



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 06:37 AM EST

PDB ID : 4HB0
Title : Crystal structure of CRM1 inhibitor Leptomycin B in complex with CRM1(K541Q,K542Q,R543S,K545Q,K548Q,K579Q)-Ran-RanBP1
Authors : Sun, Q.; Chook, Y.M.
Deposited on : 2012-09-27
Resolution : 2.20 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 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

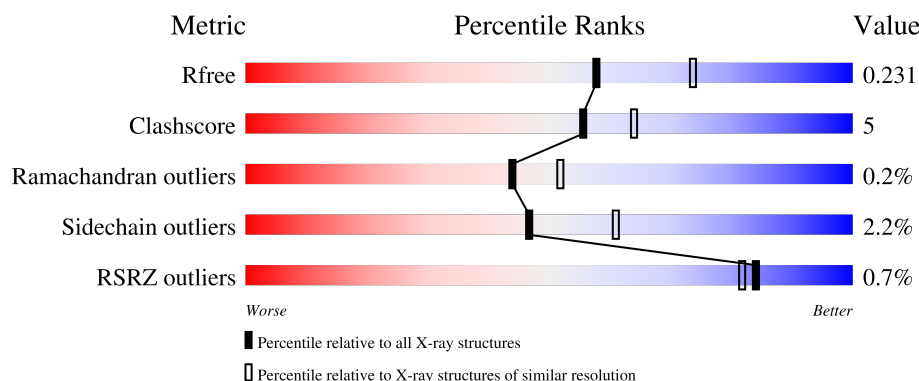
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 88% 6% • 5% </div> </div>
2	B	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 76% 9% • 14% </div> </div>
3	C	1023	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 87% 12% .. </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11869 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	205	Total	C	N	O	S	0	4	0
			1673	1080	287	300	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	1	0
			1005	636	176	189	4			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1016	Total	C	N	O	S	0	24	0
			8325	5357	1354	1571	43			

There are 10 discrepancies between the modelled and reference sequences:

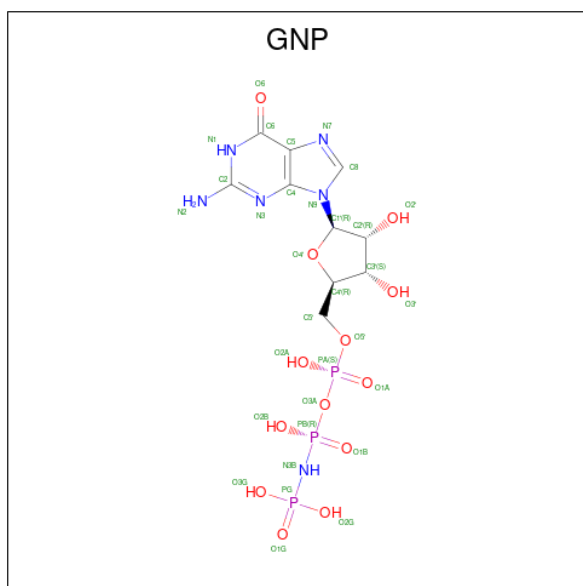
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P30822
C	0	ALA	-	expression tag	UNP P30822
C	539	CYS	THR	engineered mutation	UNP P30822
C	541	GLN	LYS	engineered mutation	UNP P30822
C	542	GLN	LYS	engineered mutation	UNP P30822
C	543	SER	ARG	engineered mutation	UNP P30822
C	545	GLN	LYS	engineered mutation	UNP P30822
C	548	GLN	LYS	engineered mutation	UNP P30822
C	579	GLN	LYS	engineered mutation	UNP P30822

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1022	CYS	TYR	engineered mutation	UNP P30822

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

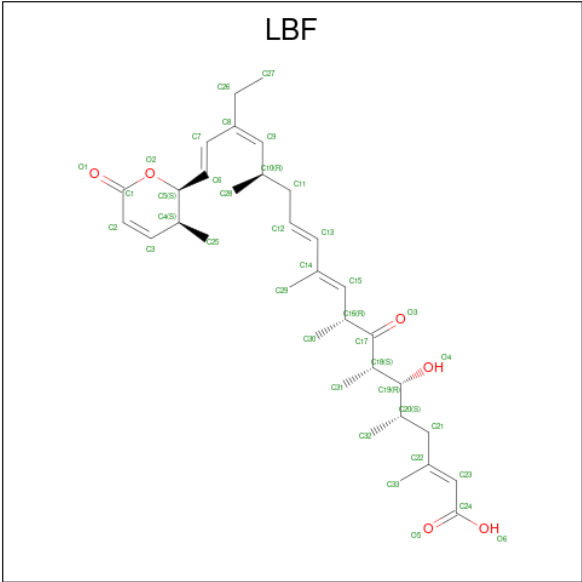


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is Leptomycin B (three-letter code: LBF) (formula: $C_{33}H_{48}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	C O	0	0
			39	33 6		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

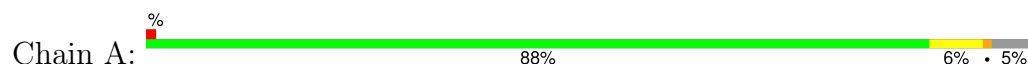
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	127	Total	O	0	0
			127	127		
8	B	45	Total	O	0	0
			45	45		
8	C	618	Total	O	0	0
			618	618		

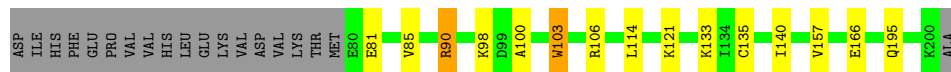
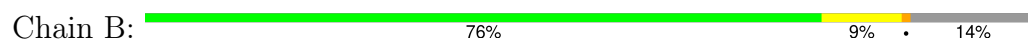
3 Residue-property plots [i](#)

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.

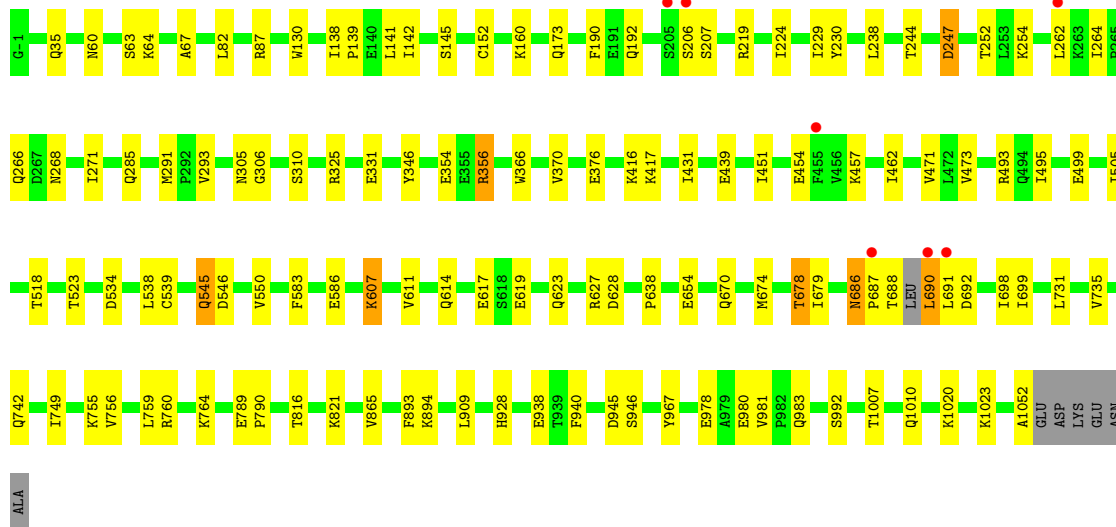
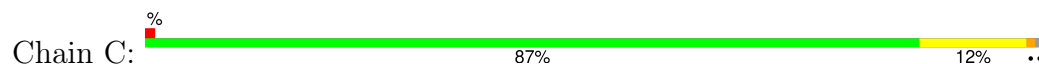
- Molecule 1: GTP-binding nuclear protein Ran



- 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	105.54Å 105.54Å 305.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.20) 98.1 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.225 0.192 , 0.231	Depositor DCC
R_{free} test set	4362 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11869	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: GNP, CL, LBF, 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	0.80	0/1721	0.86	1/2329 (0.0%)
2	B	0.70	1/1022 (0.1%)	0.85	0/1363
3	C	0.77	2/8547 (0.0%)	0.81	1/11587 (0.0%)
All	All	0.77	3/11290 (0.0%)	0.83	2/15279 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	376	GLU	C-N	6.64	1.46	1.34
2	B	103	TRP	CD2-CE2	5.27	1.47	1.41
3	C	130	TRP	CD2-CE2	5.16	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	893	PHE	CB-CA-C	-6.24	97.92	110.40
1	A	106	ARG	NE-CZ-NH1	5.77	123.19	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1673	0	1683	12	0
2	B	1005	0	1005	10	0
3	C	8325	0	8417	81	0
4	A	32	0	13	1	0
5	A	1	0	0	0	0
6	C	39	0	46	2	0
7	C	4	0	0	0	0
8	A	127	0	0	2	0
8	B	45	0	0	1	0
8	C	618	0	0	15	0
All	All	11869	0	11164	103	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 5.

All (103) 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:493:ARG:NE	3:C:499:GLU:OE2	2.08	0.85
1:A:196:GLN:HA	1:A:196:GLN:HE21	1.54	0.73
3:C:909:LEU:HD22	8:C:1808:HOH:O	1.90	0.69
3:C:293[A]:VAL:HG23	8:C:1316:HOH:O	1.92	0.68
1:A:9:VAL:N	8:A:527:HOH:O	2.28	0.66
3:C:1052:ALA:CB	8:C:1713:HOH:O	2.42	0.66
3:C:688:THR:HA	3:C:691:LEU:HD23	1.79	0.65
3:C:325:ARG:NH2	8:C:1816:HOH:O	2.30	0.64
3:C:686:ASN:HD22	3:C:688:THR:HG22	1.64	0.62
3:C:1052:ALA:HB2	8:C:1713:HOH:O	2.01	0.61
3:C:238:LEU:O	3:C:252:THR:HG21	2.01	0.60
3:C:789[B]:GLU:HB2	3:C:790:PRO:HD3	1.82	0.60
3:C:1007:THR:H	3:C:1010:GLN:HE21	1.51	0.58
3:C:244:THR:HG22	3:C:285:GLN:OE1	2.03	0.57
3:C:619:GLU:OE2	3:C:623:GLN:NE2	2.38	0.56
3:C:967:TYR:HE2	3:C:1023:LYS:HZ2	1.54	0.55
3:C:674:MET:O	3:C:678:THR:HG23	2.05	0.55
3:C:417:LYS:NZ	8:C:1330:HOH:O	2.40	0.55
3:C:293[B]:VAL:HG12	3:C:346:TYR:CE2	2.43	0.54
8:A:488:HOH:O	3:C:254:LYS:HE3	2.06	0.54
3:C:686:ASN:HD22	3:C:688:THR:CG2	2.20	0.54
3:C:1007:THR:H	3:C:1010:GLN:NE2	2.07	0.53
3:C:523:THR:CG2	8:C:1770:HOH:O	2.57	0.52
3:C:760:ARG:O	3:C:764:LYS:HG3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:LEU:O	3:C:87:ARG:NH1	2.43	0.52
3:C:244:THR:CG2	3:C:285:GLN:OE1	2.59	0.51
3:C:230:TYR:CE2	3:C:264:ILE:HD11	2.45	0.51
3:C:138:ILE:HB	3:C:139:PRO:HD3	1.91	0.51
3:C:266:GLN:NE2	8:C:1816:HOH:O	2.43	0.51
3:C:229:ILE:HG13	3:C:262:LEU:HD11	1.92	0.51
3:C:268:ASN:ND2	3:C:271:ILE:HD12	2.25	0.51
3:C:614:GLN:HB2	3:C:617:GLU:HG3	1.93	0.50
1:A:187:VAL:HG12	1:A:188:VAL:N	2.26	0.50
3:C:686:ASN:HB2	3:C:688:THR:HG22	1.94	0.49
3:C:451:ILE:HG13	3:C:550:VAL:HG23	1.93	0.49
3:C:473:VAL:HG13	3:C:518:THR:HG22	1.95	0.49
1:A:187:VAL:CG1	1:A:188:VAL:N	2.75	0.49
3:C:331:GLU:OE1	3:C:416:LYS:HE3	2.13	0.49
3:C:523:THR:HG23	8:C:1770:HOH:O	2.13	0.49
3:C:945:ASP:O	3:C:946:SER:HB2	2.13	0.48
6:C:1101:LBF:O5	6:C:1101:LBF:C33	2.60	0.48
3:C:583:PHE:O	3:C:586:GLU:HB2	2.14	0.48
1:A:166:ARG:HG2	1:A:174:LEU:HB3	1.96	0.47
3:C:607:LYS:HG3	3:C:654:GLU:CG	2.44	0.47
3:C:145:SER:O	3:C:152:CYS:HB2	2.14	0.47
3:C:247:ASP:OD2	3:C:247:ASP:N	2.47	0.47
1:A:196:GLN:HA	1:A:196:GLN:NE2	2.26	0.47
3:C:495:ILE:HD11	3:C:534:ASP:HB3	1.96	0.46
3:C:64:LYS:O	3:C:67:ALA:HB3	2.15	0.46
2:B:85:VAL:HG22	2:B:114:LEU:CD2	2.45	0.46
3:C:699:ILE:HG21	3:C:731:LEU:HD21	1.97	0.46
3:C:262:LEU:O	3:C:325:ARG:NH1	2.45	0.46
3:C:293[B]:VAL:HG12	3:C:346:TYR:CZ	2.51	0.45
3:C:173:GLN:NE2	8:C:1527:HOH:O	2.50	0.45
3:C:691:LEU:O	3:C:755:LYS:NZ	2.27	0.45
3:C:690:LEU:C	3:C:692:ASP:H	2.19	0.45
2:B:121:LYS:HD3	2:B:121:LYS:HA	1.79	0.45
3:C:789[A]:GLU:HB3	3:C:790:PRO:HD3	1.99	0.45
2:B:90:ARG:HH21	2:B:90:ARG:HG3	1.81	0.44
2:B:140:ILE:HG22	2:B:195:GLN:HG3	1.99	0.44
2:B:98:LYS:O	2:B:100:ALA:O	2.34	0.44
3:C:190:PHE:CZ	3:C:224:ILE:HG21	2.53	0.44
2:B:81:GLU:HB3	8:B:338:HOH:O	2.18	0.44
3:C:160:LYS:HD2	3:C:219:ARG:CZ	2.47	0.44
3:C:366:TRP:O	3:C:370:VAL:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:ILE:CD1	3:C:192[A]:GLN:HB3	2.49	0.43
3:C:686:ASN:C	3:C:688:THR:H	2.22	0.43
3:C:431[B]:ILE:HD11	3:C:471:VAL:HG11	1.99	0.43
3:C:439[A]:GLU:HB3	3:C:462[A]:ILE:CD1	2.49	0.43
3:C:454:GLU:OE2	3:C:457:LYS:NZ	2.46	0.43
3:C:928:HIS:HE1	8:C:1619:HOH:O	2.00	0.43
3:C:679:ILE:HD11	3:C:698:ILE:CG2	2.49	0.43
3:C:268:ASN:OD1	3:C:268:ASN:C	2.56	0.42
3:C:742:GLN:HG2	3:C:756:VAL:CG2	2.49	0.42
3:C:1020:LYS:HG3	8:C:1620:HOH:O	2.18	0.42
3:C:60:ASN:O	3:C:63:SER:HB2	2.19	0.42
3:C:545:GLN:HG3	3:C:546:ASP:N	2.35	0.42
3:C:623:GLN:O	3:C:627:ARG:HG3	2.20	0.42
3:C:978:GLU:C	3:C:980:GLU:H	2.22	0.42
3:C:142:ILE:CD1	3:C:192[B]:GLN:HB3	2.50	0.42
2:B:106:ARG:NH2	2:B:166:GLU:HG2	2.35	0.42
3:C:493:ARG:HB3	3:C:499:GLU:HG3	2.02	0.41
1:A:179:MET:HE2	2:B:133:LYS:HG2	2.02	0.41
3:C:894:LYS:NZ	3:C:938:GLU:OE1	2.50	0.41
1:A:171:ASP:HA	1:A:172:PRO:HD2	1.93	0.41
1:A:209:LEU:HD23	2:B:103:TRP:CG	2.56	0.41
1:A:182:LEU:H	1:A:182:LEU:HD12	1.85	0.41
3:C:523:THR:HG22	8:C:1770:HOH:O	2.20	0.41
3:C:356:ARG:HD2	8:C:1384:HOH:O	2.20	0.41
3:C:670:GLN:O	3:C:674:MET:HG3	2.19	0.41
3:C:462[B]:ILE:HD12	8:C:1423:HOH:O	2.20	0.41
1:A:56:ARG:HD3	1:A:171:ASP:OD2	2.21	0.41
3:C:305:ASN:O	3:C:306:GLY:C	2.59	0.41
3:C:749:ILE:HD12	3:C:749:ILE:HA	1.95	0.41
3:C:431[B]:ILE:HD11	3:C:471:VAL:CG1	2.50	0.41
3:C:505:ILE:HD12	3:C:505:ILE:HA	1.85	0.41
3:C:821:LYS:HA	3:C:821:LYS:HD3	1.94	0.41
2:B:106:ARG:NH1	2:B:135:CYS:O	2.54	0.40
3:C:735:VAL:HG13	3:C:759:LEU:HB3	2.04	0.40
3:C:141:LEU:C	3:C:141:LEU:HD23	2.41	0.40
3:C:816:THR:HG23	3:C:865:VAL:HG11	2.03	0.40
6:C:1101:LBF:H27	6:C:1101:LBF:H23	1.95	0.40
1:A:23:LYS:NZ	4:A:301:GNP:O2B	2.47	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	205/216 (95%)	196 (96%)	8 (4%)	1 (0%)	25	28
2	B	120/140 (86%)	112 (93%)	8 (7%)	0	100	100
3	C	1036/1023 (101%)	1017 (98%)	18 (2%)	1 (0%)	48	57
All	All	1361/1379 (99%)	1325 (97%)	34 (2%)	2 (0%)	44	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ALA
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	181/185 (98%)	179 (99%)	2 (1%)	70	82
2	B	105/122 (86%)	103 (98%)	2 (2%)	52	67
3	C	950/933 (102%)	928 (98%)	22 (2%)	45	59
All	All	1236/1240 (100%)	1210 (98%)	26 (2%)	47	63

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

Mol	Chain	Res	Type
1	A	179	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	GLN
2	B	90	ARG
2	B	157	VAL
3	C	35	GLN
3	C	206	SER
3	C	207	SER
3	C	247	ASP
3	C	291	MET
3	C	310	SER
3	C	354	GLU
3	C	356	ARG
3	C	538	LEU
3	C	539	CYS
3	C	545	GLN
3	C	607	LYS
3	C	611	VAL
3	C	628	ASP
3	C	638	PRO
3	C	678	THR
3	C	686	ASN
3	C	690	LEU
3	C	940	PHE
3	C	981	VAL
3	C	983	GLN
3	C	992	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	196	GLN
3	C	56	GLN
3	C	203	GLN
3	C	434	ASN
3	C	541	GLN
3	C	545	GLN
3	C	548	GLN
3	C	686	ASN
3	C	930	ASN
3	C	983	GLN
3	C	1010	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are 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	29,34,34	1.58	6 (20%)	33,54,54	1.79	7 (21%)
6	LBF	C	1101	3	38,39,39	2.29	6 (15%)	42,52,52	2.76	9 (21%)

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	-	2/14/38/38	0/3/3/3
6	LBF	C	1101	3	-	1/45/58/58	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1101	LBF	C2-C3	9.89	1.52	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1101	LBF	O2-C1	7.62	1.46	1.35
4	A	301	GNP	C5-C6	3.97	1.48	1.41
4	A	301	GNP	PG-N3B	3.25	1.71	1.63
6	C	1101	LBF	C2-C1	3.22	1.51	1.44
4	A	301	GNP	PB-O1B	2.76	1.50	1.46
4	A	301	GNP	PA-O3A	2.56	1.62	1.59
4	A	301	GNP	PB-O3A	2.49	1.62	1.59
6	C	1101	LBF	C16-C17	-2.32	1.50	1.53
6	C	1101	LBF	O6-C24	-2.28	1.24	1.30
4	A	301	GNP	PG-O2G	2.21	1.62	1.56
6	C	1101	LBF	C7-C8	2.20	1.49	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1101	LBF	C3-C2-C1	-12.53	111.34	121.39
6	C	1101	LBF	O2-C1-C2	7.46	123.20	118.00
4	A	301	GNP	O1G-PG-N3B	-4.51	105.12	111.77
6	C	1101	LBF	C4-C3-C2	-4.34	119.12	123.59
4	A	301	GNP	C2-N3-C4	3.99	119.79	115.48
4	A	301	GNP	C5-C6-N1	-3.79	118.35	123.42
6	C	1101	LBF	O1-C1-C2	-3.75	119.33	126.00
6	C	1101	LBF	C30-C16-C15	-3.59	107.29	110.73
4	A	301	GNP	C2-N1-C6	3.37	120.65	115.96
6	C	1101	LBF	C22-C23-C24	-3.18	121.34	126.94
6	C	1101	LBF	C11-C12-C13	-3.13	119.15	125.93
4	A	301	GNP	C4-C5-C6	-3.06	116.55	121.23
6	C	1101	LBF	C6-C7-C8	-2.39	121.23	126.12
4	A	301	GNP	O2G-PG-O1G	-2.37	107.50	113.45
4	A	301	GNP	O2A-PA-O1A	2.30	123.13	112.44
6	C	1101	LBF	C29-C14-C13	2.01	121.16	118.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

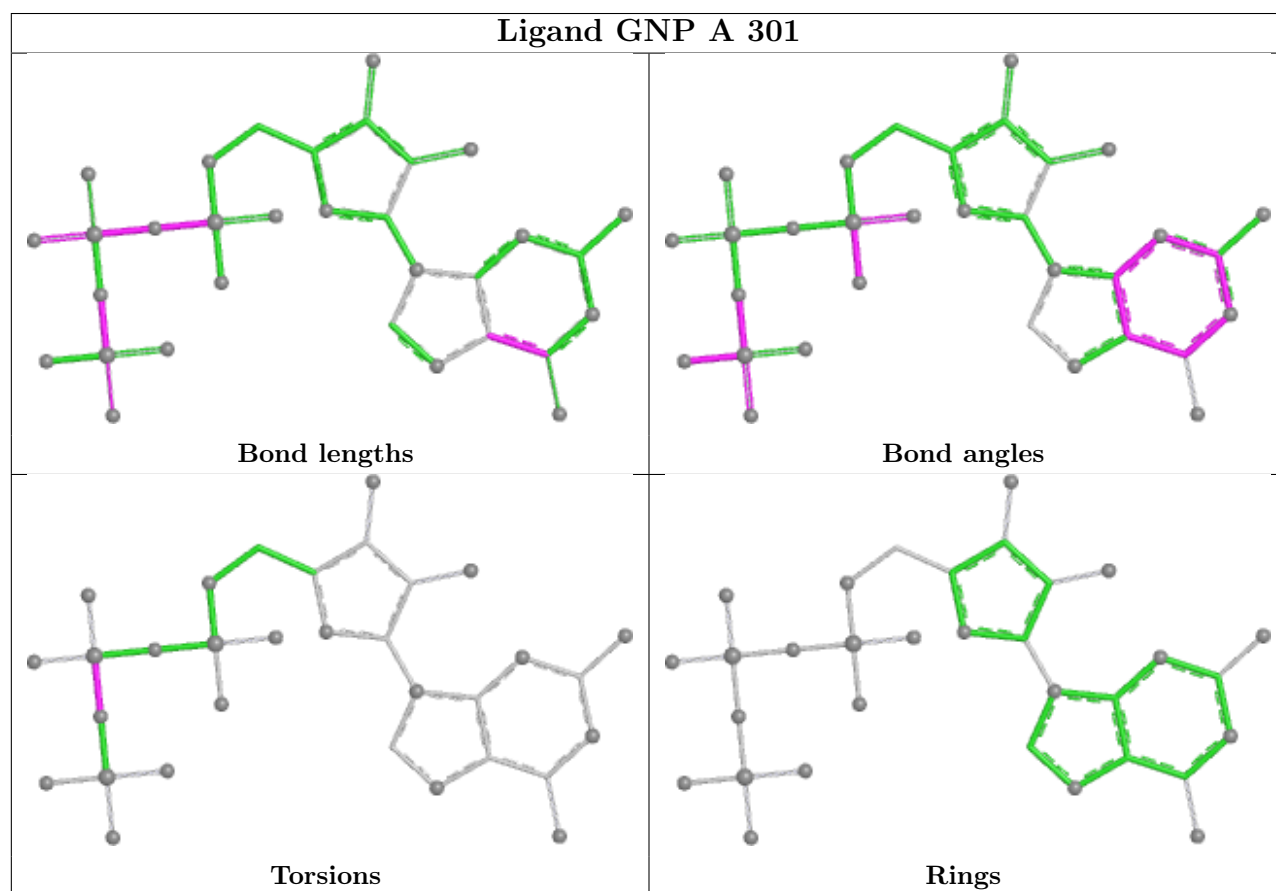
Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
4	A	301	GNP	PG-N3B-PB-O3A
6	C	1101	LBF	C27-C26-C8-C9

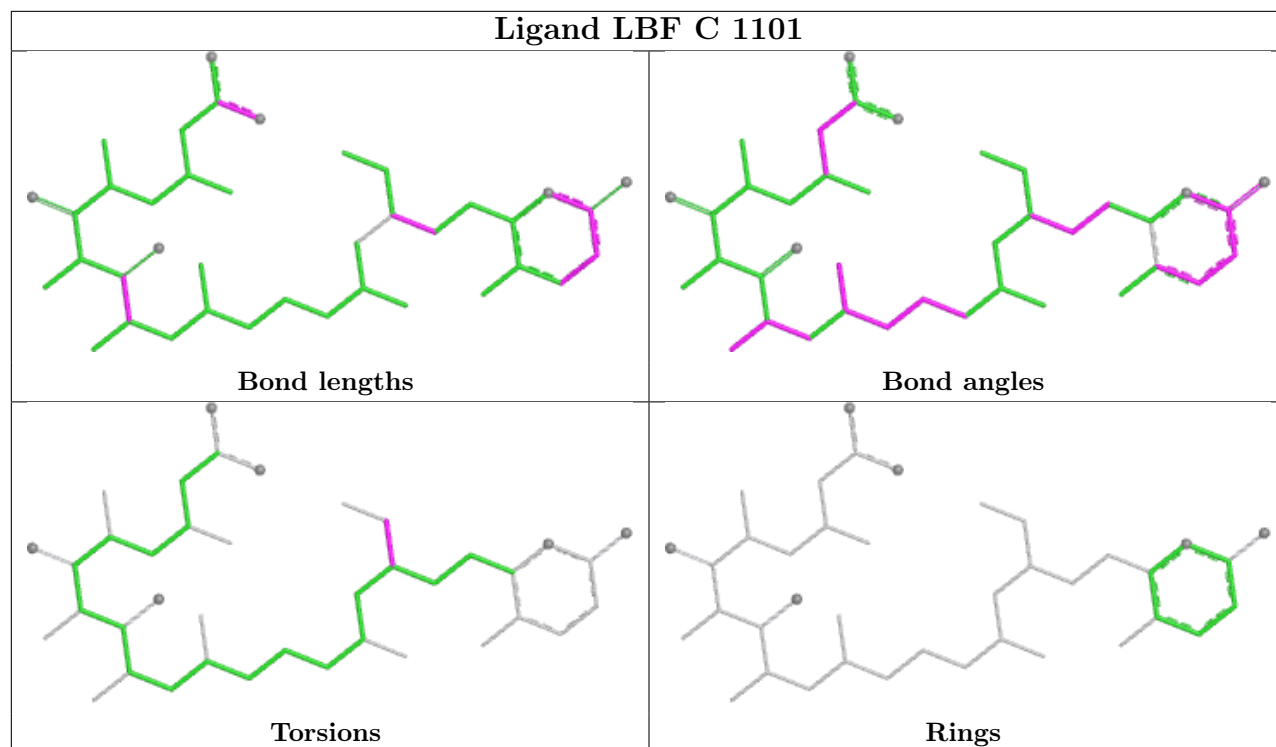
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GNP	1	0
6	C	1101	LBF	2	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	205/216 (94%)	-0.44	3 (1%) 71 68	17, 43, 88, 113	4 (1%)
2	B	121/140 (86%)	-0.38	0 100 100	37, 57, 76, 88	1 (0%)
3	C	1016/1023 (99%)	-0.48	7 (0%) 84 82	18, 46, 73, 107	24 (2%)
All	All	1342/1379 (97%)	-0.46	10 (0%) 84 82	17, 47, 75, 113	29 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	4.5
3	C	687	PRO	4.2
1	A	192	ALA	3.4
3	C	205	SER	3.2
3	C	262	LEU	2.7
3	C	691	LEU	2.5
3	C	455	PHE	2.2
3	C	690	LEU	2.2
1	A	197	TYR	2.1
3	C	206	SER	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](#)

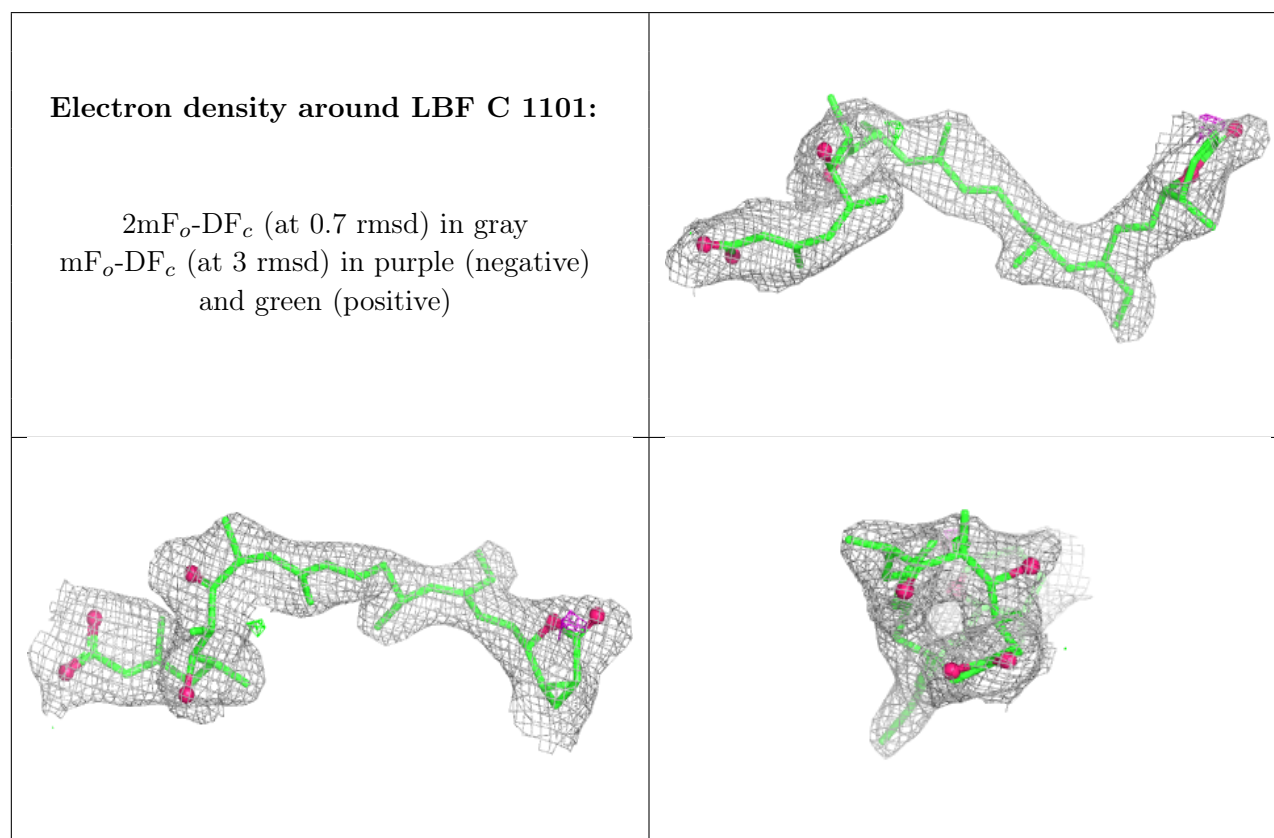
There are no monosaccharides in this entry.

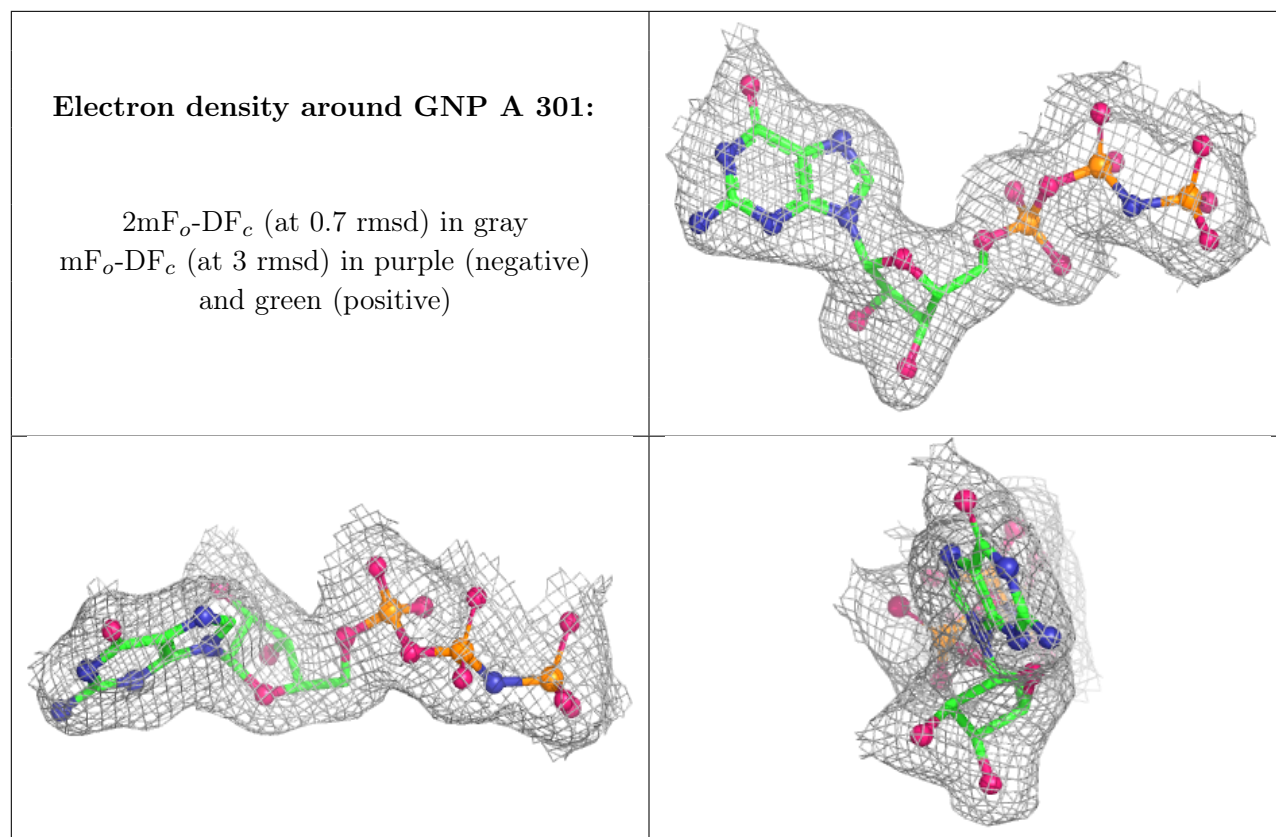
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
7	CL	C	1102	1/1	0.90	0.18	80,80,80,80	0
6	LBF	C	1101	39/39	0.93	0.09	44,54,60,61	0
7	CL	C	1105	1/1	0.93	0.08	80,80,80,80	0
7	CL	C	1103	1/1	0.94	0.11	57,57,57,57	0
7	CL	C	1104	1/1	0.95	0.11	73,73,73,73	0
5	MG	A	302	1/1	0.99	0.02	39,39,39,39	0
4	GNP	A	301	32/32	0.99	0.04	36,39,40,44	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.