C	201	NAG	C3-C2-N2-C7
4	C	202	NAG	C8-C7-N2-C2
4	C	202	NAG	O7-C7-N2-C2
4	C	202	NAG	O5-C5-C6-O6
4	P	204	NAG	C3-C2-N2-C7
4	P	201	NAG	O5-C5-C6-O6
4	P	203	NAG	C4-C5-C6-O6
4	P	202	NAG	C4-C5-C6-O6

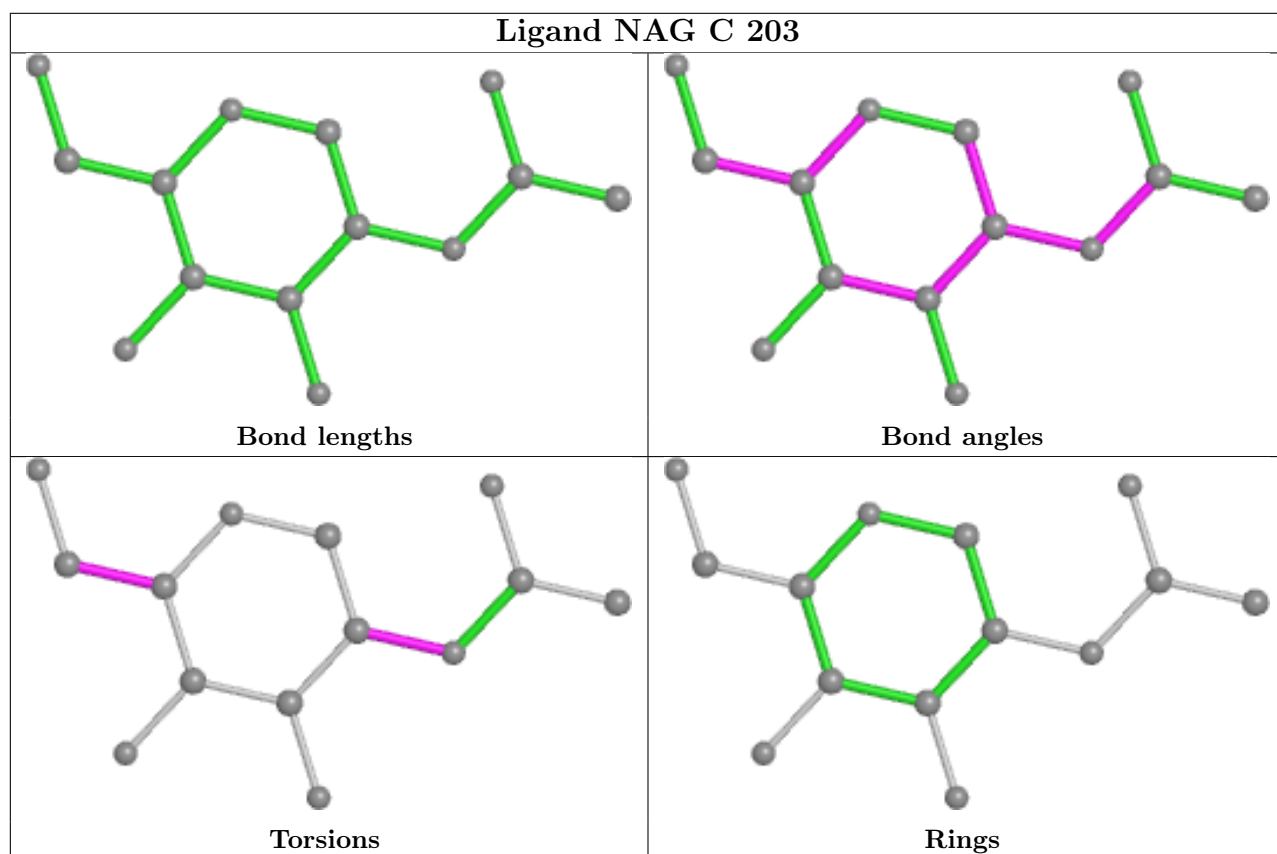
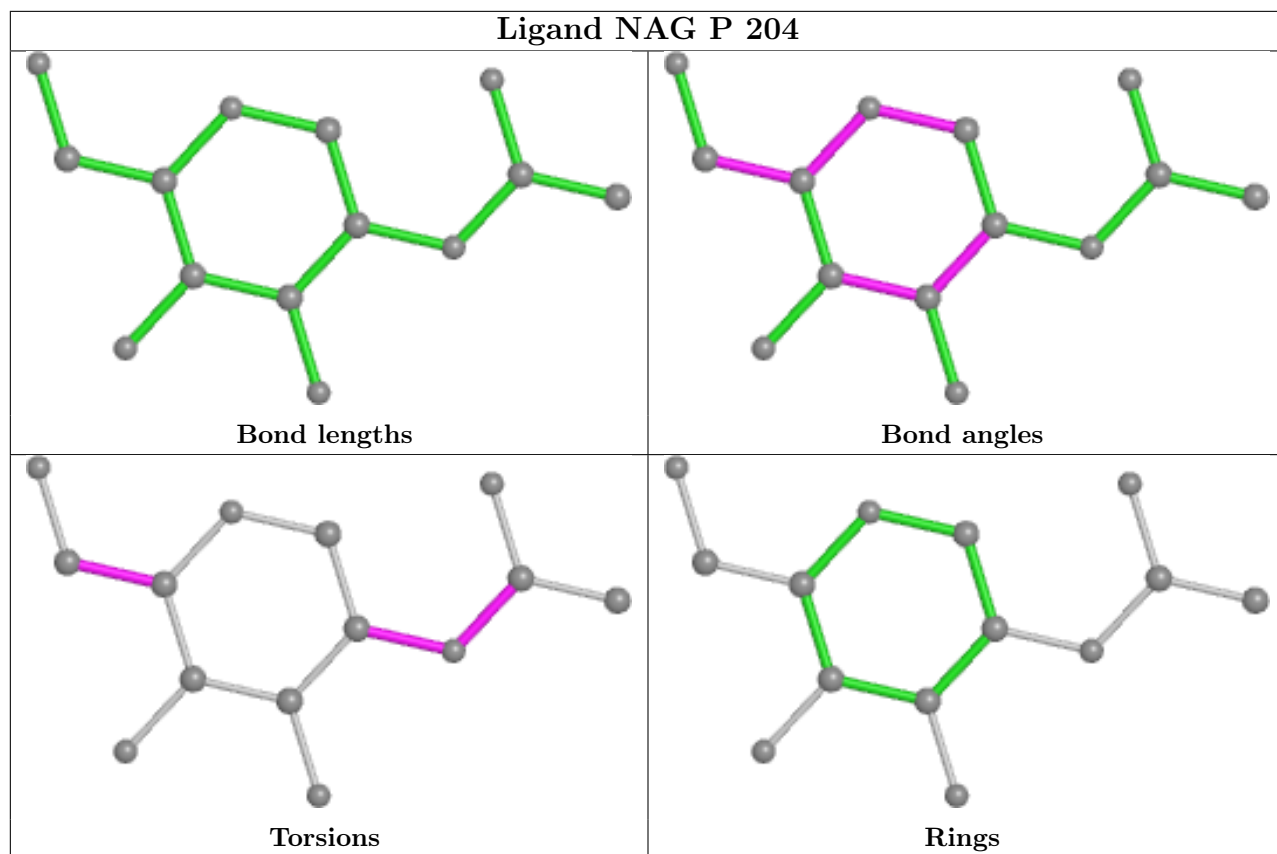
There are no ring outliers.

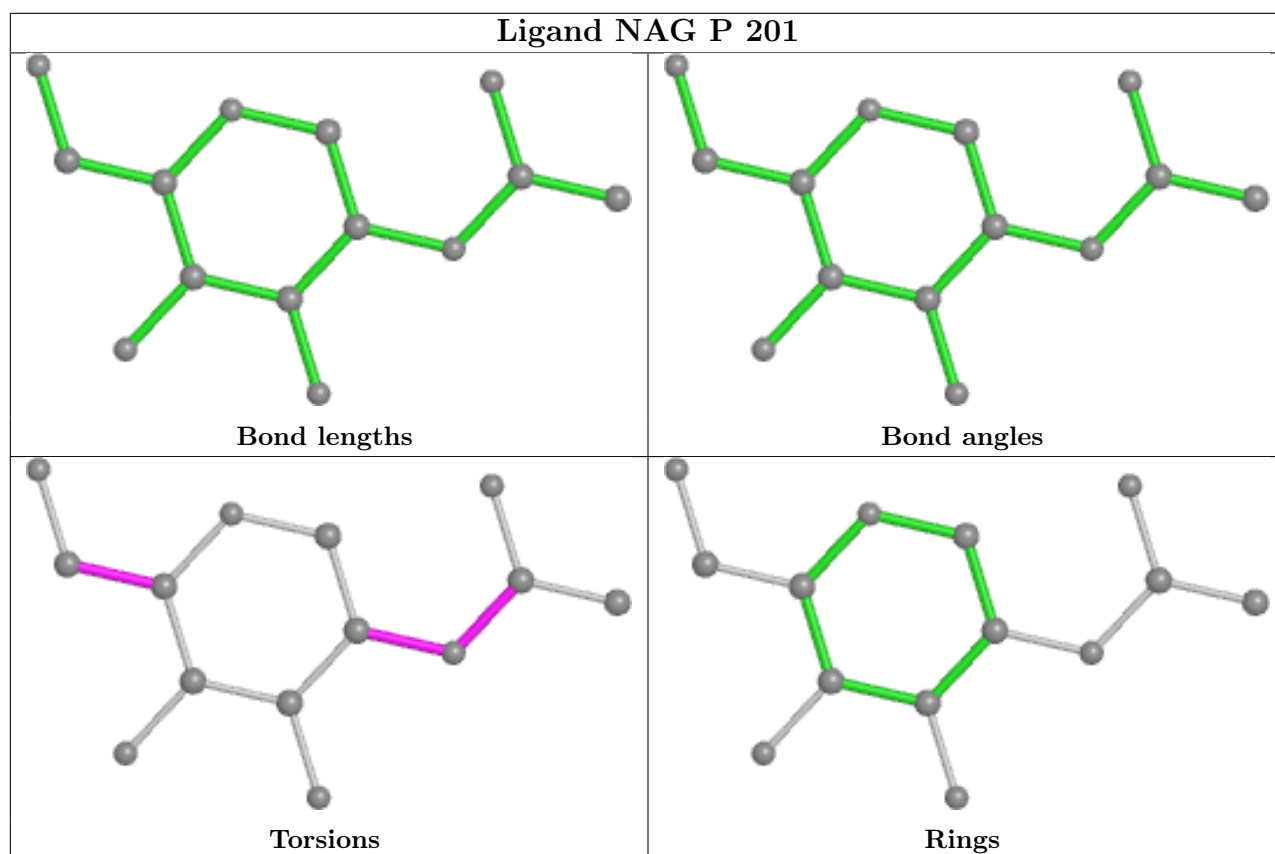
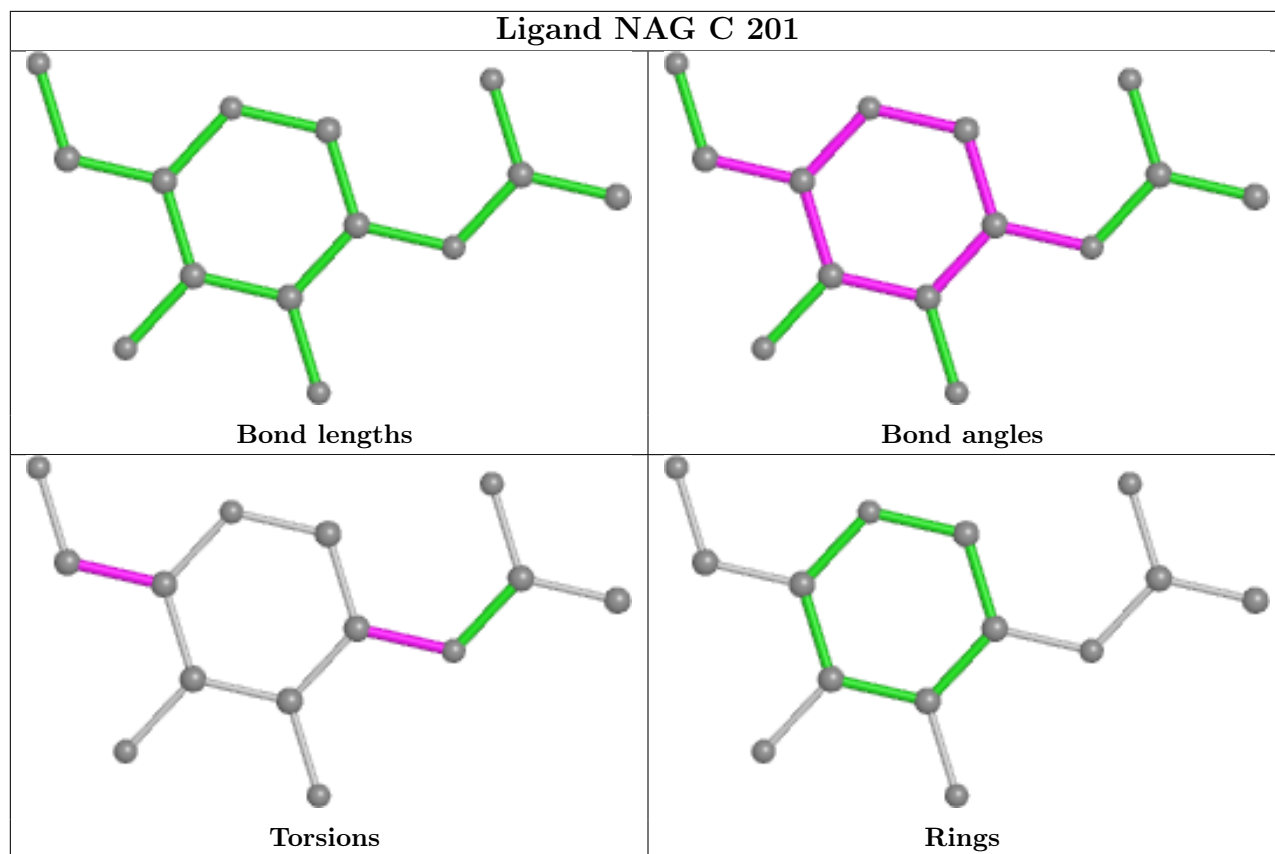
6 monomers are involved in 37 short contacts:

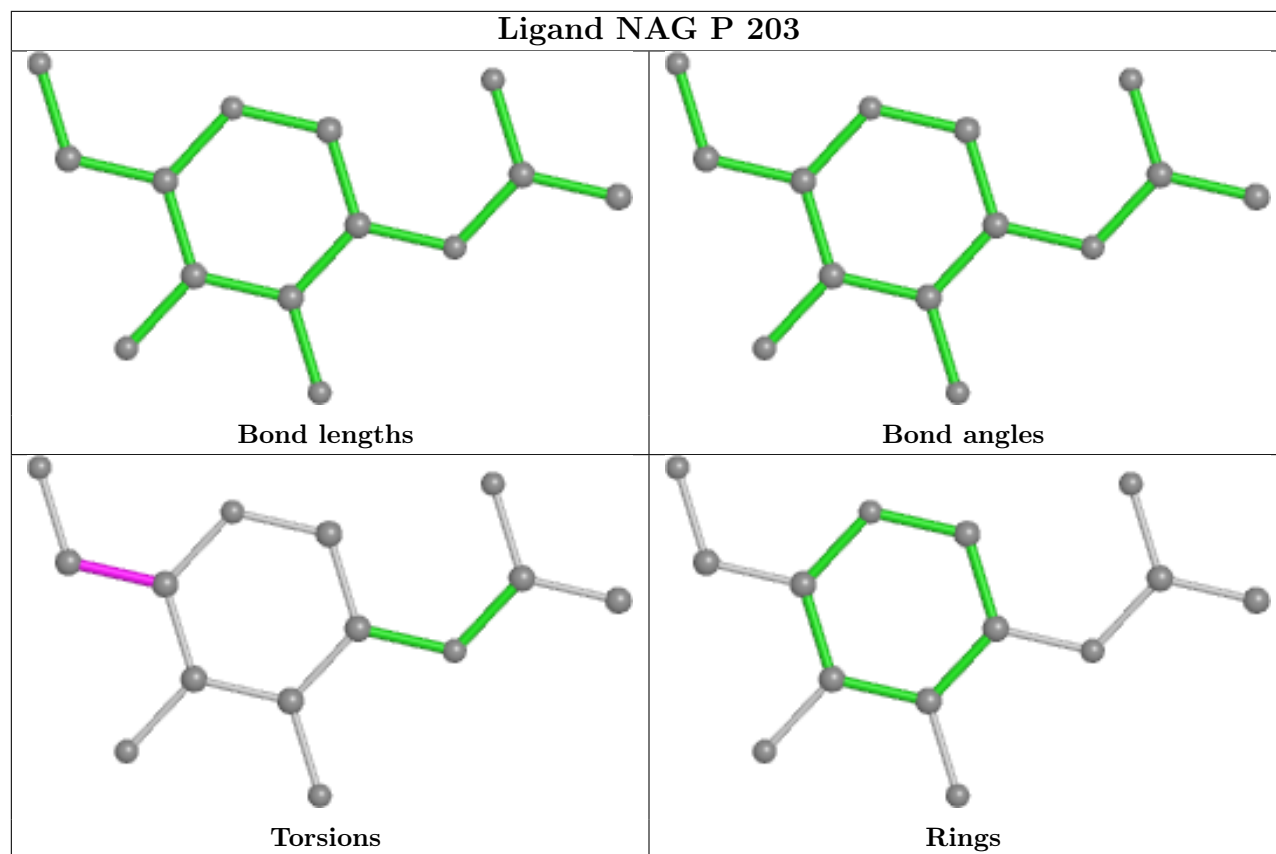
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	202	NAG	2	0
4	P	202	NAG	7	0
4	P	204	NAG	9	0
4	C	203	NAG	11	0
4	P	201	NAG	2	0
4	P	203	NAG	6	0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/228 (95%)	0.63	25 (11%) 4 3	71, 109, 147, 185	0
1	H	218/228 (95%)	0.57	12 (5%) 25 14	57, 89, 143, 161	0
2	B	214/214 (100%)	0.31	3 (1%) 75 63	60, 91, 133, 172	0
2	L	213/214 (99%)	0.57	10 (4%) 31 19	56, 93, 140, 162	0
3	C	114/151 (75%)	0.16	3 (2%) 56 40	85, 123, 163, 185	0
3	P	114/151 (75%)	0.87	14 (12%) 4 2	79, 124, 168, 187	0
All	All	1091/1186 (91%)	0.52	67 (6%) 21 12	56, 100, 151, 187	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	91	GLN	4.7
1	H	69	ILE	4.6
3	P	87	SER	4.1
1	A	18	LEU	3.8
3	P	93	CYS	3.6
3	C	91	GLN	3.6
1	H	212	VAL	3.6
1	A	82	LEU	3.4
3	P	63	PHE	3.4
1	H	24	VAL	3.4
1	A	10	GLY	3.2
3	P	112	ARG	3.2
3	C	141	GLU	3.0
3	P	65	LEU	3.0
1	A	175	LEU	3.0
3	P	97	VAL	3.0
2	B	146	VAL	3.0
3	P	110	VAL	2.9
2	L	32	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	68	THR	2.8
1	A	9	PRO	2.8
1	A	147	VAL	2.7
1	A	69	ILE	2.7
1	A	19	SER	2.6
1	A	112	THR	2.6
1	H	203	VAL	2.6
2	L	11	LEU	2.5
2	L	2	ILE	2.5
1	H	82	LEU	2.5
1	A	121	THR	2.5
1	A	114	VAL	2.5
1	A	207	PRO	2.5
2	L	196	VAL	2.5
1	H	67	VAL	2.5
1	A	204	ASP	2.4
3	P	134	ILE	2.4
1	A	20	LEU	2.4
3	P	82	PHE	2.4
2	B	111	ALA	2.4
3	P	142	LEU	2.4
3	P	88	GLN	2.4
1	A	80	LEU	2.4
2	L	104	LEU	2.4
1	A	126	VAL	2.3
1	A	132	CYS	2.3
1	A	151	PHE	2.3
2	L	92	TYR	2.3
3	P	96	ARG	2.3
1	H	29	LEU	2.3
1	A	93	TYR	2.2
1	H	105	ILE	2.2
1	H	27	PHE	2.2
1	A	174	VAL	2.2
1	A	36	TRP	2.2
3	P	100	LEU	2.2
2	L	98	PHE	2.1
1	H	211	LYS	2.1
2	B	165	GLU	2.1
1	H	36	TRP	2.1
2	L	110	VAL	2.1
1	A	218	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	27	GLU	2.0
2	L	33	VAL	2.0
3	C	65	LEU	2.0
1	A	120	SER	2.0
1	A	180	LEU	2.0
1	A	179	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](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

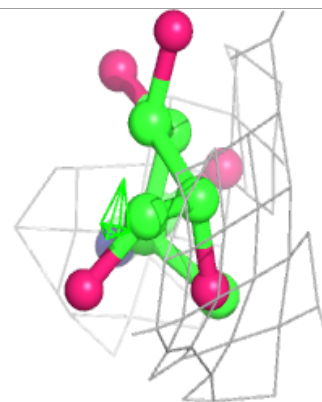
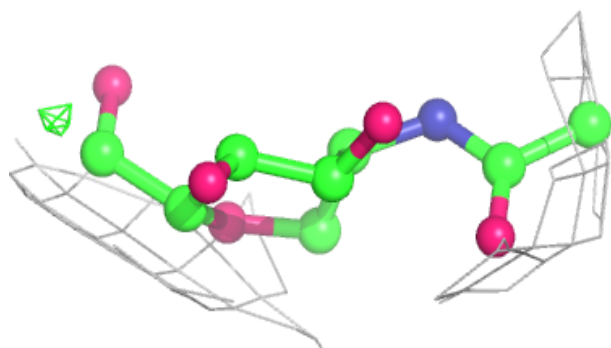
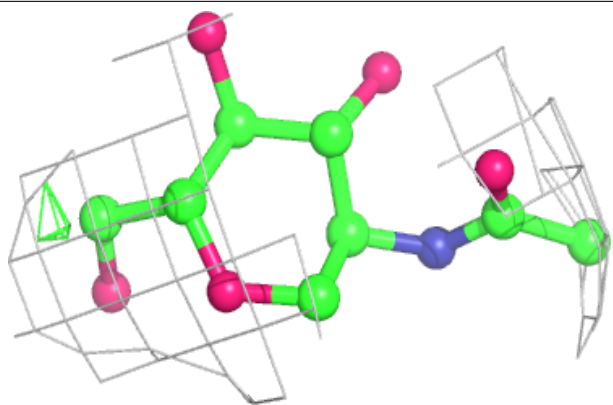
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	201	14/15	0.67	0.20	127,147,162,163	0
4	NAG	C	203	14/15	0.68	0.18	137,166,177,178	0
4	NAG	P	204	14/15	0.69	0.18	140,168,178,185	0
4	NAG	C	202	14/15	0.71	0.22	120,147,158,162	0
4	NAG	P	201	14/15	0.75	0.24	131,153,168,170	0
4	NAG	P	202	14/15	0.77	0.19	124,159,168,168	0
4	NAG	P	203	14/15	0.83	0.25	129,149,160,161	0

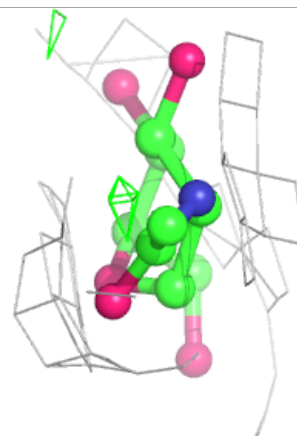
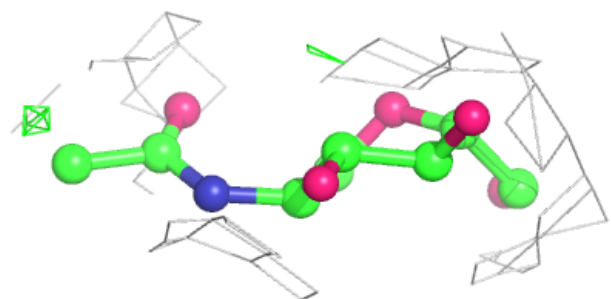
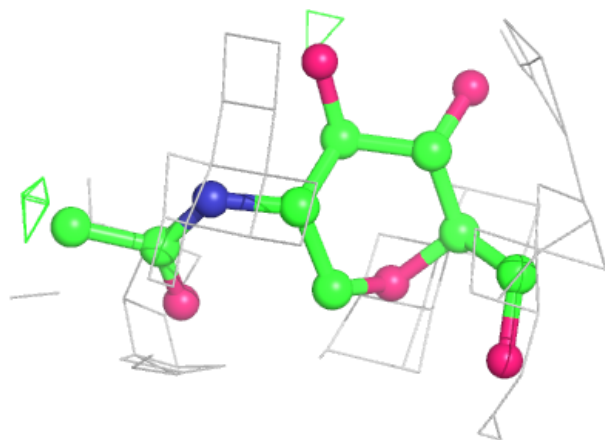
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG C 201:

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

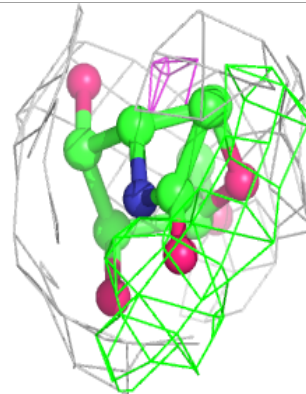
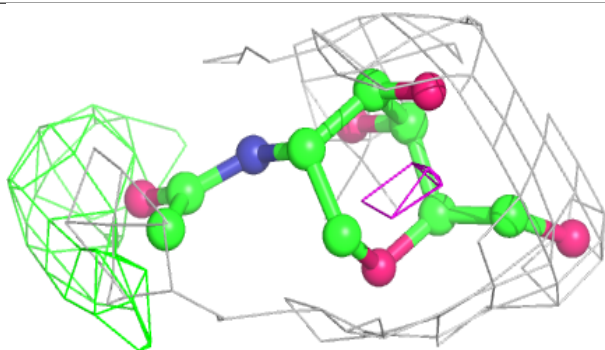
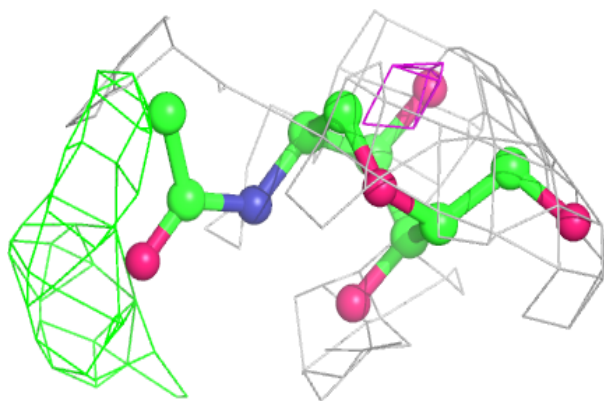
**Electron density around NAG C 203:**

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

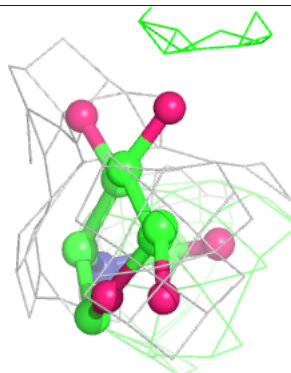
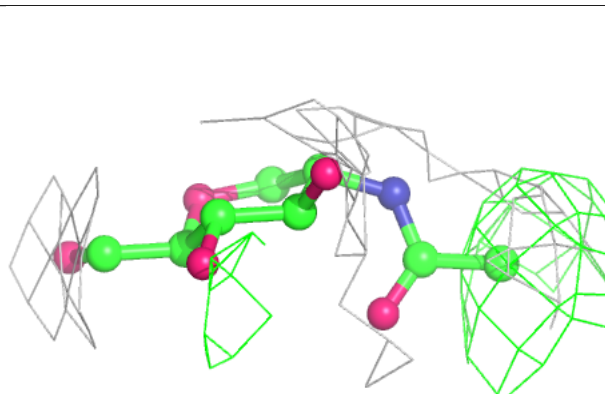
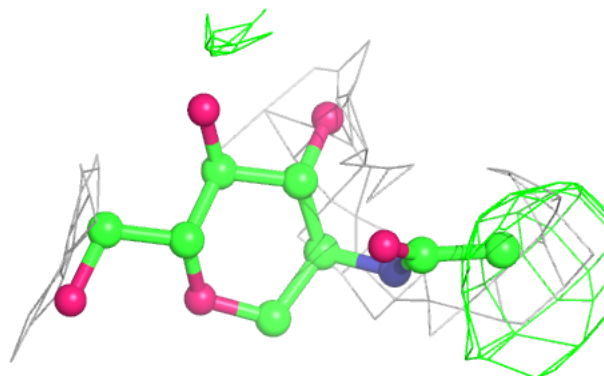


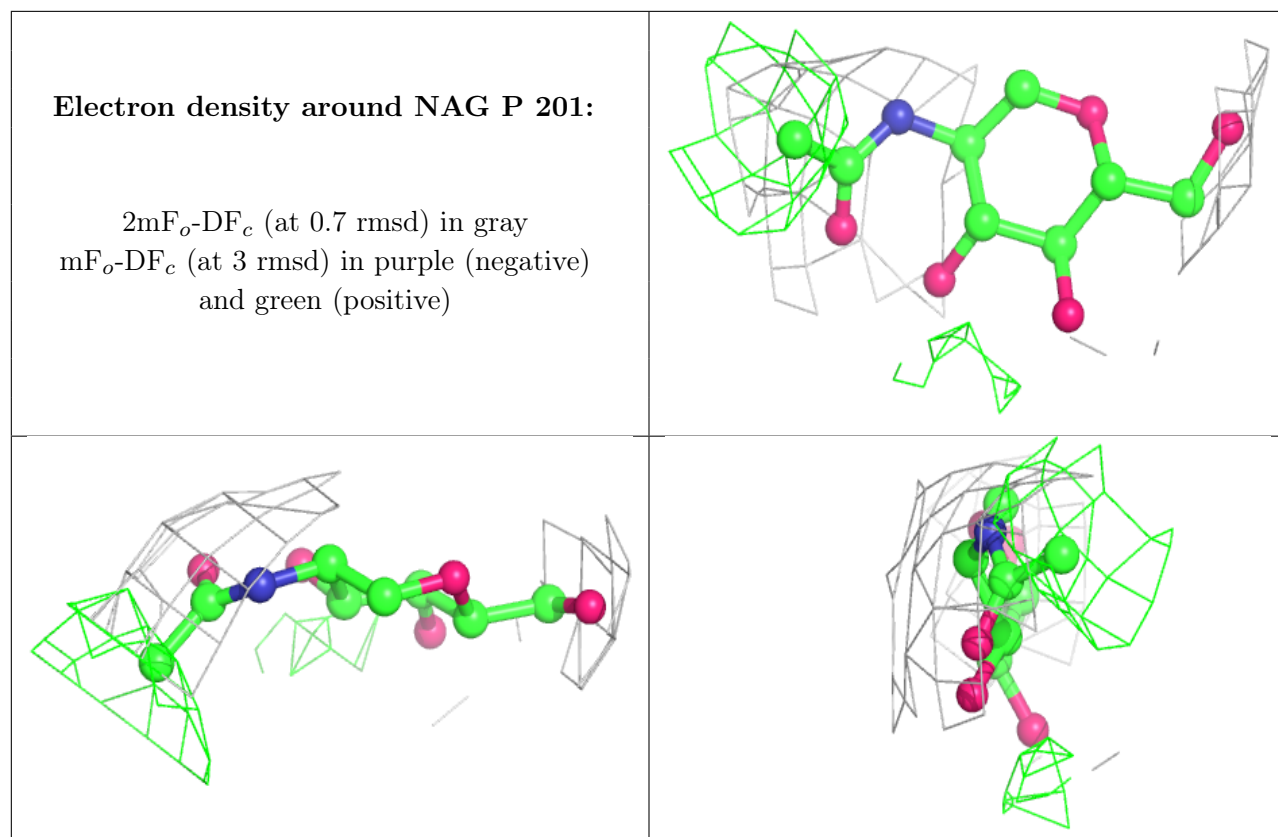
Electron density around NAG P 204:

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

**Electron density around NAG C 202:**

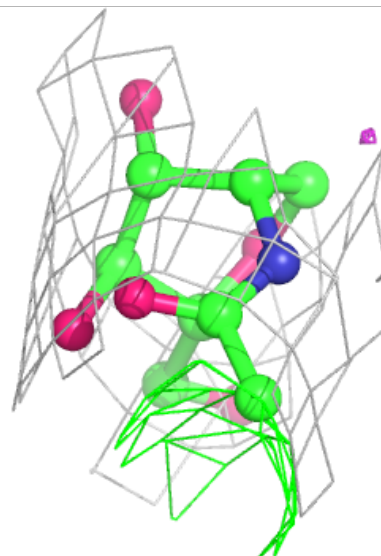
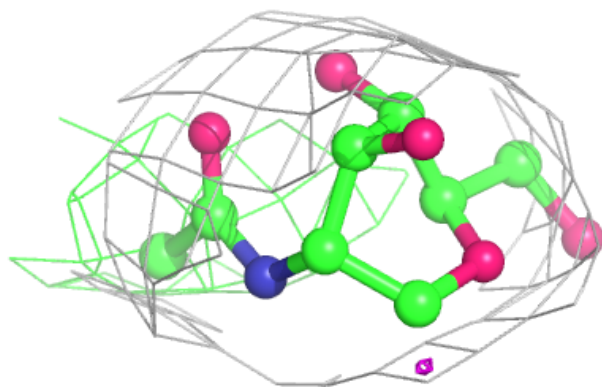
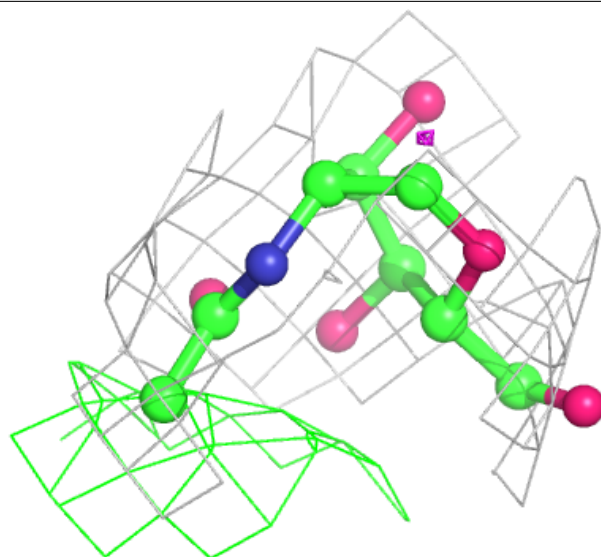
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

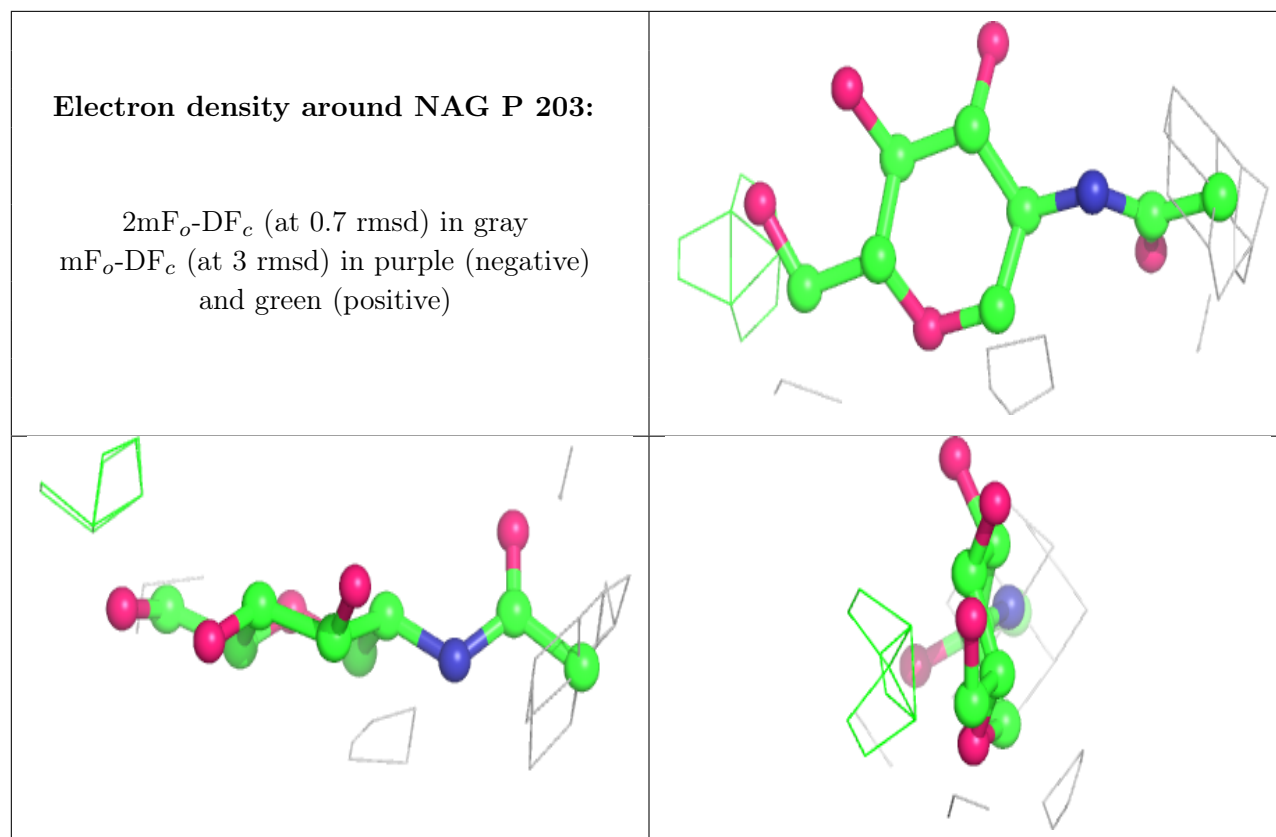




Electron density around NAG P 202:

$2mF_o-DF_c$ (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.