



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2025 – 12:13 PM JST

PDB ID : 9IIT
Title : Full length structure of FKP in complex with GTP and GDP
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Deposited on : 2024-06-21
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

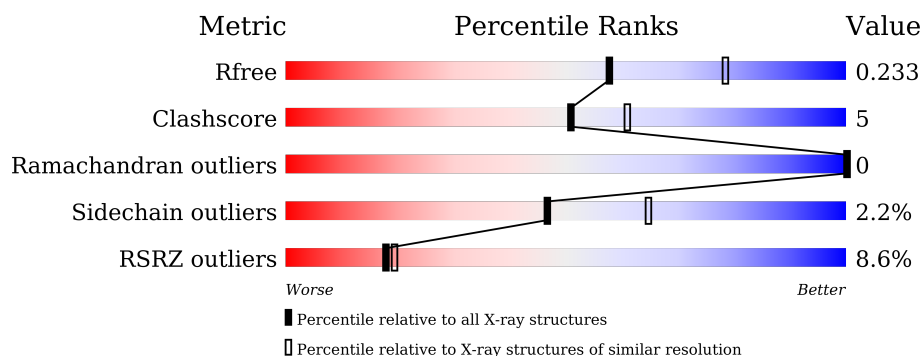
1 Overall quality at a glance

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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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	969	<div> <div>9%</div> <div>84%</div> <div>14%</div> <div>••</div> </div>
1	B	969	<div> <div>8%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15926 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 L-fucokinase/L-fucose-1-P guanylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	950	Total	C	N	O	S	0	0	0
			7457	4759	1274	1393	31			
1	B	950	Total	C	N	O	S	0	0	0
			7457	4759	1274	1393	31			

There are 40 discrepancies between the modelled and reference sequences:

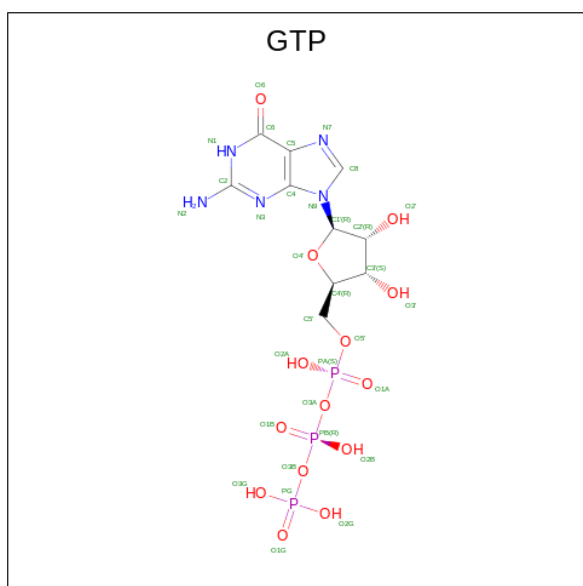
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q58T34
A	-18	GLY	-	expression tag	UNP Q58T34
A	-17	SER	-	expression tag	UNP Q58T34
A	-16	SER	-	expression tag	UNP Q58T34
A	-15	HIS	-	expression tag	UNP Q58T34
A	-14	HIS	-	expression tag	UNP Q58T34
A	-13	HIS	-	expression tag	UNP Q58T34
A	-12	HIS	-	expression tag	UNP Q58T34
A	-11	HIS	-	expression tag	UNP Q58T34
A	-10	HIS	-	expression tag	UNP Q58T34
A	-9	SER	-	expression tag	UNP Q58T34
A	-8	SER	-	expression tag	UNP Q58T34
A	-7	GLY	-	expression tag	UNP Q58T34
A	-6	LEU	-	expression tag	UNP Q58T34
A	-5	VAL	-	expression tag	UNP Q58T34
A	-4	PRO	-	expression tag	UNP Q58T34
A	-3	ARG	-	expression tag	UNP Q58T34
A	-2	GLY	-	expression tag	UNP Q58T34
A	-1	SER	-	expression tag	UNP Q58T34
A	0	HIS	-	expression tag	UNP Q58T34
B	-19	MET	-	initiating methionine	UNP Q58T34
B	-18	GLY	-	expression tag	UNP Q58T34
B	-17	SER	-	expression tag	UNP Q58T34
B	-16	SER	-	expression tag	UNP Q58T34
B	-15	HIS	-	expression tag	UNP Q58T34

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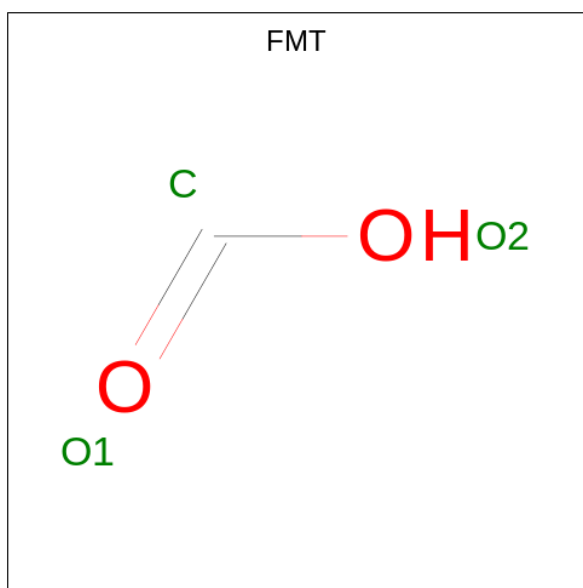
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q58T34
B	-13	HIS	-	expression tag	UNP Q58T34
B	-12	HIS	-	expression tag	UNP Q58T34
B	-11	HIS	-	expression tag	UNP Q58T34
B	-10	HIS	-	expression tag	UNP Q58T34
B	-9	SER	-	expression tag	UNP Q58T34
B	-8	SER	-	expression tag	UNP Q58T34
B	-7	GLY	-	expression tag	UNP Q58T34
B	-6	LEU	-	expression tag	UNP Q58T34
B	-5	VAL	-	expression tag	UNP Q58T34
B	-4	PRO	-	expression tag	UNP Q58T34
B	-3	ARG	-	expression tag	UNP Q58T34
B	-2	GLY	-	expression tag	UNP Q58T34
B	-1	SER	-	expression tag	UNP Q58T34
B	0	HIS	-	expression tag	UNP Q58T34

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



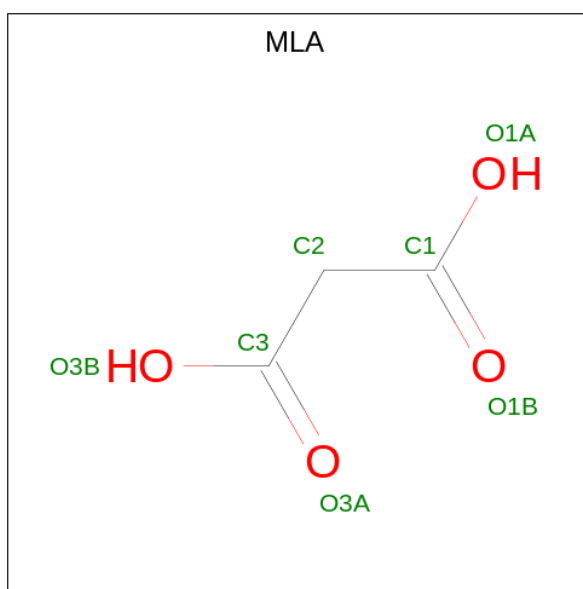
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



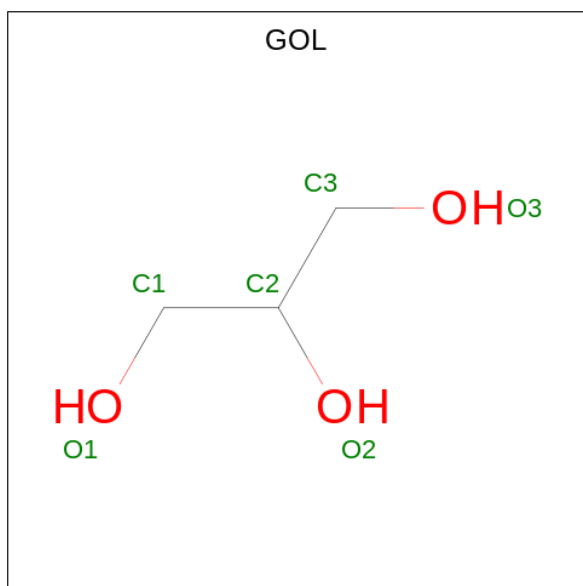
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is MALONIC ACID (three-letter code: MLA) (formula: $\text{C}_3\text{H}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



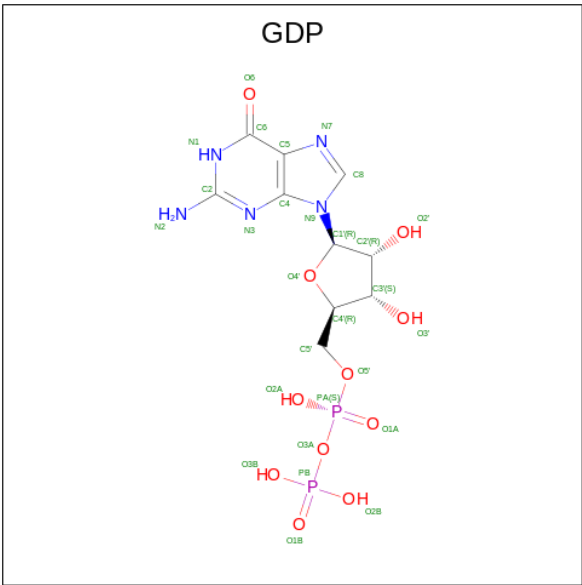
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



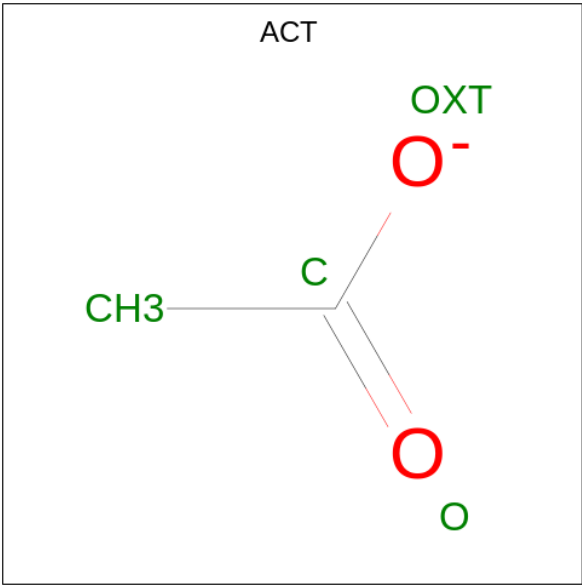
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

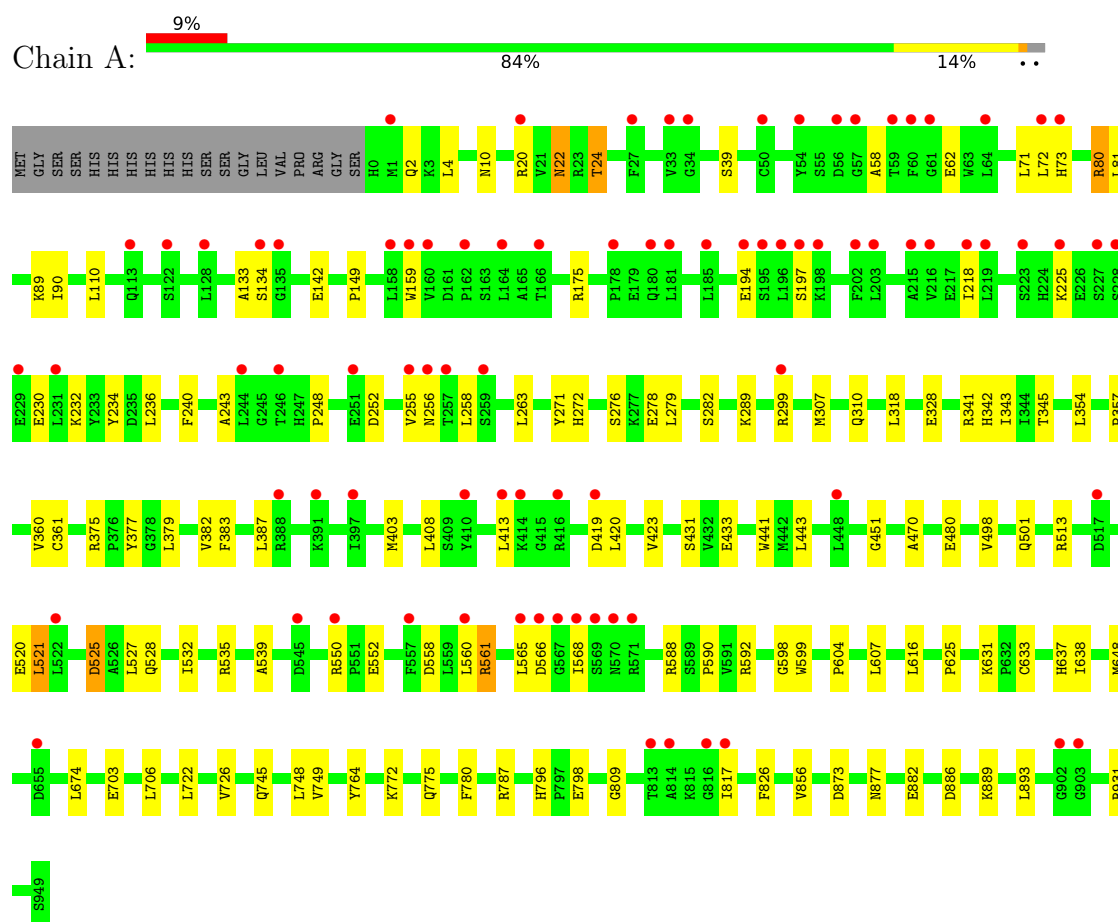
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	471	Total 471	O 471	0	0
8	B	372	Total 372	O 372	0	0

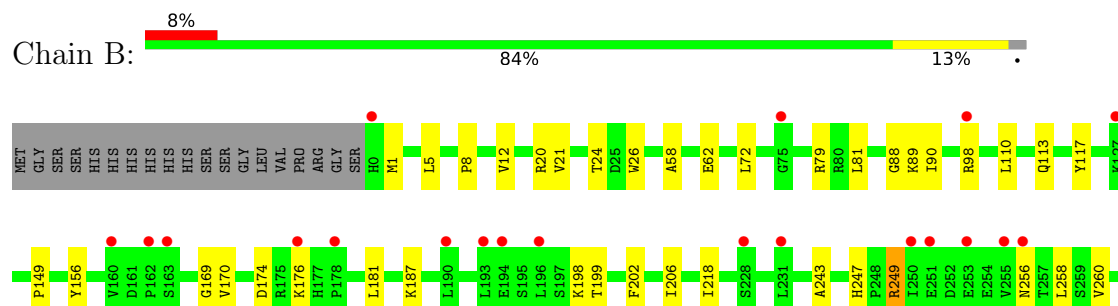
3 Residue-property plots

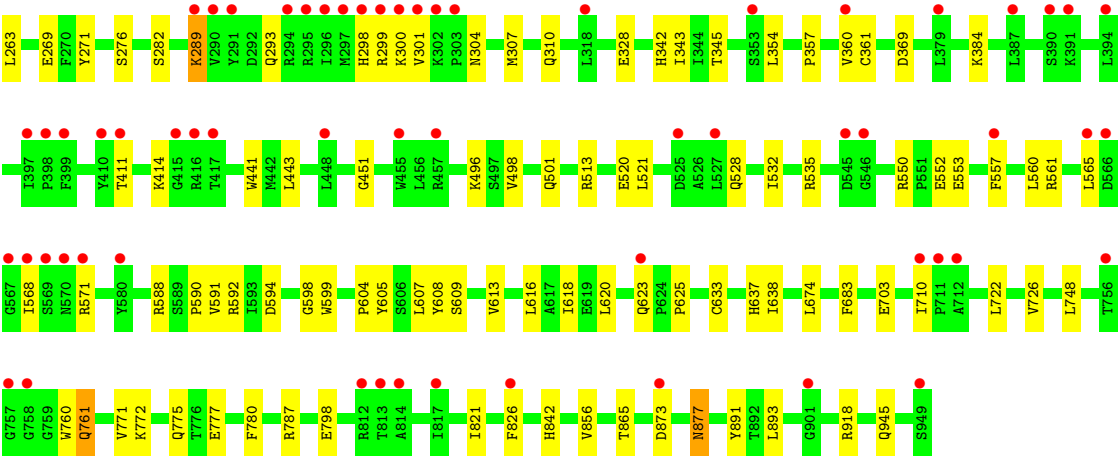
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: L-fucokinase/L-fucose-1-P guanylyltransferase



- Molecule 1: L-fucokinase/L-fucose-1-P guanylyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.82Å 96.06Å 127.37Å 90.00° 97.09° 90.00°	Depositor
Resolution (Å)	29.15 – 2.30 29.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.15-2.30) 90.0 (29.15-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.200 , 0.232 0.202 , 0.233	Depositor DCC
R_{free} test set	109354 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.9	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	0.94	EDS
Total number of atoms	15926	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, MLA, GTP, GOL, GDP, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/7632	0.43	0/10347
1	B	0.25	0/7632	0.43	0/10347
All	All	0.25	0/15264	0.43	0/20694

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7457	0	7433	83	0
1	B	7457	0	7433	73	0
2	A	64	0	24	2	0
2	B	32	0	12	0	0
3	A	6	0	2	0	0
4	A	7	0	2	0	0
5	A	12	0	16	1	0
5	B	12	0	16	1	0
6	B	28	0	12	0	0
7	B	8	0	6	0	0
8	A	471	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	372	0	0	2	0
All	All	15926	0	14956	153	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (153) 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:142:GLU:OE2	1:A:289:LYS:NZ	2.10	0.85
1:B:613:VAL:HG11	1:B:761:GLN:HG3	1.62	0.81
1:B:243:ALA:O	1:B:256:ASN:ND2	2.18	0.77
1:B:300:LYS:HE3	1:B:496:LYS:O	1.87	0.75
1:B:58:ALA:HB1	1:B:62:GLU:HG3	1.70	0.73
1:A:58:ALA:HB1	1:A:62:GLU:HG3	1.73	0.71
1:B:357:PRO:HD2	1:B:360:VAL:HG11	1.72	0.71
1:B:565:LEU:HD22	1:B:568:ILE:HD11	1.71	0.71
1:A:271:TYR:HB3	1:A:282:SER:HB3	1.74	0.70
1:B:269:GLU:OE1	1:B:289:LYS:NZ	2.24	0.69
1:A:20:ARG:NH2	1:A:480:GLU:OE2	2.26	0.67
1:A:175:ARG:HH22	1:B:299:ARG:HH12	1.42	0.67
1:B:357:PRO:O	1:B:360:VAL:HG12	1.96	0.66
1:B:90:ILE:HG12	1:B:110:LEU:HB2	1.78	0.65
1:A:403:MET:HE3	1:A:413:LEU:HD11	1.79	0.65
1:A:525:ASP:N	1:A:525:ASP:OD1	2.31	0.64
1:B:777:GLU:OE2	8:B:1101:HOH:O	2.15	0.64
1:A:566:ASP:H	1:A:568:ILE:HG13	1.65	0.61
1:A:225:LYS:HB2	1:A:230:GLU:HB3	1.81	0.61
1:A:431:SER:OG	1:A:433:GLU:OE2	2.19	0.61
1:A:565:LEU:HA	1:A:568:ILE:HD12	1.81	0.61
1:A:387:LEU:HD21	1:A:423:VAL:HG21	1.81	0.60
1:B:638:ILE:HD13	1:B:674:LEU:HD13	1.83	0.60
1:A:225:LYS:HD2	1:A:232:LYS:HB3	1.82	0.60
1:A:272:HIS:ND1	1:A:278:GLU:OE1	2.30	0.60
1:A:560:LEU:HD22	1:A:826:PHE:HZ	1.66	0.60
1:B:98:ARG:HB2	1:B:298:HIS:HB3	1.85	0.58
1:A:243:ALA:O	1:A:256:ASN:ND2	2.36	0.58
1:A:638:ILE:HD13	1:A:674:LEU:HD13	1.85	0.58
1:B:560:LEU:HD22	1:B:826:PHE:HZ	1.68	0.58
1:A:354:LEU:HD11	1:A:443:LEU:HD12	1.86	0.57
2:A:1001:GTP:O2G	8:A:1101:HOH:O	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:PRO:HA	1:B:625:PRO:HD2	1.86	0.56
1:B:354:LEU:HD11	1:B:443:LEU:HD12	1.87	0.56
1:B:633:CYS:HB2	1:B:703:GLU:HG3	1.87	0.56
1:A:856:VAL:HA	1:A:893:LEU:HD13	1.88	0.56
1:A:633:CYS:HB2	1:A:703:GLU:HG3	1.88	0.55
1:A:357:PRO:O	1:A:360:VAL:HG12	2.07	0.55
1:A:4:LEU:HB2	1:A:71:LEU:HG	1.88	0.54
1:A:175:ARG:HH22	1:B:299:ARG:NH1	2.06	0.54
1:A:590:PRO:HA	1:A:625:PRO:HD2	1.90	0.54
1:A:706:LEU:HD22	5:A:1006:GOL:H31	1.89	0.53
1:A:341:ARG:HB3	1:A:379:LEU:HD22	1.90	0.53
1:B:604:PRO:HG3	1:B:826:PHE:CD1	2.43	0.53
1:A:775:GLN:OE1	1:A:787:ARG:NH2	2.42	0.53
1:A:72:LEU:HD13	1:A:90:ILE:HD11	1.91	0.53
1:A:90:ILE:HG12	1:A:110:LEU:HB2	1.91	0.53
1:B:856:VAL:HA	1:B:893:LEU:HD13	1.90	0.52
1:A:81:LEU:HD23	1:A:89:LYS:HG2	1.92	0.52
1:B:535:ARG:NH1	1:B:552:GLU:OE1	2.33	0.52
1:A:279:LEU:HD23	1:A:343:ILE:HD13	1.92	0.52
1:B:775:GLN:OE1	1:B:787:ARG:NH1	2.43	0.52
1:A:568:ILE:HG23	1:A:749:VAL:HG13	1.92	0.52
1:A:408:LEU:HD11	1:A:441:TRP:HH2	1.75	0.51
1:A:149:PRO:HD2	1:A:263:LEU:HD11	1.91	0.51
1:A:252:ASP:HB3	1:A:255:VAL:HB	1.91	0.51
1:A:796:HIS:ND1	1:A:798:GLU:HG2	2.26	0.51
1:B:945:GLN:OE1	8:B:1102:HOH:O	2.19	0.51
1:B:181:LEU:HD22	1:B:260:VAL:HG11	1.94	0.50
1:A:194:GLU:OE2	1:B:301:VAL:HG23	2.11	0.50
1:B:607:LEU:HD22	1:B:780:PHE:HA	1.93	0.50
1:A:631:LYS:NZ	8:A:1105:HOH:O	2.30	0.50
1:B:310:GLN:O	1:B:328:GLU:HA	2.10	0.50
1:A:310:GLN:O	1:A:328:GLU:HA	2.11	0.50
1:A:22:ASN:HD22	1:A:24:THR:HG23	1.77	0.49
1:A:539:ALA:HB2	1:A:552:GLU:HB3	1.94	0.49
1:A:248:PRO:HG3	1:A:256:ASN:ND2	2.27	0.49
1:A:535:ARG:NH1	1:A:552:GLU:OE1	2.42	0.49
1:A:560:LEU:HD22	1:A:826:PHE:CZ	2.47	0.49
1:A:877:ASN:ND2	1:A:882:GLU:OE1	2.37	0.49
1:A:441:TRP:HB2	1:A:451:GLY:HA3	1.94	0.48
1:A:745:GLN:OE1	1:A:764:TYR:OH	2.28	0.48
1:A:598:GLY:O	1:A:599:TRP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:ILE:HD11	1:B:873:ASP:HB2	1.95	0.47
1:B:276:SER:HB3	1:B:343:ILE:HD12	1.97	0.47
1:A:528:GLN:O	1:A:532:ILE:HG13	2.15	0.47
1:B:625:PRO:HB3	1:B:710:ILE:HG12	1.97	0.47
1:A:175:ARG:NH2	1:A:197:SER:O	2.48	0.47
1:A:722:LEU:O	1:A:726:VAL:HG23	2.15	0.47
1:A:218:ILE:HD12	1:A:258:LEU:HD21	1.97	0.47
1:A:159:TRP:NE1	1:B:293:GLN:HG3	2.31	0.46
1:B:343:ILE:O	1:B:361:CYS:HB3	2.16	0.46
1:A:343:ILE:O	1:A:361:CYS:HB3	2.16	0.46
1:A:20:ARG:HH22	1:A:513:ARG:NH2	2.14	0.46
1:B:842:HIS:NE2	1:B:865:THR:OG1	2.47	0.45
1:B:5:LEU:HD22	1:B:72:LEU:HB2	1.99	0.45
1:B:560:LEU:HD22	1:B:826:PHE:CZ	2.50	0.45
1:B:605:TYR:HA	1:B:608:TYR:CD2	2.51	0.45
1:B:271:TYR:HB3	1:B:282:SER:HB3	1.99	0.45
1:A:342:HIS:HE1	1:A:357:PRO:O	2.00	0.45
1:B:328:GLU:O	1:B:345:THR:HA	2.17	0.45
1:A:39:SER:HB2	1:A:236:LEU:H	1.81	0.44
1:A:276:SER:HB3	1:A:343:ILE:HD12	1.98	0.44
1:B:218:ILE:HD12	1:B:258:LEU:HD21	1.99	0.44
1:A:558:ASP:O	1:A:561:ARG:HG3	2.17	0.44
1:B:561:ARG:O	1:B:565:LEU:HG	2.16	0.44
1:B:620:LEU:O	1:B:623:GLN:HG2	2.17	0.44
1:A:521:LEU:HD21	1:A:535:ARG:CZ	2.48	0.44
1:A:480:GLU:OE2	1:A:513:ARG:NH2	2.46	0.44
1:B:342:HIS:HE1	1:B:357:PRO:O	2.01	0.44
1:A:22:ASN:ND2	1:A:24:THR:HG23	2.33	0.44
1:B:598:GLY:O	1:B:599:TRP:HB2	2.17	0.44
1:B:748:LEU:HD11	1:B:760:TRP:HB3	1.99	0.44
1:A:383:PHE:HA	1:A:420:LEU:HD23	1.98	0.44
1:B:79:ARG:NH1	1:B:384:LYS:HG2	2.33	0.43
1:B:156:TYR:HB3	1:B:206:ILE:HD11	2.00	0.43
1:A:809:GLY:O	1:A:931:ARG:NH1	2.36	0.43
1:B:304:ASN:HB3	1:B:307:MET:HG3	2.00	0.43
1:A:498:VAL:O	1:A:501:GLN:HG2	2.18	0.43
1:A:604:PRO:HG3	1:A:826:PHE:CD1	2.54	0.43
1:B:174:ASP:OD1	1:B:176:LYS:N	2.38	0.43
1:B:411:THR:O	1:B:414:LYS:NZ	2.52	0.43
1:B:498:VAL:O	1:B:501:GLN:HG2	2.18	0.43
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:ND2	1:A:470:ALA:O	2.35	0.43
1:B:88:GLY:O	1:B:90:ILE:N	2.45	0.43
1:B:20:ARG:HH22	1:B:513:ARG:NH2	2.17	0.43
1:B:198:LYS:HG3	1:B:199:THR:HG23	2.00	0.43
1:B:113:GLN:HG3	1:B:117:TYR:CE2	2.54	0.43
1:A:817:ILE:HD12	1:A:873:ASP:OD1	2.19	0.43
1:A:73:HIS:CE1	1:A:134:SER:HB3	2.54	0.43
1:B:300:LYS:HE2	1:B:496:LYS:HB3	2.01	0.43
1:B:722:LEU:O	1:B:726:VAL:HG23	2.19	0.43
1:A:80:ARG:HD3	1:A:382:VAL:HG13	2.00	0.42
1:B:441:TRP:HB2	1:B:451:GLY:HA3	2.01	0.42
1:B:591:VAL:HG23	1:B:618:ILE:HG13	2.01	0.42
1:A:328:GLU:O	1:A:345:THR:HA	2.19	0.42
1:B:553:GLU:HG2	1:B:557:PHE:CE2	2.54	0.42
1:B:891:TYR:CE1	1:B:918:ARG:HG2	2.55	0.42
1:A:307:MET:HE2	1:A:318:LEU:HD13	2.02	0.42
1:B:21:VAL:HB	1:B:26:TRP:CD1	2.55	0.42
1:B:81:LEU:HD23	1:B:89:LYS:HG2	2.02	0.41
1:B:568:ILE:HG23	1:B:683:PHE:CE1	2.55	0.41
1:A:299:ARG:NH1	1:A:527:LEU:HD11	2.34	0.41
1:A:419:ASP:O	1:A:423:VAL:HG23	2.21	0.41
1:B:247:HIS:O	1:B:249:ARG:NH2	2.53	0.41
1:A:234:TYR:CE2	1:A:240:PHE:HB2	2.56	0.41
1:A:289:LYS:HE2	1:A:289:LYS:HB3	1.78	0.41
1:B:877:ASN:N	1:B:877:ASN:HD22	2.19	0.41
1:A:72:LEU:HD23	1:A:133:ALA:HB3	2.03	0.41
1:B:293:GLN:O	1:B:299:ARG:NH2	2.53	0.41
1:A:360:VAL:HG23	1:A:377:TYR:O	2.20	0.41
1:A:375:ARG:NH2	8:A:1116:HOH:O	2.47	0.41
1:B:149:PRO:HD2	1:B:263:LEU:HD11	2.03	0.41
1:B:528:GLN:O	1:B:532:ILE:HG13	2.21	0.41
1:B:594:ASP:HB3	1:B:761:GLN:OE1	2.21	0.41
1:A:565:LEU:HD23	1:A:568:ILE:HD12	2.03	0.41
1:B:8:PRO:O	1:B:12:VAL:HG23	2.21	0.41
1:B:170:VAL:CG1	1:B:202:PHE:HB2	2.51	0.41
1:A:607:LEU:HD22	1:A:780:PHE:HA	2.03	0.40
1:A:886:ASP:HA	1:A:889:LYS:HD2	2.04	0.40
1:A:73:HIS:CE1	2:A:1001:GTP:H4'	2.57	0.40
1:B:169:GLY:N	5:B:1005:GOL:O3	2.44	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	948/969 (98%)	917 (97%)	31 (3%)	0	100	100
1	B	948/969 (98%)	923 (97%)	25 (3%)	0	100	100
All	All	1896/1938 (98%)	1840 (97%)	56 (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	806/822 (98%)	790 (98%)	16 (2%)	50	68
1	B	806/822 (98%)	787 (98%)	19 (2%)	44	61
All	All	1612/1644 (98%)	1577 (98%)	35 (2%)	47	65

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	22	ASN
1	A	24	THR
1	A	80	ARG
1	A	520	GLU
1	A	521	LEU
1	A	525	ASP
1	A	550	ARG

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Mol	Chain	Res	Type
1	A	561	ARG
1	A	588	ARG
1	A	592	ARG
1	A	616	LEU
1	A	637	HIS
1	A	648	MET
1	A	748	LEU
1	A	772	LYS
1	B	1	MET
1	B	24	THR
1	B	187	LYS
1	B	249	ARG
1	B	289	LYS
1	B	369	ASP
1	B	520	GLU
1	B	550	ARG
1	B	571	ARG
1	B	588	ARG
1	B	592	ARG
1	B	609	SER
1	B	616	LEU
1	B	637	HIS
1	B	761	GLN
1	B	771	VAL
1	B	772	LYS
1	B	798	GLU
1	B	877	ASN

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	2	GLN
1	A	16	HIS
1	A	22	ASN
1	A	77	GLN
1	A	256	ASN
1	A	792	HIS
1	A	851	GLN
1	B	256	ASN
1	B	745	GLN
1	B	851	GLN
1	B	877	ASN

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 ⓘ

13 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	GTP	B	1001	-	26,34,34	1.11	2 (7%)	32,54,54	1.56	7 (21%)
5	GOL	B	1006	-	5,5,5	0.90	0	5,5,5	1.00	0
6	GDP	B	1002	-	24,30,30	0.93	1 (4%)	30,47,47	1.28	4 (13%)
3	FMT	A	1004	-	2,2,2	0.71	0	1,1,1	0.23	0
3	FMT	A	1003	-	2,2,2	0.72	0	1,1,1	0.24	0
2	GTP	A	1001	-	26,34,34	1.12	2 (7%)	32,54,54	1.58	7 (21%)
4	MLA	A	1005	-	6,6,6	1.28	0	7,7,7	1.25	0
5	GOL	A	1006	-	5,5,5	0.87	0	5,5,5	1.03	0
7	ACT	B	1004	-	3,3,3	1.28	0	3,3,3	1.39	0
7	ACT	B	1003	-	3,3,3	1.32	0	3,3,3	1.38	0
5	GOL	A	1007	-	5,5,5	1.00	0	5,5,5	0.83	0
2	GTP	A	1002	-	26,34,34	1.13	2 (7%)	32,54,54	1.52	7 (21%)
5	GOL	B	1005	-	5,5,5	0.86	0	5,5,5	1.08	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	GTP	B	1001	-	-	5/18/38/38	0/3/3/3
5	GOL	B	1006	-	-	0/4/4/4	-
6	GDP	B	1002	-	-	5/12/32/32	0/3/3/3
2	GTP	A	1001	-	-	5/18/38/38	0/3/3/3
4	MLA	A	1005	-	-	4/4/4/4	-
5	GOL	A	1006	-	-	4/4/4/4	-
5	GOL	A	1007	-	-	2/4/4/4	-
2	GTP	A	1002	-	-	2/18/38/38	0/3/3/3
5	GOL	B	1005	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	GTP	C5-C6	-4.05	1.39	1.47
2	B	1001	GTP	C5-C6	-3.95	1.39	1.47
2	A	1001	GTP	C5-C6	-3.88	1.39	1.47
6	B	1002	GDP	C6-N1	-2.32	1.34	1.37
2	B	1001	GTP	C2-N3	2.24	1.38	1.33
2	A	1001	GTP	C2-N3	2.21	1.38	1.33
2	A	1002	GTP	C2-N3	2.21	1.38	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	GTP	PA-O3A-PB	-3.85	119.60	132.83
2	B	1001	GTP	PB-O3B-PG	-3.46	120.97	132.83
2	B	1001	GTP	C3'-C2'-C1'	3.38	106.07	100.98
2	A	1001	GTP	C5-C6-N1	3.25	119.69	113.95
6	B	1002	GDP	C3'-C2'-C1'	3.23	105.84	100.98
2	A	1001	GTP	C3'-C2'-C1'	3.20	105.80	100.98
2	B	1001	GTP	C5-C6-N1	3.19	119.58	113.95
6	B	1002	GDP	PA-O3A-PB	-3.16	121.99	132.83
2	A	1002	GTP	C5-C6-N1	3.12	119.45	113.95
2	A	1001	GTP	PB-O3B-PG	-3.10	122.18	132.83
2	A	1001	GTP	PA-O3A-PB	-3.09	122.21	132.83
2	A	1001	GTP	C8-N7-C5	3.04	108.78	102.99
2	B	1001	GTP	C8-N7-C5	3.04	108.78	102.99
2	A	1002	GTP	C8-N7-C5	3.01	108.72	102.99
2	A	1002	GTP	PB-O3B-PG	-2.93	122.78	132.83
2	B	1001	GTP	C2-N1-C6	-2.84	119.88	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GTP	C2-N1-C6	-2.77	119.99	125.10
2	A	1002	GTP	C2-N1-C6	-2.77	119.99	125.10
2	A	1002	GTP	C3'-C2'-C1'	2.77	105.14	100.98
2	B	1001	GTP	PA-O3A-PB	-2.33	124.85	132.83
6	B	1002	GDP	C8-N7-C5	2.30	107.38	102.99
6	B	1002	GDP	C5-C6-N1	2.21	117.85	113.95
2	B	1001	GTP	O6-C6-C5	-2.15	120.17	124.37
2	A	1002	GTP	O6-C6-C5	-2.10	120.26	124.37
2	A	1001	GTP	O6-C6-C5	-2.09	120.28	124.37

There are no chirality outliers.

All (27) torsion outliers are listed below:

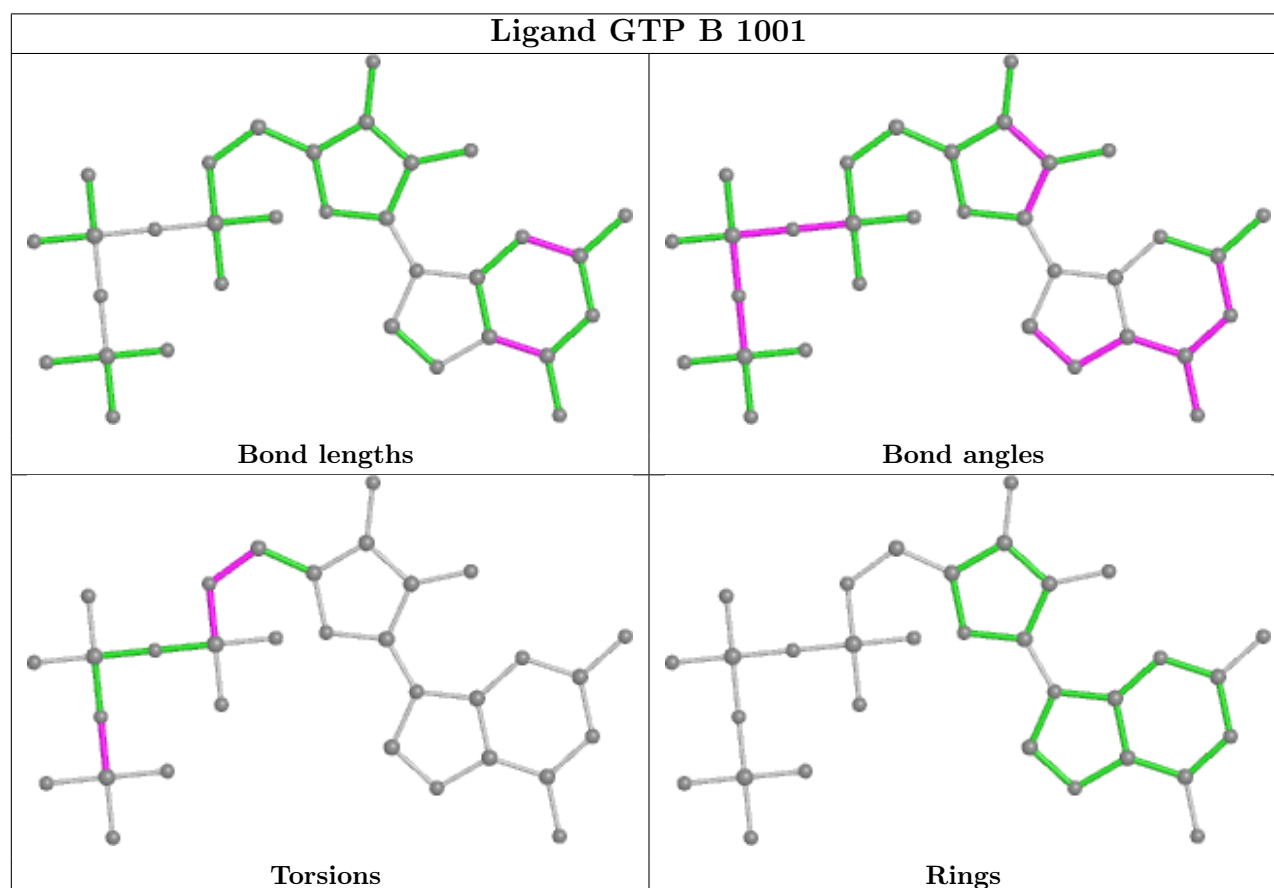
Mol	Chain	Res	Type	Atoms
2	A	1001	GTP	PB-O3B-PG-O2G
2	A	1001	GTP	C5'-O5'-PA-O1A
2	A	1001	GTP	C5'-O5'-PA-O2A
2	A	1002	GTP	PB-O3B-PG-O3G
2	B	1001	GTP	C5'-O5'-PA-O1A
2	B	1001	GTP	C5'-O5'-PA-O2A
5	A	1006	GOL	C1-C2-C3-O3
5	A	1007	GOL	C1-C2-C3-O3
6	B	1002	GDP	C5'-O5'-PA-O2A
5	A	1007	GOL	O2-C2-C3-O3
5	A	1006	GOL	O1-C1-C2-C3
5	A	1006	GOL	O2-C2-C3-O3
2	B	1001	GTP	PB-O3B-PG-O1G
2	B	1001	GTP	C4'-C5'-O5'-PA
6	B	1002	GDP	O4'-C4'-C5'-O5'
2	A	1002	GTP	PB-O3B-PG-O2G
6	B	1002	GDP	C5'-O5'-PA-O3A
2	A	1001	GTP	C4'-C5'-O5'-PA
6	B	1002	GDP	C5'-O5'-PA-O1A
4	A	1005	MLA	O1B-C1-C2-C3
6	B	1002	GDP	C3'-C4'-C5'-O5'
4	A	1005	MLA	O1A-C1-C2-C3
4	A	1005	MLA	C1-C2-C3-O3A
4	A	1005	MLA	C1-C2-C3-O3B
2	A	1001	GTP	C5'-O5'-PA-O3A
2	B	1001	GTP	C5'-O5'-PA-O3A
5	A	1006	GOL	O1-C1-C2-O2

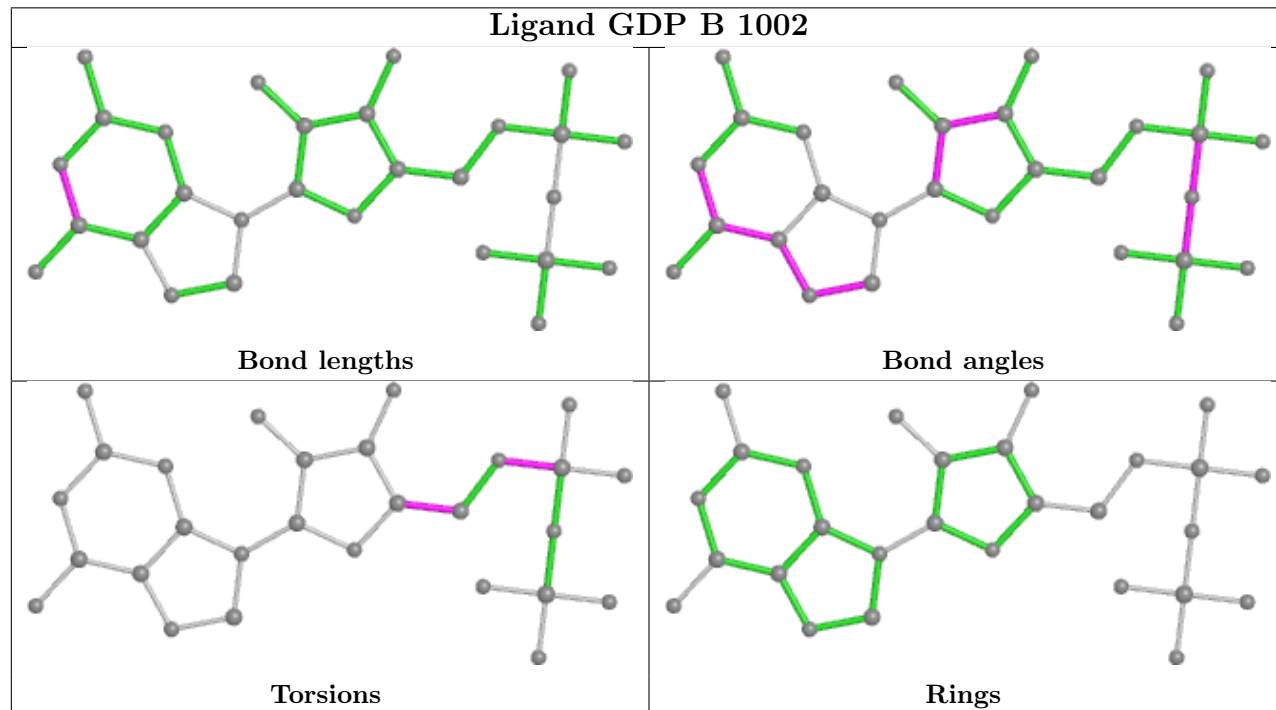
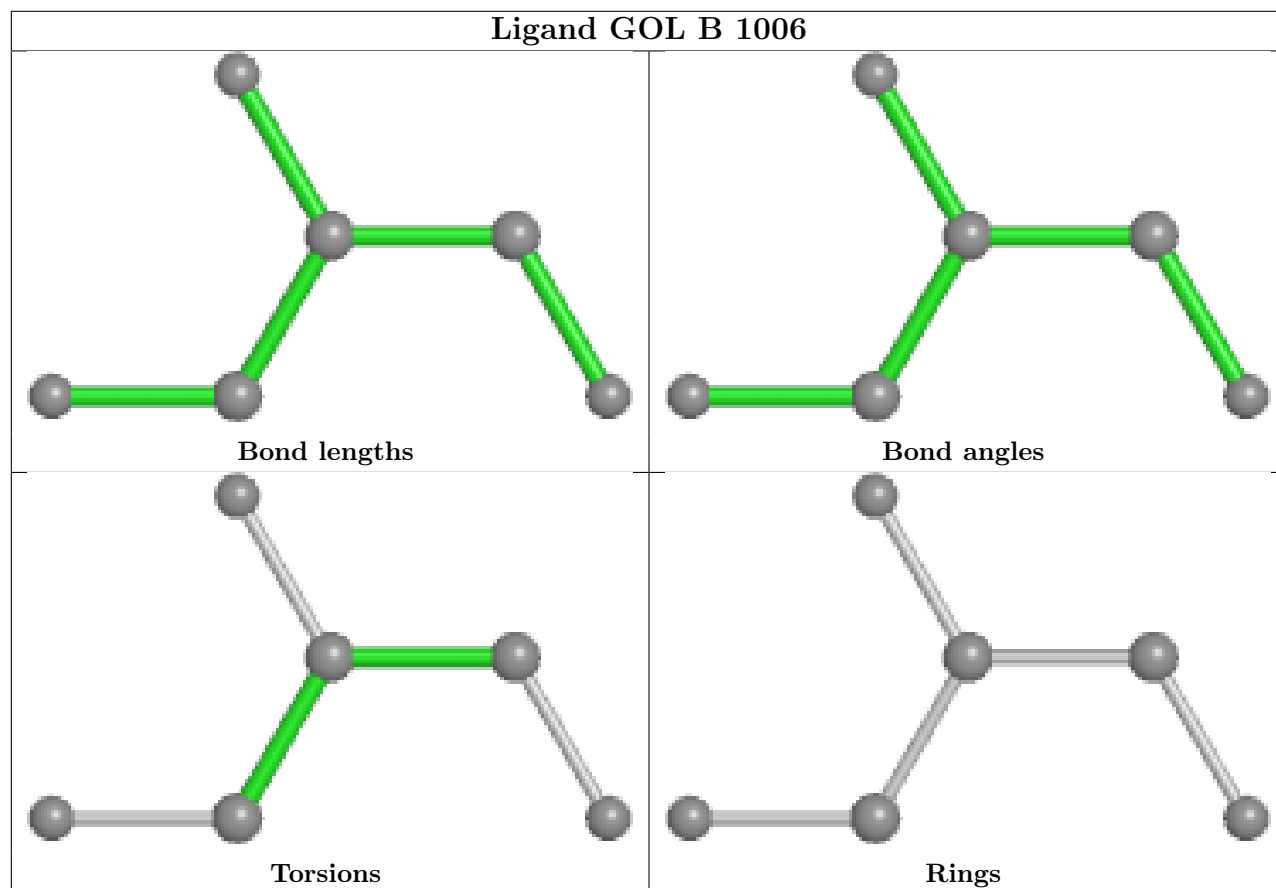
There are no ring outliers.

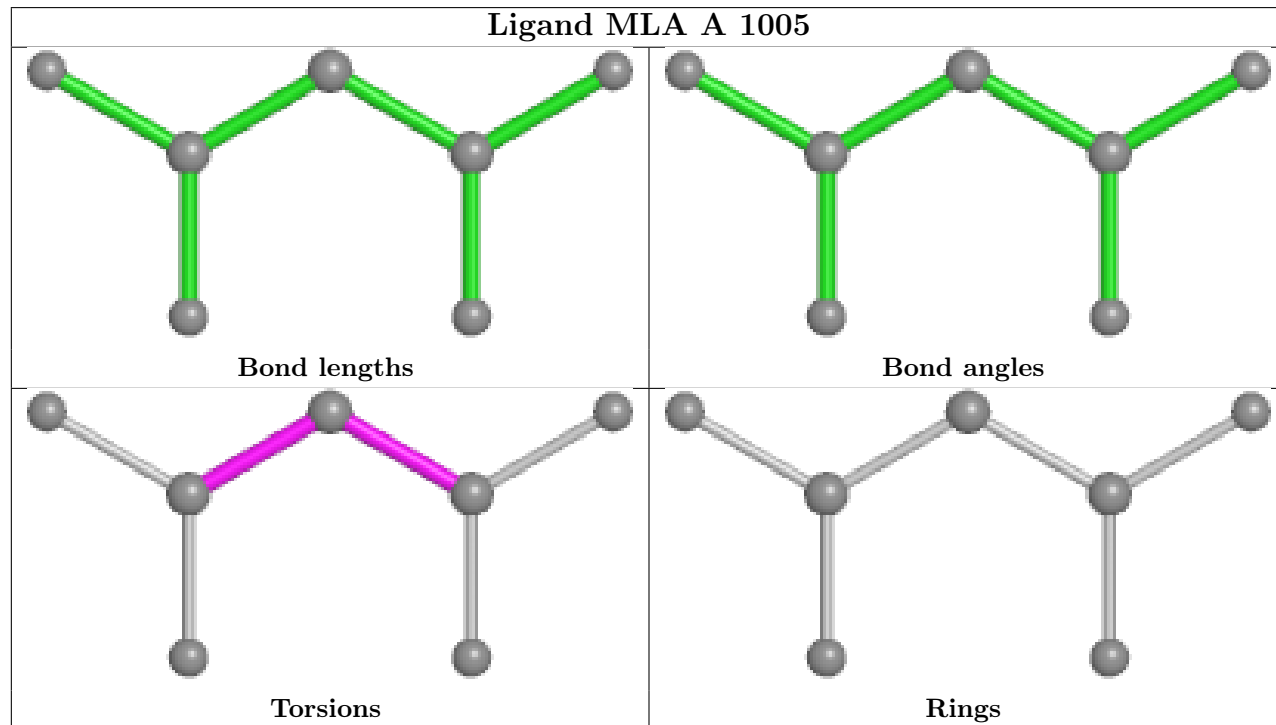
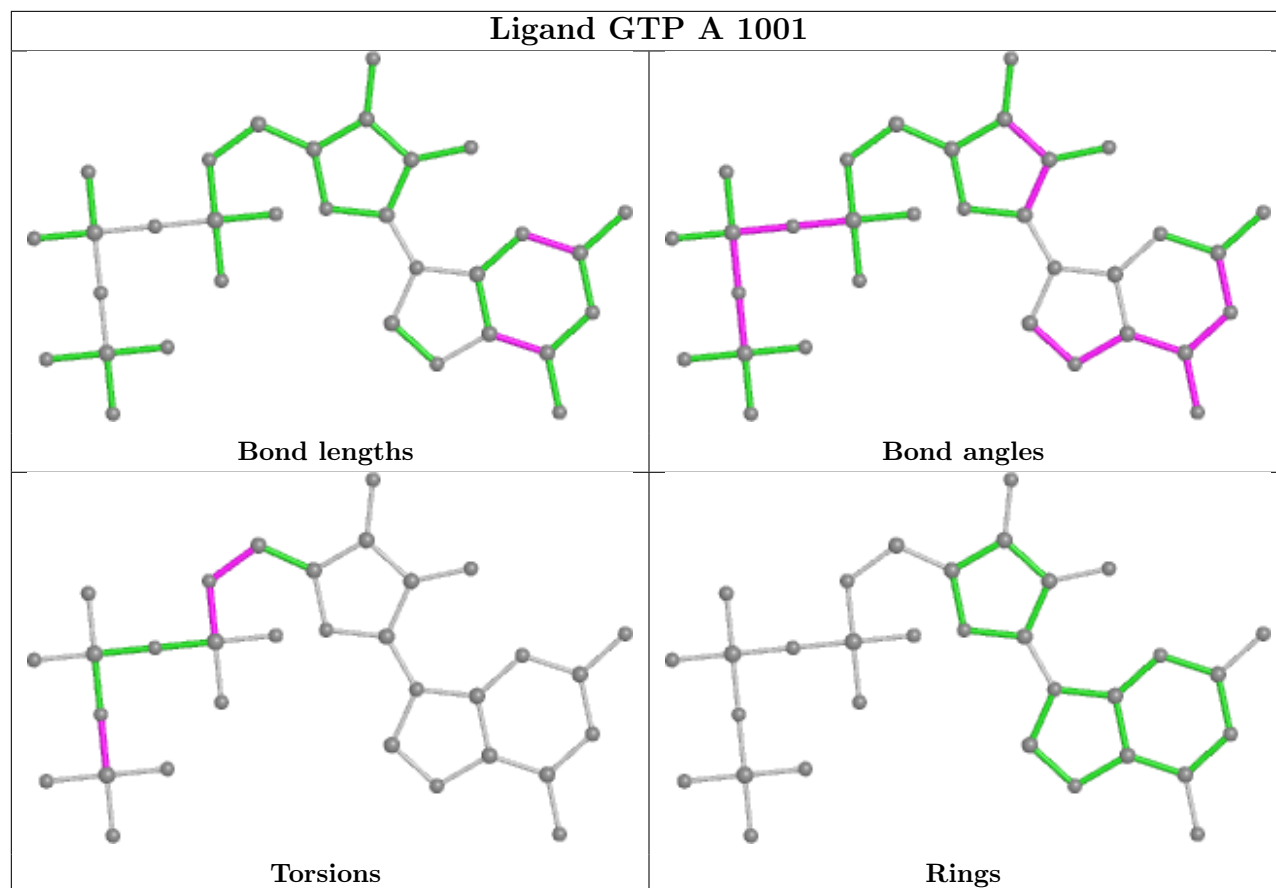
3 monomers are involved in 4 short contacts:

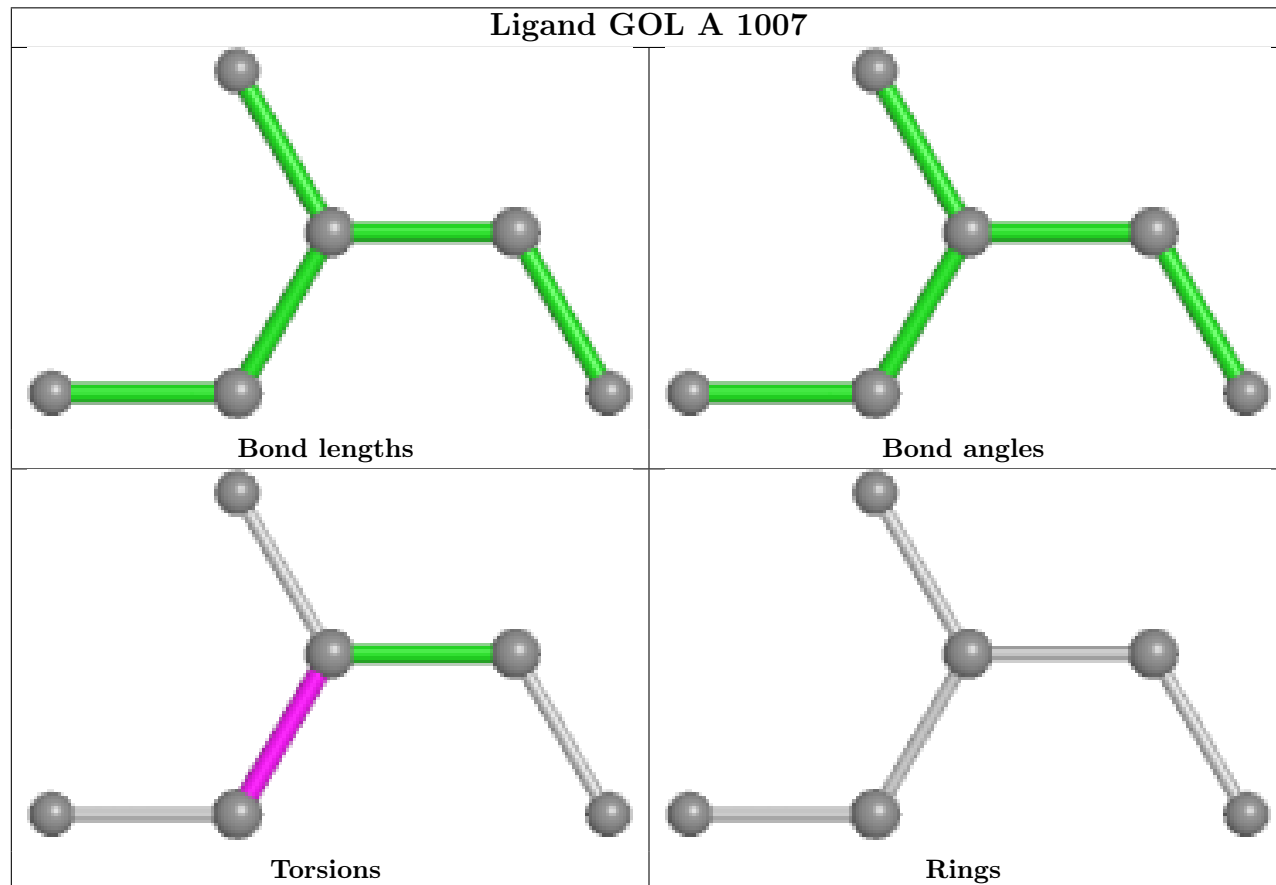
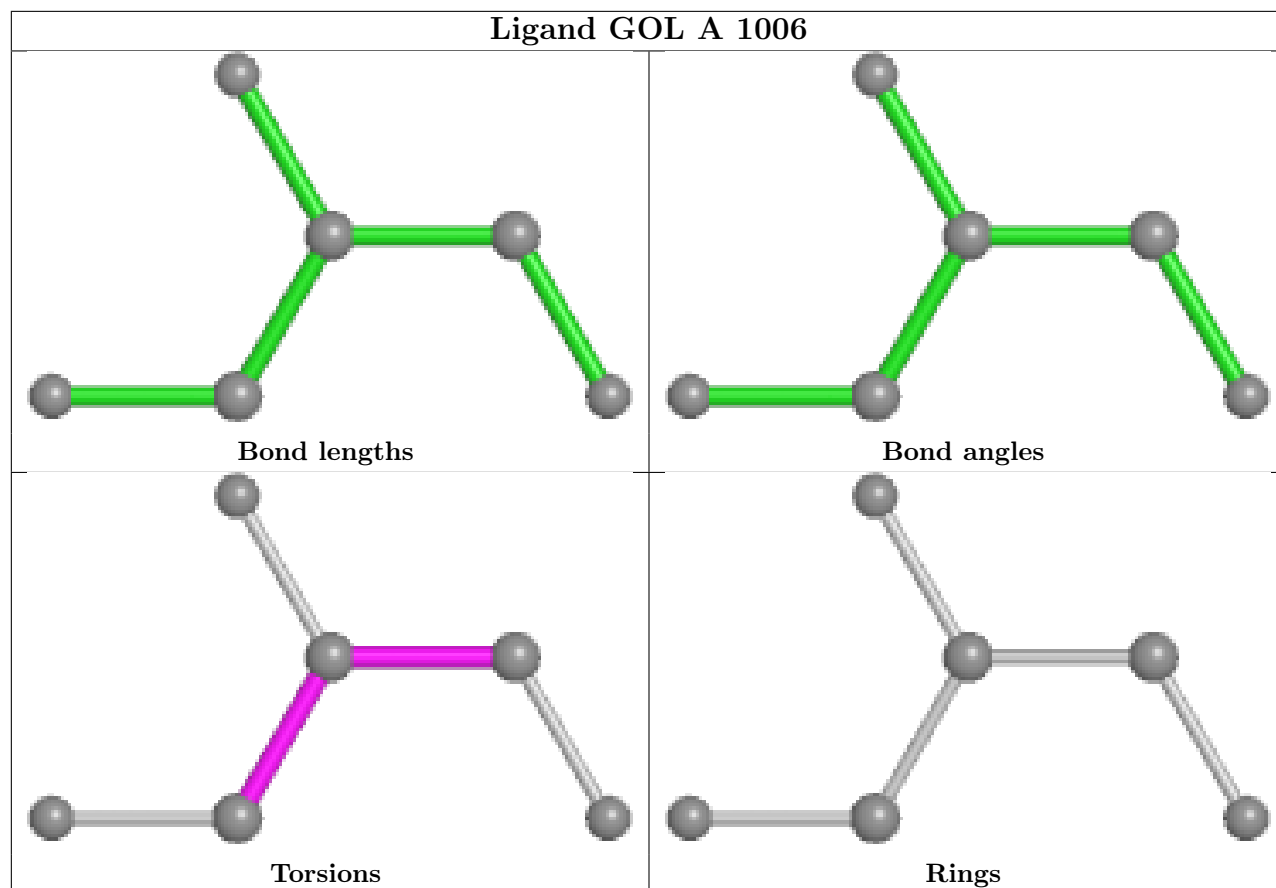
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GTP	2	0
5	A	1006	GOL	1	0
5	B	1005	GOL	1	0

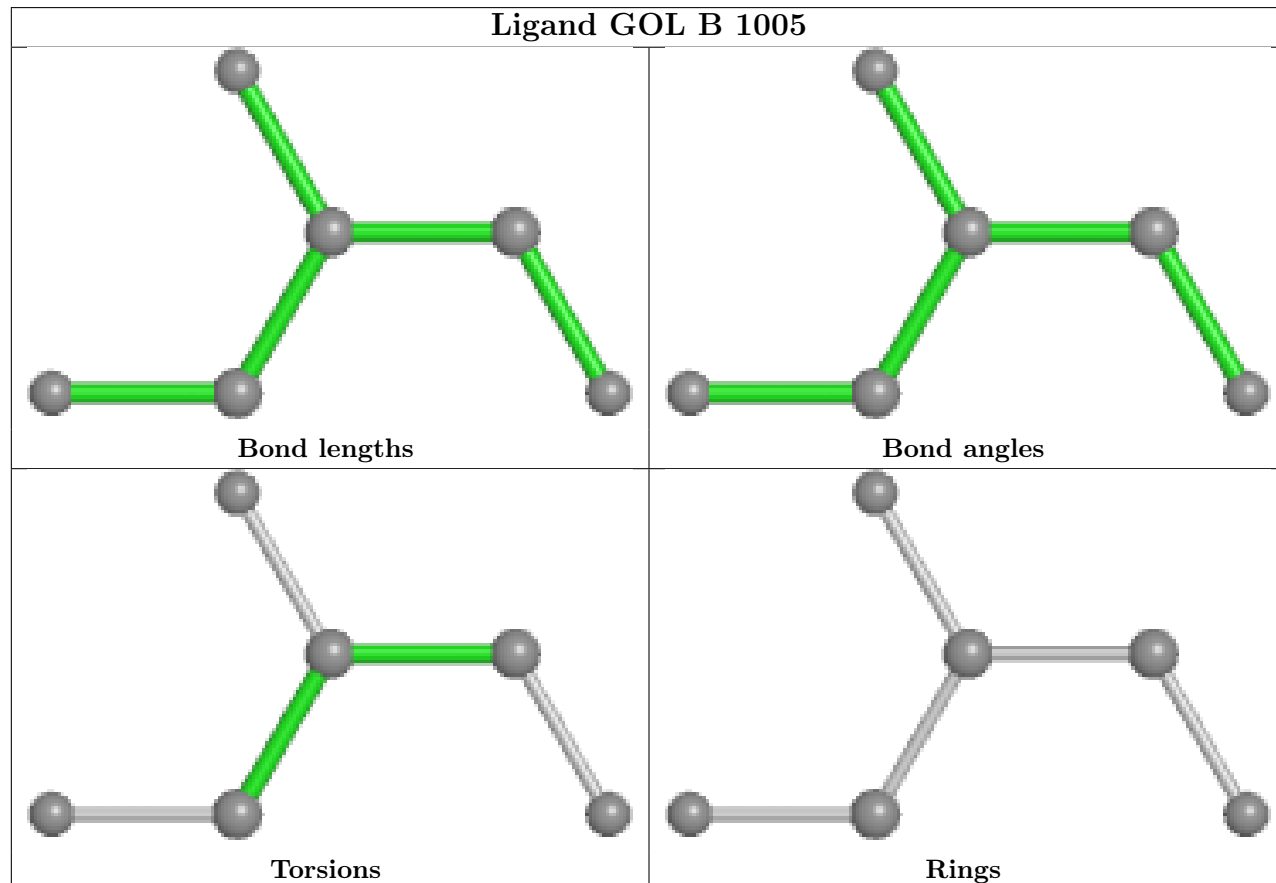
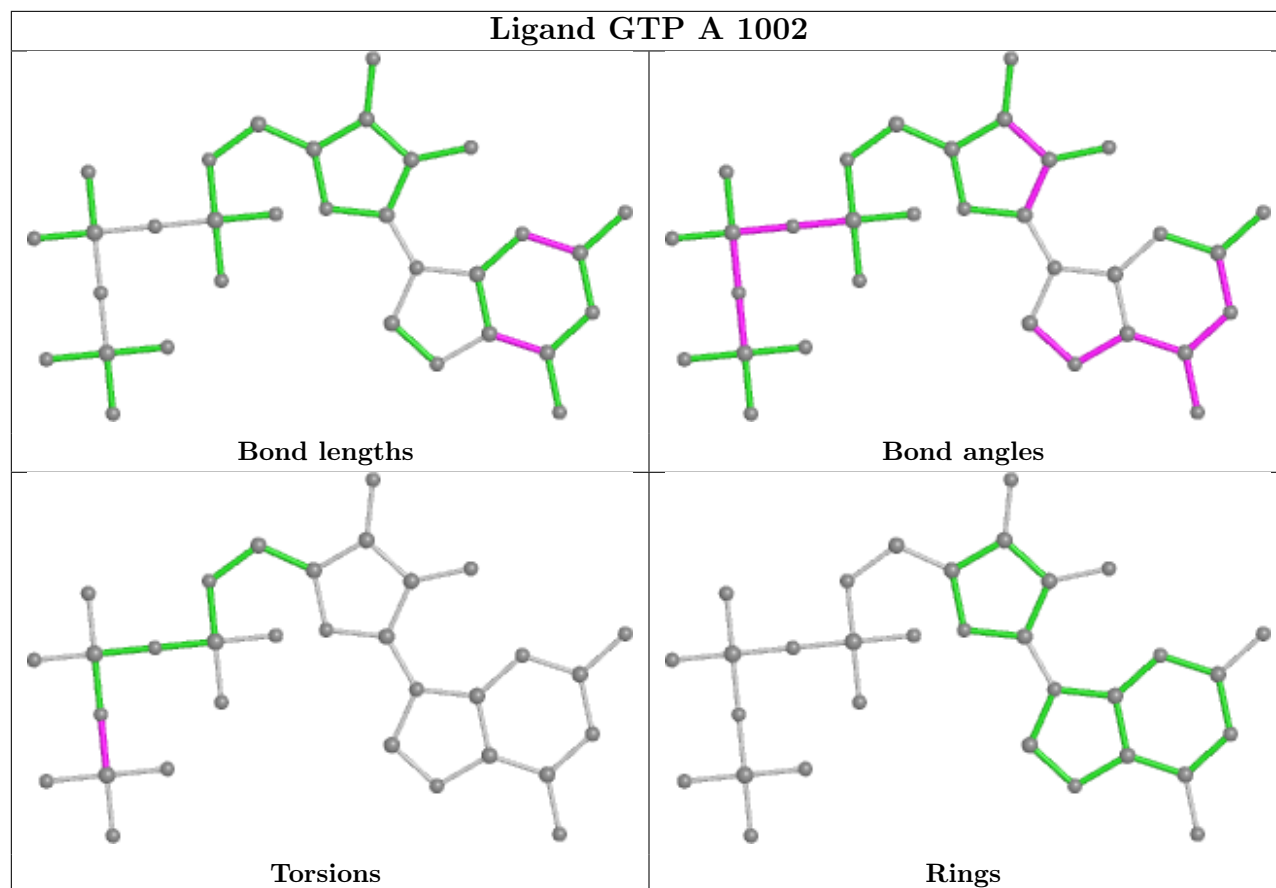
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	950/969 (98%)	0.57	84 (8%) 17 19	25, 61, 129, 210	0
1	B	950/969 (98%)	0.60	80 (8%) 18 20	30, 61, 120, 206	0
All	All	1900/1938 (98%)	0.59	164 (8%) 18 19	25, 61, 125, 210	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	ILE	7.7
1	B	290	VAL	6.0
1	B	568	ILE	5.9
1	B	298	HIS	5.5
1	A	216	VAL	5.4
1	B	565	LEU	4.9
1	B	296	ILE	4.8
1	A	567	GLY	4.8
1	A	565	LEU	4.7
1	A	570	ASN	4.3
1	A	569	SER	4.3
1	A	817	ILE	4.3
1	B	569	SER	4.2
1	B	301	VAL	4.1
1	B	756	THR	4.1
1	B	710	ILE	4.0
1	B	757	GLY	4.0
1	A	814	ALA	3.9
1	A	160	VAL	3.8
1	B	567	GLY	3.7
1	B	712	ALA	3.6
1	A	135	GLY	3.6
1	B	397	ILE	3.5
1	B	194	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	814	ALA	3.5
1	A	566	ASP	3.5
1	B	228	SER	3.4
1	A	448	LEU	3.4
1	A	202	PHE	3.4
1	A	178	PRO	3.4
1	A	903	GLY	3.4
1	B	297	MET	3.4
1	A	816	GLY	3.3
1	A	218	ILE	3.3
1	B	291	TYR	3.2
1	A	57	GLY	3.1
1	B	176	LYS	3.1
1	A	1	MET	3.1
1	B	196	LEU	3.1
1	A	255	VAL	3.1
1	A	228	SER	3.0
1	B	711	PRO	3.0
1	A	215	ALA	3.0
1	A	159	TRP	2.9
1	A	219	LEU	2.9
1	A	20	ARG	2.9
1	B	300	LYS	2.8
1	B	302	LYS	2.8
1	A	164	LEU	2.8
1	A	571	ARG	2.8
1	A	50	CYS	2.8
1	B	758	GLY	2.8
1	A	180	GLN	2.8
1	A	195	SER	2.8
1	A	251	GLU	2.8
1	B	98	ARG	2.8
1	A	60	PHE	2.8
1	B	417	THR	2.8
1	B	299	ARG	2.7
1	A	517	ASP	2.7
1	A	54	TYR	2.7
1	B	410	TYR	2.7
1	B	289	LYS	2.7
1	A	227	SER	2.7
1	A	73	HIS	2.7
1	A	397	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	353	SER	2.6
1	A	197	SER	2.6
1	B	163	SER	2.6
1	A	59	THR	2.5
1	B	812	ARG	2.5
1	A	246	THR	2.5
1	A	198	LYS	2.5
1	B	525	ASP	2.5
1	B	873	ASP	2.5
1	A	194	GLU	2.5
1	B	415	GLY	2.5
1	B	901	GLY	2.5
1	A	550	ARG	2.5
1	B	295	ARG	2.5
1	A	162	PRO	2.5
1	B	398	PRO	2.5
1	B	566	ASP	2.4
1	A	256	ASN	2.4
1	B	457	ARG	2.4
1	B	571	ARG	2.4
1	B	813	THR	2.4
1	B	162	PRO	2.4
1	A	56	ASP	2.4
1	A	902	GLY	2.4
1	A	166	THR	2.4
1	A	419	ASP	2.4
1	B	545	ASP	2.4
1	A	185	LEU	2.4
1	B	570	ASN	2.4
1	A	33	VAL	2.3
1	A	223	SER	2.3
1	A	231	LEU	2.3
1	A	522	LEU	2.3
1	B	394	LEU	2.3
1	A	257	THR	2.3
1	B	178	PRO	2.3
1	A	122	SER	2.3
1	B	253	GLU	2.3
1	B	387	LEU	2.3
1	B	411	THR	2.3
1	B	817	ILE	2.3
1	A	244	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	813	THR	2.2
1	A	113	GLN	2.2
1	B	949	SER	2.2
1	A	560	LEU	2.2
1	B	231	LEU	2.2
1	B	255	VAL	2.2
1	B	826	PHE	2.2
1	A	655	ASP	2.2
1	B	391	LYS	2.2
1	A	128	LEU	2.2
1	A	158	LEU	2.2
1	A	196	LEU	2.2
1	A	388	ARG	2.2
1	B	193	LEU	2.2
1	B	294	ARG	2.2
1	B	416	ARG	2.2
1	B	623	GLN	2.2
1	A	61	GLY	2.2
1	B	250	ILE	2.2
1	A	181	LEU	2.2
1	B	527	LEU	2.2
1	B	160	VAL	2.2
1	B	399	PHE	2.2
1	B	251	GLU	2.1
1	B	455	TRP	2.1
1	B	318	LEU	2.1
1	B	379	LEU	2.1
1	B	448	LEU	2.1
1	B	303	PRO	2.1
1	A	27	PHE	2.1
1	B	75	GLY	2.1
1	B	546	GLY	2.1
1	A	416	ARG	2.1
1	B	256	ASN	2.1
1	B	360	VAL	2.1
1	A	134	SER	2.1
1	A	259	SER	2.1
1	A	299	ARG	2.1
1	B	0	HIS	2.1
1	A	203	LEU	2.1
1	A	391	LYS	2.1
1	B	580	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	557	PHE	2.1
1	A	34	GLY	2.1
1	A	64	LEU	2.1
1	A	410	TYR	2.0
1	B	557	PHE	2.0
1	A	545	ASP	2.0
1	A	225	LYS	2.0
1	A	414	LYS	2.0
1	A	413	LEU	2.0
1	A	229	GLU	2.0
1	B	127	LYS	2.0
1	B	390	SER	2.0
1	A	72	LEU	2.0
1	B	190	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

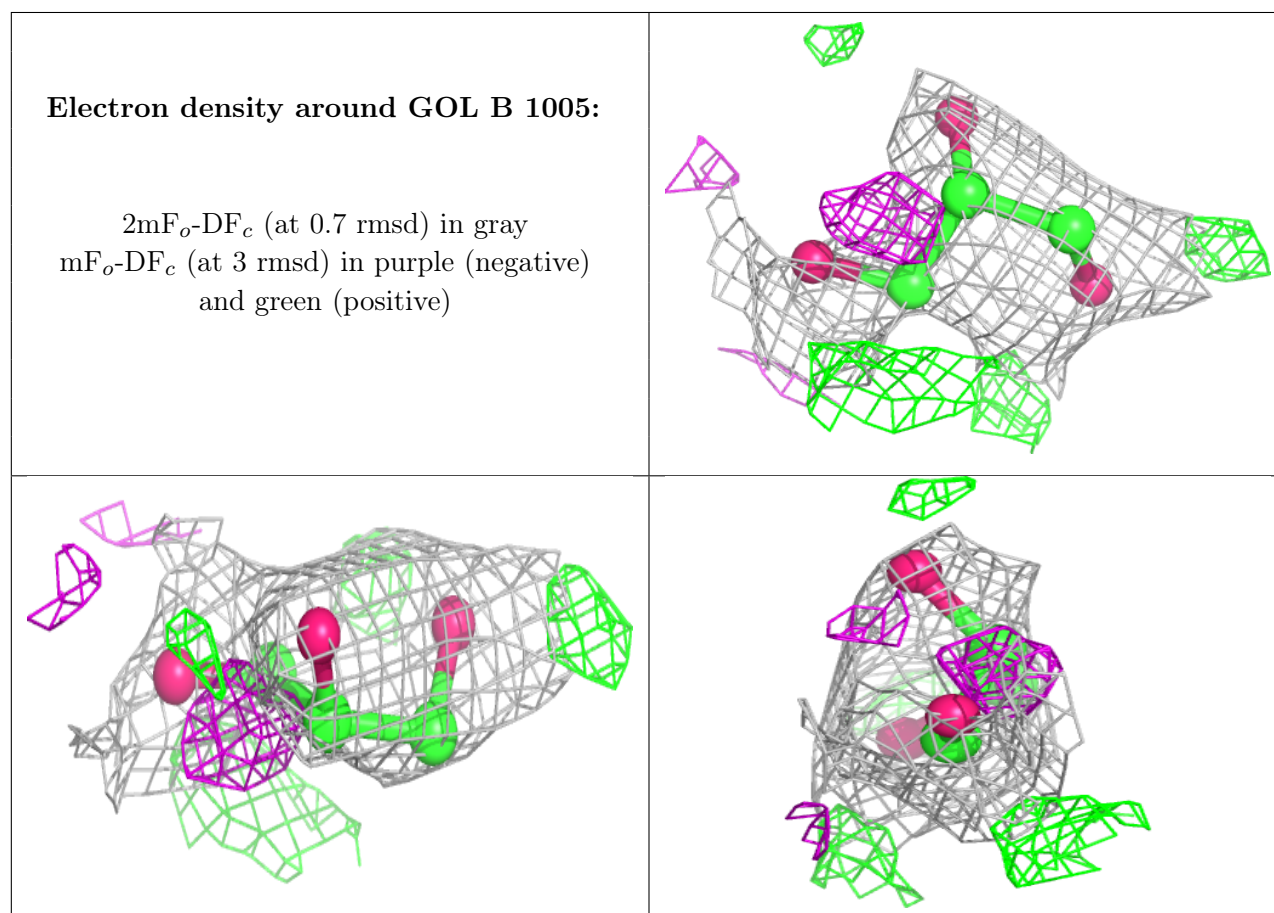
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ACT	B	1003	4/4	0.65	0.19	74,74,75,75	0
5	GOL	B	1005	6/6	0.71	0.22	73,76,81,83	0
2	GTP	B	1001	32/32	0.72	0.16	104,120,144,145	0
3	FMT	A	1003	3/3	0.79	0.17	69,69,71,72	0
7	ACT	B	1004	4/4	0.79	0.19	79,80,81,82	0
5	GOL	A	1007	6/6	0.81	0.18	40,52,54,54	0
3	FMT	A	1004	3/3	0.82	0.17	62,62,63,66	0
2	GTP	A	1001	32/32	0.84	0.13	75,94,119,121	0
4	MLA	A	1005	7/7	0.88	0.12	39,44,50,50	0

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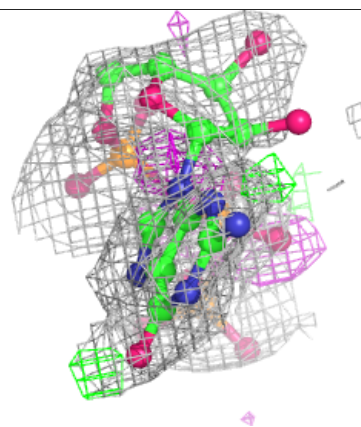
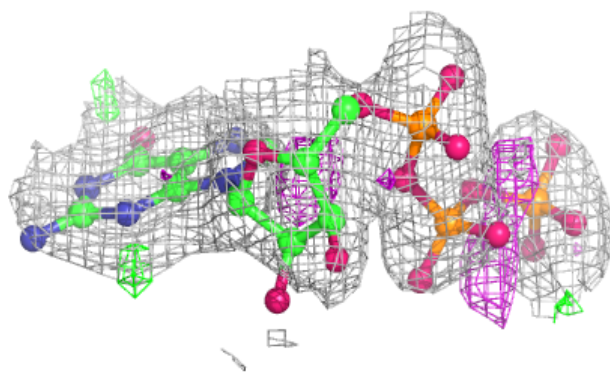
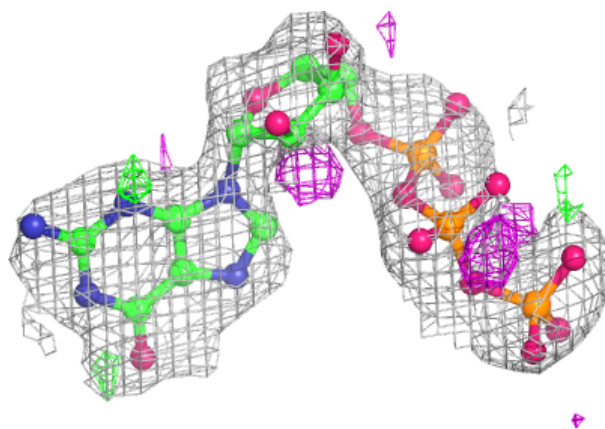
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GDP	B	1002	28/28	0.92	0.09	47,60,80,82	0
5	GOL	B	1006	6/6	0.93	0.09	34,42,47,51	0
2	GTP	A	1002	32/32	0.94	0.09	34,43,94,101	0
5	GOL	A	1006	6/6	0.96	0.07	27,33,34,40	0

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.



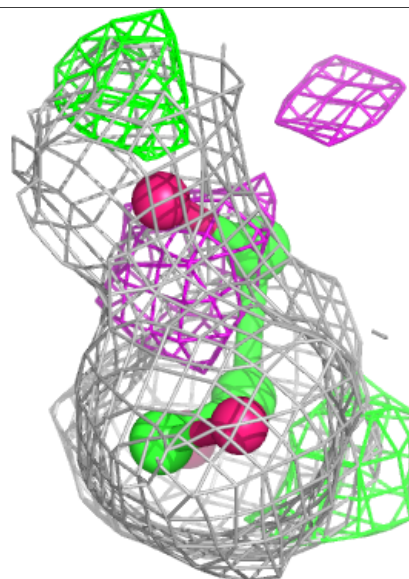
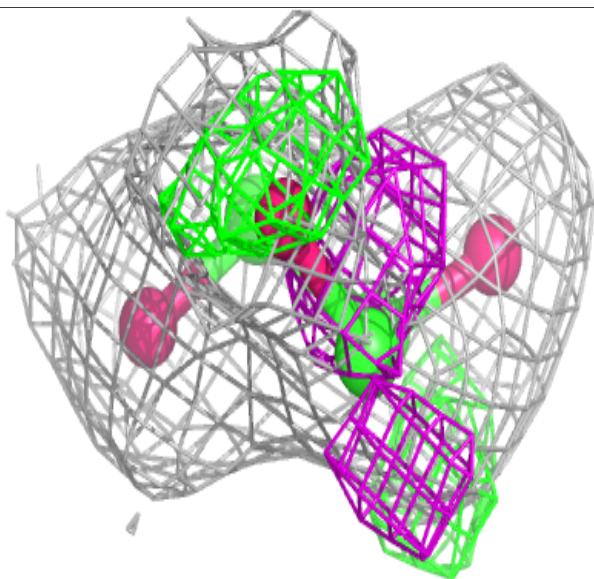
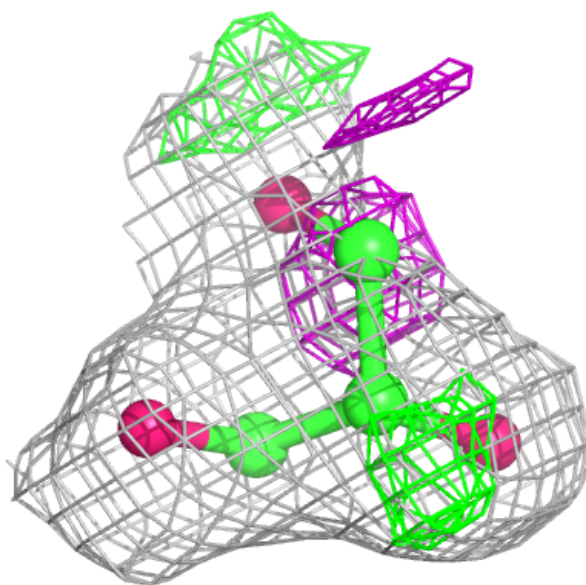
Electron density around GTP B 1001:

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



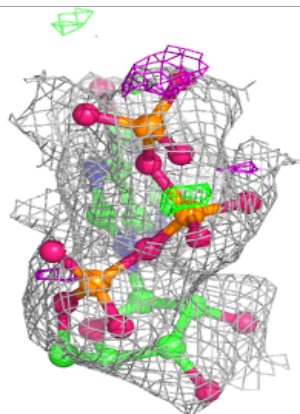
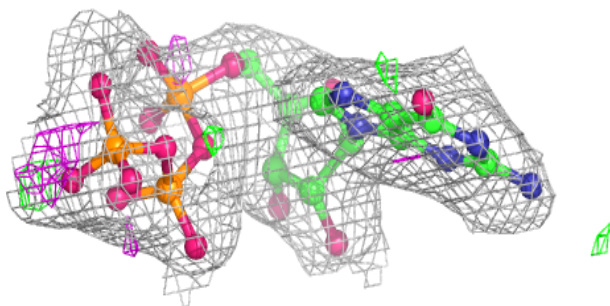
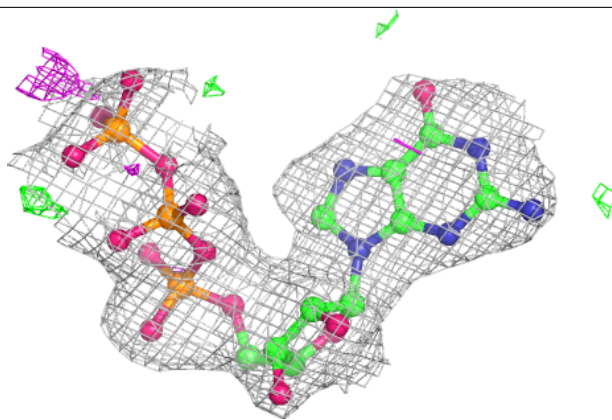
Electron density around GOL A 1007:

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

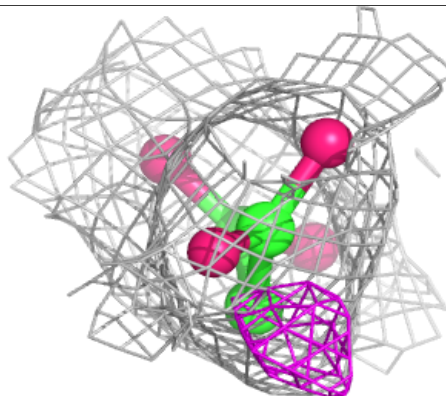
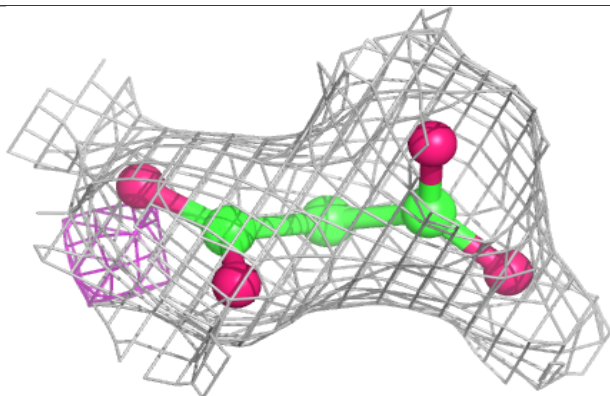
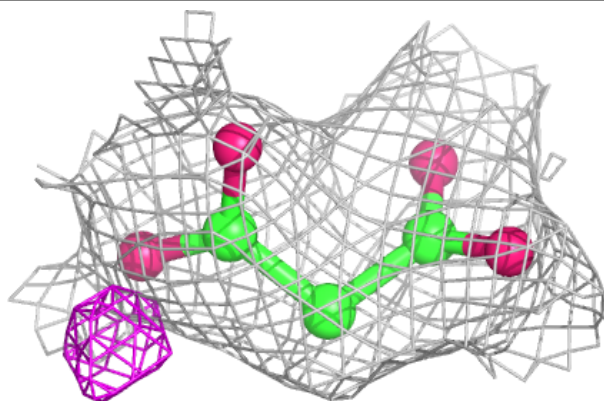


Electron density around GTP A 1001:

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

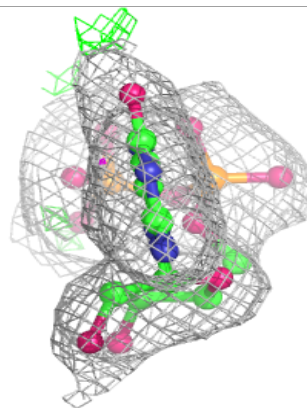
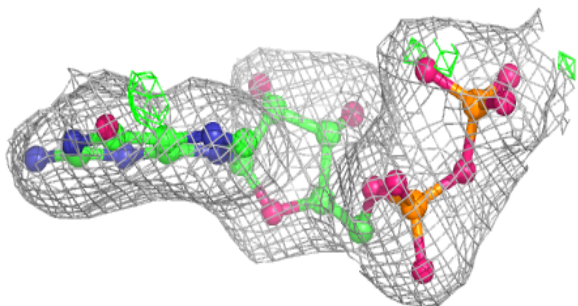
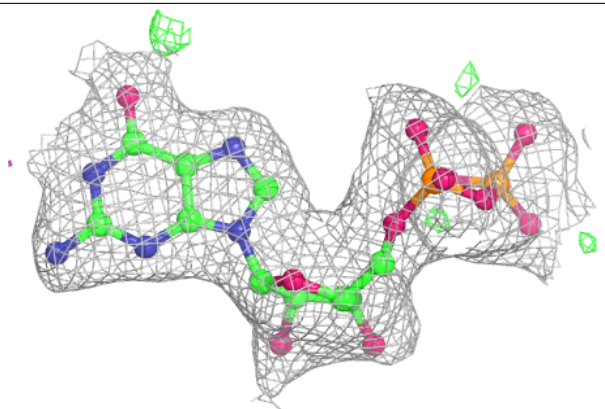
**Electron density around MLA A 1005:**

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



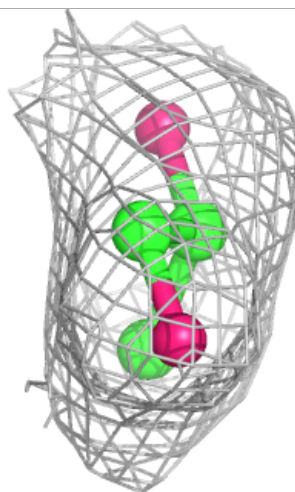
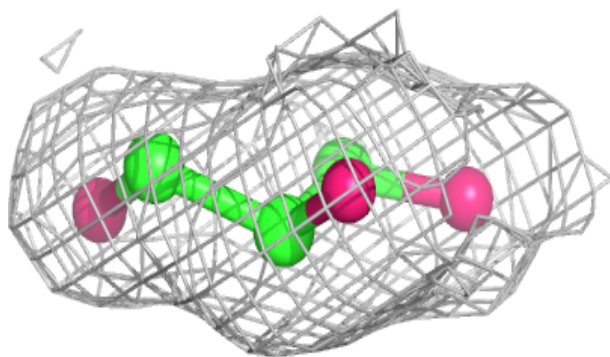
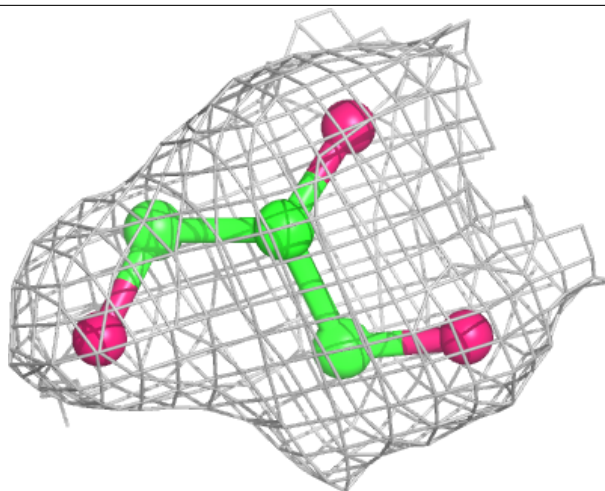
Electron density around GDP B 1002:

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



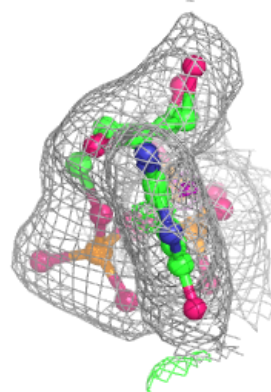
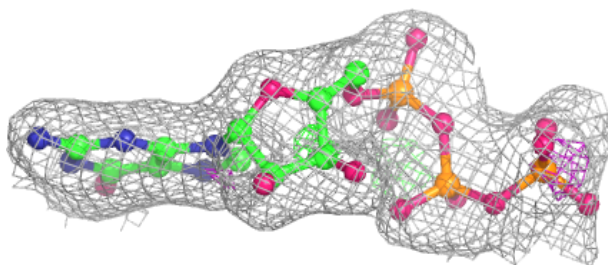
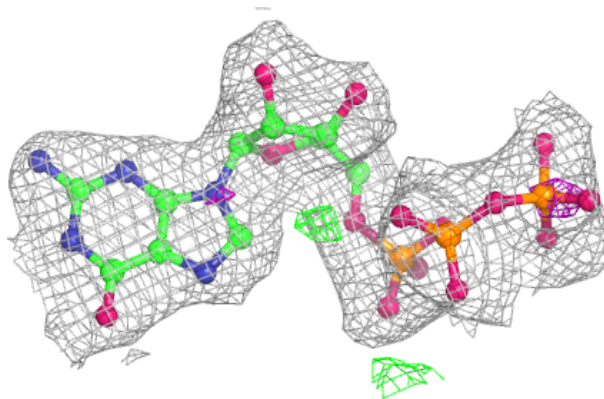
Electron density around GOL B 1006:

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



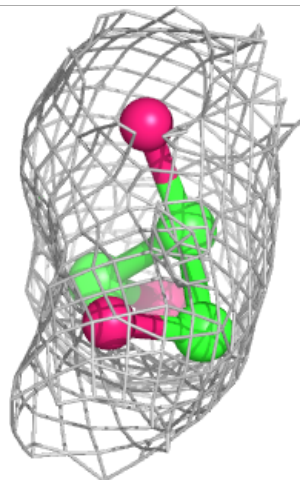
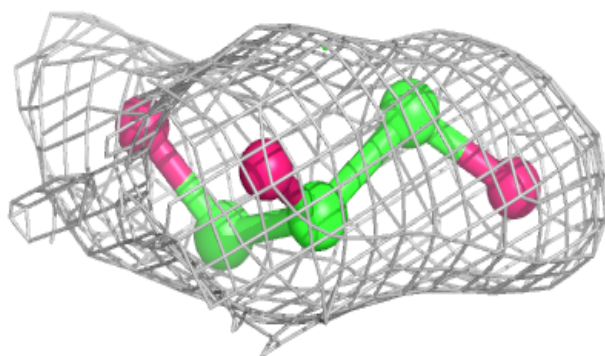
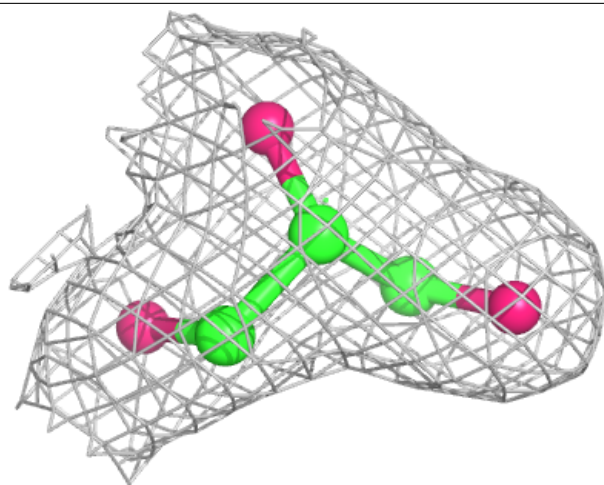
Electron density around GTP A 1002:

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



Electron density around GOL A 1006:

$2mF_o-DF_c$ (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.