



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:37 am BST

PDB ID : 3R9X
Title : Crystal structure of Era in complex with MgGDPNP, nucleotides 1506-1542 of 16S ribosomal RNA, and KsgA
Authors : Tu, C.; Ji, X.
Deposited on : 2011-03-26
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

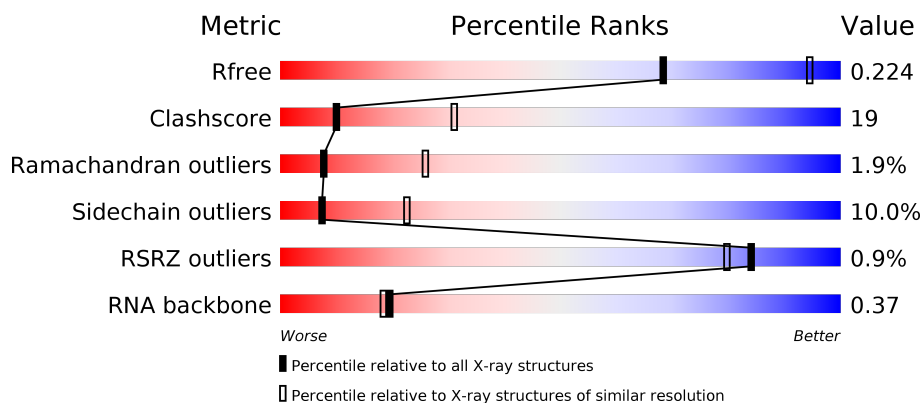
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



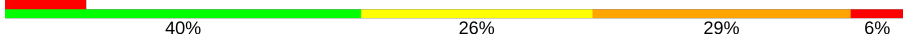
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 on 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	307	
2	B	248	
3	C	35	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5208 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 GTPase Era.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	1	4	0
			2430	1575	419	428	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP O67800
A	-4	HIS	-	EXPRESSION TAG	UNP O67800
A	-3	HIS	-	EXPRESSION TAG	UNP O67800
A	-2	HIS	-	EXPRESSION TAG	UNP O67800
A	-1	HIS	-	EXPRESSION TAG	UNP O67800
A	0	HIS	-	EXPRESSION TAG	UNP O67800

- Molecule 2 is a protein called Ribosomal RNA small subunit methyltransferase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	1	0
			1894	1229	313	347	5			

- Molecule 3 is a RNA chain called RNA301.

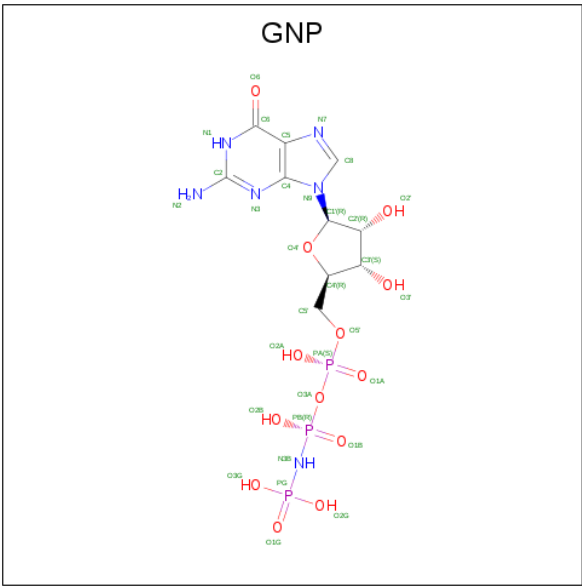
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	P	0	0	0
			744	332	132	245	35			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

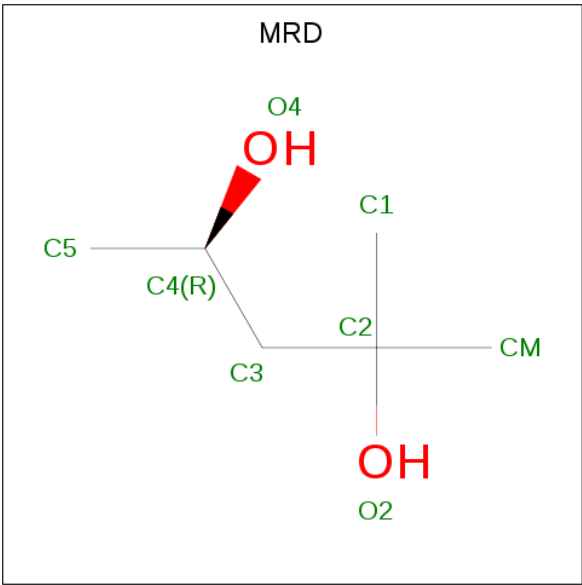
- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter

code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



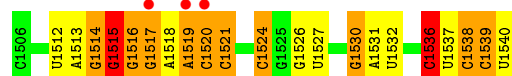
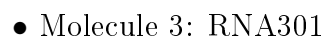
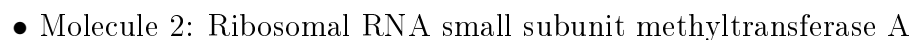
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	62	Total	O	0	0
			62	62		
8	B	14	Total	O	0	0
			14	14		
8	C	7	Total	O	0	0
			7	7		

These plots are drawn for all protein, RNA and DNA 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.

Chain A: 69% 27% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.50 Å 68.09 Å 73.59 Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	28.69 – 2.80 28.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (28.69-2.80) 95.4 (28.69-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.80 Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, R_{free}	0.171 , 0.226 0.170 , 0.224	Depositor DCC
R_{free} test set	975 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 62.5	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	5208	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: MRD, GNP, MG, ACT

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	0.42	0/2488	0.63	0/3367
2	B	0.34	0/1930	0.58	0/2603
3	C	0.53	0/830	1.24	8/1291 (0.6%)
All	All	0.41	0/5248	0.76	8/7261 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1536	C	N1-C1'-C2'	-10.27	100.65	114.00
3	C	1530	G	P-O3'-C3'	8.37	129.74	119.70
3	C	1515	G	P-O3'-C3'	6.95	128.04	119.70
3	C	1536	C	P-O3'-C3'	-6.76	111.59	119.70
3	C	1536	C	O4'-C1'-N1	6.33	113.27	108.20
3	C	1536	C	C3'-C2'-C1'	5.07	105.56	101.50
3	C	1524	C	O4'-C1'-N1	5.07	112.25	108.20
3	C	1538	C	O4'-C1'-N1	5.04	112.23	108.20

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	2430	0	2607	70	0
2	B	1894	0	1982	93	0
3	C	744	0	379	31	0
4	A	1	0	0	0	0
5	A	32	0	13	1	0
6	A	16	0	28	7	0
7	B	8	0	6	1	0
8	A	62	0	0	2	0
8	B	14	0	0	3	0
8	C	7	0	0	0	0
All	All	5208	0	5015	193	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 19.

All (193) 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:B:171:LYS:HD3	2:B:171:LYS:H	1.25	1.02
2:B:203:ASN:HB3	2:B:206:LYS:HG3	1.54	0.88
1:A:100[A]:ARG:HG3	1:A:100[A]:ARG:HH11	1.34	0.88
1:A:295[A]:ARG:HG2	1:A:295[A]:ARG:HH11	1.35	0.88
1:A:118:VAL:H	6:A:503:MRD:HMC2	1.38	0.88
3:C:1520:C:H2'	3:C:1521:C:H5''	1.53	0.86
1:A:117:PRO:HA	6:A:503:MRD:H3C2	1.58	0.86
3:C:1520:C:C2'	3:C:1521:C:H5''	2.08	0.84
2:B:140:LYS:O	2:B:141:ASP:HB2	1.78	0.83
3:C:1521:C:H6	3:C:1521:C:H5'	1.45	0.82
2:B:205:ARG:HG3	2:B:205:ARG:HH11	1.48	0.78
2:B:40:GLY:HA3	2:B:42:GLY:H	1.50	0.77
2:B:150:ARG:O	2:B:184:LYS:HE2	1.84	0.77
1:A:220:GLU:OE2	1:A:222:LYS:HD3	1.84	0.77
1:A:105:GLU:HB3	6:A:504:MRD:H1C3	1.67	0.77
1:A:100[A]:ARG:HH11	1:A:100[A]:ARG:CG	1.98	0.76
1:A:241:ARG:NH2	3:C:1530:G:O6	2.21	0.73
2:B:68:ASN:O	2:B:71:SER:HB3	1.88	0.73
1:A:27:LYS:HE2	8:A:662:HOH:O	1.90	0.72
2:B:171:LYS:N	2:B:171:LYS:HD3	2.03	0.71
1:A:295[A]:ARG:NH1	1:A:295[A]:ARG:HG2	2.00	0.68
2:B:87:PHE:HE2	2:B:92:LEU:HD11	1.59	0.67
3:C:1512:U:H2'	3:C:1513:A:H8	1.59	0.67
3:C:1518:A:H2'	3:C:1519:A:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HD12	1:A:271:LEU:HD13	1.77	0.65
3:C:1538:C:C5	3:C:1539:C:C4	2.84	0.65
2:B:65:MET:O	2:B:69:LEU:HD13	1.96	0.64
2:B:40:GLY:HA3	2:B:42:GLY:N	2.11	0.64
2:B:171:LYS:CD	2:B:171:LYS:H	1.98	0.63
2:B:239:LEU:O	2:B:243:ILE:HG13	1.98	0.63
3:C:1512:U:H2'	3:C:1513:A:C8	2.33	0.63
2:B:203:ASN:HB3	2:B:206:LYS:CG	2.27	0.62
2:B:205:ARG:CG	2:B:205:ARG:HH11	2.12	0.62
2:B:207:VAL:HG11	2:B:225:ASP:HB2	1.82	0.62
2:B:213:PRO:HD2	2:B:216:LEU:HD21	1.81	0.61
2:B:101:ASN:HD22	2:B:102:LEU:N	1.98	0.60
1:A:55:ILE:HD13	1:A:180:PHE:HE2	1.66	0.60
2:B:207:VAL:CG1	2:B:225:ASP:HB2	2.31	0.60
2:B:203:ASN:CB	2:B:206:LYS:HG3	2.28	0.60
1:A:63:TYR:O	1:A:65:PRO:HD3	2.02	0.59
2:B:19:LEU:HD22	2:B:44:LEU:HB2	1.84	0.59
2:B:28:ILE:HG21	2:B:53:LEU:HD23	1.85	0.59
1:A:100[B]:ARG:HA	1:A:100[B]:ARG:NE	2.18	0.58
2:B:54:LYS:O	2:B:55:LYS:HB2	2.01	0.58
2:B:129:GLN:HE22	2:B:131:GLU:HG2	1.68	0.58
2:B:200:ILE:O	2:B:228:VAL:HG21	2.04	0.57
3:C:1521:C:H6	3:C:1521:C:C5'	2.15	0.57
1:A:112:LYS:N	1:A:113:PRO:CD	2.68	0.57
2:B:54:LYS:O	2:B:54:LYS:HG2	2.03	0.57
1:A:243:ASN:HB3	3:C:1530:G:N7	2.19	0.57
2:B:138:GLY:HA2	2:B:142:THR:HG23	1.87	0.57
2:B:235:ASP:O	2:B:239:LEU:HD22	2.04	0.57
1:A:55:ILE:HD13	1:A:180:PHE:CE2	2.39	0.56
3:C:1516:G:C2	3:C:1518:A:OP2	2.59	0.56
1:A:118:VAL:N	6:A:503:MRD:HMC2	2.13	0.56
2:B:101:ASN:ND2	2:B:127:MET:HG2	2.21	0.55
3:C:1519:A:N6	3:C:1520:C:H1'	2.21	0.55
3:C:1515:G:H2'	3:C:1516:G:C8	2.42	0.55
1:A:287:TRP:HA	1:A:290:ARG:HD3	1.89	0.54
3:C:1514:G:H2'	3:C:1515:G:H5'	1.90	0.54
1:A:210:VAL:HB	1:A:211:PRO:HD3	1.91	0.53
3:C:1531:A:O2'	3:C:1532:U:H5'	2.08	0.53
3:C:1536:C:O2'	3:C:1537:U:H5'	2.08	0.53
1:A:43:LEU:C	1:A:43:LEU:HD23	2.29	0.53
2:B:87:PHE:CD1	2:B:88:PRO:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1518:A:H2'	3:C:1519:A:H8	1.74	0.53
1:A:261:LYS:O	1:A:265:GLN:HG3	2.09	0.52
1:A:100[A]:ARG:HB3	1:A:101:PRO:HD2	1.92	0.52
2:B:122:PRO:HA	2:B:181:LYS:HB2	1.91	0.52
2:B:104:TYR:CD1	2:B:129:GLN:HB2	2.45	0.52
2:B:144:TRP:CG	2:B:145:LEU:N	2.78	0.52
1:A:226:ALA:O	1:A:227:ASN:HB2	2.10	0.52
1:A:29:SER:HB2	1:A:42:VAL:HG11	1.92	0.51
3:C:1521:C:H5'	3:C:1521:C:C6	2.36	0.51
1:A:78:ILE:HG12	1:A:301:LEU:HD13	1.93	0.51
2:B:65:MET:HA	2:B:68:ASN:OD1	2.11	0.51
1:A:291:PRO:O	1:A:295[B]:ARG:HB2	2.11	0.51
1:A:190:LEU:HD23	1:A:221:ILE:HD13	1.92	0.51
2:B:188:LYS:O	2:B:189:ASP:HB3	2.10	0.50
2:B:23:ALA:HB2	2:B:48:LEU:HD23	1.94	0.50
2:B:205:ARG:CG	2:B:205:ARG:NH1	2.75	0.49
2:B:101:ASN:HA	2:B:127:MET:HB3	1.95	0.49
2:B:232:SER:HB2	8:B:679:HOH:O	2.12	0.49
1:A:243:ASN:ND2	1:A:243:ASN:H	2.11	0.49
2:B:26:LEU:HD11	2:B:99:VAL:HB	1.95	0.49
3:C:1520:C:C3'	3:C:1521:C:H5''	2.43	0.48
1:A:105:GLU:OE1	6:A:504:MRD:HMC2	2.13	0.48
1:A:201:LYS:HD2	1:A:262:ARG:HB3	1.96	0.48
3:C:1517:G:C6	3:C:1518:A:C2	3.01	0.48
2:B:14:VAL:HG12	2:B:166:PHE:HD2	1.78	0.48
1:A:256:LEU:HD22	1:A:256:LEU:O	2.14	0.48
1:A:286:ASP:HB3	1:A:289:ARG:HD3	1.95	0.48
2:B:105:ASN:OD1	2:B:106:VAL:HG22	2.14	0.48
2:B:168:PRO:O	2:B:170:PRO:HD3	2.14	0.48
3:C:1514:G:C2'	3:C:1515:G:H5'	2.45	0.47
2:B:156:ASN:HB2	2:B:178:LYS:HB3	1.96	0.47
1:A:133:ASN:O	1:A:136:PRO:HD2	2.14	0.47
1:A:17:SER:OG	1:A:58:ASP:OD2	2.33	0.47
2:B:195:LYS:O	2:B:198:THR:HG22	2.15	0.47
3:C:1539:C:N4	3:C:1540:U:O4	2.48	0.47
2:B:121:VAL:HG22	2:B:121:VAL:O	2.14	0.47
2:B:43:ASN:N	2:B:43:ASN:OD1	2.47	0.47
1:A:197:ILE:O	1:A:201:LYS:HG2	2.14	0.47
1:A:226:ALA:O	1:A:227:ASN:CB	2.63	0.47
2:B:103:PRO:O	2:B:104:TYR:C	2.53	0.47
1:A:40:MET:HA	1:A:78:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:LEU:O	2:B:150:ARG:HD2	2.14	0.47
2:B:228:VAL:HG23	8:B:672:HOH:O	2.14	0.47
2:B:87:PHE:HZ	2:B:92:LEU:HD21	1.80	0.46
1:A:100[A]:ARG:HG3	1:A:100[A]:ARG:NH1	2.13	0.46
2:B:121:VAL:HA	2:B:122:PRO:HD3	1.79	0.46
2:B:207:VAL:HB	2:B:225:ASP:HA	1.96	0.46
1:A:249:ILE:HA	1:A:256:LEU:HB2	1.95	0.46
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.63	0.46
2:B:135:LYS:O	2:B:146:SER:HB2	2.15	0.46
2:B:123:LEU:HA	2:B:179:LEU:O	2.15	0.46
2:B:152:PHE:CZ	2:B:190:LEU:HD22	2.51	0.46
3:C:1526:G:O2'	3:C:1527:U:H5'	2.16	0.46
2:B:220:ALA:HB2	2:B:242:LEU:HD12	1.97	0.45
2:B:112:GLU:HG2	2:B:116:TYR:HE2	1.82	0.45
2:B:234:GLU:H	2:B:234:GLU:HG2	1.57	0.45
1:A:14:VAL:CG2	1:A:92:MET:HG2	2.47	0.45
1:A:43:LEU:HD23	1:A:44:GLY:N	2.32	0.45
2:B:101:ASN:CG	2:B:127:MET:HG2	2.37	0.45
2:B:33:THR:HG23	2:B:55:LYS:HB3	1.98	0.45
2:B:40:GLY:CA	2:B:42:GLY:H	2.25	0.45
1:A:120:VAL:HG21	1:A:148:LEU:HD13	1.99	0.44
2:B:101:ASN:C	2:B:101:ASN:HD22	2.18	0.44
2:B:77:LEU:HD12	2:B:78:GLU:O	2.16	0.44
2:B:129:GLN:NE2	2:B:131:GLU:HG2	2.32	0.44
2:B:227:ARG:O	2:B:230:GLN:HG3	2.17	0.44
1:A:204:MET:HE1	8:A:605:HOH:O	2.18	0.44
2:B:118:LYS:O	2:B:181:LYS:HE3	2.17	0.44
1:A:107:TYR:CE2	1:A:112:LYS:HD2	2.53	0.44
2:B:188:LYS:O	2:B:189:ASP:CB	2.66	0.44
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.77	0.43
3:C:1512:U:O2'	3:C:1513:A:H5'	2.18	0.43
3:C:1519:A:C6	3:C:1520:C:H1'	2.53	0.43
2:B:26:LEU:O	2:B:27:ASN:C	2.56	0.43
2:B:233:LEU:HD13	2:B:237:PHE:CZ	2.53	0.43
1:A:30:ILE:HB	1:A:200:GLU:HG3	2.01	0.43
1:A:219:ASN:HD21	1:A:236:GLU:HG3	1.83	0.43
1:A:205:LEU:HD12	1:A:259:ILE:HG13	2.01	0.43
1:A:296:LEU:O	1:A:296:LEU:HG	2.18	0.43
3:C:1530:G:HO2'	3:C:1531:A:H8	1.64	0.43
1:A:16:LYS:HB2	1:A:16:LYS:HE2	1.75	0.43
2:B:99:VAL:HA	2:B:125:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HB2	6:A:504:MRD:H3C2	2.00	0.42
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.88	0.42
3:C:1518:A:C2	3:C:1519:A:C6	3.08	0.42
2:B:104:TYR:HD1	2:B:129:GLN:HB2	1.84	0.42
2:B:13:LEU:O	2:B:166:PHE:HB3	2.19	0.42
3:C:1518:A:C2	3:C:1519:A:C5	3.08	0.42
1:A:112:LYS:N	1:A:113:PRO:HD3	2.35	0.42
1:A:188:LEU:HA	1:A:189:PRO:HD3	1.76	0.42
2:B:213:PRO:O	2:B:216:LEU:HD22	2.20	0.42
2:B:51:HIS:HA	2:B:52:PRO:HD3	1.82	0.42
2:B:144:TRP:CD2	2:B:145:LEU:N	2.88	0.42
2:B:188:LYS:HD2	2:B:188:LYS:HA	1.75	0.42
2:B:233:LEU:HD13	2:B:237:PHE:HZ	1.84	0.42
2:B:214:GLU:O	2:B:217:LEU:HB2	2.20	0.42
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.64	0.42
1:A:243:ASN:HD22	1:A:243:ASN:H	1.66	0.42
1:A:242:GLU:O	1:A:246:PRO:HD2	2.19	0.42
2:B:211:LYS:O	2:B:212:ILE:HD13	2.20	0.42
7:B:502:ACT:H2	8:B:673:HOH:O	2.19	0.42
2:B:197:LEU:HA	2:B:197:LEU:HD23	1.88	0.42
1:A:190:LEU:HD13	1:A:271:LEU:HD21	2.02	0.41
2:B:142:THR:HG22	2:B:146:SER:HB3	2.02	0.41
1:A:19:LEU:HD22	1:A:92:MET:HE1	2.01	0.41
1:A:290:ARG:HA	1:A:291:PRO:HD3	1.88	0.41
1:A:245:LYS:N	1:A:246:PRO:HD2	2.36	0.41
2:B:85:SER:HB3	2:B:110:ILE:HD12	2.02	0.41
1:A:224:GLY:HA2	1:A:232:VAL:HG12	2.02	0.41
2:B:59:ILE:O	2:B:59:ILE:HG22	2.20	0.41
3:C:1515:G:N2	3:C:1521:C:C2	2.88	0.41
3:C:1530:G:O2'	3:C:1531:A:C8	2.73	0.41
2:B:105:ASN:ND2	2:B:106:VAL:HG13	2.36	0.41
2:B:106:VAL:O	2:B:110:ILE:HD13	2.19	0.41
1:A:100[A]:ARG:HB3	1:A:101:PRO:CD	2.50	0.41
1:A:117:PRO:HA	6:A:503:MRD:C3	2.39	0.41
1:A:295[A]:ARG:NH1	1:A:295[A]:ARG:CG	2.75	0.41
2:B:112:GLU:HG2	2:B:116:TYR:CE2	2.56	0.41
2:B:40:GLY:N	2:B:41:THR:HA	2.34	0.41
2:B:189:ASP:OD1	2:B:192:ASN:HB2	2.21	0.41
1:A:157:LEU:HB2	5:A:402:GNP:C6	2.51	0.41
2:B:37:VAL:HG23	2:B:38:GLY:N	2.35	0.41
1:A:219:ASN:ND2	1:A:236:GLU:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:HB2	1:A:251:LYS:HE2	1.88	0.40
2:B:163:PRO:HA	2:B:166:PHE:HE1	1.85	0.40
2:B:109:LEU:N	2:B:109:LEU:HD22	2.37	0.40
2:B:185:PHE:CD1	2:B:237:PHE:HB3	2.57	0.40
3:C:1515:G:C2	3:C:1521:C:N3	2.90	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	304/307 (99%)	285 (94%)	16 (5%)	3 (1%)	15	44
2	B	234/248 (94%)	198 (85%)	29 (12%)	7 (3%)	4	15
All	All	538/555 (97%)	483 (90%)	45 (8%)	10 (2%)	8	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	227	ASN
2	B	141	ASP
2	B	53	LEU
1	A	41	ARG
2	B	39	GLY
2	B	54	LYS
2	B	55	LYS
2	B	30	GLU
2	B	104	TYR

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	271/272 (100%)	251 (93%)	20 (7%)	13	37
2	B	215/226 (95%)	184 (86%)	31 (14%)	3	10
All	All	486/498 (98%)	435 (90%)	51 (10%)	7	20

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	26	THR
1	A	27	LYS
1	A	34	LYS
1	A	40	MET
1	A	81	GLN
1	A	90	LEU
1	A	93	ILE
1	A	100[A]	ARG
1	A	100[B]	ARG
1	A	102[A]	ARG
1	A	102[B]	ARG
1	A	147	GLU
1	A	170	LEU
1	A	183	ASP
1	A	184	MET
1	A	188	LEU
1	A	232	VAL
1	A	256	LEU
1	A	292	GLU
2	B	18	VAL
2	B	20	LYS
2	B	24	GLU
2	B	34	VAL
2	B	36	GLU
2	B	37	VAL
2	B	56	LEU

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Mol	Chain	Res	Type
2	B	63	ARG
2	B	71	SER
2	B	74	ASP
2	B	101	ASN
2	B	109	LEU
2	B	118	LYS
2	B	119[A]	ASP
2	B	119[B]	ASP
2	B	121	VAL
2	B	123	LEU
2	B	142	THR
2	B	166	PHE
2	B	167	VAL
2	B	171	LYS
2	B	179	LEU
2	B	188	LYS
2	B	191	LYS
2	B	205	ARG
2	B	206	LYS
2	B	216	LEU
2	B	230	GLN
2	B	233	LEU
2	B	239	LEU
2	B	241	ARG

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

Mol	Chain	Res	Type
1	A	109	ASN
1	A	219	ASN
1	A	243	ASN
2	B	101	ASN
2	B	202	GLN
2	B	230	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	34/35 (97%)	10 (29%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	1514	G
3	C	1515	G
3	C	1516	G
3	C	1517	G
3	C	1519	A
3	C	1520	C
3	C	1521	C
3	C	1524	C
3	C	1536	C
3	C	1539	C

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
5	GNP	A	402	4	28,34,34	2.47	10 (35%)	30,54,54	2.17	9 (30%)
7	ACT	B	502	-	1,3,3	1.53	0	0,3,3	0.00	-
7	ACT	B	501	-	1,3,3	1.33	0	0,3,3	0.00	-
6	MRD	A	504	-	7,7,7	0.35	0	9,10,10	0.34	0
6	MRD	A	503	-	7,7,7	0.28	0	9,10,10	0.74	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
5	GNP	A	402	4	-	4/17/38/38	0/3/3/3
6	MRD	A	504	-	-	4/5/5/5	-
6	MRD	A	503	-	-	2/5/5/5	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	GNP	C4-N9	-7.19	1.38	1.47
5	A	402	GNP	C5-C6	-6.68	1.41	1.52
5	A	402	GNP	PB-O3A	-3.59	1.54	1.59
5	A	402	GNP	C6-N1	3.53	1.39	1.33
5	A	402	GNP	PB-O2B	-3.30	1.47	1.56
5	A	402	GNP	PG-O1G	2.73	1.50	1.46
5	A	402	GNP	C5-C4	-2.38	1.38	1.53
5	A	402	GNP	PG-O3G	-2.29	1.50	1.56
5	A	402	GNP	C8-N9	-2.21	1.38	1.45
5	A	402	GNP	PG-O2G	-2.15	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	GNP	C4-C5-N7	6.57	111.17	102.46
5	A	402	GNP	C5-C6-N1	-5.08	111.92	118.19
5	A	402	GNP	O6-C6-C5	4.08	128.18	119.86
5	A	402	GNP	O2B-PB-O1B	3.20	116.63	109.92
5	A	402	GNP	O1B-PB-N3B	-2.47	108.14	111.77
5	A	402	GNP	O3A-PB-N3B	2.42	113.32	106.59
5	A	402	GNP	O3G-PG-O1G	-2.26	107.77	113.45
5	A	402	GNP	O6-C6-N1	-2.08	119.89	122.69
5	A	402	GNP	O1G-PG-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	402	GNP	PB-N3B-PG-O1G
5	A	402	GNP	PG-N3B-PB-O1B

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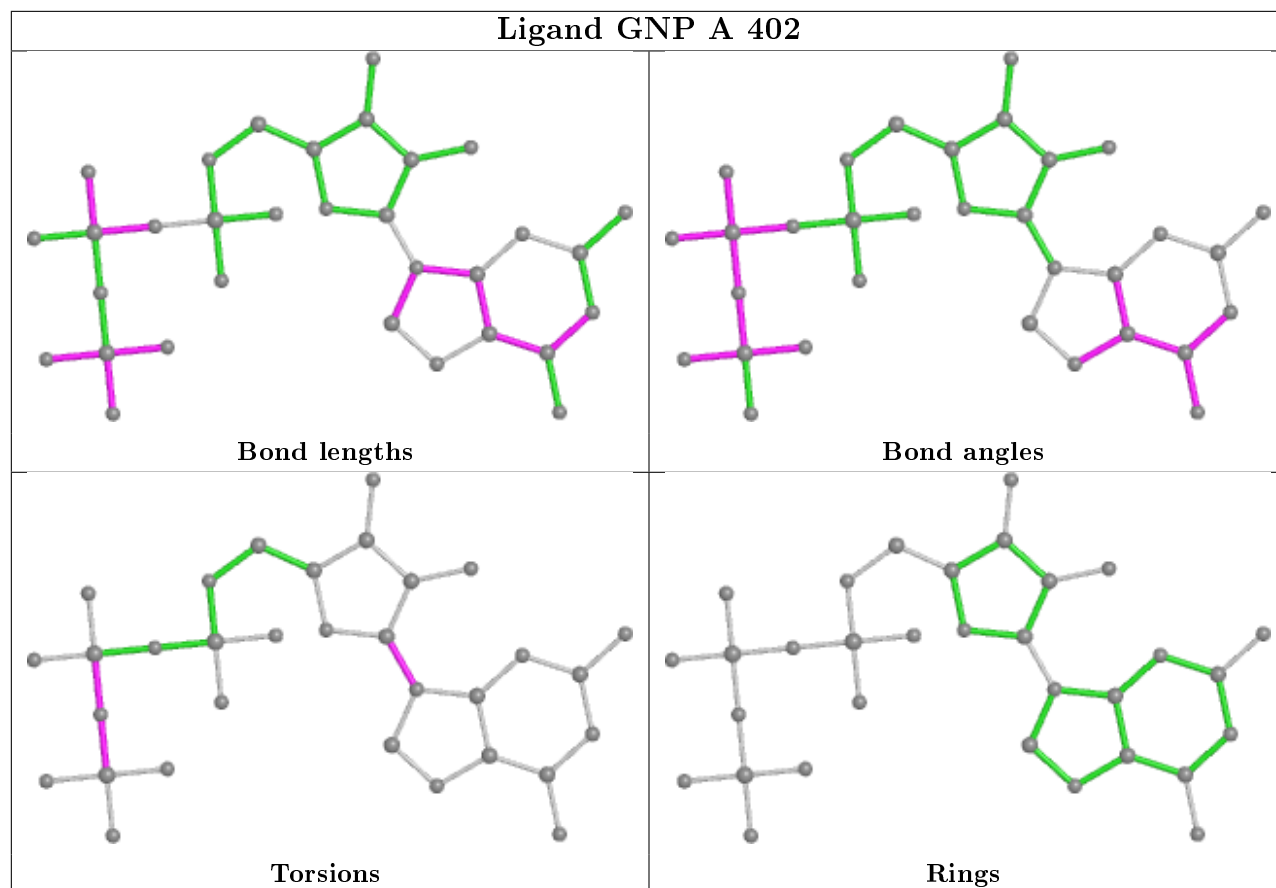
Mol	Chain	Res	Type	Atoms
5	A	402	GNP	PG-N3B-PB-O3A
5	A	402	GNP	C2'-C1'-N9-C4
6	A	504	MRD	O2-C2-C3-C4
6	A	504	MRD	C2-C3-C4-O4
6	A	503	MRD	C2-C3-C4-O4
6	A	504	MRD	C1-C2-C3-C4
6	A	504	MRD	CM-C2-C3-C4
6	A	503	MRD	CM-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	GNP	1	0
7	B	502	ACT	1	0
6	A	504	MRD	3	0
6	A	503	MRD	4	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	302/307 (98%)	-0.83	0 100 100	21, 47, 84, 125	12 (3%)
2	B	235/248 (94%)	-0.47	2 (0%) 84 80	42, 86, 147, 172	7 (2%)
3	C	35/35 (100%)	0.24	3 (8%) 10 5	58, 107, 226, 232	0
All	All	572/590 (96%)	-0.62	5 (0%) 84 80	21, 63, 142, 232	19 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1520	C	2.9
2	B	61	LEU	2.9
3	C	1519	A	2.8
3	C	1517	G	2.5
2	B	63	ARG	2.2

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](#)

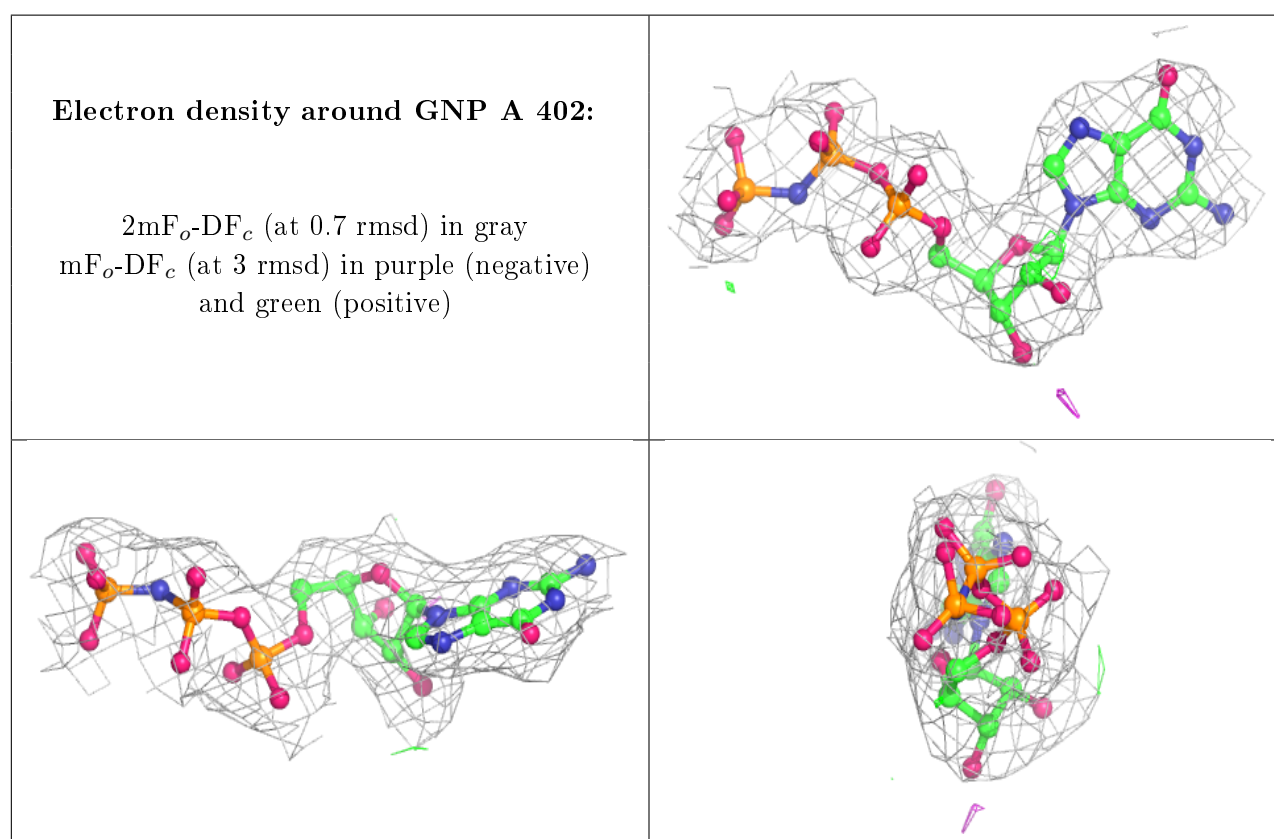
There are no carbohydrates in this entry.

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	ACT	B	502	4/4	0.81	0.21	81,81,90,98	0
6	MRD	A	504	8/8	0.87	0.28	70,87,92,98	0
6	MRD	A	503	8/8	0.91	0.22	45,80,89,94	0
7	ACT	B	501	4/4	0.97	0.21	64,69,70,71	0
5	GNP	A	402	32/32	0.98	0.14	23,36,48,55	0
4	MG	A	401	1/1	0.99	0.20	23,23,23,23	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.