



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 PM UTC

PDB ID : 2IEZ / pdb_00002iez
Title : Crystal Structure of mouse Rab27b bound to GDP in monoclinic space group
Authors : Chavas, L.M.G.; Torii, S.; Kamikubo, H.; Kawasaki, M.; Ihara, K.; Kato, R.; Kataoka, M.; Izumi, T.; Wakatsuki, S.
Deposited on : 2006-09-19
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 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

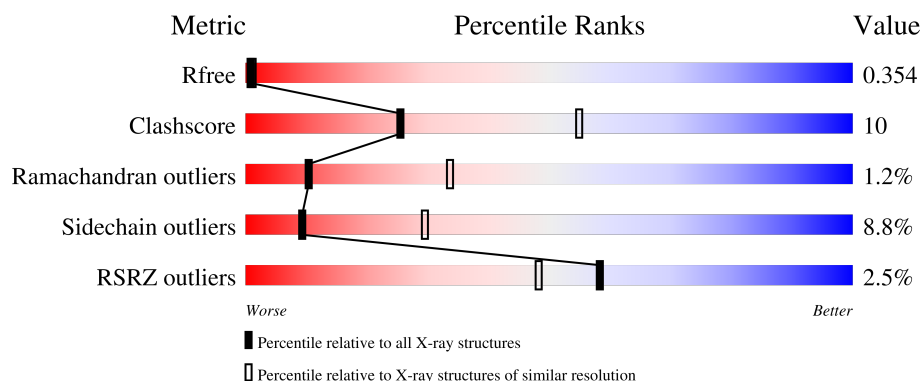
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	220	3% 57% 20% • 19%
1	B	220	0% 56% 20% • 22%
1	H	220	2% 58% 17% • 23%
1	I	220	2% 58% 20% • 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5754 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ras-related protein Rab-27B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1448	926	244	271	7			
1	B	171	Total	C	N	O	S	0	0	0
			1388	884	235	262	7			
1	H	169	Total	C	N	O	S	0	0	0
			1372	875	234	256	7			
1	I	173	Total	C	N	O	S	0	0	0
			1392	888	232	265	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q99P58
A	0	SER	-	expression tag	UNP Q99P58
A	78	LEU	GLN	engineered mutation	UNP Q99P58
B	-1	GLY	-	expression tag	UNP Q99P58
B	0	SER	-	expression tag	UNP Q99P58
B	78	LEU	GLN	engineered mutation	UNP Q99P58
H	-1	GLY	-	expression tag	UNP Q99P58
H	0	SER	-	expression tag	UNP Q99P58
H	78	LEU	GLN	engineered mutation	UNP Q99P58
I	-1	GLY	-	expression tag	UNP Q99P58
I	0	SER	-	expression tag	UNP Q99P58
I	78	LEU	GLN	engineered mutation	UNP Q99P58

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

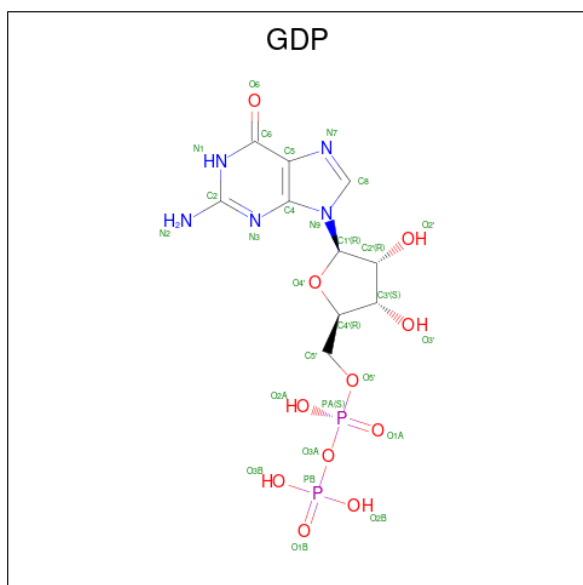
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 28 10 5 11 2	0	0
3	B	1	Total C N O P 28 10 5 11 2	0	0
3	H	1	Total C N O P 28 10 5 11 2	0	0
3	I	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	10	Total O 10 10	0	0
4	H	9	Total O 9 9	0	0

Continued on next page...

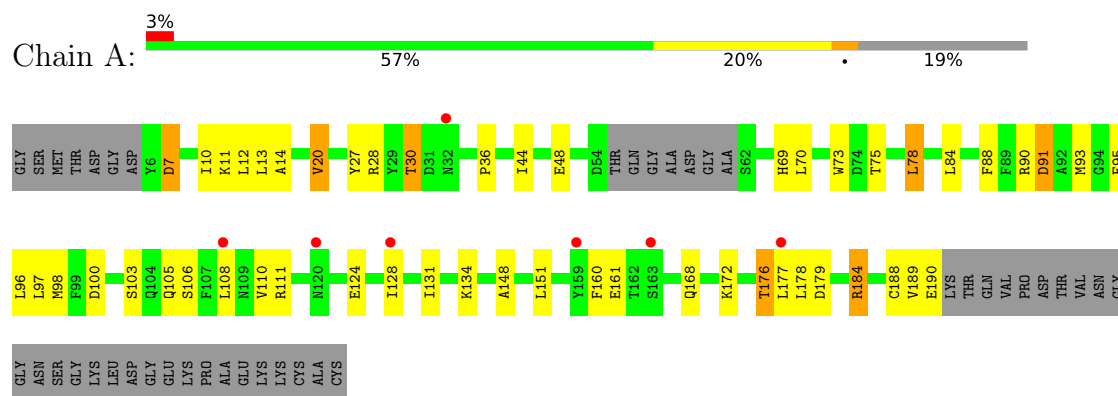
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	5	Total	O	0	0
			5	5		

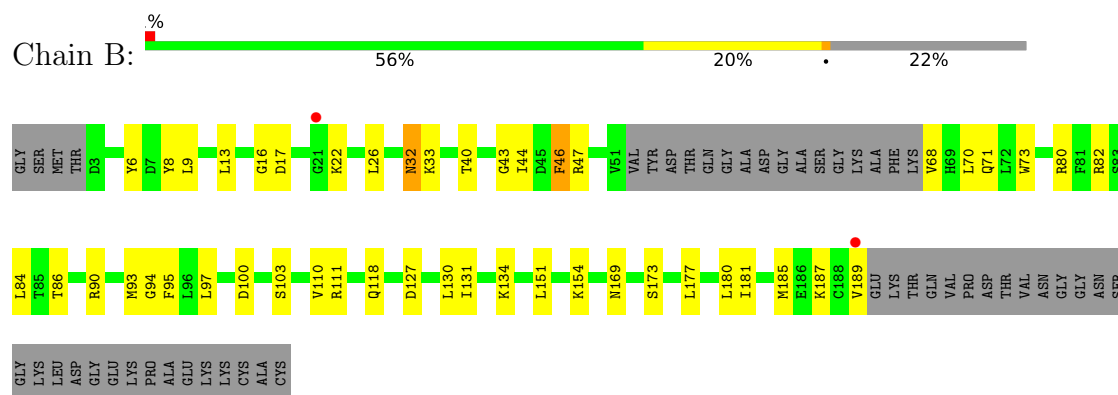
3 Residue-property plots [i](#)

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.

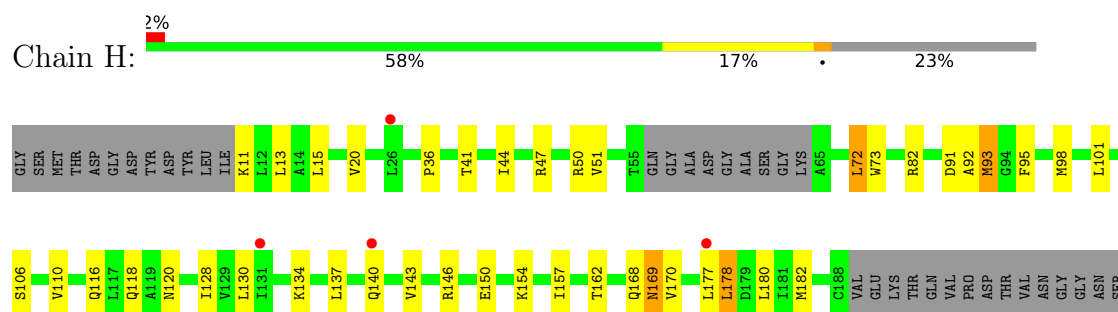
• Molecule 1: Ras-related protein Rab-27B



• Molecule 1: Ras-related protein Rab-27B



• Molecule 1: Ras-related protein Rab-27B



GLY
LYS
LEU
ASP
GLY
GLY
LYS
PRO
ALA
GLY
LYS
CYS
ALA
CYS

● Molecule 1: Ras-related protein Rab-27B



GLY	SER	THR	D3	G4	D5	Y6	D7	I10	K11	L12	D17	V20	G21	K22	T23	T24	F25	L26	T30	F34	N35	P36	V42	D45	F46	ARG	GLU	LYS	ARG	VAL	VAL	TYR	ASP	THR	GLN	GLY	ALA	ASP	GLY	A61	K64	A65	F66	K67	VAL	H69	L70	Q71	L72	W73
-----	-----	-----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

D74	T75	T86	R90	H98	T102	L108	N109	V110	M114	E124	V129	L130	Q140	M144	E145	R146	Q147	E153	K154	P158	Y159	F160	E161	M182	K183	K187	E190	LYS	THR	GLN	VAL	VAL	PRO	ASP	THR	VAL	ASN	GLY	GLY	ASN	SER	GLY	LYS	LEU	ASP
-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY
GLU
LYS
PRO
ALA
GLY
LYS
CYS
ALA
CYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.50Å 63.35Å 80.84Å 90.00° 98.45° 90.00°	Depositor
Resolution (Å)	35.60 – 2.80 35.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.4 (35.60-2.80) 87.3 (35.60-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.262 , 0.363 0.258 , 0.354	Depositor DCC
R_{free} test set	1033 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.2	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	0.91	EDS
Total number of atoms	5754	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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: CA, GDP

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	0.49	0/1475	0.83	1/1987 (0.1%)
1	B	0.59	0/1413	0.85	1/1905 (0.1%)
1	H	0.48	0/1397	0.80	0/1882
1	I	0.57	0/1417	0.90	1/1908 (0.1%)
All	All	0.54	0/5702	0.84	3/7682 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ALA	N-CA-C	-6.45	107.27	114.62
1	I	98	MET	N-CA-C	5.83	118.91	109.40
1	B	46	PHE	N-CA-C	5.13	116.88	109.07

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	1448	0	1432	46	0
1	B	1388	0	1367	30	0
1	H	1372	0	1359	25	0
1	I	1392	0	1363	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	28	0	12	2	0
3	B	28	0	12	1	0
3	H	28	0	12	1	0
3	I	28	0	12	0	0
4	A	14	0	0	0	0
4	B	10	0	0	0	0
4	H	9	0	0	0	0
4	I	5	0	0	0	0
All	All	5754	0	5569	108	0

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

All (108) 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)
1:B:16:GLY:O	1:B:22:LYS:NZ	2.15	0.78
1:B:169:ASN:O	1:B:173:SER:HB2	1.85	0.77
1:H:50:ARG:HH12	1:I:6:TYR:HB3	1.49	0.77
1:A:184:ARG:HH11	1:A:184:ARG:HG3	1.51	0.75
1:B:111:ARG:HG3	1:B:151:LEU:HD13	1.69	0.73
1:A:95:PHE:HB2	1:A:128:ILE:HG12	1.72	0.71
1:I:144:ASN:HD22	1:I:147:GLN:H	1.37	0.71
1:B:86:THR:HG22	1:B:90:ARG:NH1	2.05	0.71
1:I:182:MET:HE2	1:I:182:MET:HA	1.71	0.71
1:H:146:ARG:O	1:H:150:GLU:HG2	1.90	0.71
1:H:150:GLU:HB3	1:H:154:LYS:HE3	1.78	0.66
1:A:178:LEU:CD2	1:B:70:LEU:HD21	2.26	0.65
1:A:10:ILE:HD12	1:B:68:VAL:HG11	1.77	0.65
1:A:134:LYS:HG2	3:A:2001:GDP:C6	2.32	0.64
1:A:14:ALA:HA	1:A:96:LEU:HB2	1.81	0.63
1:A:48:GLU:OE2	1:A:69:HIS:ND1	2.29	0.63
1:A:178:LEU:HD21	1:B:70:LEU:HD21	1.80	0.63
1:A:13:LEU:HD23	1:B:73:TRP:HB2	1.81	0.61
1:A:96:LEU:HD21	1:A:177:LEU:CD1	2.31	0.60
1:A:100:ASP:HB3	1:A:103:SER:HB3	1.84	0.60
1:I:144:ASN:HD22	1:I:147:GLN:N	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:GLN:HG2	1:H:169:ASN:HD22	1.68	0.58
1:A:84:LEU:HD11	1:B:43:GLY:HA2	1.84	0.58
1:I:102:THR:HG23	1:I:140:GLN:HB3	1.85	0.58
1:A:98:MET:HB3	1:A:131:ILE:HB	1.86	0.58
1:A:98:MET:HA	1:A:131:ILE:O	2.03	0.58
1:I:110:VAL:O	1:I:114:MET:HG3	2.04	0.57
1:A:96:LEU:CD2	1:A:177:LEU:HD11	2.34	0.57
1:I:129:VAL:HG12	1:I:158:PRO:HG2	1.86	0.57
1:A:88:PHE:HB2	1:B:44:ILE:HG21	1.87	0.56
1:A:44:ILE:HG22	1:A:75:THR:HG22	1.88	0.55
1:H:162:THR:HG22	1:H:169:ASN:HB2	1.89	0.55
1:A:160:PHE:HE1	1:A:176:THR:HG21	1.71	0.54
1:H:168:GLN:HG2	1:H:169:ASN:ND2	2.21	0.54
1:A:7:ASP:HB2	1:B:68:VAL:HA	1.91	0.52
1:I:34:PHE:CZ	1:I:36:PRO:HG3	2.44	0.52
1:B:95:PHE:N	1:B:127:ASP:O	2.43	0.52
1:A:27:TYR:HD2	1:A:28:ARG:HG3	1.74	0.51
1:A:160:PHE:CE1	1:A:176:THR:HG21	2.45	0.51
1:A:111:ARG:HG3	1:A:151:LEU:HD12	1.91	0.51
1:A:96:LEU:HD21	1:A:177:LEU:HD11	1.92	0.51
1:A:97:LEU:HD21	1:A:110:VAL:HG13	1.92	0.51
1:I:45:ASP:CG	1:I:74:ASP:HB3	2.36	0.50
1:A:20:VAL:HG22	1:A:100:ASP:HB2	1.92	0.50
1:I:26:LEU:O	1:I:30:THR:HB	2.11	0.50
1:A:13:LEU:HD12	1:A:95:PHE:CE2	2.47	0.50
1:A:96:LEU:HD21	1:A:177:LEU:HD12	1.92	0.50
1:H:11:LYS:N	1:H:93:MET:HG2	2.28	0.49
1:I:10:ILE:HD11	1:I:182:MET:HE1	1.95	0.48
1:A:69:HIS:CD2	1:B:6:TYR:HB3	2.49	0.48
1:A:161:GLU:O	1:A:168:GLN:NE2	2.46	0.48
1:I:183:LYS:O	1:I:187:LYS:HB2	2.13	0.48
1:A:7:ASP:HB2	1:B:68:VAL:N	2.29	0.48
1:B:86:THR:HG22	1:B:90:ARG:HH11	1.77	0.47
1:H:178:LEU:O	1:H:182:MET:HG2	2.14	0.47
1:I:154:LYS:HG2	1:I:154:LYS:O	2.15	0.47
1:H:150:GLU:HB3	1:H:154:LYS:CE	2.44	0.47
1:H:72:LEU:HD12	1:I:12:LEU:HD12	1.97	0.47
1:B:134:LYS:HD3	3:B:1001:GDP:C4	2.50	0.47
1:I:17:ASP:O	1:I:22:LYS:NZ	2.47	0.47
1:A:30:THR:HG21	1:B:47:ARG:HD3	1.95	0.46
1:H:134:LYS:HG2	3:H:4001:GDP:C5	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:ASN:HD21	1:I:146:ARG:HB3	1.80	0.46
1:A:12:LEU:HD22	1:A:177:LEU:HD13	1.97	0.46
1:H:44:ILE:HD12	1:H:73:TRP:HZ3	1.81	0.46
1:I:144:ASN:ND2	1:I:147:GLN:H	2.08	0.46
1:B:94:GLY:HA3	1:B:181:ILE:HD11	1.97	0.45
1:B:97:LEU:HD21	1:B:110:VAL:HG13	1.98	0.45
1:B:32:ASN:HD22	1:B:32:ASN:C	2.25	0.45
1:H:101:LEU:HD23	1:H:143:VAL:HB	1.99	0.45
1:I:159:TYR:OH	1:I:161:GLU:HG2	2.17	0.45
1:B:8:TYR:CE2	1:B:185:MET:HE1	2.52	0.44
1:A:13:LEU:HD22	1:A:88:PHE:CE2	2.52	0.44
1:H:44:ILE:HD12	1:H:73:TRP:CZ3	2.52	0.44
1:A:48:GLU:HA	1:A:70:LEU:O	2.18	0.44
1:B:44:ILE:HD12	1:B:73:TRP:HZ3	1.83	0.44
1:I:45:ASP:OD2	1:I:74:ASP:HB3	2.16	0.44
1:A:90:ARG:O	1:A:91:ASP:C	2.61	0.44
1:H:13:LEU:HD12	1:H:95:PHE:CE2	2.53	0.44
1:H:128:ILE:HB	1:H:157:ILE:HG21	1.99	0.44
1:A:73:TRP:HB2	1:B:13:LEU:HD23	1.99	0.43
1:B:22:LYS:O	1:B:26:LEU:HG	2.18	0.43
1:A:172:LYS:O	1:A:176:THR:HB	2.18	0.43
1:A:184:ARG:HG3	1:A:184:ARG:NH1	2.26	0.43
1:A:105:GLN:HA	1:A:108:LEU:HB2	2.01	0.43
1:H:11:LYS:N	1:H:92:ALA:HA	2.34	0.43
1:H:36:PRO:HD2	1:I:46:PHE:O	2.18	0.43
1:B:177:LEU:O	1:B:180:LEU:HB2	2.19	0.42
1:B:130:LEU:C	1:B:131:ILE:HG13	2.44	0.42
1:B:154:LYS:HB2	1:B:154:LYS:HE3	1.89	0.42
1:I:86:THR:O	1:I:90:ARG:HB3	2.20	0.42
1:A:11:LYS:H	1:A:93:MET:HE3	1.85	0.42
1:A:100:ASP:H	1:A:106:SER:HB3	1.85	0.41
1:B:185:MET:C	1:B:187:LYS:N	2.78	0.41
1:H:134:LYS:HB3	1:H:137:LEU:HD12	2.02	0.41
1:H:180:LEU:HD23	1:H:180:LEU:HA	1.93	0.41
1:A:13:LEU:HD12	1:A:95:PHE:HE2	1.84	0.41
1:H:11:LYS:HD3	1:I:73:TRP:NE1	2.35	0.41
1:H:50:ARG:NH1	1:I:6:TYR:HB3	2.26	0.41
1:A:134:LYS:HE2	3:A:2001:GDP:C4	2.56	0.41
1:H:47:ARG:HD2	1:I:30:THR:HG21	2.03	0.40
1:A:13:LEU:HD21	1:A:88:PHE:O	2.21	0.40
1:A:100:ASP:H	1:A:106:SER:CB	2.34	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:ILE:HD11	1:I:182:MET:CE	2.51	0.40
1:A:36:PRO:HD2	1:B:46:PHE:O	2.21	0.40
1:H:168:GLN:O	1:H:170:VAL:N	2.54	0.40
1:B:100:ASP:HB3	1:B:103:SER:HB3	2.02	0.40
1:H:98:MET:HE2	1:H:98:MET:HB3	1.88	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	174/220 (79%)	161 (92%)	9 (5%)	4 (2%)	5	18
1	B	167/220 (76%)	156 (93%)	10 (6%)	1 (1%)	21	51
1	H	165/220 (75%)	155 (94%)	9 (6%)	1 (1%)	21	51
1	I	167/220 (76%)	152 (91%)	13 (8%)	2 (1%)	10	34
All	All	673/880 (76%)	624 (93%)	41 (6%)	8 (1%)	10	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	B	17	ASP
1	I	65	ALA
1	H	169	ASN
1	I	66	PHE
1	A	91	ASP
1	A	189	VAL
1	A	7	ASP

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	156/186 (84%)	147 (94%)	9 (6%)	18	49
1	B	150/186 (81%)	139 (93%)	11 (7%)	13	38
1	H	148/186 (80%)	131 (88%)	17 (12%)	5	18
1	I	149/186 (80%)	133 (89%)	16 (11%)	6	21
All	All	603/744 (81%)	550 (91%)	53 (9%)	9	29

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	30	THR
1	A	78	LEU
1	A	124	GLU
1	A	176	THR
1	A	179	ASP
1	A	184	ARG
1	A	188	CYS
1	A	190	GLU
1	B	9	LEU
1	B	32	ASN
1	B	33	LYS
1	B	40	THR
1	B	71	GLN
1	B	80	ARG
1	B	82	ARG
1	B	84	LEU
1	B	93	MET
1	B	118	GLN
1	B	189	VAL
1	H	15	LEU
1	H	20	VAL
1	H	41	THR
1	H	51	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	72	LEU
1	H	82	ARG
1	H	91	ASP
1	H	93	MET
1	H	106	SER
1	H	110	VAL
1	H	116	GLN
1	H	118	GLN
1	H	120	ASN
1	H	130	LEU
1	H	140	GLN
1	H	177	LEU
1	H	178	LEU
1	I	5	ASP
1	I	7	ASP
1	I	20	VAL
1	I	24	THR
1	I	30	THR
1	I	42	VAL
1	I	67	LYS
1	I	69	HIS
1	I	70	LEU
1	I	75	THR
1	I	86	THR
1	I	108	LEU
1	I	124	GLU
1	I	130	LEU
1	I	153	GLU
1	I	187	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	71	GLN
1	A	168	GLN
1	A	169	ASN
1	B	32	ASN
1	B	35	ASN
1	B	69	HIS
1	B	71	GLN
1	B	109	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	168	GLN
1	H	71	GLN
1	H	109	ASN
1	H	116	GLN
1	H	140	GLN
1	H	168	GLN
1	H	169	ASN
1	I	140	GLN
1	I	144	ASN
1	I	168	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GDP	I	3001	2	29,30,30	1.15	2 (6%)	45,47,47	1.92	8 (17%)
3	GDP	B	1001	2	29,30,30	1.21	4 (13%)	45,47,47	1.64	6 (13%)
3	GDP	H	4001	2	29,30,30	1.06	2 (6%)	45,47,47	1.95	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDP	A	2001	2	29,30,30	1.16	2 (6%)	45,47,47	1.74	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	I	3001	2	-	3/16/32/32	0/3/3/3
3	GDP	B	1001	2	-	4/16/32/32	0/3/3/3
3	GDP	H	4001	2	-	1/16/32/32	0/3/3/3
3	GDP	A	2001	2	-	5/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	GDP	C5-C4	3.25	1.47	1.38
3	B	1001	GDP	C5-C4	3.19	1.47	1.38
3	I	3001	GDP	C5-C4	3.11	1.47	1.38
3	H	4001	GDP	C5-C4	3.07	1.47	1.38
3	I	3001	GDP	C6-N1	-2.81	1.33	1.38
3	A	2001	GDP	C6-N1	-2.46	1.34	1.38
3	B	1001	GDP	C6-N1	-2.34	1.34	1.38
3	H	4001	GDP	C6-N1	-2.26	1.34	1.38
3	B	1001	GDP	C4-N9	-2.23	1.32	1.38
3	B	1001	GDP	C5-N7	-2.16	1.34	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3001	GDP	C5-C4-N3	-6.75	117.65	128.39
3	A	2001	GDP	C5-C4-N3	-6.22	118.50	128.39
3	H	4001	GDP	C5-C4-N3	-5.66	119.38	128.39
3	I	3001	GDP	C2-N3-C4	5.61	121.96	112.30
3	B	1001	GDP	C5-C4-N3	-5.45	119.71	128.39
3	H	4001	GDP	C2-N3-C4	5.13	121.14	112.30
3	A	2001	GDP	C2-N3-C4	4.97	120.86	112.30
3	I	3001	GDP	N9-C4-N3	4.63	135.22	125.95
3	B	1001	GDP	C2-N3-C4	4.61	120.24	112.30
3	A	2001	GDP	N9-C4-N3	4.59	135.13	125.95
3	H	4001	GDP	N9-C4-N3	4.17	134.30	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	GDP	N9-C4-N3	4.04	134.04	125.95
3	H	4001	GDP	C6-C5-N7	3.94	137.46	130.29
3	H	4001	GDP	C2'-C1'-N9	-3.94	102.29	113.25
3	I	3001	GDP	C6-C5-N7	3.90	137.40	130.29
3	I	3001	GDP	C4-C5-N7	-3.21	105.58	110.67
3	B	1001	GDP	C6-C5-N7	3.12	135.98	130.29
3	A	2001	GDP	C6-C5-N7	3.09	135.92	130.29
3	H	4001	GDP	C4-C5-N7	-2.75	106.32	110.67
3	A	2001	GDP	C4-C5-N7	-2.52	106.68	110.67
3	H	4001	GDP	C3'-C2'-C1'	2.38	105.97	101.46
3	B	1001	GDP	C4-C5-N7	-2.33	106.98	110.67
3	I	3001	GDP	C8-N7-C5	2.33	108.41	104.26
3	B	1001	GDP	O6-C6-C5	-2.29	120.48	126.53
3	I	3001	GDP	C5-C6-N1	2.19	118.83	113.25
3	A	2001	GDP	O6-C6-C5	-2.15	120.87	126.53
3	H	4001	GDP	O6-C6-C5	-2.12	120.93	126.53
3	H	4001	GDP	C5-C6-N1	2.11	118.63	113.25
3	I	3001	GDP	C2-N1-C6	-2.04	121.41	125.11

There are no chirality outliers.

All (13) torsion outliers are listed below:

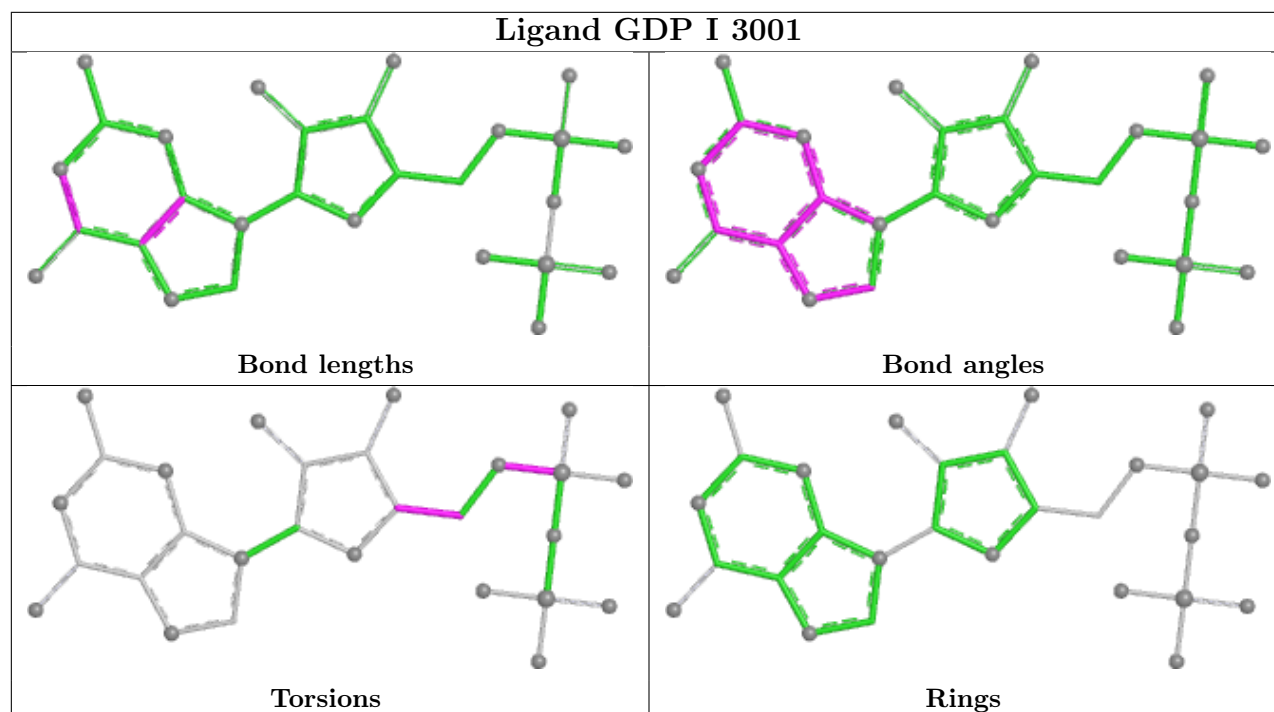
Mol	Chain	Res	Type	Atoms
3	A	2001	GDP	C5'-O5'-PA-O3A
3	A	2001	GDP	C5'-O5'-PA-O1A
3	A	2001	GDP	C5'-O5'-PA-O2A
3	B	1001	GDP	PA-O3A-PB-O3B
3	B	1001	GDP	C5'-O5'-PA-O2A
3	I	3001	GDP	C5'-O5'-PA-O1A
3	I	3001	GDP	O4'-C4'-C5'-O5'
3	I	3001	GDP	C3'-C4'-C5'-O5'
3	A	2001	GDP	O4'-C4'-C5'-O5'
3	B	1001	GDP	C5'-O5'-PA-O3A
3	H	4001	GDP	C5'-O5'-PA-O3A
3	A	2001	GDP	C3'-C4'-C5'-O5'
3	B	1001	GDP	PA-O3A-PB-O2B

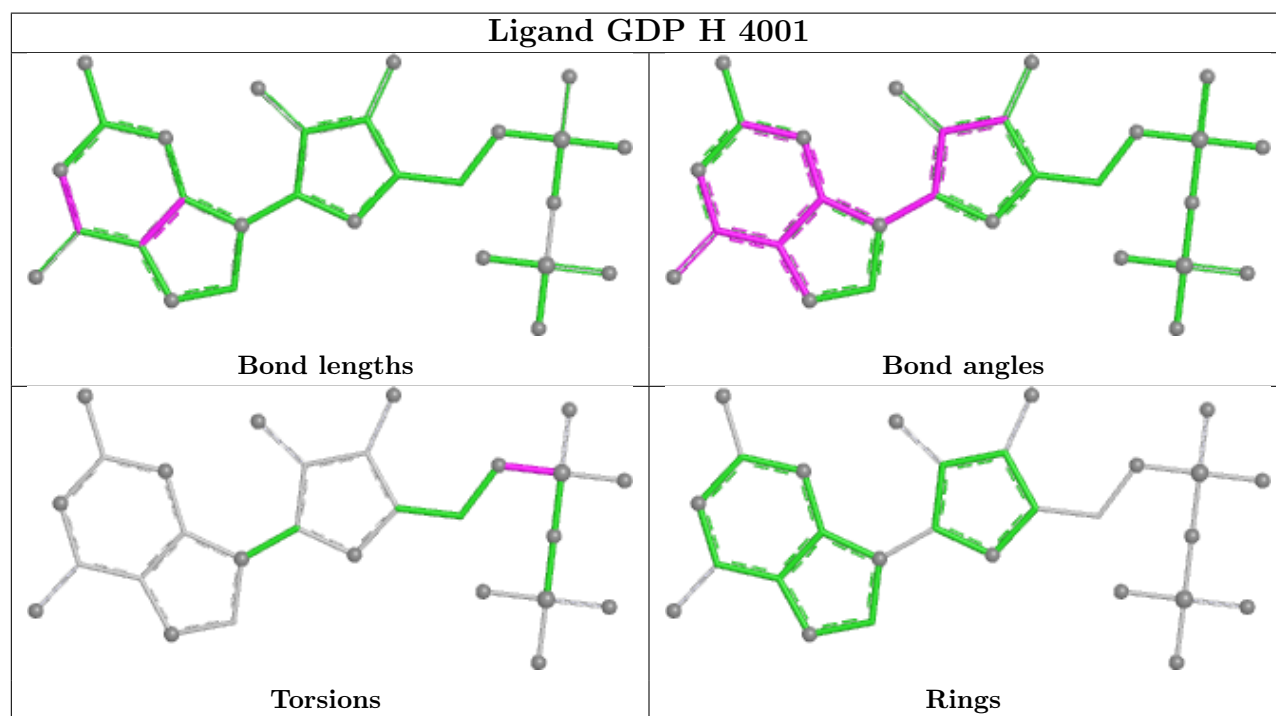
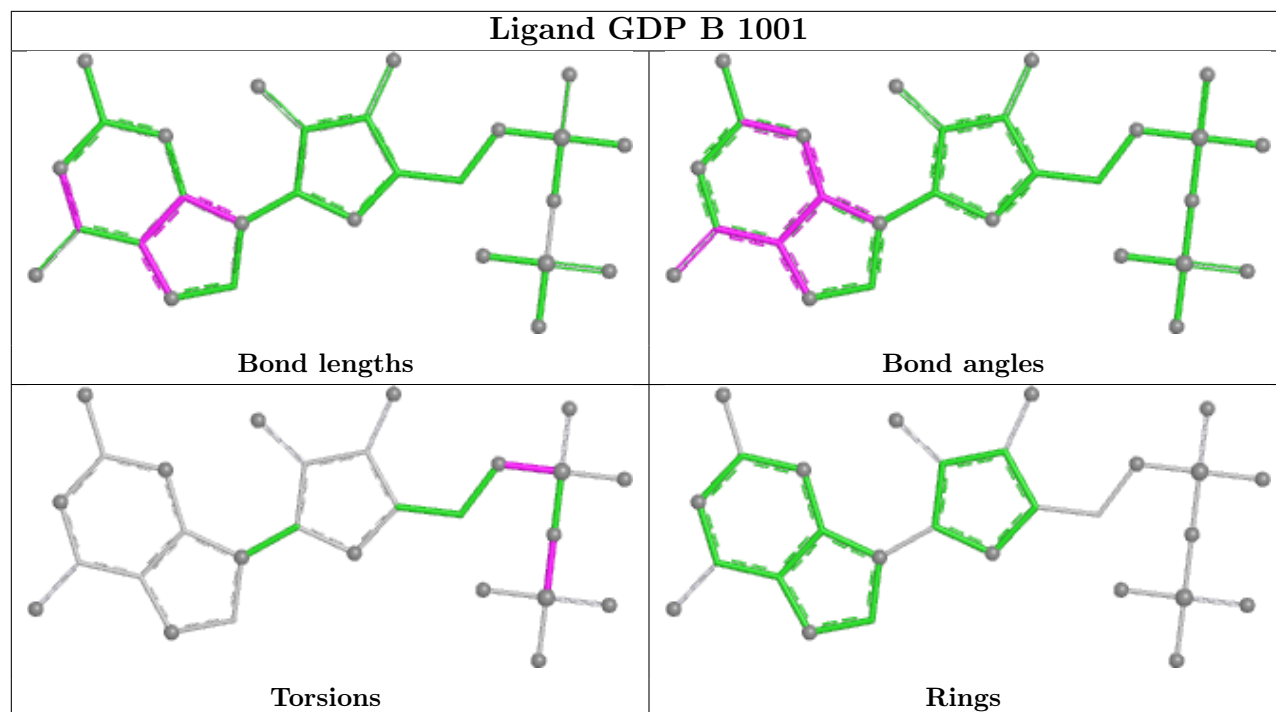
There are no ring outliers.

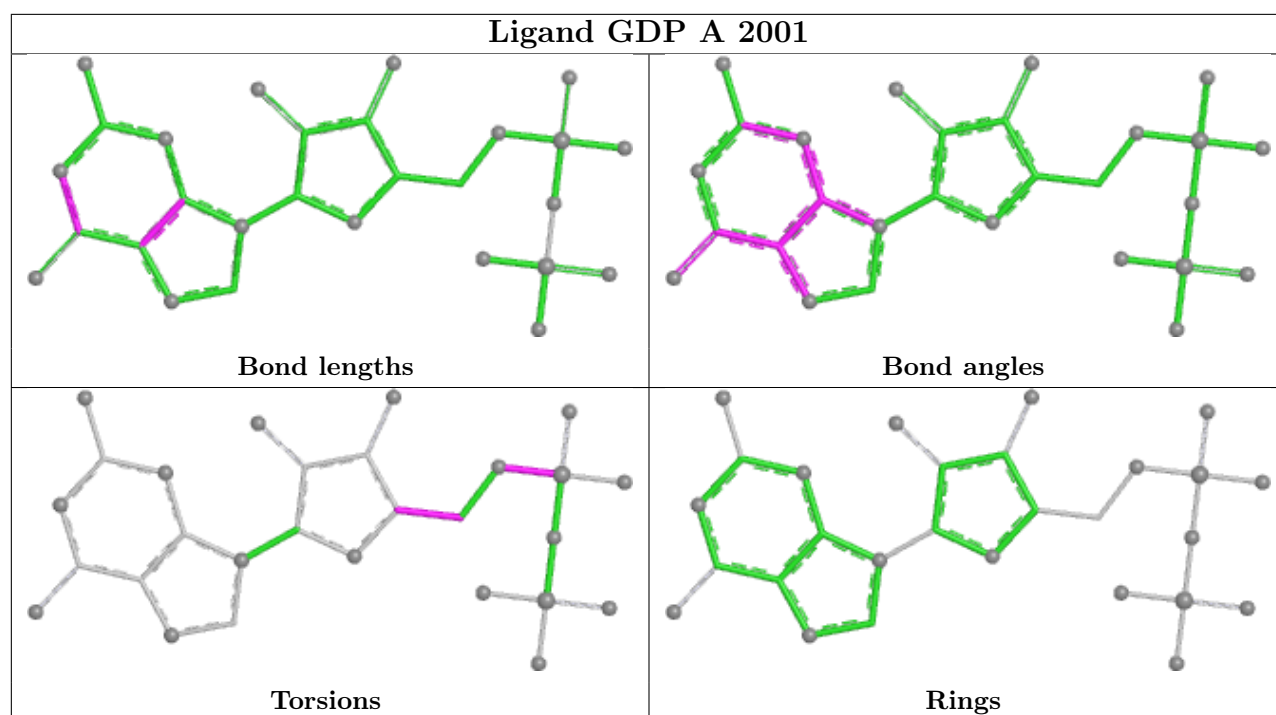
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	GDP	1	0
3	H	4001	GDP	1	0
3	A	2001	GDP	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	178/220 (80%)	0.49	7 (3%) 43 34	40, 66, 85, 89	0
1	B	171/220 (77%)	0.05	2 (1%) 76 68	32, 42, 56, 67	0
1	H	169/220 (76%)	0.39	4 (2%) 59 49	44, 65, 78, 82	0
1	I	173/220 (78%)	0.25	4 (2%) 61 51	32, 50, 78, 82	0
All	All	691/880 (78%)	0.30	17 (2%) 58 48	32, 55, 80, 89	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	26	LEU	3.6
1	A	159	TYR	3.1
1	A	108	LEU	2.9
1	B	189	VAL	2.8
1	A	163	SER	2.8
1	H	140	GLN	2.7
1	I	187	LYS	2.4
1	I	61	ALA	2.4
1	A	177	LEU	2.3
1	I	64	LYS	2.2
1	A	32	ASN	2.2
1	B	21	GLY	2.2
1	H	177	LEU	2.1
1	I	72	LEU	2.0
1	A	128	ILE	2.0
1	H	131	ILE	2.0
1	A	120	ASN	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](#)

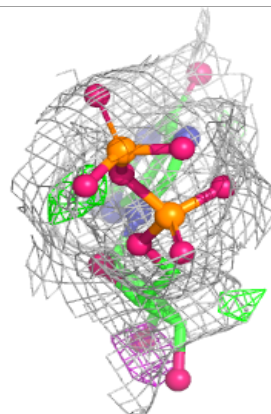
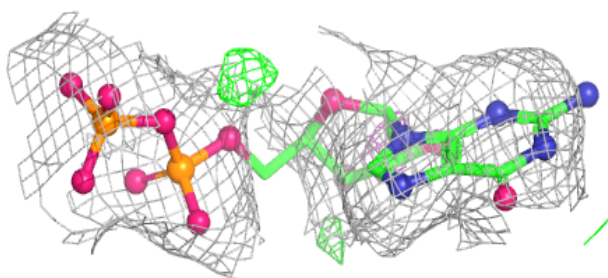
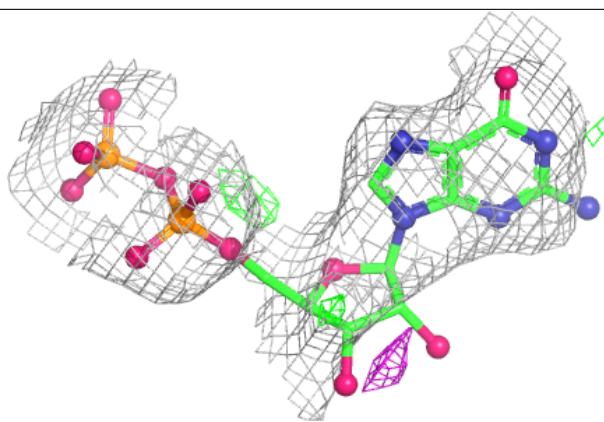
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	CA	H	401	1/1	0.77	0.09	47,47,47,47	0
2	CA	B	219	1/1	0.84	0.07	27,27,27,27	0
3	GDP	H	4001	28/28	0.86	0.10	56,58,59,59	0
2	CA	I	301	1/1	0.87	0.10	52,52,52,52	0
2	CA	A	219	1/1	0.87	0.06	44,44,44,44	0
3	GDP	A	2001	28/28	0.94	0.09	42,56,59,59	0
3	GDP	I	3001	28/28	0.94	0.07	31,32,36,38	0
3	GDP	B	1001	28/28	0.95	0.08	31,34,37,37	0

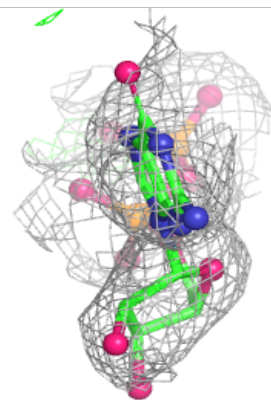
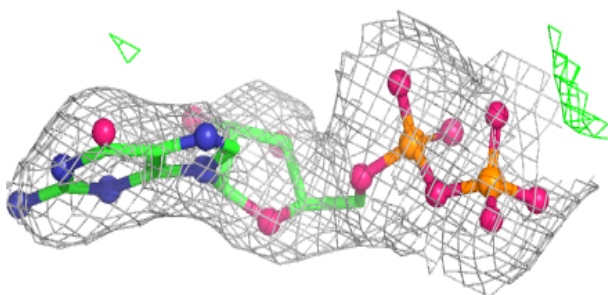
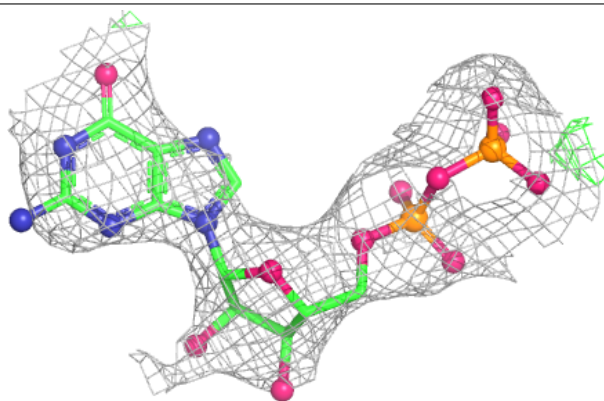
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP H 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

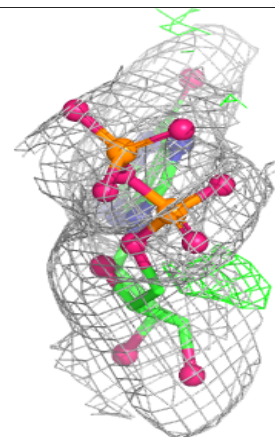
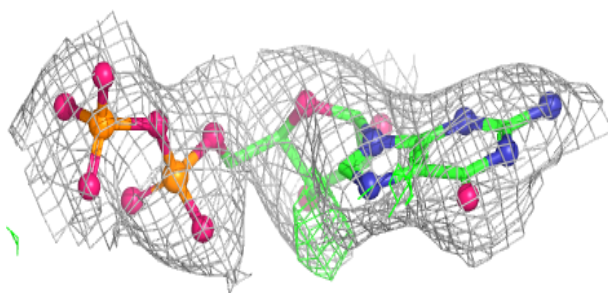
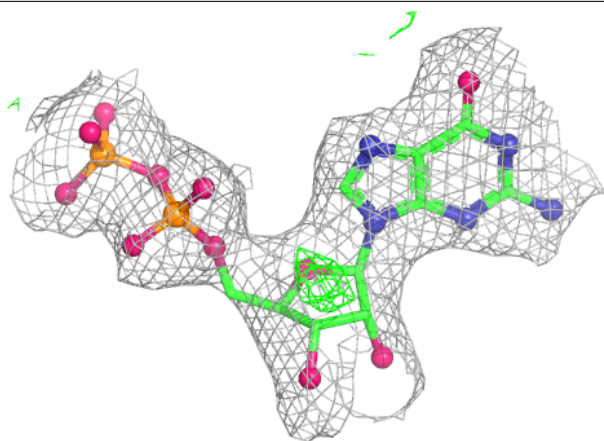
**Electron density around GDP A 2001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

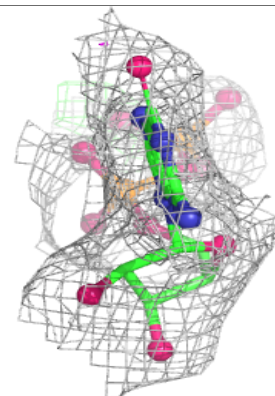
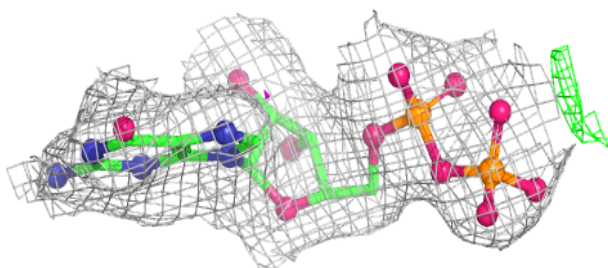
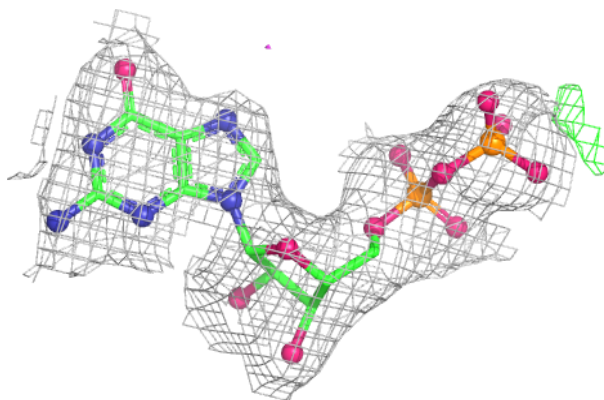


Electron density around GDP I 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP B 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.