



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:16 PM UTC

PDB ID : 6ZSI / pdb_00006zsi
Title : The mechanism of activation of the actin binding protein EHBP1 by Rab8 family members.
Authors : Rai, A.; Bleimling, N.; Vetter, I.R.; Goody, R.S.
Deposited on : 2020-07-15
Resolution : 1.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

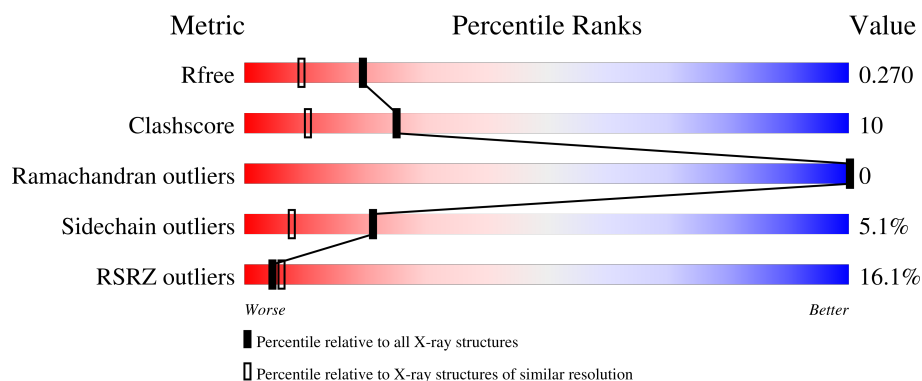
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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

Mol	Chain	Length	Quality of chain
1	A	178	26% 72% 20% • •
1	B	178	3% 90% 7% •
2	C	156	16% 58% 17% 6% • 17%
2	D	156	13% 65% 18% • 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5111 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 Ras-related protein Rab-8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	2	0
			1392	887	236	262	7			
1	B	173	Total	C	N	O	S	0	1	0
			1408	896	243	262	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P61006
A	0	HIS	-	expression tag	UNP P61006
B	-1	GLY	-	expression tag	UNP P61006
B	0	HIS	-	expression tag	UNP P61006

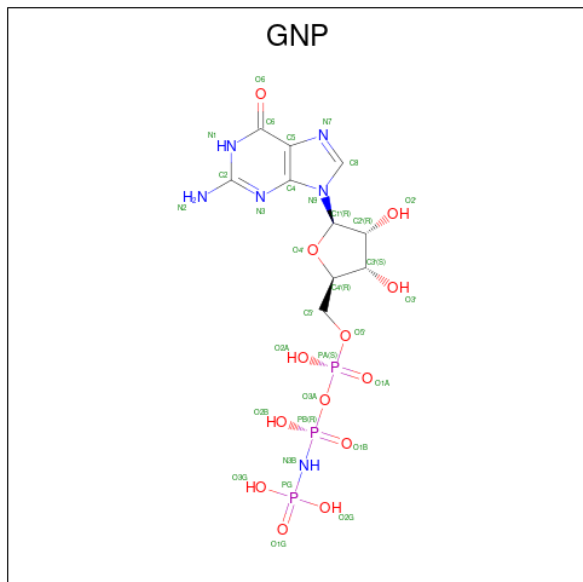
- Molecule 2 is a protein called EH domain-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	130	Total	C	N	O	S	0	0	0
			1081	668	201	207	5			
2	D	133	Total	C	N	O	S	0	0	0
			1108	683	204	216	5			

There are 8 discrepancies between the modelled and reference sequences:

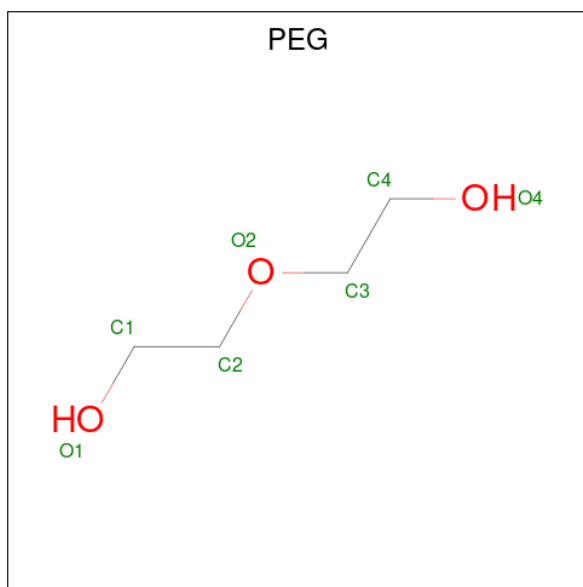
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	GLY	-	expression tag	UNP Q8NDI1
C	1058	HIS	-	expression tag	UNP Q8NDI1
C	1059	MET	-	expression tag	UNP Q8NDI1
C	1116	ALA	MET	engineered mutation	UNP Q8NDI1
D	1057	GLY	-	expression tag	UNP Q8NDI1
D	1058	HIS	-	expression tag	UNP Q8NDI1
D	1059	MET	-	expression tag	UNP Q8NDI1
D	1116	ALA	MET	engineered mutation	UNP Q8NDI1

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

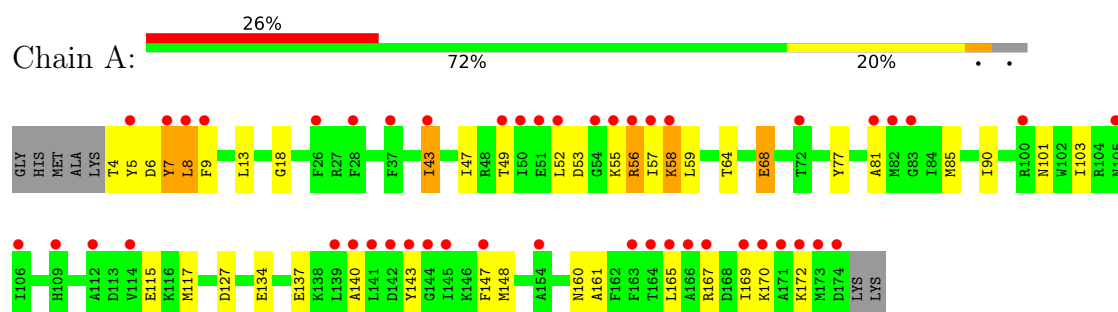
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	18	Total O 18 18	0	0
6	B	22	Total O 22 22	0	0
6	D	2	Total O 2 2	0	0

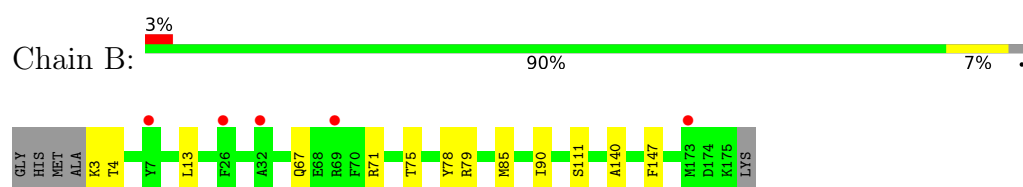
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

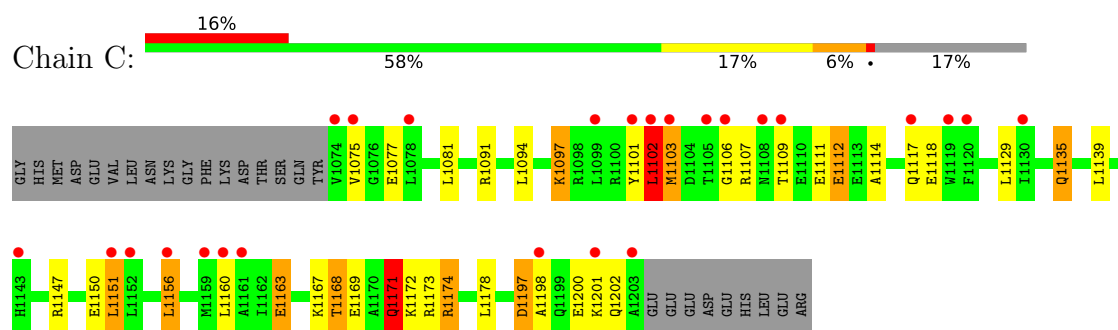
• Molecule 1: Ras-related protein Rab-8A



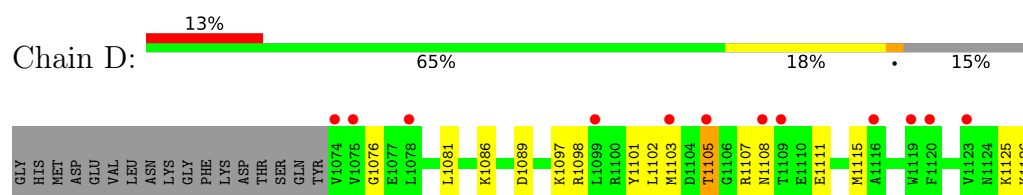
• Molecule 1: Ras-related protein Rab-8A



• Molecule 2: EH domain-binding protein 1



• Molecule 2: EH domain-binding protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.36Å 35.38Å 165.67Å 90.00° 93.76° 90.00°	Depositor
Resolution (Å)	46.11 – 1.91 46.11 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.11-1.91) 99.4 (46.11-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.267 0.230 , 0.270	Depositor DCC
R_{free} test set	2630 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5111	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, GNP, MG

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	0.63	0/1419	0.89	1/1904 (0.1%)
1	B	0.62	0/1432	0.81	0/1918
2	C	0.50	0/1088	0.95	4/1457 (0.3%)
2	D	0.44	0/1115	0.85	2/1493 (0.1%)
All	All	0.56	0/5054	0.87	7/6772 (0.1%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1205	GLU	N-CA-C	-8.42	102.02	113.30
2	C	1112	GLU	N-CA-C	7.16	118.73	111.07
2	D	1076	GLY	N-CA-C	-7.05	105.92	114.66
2	C	1171	GLN	N-CA-C	6.96	121.03	112.54
2	C	1106	GLY	N-CA-C	-6.54	106.08	115.64
1	A	7	TYR	N-CA-C	6.17	118.33	109.14
2	C	1102	LEU	N-CA-C	-5.05	103.81	110.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1204	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1392	0	1401	40	0
1	B	1408	0	1425	9	0
2	C	1081	0	1104	28	0
2	D	1108	0	1122	25	0
3	A	32	0	13	1	0
3	B	32	0	13	0	0
4	A	7	0	10	1	0
4	B	7	0	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	18	0	0	1	0
6	B	22	0	0	1	0
6	D	2	0	0	0	0
All	All	5111	0	5098	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1169:GLU:HA	2:C:1172:LYS:HD2	1.44	0.95
1:A:7:TYR:CE2	1:A:55:LYS:HE3	2.10	0.86
2:C:1091:ARG:NH2	2:C:1118:GLU:OE2	2.09	0.85
2:C:1103:MET:HE1	2:C:1112:GLU:HG3	1.58	0.84
2:D:1101:TYR:OH	2:D:1107:ARG:NH1	2.11	0.82
1:A:4:THR:HG23	1:A:56:ARG:NH1	1.99	0.78
1:A:81:ALA:O	6:A:301:HOH:O	2.04	0.75
1:A:68:GLU:N	1:A:68:GLU:OE1	2.19	0.75
1:B:67:GLN:HG3	6:B:318:HOH:O	1.87	0.73
1:A:7:TYR:HD2	1:A:57[A]:ILE:HG13	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1169:GLU:OE1	2:D:1173:ARG:NH1	2.22	0.72
1:A:115:GLU:OE1	1:A:172:LYS:NZ	2.22	0.72
1:A:53:ASP:OD1	1:A:167:ARG:NH2	2.29	0.66
1:A:169:ILE:HA	1:A:172:LYS:HZ1	1.60	0.66
1:A:4:THR:HG23	1:A:56:ARG:HH12	1.61	0.65
2:D:1162:ILE:HD11	2:D:1167:LYS:HG2	1.76	0.65
2:D:1102:LEU:HD22	2:D:1108:ASN:HB2	1.80	0.64
1:A:5:TYR:OH	2:C:1197:ASP:HB2	1.98	0.63
1:A:169:ILE:HA	1:A:172:LYS:NZ	2.14	0.62
2:C:1198:ALA:O	2:C:1201:LYS:HD2	2.00	0.61
1:A:7:TYR:CD2	1:A:57[A]:ILE:HG13	2.36	0.60
1:A:13:LEU:HD23	1:A:85:MET:HB2	1.83	0.60
2:C:1169:GLU:OE2	2:C:1173:ARG:HB2	2.01	0.60
2:D:1111:GLU:H	2:D:1111:GLU:CD	2.08	0.60
2:D:1169:GLU:HA	2:D:1172:LYS:HE2	1.86	0.58
1:A:52:LEU:HB3	1:A:57[A]:ILE:HD13	1.86	0.57
2:D:1108:ASN:HB3	2:D:1111:GLU:OE1	2.04	0.57
1:A:6:ASP:HB3	1:A:7:TYR:CZ	2.40	0.57
2:D:1167:LYS:O	2:D:1172:LYS:NZ	2.37	0.56
1:A:8:LEU:HD23	1:A:58:LYS:HE2	1.87	0.56
1:A:165:LEU:O	1:A:169:ILE:HG12	2.06	0.55
2:C:1198:ALA:HA	2:C:1201:LYS:HE3	1.89	0.54
1:B:71:ARG:O	1:B:75:THR:HG23	2.07	0.54
2:D:1164:ASP:O	2:D:1172:LYS:NZ	2.41	0.54
1:A:140:ALA:CB	1:A:147:PHE:HB2	2.38	0.54
2:C:1077:GLU:O	2:C:1081:LEU:HD13	2.08	0.53
1:A:5:TYR:HA	1:A:56:ARG:NE	2.24	0.52
2:D:1171:GLN:HG3	2:D:1174:ARG:HH12	1.74	0.52
2:D:1127:ASN:O	2:D:1130:ILE:HG13	2.10	0.52
2:C:1102:LEU:HD23	2:C:1112:GLU:HB2	1.92	0.51
1:A:7:TYR:HE2	1:A:55:LYS:HG3	1.75	0.51
2:C:1094:LEU:HA	2:C:1097:LYS:HE3	1.91	0.51
2:C:1101:TYR:OH	2:C:1107:ARG:NH1	2.44	0.50
1:A:43:ILE:HD13	1:A:77:TYR:CD2	2.47	0.49
2:C:1168:THR:OG1	2:C:1171:GLN:HG3	2.13	0.49
1:B:4:THR:OG1	2:D:1200:GLU:OE2	2.22	0.49
1:A:9:PHE:HB2	1:A:59:LEU:HD23	1.94	0.49
1:B:13:LEU:HD23	1:B:85:MET:HB2	1.94	0.49
1:A:101:ASN:HB3	4:A:202:PEG:H22	1.93	0.49
1:B:75:THR:HA	1:B:78:TYR:CE1	2.48	0.49
1:A:6:ASP:HB2	1:A:56:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HE2	1:A:170:LYS:CE	2.43	0.48
1:B:75:THR:HA	1:B:78:TYR:CD1	2.49	0.48
2:D:1089:ASP:HB3	2:D:1126:LYS:HE3	1.96	0.48
2:D:1107:ARG:O	2:D:1108:ASN:ND2	2.47	0.47
2:D:1105:THR:C	2:D:1107:ARG:H	2.22	0.47
1:A:117:MET:HE1	1:A:161:ALA:HA	1.97	0.46
1:A:7:TYR:CZ	1:A:55:LYS:HE3	2.49	0.46
2:D:1171:GLN:HG3	2:D:1174:ARG:NH1	2.30	0.46
1:B:140:ALA:CB	1:B:147:PHE:HB2	2.46	0.45
2:C:1156:LEU:HD22	2:C:1160:LEU:HG	1.98	0.45
1:A:5:TYR:HA	1:A:56:ARG:CD	2.46	0.45
1:A:43:ILE:HD12	1:A:64:THR:HG22	1.98	0.45
1:A:127:ASP:OD1	1:A:127:ASP:N	2.50	0.45
2:C:1168:THR:HG23	2:C:1171:GLN:NE2	2.32	0.45
2:D:1103:MET:HB3	2:D:1103:MET:HE2	1.62	0.45
2:C:1135:GLN:O	2:C:1139:LEU:HD23	2.17	0.44
2:C:1163:GLU:CD	2:C:1163:GLU:H	2.24	0.44
2:D:1167:LYS:C	2:D:1172:LYS:HZ3	2.23	0.44
1:A:4:THR:HA	2:C:1200:GLU:OE2	2.18	0.44
1:B:79:ARG:NH1	1:B:111:SER:OG	2.51	0.43
2:C:1103:MET:HB2	2:C:1103:MET:HE2	1.61	0.43
1:A:49:THR:HA	1:A:58:LYS:HA	2.00	0.43
1:A:5:TYR:CD1	1:A:5:TYR:C	2.96	0.43
2:C:1156:LEU:CD2	2:C:1160:LEU:HG	2.49	0.43
2:D:1086:LYS:HA	2:D:1089:ASP:OD1	2.19	0.43
2:D:1125:LYS:O	2:D:1129:LEU:HB2	2.18	0.42
2:D:1089:ASP:OD1	2:D:1089:ASP:N	2.50	0.42
2:D:1098:ARG:HB3	2:D:1115:MET:HE2	2.00	0.42
1:A:148:MET:HE1	1:A:160:ASN:HB3	2.01	0.42
2:C:1198:ALA:HA	2:C:1201:LYS:CE	2.49	0.42
2:C:1147:ARG:O	2:C:1151:LEU:HG	2.19	0.42
2:C:1109:THR:HA	2:C:1112:GLU:HB3	2.02	0.42
2:C:1102:LEU:HD21	2:C:1111:GLU:HG2	2.01	0.42
1:A:52:LEU:HD11	1:A:167:ARG:CG	2.49	0.42
2:C:1111:GLU:O	2:C:1114:ALA:HB3	2.20	0.41
2:C:1081:LEU:HB3	2:C:1129:LEU:HD11	2.01	0.41
2:C:1103:MET:HE1	2:C:1112:GLU:CG	2.39	0.41
2:C:1150:GLU:HG2	2:C:1151:LEU:HD23	2.03	0.41
1:A:6:ASP:CB	1:A:7:TYR:CE2	3.03	0.41
2:D:1081:LEU:HD13	2:D:1132:ARG:HG2	2.02	0.41
2:C:1174:ARG:O	2:C:1178:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HD2	1:B:3:LYS:HA	1.73	0.40
2:D:1097:LYS:HA	2:D:1097:LYS:HD2	1.95	0.40
1:A:103:ILE:HD13	1:A:143:TYR:CZ	2.56	0.40
2:D:1111:GLU:CD	2:D:1111:GLU:N	2.79	0.40
1:A:6:ASP:HB3	1:A:7:TYR:CE2	2.56	0.40
1:A:18:GLY:H	3:A:201:GNP:HNB3	1.68	0.40
1:A:137:GLU:HG3	1:A:147:PHE:CD2	2.57	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	171/178 (96%)	167 (98%)	4 (2%)	0	100	100
1	B	172/178 (97%)	170 (99%)	2 (1%)	0	100	100
2	C	128/156 (82%)	124 (97%)	4 (3%)	0	100	100
2	D	131/156 (84%)	128 (98%)	3 (2%)	0	100	100
All	All	602/668 (90%)	589 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	150/153 (98%)	142 (95%)	8 (5%)	20	7
1	B	151/153 (99%)	150 (99%)	1 (1%)	76	73
2	C	114/138 (83%)	99 (87%)	15 (13%)	4	0
2	D	117/138 (85%)	114 (97%)	3 (3%)	40	24
All	All	532/582 (91%)	505 (95%)	27 (5%)	21	8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	43	ILE
1	A	47	ILE
1	A	56	ARG
1	A	58	LYS
1	A	68	GLU
1	A	90	ILE
1	A	134	GLU
1	B	90	ILE
2	C	1075	VAL
2	C	1097	LYS
2	C	1102	LEU
2	C	1103	MET
2	C	1117	GLN
2	C	1135	GLN
2	C	1151	LEU
2	C	1156	LEU
2	C	1163	GLU
2	C	1167	LYS
2	C	1168	THR
2	C	1171	GLN
2	C	1174	ARG
2	C	1197	ASP
2	C	1202	GLN
2	D	1105	THR
2	D	1162	ILE
2	D	1171	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	GLN

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Mol	Chain	Res	Type
2	C	1143	HIS
2	D	1108	ASN
2	D	1117	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GNP	B	201	5	34,34,34	1.35	3 (8%)	47,54,54	1.13	4 (8%)
3	GNP	A	201	5	34,34,34	1.46	5 (14%)	47,54,54	1.35	6 (12%)
4	PEG	A	202	-	6,6,6	0.49	0	5,5,5	0.38	0
4	PEG	B	202	-	6,6,6	0.52	0	5,5,5	0.32	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
3	GNP	B	201	5	-	3/18/38/38	0/3/3/3
3	GNP	A	201	5	-	3/18/38/38	0/3/3/3
4	PEG	A	202	-	-	3/4/4/4	-
4	PEG	B	202	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GNP	PG-O1G	4.67	1.53	1.46
3	B	201	GNP	PG-O1G	4.20	1.52	1.46
3	A	201	GNP	PB-O2B	-3.93	1.46	1.56
3	B	201	GNP	PB-O3A	-3.46	1.54	1.59
3	B	201	GNP	PB-O2B	-2.84	1.49	1.56
3	A	201	GNP	PG-O2G	-2.47	1.50	1.56
3	A	201	GNP	PA-O3A	-2.22	1.57	1.59
3	A	201	GNP	PB-O1B	2.12	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	GNP	O1G-PG-N3B	-4.95	104.48	111.77
3	B	201	GNP	O2B-PB-O1B	3.42	117.19	109.87
3	A	201	GNP	O2B-PB-O1B	3.31	116.97	109.87
3	A	201	GNP	O1B-PB-N3B	-3.24	107.00	111.77
3	B	201	GNP	O1G-PG-N3B	-3.11	107.19	111.77
3	A	201	GNP	O2G-PG-O3G	2.70	114.85	107.59
3	B	201	GNP	O3G-PG-O1G	-2.68	106.73	113.45
3	B	201	GNP	O2B-PB-O3A	2.60	113.33	104.64
3	A	201	GNP	O3G-PG-O1G	-2.43	107.37	113.45
3	A	201	GNP	O2B-PB-O3A	2.39	112.62	104.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GNP	PG-N3B-PB-O1B
3	A	201	GNP	PA-O3A-PB-O2B
3	B	201	GNP	PG-N3B-PB-O1B
3	B	201	GNP	PA-O3A-PB-O2B
4	B	202	PEG	O1-C1-C2-O2
4	A	202	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	202	PEG	C1-C2-O2-C3
4	A	202	PEG	O2-C3-C4-O4
4	B	202	PEG	O2-C3-C4-O4
3	A	201	GNP	PA-O3A-PB-O1B
3	B	201	GNP	PA-O3A-PB-O1B

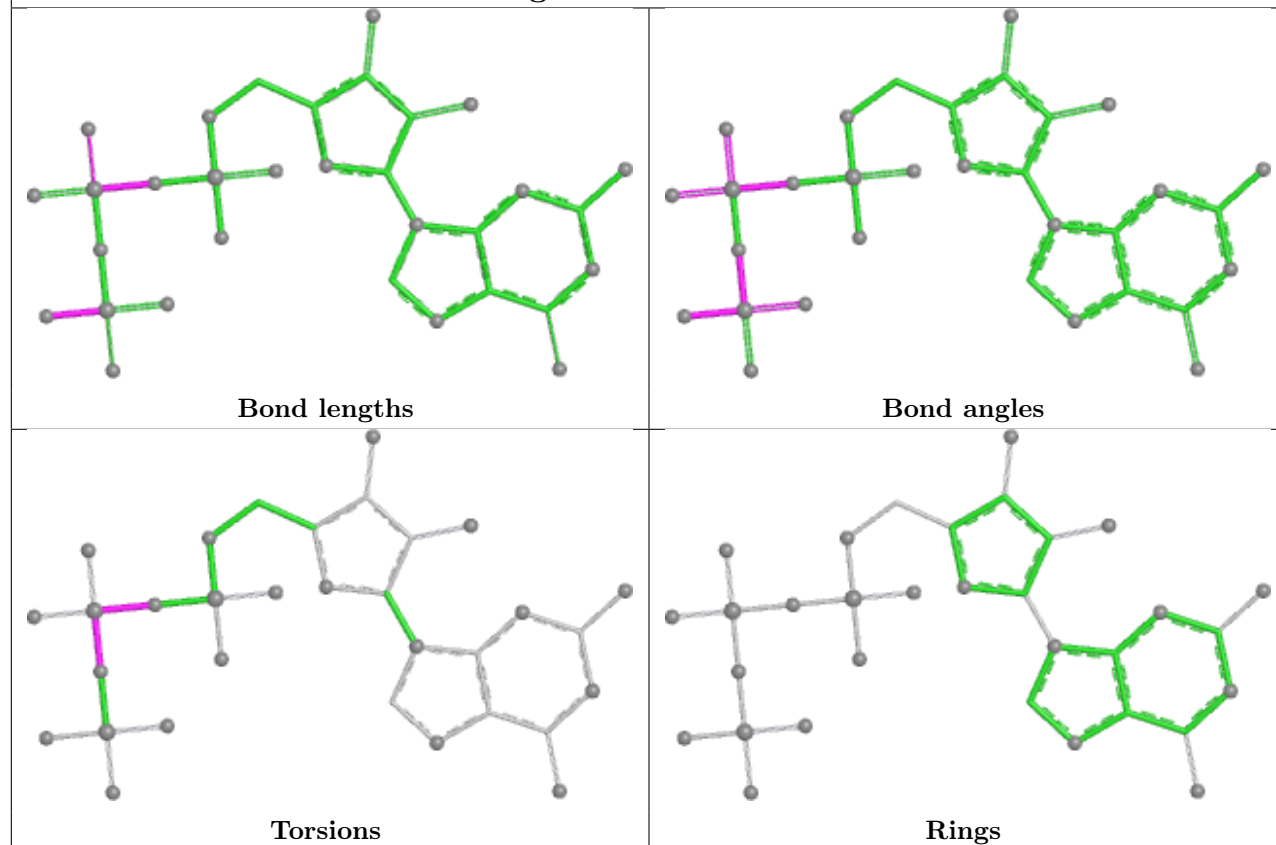
There are no ring outliers.

2 monomers are involved in 2 short contacts:

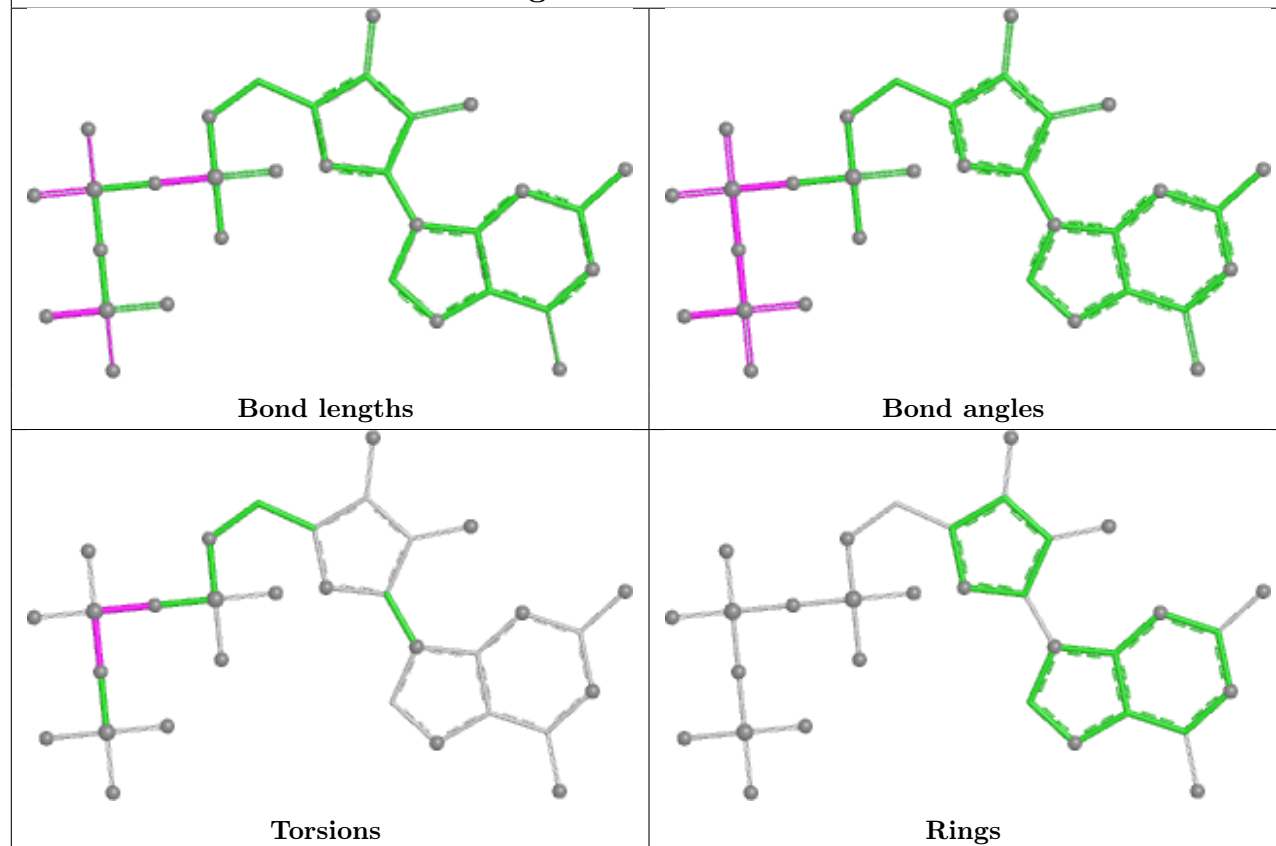
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	GNP	1	0
4	A	202	PEG	1	0

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 GNP B 201



Ligand GNP A 201



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	171/178 (96%)	1.32	47 (27%) 1 1	31, 61, 124, 162	2 (1%)
1	B	173/178 (97%)	0.31	5 (2%) 53 60	29, 46, 69, 94	1 (0%)
2	C	130/156 (83%)	1.39	25 (19%) 3 4	47, 88, 139, 151	0
2	D	133/156 (85%)	1.23	21 (15%) 5 6	43, 79, 123, 142	0
All	All	607/668 (90%)	1.03	98 (16%) 4 6	29, 66, 126, 162	3 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	GLY	6.7
1	A	52	LEU	5.2
2	D	1075	VAL	4.9
1	A	50	ILE	4.8
1	A	7	TYR	4.6
1	A	171	ALA	4.5
1	A	167	ARG	4.3
1	A	169	ILE	4.3
1	A	141	LEU	4.2
2	D	1074	VAL	4.2
2	C	1074	VAL	4.1
1	A	166	ALA	4.1
2	C	1109	THR	4.1
2	C	1203	ALA	4.0
1	A	145	ILE	3.9
1	A	112	ALA	3.7
2	D	1108	ASN	3.6
1	A	174	ASP	3.6
1	A	163	PHE	3.6
1	A	9	PHE	3.5
1	A	105	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	1203	ALA	3.4
1	A	57[A]	ILE	3.3
2	D	1120	PHE	3.3
1	B	26	PHE	3.3
1	A	140	ALA	3.2
2	D	1130	ILE	3.2
1	A	144	GLY	3.2
1	A	170	LYS	3.1
1	A	83	GLY	3.1
2	C	1101	TYR	3.1
2	D	1158	ALA	3.1
2	C	1151	LEU	3.0
1	B	7	TYR	2.9
1	B	32	ALA	2.9
1	A	139	LEU	2.9
2	C	1159	MET	2.8
1	A	8	LEU	2.8
1	A	5	TYR	2.8
2	D	1109	THR	2.8
2	C	1102	LEU	2.8
1	A	114	VAL	2.8
1	A	81	ALA	2.7
2	C	1099	LEU	2.7
2	C	1106	GLY	2.7
1	A	26	PHE	2.7
1	A	43	ILE	2.6
2	C	1075	VAL	2.6
2	C	1120	PHE	2.6
1	A	173	MET	2.6
1	A	143	TYR	2.6
2	C	1105	THR	2.6
2	C	1119	TRP	2.5
2	D	1165	TRP	2.5
2	D	1160	LEU	2.5
2	D	1162	ILE	2.5
1	A	164	THR	2.5
2	D	1159	MET	2.5
1	A	142[A]	ASP	2.5
1	A	165	LEU	2.5
2	C	1160	LEU	2.5
2	D	1119	TRP	2.5
2	D	1078	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	1117	GLN	2.4
1	A	49	THR	2.4
2	D	1105	THR	2.4
1	A	28	PHE	2.4
2	D	1161	ALA	2.4
2	C	1152	LEU	2.3
1	A	56	ARG	2.3
2	D	1116	ALA	2.3
2	C	1078	LEU	2.3
1	A	82	MET	2.3
1	A	100	ARG	2.3
1	B	69[A]	ARG	2.3
1	A	72	THR	2.3
1	B	173	MET	2.3
2	C	1156	LEU	2.3
2	D	1123	VAL	2.2
1	A	106	ILE	2.2
2	C	1143	HIS	2.2
1	A	172	LYS	2.2
2	C	1103	MET	2.2
2	D	1103	MET	2.2
2	C	1130	ILE	2.2
1	A	51	GLU	2.2
2	D	1206	GLU	2.2
1	A	37	PHE	2.1
1	A	58	LYS	2.1
2	C	1201	LYS	2.1
1	A	154	ALA	2.1
2	C	1161	ALA	2.1
2	C	1198	ALA	2.1
1	A	55	LYS	2.1
1	A	147	PHE	2.0
1	A	109	HIS	2.0
2	C	1108	ASN	2.0
2	D	1099	LEU	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](#)

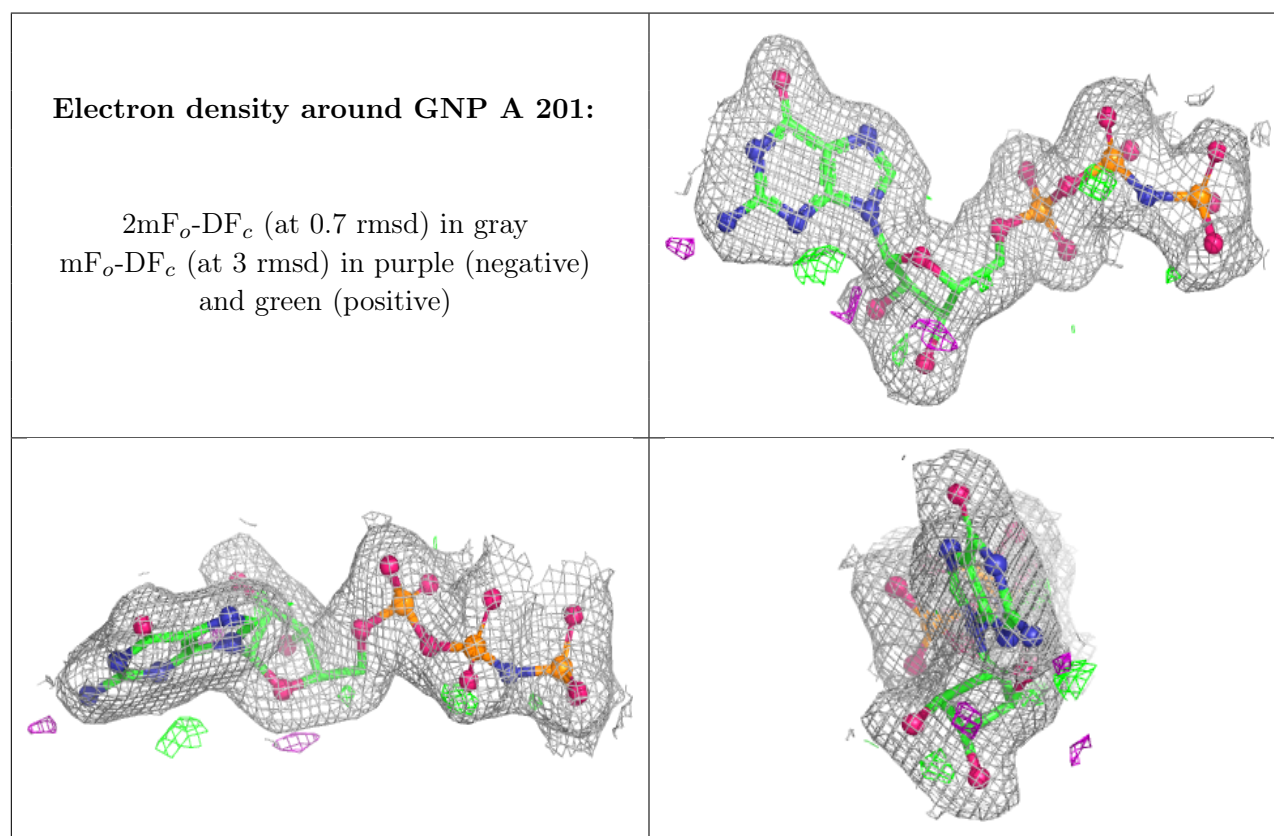
There are no oligosaccharides in this entry.

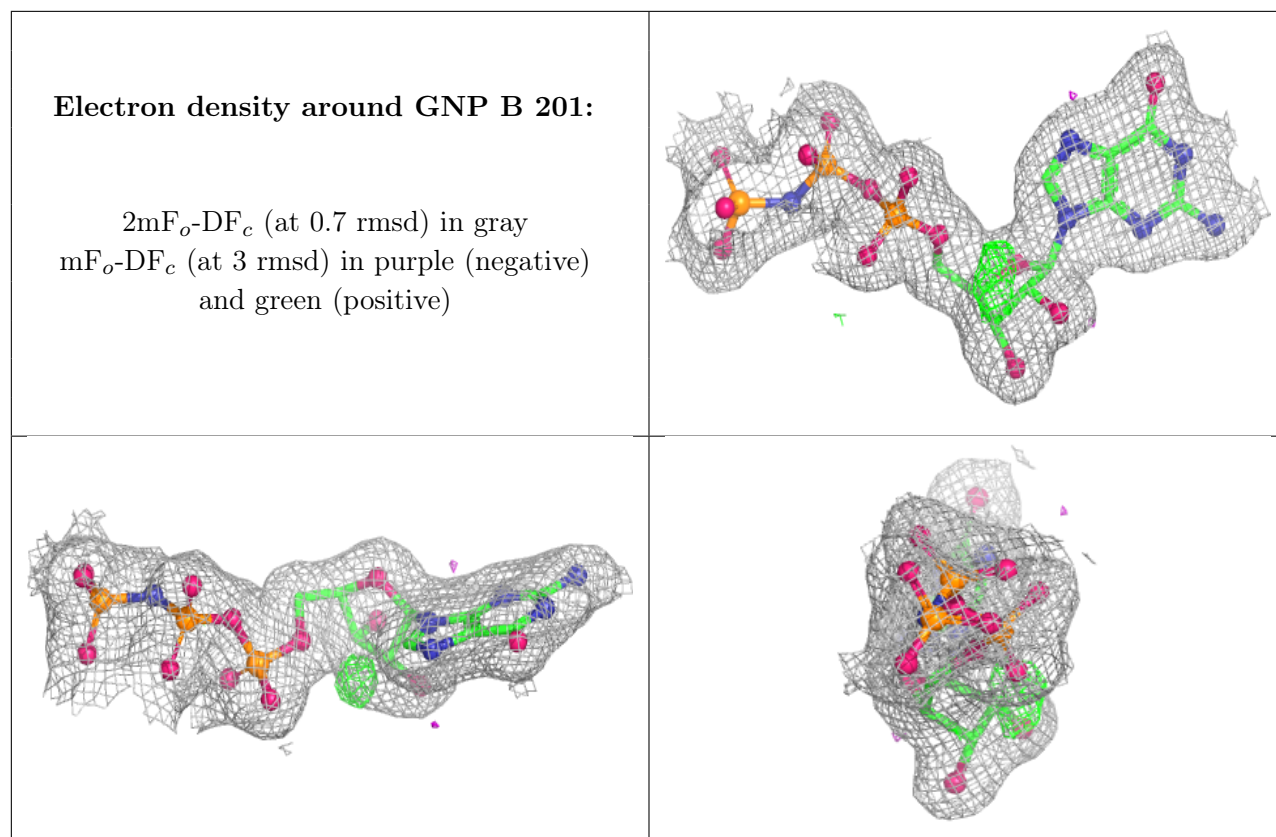
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	A	202	7/7	0.87	0.14	51,67,70,76	0
4	PEG	B	202	7/7	0.92	0.10	44,47,51,56	0
3	GNP	A	201	32/32	0.97	0.06	30,34,45,46	0
3	GNP	B	201	32/32	0.98	0.06	28,33,40,44	0
5	MG	A	203	1/1	0.99	0.04	37,37,37,37	0
5	MG	B	203	1/1	0.99	0.05	35,35,35,35	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.