



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:11 PM UTC

PDB ID : 9IIT / pdb_00009iit
Title : Full length structure of FKP in complex with GTP and GDP
Authors : Ko, T.P.; Lin, S.W.; Hsu, M.F.; Lin, C.H.
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

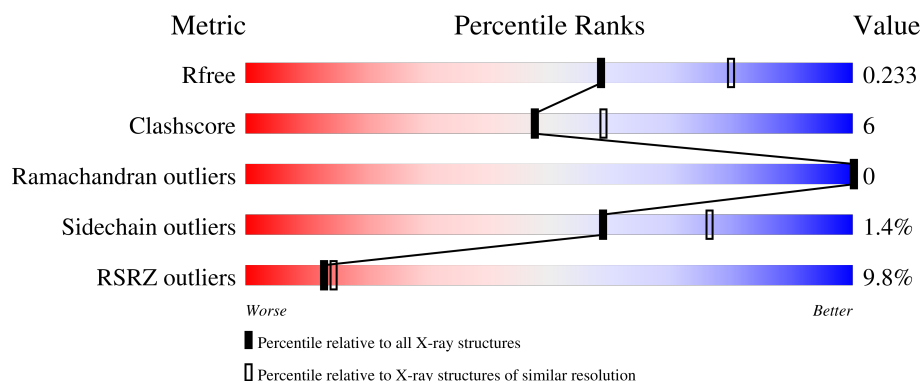
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	969	10% 83% 14% ..
1	B	969	10% 84% 14% .

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:

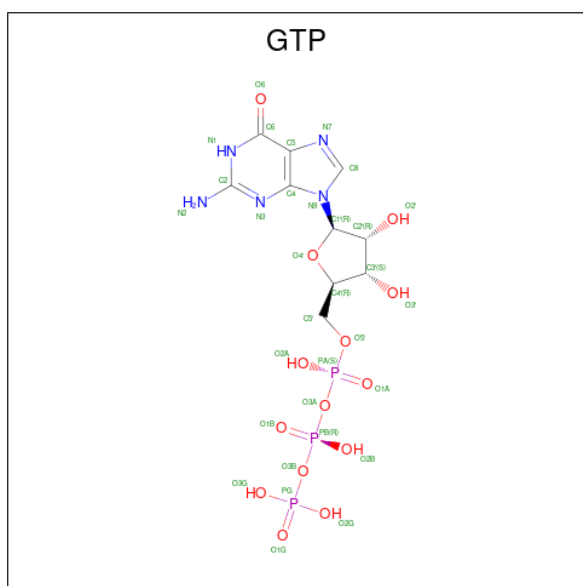
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q58T34
A	-18	GLY	-	expression tag	UNP Q58T34
A	-17	SER	-	expression tag	UNP Q58T34
A	-16	SER	-	expression tag	UNP Q58T34
A	-15	HIS	-	expression tag	UNP Q58T34
A	-14	HIS	-	expression tag	UNP Q58T34
A	-13	HIS	-	expression 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

Continued on next page...

Continued from previous page...

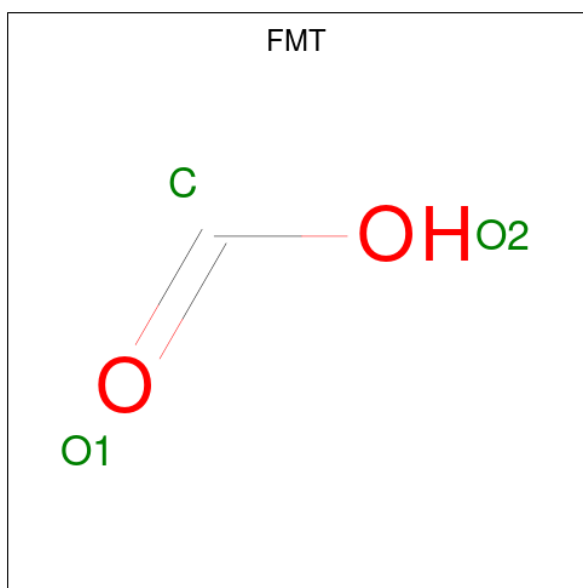
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q58T34
B	-13	HIS	-	expression tag	UNP Q58T34
B	-12	HIS	-	expression tag	UNP Q58T34
B	-11	HIS	-	expression tag	UNP Q58T34
B	-10	HIS	-	expression tag	UNP Q58T34
B	-9	SER	-	expression tag	UNP Q58T34
B	-8	SER	-	expression tag	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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



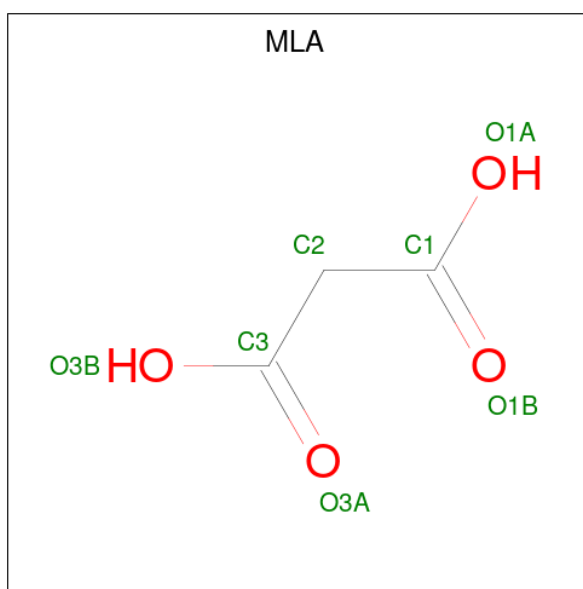
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			32	10	5	14	3	0
2	A	1	Total	C	N	O	P	
			32	10	5	14	3	0
2	B	1	Total	C	N	O	P	
			32	10	5	14	3	0

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



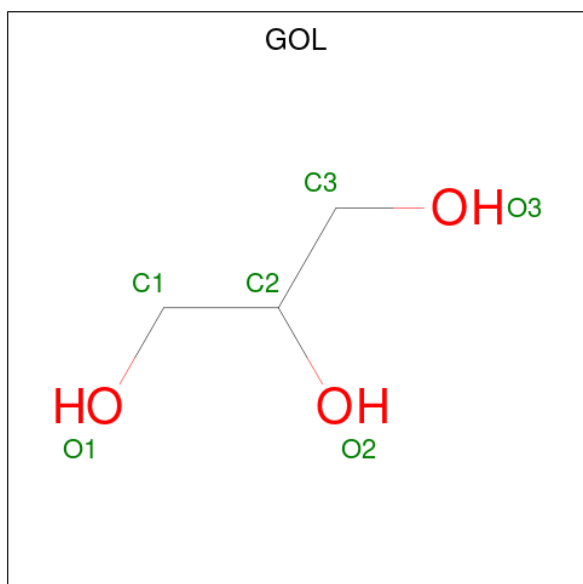
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		

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



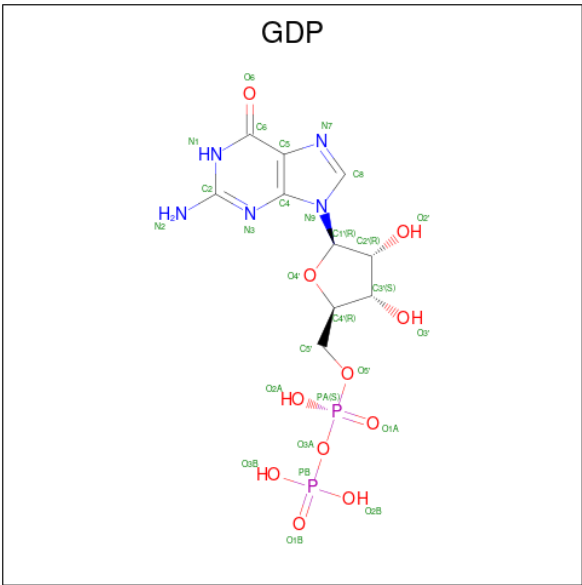
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		

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



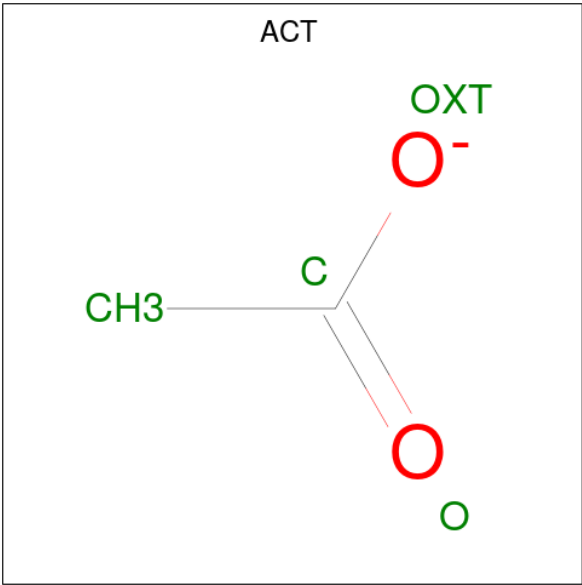
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

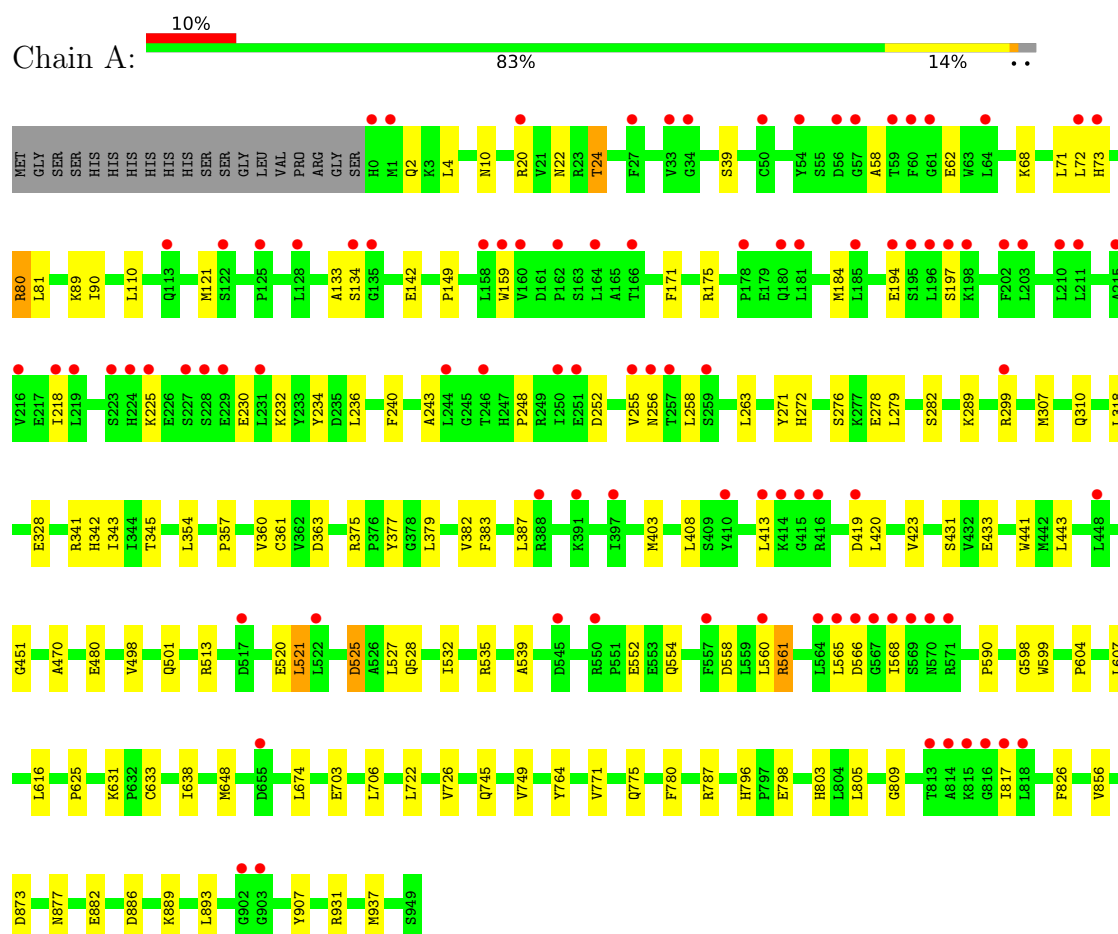
- Molecule 8 is water.

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

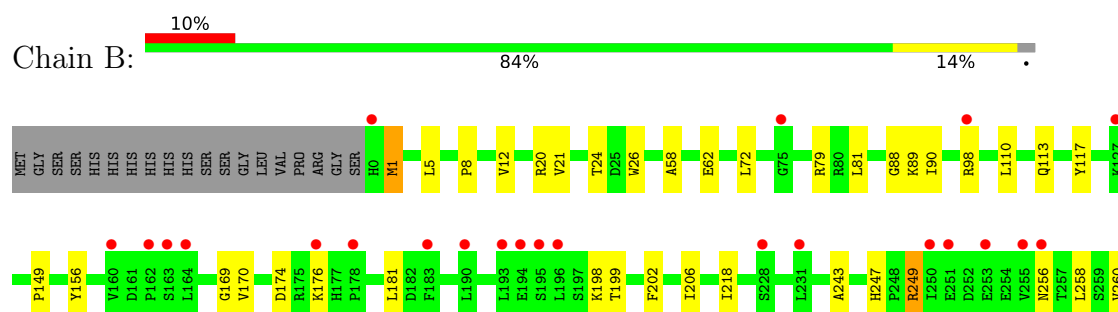
3 Residue-property plots

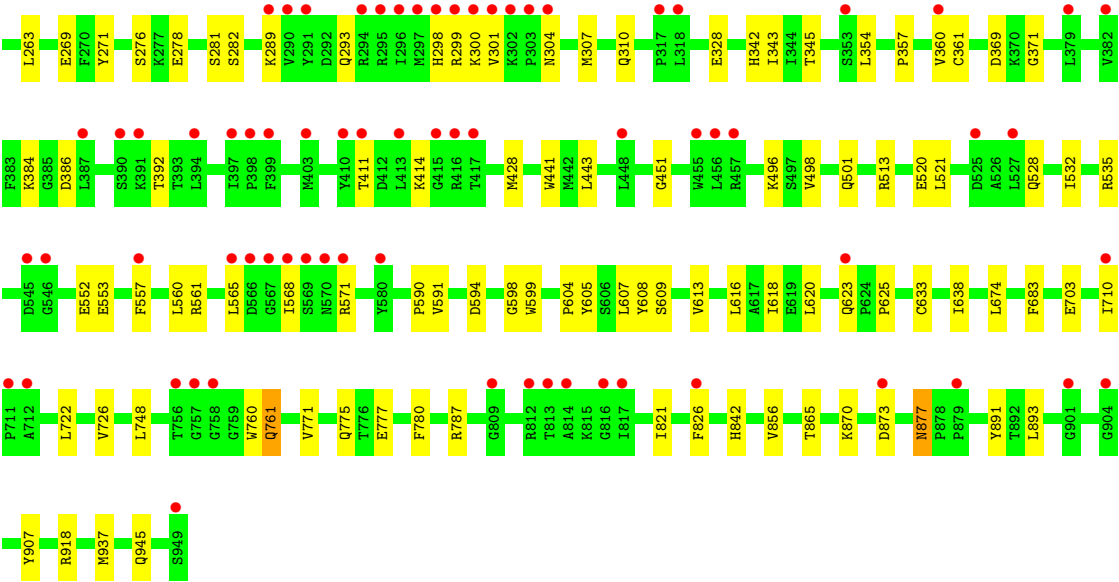
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	1989 reflections (1.79%)	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: GTP, FMT, MLA, GDP, GOL, 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	0.12	0/7632	0.32	0/10347
1	B	0.11	0/7632	0.31	0/10347
All	All	0.12	0/15264	0.31	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	90	0
1	B	7457	0	7433	81	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	2	0
6	B	28	0	12	0	0
7	B	8	0	6	0	0
8	A	471	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	372	0	0	3	0
All	All	15926	0	14956	168	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 (168) 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:307:MET:HE1	1:A:318:LEU:HB3	1.78	0.64
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:631:LYS:NZ	8:A:1105:HOH:O	2.30	0.62
1:A:907:TYR:CD1	1:A:937:MET:HE1	2.35	0.62
1:A:403:MET:HE3	1:A:413:LEU:HD11	1.82	0.62
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:68:LYS:HB3	1:A:121:MET:HE3	1.84	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:907:TYR:CD1	1:B:937:MET:HE1	2.37	0.59
1:B:98:ARG:HB2	1:B:298:HIS:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:907:TYR:HD1	1:A:937:MET:HE1	1.72	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:907:TYR:HD1	1:B:937:MET:HE1	1.74	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:371:GLY:HA3	1:B:428:MET:HE2	1.97	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:171:PHE:HE1	1:A:184:MET:HE2	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:GLY:O	1:A:931:ARG:NH1	2.36	0.43
1:A:345:THR:OG1	1:A:363:ASP:OD1	2.32	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
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:A:805:LEU:HB2	1:A:937:MET:HE2	2.02	0.42
1:B:278:GLU:HA	1:B:281:SER:HG	1.85	0.42
1:B:386:ASP:O	1:B:392:THR:OG1	2.33	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:B:21:VAL:HB	1:B:26:TRP:CD1	2.55	0.42
1:B:870:LYS:NZ	8:B:1115:HOH:O	2.50	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:1:MET:HB2	1:B:1:MET:HE2	1.68	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:803:HIS:C	1:A:937:MET:HE3	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLY:H	5:B:1005:GOL:HO3	1.63	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 [i](#)

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%)	795 (99%)	11 (1%)	59	76
1	B	806/822 (98%)	795 (99%)	11 (1%)	59	76
All	All	1612/1644 (98%)	1590 (99%)	22 (1%)	59	76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	24	THR
1	A	80	ARG
1	A	520	GLU
1	A	521	LEU
1	A	525	ASP
1	A	554	GLN
1	A	561	ARG
1	A	616	LEU
1	A	648	MET
1	A	771	VAL
1	B	1	MET
1	B	24	THR
1	B	249	ARG
1	B	369	ASP
1	B	520	GLU
1	B	571	ARG
1	B	609	SER
1	B	616	LEU
1	B	761	GLN
1	B	771	VAL
1	B	877	ASN

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	2	GLN
1	A	22	ASN
1	A	77	GLN
1	A	167	HIS
1	A	256	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	792	HIS
1	A	834	ASN
1	A	851	GLN
1	B	186	GLN
1	B	256	ASN
1	B	570	ASN
1	B	637	HIS
1	B	745	GLN
1	B	796	HIS
1	B	834	ASN
1	B	851	GLN
1	B	877	ASN

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](#)

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	$\# Z > 2$
3	FMT	A	1003	-	2,2,2	0.74	0	1,1,1	0.23	0
4	MLA	A	1005	-	6,6,6	1.31	0	7,7,7	1.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GTP	A	1002	-	33,34,34	0.97	1 (3%)	50,54,54	1.54	8 (16%)
5	GOL	B	1005	-	5,5,5	0.89	0	5,5,5	1.16	1 (20%)
5	GOL	B	1006	-	5,5,5	0.93	0	5,5,5	1.08	0
7	ACT	B	1003	-	3,3,3	1.40	1 (33%)	3,3,3	1.36	0
6	GDP	B	1002	-	29,30,30	1.17	4 (13%)	45,47,47	1.76	7 (15%)
3	FMT	A	1004	-	2,2,2	0.73	0	1,1,1	0.22	0
5	GOL	A	1006	-	5,5,5	0.90	0	5,5,5	1.10	0
2	GTP	B	1001	-	33,34,34	0.98	2 (6%)	50,54,54	1.62	9 (18%)
2	GTP	A	1001	-	33,34,34	0.88	1 (3%)	50,54,54	1.61	9 (18%)
5	GOL	A	1007	-	5,5,5	1.04	0	5,5,5	0.90	0
7	ACT	B	1004	-	3,3,3	1.36	0	3,3,3	1.38	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
4	MLA	A	1005	-	-	4/4/4/4	-
2	GTP	A	1002	-	-	2/22/38/38	0/3/3/3
5	GOL	B	1005	-	-	0/4/4/4	-
5	GOL	B	1006	-	-	0/4/4/4	-
6	GDP	B	1002	-	-	5/16/32/32	0/3/3/3
5	GOL	A	1006	-	-	4/4/4/4	-
2	GTP	B	1001	-	-	5/22/38/38	0/3/3/3
2	GTP	A	1001	-	-	5/22/38/38	0/3/3/3
5	GOL	A	1007	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1002	GDP	C5-C4	3.17	1.47	1.38
6	B	1002	GDP	C6-N1	-2.37	1.34	1.38
2	B	1001	GTP	C2-N3	2.23	1.38	1.33
2	A	1002	GTP	C2-N3	2.21	1.38	1.33
2	A	1001	GTP	C2-N3	2.21	1.38	1.33
2	B	1001	GTP	PA-O3A	2.05	1.61	1.59
7	B	1003	ACT	CH3-C	2.03	1.57	1.49
6	B	1002	GDP	C5-N7	-2.02	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1002	GDP	PA-O3A	2.01	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1002	GDP	C5-C4-N3	-6.08	118.72	128.39
2	B	1001	GTP	C5-C4-N3	-5.08	120.30	128.39
2	A	1002	GTP	C5-C4-N3	-5.07	120.32	128.39
2	A	1001	GTP	C5-C4-N3	-4.99	120.44	128.39
6	B	1002	GDP	C2-N3-C4	4.98	120.88	112.30
2	A	1001	GTP	C2-N3-C4	4.73	120.44	112.30
2	B	1001	GTP	C2-N3-C4	4.64	120.29	112.30
2	A	1002	GTP	C2-N3-C4	4.60	120.23	112.30
6	B	1002	GDP	N9-C4-N3	4.53	135.01	125.95
2	B	1001	GTP	N9-C4-N3	3.28	132.51	125.95
2	A	1002	GTP	N9-C4-N3	3.27	132.50	125.95
6	B	1002	GDP	C6-C5-N7	3.17	136.07	130.29
2	A	1001	GTP	N9-C4-N3	3.15	132.25	125.95
2	B	1001	GTP	C2-N1-C6	-2.89	119.88	125.11
2	A	1001	GTP	C2-N1-C6	-2.82	119.99	125.11
2	A	1002	GTP	C2-N1-C6	-2.82	119.99	125.11
2	A	1001	GTP	N9-C8-N7	-2.67	108.45	113.40
2	B	1001	GTP	N9-C8-N7	-2.63	108.52	113.40
2	A	1002	GTP	N9-C8-N7	-2.59	108.60	113.40
2	A	1001	GTP	C8-N7-C5	2.54	108.78	104.26
2	B	1001	GTP	C8-N7-C5	2.54	108.78	104.26
6	B	1002	GDP	C4-C5-N7	-2.53	106.66	110.67
2	A	1001	GTP	C5-C6-N1	2.53	119.68	113.25
2	A	1002	GTP	C8-N7-C5	2.50	108.72	104.26
2	B	1001	GTP	C5-C6-N1	2.49	119.58	113.25
2	B	1001	GTP	C3'-C2'-C1'	2.44	106.07	101.46
2	A	1002	GTP	C5-C6-N1	2.44	119.46	113.25
2	B	1001	GTP	O6-C6-C5	-2.41	120.17	126.53
2	A	1002	GTP	O6-C6-C5	-2.38	120.26	126.53
2	A	1001	GTP	O6-C6-C5	-2.37	120.29	126.53
6	B	1002	GDP	C3'-C2'-C1'	2.32	105.85	101.46
2	A	1001	GTP	C3'-C2'-C1'	2.29	105.80	101.46
6	B	1002	GDP	O6-C6-C5	-2.16	120.83	126.53
5	B	1005	GOL	C3-C2-C1	-2.12	104.01	111.80

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-O3A
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-O3A
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-O3A
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
6	B	1002	GDP	O4'-C4'-C5'-O5'
2	A	1002	GTP	PB-O3B-PG-O2G
6	B	1002	GDP	C3'-C4'-C5'-O5'
6	B	1002	GDP	C5'-O5'-PA-O1A
2	B	1001	GTP	C4'-C5'-O5'-PA
4	A	1005	MLA	C1-C2-C3-O3A
4	A	1005	MLA	C1-C2-C3-O3B
2	A	1001	GTP	C4'-C5'-O5'-PA
4	A	1005	MLA	O1B-C1-C2-C3
4	A	1005	MLA	O1A-C1-C2-C3
5	A	1006	GOL	O1-C1-C2-O2

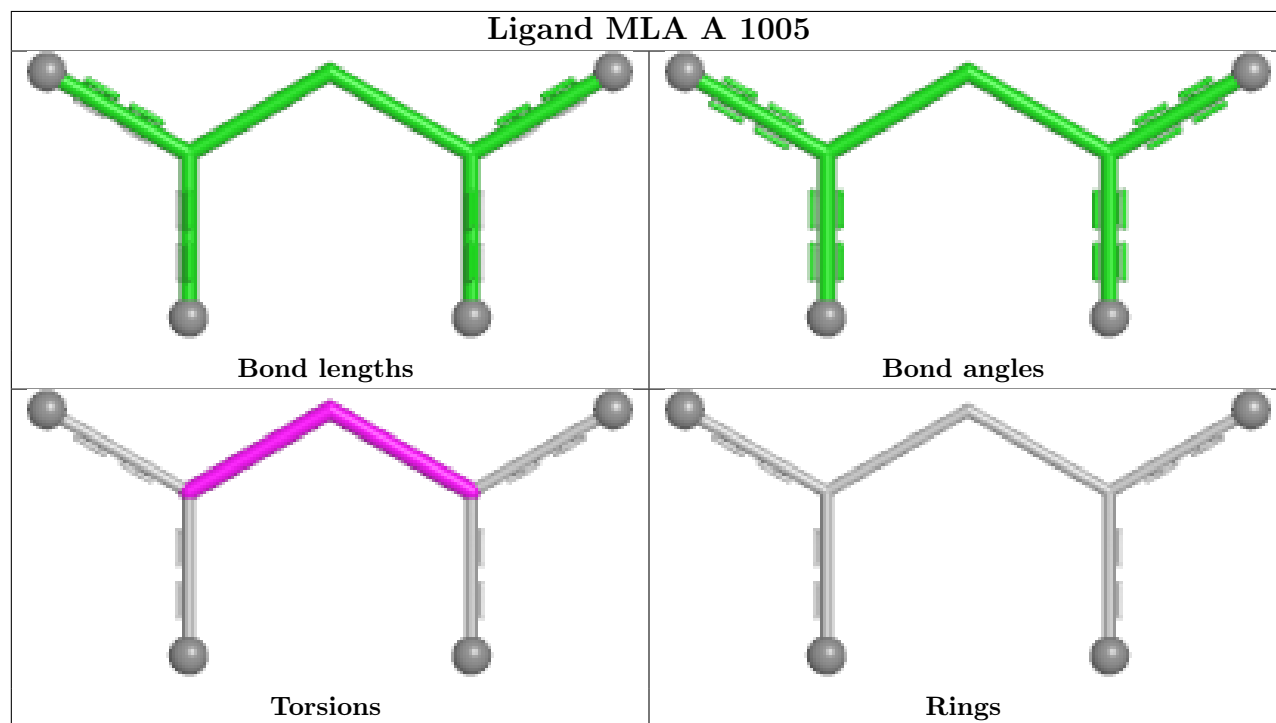
There are no ring outliers.

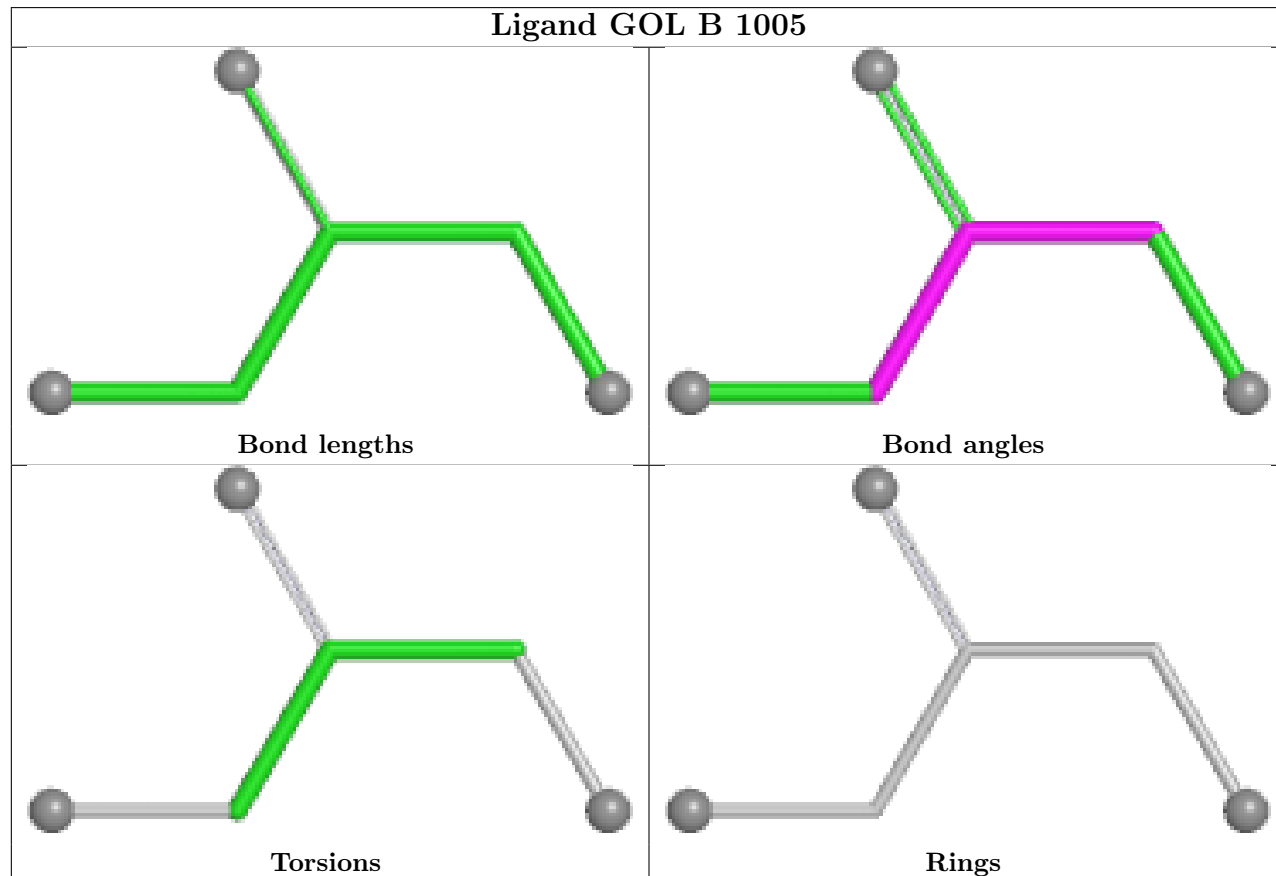
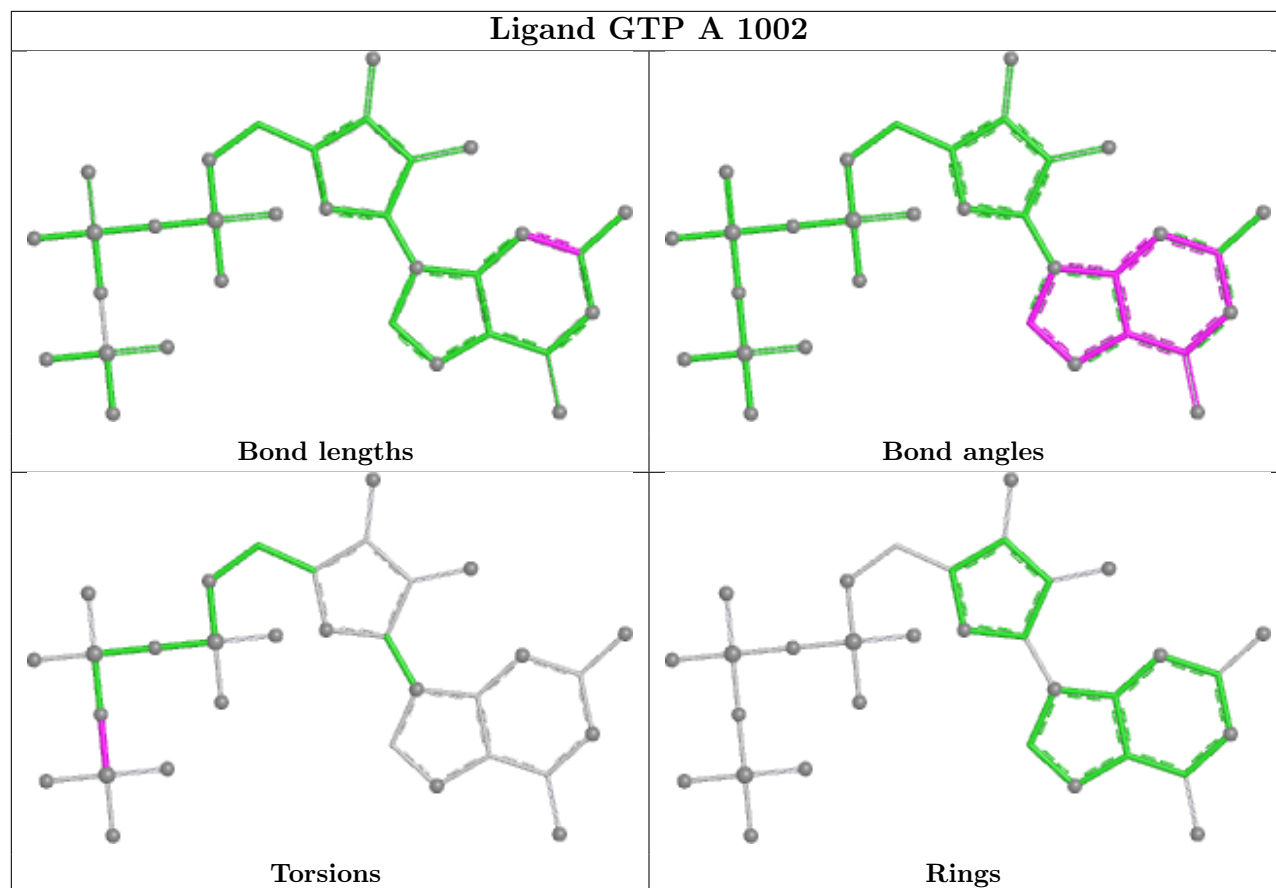
3 monomers are involved in 5 short contacts:

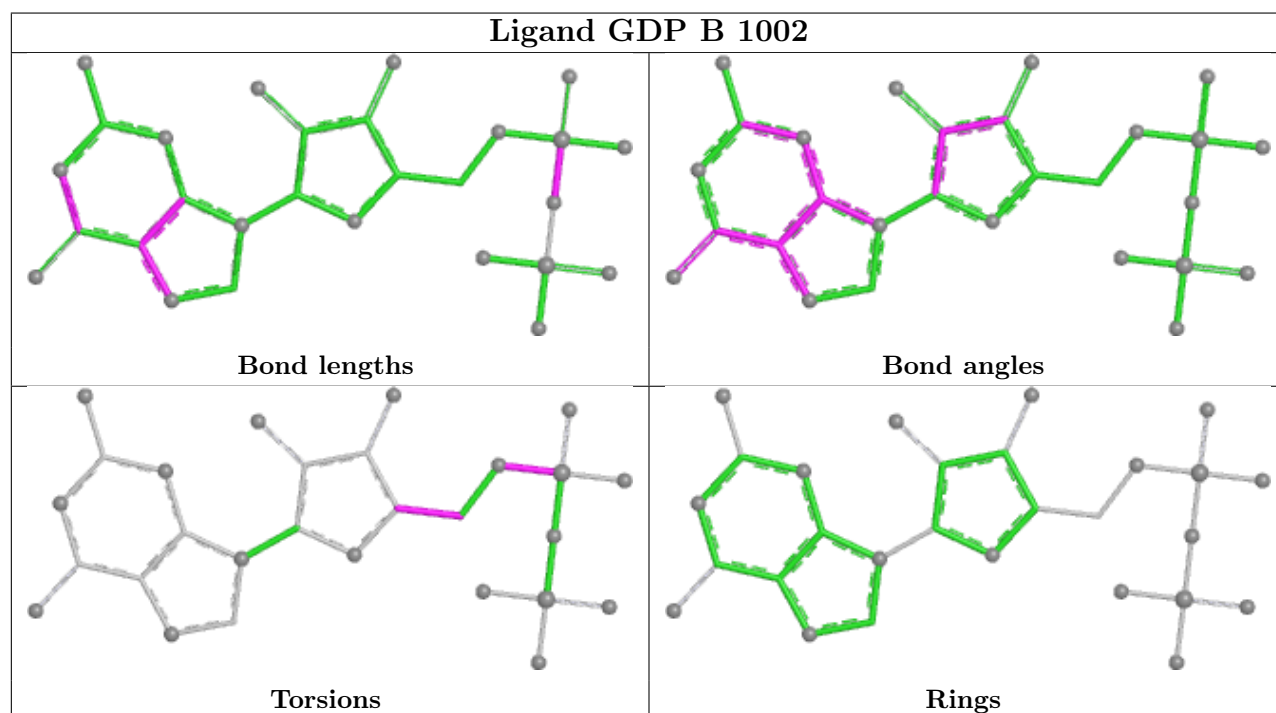
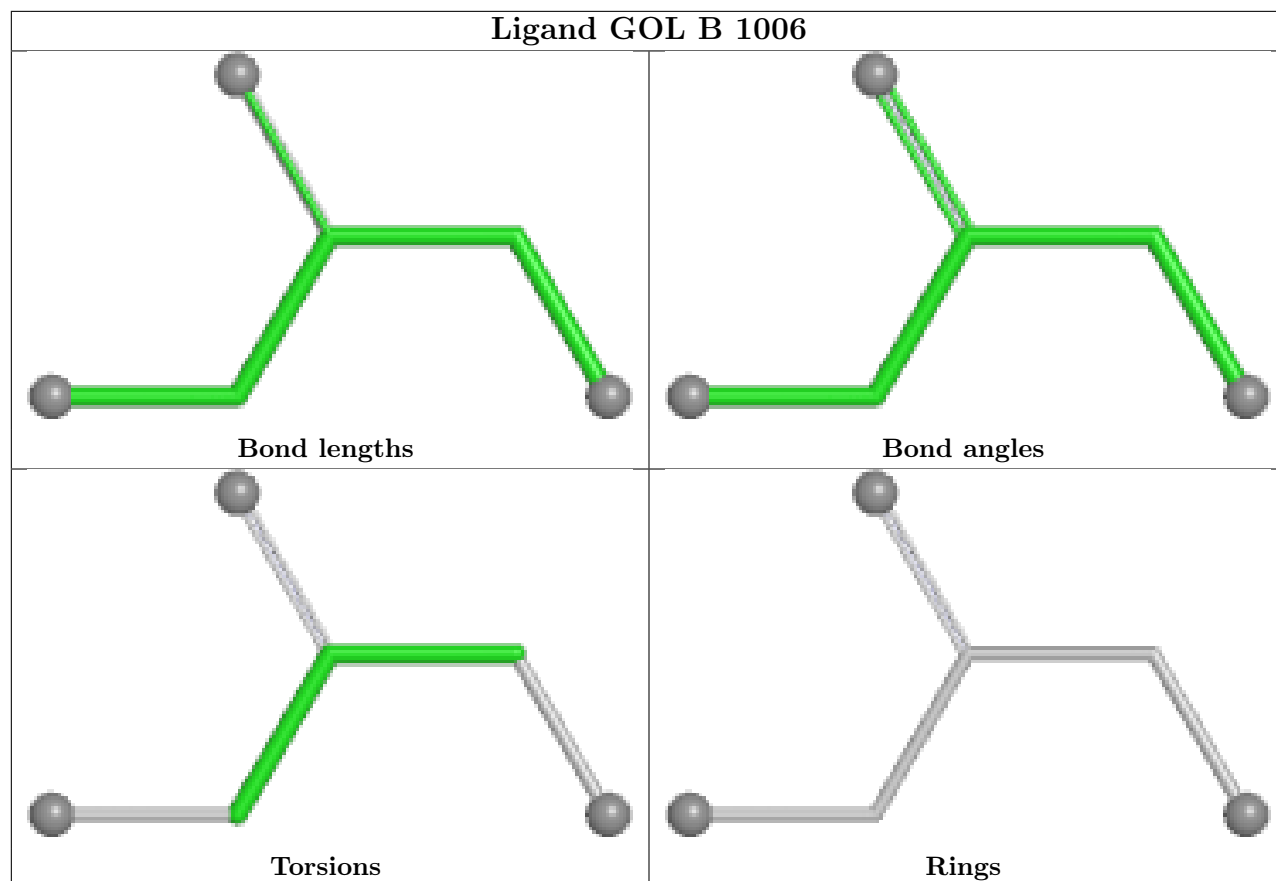
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1005	GOL	2	0
5	A	1006	GOL	1	0
2	A	1001	GTP	2	0

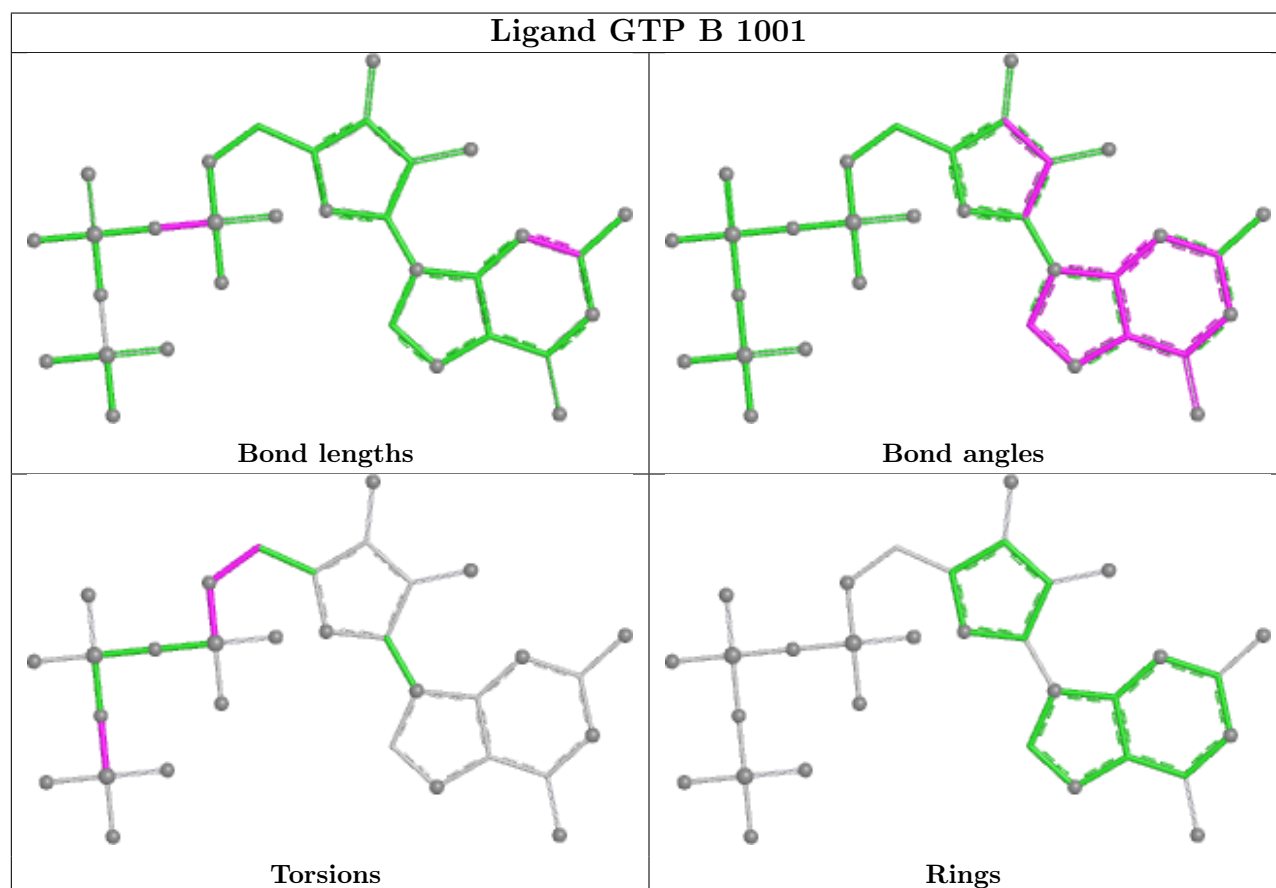
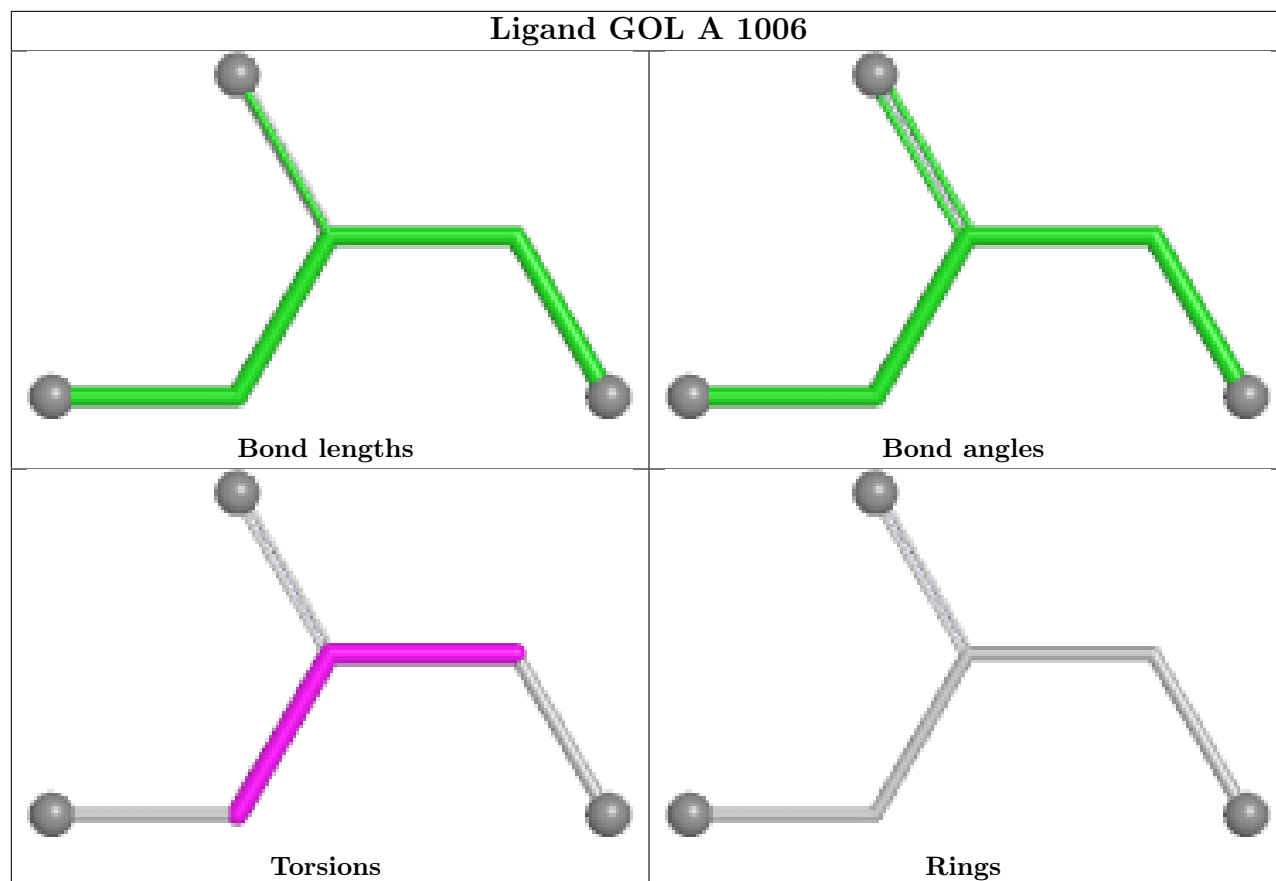
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

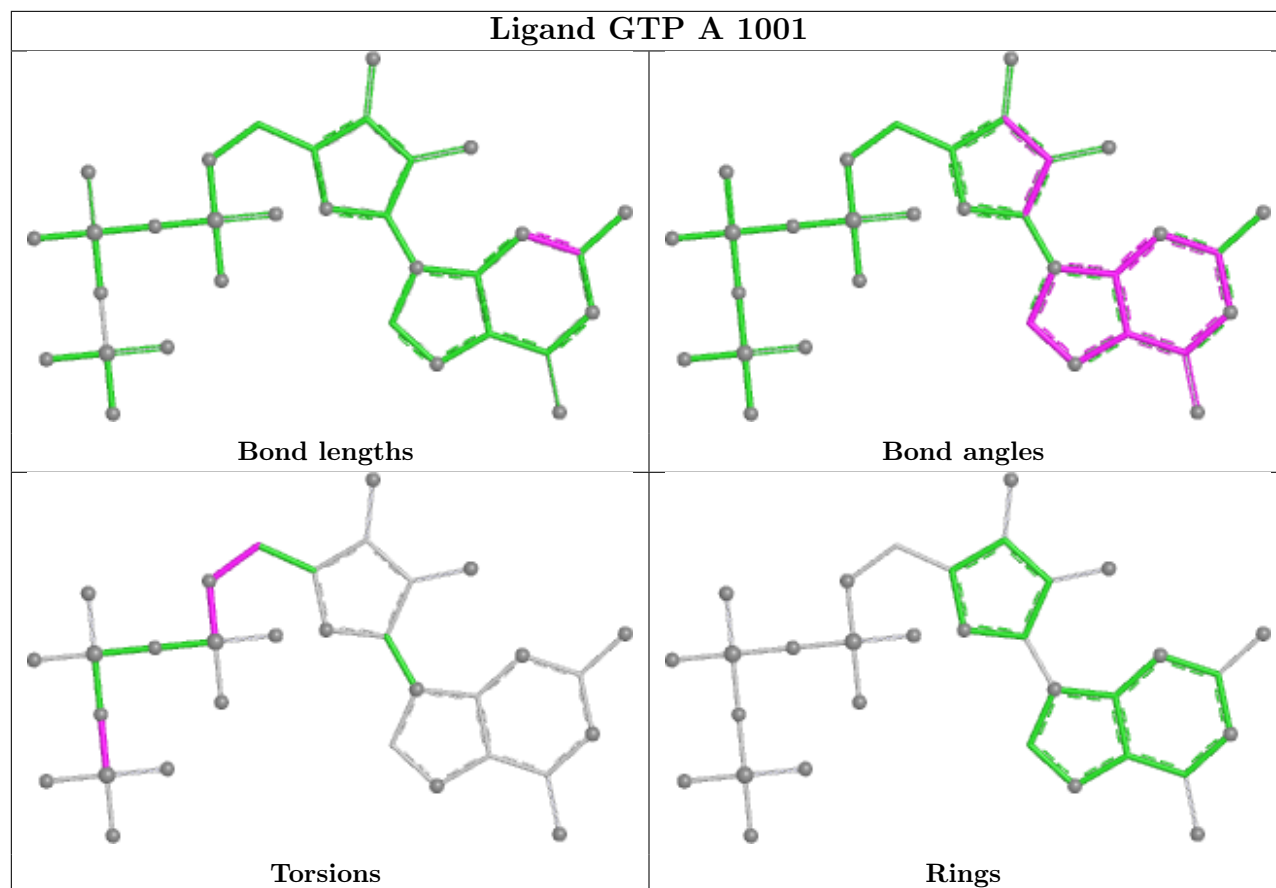




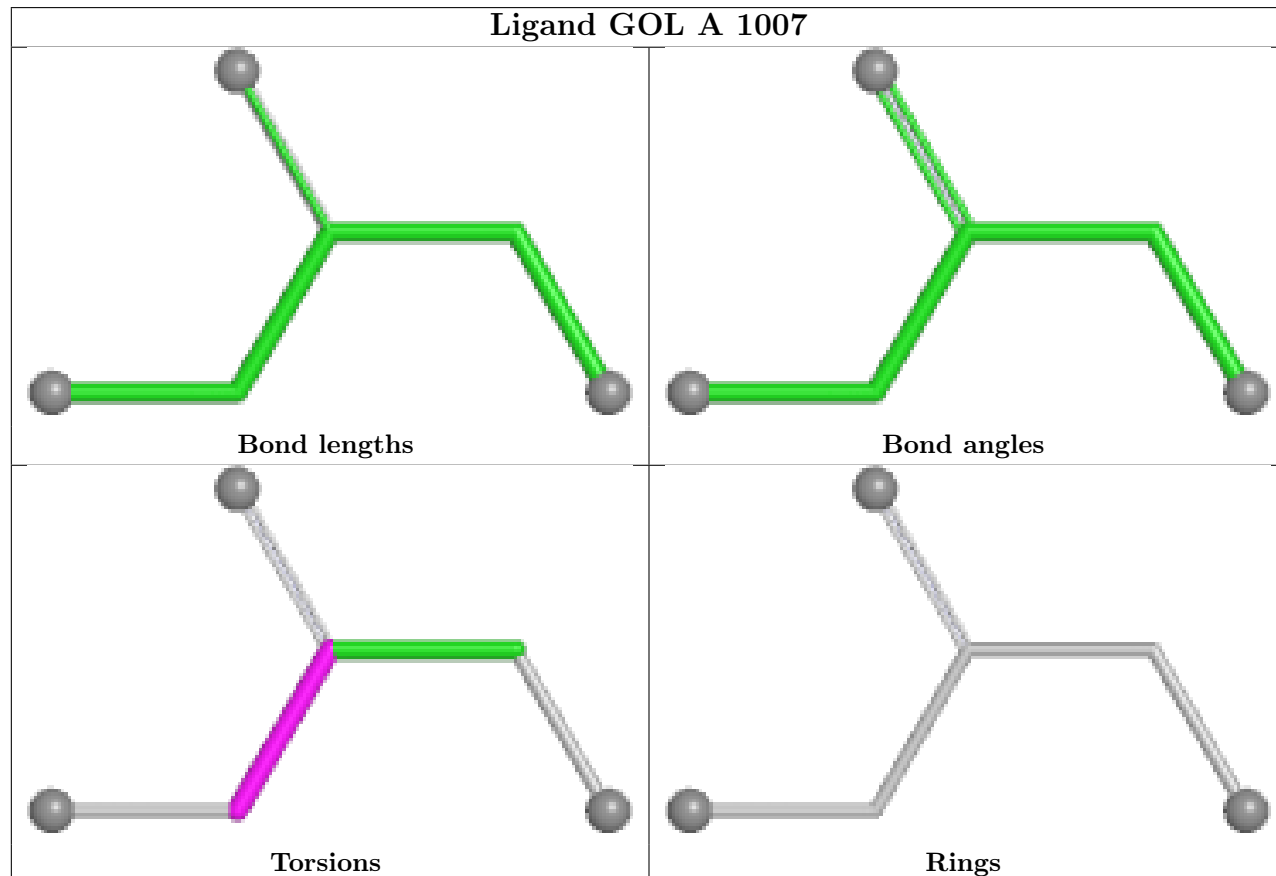




Ligand GTP A 1001



Ligand GOL A 1007



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.67	94 (9%)	13 14	25, 61, 129, 210	0
1	B	950/969 (98%)	0.70	93 (9%)	13 14	30, 61, 120, 206	0
All	All	1900/1938 (98%)	0.69	187 (9%)	13 14	25, 61, 125, 210	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	ILE	7.8
1	B	290	VAL	6.2
1	B	568	ILE	6.0
1	A	216	VAL	5.6
1	B	298	HIS	5.6
1	B	565	LEU	5.0
1	A	567	GLY	4.9
1	B	296	ILE	4.9
1	A	565	LEU	4.8
1	A	817	ILE	4.4
1	A	570	ASN	4.4
1	A	569	SER	4.4
1	B	569	SER	4.3
1	B	301	VAL	4.2
1	B	756	THR	4.2
1	B	757	GLY	4.1
1	B	710	ILE	4.1
1	A	814	ALA	4.0
1	A	160	VAL	3.9
1	B	567	GLY	3.8
1	B	712	ALA	3.7
1	A	135	GLY	3.7
1	B	814	ALA	3.7
1	B	397	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	448	LEU	3.5
1	B	194	GLU	3.5
1	B	228	SER	3.5
1	A	202	PHE	3.5
1	A	566	ASP	3.5
1	A	903	GLY	3.5
1	A	178	PRO	3.5
1	B	297	MET	3.4
1	A	816	GLY	3.4
1	A	218	ILE	3.4
1	B	291	TYR	3.3
1	A	57	GLY	3.2
1	A	255	VAL	3.2
1	B	196	LEU	3.2
1	A	1	MET	3.2
1	A	215	ALA	3.1
1	B	711	PRO	3.1
1	A	159	TRP	3.1
1	B	176	LYS	3.1
1	A	228	SER	3.1
1	A	219	LEU	3.1
1	A	164	LEU	2.9
1	B	758	GLY	2.9
1	A	60	PHE	2.9
1	A	20	ARG	2.9
1	A	50	CYS	2.9
1	B	417	THR	2.9
1	A	195	SER	2.8
1	A	54	TYR	2.8
1	A	180	GLN	2.8
1	B	300	LYS	2.8
1	B	302	LYS	2.8
1	A	571	ARG	2.8
1	B	410	TYR	2.8
1	B	98	ARG	2.8
1	A	517	ASP	2.8
1	A	251	GLU	2.8
1	B	299	ARG	2.8
1	A	73	HIS	2.7
1	A	397	ILE	2.7
1	A	227	SER	2.7
1	B	289	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	353	SER	2.7
1	A	197	SER	2.7
1	A	59	THR	2.6
1	B	163	SER	2.6
1	A	246	THR	2.6
1	B	415	GLY	2.6
1	B	901	GLY	2.6
1	B	812	ARG	2.6
1	B	525	ASP	2.6
1	B	873	ASP	2.6
1	A	162	PRO	2.6
1	B	398	PRO	2.6
1	A	198	LYS	2.5
1	A	194	GLU	2.5
1	A	550	ARG	2.5
1	A	256	ASN	2.5
1	B	566	ASP	2.5
1	A	902	GLY	2.5
1	B	162	PRO	2.5
1	B	813	THR	2.5
1	B	295	ARG	2.5
1	A	166	THR	2.5
1	A	33	VAL	2.5
1	B	457	ARG	2.5
1	B	571	ARG	2.5
1	A	185	LEU	2.5
1	A	56	ASP	2.5
1	A	419	ASP	2.4
1	B	545	ASP	2.4
1	B	570	ASN	2.4
1	A	231	LEU	2.4
1	A	522	LEU	2.4
1	B	394	LEU	2.4
1	B	178	PRO	2.4
1	A	257	THR	2.4
1	A	223	SER	2.4
1	B	387	LEU	2.4
1	B	411	THR	2.4
1	A	122	SER	2.4
1	B	817	ILE	2.4
1	A	244	LEU	2.4
1	A	813	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	255	VAL	2.3
1	B	826	PHE	2.3
1	A	560	LEU	2.3
1	B	231	LEU	2.3
1	B	949	SER	2.3
1	A	113	GLN	2.3
1	B	253	GLU	2.3
1	A	128	LEU	2.3
1	A	158	LEU	2.3
1	A	196	LEU	2.3
1	B	193	LEU	2.3
1	A	61	GLY	2.3
1	B	455	TRP	2.3
1	B	250	ILE	2.3
1	B	160	VAL	2.3
1	B	399	PHE	2.3
1	A	181	LEU	2.3
1	B	527	LEU	2.3
1	A	655	ASP	2.3
1	B	623	GLN	2.3
1	A	27	PHE	2.2
1	B	318	LEU	2.2
1	B	379	LEU	2.2
1	B	448	LEU	2.2
1	B	303	PRO	2.2
1	A	388	ARG	2.2
1	B	75	GLY	2.2
1	B	294	ARG	2.2
1	B	416	ARG	2.2
1	B	546	GLY	2.2
1	B	391	LYS	2.2
1	B	360	VAL	2.2
1	B	580	TYR	2.2
1	A	203	LEU	2.2
1	A	557	PHE	2.2
1	B	256	ASN	2.2
1	A	34	GLY	2.2
1	B	0	HIS	2.2
1	B	251	GLU	2.2
1	A	134	SER	2.2
1	A	259	SER	2.2
1	A	410	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	2.2
1	A	416	ARG	2.2
1	B	557	PHE	2.2
1	A	299	ARG	2.1
1	A	413	LEU	2.1
1	A	72	LEU	2.1
1	A	391	LYS	2.1
1	B	190	LEU	2.1
1	A	545	ASP	2.1
1	B	390	SER	2.1
1	A	210	LEU	2.1
1	A	211	LEU	2.1
1	A	564	LEU	2.1
1	A	818	LEU	2.1
1	B	413	LEU	2.1
1	B	456	LEU	2.1
1	B	816	GLY	2.1
1	B	904	GLY	2.1
1	A	225	LYS	2.1
1	A	414	LYS	2.1
1	A	229	GLU	2.1
1	A	0	HIS	2.1
1	A	224	HIS	2.1
1	A	250	ILE	2.1
1	A	415	GLY	2.1
1	B	183	PHE	2.1
1	B	809	GLY	2.1
1	B	127	LYS	2.0
1	B	195	SER	2.0
1	B	403	MET	2.0
1	B	164	LEU	2.0
1	B	304	ASN	2.0
1	A	125	PRO	2.0
1	B	879	PRO	2.0
1	B	382	VAL	2.0
1	A	815	LYS	2.0
1	B	317	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

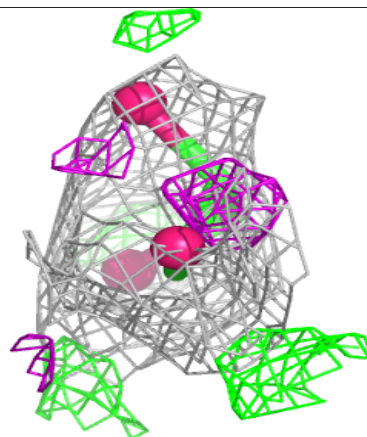
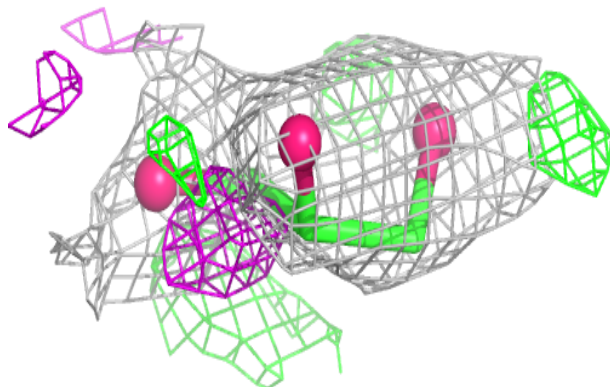
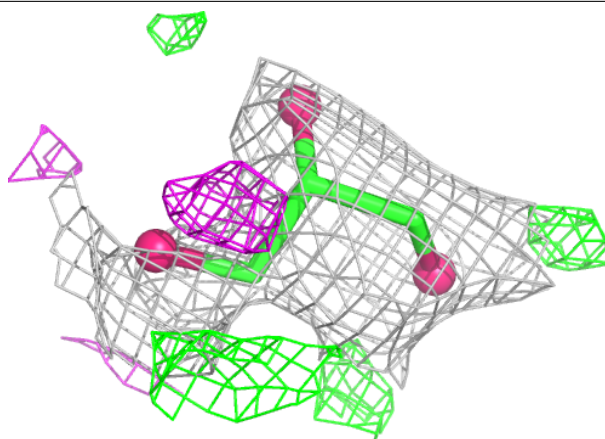
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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.

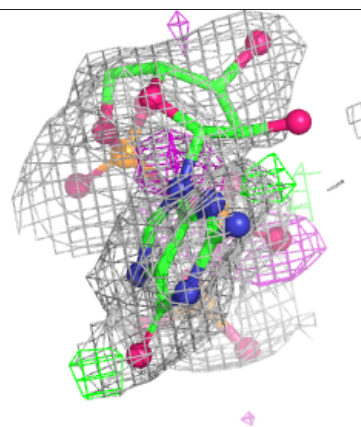
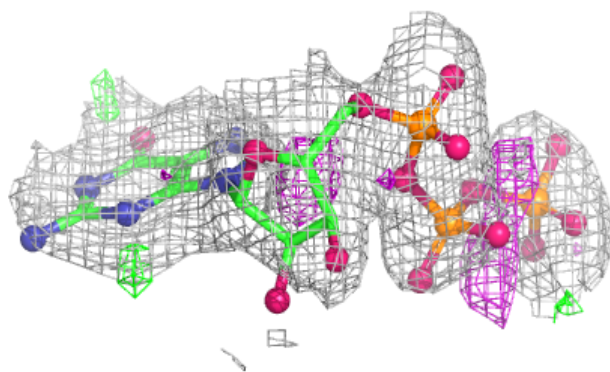
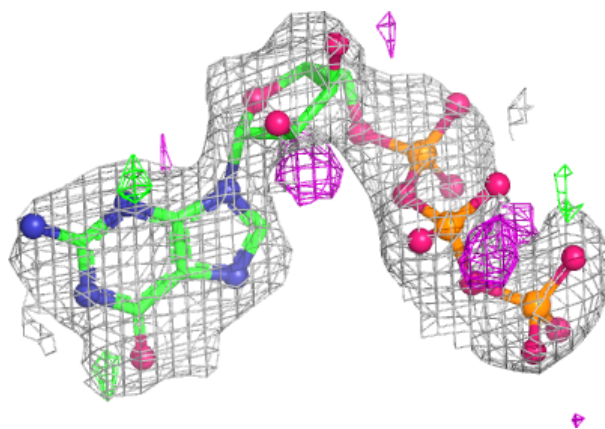
Electron density around GOL B 1005:

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



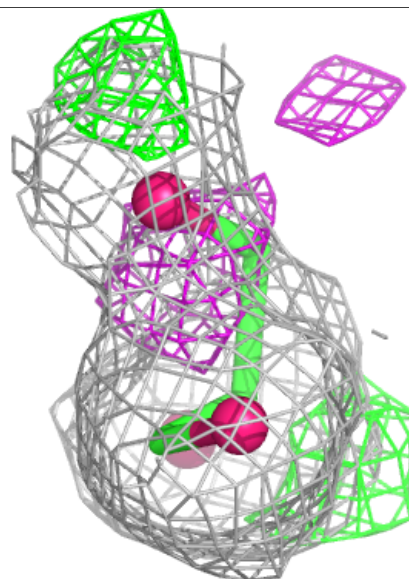
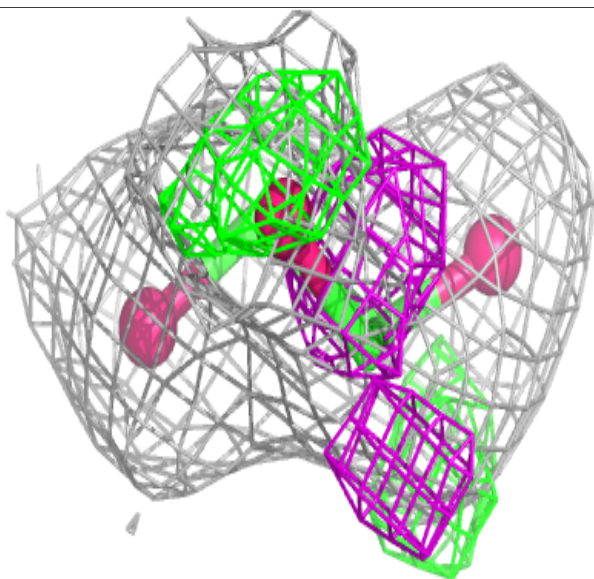
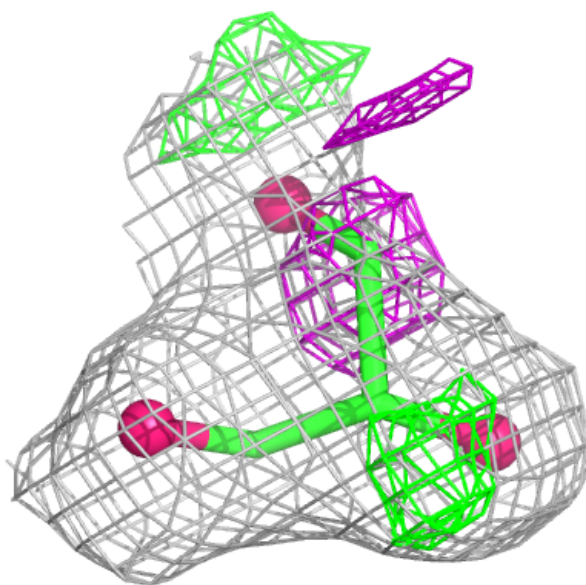
Electron density around GTP B 1001:

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



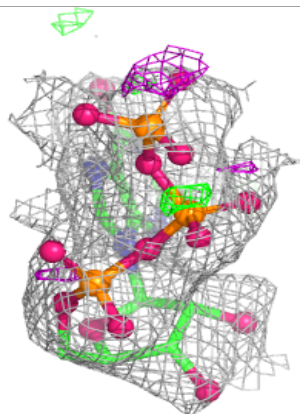
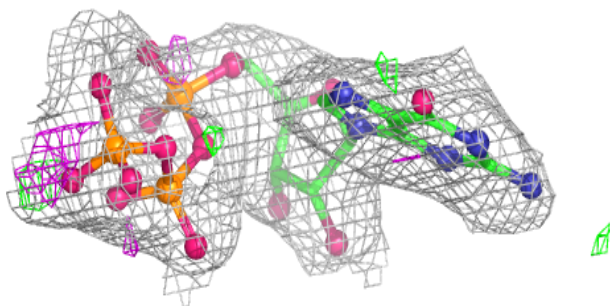
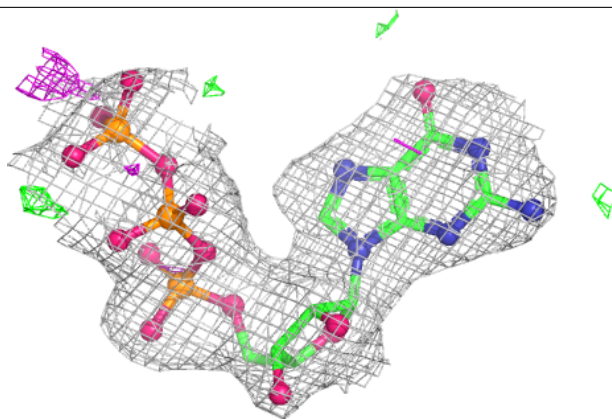
Electron density around GOL A 1007:

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

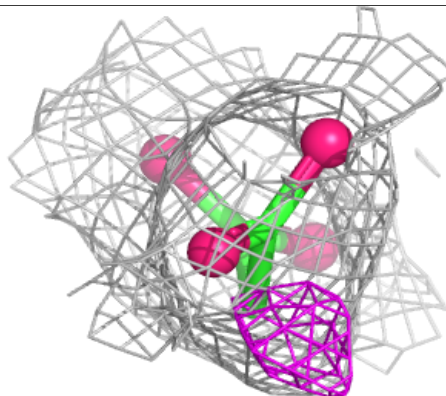
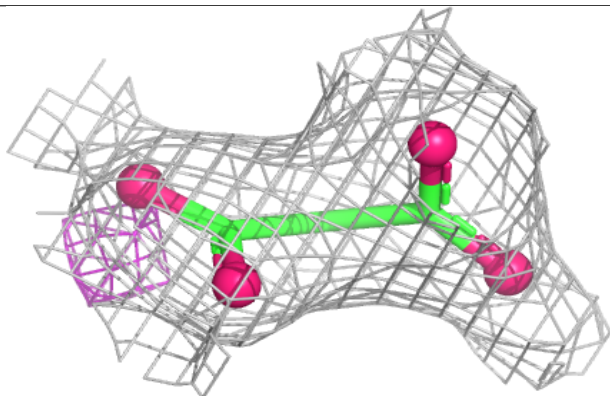
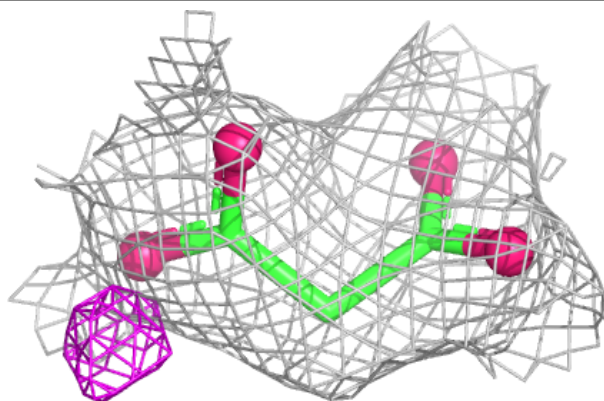


Electron density around GTP A 1001:

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

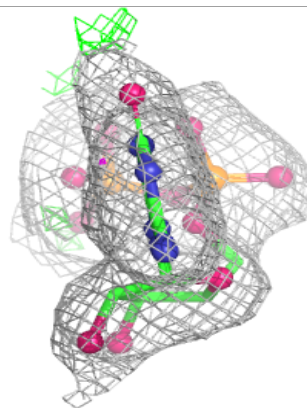
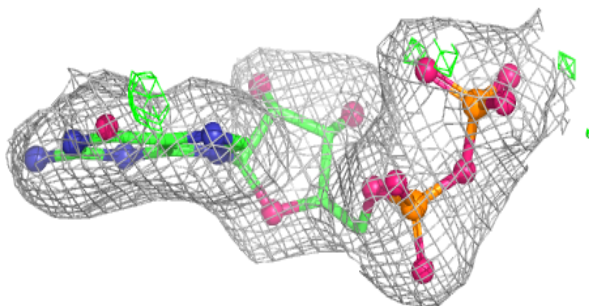
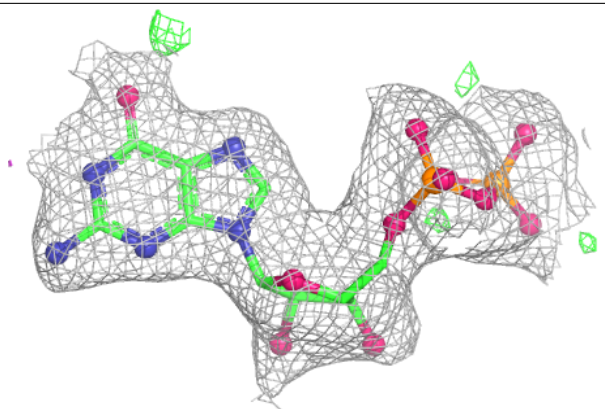
**Electron density around MLA A 1005:**

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



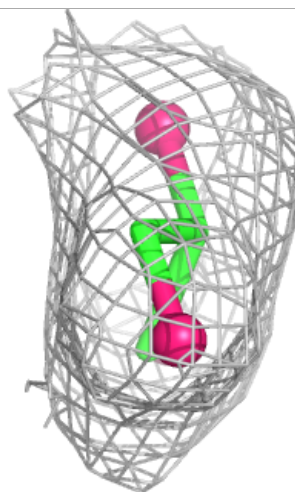
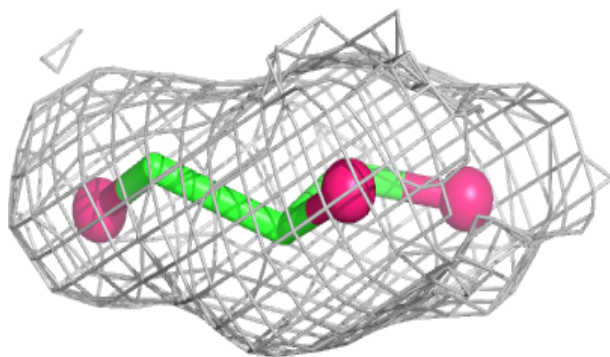
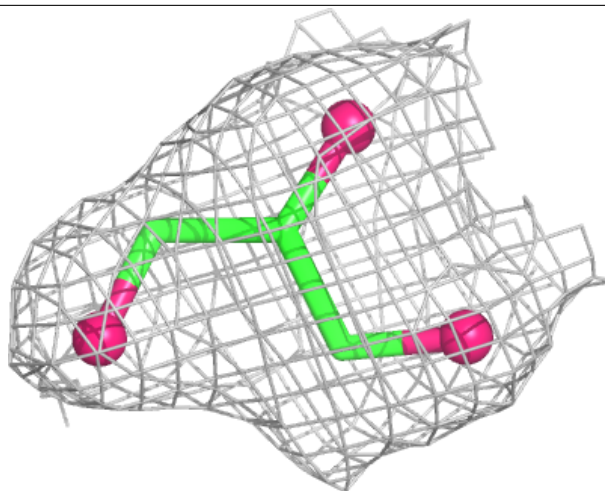
Electron density around GDP B 1002:

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



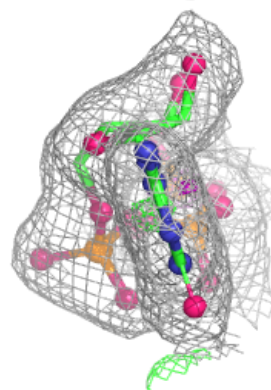
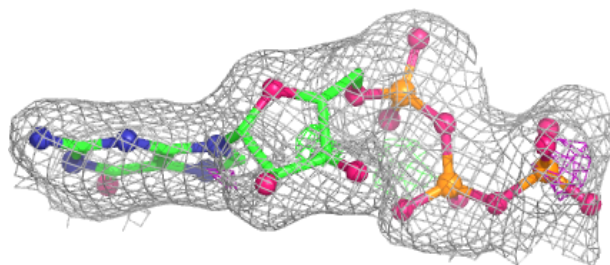
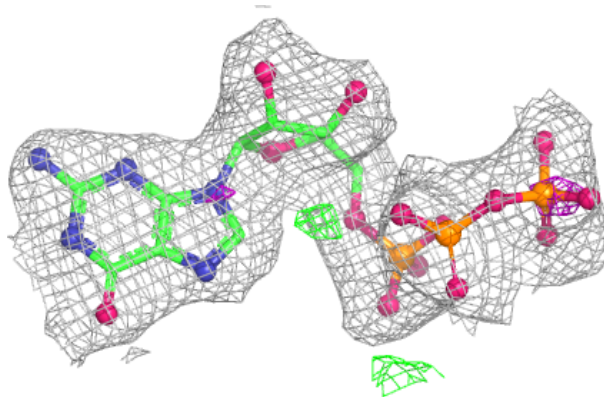
Electron density around GOL B 1006:

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



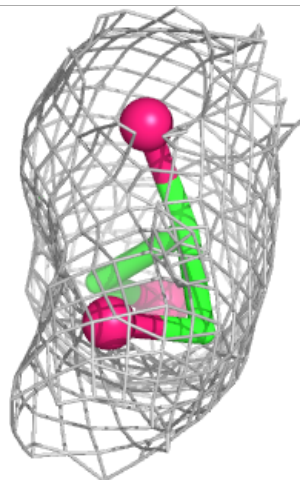
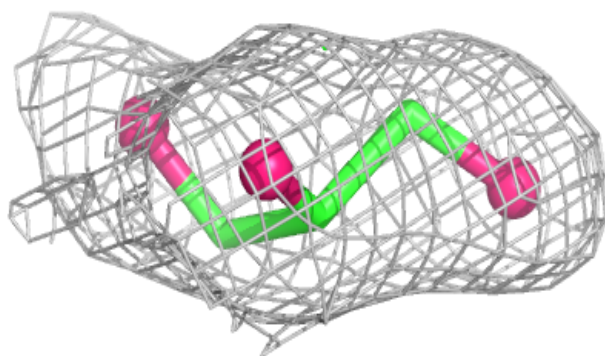
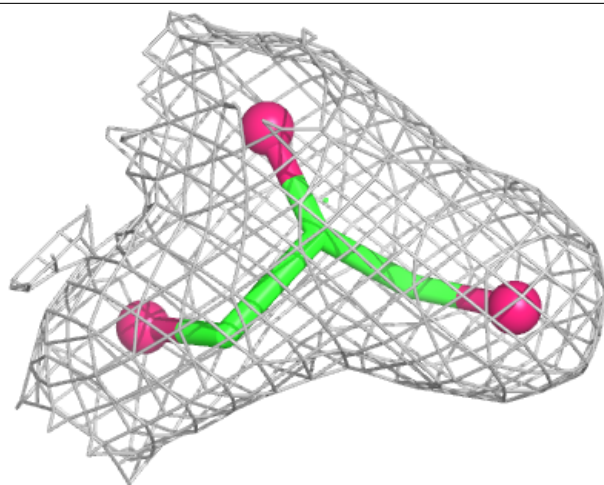
Electron density around GTP A 1002:

$2mF_o - DF_c$ (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.