



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:39 PM UTC

PDB ID : 4GPT / pdb_00004gpt
Title : Crystal structure of KPT251 in complex with CRM1-Ran-RanBP1
Authors : Sun, Q.; Chook, Y.M.
Deposited on : 2012-08-21
Resolution : 2.22 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

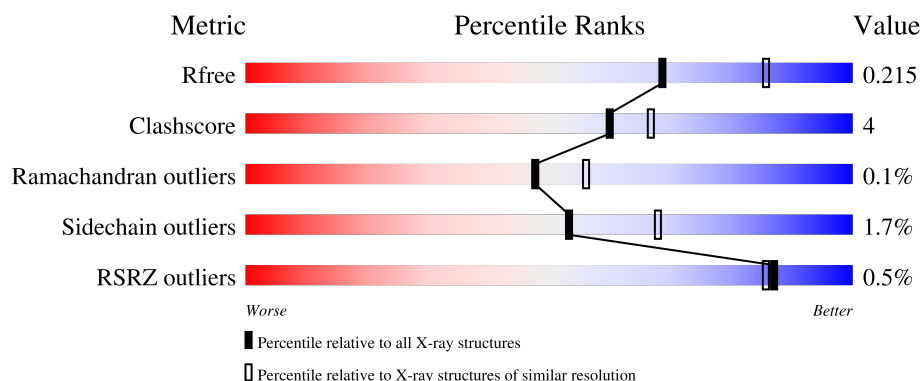
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	216	
2	B	140	
3	C	1060	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12518 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	4	0
			1700	1097	291	305	7			

- 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	1	0
			1016	642	178	192	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	ALA	MET	conflict	UNP P41920
B	98	LYS	ALA	conflict	UNP P41920

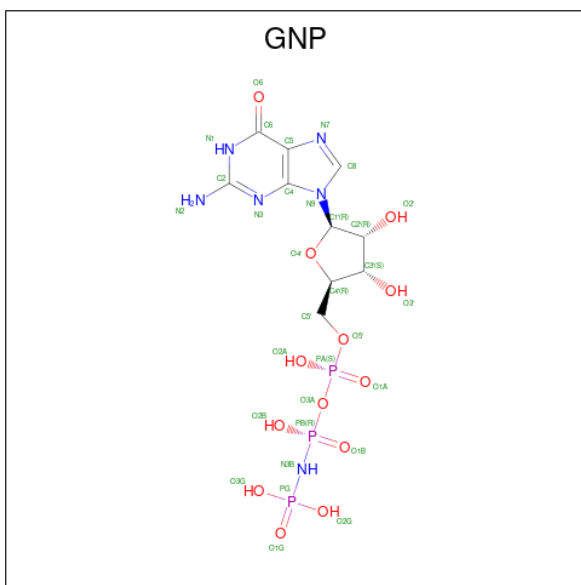
- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1017	Total	C	N	O	S	0	35	0
			8425	5426	1372	1584	43			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P30822
C	0	ALA	-	expression tag	UNP P30822
C	539	CYS	THR	engineered mutation	UNP P30822
C	1022	CYS	TYR	engineered mutation	UNP P30822

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

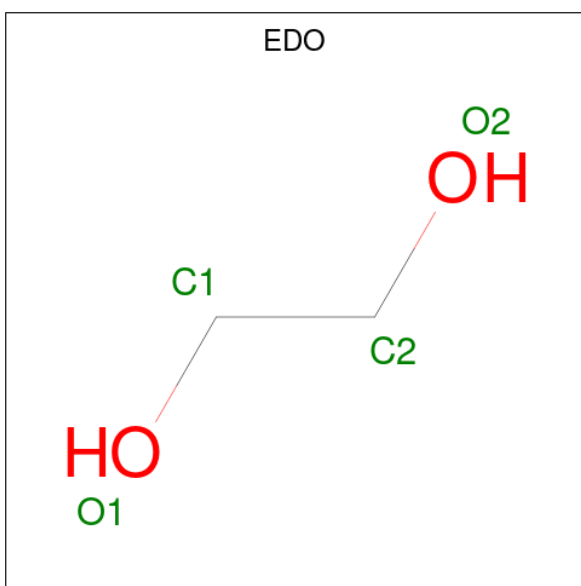


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).

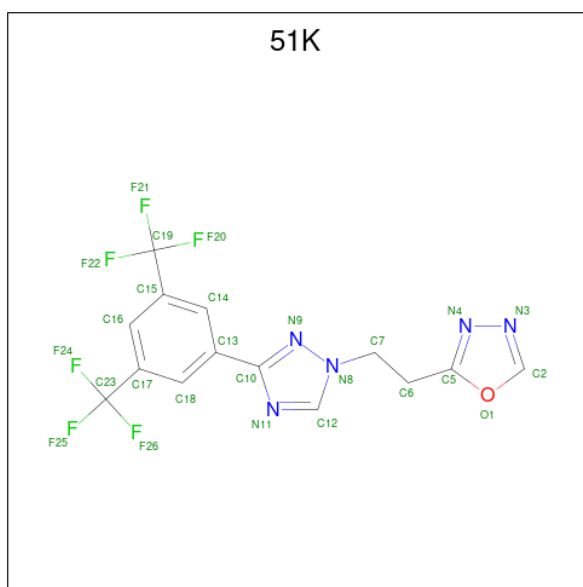


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	C	4	Total	Cl	0	0
			4	4		

- Molecule 8 is 2-(2-{3-[3,5-bis(trifluoromethyl)phenyl]-1H-1,2,4-triazol-1-yl}ethyl)-1,3,4-oxadiazole (CCD ID: 51K) (formula: C₁₄H₉F₆N₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	F	N	O	0	0
			26	14	6	5	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	215	Total	O	0	0
			215	215		
10	B	66	Total	O	0	0
			66	66		
10	C	1006	Total	O	0	0
			1006	1006		

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: GTP-binding nuclear protein Ran

Chain A: 



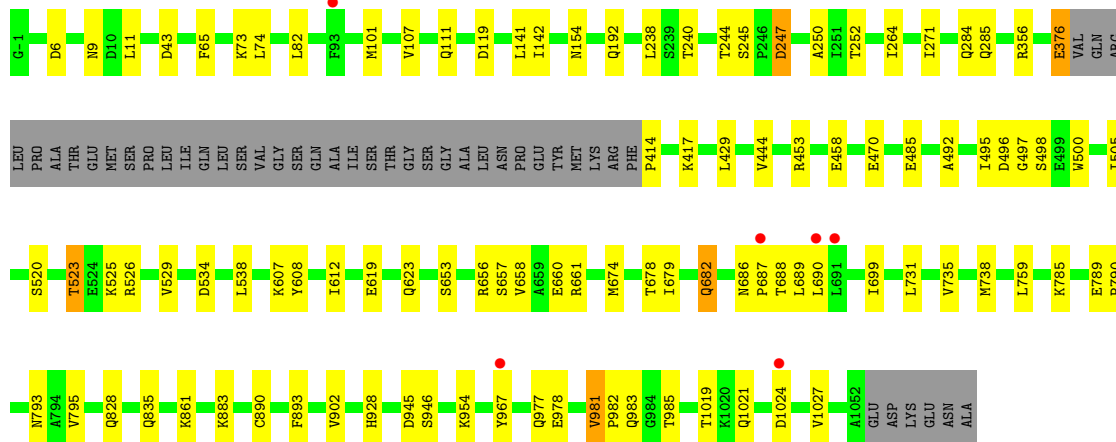
- Molecule 2: Ran-specific GTPase-activating protein 1

Chain B: 



- Molecule 3: Exportin-1

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.94Å 105.94Å 305.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.22 50.00 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.22) 99.3 (50.00-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.165 , 0.210 0.172 , 0.215	Depositor DCC
R_{free} test set	4331 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12518	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: MG, CL, EDO, GNP, GOL, 51K

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	0.74	0/1744	0.78	0/2361
2	B	0.58	0/1033	0.69	0/1378
3	C	0.79	1/8658 (0.0%)	0.81	3/11732 (0.0%)
All	All	0.77	1/11435 (0.0%)	0.80	3/15471 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	376	GLU	C-N	32.00	1.76	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	376	GLU	CA-C-N	-9.43	110.06	119.78
3	C	376	GLU	C-N-CA	-9.43	110.06	119.78
3	C	376	GLU	CA-C-O	6.79	124.69	119.46

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	1700	0	1709	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1016	0	1013	8	0
3	C	8425	0	8547	80	0
4	A	32	0	13	0	0
5	A	1	0	0	0	0
6	A	4	0	6	0	0
6	C	4	0	6	0	0
7	A	1	0	0	0	0
7	C	4	0	0	0	0
8	C	26	0	7	0	0
9	C	18	0	24	0	0
10	A	215	0	0	2	0
10	B	66	0	0	1	0
10	C	1006	0	0	17	0
All	All	12518	0	11325	96	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 (96) 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:C	3:C:414:PRO:N	1.76	1.40
3:C:429:LEU:HD22	10:C:2181:HOH:O	1.48	1.11
3:C:690:LEU:HD23	3:C:738:MET:HE1	1.39	1.02
3:C:523:THR:HB	10:C:2122:HOH:O	1.66	0.95
3:C:967[B]:TYR:CZ	3:C:1019[B]:THR:HG21	2.03	0.93
3:C:967[B]:TYR:CE1	3:C:1019[B]:THR:HG21	2.05	0.90
3:C:520:SER:HG	3:C:523:THR:HG1	1.20	0.76
3:C:967[B]:TYR:CE1	3:C:1019[B]:THR:CG2	2.70	0.73
3:C:376:GLU:C	3:C:414:PRO:CA	2.64	0.70
3:C:690:LEU:CD2	3:C:738:MET:HE1	2.19	0.70
3:C:1024:ASP:HB2	10:C:2180:HOH:O	1.94	0.66
3:C:793:ASN:HB3	10:C:1766:HOH:O	1.95	0.65
3:C:682:GLN:HG2	3:C:689:LEU:HD22	1.79	0.64
3:C:690:LEU:HD23	3:C:738:MET:CE	2.20	0.64
3:C:967[B]:TYR:CZ	3:C:1019[B]:THR:CG2	2.79	0.63
1:A:179:MET:HE3	2:B:133:LYS:HG2	1.79	0.63
3:C:250:ALA:HB3	10:C:1775:HOH:O	2.00	0.61
3:C:660[A]:GLU:OE1	3:C:660[A]:GLU:N	2.31	0.60
3:C:111[A]:GLN:HA	3:C:111[A]:GLN:OE1	2.02	0.60
3:C:902:VAL:HG13	3:C:954:LYS:HZ2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:981:VAL:HG13	3:C:982:PRO:HD2	1.85	0.58
3:C:658[B]:VAL:HG22	3:C:661:ARG:HH22	1.68	0.58
3:C:444:VAL:HG11	10:C:2004:HOH:O	2.06	0.56
3:C:523:THR:HG22	3:C:526:ARG:NH1	2.21	0.56
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.37	0.55
2:B:90:ARG:NH2	2:B:129:ASP:OD2	2.41	0.53
3:C:244:THR:HG22	3:C:285:GLN:OE1	2.09	0.53
3:C:356:ARG:NH1	10:C:1400:HOH:O	2.42	0.53
3:C:828:GLN:HG2	10:C:2186:HOH:O	2.09	0.52
3:C:496:ASP:OD1	3:C:497:GLY:N	2.43	0.52
3:C:523:THR:HG21	10:C:2202:HOH:O	2.09	0.51
3:C:141:LEU:C	3:C:141:LEU:HD23	2.35	0.51
2:B:82:ASP:OD2	2:B:118:LYS:NZ	2.42	0.51
2:B:78:THR:HG22	10:B:364:HOH:O	2.10	0.51
1:A:95:ARG:O	1:A:99[B]:LYS:HE2	2.11	0.50
3:C:496:ASP:OD1	3:C:498:SER:N	2.37	0.50
3:C:245:SER:HB2	3:C:247[A]:ASP:OD2	2.12	0.49
3:C:523:THR:HG22	3:C:526:ARG:HH12	1.78	0.49
2:B:188:LYS:NZ	2:B:192:GLU:OE1	2.43	0.49
1:A:9:VAL:N	10:A:604:HOH:O	2.47	0.48
3:C:653:SER:O	3:C:656:ARG:NH1	2.43	0.48
3:C:890:CYS:O	3:C:893[B]:PHE:HB2	2.13	0.48
3:C:492:ALA:HA	3:C:495:ILE:HD12	1.95	0.48
3:C:43:ASP:OD2	3:C:73:LYS:NZ	2.48	0.47
3:C:699:ILE:HG21	3:C:731:LEU:HD21	1.96	0.47
3:C:674:MET:O	3:C:678:THR:HG23	2.15	0.47
3:C:789[B]:GLU:HB2	3:C:790:PRO:HD3	1.97	0.47
3:C:238:LEU:O	3:C:252:THR:HG21	2.15	0.47
1:A:99[B]:LYS:NZ	10:A:476:HOH:O	2.47	0.47
3:C:679:ILE:HD13	3:C:699:ILE:HG13	1.96	0.47
3:C:619:GLU:OE2	3:C:623[A]:GLN:NE2	2.43	0.46
3:C:376:GLU:CA	3:C:414:PRO:N	2.70	0.46
1:A:180:PRO:HA	2:B:78:THR:O	2.15	0.46
3:C:981:VAL:HG11	3:C:985:THR:HG21	1.96	0.46
3:C:101[A]:MET:HG2	3:C:107:VAL:HG11	1.98	0.46
1:A:179:MET:HE3	2:B:133:LYS:HA	1.98	0.46
3:C:6:ASP:OD2	3:C:9:ASN:ND2	2.49	0.45
3:C:470[B]:GLU:HG3	10:C:1750:HOH:O	2.16	0.45
3:C:690:LEU:HB3	3:C:738:MET:HE1	1.99	0.45
1:A:179:MET:HE3	2:B:133:LYS:CG	2.45	0.45
3:C:74:LEU:HD11	3:C:82:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1021:GLN:CD	3:C:1027:VAL:HG12	2.41	0.45
3:C:142:ILE:CD1	3:C:192[B]:GLN:HB3	2.47	0.44
3:C:657:SER:OG	3:C:660[A]:GLU:OE1	2.31	0.44
3:C:458[A]:GLU:OE2	3:C:458[A]:GLU:HA	2.17	0.44
3:C:505:ILE:HD12	3:C:505:ILE:HA	1.87	0.44
3:C:240:THR:O	3:C:244:THR:HG23	2.17	0.44
3:C:835:GLN:HG3	10:C:1705:HOH:O	2.18	0.44
3:C:679:ILE:HD13	3:C:699:ILE:CG1	2.48	0.44
3:C:735[A]:VAL:HG13	3:C:759:LEU:HB3	2.00	0.44
3:C:623[B]:GLN:NE2	10:C:1642:HOH:O	2.50	0.43
3:C:688:THR:HG23	3:C:689:LEU:N	2.34	0.43
3:C:496:ASP:OD1	3:C:496:ASP:C	2.61	0.43
1:A:13:LEU:C	1:A:13:LEU:HD23	2.43	0.43
3:C:686:ASN:OD1	3:C:686:ASN:N	2.52	0.42
3:C:417:LYS:NZ	10:C:1338:HOH:O	2.53	0.42
1:A:81:ILE:HD11	3:C:65:PHE:CG	2.54	0.42
3:C:608:TYR:CE2	3:C:612:ILE:HD13	2.53	0.42
3:C:485:GLU:HG3	10:C:1605:HOH:O	2.19	0.42
3:C:525:LYS:O	3:C:529:VAL:HG23	2.20	0.42
3:C:500:TRP:CZ3	3:C:538:LEU:HD12	2.55	0.41
3:C:789[A]:GLU:HB3	3:C:790:PRO:HD3	2.02	0.41
3:C:11:LEU:HD13	10:C:2115:HOH:O	2.20	0.41
3:C:967[B]:TYR:CD1	3:C:1019[B]:THR:CG2	3.02	0.41
1:A:77:ASP:HA	1:A:80:TYR:CE2	2.56	0.41
3:C:264:ILE:CG2	3:C:271:ILE:HG21	2.51	0.41
3:C:495:ILE:HD11	3:C:534:ASP:HB3	2.02	0.41
1:A:99[B]:LYS:HA	1:A:99[B]:LYS:HD3	1.90	0.41
3:C:861:LYS:NZ	10:C:1794:HOH:O	2.53	0.40
1:A:159:LYS:HB2	1:A:160:PRO:HD3	2.03	0.40
3:C:495:ILE:HD11	3:C:534:ASP:CG	2.46	0.40
3:C:928:HIS:HE1	10:C:1739:HOH:O	2.03	0.40
1:A:171:ASP:OD1	1:A:171:ASP:C	2.64	0.40
3:C:690:LEU:CB	3:C:738:MET:HE1	2.52	0.40
3:C:945:ASP:O	3:C:946:SER:HB2	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	210/216 (97%)	206 (98%)	4 (2%)	0	100	100
2	B	122/140 (87%)	116 (95%)	6 (5%)	0	100	100
3	C	1050/1060 (99%)	1033 (98%)	16 (2%)	1 (0%)	48	56
All	All	1382/1416 (98%)	1355 (98%)	26 (2%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	687	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	184/185 (100%)	179 (97%)	5 (3%)	39	52
2	B	106/121 (88%)	103 (97%)	3 (3%)	38	50
3	C	963/964 (100%)	948 (98%)	15 (2%)	55	70
All	All	1253/1270 (99%)	1230 (98%)	23 (2%)	53	66

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

Mol	Chain	Res	Type
1	A	54	THR
1	A	70	GLU

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Mol	Chain	Res	Type
1	A	182	LEU
1	A	186	GLU
1	A	202	GLU
2	B	78	THR
2	B	143	GLU
2	B	157	VAL
3	C	247[A]	ASP
3	C	247[B]	ASP
3	C	284	GLN
3	C	453	ARG
3	C	523	THR
3	C	607	LYS
3	C	682	GLN
3	C	785[A]	LYS
3	C	785[B]	LYS
3	C	795	VAL
3	C	883	LYS
3	C	977	GLN
3	C	978	GLU
3	C	981	VAL
3	C	983	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	62	ASN
1	A	105	HIS
1	A	143	ASN
1	A	196	GLN
1	A	205	GLN
3	C	9	ASN
3	C	31	GLN
3	C	49	GLN
3	C	173	GLN
3	C	203	GLN
3	C	284	GLN
3	C	313	GLN
3	C	434	ASN
3	C	494	GLN
3	C	701	ASN
3	C	828	GLN

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Mol	Chain	Res	Type
3	C	835	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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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$
8	51K	C	1101	3	26,28,28	1.33	3 (11%)	37,42,42	2.64	15 (40%)
6	EDO	A	303	-	3,3,3	0.55	0	2,2,2	0.07	0
9	GOL	C	1102	-	5,5,5	0.39	0	5,5,5	0.35	0
4	GNP	A	301	5	34,34,34	1.56	6 (17%)	47,54,54	1.66	5 (10%)
9	GOL	C	1108	-	5,5,5	0.45	0	5,5,5	0.64	0
6	EDO	C	1104	-	3,3,3	0.46	0	2,2,2	0.47	0
9	GOL	C	1103	-	5,5,5	0.44	0	5,5,5	0.37	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
8	51K	C	1101	3	-	1/21/21/21	0/3/3/3
6	EDO	A	303	-	-	0/1/1/1	-
9	GOL	C	1102	-	-	2/4/4/4	-
4	GNP	A	301	5	-	3/18/38/38	0/3/3/3
9	GOL	C	1108	-	-	3/4/4/4	-
6	EDO	C	1104	-	-	1/1/1/1	-
9	GOL	C	1103	-	-	1/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1101	51K	C5-N4	5.43	1.35	1.28
4	A	301	GNP	PG-N3B	4.06	1.74	1.63
4	A	301	GNP	C5-C4	3.62	1.48	1.38
4	A	301	GNP	PB-N3B	3.24	1.71	1.63
4	A	301	GNP	C6-N1	-2.55	1.34	1.38
4	A	301	GNP	C4-N9	-2.42	1.31	1.38
8	C	1101	51K	N8-N9	2.24	1.38	1.35
4	A	301	GNP	C5-N7	-2.16	1.34	1.39
8	C	1101	51K	O1-C2	2.12	1.39	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1101	51K	N8-C12-N11	-7.87	106.62	110.82
8	C	1101	51K	C12-N11-C10	6.45	108.26	102.71
4	A	301	GNP	C5-C4-N3	-5.24	120.05	128.39
8	C	1101	51K	O1-C5-N4	-4.83	108.88	112.75
8	C	1101	51K	C6-C5-N4	-4.30	126.00	129.47
4	A	301	GNP	O1G-PG-N3B	-4.29	105.46	111.77
8	C	1101	51K	C7-N8-N9	-4.27	115.25	119.56
4	A	301	GNP	N9-C4-N3	3.99	133.92	125.95
4	A	301	GNP	C2-N3-C4	3.84	118.91	112.30
8	C	1101	51K	C5-N4-N3	3.72	108.27	106.25
8	C	1101	51K	O1-C5-C6	3.17	125.12	117.96
4	A	301	GNP	C6-C5-N7	3.03	135.80	130.29
8	C	1101	51K	C16-C17-C23	-2.52	116.24	119.57
8	C	1101	51K	C18-C17-C23	2.48	122.85	119.57
8	C	1101	51K	F25-C23-C17	-2.48	107.59	112.90
8	C	1101	51K	F24-C23-F26	2.28	114.02	105.77
8	C	1101	51K	N9-C10-N11	-2.22	110.11	114.62
8	C	1101	51K	F24-C23-C17	-2.16	108.28	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1101	51K	F22-C19-C15	-2.14	108.31	112.90
8	C	1101	51K	F20-C19-F22	2.02	113.05	105.77

There are no chirality outliers.

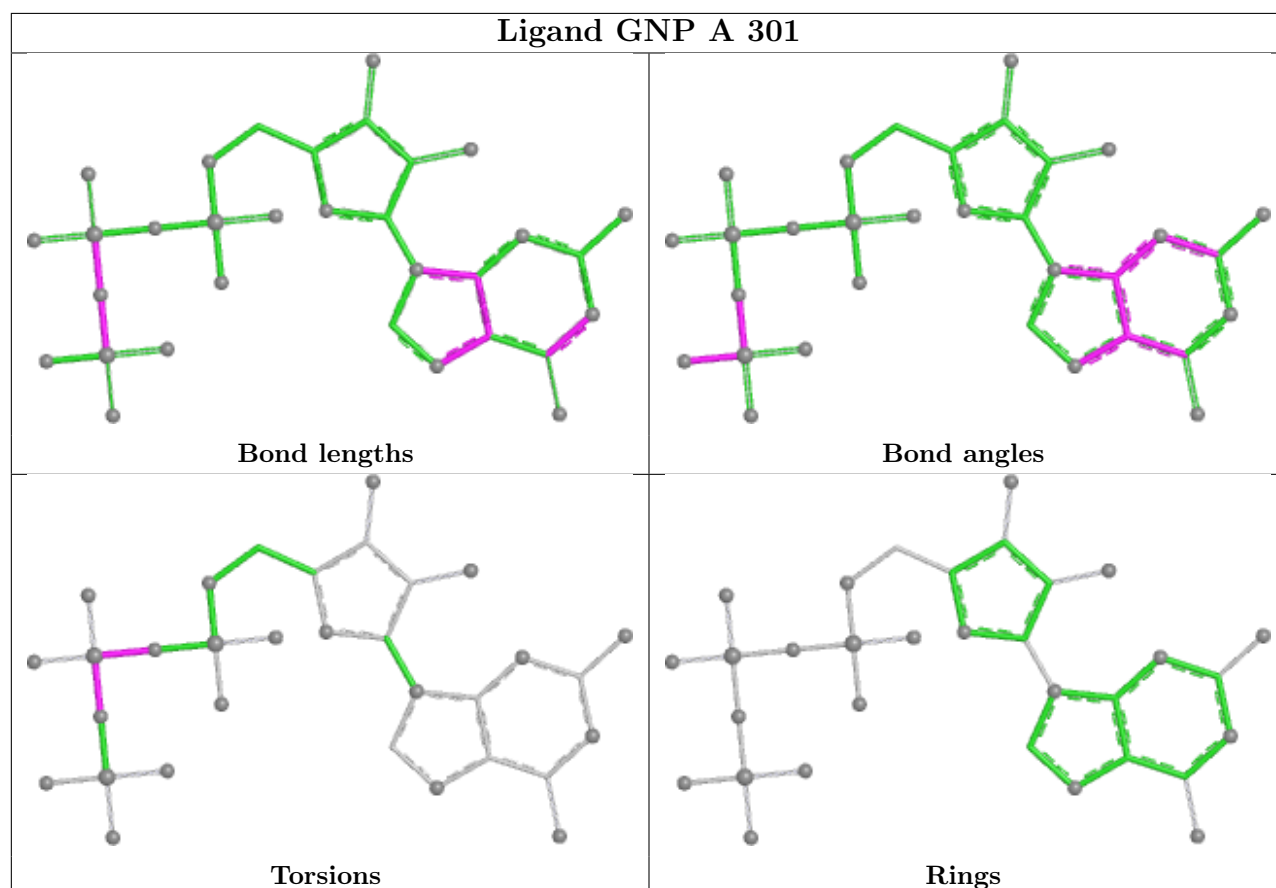
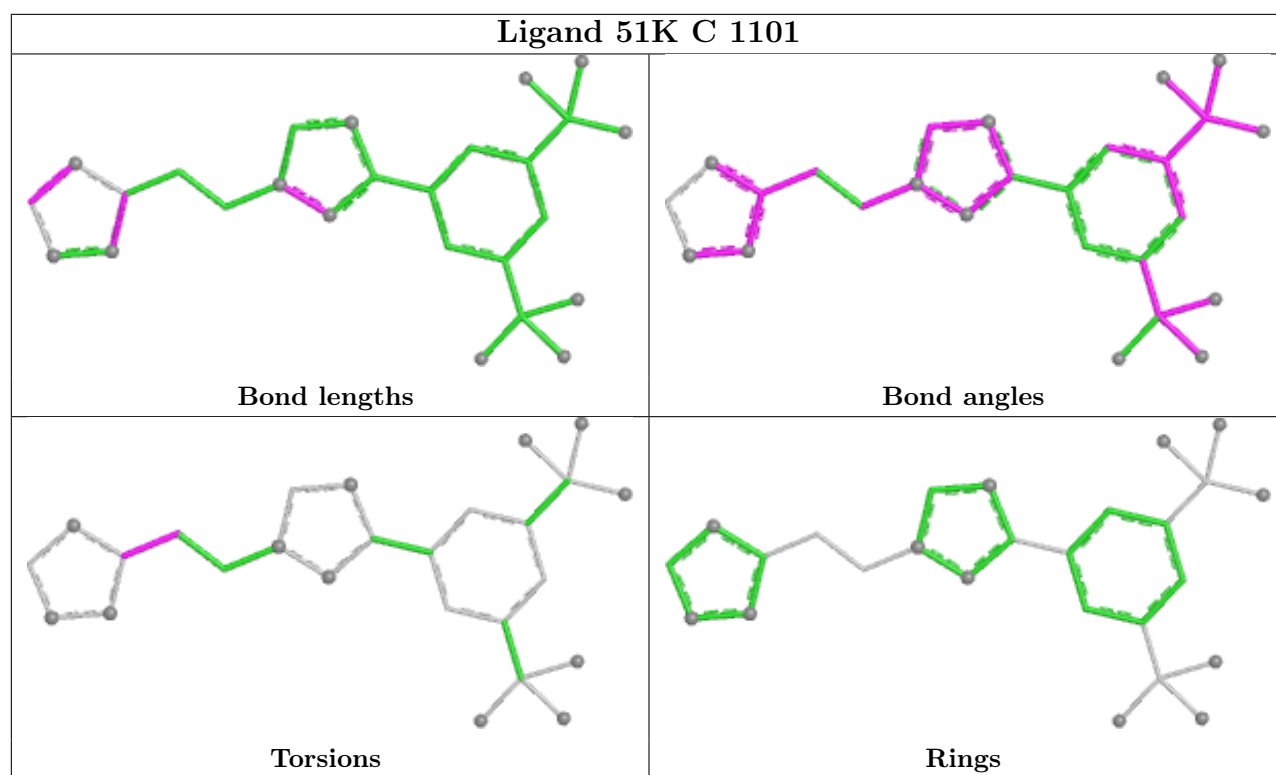
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
9	C	1102	GOL	C1-C2-C3-O3
9	C	1108	GOL	O1-C1-C2-C3
9	C	1102	GOL	O2-C2-C3-O3
9	C	1108	GOL	O1-C1-C2-O2
8	C	1101	51K	O1-C5-C6-C7
6	C	1104	EDO	O1-C1-C2-O2
9	C	1103	GOL	O1-C1-C2-O2
4	A	301	GNP	PA-O3A-PB-O1B
4	A	301	GNP	PG-N3B-PB-O3A
9	C	1108	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.36	1 (0%) 87 86	19, 50, 101, 123	4 (1%)
2	B	123/140 (87%)	-0.34	0 100 100	44, 63, 87, 103	1 (0%)
3	C	1017/1060 (95%)	-0.43	6 (0%) 85 84	20, 52, 81, 128	35 (3%)
All	All	1348/1416 (95%)	-0.41	7 (0%) 87 86	19, 53, 83, 128	40 (2%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	967[A]	TYR	4.1
3	C	690	LEU	3.3
3	C	691	LEU	3.0
1	A	189	MET	2.9
3	C	687	PRO	2.8
3	C	93	PHE	2.1
3	C	1024	ASP	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.

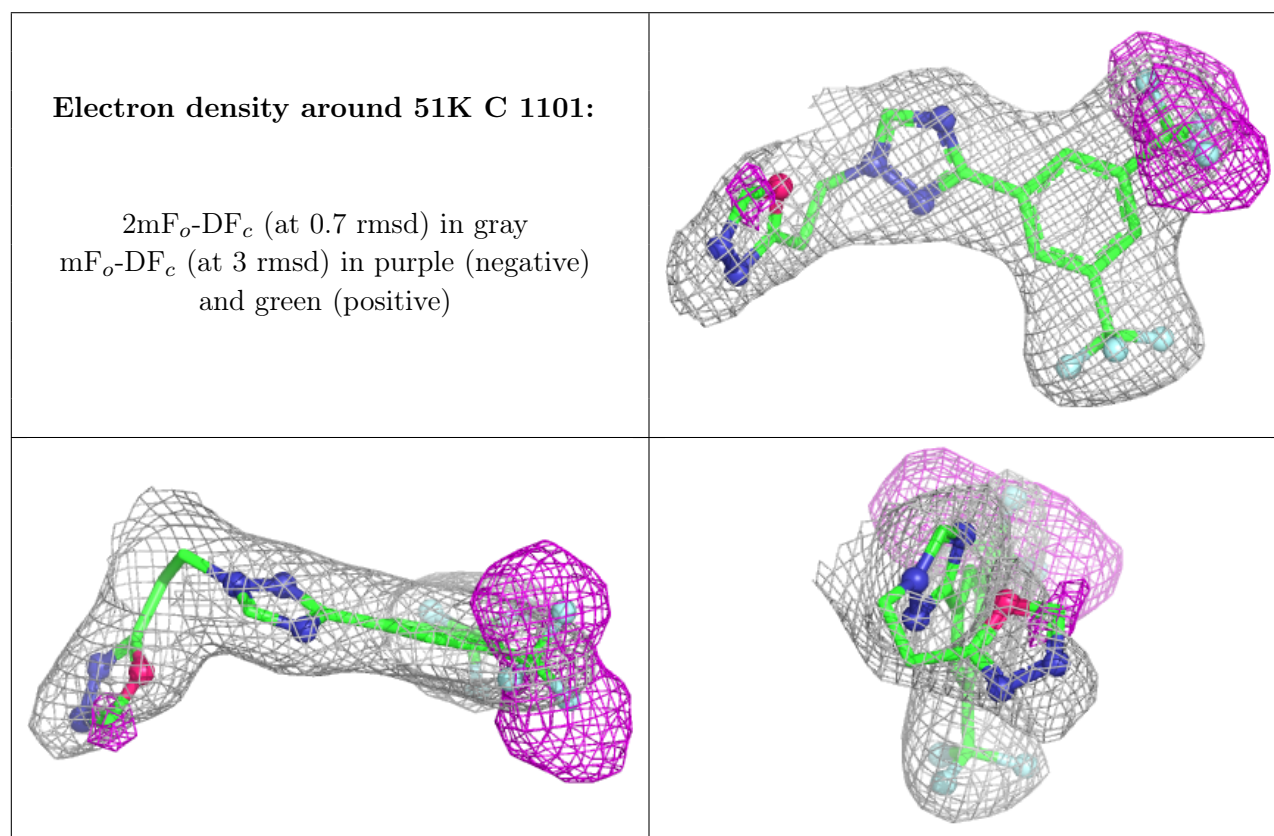
6.4 Ligands [i](#)

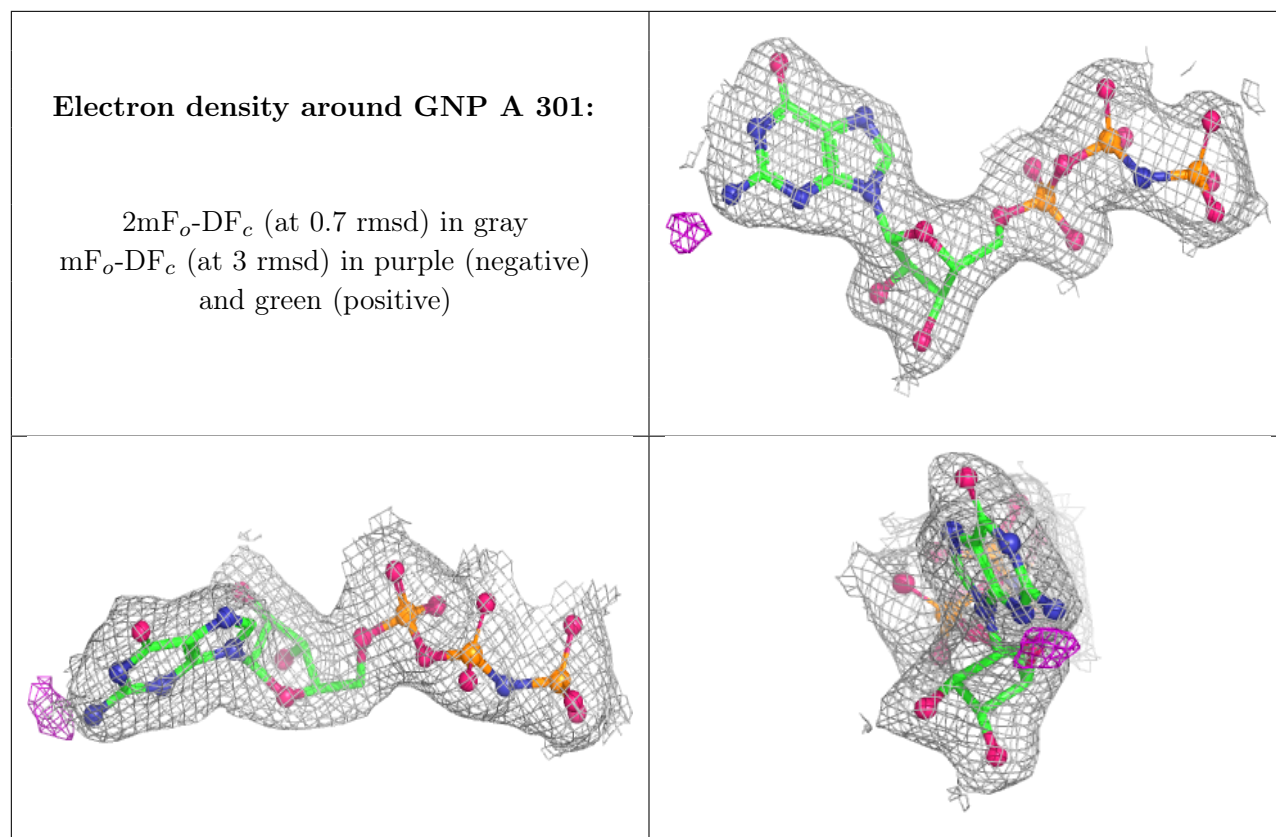
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(Å ²)	Q<0.9
9	GOL	C	1103	6/6	0.71	0.14	80,86,90,95	0
6	EDO	C	1104	4/4	0.81	0.21	81,83,84,92	0
9	GOL	C	1108	6/6	0.83	0.08	69,77,82,86	0
7	CL	C	1109	1/1	0.86	0.14	95,95,95,95	0
6	EDO	A	303	4/4	0.91	0.17	67,72,73,75	0
9	GOL	C	1102	6/6	0.91	0.11	73,74,76,80	0
8	51K	C	1101	26/26	0.92	0.09	56,63,84,90	0
7	CL	C	1107	1/1	0.92	0.13	89,89,89,89	0
7	CL	A	304	1/1	0.95	0.07	65,65,65,65	0
7	CL	C	1106	1/1	0.95	0.09	72,72,72,72	0
7	CL	C	1105	1/1	0.96	0.08	81,81,81,81	0
5	MG	A	302	1/1	0.99	0.03	45,45,45,45	0
4	GNP	A	301	32/32	0.99	0.04	42,45,47,48	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.