



Full wwPDB X-ray Structure Validation Report ⓘ

May 10, 2026 – 01:01 AM JST

PDB ID : 22HQ / pdb_000022hq
Title : Crystal structure of GDP-bound FtsZ from *Acinetobacter baumannii*
Authors : Yadav, A.K.; Madhuri, M.; Saini, C.; Singh, A.; Kumar, M.; Kaur, P.; Singh, T.P.; Ethayathulla, A.S.
Deposited on : 2026-01-11
Resolution : 2.30 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	:	1.8.5 (274361), CSD as541be (2020)
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

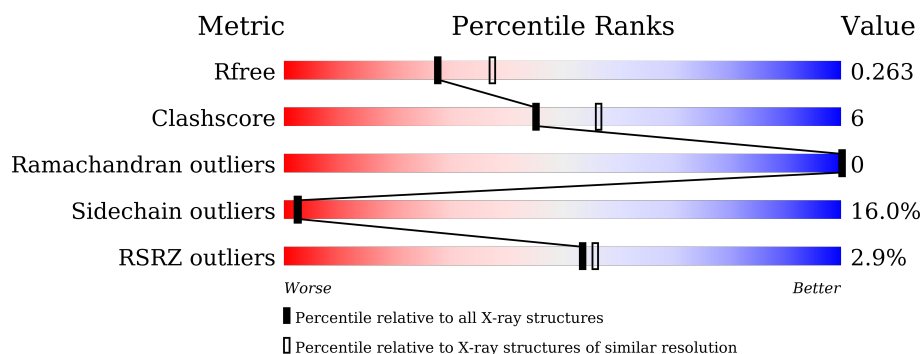
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	306	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>5%</div> <div></div> </div> </div>
1	B	306	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div></div> </div> </div>
1	C	306	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div></div> </div> </div>
1	D	306	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

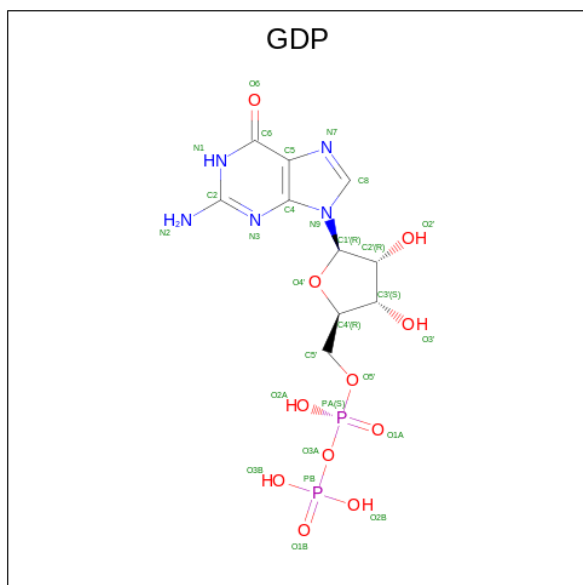
There are 3 unique types of molecules in this entry. The entry contains 8948 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cell division protein FtsZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2121	1322	374	415	10			
1	B	297	Total	C	N	O	S	0	1	0
			2177	1352	387	428	10			
1	C	303	Total	C	N	O	S	0	1	0
			2180	1358	388	423	11			
1	D	297	Total	C	N	O	S	0	0	0
			2164	1347	382	424	11			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

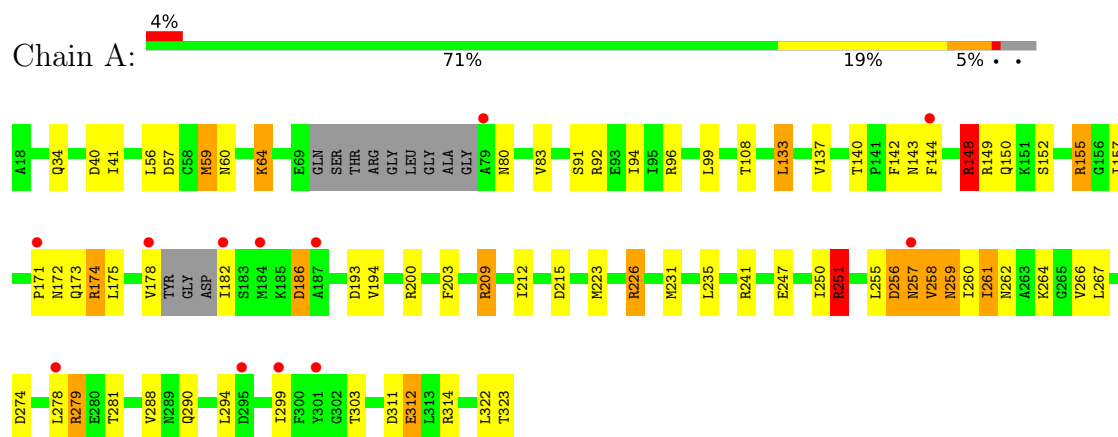
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	63	Total	O	0	0
			63	63		
3	C	44	Total	O	0	0
			44	44		
3	D	63	Total	O	0	0
			63	63		

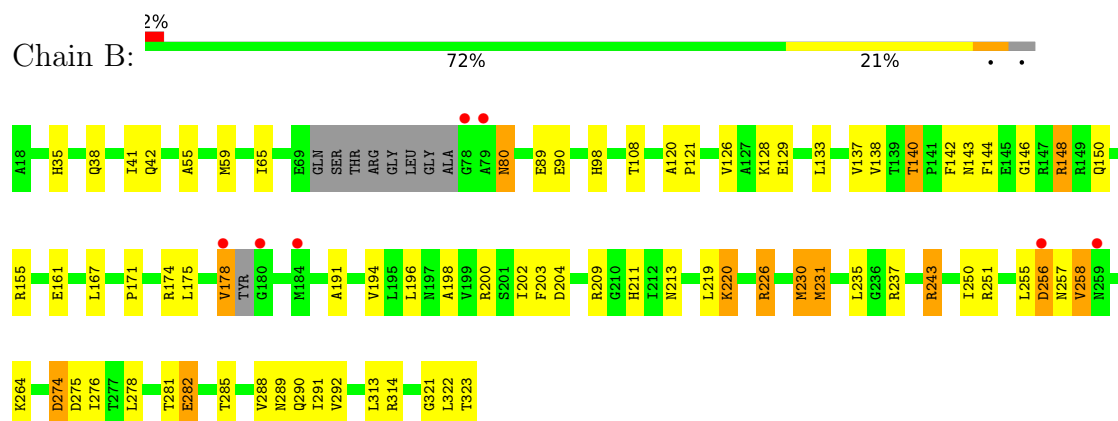
3 Residue-property plots

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.

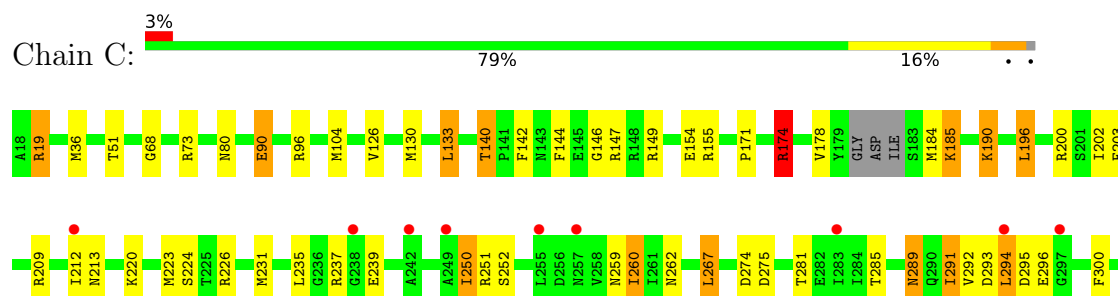
- Molecule 1: Cell division protein FtsZ



- Molecule 1: Cell division protein FtsZ

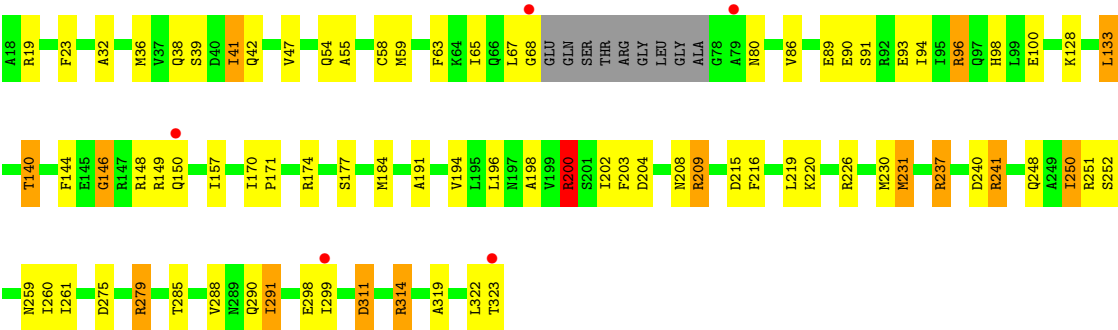


- Molecule 1: Cell division protein FtsZ





● Molecule 1: Cell division protein FtsZ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.27Å 80.84Å 84.07Å 101.73° 98.66° 92.52°	Depositor
Resolution (Å)	79.04 – 2.30 79.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (79.04-2.30) 93.7 (79.04-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.214 , 0.260 0.218 , 0.263	Depositor DCC
R_{free} test set	2359 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8948	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2279e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.88	0/2143	1.32	4/2911 (0.1%)
1	B	0.86	0/2199	1.29	4/2979 (0.1%)
1	C	0.89	0/2203	1.31	5/2989 (0.2%)
1	D	0.88	0/2187	1.30	6/2965 (0.2%)
All	All	0.88	0/8732	1.30	19/11844 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	8
1	C	0	13
1	D	0	12
All	All	0	42

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	PHE	CA-CB-CG	8.23	122.03	113.80
1	A	144	PHE	CA-CB-CG	7.08	120.89	113.80
1	B	203	PHE	CA-CB-CG	6.97	120.77	113.80
1	D	203	PHE	CA-CB-CG	6.72	120.52	113.80
1	B	144	PHE	CA-CB-CG	6.63	120.43	113.80
1	A	203	PHE	CA-CB-CG	6.37	120.17	113.80
1	D	311	ASP	N-CA-C	-6.17	105.72	113.18
1	C	239	GLU	N-CA-C	-5.96	105.50	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	259	ASN	N-CA-C	-5.69	105.74	114.16
1	A	142	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	146	GLY	CA-C-O	-5.62	118.08	122.52
1	B	142	PHE	CA-CB-CG	5.50	119.30	113.80
1	C	142	PHE	CA-CB-CG	5.45	119.25	113.80
1	C	146	GLY	CA-C-O	-5.38	118.72	122.22
1	D	146	GLY	CA-C-O	-5.37	118.28	122.52
1	D	215	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	23	PHE	CA-CB-CG	5.05	118.85	113.80
1	C	51	THR	N-CA-C	-5.04	107.14	113.28

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	155	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	241	ARG	Sidechain
1	A	251	ARG	Sidechain
1	A	279	ARG	Sidechain
1	A	314	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	148	ARG	Sidechain
1	B	155	ARG	Sidechain
1	B	174	ARG	Sidechain
1	B	209	ARG	Sidechain
1	B	226	ARG	Sidechain
1	B	243	ARG	Sidechain
1	B	251	ARG	Sidechain
1	B	314	ARG	Sidechain
1	C	147	ARG	Sidechain
1	C	149	ARG	Sidechain
1	C	155	ARG	Sidechain
1	C	174	ARG	Sidechain
1	C	19	ARG	Sidechain
1	C	200	ARG	Sidechain
1	C	209	ARG	Sidechain
1	C	226	ARG	Sidechain
1	C	251	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	73	ARG	Sidechain
1	C	80[A]	ASN	Mainchain
1	C	80[B]	ASN	Mainchain
1	C	96	ARG	Sidechain
1	D	148	ARG	Sidechain
1	D	149	ARG	Sidechain
1	D	19	ARG	Sidechain
1	D	200	ARG	Sidechain
1	D	209	ARG	Sidechain
1	D	226	ARG	Sidechain
1	D	237	ARG	Sidechain
1	D	241	ARG	Sidechain
1	D	251	ARG	Sidechain
1	D	279	ARG	Sidechain
1	D	314	ARG	Sidechain
1	D	96	ARG	Sidechain

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	2121	0	2058	26	0
1	B	2177	0	2130	31	0
1	C	2180	0	2129	22	0
1	D	2164	0	2125	23	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	0	0
3	A	24	0	0	0	0
3	B	63	0	0	0	0
3	C	44	0	0	1	0
3	D	63	0	0	0	0
All	All	8948	0	8490	102	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 6.

All (102) 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:140:THR:HG23	1:B:171:PRO:HA	1.58	0.86
1:B:133:LEU:HD22	1:B:220:LYS:HG2	1.71	0.72
1:B:278:LEU:O	1:B:282:GLU:HG2	1.90	0.71
1:C:289:ASN:HD21	1:C:294:LEU:HA	1.54	0.70
1:C:104:MET:HE2	1:C:133:LEU:HD22	1.80	0.63
1:D:36:MET:HG2	1:D:196:LEU:HD13	1.81	0.62
1:A:175:LEU:HD21	1:A:194:VAL:HG21	1.82	0.61
1:C:291:ILE:HG13	1:C:292:VAL:HG13	1.82	0.61
1:C:68:GLY:HA2	1:C:90:GLU:CD	2.26	0.60
1:B:198:ALA:HA	1:B:231:MET:HE1	1.84	0.60
1:D:140:THR:OG1	1:D:171:PRO:HA	2.03	0.58
1:D:202:ILE:HG23	1:D:219:LEU:HD11	1.85	0.57
1:C:202:ILE:HG21	1:C:223:MET:HE2	1.86	0.57
1:A:171:PRO:HB2	1:A:174:ARG:HG3	1.87	0.57
1:B:202:ILE:HG23	1:B:219:LEU:HD11	1.87	0.57
1:B:143:ASN:HA	1:B:150:GLN:HE22	1.71	0.55
1:A:34:GLN:HE22	1:A:59:MET:HA	1.72	0.55
1:D:146:GLY:O	1:D:150:GLN:HG2	2.09	0.53
1:C:231:MET:HG3	1:C:318:ILE:HG13	1.91	0.52
1:D:91:SER:O	1:D:94:ILE:HG22	2.10	0.52
1:A:212:ILE:HB	1:A:303:THR:HG23	1.91	0.51
1:B:80:ASN:OD1	1:B:80:ASN:N	2.45	0.50
1:B:250:ILE:HB	1:B:291:ILE:HG21	1.94	0.50
1:B:55:ALA:O	1:B:59:MET:HG2	2.13	0.48
1:D:96:ARG:O	1:D:100:GLU:HG2	2.14	0.48
1:D:250:ILE:HD11	1:D:288:VAL:HG22	1.95	0.48
1:B:291:ILE:HG13	1:B:292:VAL:HG13	1.96	0.48
1:D:216:PHE:CE2	1:D:220:LYS:HD2	2.48	0.48
1:A:56:LEU:HG	1:A:64:LYS:HG2	1.97	0.47
1:B:126:VAL:O	1:B:129:GLU:HG2	2.14	0.47
1:D:231:MET:HB2	1:D:231:MET:HE2	1.59	0.47
1:D:191:ALA:O	1:D:194:VAL:HG12	2.15	0.47
1:B:256:ASP:C	1:B:258:VAL:H	2.23	0.46
1:C:171:PRO:HB2	1:C:174:ARG:HG3	1.96	0.46
1:C:190:LYS:HB2	1:C:190:LYS:HE2	1.69	0.46
1:A:247:GLU:HB3	1:A:251:ARG:HH12	1.80	0.46
1:A:140:THR:O	1:A:172:ASN:HB2	2.16	0.45
1:B:35:HIS:O	1:B:38:GLN:HG3	2.16	0.45
1:B:235:LEU:HD21	1:B:237:ARG:HH22	1.82	0.45
1:C:140:THR:OG1	1:C:171:PRO:HA	2.16	0.45
1:A:264:LYS:HA	1:A:294:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASN:O	1:A:175:LEU:HB2	2.16	0.45
1:D:32:ALA:O	1:D:36:MET:HG3	2.17	0.45
1:D:198:ALA:HA	1:D:231:MET:HE1	1.99	0.45
1:B:264:LYS:HB2	1:B:321:GLY:HA3	1.99	0.45
1:C:133:LEU:HD11	1:C:224:SER:OG	2.17	0.45
1:D:39:SER:HB2	1:D:41:ILE:HD12	1.99	0.45
1:A:57:ASP:C	1:A:59:MET:H	2.25	0.44
1:A:80:ASN:HB3	1:A:83:VAL:HG23	1.97	0.44
1:C:174:ARG:HD3	3:C:534:HOH:O	2.17	0.44
1:A:133:LEU:HD22	1:A:133:LEU:HA	1.81	0.44
1:B:220:LYS:HB3	1:B:220:LYS:HE2	1.56	0.44
1:D:55:ALA:O	1:D:59:MET:HG2	2.18	0.44
1:A:59:MET:HE2	1:A:59:MET:HB3	1.45	0.43
1:B:175:LEU:HA	1:B:178:VAL:HG23	1.99	0.43
1:C:260:ILE:HD13	1:C:291:ILE:HD12	2.00	0.43
1:D:65:ILE:HD11	1:D:98:HIS:CG	2.53	0.43
1:A:186:ASP:OD1	1:A:186:ASP:N	2.51	0.43
1:D:86:VAL:O	1:D:90:GLU:HG2	2.18	0.43
1:A:259:ASN:O	1:A:262:ASN:N	2.45	0.43
1:B:143:ASN:HA	1:B:150:GLN:NE2	2.34	0.43
1:A:143:ASN:H	1:A:173:GLN:HG2	1.83	0.43
1:C:36:MET:HA	1:C:196:LEU:HD12	2.00	0.43
1:A:257:ASN:O	1:A:258:VAL:C	2.62	0.43
1:A:209:ARG:HE	1:A:209:ARG:HB2	1.62	0.43
1:C:220:LYS:HB3	1:C:220:LYS:HE3	1.73	0.42
1:B:65:ILE:HG12	1:B:98:HIS:CE1	2.54	0.42
1:A:256:ASP:C	1:A:258:VAL:H	2.27	0.42
1:D:133:LEU:HD22	1:D:133:LEU:HA	1.89	0.42
1:D:319:ALA:HB3	1:D:322:LEU:HD11	2.02	0.42
1:A:312:GLU:H	1:A:312:GLU:HG3	1.64	0.42
1:A:148:ARG:HE	1:A:148:ARG:HB3	1.39	0.42
1:B:161:GLU:O	1:B:226:ARG:NH2	2.53	0.42
1:B:213:ASN:OD1	1:B:213:ASN:N	2.51	0.42
1:C:289:ASN:ND2	1:C:294:LEU:HA	2.28	0.42
1:B:276:ILE:HG12	1:B:313:LEU:HD11	2.01	0.42
1:D:47:VAL:HG22	1:D:63:PHE:HB2	2.01	0.42
1:A:247:GLU:HA	1:A:250:ILE:HG12	2.02	0.41
1:A:259:ASN:C	1:A:261:ILE:N	2.74	0.41
1:D:67:LEU:O	1:D:68:GLY:C	2.63	0.41
1:D:204:ASP:OD1	1:D:208:ASN:ND2	2.52	0.41
1:A:108:THR:HA	1:A:137:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:O	1:B:204:ASP:HB2	2.21	0.41
1:C:295:ASP:O	1:C:296:GLU:C	2.63	0.41
1:C:126:VAL:O	1:C:130:MET:HG3	2.20	0.41
1:C:250:ILE:HG21	1:C:291:ILE:HG21	2.03	0.41
1:D:200:ARG:O	1:D:204:ASP:HB2	2.20	0.41
1:B:191:ALA:HA	1:B:194:VAL:HG12	2.02	0.41
1:C:267:LEU:HD23	1:C:300:PHE:HB2	2.02	0.41
1:B:230:MET:HB3	1:B:255:LEU:HD23	2.03	0.41
1:C:250:ILE:HD12	1:C:250:ILE:HA	1.85	0.41
1:B:313:LEU:HD12	1:B:313:LEU:HA	1.84	0.41
1:C:289:ASN:HD22	1:C:289:ASN:HA	1.55	0.41
1:B:288:VAL:O	1:B:291:ILE:HG12	2.20	0.40
1:D:250:ILE:HG13	1:D:291:ILE:HG21	2.02	0.40
1:B:108:THR:HA	1:B:137:VAL:O	2.20	0.40
1:B:120:ALA:HB3	1:B:121:PRO:HD3	2.03	0.40
1:C:185:LYS:HE3	1:C:185:LYS:HB2	1.40	0.40
1:A:223:MET:HE3	1:A:267:LEU:HD22	2.03	0.40
1:A:266:VAL:HG11	1:A:288:VAL:HG11	2.03	0.40
1:B:138:VAL:HG22	1:B:167:LEU:HD11	2.03	0.40
1:B:211:HIS:HE2	1:B:274:ASP:CG	2.27	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	288/306 (94%)	273 (95%)	15 (5%)	0	100	100
1	B	292/306 (95%)	289 (99%)	3 (1%)	0	100	100
1	C	300/306 (98%)	290 (97%)	10 (3%)	0	100	100
1	D	293/306 (96%)	286 (98%)	7 (2%)	0	100	100
All	All	1173/1224 (96%)	1138 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	212/239 (89%)	169 (80%)	43 (20%)	1	1
1	B	221/239 (92%)	194 (88%)	27 (12%)	5	5
1	C	216/239 (90%)	185 (86%)	31 (14%)	3	3
1	D	220/239 (92%)	181 (82%)	39 (18%)	2	2
All	All	869/956 (91%)	729 (84%)	140 (16%)	2	2

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	41	ILE
1	A	59	MET
1	A	60	ASN
1	A	64	LYS
1	A	91	SER
1	A	92	ARG
1	A	94	ILE
1	A	99	LEU
1	A	133	LEU
1	A	148	ARG
1	A	150	GLN
1	A	152	SER
1	A	155	ARG
1	A	157	ILE
1	A	174	ARG
1	A	178	VAL
1	A	182	ILE
1	A	186	ASP
1	A	193	ASP
1	A	200	ARG
1	A	209	ARG

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Mol	Chain	Res	Type
1	A	215	ASP
1	A	226	ARG
1	A	231	MET
1	A	235	LEU
1	A	251	ARG
1	A	255	LEU
1	A	256	ASP
1	A	257	ASN
1	A	258	VAL
1	A	260	ILE
1	A	261	ILE
1	A	274	ASP
1	A	278	LEU
1	A	279	ARG
1	A	281	THR
1	A	290	GLN
1	A	299	ILE
1	A	311	ASP
1	A	312	GLU
1	A	322	LEU
1	A	323	THR
1	B	41	ILE
1	B	42	GLN
1	B	80	ASN
1	B	89	GLU
1	B	90	GLU
1	B	128	LYS
1	B	140	THR
1	B	148	ARG
1	B	178	VAL
1	B	196	LEU
1	B	220	LYS
1	B	230	MET
1	B	231	MET
1	B	243	ARG
1	B	256	ASP
1	B	257	ASN
1	B	258	VAL
1	B	274	ASP
1	B	275	ASP
1	B	281	THR
1	B	282	GLU

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Mol	Chain	Res	Type
1	B	285	THR
1	B	289[A]	ASN
1	B	289[B]	ASN
1	B	290	GLN
1	B	322	LEU
1	B	323	THR
1	C	19	ARG
1	C	90	GLU
1	C	133	LEU
1	C	140	THR
1	C	144	PHE
1	C	154	GLU
1	C	174	ARG
1	C	178	VAL
1	C	184	MET
1	C	185	LYS
1	C	190	LYS
1	C	196	LEU
1	C	212	ILE
1	C	213	ASN
1	C	235	LEU
1	C	237	ARG
1	C	250	ILE
1	C	252	SER
1	C	259	ASN
1	C	260	ILE
1	C	262	ASN
1	C	267	LEU
1	C	274	ASP
1	C	275	ASP
1	C	281	THR
1	C	285	THR
1	C	289	ASN
1	C	291	ILE
1	C	293	ASP
1	C	294	LEU
1	C	308	ASP
1	D	38	GLN
1	D	41	ILE
1	D	42	GLN
1	D	54	GLN
1	D	58	CYS

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Mol	Chain	Res	Type
1	D	80	ASN
1	D	89	GLU
1	D	93	GLU
1	D	128	LYS
1	D	133	LEU
1	D	140	THR
1	D	157	ILE
1	D	170	ILE
1	D	174	ARG
1	D	177	SER
1	D	184	MET
1	D	200	ARG
1	D	209	ARG
1	D	230	MET
1	D	231	MET
1	D	237	ARG
1	D	240	ASP
1	D	241	ARG
1	D	248	GLN
1	D	250	ILE
1	D	252	SER
1	D	259	ASN
1	D	260	ILE
1	D	261	ILE
1	D	275	ASP
1	D	279	ARG
1	D	285	THR
1	D	290	GLN
1	D	291	ILE
1	D	298	GLU
1	D	299	ILE
1	D	311	ASP
1	D	314	ARG
1	D	323	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	42	GLN
1	A	80	ASN
1	A	262	ASN

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Mol	Chain	Res	Type
1	B	42	GLN
1	B	150	GLN
1	B	163	HIS
1	B	172	ASN
1	B	290	GLN
1	C	66	GLN
1	C	211	HIS
1	C	289	ASN
1	C	290	GLN
1	D	54	GLN
1	D	60	ASN
1	D	259	ASN
1	D	290	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](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	GDP	A	401	-	28,30,30	0.51	0	44,47,47	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	D	401	-	28,30,30	0.54	0	44,47,47	0.45	0
2	GDP	B	401	-	28,30,30	0.54	0	44,47,47	0.42	0
2	GDP	C	401	-	28,30,30	0.53	0	44,47,47	0.45	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
2	GDP	A	401	-	-	0/16/32/32	0/3/3/3
2	GDP	D	401	-	-	0/16/32/32	0/3/3/3
2	GDP	B	401	-	-	0/16/32/32	0/3/3/3
2	GDP	C	401	-	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

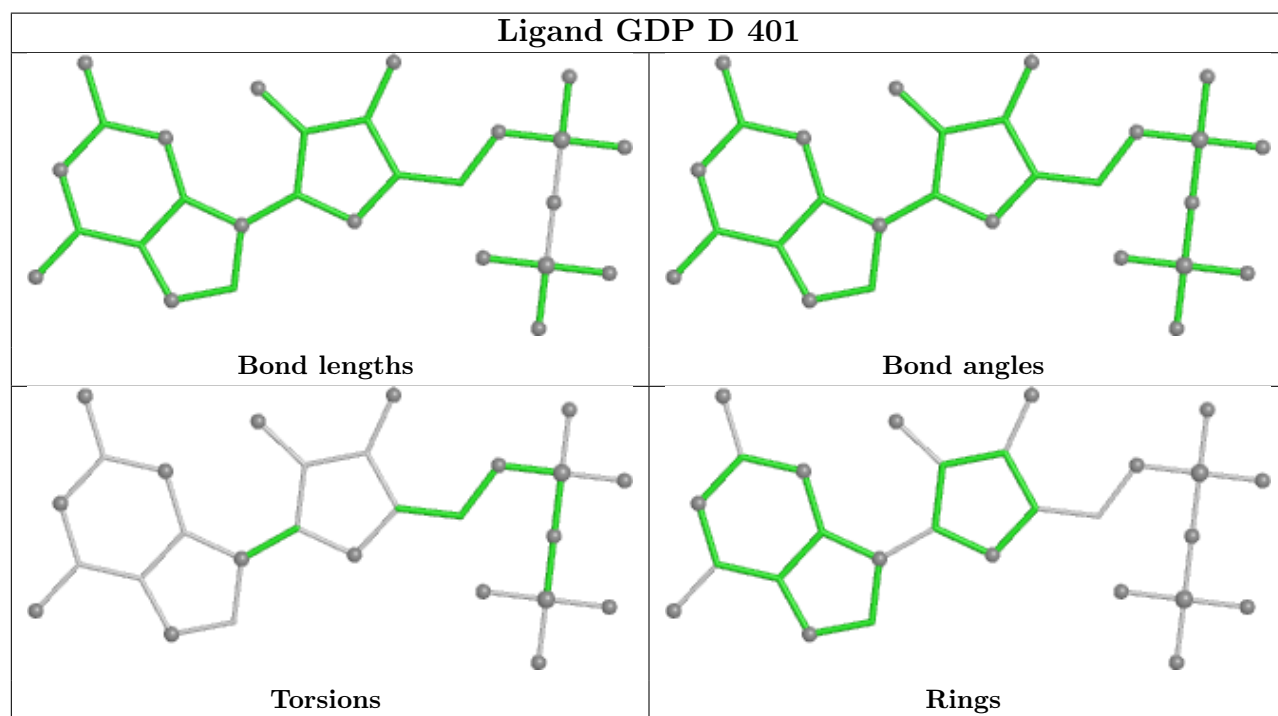
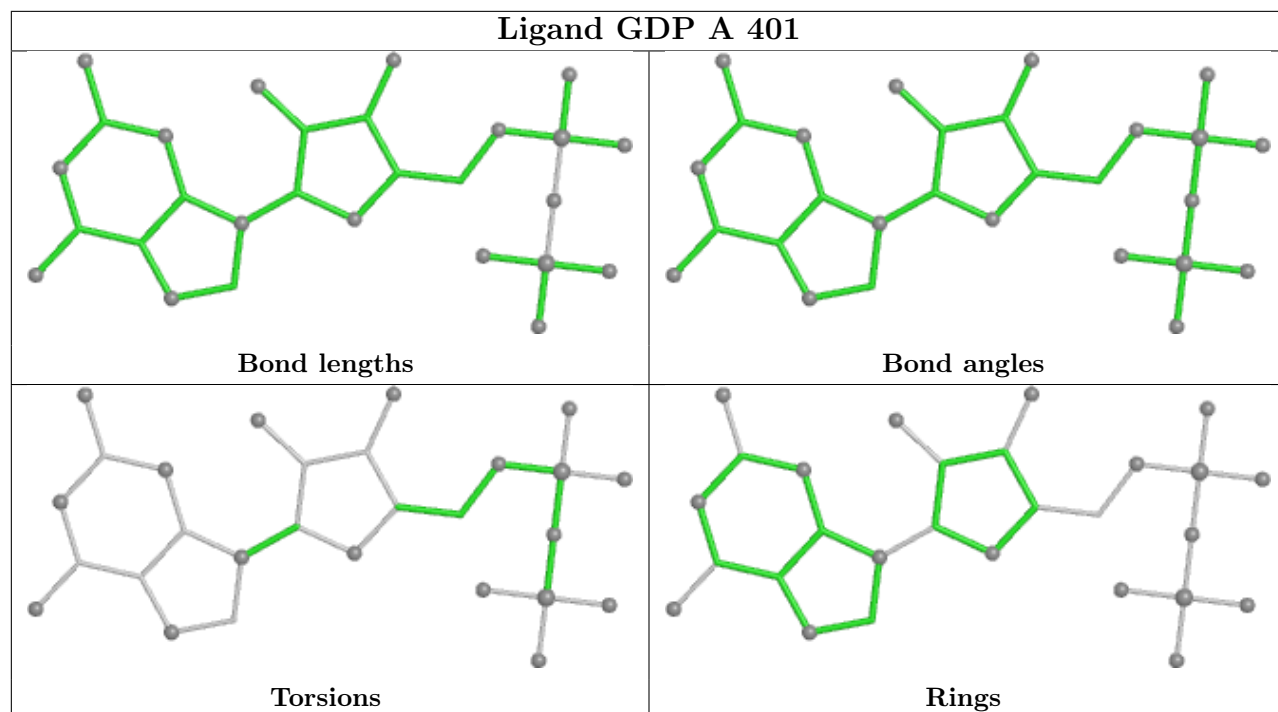
There are no chirality outliers.

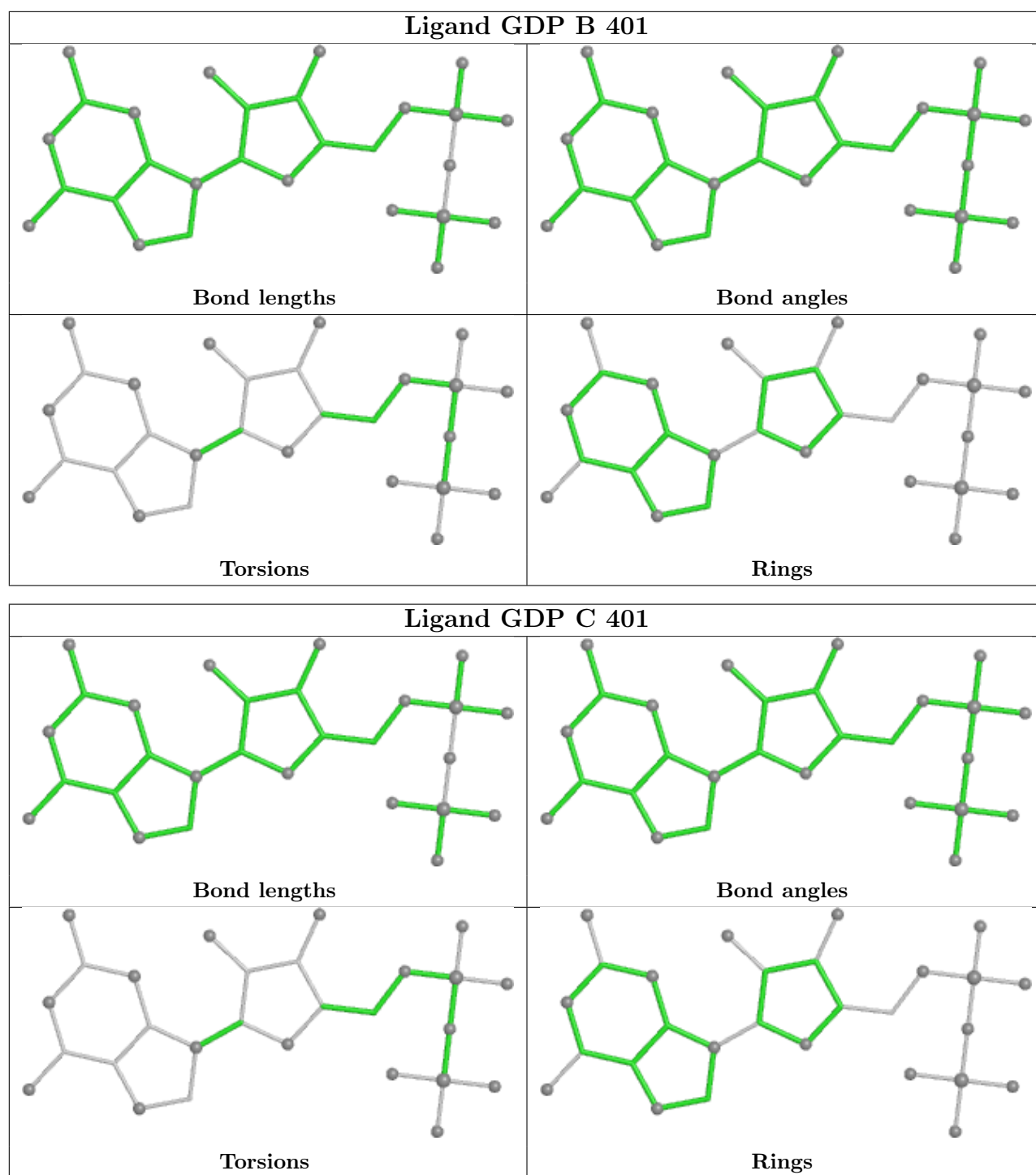
There are no torsion outliers.

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

6.1 Protein, DNA and RNA chains

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	294/306 (96%)	0.58	12 (4%) 41 43	42, 65, 99, 134	0
1	B	297/306 (97%)	0.26	7 (2%) 59 62	31, 47, 80, 122	1 (0%)
1	C	303/306 (99%)	0.52	10 (3%) 49 51	24, 57, 109, 119	1 (0%)
1	D	297/306 (97%)	0.45	5 (1%) 69 70	31, 53, 96, 117	0
All	All	1191/1224 (97%)	0.45	34 (2%) 53 56	24, 56, 99, 134	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	323	THR	5.5
1	B	178	VAL	3.8
1	A	182	ILE	3.8
1	B	78	GLY	3.7
1	D	79	ALA	3.4
1	C	212	ILE	3.0
1	C	255	LEU	2.9
1	A	178	VAL	2.8
1	C	257	ASN	2.7
1	A	79	ALA	2.7
1	B	184	MET	2.6
1	A	299	ILE	2.5
1	A	257	ASN	2.5
1	A	187	ALA	2.4
1	C	238	GLY	2.4
1	B	180	GLY	2.4
1	D	68	GLY	2.3
1	A	144	PHE	2.3
1	B	79	ALA	2.3
1	C	283	ILE	2.3
1	A	301	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	150	GLN	2.2
1	C	242	ALA	2.2
1	A	171	PRO	2.2
1	C	297	GLY	2.2
1	C	294	LEU	2.2
1	A	295	ASP	2.1
1	C	249	ALA	2.1
1	A	184	MET	2.1
1	B	256	ASP	2.1
1	B	259	ASN	2.1
1	D	299	ILE	2.1
1	A	278	LEU	2.0
1	C	305	PHE	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](#)

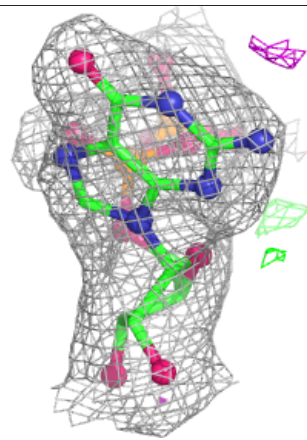
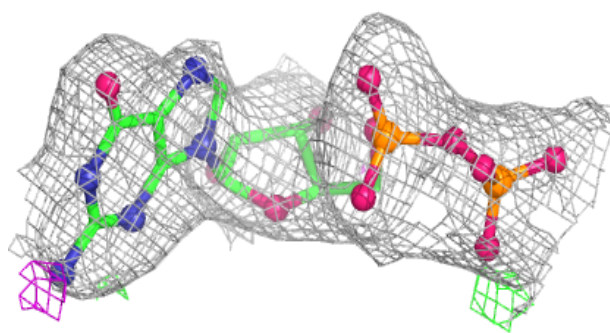
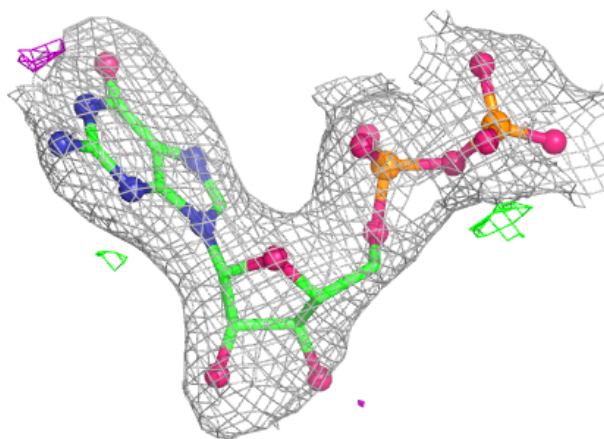
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GDP	A	401	28/28	0.91	0.08	57,67,73,81	0
2	GDP	D	401	28/28	0.96	0.06	40,46,53,60	0
2	GDP	C	401	28/28	0.97	0.05	34,40,44,47	0
2	GDP	B	401	28/28	0.97	0.05	33,39,43,44	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.

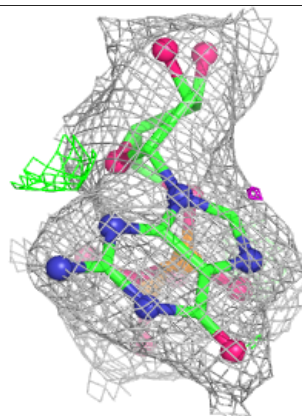
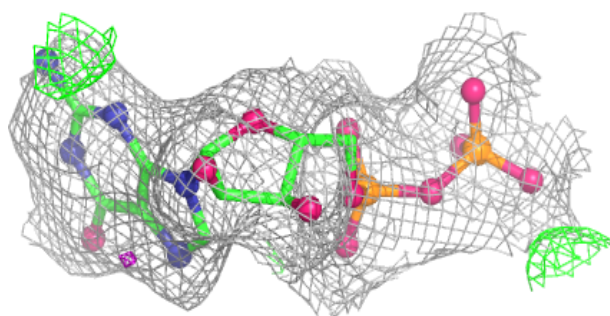
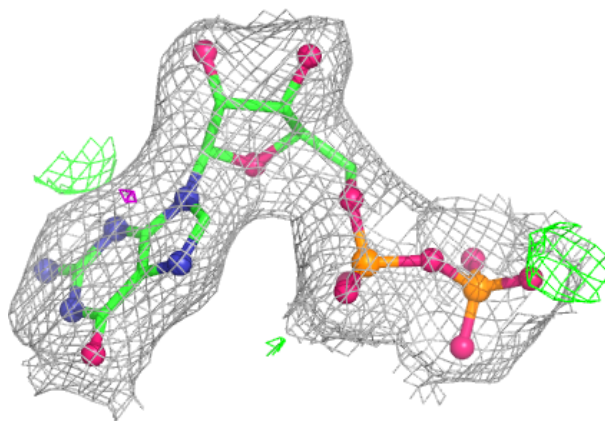
Electron density around GDP A 401:

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



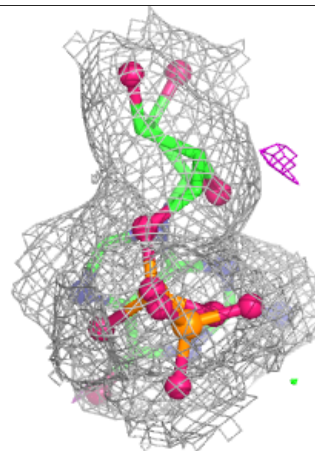
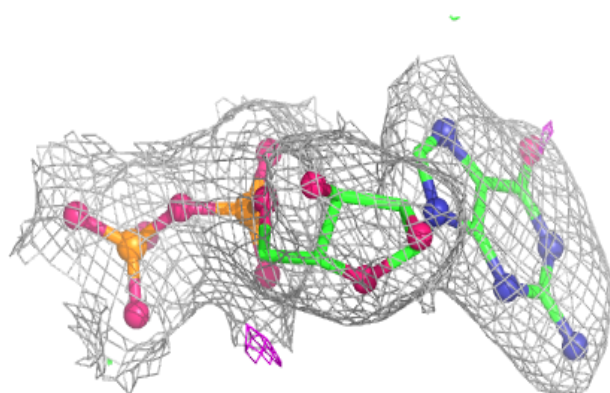
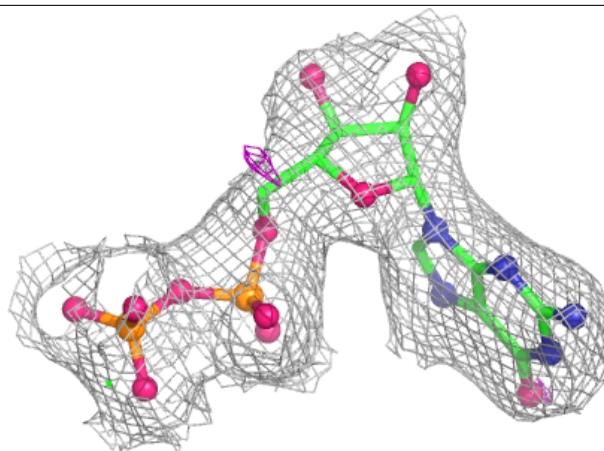
Electron density around GDP D 401:

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



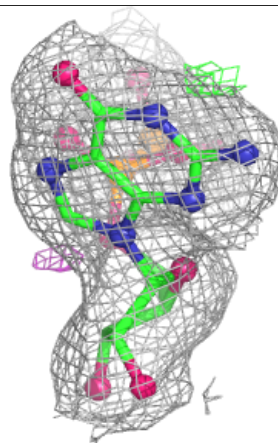
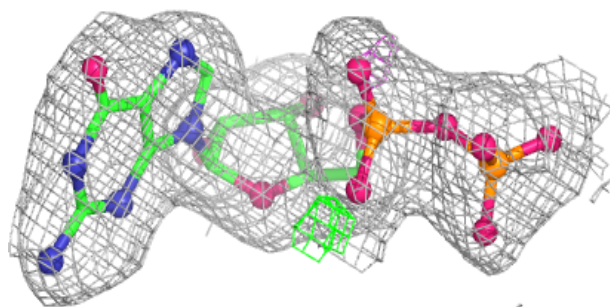
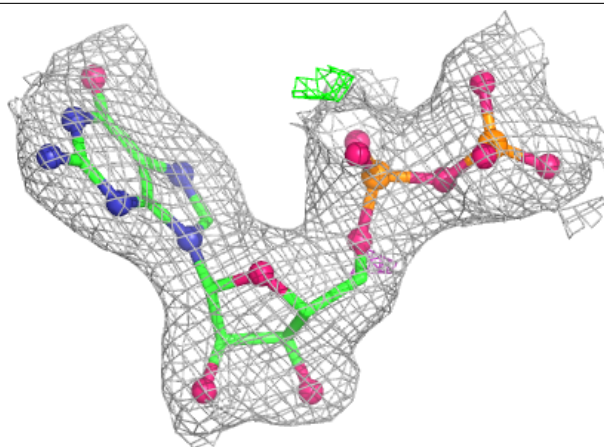
Electron density around GDP C 401:

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



Electron density around GDP B 401:

$2mF_o-DF_c$ (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.