



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:49 PM UTC

PDB ID : 4ZCL / pdb_00004zcl
Title : Crystal Structure of Escherichia coli GTPase BipA/TypA Complexed with GDP
Authors : Fan, H.T.; Hahm, J.; Diggs, S.; Blaha, G.
Deposited on : 2015-04-16
Resolution : 3.06 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

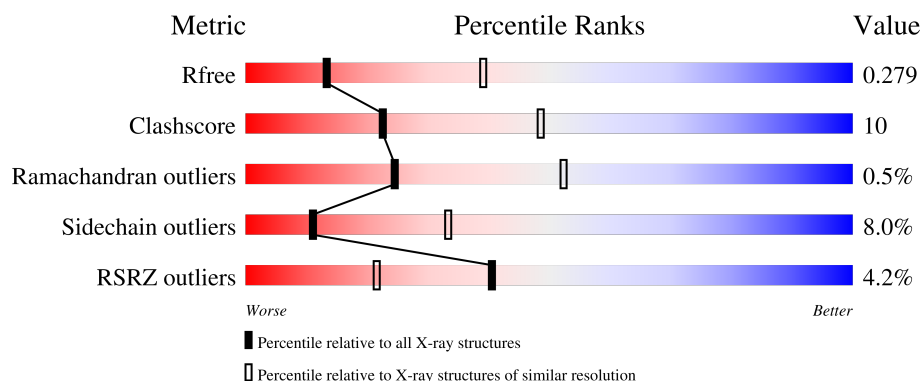
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	635	 3% 66% 20% 12%
1	B	635	 4% 65% 21% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8524 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 protein TypA/BipA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4236	2653	749	817	17			
1	B	561	Total	C	N	O	S	0	0	0
			4203	2630	744	812	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP P32132
A	-32	GLY	-	expression tag	UNP P32132
A	-31	SER	-	expression tag	UNP P32132
A	-30	SER	-	expression tag	UNP P32132
A	-29	HIS	-	expression tag	UNP P32132
A	-28	HIS	-	expression tag	UNP P32132
A	-27	HIS	-	expression tag	UNP P32132
A	-26	HIS	-	expression tag	UNP P32132
A	-25	HIS	-	expression tag	UNP P32132
A	-24	HIS	-	expression tag	UNP P32132
A	-23	SER	-	expression tag	UNP P32132
A	-22	SER	-	expression tag	UNP P32132
A	-21	GLY	-	expression tag	UNP P32132
A	-20	LEU	-	expression tag	UNP P32132
A	-19	VAL	-	expression tag	UNP P32132
A	-18	PRO	-	expression tag	UNP P32132
A	-17	ARG	-	expression tag	UNP P32132
A	-16	GLY	-	expression tag	UNP P32132
A	-15	SER	-	expression tag	UNP P32132
A	-14	HIS	-	expression tag	UNP P32132
A	-13	MET	-	expression tag	UNP P32132
A	-12	ALA	-	expression tag	UNP P32132
A	-11	SER	-	expression tag	UNP P32132
A	-10	MET	-	expression tag	UNP P32132
A	-9	THR	-	expression tag	UNP P32132

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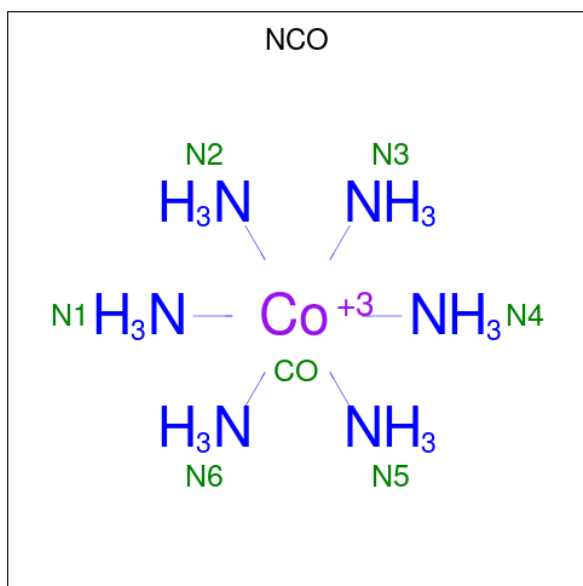
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P32132
A	-7	GLY	-	expression tag	UNP P32132
A	-6	GLN	-	expression tag	UNP P32132
A	-5	GLN	-	expression tag	UNP P32132
A	-4	MET	-	expression tag	UNP P32132
A	-3	GLY	-	expression tag	UNP P32132
A	-2	ARG	-	expression tag	UNP P32132
A	-1	GLY	-	expression tag	UNP P32132
A	0	SER	-	expression tag	UNP P32132
B	-33	MET	-	initiating methionine	UNP P32132
B	-32	GLY	-	expression tag	UNP P32132
B	-31	SER	-	expression tag	UNP P32132
B	-30	SER	-	expression tag	UNP P32132
B	-29	HIS	-	expression tag	UNP P32132
B	-28	HIS	-	expression tag	UNP P32132
B	-27	HIS	-	expression tag	UNP P32132
B	-26	HIS	-	expression tag	UNP P32132
B	-25	HIS	-	expression tag	UNP P32132
B	-24	HIS	-	expression tag	UNP P32132
B	-23	SER	-	expression tag	UNP P32132
B	-22	SER	-	expression tag	UNP P32132
B	-21	GLY	-	expression tag	UNP P32132
B	-20	LEU	-	expression tag	UNP P32132
B	-19	VAL	-	expression tag	UNP P32132
B	-18	PRO	-	expression tag	UNP P32132
B	-17	ARG	-	expression tag	UNP P32132
B	-16	GLY	-	expression tag	UNP P32132
B	-15	SER	-	expression tag	UNP P32132
B	-14	HIS	-	expression tag	UNP P32132
B	-13	MET	-	expression tag	UNP P32132
B	-12	ALA	-	expression tag	UNP P32132
B	-11	SER	-	expression tag	UNP P32132
B	-10	MET	-	expression tag	UNP P32132
B	-9	THR	-	expression tag	UNP P32132
B	-8	GLY	-	expression tag	UNP P32132
B	-7	GLY	-	expression tag	UNP P32132
B	-6	GLN	-	expression tag	UNP P32132
B	-5	GLN	-	expression tag	UNP P32132
B	-4	MET	-	expression tag	UNP P32132
B	-3	GLY	-	expression tag	UNP P32132
B	-2	ARG	-	expression tag	UNP P32132
B	-1	GLY	-	expression tag	UNP P32132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P32132

- Molecule 2 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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

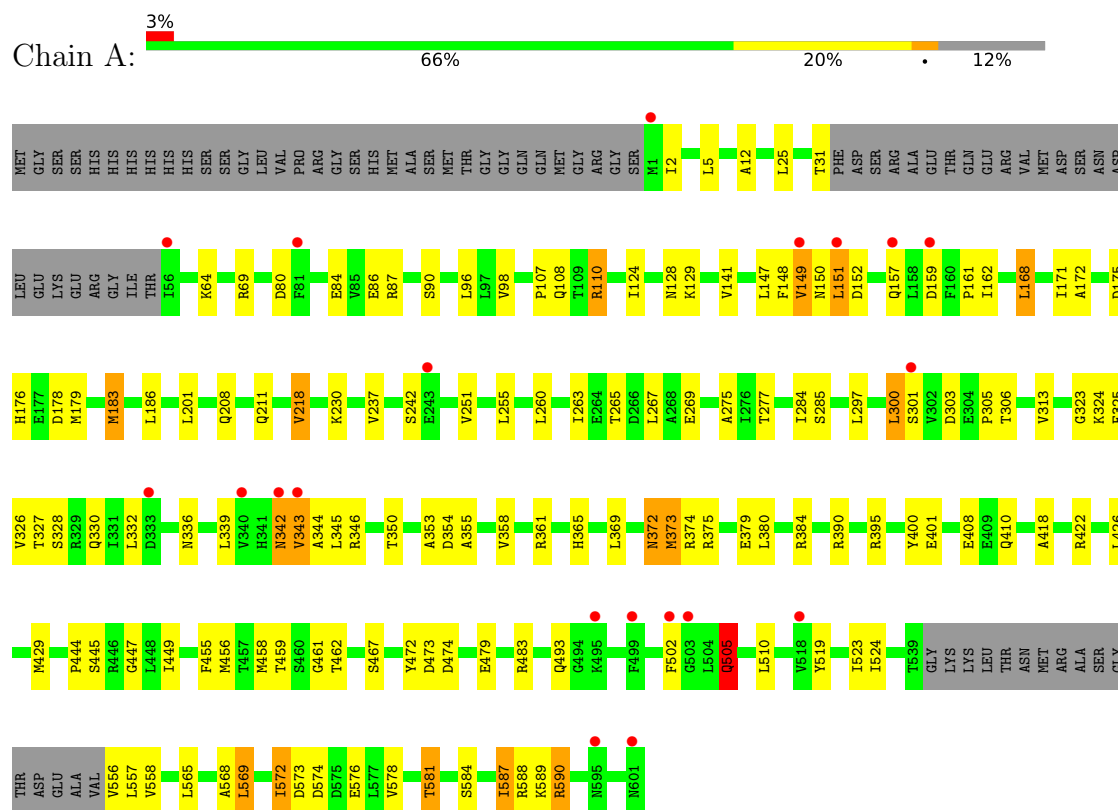
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

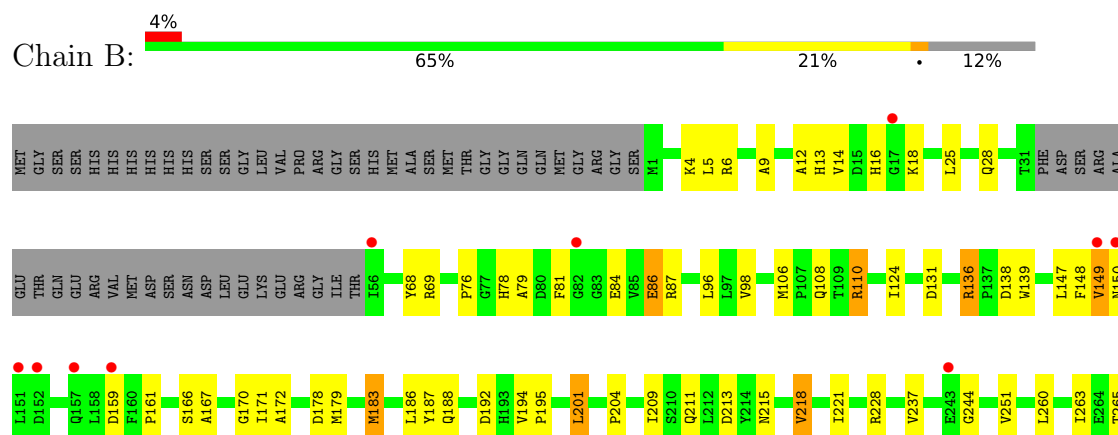
3 Residue-property plots

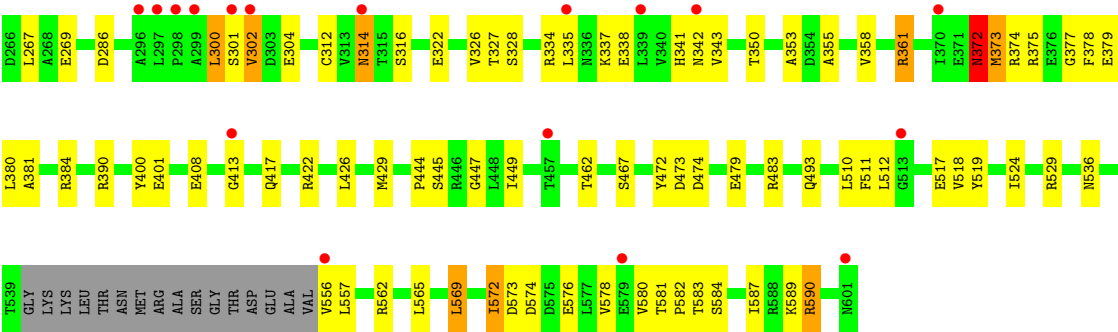
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: GTP-binding protein TypA/BipA



• Molecule 1: GTP-binding protein TypA/BipA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.43Å 160.01Å 90.02Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	48.18 – 3.06 48.18 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.18-3.06) 100.0 (48.18-3.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.07Å)	Xtriage
Refinement program	PHENIX dev_1819	Depositor
R, R_{free}	0.232 , 0.271 0.240 , 0.279	Depositor DCC
R_{free} test set	1450 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.8	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	0.92	EDS
Total number of atoms	8524	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: MG, NCO, 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	0.30	0/4303	0.76	3/5840 (0.1%)
1	B	0.32	0/4270	0.77	4/5805 (0.1%)
All	All	0.31	0/8573	0.76	7/11645 (0.1%)

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	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	GLN	N-CA-C	-8.84	102.50	113.28
1	A	373	MET	N-CA-C	-8.05	102.08	112.23
1	B	373	MET	N-CA-C	-6.21	105.53	113.23
1	B	335	LEU	N-CA-C	-5.81	105.95	113.16
1	A	242	SER	N-CA-C	5.04	117.50	111.71
1	B	136	ARG	CA-C-N	5.01	124.18	118.97
1	B	136	ARG	C-N-CA	5.01	124.18	118.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	372	ASN	Peptide

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	4236	0	4128	84	0
1	B	4203	0	4050	91	0
2	A	14	0	0	1	0
2	B	14	0	0	1	0
3	A	28	0	12	4	0
3	B	28	0	12	1	0
4	A	1	0	0	0	0
All	All	8524	0	8202	175	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 (175) 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:A:150:ASN:O	1:A:152:ASP:N	1.83	1.12
1:B:334:ARG:HE	1:B:337:LYS:HD2	1.26	1.01
1:B:372:ASN:O	1:B:372:ASN:ND2	1.97	0.96
1:A:150:ASN:O	1:A:151:LEU:C	2.26	0.79
1:B:334:ARG:NE	1:B:337:LYS:HD2	1.98	0.78
1:A:343:VAL:O	1:A:346:ARG:NH2	2.16	0.77
1:A:150:ASN:C	1:A:152:ASP:N	2.44	0.75
1:B:337:LYS:HE2	1:B:338:GLU:HG3	1.71	0.71
1:A:124:ILE:HG23	1:A:161:PRO:HG2	1.73	0.71
1:A:342:ASN:OD1	1:A:344:ALA:N	2.25	0.70
1:B:334:ARG:HD3	1:B:378:PHE:CZ	2.30	0.67
1:A:148:PHE:C	1:A:150:ASN:H	2.03	0.65
1:B:334:ARG:HG3	1:B:337:LYS:HG3	1.79	0.65
1:B:215:ASN:HB3	1:B:218:VAL:HG22	1.79	0.64
1:B:578:VAL:HG12	1:B:587:ILE:HG22	1.80	0.64
1:A:361:ARG:H	1:A:365:HIS:HD2	1.45	0.64
1:B:124:ILE:HG23	1:B:161:PRO:HG2	1.78	0.63
1:A:372:ASN:HA	1:A:375:ARG:H	1.63	0.62
1:B:84:GLU:HA	1:B:87:ARG:HD2	1.81	0.62
1:B:372:ASN:HD22	1:B:372:ASN:C	2.05	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:O	1:A:149:VAL:HG22	2.00	0.62
1:B:576:GLU:HG2	1:B:589:LYS:HD3	1.81	0.62
1:A:300:LEU:HD23	1:A:300:LEU:H	1.65	0.62
1:A:110:ARG:NH1	1:A:467:SER:O	2.34	0.60
1:B:110:ARG:NH1	1:B:467:SER:O	2.34	0.60
1:B:149:VAL:O	1:B:149:VAL:HG22	2.01	0.60
1:A:84:GLU:HA	1:A:87:ARG:HD2	1.84	0.59
1:B:417:GLN:OE1	1:B:417:GLN:N	2.27	0.59
1:A:374:ARG:NH1	1:A:581:THR:O	2.34	0.58
1:A:523:ILE:HB	1:A:587:ILE:HG23	1.86	0.58
1:A:171:ILE:HG22	1:A:179:MET:HE3	1.86	0.57
1:B:338:GLU:O	1:B:342:ASN:ND2	2.37	0.57
1:A:401:GLU:OE1	1:A:467:SER:OG	2.21	0.57
1:B:328:SER:OG	1:B:353:ALA:O	2.19	0.57
1:B:148:PHE:C	1:B:150:ASN:H	2.13	0.57
1:B:312:CYS:HB2	1:B:381:ALA:HB3	1.86	0.57
1:A:150:ASN:C	1:A:152:ASP:H	2.09	0.57
1:A:12:ALA:HB2	1:A:98:VAL:HB	1.86	0.57
1:B:334:ARG:HD3	1:B:378:PHE:CE1	2.41	0.56
1:B:401:GLU:OE1	1:B:467:SER:OG	2.22	0.56
1:B:350:THR:OG1	1:B:355:ALA:O	2.21	0.56
1:B:172:ALA:HB2	1:B:183:MET:HE2	1.88	0.55
1:B:334:ARG:HG3	1:B:337:LYS:CG	2.37	0.54
1:B:372:ASN:HB2	1:B:375:ARG:NH1	2.23	0.54
1:A:408:GLU:OE1	1:A:410:GLN:NE2	2.37	0.54
1:A:25:LEU:HD21	1:A:186:LEU:HD23	1.89	0.53
1:B:334:ARG:HG3	1:B:337:LYS:CD	2.39	0.53
1:B:374:ARG:NH1	1:B:581:THR:O	2.39	0.53
1:A:384:ARG:HB3	1:A:572:ILE:HG22	1.90	0.53
1:B:13:HIS:CD2	1:B:106:MET:HG3	2.44	0.52
1:B:379:GLU:HA	1:B:580:VAL:O	2.09	0.52
1:B:5:LEU:HD23	1:B:69:ARG:HB2	1.91	0.52
1:B:322:GLU:HB2	1:B:581:THR:OG1	2.10	0.52
1:B:384:ARG:HB3	1:B:572:ILE:HG22	1.91	0.52
1:A:255:LEU:HB2	1:A:275:ALA:HB3	1.92	0.52
1:A:576:GLU:HG2	1:A:589:LYS:HD3	1.91	0.51
1:B:108:GLN:N	1:B:108:GLN:OE1	2.43	0.51
1:B:422:ARG:NH1	1:B:447:GLY:O	2.34	0.51
1:B:473:ASP:OD1	1:B:474:ASP:N	2.43	0.51
1:B:400:TYR:HA	1:B:444:PRO:HA	1.91	0.51
1:B:300:LEU:HD23	1:B:300:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:C	1:B:149:VAL:H	2.19	0.50
1:A:108:GLN:OE1	1:A:108:GLN:N	2.44	0.50
1:B:12:ALA:HB2	1:B:98:VAL:HB	1.93	0.50
1:A:159:ASP:OD1	2:A:1002:NCO:N4	2.45	0.50
1:B:378:PHE:O	1:B:582:PRO:HD3	2.12	0.49
1:A:323:GLY:HA3	1:A:379:GLU:HB2	1.94	0.49
1:B:138:ASP:OD1	1:B:138:ASP:N	2.42	0.49
1:A:400:TYR:HA	1:A:444:PRO:HA	1.93	0.49
1:B:4:LYS:HB3	1:B:68:TYR:CD2	2.48	0.48
1:B:149:VAL:O	1:B:149:VAL:HG13	2.13	0.48
1:A:305:PRO:HG3	1:A:346:ARG:HG2	1.96	0.48
1:A:327:THR:OG1	1:A:328:SER:N	2.45	0.48
1:B:209:ILE:HD13	1:B:286:ASP:HB2	1.96	0.48
1:B:304:GLU:O	1:B:361:ARG:NH1	2.46	0.48
1:B:390:ARG:NH1	1:B:472:TYR:OH	2.46	0.48
1:B:413:GLY:O	1:B:417:GLN:NE2	2.32	0.48
1:B:25:LEU:O	1:B:187:TYR:OH	2.30	0.48
1:A:148:PHE:C	1:A:150:ASN:N	2.69	0.48
1:A:568:ALA:O	1:A:572:ILE:HD13	2.13	0.48
1:A:422:ARG:NH1	1:A:447:GLY:O	2.35	0.47
1:B:372:ASN:ND2	1:B:372:ASN:C	2.70	0.47
1:A:172:ALA:HB2	1:A:183:MET:HE2	1.97	0.47
1:B:572:ILE:HG12	1:B:578:VAL:HG13	1.96	0.46
1:B:213:ASP:HB3	1:B:221:ILE:HB	1.96	0.46
1:A:372:ASN:OD1	1:A:372:ASN:N	2.46	0.46
1:A:87:ARG:O	1:A:90:SER:OG	2.29	0.46
1:A:505:GLN:HE22	1:A:558:VAL:HG13	1.81	0.46
1:A:175:ASP:OD1	1:A:176:HIS:N	2.48	0.46
1:B:493:GLN:HA	1:B:519:TYR:HA	1.98	0.46
1:A:129:LYS:HG2	3:A:1003:GDP:C5	2.51	0.46
1:B:312:CYS:HA	1:B:355:ALA:HA	1.97	0.45
1:A:342:ASN:HD21	1:A:345:LEU:HB2	1.81	0.45
1:B:86:GLU:H	1:B:86:GLU:HG2	1.43	0.45
1:B:377:GLY:HA2	1:B:582:PRO:HG3	1.97	0.45
1:A:581:THR:HG23	1:A:584:SER:O	2.17	0.45
1:B:300:LEU:HG	1:B:301:SER:H	1.81	0.45
1:B:131:ASP:OD2	1:B:166:SER:OG	2.30	0.45
1:A:574:ASP:O	1:A:590:ARG:NH1	2.50	0.45
1:B:79:ALA:HB3	1:B:81:PHE:HE1	1.81	0.45
1:B:167:ALA:HB3	3:B:1003:GDP:N7	2.32	0.45
1:B:78:HIS:O	1:B:78:HIS:ND1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ASP:O	1:B:590:ARG:NH1	2.50	0.45
1:A:328:SER:OG	1:A:353:ALA:O	2.35	0.45
1:B:136:ARG:HB2	1:B:139:TRP:HB3	1.98	0.45
1:B:556:VAL:HG22	1:B:557:LEU:H	1.82	0.44
1:B:9:ALA:O	1:B:96:LEU:N	2.44	0.44
1:B:581:THR:HG23	1:B:584:SER:H	1.83	0.44
1:A:369:LEU:O	1:A:373:MET:HB2	2.17	0.44
1:A:445:SER:O	1:A:449:ILE:HG13	2.18	0.44
1:A:230:LYS:HA	1:A:269:GLU:HA	2.00	0.44
1:A:426:LEU:HD21	1:A:429:MET:HE2	1.99	0.44
1:B:314:ASN:OD1	1:B:316:SER:HB3	2.18	0.44
1:B:408:GLU:OE2	1:B:462:THR:HG21	2.17	0.44
1:A:303:ASP:O	1:A:344:ALA:HA	2.17	0.44
1:B:265:THR:HG22	1:B:267:LEU:H	1.83	0.44
1:A:325:PHE:O	1:A:330:GLN:NE2	2.51	0.44
1:A:418:ALA:HB2	1:A:458:MET:HE1	2.00	0.43
1:A:456:MET:O	1:A:461:GLY:N	2.49	0.43
1:A:502:PHE:O	1:A:505:GLN:HG3	2.18	0.43
1:A:455:PHE:O	1:A:459:THR:HG22	2.18	0.43
1:A:300:LEU:HG	1:A:301:SER:H	1.83	0.43
1:A:5:LEU:HD23	1:A:69:ARG:HB2	2.01	0.43
1:A:168:LEU:HD22	3:A:1003:GDP:N1	2.33	0.43
1:A:459:THR:O	1:A:462:THR:HG22	2.18	0.43
1:B:201:LEU:HD21	1:B:269:GLU:HB3	2.00	0.43
1:A:572:ILE:HG12	1:A:578:VAL:HG13	2.00	0.43
1:B:426:LEU:HD21	1:B:429:MET:HE2	2.01	0.43
1:B:171:ILE:HG22	1:B:179:MET:HE3	2.01	0.43
1:A:342:ASN:ND2	1:A:365:HIS:NE2	2.67	0.42
1:B:148:PHE:C	1:B:150:ASN:N	2.75	0.42
1:B:334:ARG:HG3	1:B:337:LYS:HD2	1.99	0.42
1:A:556:VAL:HG22	1:A:557:LEU:H	1.84	0.42
1:A:336:ASN:HA	1:A:339:LEU:HD12	2.01	0.42
1:A:147:LEU:C	1:A:149:VAL:H	2.27	0.42
1:B:188:GLN:NE2	1:B:192:ASP:OD1	2.53	0.42
1:A:96:LEU:HD12	1:A:124:ILE:HB	2.02	0.42
1:B:194:VAL:HA	1:B:195:PRO:HD3	1.91	0.42
1:B:338:GLU:HB3	1:B:342:ASN:ND2	2.35	0.41
1:A:150:ASN:O	1:A:152:ASP:CA	2.63	0.41
1:B:6:ARG:HD2	1:B:194:VAL:HB	2.01	0.41
1:A:218:VAL:HG22	1:A:277:THR:HG21	2.03	0.41
1:B:204:PRO:HG2	1:B:228:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:HG22	1:A:267:LEU:H	1.85	0.41
1:A:313:VAL:HG22	1:A:354:ASP:HB3	2.03	0.41
1:A:129:LYS:HG2	3:A:1003:GDP:C6	2.55	0.41
1:B:483:ARG:NH1	1:B:573:ASP:HB2	2.35	0.41
1:A:565:LEU:O	1:A:569:LEU:HB2	2.19	0.41
1:B:25:LEU:HD21	1:B:186:LEU:HD23	2.03	0.41
1:B:565:LEU:O	1:B:569:LEU:HB2	2.21	0.41
1:A:473:ASP:OD1	1:A:474:ASP:N	2.47	0.41
1:A:572:ILE:HD11	1:A:587:ILE:CD1	2.50	0.41
1:B:338:GLU:HA	1:B:341:HIS:HB2	2.02	0.41
1:A:208:GLN:HB2	1:A:297:LEU:HD12	2.03	0.41
1:A:390:ARG:NH1	1:A:472:TYR:OH	2.53	0.41
1:B:28:GLN:NE2	1:B:170:GLY:HA3	2.34	0.41
1:B:159:ASP:OD1	2:B:1002:NCO:N4	2.53	0.41
1:A:31:THR:HB	1:A:64:LYS:HB2	2.01	0.41
1:A:107:PRO:O	1:A:110:ARG:HB2	2.21	0.41
1:B:76:PRO:HB3	1:B:81:PHE:CD2	2.56	0.41
1:B:314:ASN:ND2	1:B:379:GLU:HG2	2.35	0.41
1:B:337:LYS:HE2	1:B:338:GLU:CG	2.46	0.41
1:B:373:MET:O	1:B:378:PHE:HB2	2.21	0.41
1:A:168:LEU:HB3	3:A:1003:GDP:C5	2.57	0.41
1:A:587:ILE:HD12	1:A:588:ARG:H	1.86	0.41
1:B:445:SER:O	1:B:449:ILE:HG13	2.20	0.40
1:B:483:ARG:NH1	1:B:576:GLU:OE1	2.54	0.40
1:B:511:PHE:CE2	1:B:587:ILE:HD11	2.56	0.40
1:A:141:VAL:HG22	1:A:162:ILE:HD13	2.03	0.40
1:A:284:ILE:O	1:A:285:SER:HB2	2.22	0.40
1:A:306:THR:OG1	1:A:361:ARG:O	2.39	0.40
1:A:483:ARG:NH1	1:A:573:ASP:HB2	2.36	0.40
1:A:342:ASN:OD1	1:A:342:ASN:C	2.64	0.40
1:A:350:THR:OG1	1:A:355:ALA:O	2.31	0.40
1:A:493:GLN:HA	1:A:519:TYR:HA	2.03	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	555/635 (87%)	524 (94%)	28 (5%)	3 (0%)	24	52
1	B	555/635 (87%)	521 (94%)	31 (6%)	3 (0%)	24	52
All	All	1110/1270 (87%)	1045 (94%)	59 (5%)	6 (0%)	24	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	B	149	VAL
1	A	149	VAL
1	B	302	VAL
1	A	2	ILE
1	B	244	GLY

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	447/540 (83%)	413 (92%)	34 (8%)	12	35
1	B	438/540 (81%)	401 (92%)	37 (8%)	10	31
All	All	885/1080 (82%)	814 (92%)	71 (8%)	11	33

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	A	86	GLU
1	A	110	ARG
1	A	128	ASN
1	A	157	GLN
1	A	168	LEU

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Mol	Chain	Res	Type
1	A	178	ASP
1	A	183	MET
1	A	201	LEU
1	A	211	GLN
1	A	218	VAL
1	A	237	VAL
1	A	251	VAL
1	A	260	LEU
1	A	263	ILE
1	A	300	LEU
1	A	324	LYS
1	A	326	VAL
1	A	332	LEU
1	A	342	ASN
1	A	343	VAL
1	A	358	VAL
1	A	372	ASN
1	A	380	LEU
1	A	395	ARG
1	A	479	GLU
1	A	505	GLN
1	A	510	LEU
1	A	524	ILE
1	A	569	LEU
1	A	572	ILE
1	A	581	THR
1	A	587	ILE
1	A	590	ARG
1	B	14	VAL
1	B	16	HIS
1	B	18	LYS
1	B	86	GLU
1	B	110	ARG
1	B	178	ASP
1	B	183	MET
1	B	201	LEU
1	B	211	GLN
1	B	218	VAL
1	B	237	VAL
1	B	251	VAL
1	B	260	LEU
1	B	263	ILE

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Mol	Chain	Res	Type
1	B	300	LEU
1	B	302	VAL
1	B	314	ASN
1	B	326	VAL
1	B	327	THR
1	B	343	VAL
1	B	358	VAL
1	B	361	ARG
1	B	372	ASN
1	B	380	LEU
1	B	479	GLU
1	B	510	LEU
1	B	512	LEU
1	B	517	GLU
1	B	518	VAL
1	B	524	ILE
1	B	529	ARG
1	B	536	ASN
1	B	562	ARG
1	B	569	LEU
1	B	572	ILE
1	B	583	THR
1	B	590	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	157	GLN
1	A	236	GLN
1	A	336	ASN
1	A	397	GLN
1	A	505	GLN
1	B	150	ASN
1	B	188	GLN
1	B	193	HIS
1	B	410	GLN
1	B	505	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, 1 is monoatomic - leaving 6 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	A	1003	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	6 (13%)
2	NCO	A	1001	-	6,6,6	0.49	0	-		
3	GDP	B	1003	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
2	NCO	B	1002	-	6,6,6	0.50	0	-		
2	NCO	A	1002	-	6,6,6	0.49	0	-		
2	NCO	B	1001	-	6,6,6	0.47	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
3	GDP	B	1003	-	-	3/16/32/32	0/3/3/3
3	GDP	A	1003	-	-	6/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1003	GDP	C5-C4	3.18	1.47	1.38
3	A	1003	GDP	C5-C4	3.13	1.47	1.38
3	B	1003	GDP	C6-N1	-2.49	1.34	1.38
3	A	1003	GDP	C6-N1	-2.38	1.34	1.38
3	B	1003	GDP	C5-N7	-2.09	1.34	1.39
3	A	1003	GDP	C5-N7	-2.03	1.35	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	GDP	C5-C4-N3	-6.32	118.33	128.39
3	A	1003	GDP	C5-C4-N3	-6.06	118.75	128.39
3	A	1003	GDP	C2-N3-C4	5.07	121.04	112.30
3	B	1003	GDP	C2-N3-C4	5.07	121.03	112.30
3	B	1003	GDP	N9-C4-N3	4.78	135.51	125.95
3	A	1003	GDP	N9-C4-N3	4.45	134.85	125.95
3	A	1003	GDP	C6-C5-N7	3.39	136.46	130.29
3	B	1003	GDP	C6-C5-N7	3.06	135.85	130.29
3	A	1003	GDP	C4-C5-N7	-2.62	106.52	110.67
3	B	1003	GDP	C4-C5-N7	-2.52	106.68	110.67
3	B	1003	GDP	C3'-C2'-C1'	2.31	105.84	101.46
3	A	1003	GDP	O6-C6-C5	-2.14	120.87	126.53
3	B	1003	GDP	O6-C6-C5	-2.14	120.89	126.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

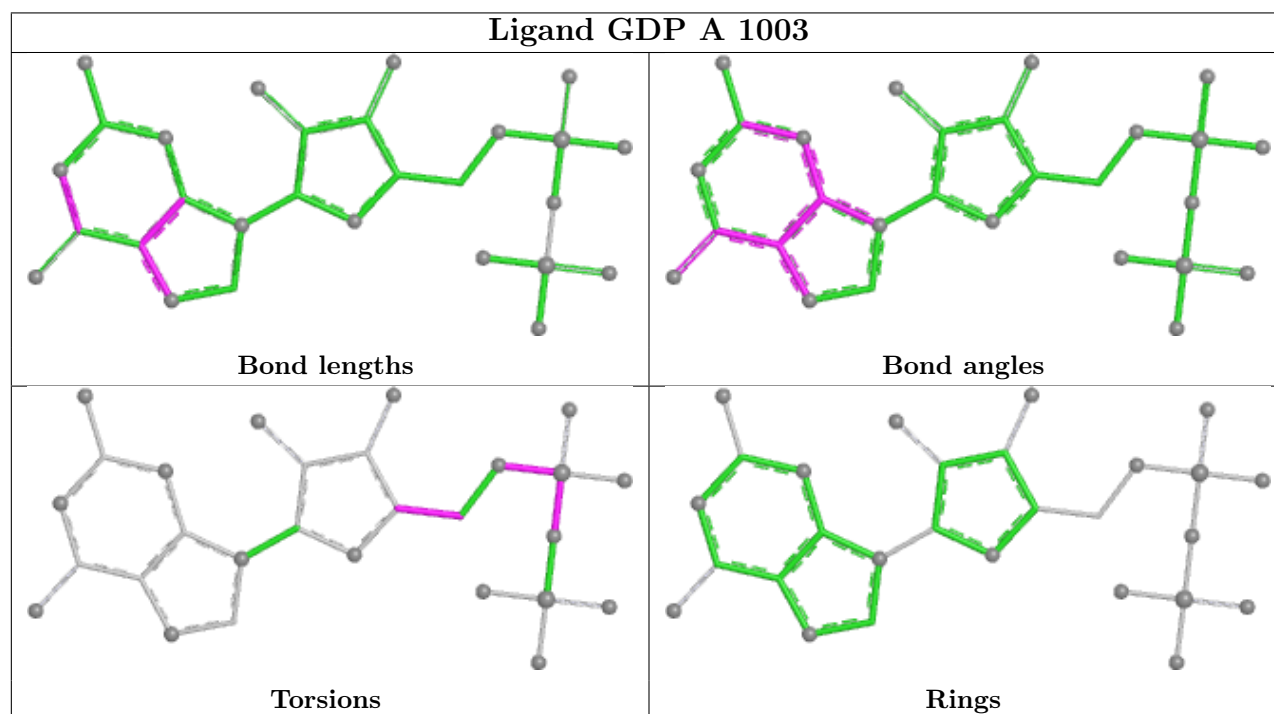
Mol	Chain	Res	Type	Atoms
3	A	1003	GDP	C5'-O5'-PA-O3A
3	A	1003	GDP	C5'-O5'-PA-O1A
3	A	1003	GDP	C5'-O5'-PA-O2A
3	B	1003	GDP	C5'-O5'-PA-O3A
3	B	1003	GDP	C5'-O5'-PA-O1A
3	B	1003	GDP	C5'-O5'-PA-O2A
3	A	1003	GDP	O4'-C4'-C5'-O5'
3	A	1003	GDP	PB-O3A-PA-O1A
3	A	1003	GDP	PB-O3A-PA-O2A

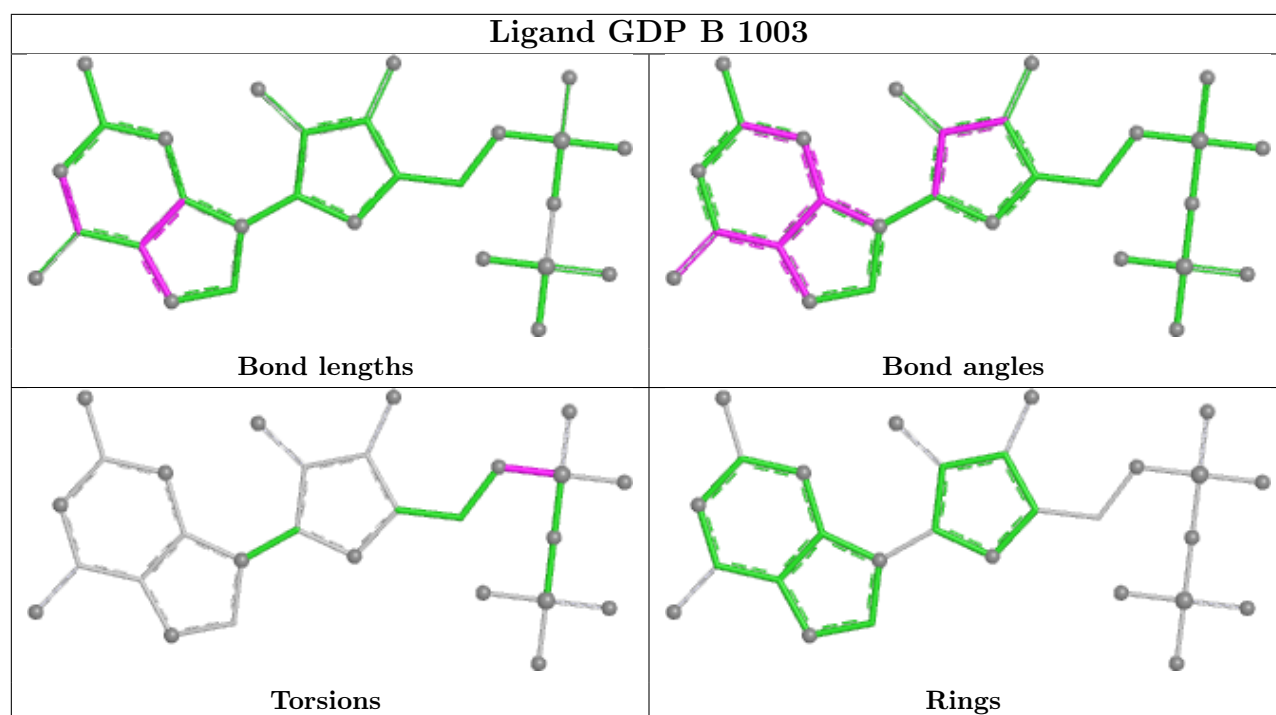
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	GDP	4	0
3	B	1003	GDP	1	0
2	B	1002	NCO	1	0
2	A	1002	NCO	1	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 ⓘ

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	561/635 (88%)	0.17	20 (3%)	46 25	34, 81, 154, 201	0
1	B	561/635 (88%)	0.42	27 (4%)	35 18	58, 101, 162, 226	0
All	All	1122/1270 (88%)	0.29	47 (4%)	40 21	34, 94, 158, 226	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	513	GLY	3.0
1	B	243	GLU	3.0
1	B	297	LEU	2.9
1	A	149	VAL	2.8
1	A	601	ASN	2.8
1	B	335	LEU	2.8
1	B	339	LEU	2.8
1	B	601	ASN	2.7
1	B	296	ALA	2.7
1	B	150	ASN	2.7
1	B	17	GLY	2.7
1	A	56	ILE	2.6
1	B	157	GLN	2.6
1	B	413	GLY	2.5
1	A	159	ASP	2.5
1	B	298	PRO	2.4
1	A	343	VAL	2.4
1	B	82	GLY	2.4
1	A	342	ASN	2.4
1	B	299	ALA	2.4
1	B	56	ILE	2.3
1	A	243	GLU	2.3
1	B	302	VAL	2.3
1	A	1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	502	PHE	2.3
1	A	157	GLN	2.3
1	A	340	VAL	2.2
1	B	152	ASP	2.2
1	A	151	LEU	2.2
1	A	499	PHE	2.2
1	A	518	VAL	2.2
1	B	301	SER	2.2
1	B	159	ASP	2.2
1	B	151	LEU	2.2
1	A	495	LYS	2.2
1	A	595	ASN	2.2
1	B	342	ASN	2.2
1	A	301	SER	2.1
1	B	370	ILE	2.1
1	A	333	ASP	2.1
1	B	579	GLU	2.1
1	B	314	ASN	2.0
1	B	457	THR	2.0
1	A	81	PHE	2.0
1	A	503	GLY	2.0
1	B	149	VAL	2.0
1	B	556	VAL	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.

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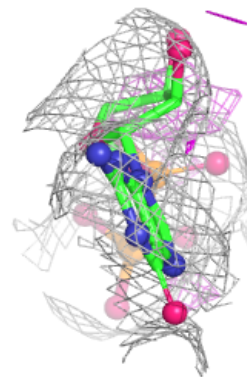
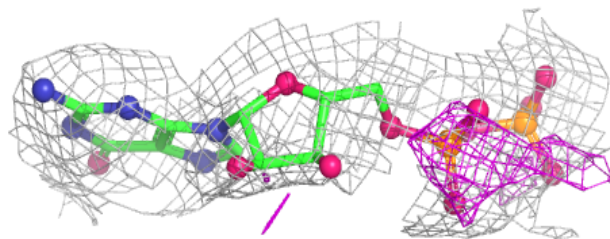
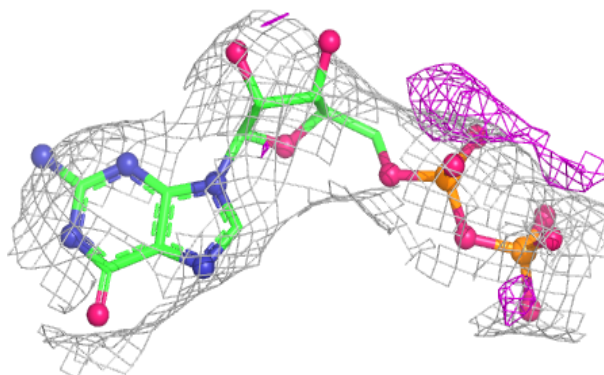
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NCO	B	1002	7/7	0.81	0.11	110,118,124,124	0
4	MG	A	1004	1/1	0.83	0.45	72,72,72,72	0
3	GDP	B	1003	28/28	0.84	0.12	81,103,111,121	0
2	NCO	A	1002	7/7	0.88	0.17	95,98,107,110	0
2	NCO	A	1001	7/7	0.93	0.13	93,98,103,103	0
3	GDP	A	1003	28/28	0.95	0.07	45,56,70,78	0
2	NCO	B	1001	7/7	0.97	0.10	56,62,74,82	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.

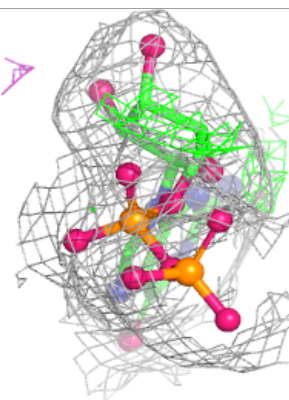
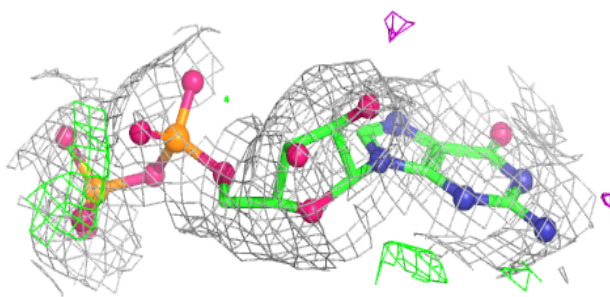
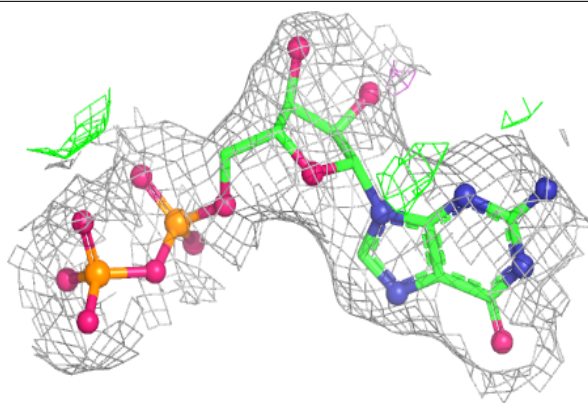
Electron density around GDP B 1003:

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 1003:

$2mF_o-DF_c$ (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.