



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:09 AM UTC

PDB ID : 6X2M / pdb_00006x2m
Title : Crystal Structure of unliganded CRM1-Ran-RanBP1
Authors : Baumhardt, J.M.
Deposited on : 2020-05-20
Resolution : 2.35 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

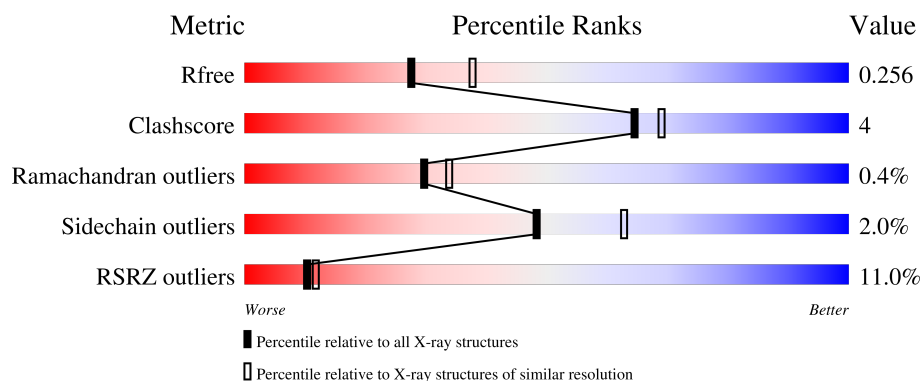
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	216	9% 87% 8% .
2	B	140	6% 79% 9% 12%
3	C	1024	12% 88% 11% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11210 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	3	0
			1694	1093	291	304	6			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	2	0
			1029	652	181	191	5			

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1011	Total	C	N	O	S	8	25	0
			8310	5336	1367	1562	45			

There are 45 discrepancies between the modelled and reference sequences:

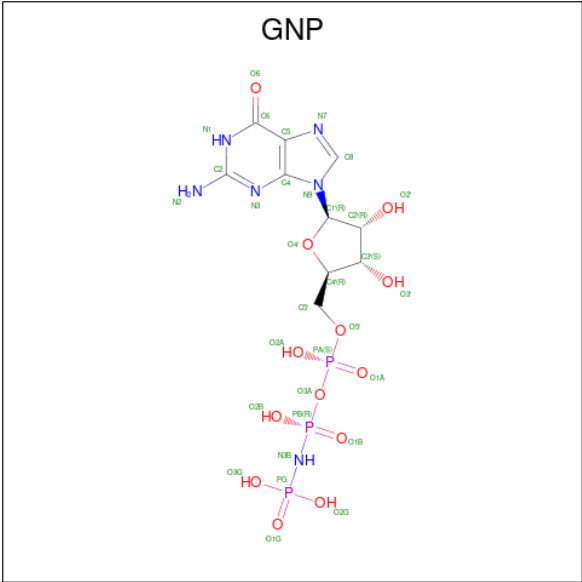
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P30822
C	-1	GLY	-	expression tag	UNP P30822
C	0	SER	-	expression tag	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	ASN	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	TYR	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	LYS	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	PHE	deletion	UNP P30822
C	537	GLY	ASP	conflict	UNP P30822
C	539	CYS	THR	conflict	UNP P30822
C	540	GLU	VAL	conflict	UNP P30822
C	541	GLN	LYS	conflict	UNP P30822
C	1022	CYS	TYR	conflict	UNP P30822

- Molecule 4 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).

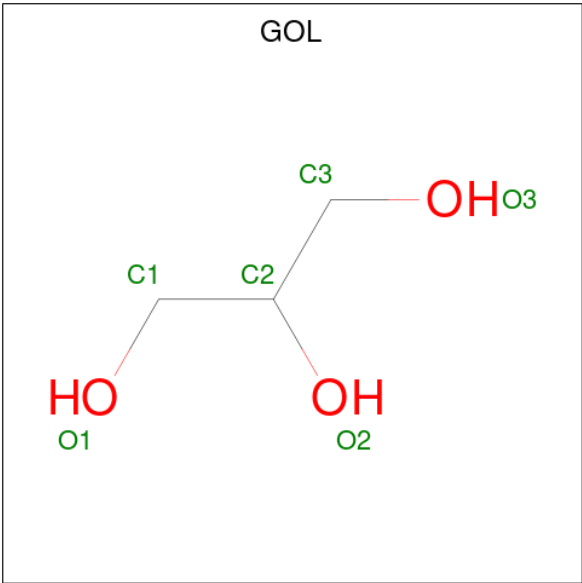


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	6	0
			6	3	3		

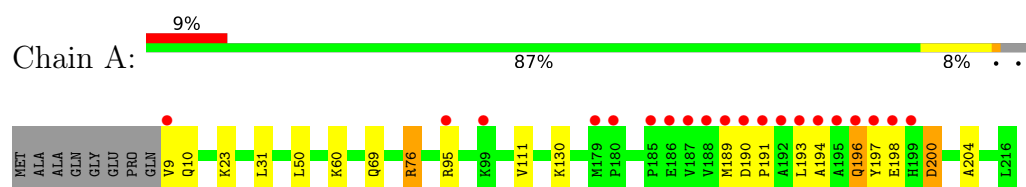
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	25	Total	O	0	0
			25	25		
7	B	8	Total	O	0	0
			8	8		
7	C	105	Total	O	0	0
			105	105		

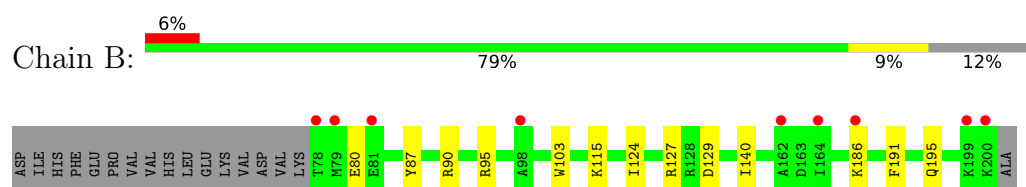
3 Residue-property plots [i](#)

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.

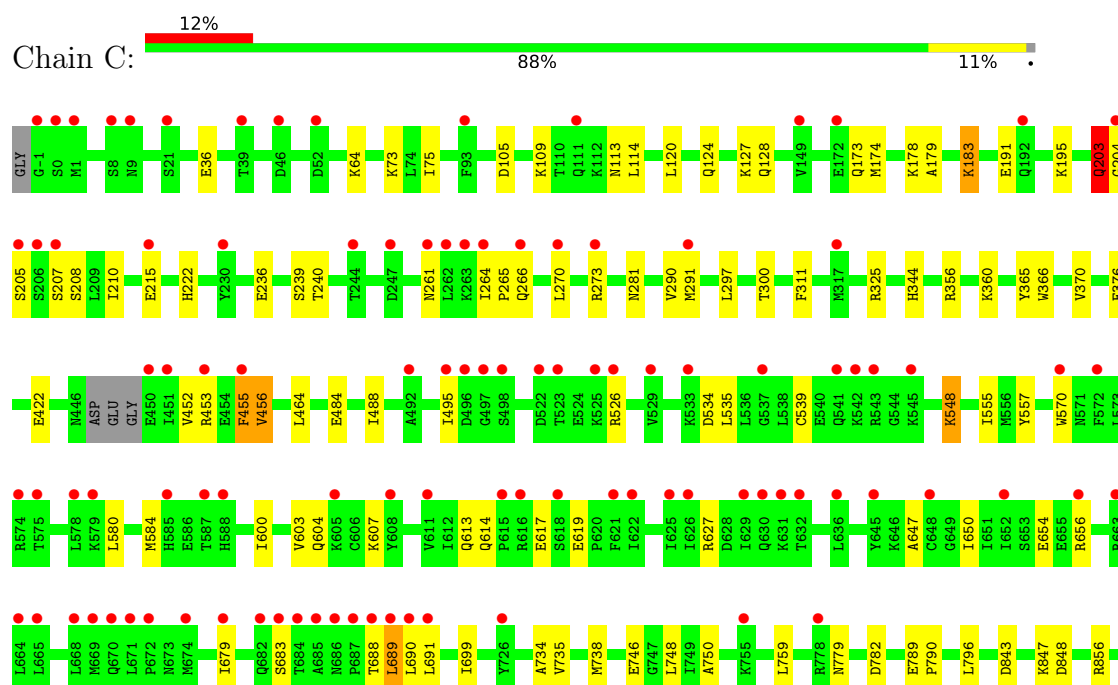
- Molecule 1: GTP-binding nuclear protein Ran

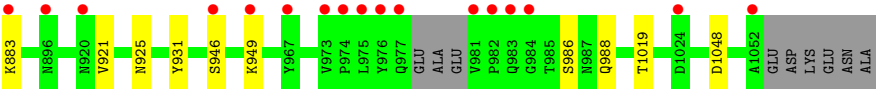


- Molecule 2: Ran-specific GTPase-activating protein 1



- Molecule 3: Exportin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.31Å 105.31Å 306.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.23 – 2.35 37.23 – 2.35	Depositor EDS
% Data completeness (in resolution range)	64.1 (37.23-2.35) 82.2 (37.23-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.232 , 0.261 0.230 , 0.256	Depositor DCC
R_{free} test set	57896 reflections (96.66%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11210	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: GOL, 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	0.13	0/1736	0.32	0/2356
2	B	0.11	0/1047	0.31	0/1397
3	C	0.12	0/8477	0.29	0/11484
All	All	0.12	0/11260	0.30	0/15237

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
3	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	203	GLN	Peptide

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	1694	0	1693	16	0
2	B	1029	0	1029	8	0
3	C	8310	0	8387	64	0
4	A	32	0	12	1	0
5	A	1	0	0	0	0
6	C	6	0	7	0	0
7	A	25	0	0	3	0
7	B	8	0	0	2	0
7	C	105	0	0	12	0
All	All	11210	0	11128	86	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 4.

All (86) 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:C:376:GLU:O	7:C:1201:HOH:O	1.94	0.86
3:C:679:ILE:HD12	3:C:699:ILE:HG12	1.65	0.79
3:C:1048:ASP:O	7:C:1202:HOH:O	2.06	0.72
2:B:95[B]:ARG:NH1	7:B:301:HOH:O	2.22	0.71
3:C:178:LYS:NZ	7:C:1210:HOH:O	2.23	0.71
3:C:600:ILE:HG12	3:C:647:ALA:HB2	1.73	0.71
3:C:204[B]:GLY:HA2	3:C:210:ILE:HD11	1.75	0.69
3:C:204[A]:GLY:HA2	3:C:210:ILE:HD11	1.76	0.67
3:C:607:LYS:NZ	3:C:654:GLU:OE1	2.30	0.65
1:A:9:VAL:N	7:A:402:HOH:O	2.30	0.64
1:A:23:LYS:NZ	4:A:301:GNP:O2G	2.31	0.64
3:C:619:GLU:OE1	3:C:627:ARG:NH2	2.31	0.63
2:B:87:TYR:OH	2:B:186:LYS:NZ	2.32	0.61
3:C:931:TYR:OH	7:C:1203:HOH:O	2.14	0.60
3:C:207[A]:SER:O	3:C:210:ILE:N	2.36	0.59
3:C:173:GLN:NE2	7:C:1216:HOH:O	2.37	0.58
3:C:557:TYR:OH	7:C:1205:HOH:O	2.17	0.57
3:C:356:ARG:HD2	3:C:464:LEU:HD22	1.87	0.57
3:C:325:ARG:NH1	7:C:1217:HOH:O	2.38	0.56
1:A:189:MET:HE3	1:A:197:TYR:HD2	1.72	0.55
3:C:688:THR:O	3:C:691:LEU:HG	2.06	0.55
1:A:196:GLN:C	1:A:198:GLU:H	2.16	0.54
3:C:261:ASN:OD1	3:C:325:ARG:NH1	2.41	0.54
1:A:196:GLN:O	1:A:196:GLN:NE2	2.39	0.54
3:C:484:GLU:OE2	3:C:526:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:452:VAL:HG22	3:C:453:ARG:H	1.74	0.53
3:C:925:ASN:OD1	7:C:1206:HOH:O	2.18	0.53
1:A:200:ASP:N	1:A:200:ASP:OD1	2.42	0.53
3:C:64:LYS:HD2	3:C:114:LEU:HD21	1.91	0.53
3:C:455:PHE:HD2	3:C:456:VAL:HG22	1.74	0.53
3:C:495:ILE:HD11	3:C:534:ASP:HB3	1.90	0.52
3:C:789:GLU:HG3	3:C:790:PRO:HD3	1.92	0.52
1:A:10:GLN:OE1	1:A:60:LYS:NZ	2.43	0.52
3:C:222:HIS:NE2	7:C:1215:HOH:O	2.34	0.51
3:C:207[B]:SER:O	3:C:210:ILE:N	2.42	0.51
3:C:191:GLU:O	3:C:195:LYS:HG2	2.09	0.51
3:C:127:LYS:HE3	3:C:174:MET:HE2	1.94	0.50
1:A:95:ARG:HD3	1:A:130:LYS:HB3	1.94	0.49
3:C:779:ASN:ND2	3:C:782:ASP:OD2	2.46	0.48
3:C:746:GLU:HB2	3:C:750:ALA:HB2	1.94	0.48
3:C:291[A]:MET:HE1	3:C:300:THR:HG21	1.95	0.48
3:C:883:LYS:HG3	3:C:931:TYR:OH	2.13	0.48
3:C:366:TRP:O	3:C:370:VAL:HG22	2.14	0.47
3:C:782:ASP:OD2	7:C:1209:HOH:O	2.20	0.47
1:A:190:ASP:OD2	1:A:193:LEU:N	2.48	0.46
1:A:31:LEU:HD23	1:A:50:LEU:HD13	1.97	0.46
3:C:539:CYS:SG	3:C:548:LYS:HG3	2.56	0.46
3:C:236:GLU:O	3:C:240:THR:OG1	2.25	0.46
3:C:291[A]:MET:HE3	3:C:297:LEU:HD22	1.99	0.45
2:B:95[A]:ARG:NE	7:B:302:HOH:O	2.33	0.45
3:C:105:ASP:O	3:C:109:LYS:HG2	2.17	0.44
3:C:779:ASN:HB3	7:C:1209:HOH:O	2.15	0.44
3:C:679:ILE:O	3:C:683:SER:OG	2.27	0.44
3:C:203:GLN:HE21	3:C:203:GLN:HB3	1.62	0.44
1:A:76:ARG:NH2	7:A:409:HOH:O	2.51	0.44
3:C:344:HIS:NE2	3:C:365:TYR:OH	2.48	0.44
1:A:197:TYR:HB3	7:A:410:HOH:O	2.18	0.44
2:B:80:GLU:OE1	2:B:127:ARG:NH2	2.44	0.44
1:A:189:MET:O	1:A:191:PRO:HD3	2.18	0.43
3:C:580:LEU:O	3:C:584:MET:HG3	2.18	0.43
3:C:848:ASP:O	3:C:856:ARG:NH2	2.43	0.43
3:C:986:SER:OG	3:C:988:GLN:OE1	2.35	0.43
2:B:90:ARG:HH12	2:B:129:ASP:CG	2.26	0.43
2:B:124:ILE:HG13	2:B:140:ILE:HG12	2.00	0.43
3:C:688:THR:O	3:C:690:LEU:N	2.52	0.43
2:B:191:PHE:O	2:B:195:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:SER:HB2	3:C:281:ASN:HB2	2.00	0.42
3:C:735[B]:VAL:HG13	3:C:759:LEU:HB3	2.02	0.42
3:C:748:LEU:HD23	3:C:748:LEU:HA	1.89	0.42
1:A:191:PRO:HA	1:A:194:ALA:HB3	2.02	0.42
3:C:796:LEU:HD23	3:C:796:LEU:HA	1.86	0.42
3:C:843:ASP:O	3:C:847:LYS:NZ	2.50	0.42
1:A:204:ALA:HB1	2:B:103:TRP:CZ2	2.54	0.42
3:C:789:GLU:CG	3:C:790:PRO:HD3	2.49	0.42
3:C:179:ALA:O	3:C:183:LYS:HB2	2.20	0.41
3:C:604:GLN:HG3	3:C:650:ILE:HD13	2.02	0.41
3:C:946:SER:HA	3:C:949:LYS:HE3	2.02	0.41
1:A:111:VAL:HA	3:C:113[B]:ASN:ND2	2.35	0.41
3:C:183:LYS:NZ	7:C:1229:HOH:O	2.52	0.41
3:C:75:ILE:O	3:C:128:GLN:NE2	2.54	0.41
3:C:570:TRP:CE2	3:C:614:GLN:HG3	2.56	0.41
3:C:734:ALA:O	3:C:738:MET:HG3	2.21	0.41
3:C:290:VAL:HG11	3:C:311:PHE:CE2	2.55	0.41
3:C:535:LEU:HB3	3:C:555:ILE:HG12	2.03	0.41
3:C:613:GLN:NE2	3:C:617:GLU:O	2.54	0.41
3:C:120:LEU:O	3:C:124:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	209/216 (97%)	200 (96%)	9 (4%)	0	100	100
2	B	123/140 (88%)	117 (95%)	6 (5%)	0	100	100
3	C	1030/1024 (101%)	992 (96%)	32 (3%)	6 (1%)	21	24
All	All	1362/1380 (99%)	1309 (96%)	47 (4%)	6 (0%)	30	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	205[A]	SER
3	C	205[B]	SER
3	C	208	SER
3	C	689	LEU
3	C	266	GLN
3	C	265	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/185 (99%)	178 (97%)	5 (3%)	39	52
2	B	107/121 (88%)	106 (99%)	1 (1%)	70	82
3	C	944/933 (101%)	924 (98%)	20 (2%)	47	61
All	All	1234/1239 (100%)	1208 (98%)	26 (2%)	48	61

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69[A]	GLN
1	A	69[B]	GLN
1	A	76	ARG
1	A	196	GLN
1	A	200	ASP
2	B	115	LYS
3	C	36	GLU
3	C	73	LYS
3	C	183	LYS
3	C	203	GLN
3	C	215[A]	GLU
3	C	215[B]	GLU
3	C	264	ILE
3	C	270	LEU
3	C	273	ARG

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Mol	Chain	Res	Type
3	C	360	LYS
3	C	422	GLU
3	C	455	PHE
3	C	456	VAL
3	C	488	ILE
3	C	548	LYS
3	C	603	VAL
3	C	656	ARG
3	C	689	LEU
3	C	921	VAL
3	C	1019	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	143	ASN
1	A	205	GLN
2	B	198	ASN
3	C	49	GLN
3	C	62	GLN
3	C	281	ASN
3	C	313	GLN
3	C	326	ASN
3	C	345	GLN
3	C	426	GLN
3	C	463	GLN
3	C	630	GLN
3	C	640	GLN
3	C	730	GLN
3	C	906	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
4	GNP	A	301	5	34,34,34	3.70	16 (47%)	47,54,54	1.66	8 (17%)
6	GOL	C	1101	-	5,5,5	0.49	0	5,5,5	0.26	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	GNP	A	301	5	-	7/18/38/38	0/3/3/3
6	GOL	C	1101	-	-	4/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	C2-N2	8.81	1.54	1.34
4	A	301	GNP	O4'-C1'	8.57	1.61	1.42
4	A	301	GNP	PA-O3A	7.32	1.67	1.59
4	A	301	GNP	C2'-C1'	-7.09	1.31	1.53
4	A	301	GNP	PB-O3A	6.91	1.67	1.59
4	A	301	GNP	PB-O1B	5.74	1.54	1.46
4	A	301	GNP	O4'-C4'	-5.37	1.33	1.45
4	A	301	GNP	PG-O1G	4.04	1.52	1.46
4	A	301	GNP	O2'-C2'	4.01	1.52	1.43
4	A	301	GNP	C6-N1	-3.18	1.32	1.38
4	A	301	GNP	O3'-C3'	-2.95	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	PB-N3B	2.71	1.70	1.63
4	A	301	GNP	O6-C6	-2.57	1.18	1.23
4	A	301	GNP	PA-O5'	2.42	1.68	1.59
4	A	301	GNP	PG-N3B	2.36	1.69	1.63
4	A	301	GNP	PB-O2B	-2.07	1.51	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	GNP	C5-C4-N3	-5.15	120.20	128.39
4	A	301	GNP	C2-N3-C4	4.42	119.91	112.30
4	A	301	GNP	N9-C8-N7	-2.99	107.86	113.40
4	A	301	GNP	N9-C4-N3	2.88	131.71	125.95
4	A	301	GNP	C2-N1-C6	-2.80	120.03	125.11
4	A	301	GNP	C5-C6-N1	2.64	119.98	113.25
4	A	301	GNP	O6-C6-C5	-2.49	119.96	126.53
4	A	301	GNP	C8-N7-C5	2.11	108.01	104.26

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
6	C	1101	GOL	C1-C2-C3-O3
4	A	301	GNP	C3'-C4'-C5'-O5'
6	C	1101	GOL	O1-C1-C2-C3
6	C	1101	GOL	O2-C2-C3-O3
4	A	301	GNP	O4'-C4'-C5'-O5'
6	C	1101	GOL	O1-C1-C2-O2
4	A	301	GNP	C5'-O5'-PA-O3A
4	A	301	GNP	C5'-O5'-PA-O1A
4	A	301	GNP	C5'-O5'-PA-O2A
4	A	301	GNP	PG-N3B-PB-O3A

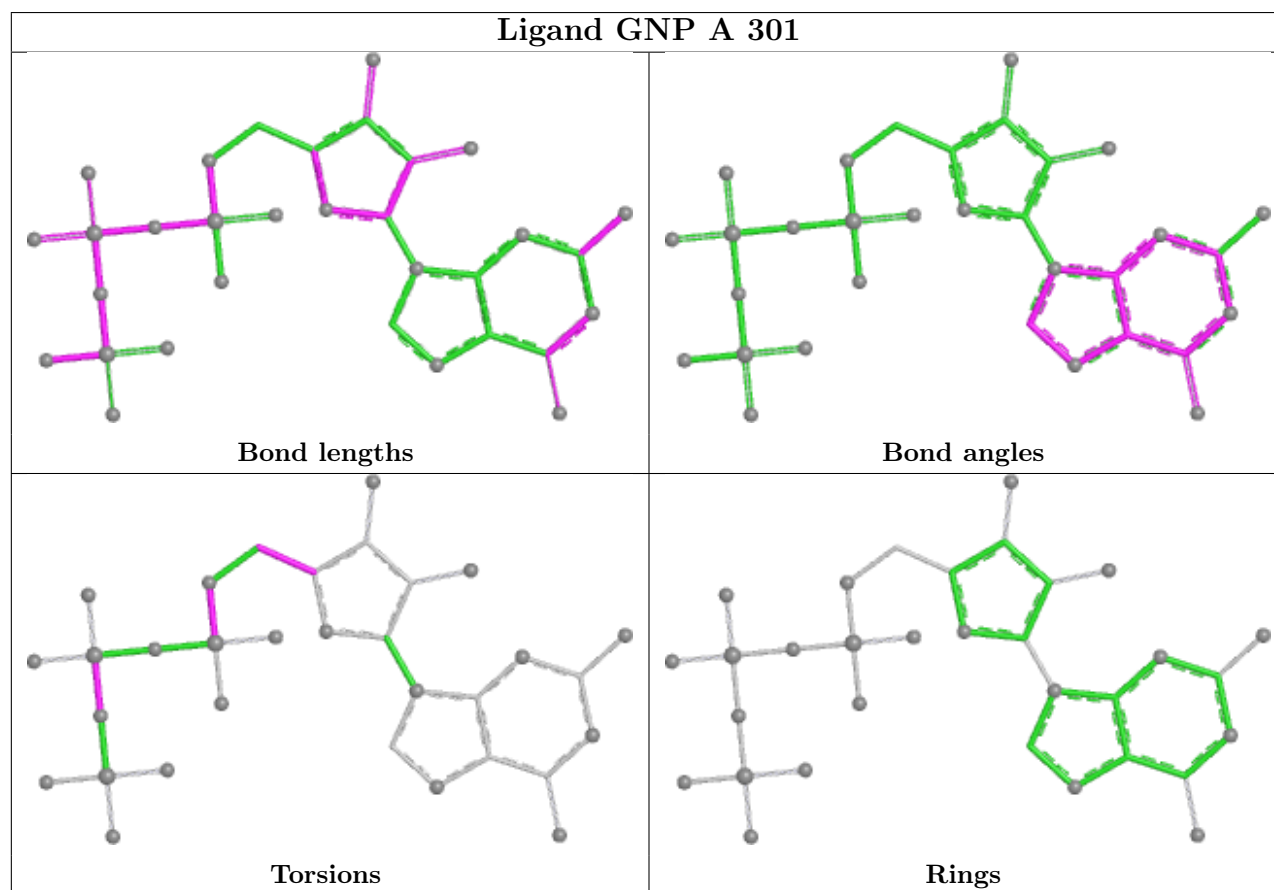
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GNP	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	208/216 (96%)	0.50	20 (9%) 13 16	9, 22, 97, 161	3 (1%)
2	B	123/140 (87%)	0.83	9 (7%) 21 24	17, 41, 61, 83	2 (1%)
3	C	1011/1024 (98%)	0.70	119 (11%) 9 10	3, 32, 66, 95	26 (2%)
All	All	1342/1380 (97%)	0.68	148 (11%) 10 12	3, 32, 66, 161	31 (2%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	39[A]	THR	9.5
1	A	195	ALA	7.8
1	A	197	TYR	6.8
3	C	206[A]	SER	6.8
1	A	194	ALA	6.2
3	C	317	MET	6.2
3	C	215[A]	GLU	6.1
3	C	291[A]	MET	5.6
3	C	684	THR	5.6
1	A	188	VAL	5.4
1	A	191	PRO	5.3
3	C	664	LEU	5.3
3	C	205[A]	SER	4.9
1	A	193	LEU	4.9
1	A	187	VAL	4.9
3	C	629	ILE	4.8
1	A	189	MET	4.6
3	C	455	PHE	4.5
3	C	611	VAL	4.3
3	C	668	LEU	4.3
1	A	190	ASP	4.2
3	C	-1	GLY	4.2
3	C	665	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
3	C	8	SER	4.0
3	C	778	ARG	4.0
3	C	572	PHE	3.9
3	C	691	LEU	3.9
1	A	192	ALA	3.9
3	C	270	LEU	3.9
3	C	9	ASN	3.7
3	C	685	ALA	3.6
1	A	179	MET	3.6
3	C	525	LYS	3.6
3	C	264	ILE	3.5
3	C	587	THR	3.5
3	C	172	GLU	3.5
3	C	981	VAL	3.5
3	C	622	ILE	3.5
3	C	625	ILE	3.5
3	C	626	ILE	3.5
3	C	93	PHE	3.5
3	C	883	LYS	3.4
3	C	983	GLN	3.4
2	B	79	MET	3.4
2	B	200	LYS	3.4
3	C	618	SER	3.3
3	C	497	GLY	3.3
3	C	204[A]	GLY	3.3
1	A	196	GLN	3.3
3	C	522	ASP	3.2
3	C	608	TYR	3.2
3	C	690	LEU	3.2
3	C	652	ILE	3.2
3	C	207[A]	SER	3.1
3	C	670	GLN	3.1
3	C	570	TRP	3.1
3	C	533	LYS	3.1
2	B	78	THR	3.1
3	C	974	PRO	3.1
2	B	81	GLU	3.0
1	A	199	HIS	3.0
3	C	632	THR	3.0
3	C	526	ARG	3.0
1	A	180	PRO	3.0
3	C	621	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	578	LEU	2.9
3	C	542	LYS	2.9
3	C	682	GLN	2.9
3	C	683	SER	2.9
2	B	162	ALA	2.9
3	C	967	TYR	2.9
3	C	52	ASP	2.8
2	B	199	LYS	2.8
3	C	679	ILE	2.8
3	C	261	ASN	2.8
3	C	575	THR	2.7
3	C	496	ASP	2.7
1	A	186	GLU	2.7
3	C	949	LYS	2.7
3	C	230	TYR	2.7
3	C	111	GLN	2.7
3	C	21	SER	2.7
3	C	636	LEU	2.7
3	C	585	HIS	2.7
3	C	523	THR	2.7
3	C	545	LYS	2.7
3	C	605	LYS	2.7
3	C	686	ASN	2.7
3	C	984	GLY	2.6
3	C	262	LEU	2.6
2	B	98	ALA	2.6
3	C	450	GLU	2.6
3	C	663	ARG	2.6
3	C	674	MET	2.6
3	C	669	MET	2.6
1	A	185	PRO	2.6
3	C	495	ILE	2.6
1	A	198	GLU	2.6
3	C	615	PRO	2.5
3	C	543	ARG	2.5
3	C	689	LEU	2.5
3	C	529	VAL	2.5
3	C	263	LYS	2.5
1	A	9	VAL	2.5
3	C	498	SER	2.5
3	C	574	ARG	2.5
3	C	616	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	1052	ALA	2.5
3	C	687	PRO	2.5
3	C	977	GLN	2.5
2	B	186	LYS	2.4
3	C	541	GLN	2.4
3	C	656	ARG	2.4
3	C	755	LYS	2.4
3	C	192[A]	GLN	2.4
3	C	46	ASP	2.4
3	C	982	PRO	2.4
3	C	645	TYR	2.3
3	C	648	CYS	2.3
3	C	266	GLN	2.3
3	C	492	ALA	2.3
3	C	588	HIS	2.3
1	A	95	ARG	2.3
3	C	273	ARG	2.3
3	C	946	SER	2.3
3	C	976	TYR	2.3
3	C	688	THR	2.2
3	C	726	TYR	2.2
3	C	631	LYS	2.2
3	C	1024	ASP	2.2
3	C	672	PRO	2.2
3	C	671	LEU	2.2
3	C	630	GLN	2.1
3	C	1	MET	2.1
1	A	99	LYS	2.1
3	C	973	VAL	2.1
3	C	453	ARG	2.1
3	C	579	LYS	2.1
2	B	164	ILE	2.1
3	C	149	VAL	2.1
3	C	244	THR	2.1
3	C	975	LEU	2.1
3	C	247	ASP	2.1
3	C	537	GLY	2.1
3	C	0	SER	2.0
3	C	896	ASN	2.0
3	C	920	ASN	2.0
3	C	451	ILE	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](#)

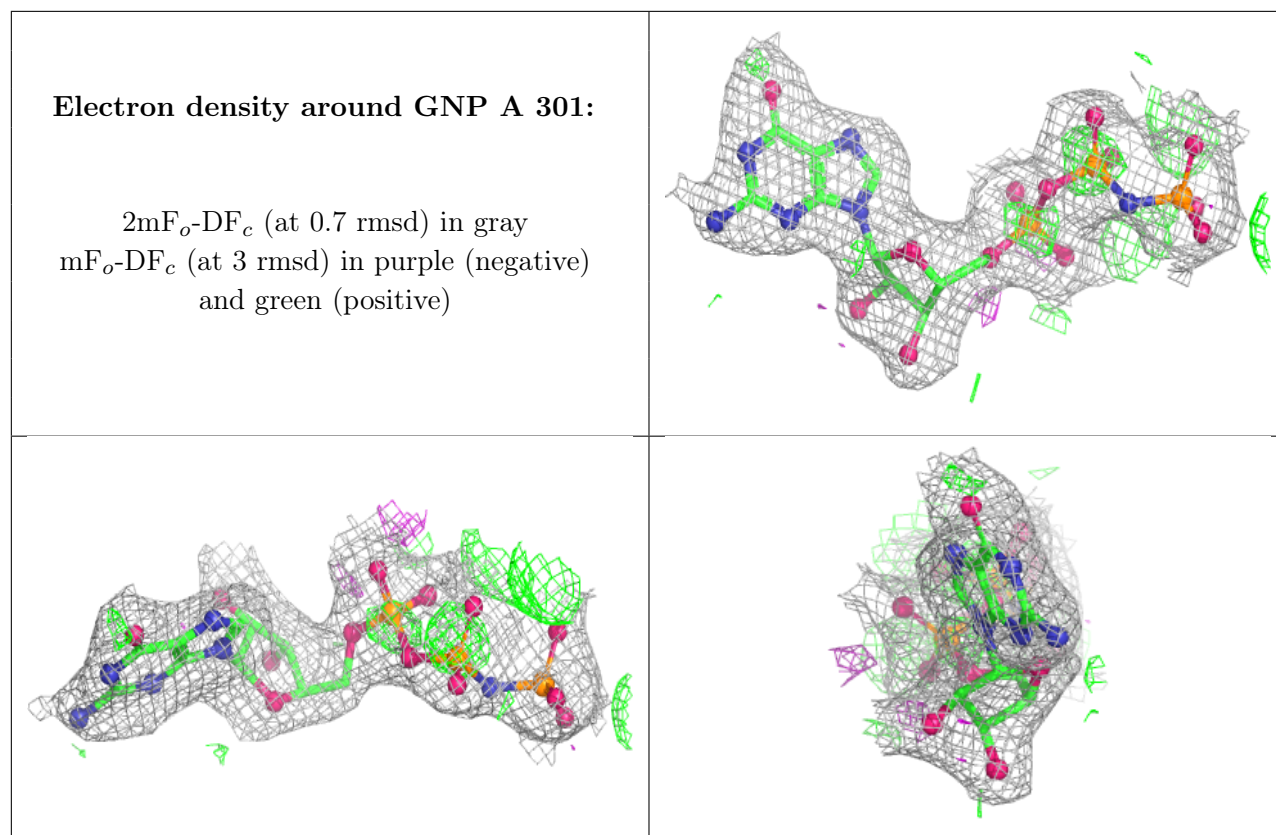
There are no oligosaccharides in this entry.

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
5	MG	A	302	1/1	0.80	0.19	38,38,38,38	0
4	GNP	A	301	32/32	0.94	0.09	17,23,25,41	0
6	GOL	C	1101	6/6	-	-	11,14,18,21	6

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.