



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:18 PM UTC

PDB ID : 9KFD / pdb_00009kfd
Title : Truncated Fzo1,GTP-bound
Authors : Yan, L.-M.; Gao, S.; Huang, S.-J.
Deposited on : 2024-11-06
Resolution : 2.73 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

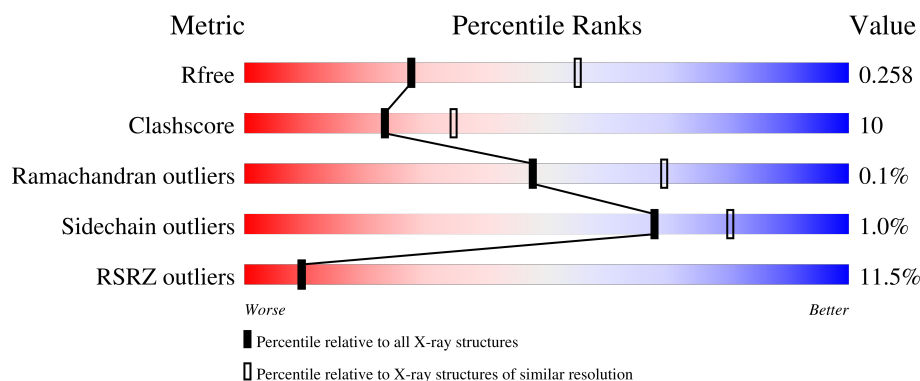
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	468	9% 66% 24% 9%
1	B	468	11% 68% 21% 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6851 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 Mitofusin FZO1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	Se	0	0	0
			3415	2167	580	656	3	9			
1	B	416	Total	C	N	O	S	Se	0	0	0
			3348	2121	570	645	3	9			

There are 32 discrepancies between the modelled and reference sequences:

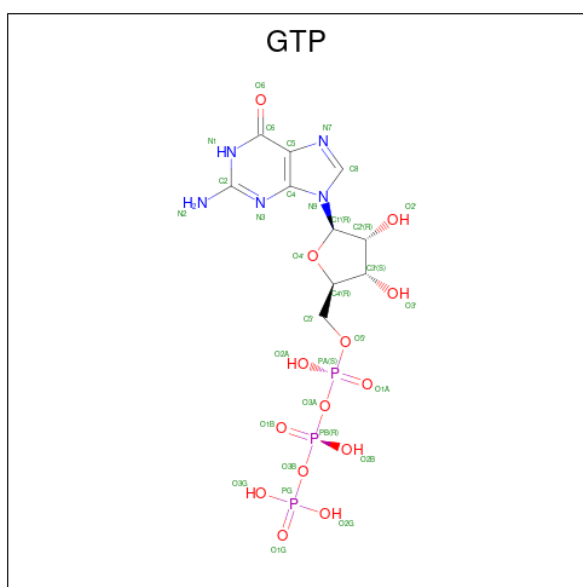
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLY	-	expression tag	UNP P38297
A	77	PRO	-	expression tag	UNP P38297
A	78	HIS	-	expression tag	UNP P38297
A	79	MSE	-	expression tag	UNP P38297
A	80	GLY	-	expression tag	UNP P38297
A	81	GLY	-	expression tag	UNP P38297
A	82	SER	-	expression tag	UNP P38297
A	806	GLY	-	linker	UNP P38297
A	807	SER	-	linker	UNP P38297
A	808	GLY	-	linker	UNP P38297
A	809	SER	-	linker	UNP P38297
A	810	GLY	-	linker	UNP P38297
A	811	SER	-	linker	UNP P38297
A	812	GLY	-	linker	UNP P38297
A	813	GLY	-	linker	UNP P38297
A	814	SER	-	linker	UNP P38297
B	76	GLY	-	expression tag	UNP P38297
B	77	PRO	-	expression tag	UNP P38297
B	78	HIS	-	expression tag	UNP P38297
B	79	MSE	-	expression tag	UNP P38297
B	80	GLY	-	expression tag	UNP P38297
B	81	GLY	-	expression tag	UNP P38297
B	82	SER	-	expression tag	UNP P38297
B	806	GLY	-	linker	UNP P38297
B	807	SER	-	linker	UNP P38297

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	808	GLY	-	linker	UNP P38297
B	809	SER	-	linker	UNP P38297
B	810	GLY	-	linker	UNP P38297
B	811	SER	-	linker	UNP P38297
B	812	GLY	-	linker	UNP P38297
B	813	GLY	-	linker	UNP P38297
B	814	SER	-	linker	UNP P38297

- 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	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	B	1	Total 1	Na 1	0	0

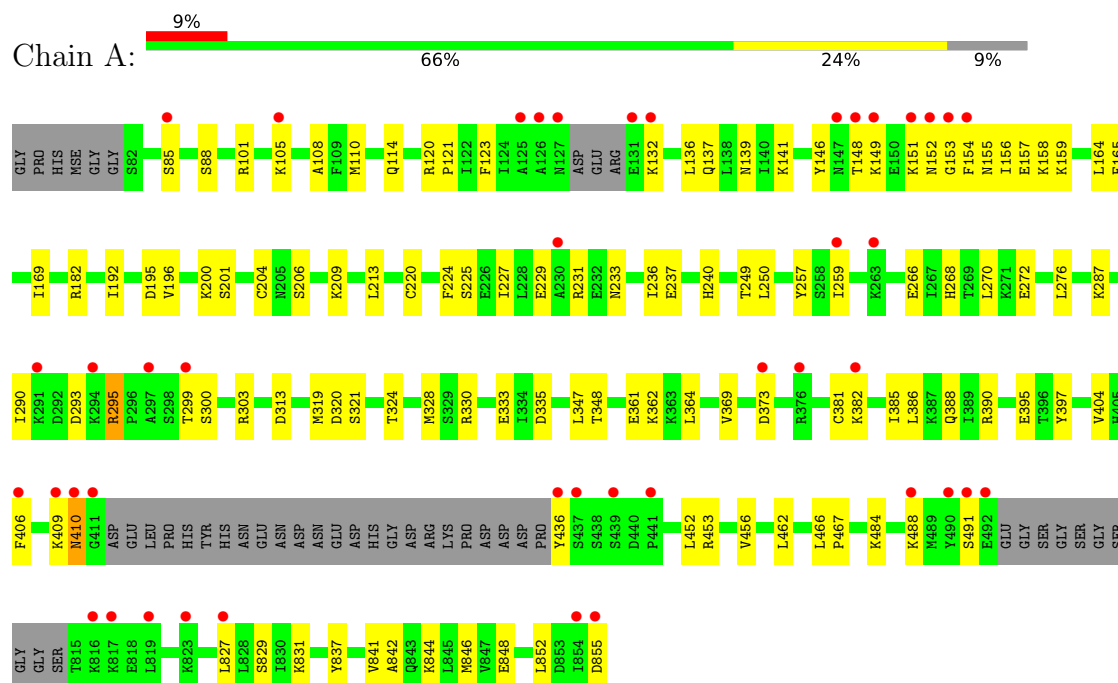
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total 12	O 12	0	0
5	B	8	Total 8	O 8	0	0

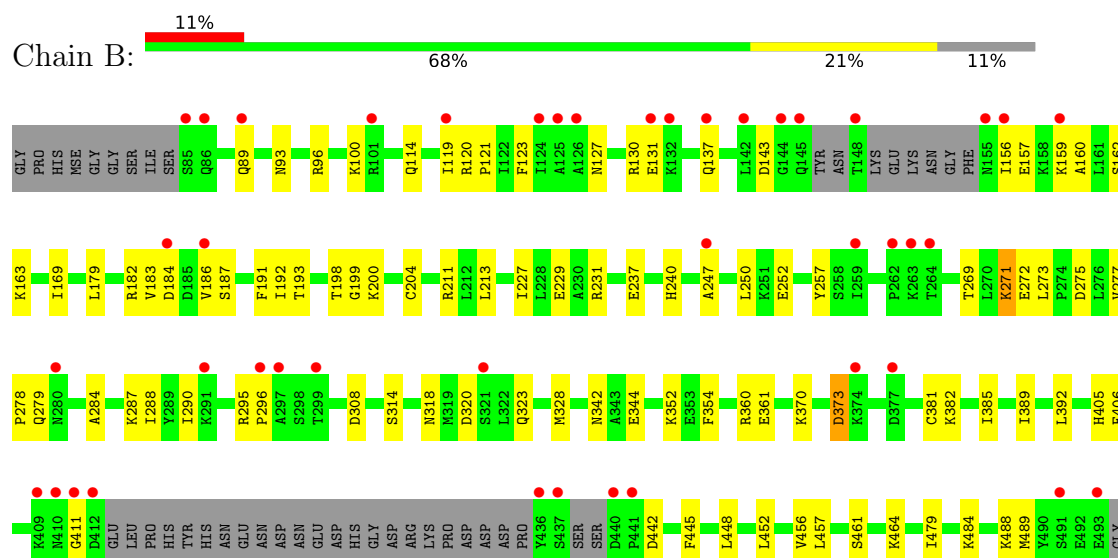
3 Residue-property plots [i](#)

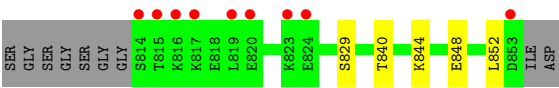
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Mitofusin FZO1



• Molecule 1: Mitofusin FZO1





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	174.40Å 174.40Å 127.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.46 – 2.73 66.46 – 2.73	Depositor EDS
% Data completeness (in resolution range)	97.8 (66.46-2.73) 97.8 (66.46-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.19-4092	Depositor
R, R_{free}	0.233 , 0.263 0.238 , 0.258	Depositor DCC
R_{free} test set	2475 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6851	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, NA, GTP

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	0.14	0/3452	0.31	0/4627
1	B	0.13	0/3381	0.32	0/4529
All	All	0.14	0/6833	0.31	0/9156

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

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	3415	0	3519	84	0
1	B	3348	0	3444	66	0
2	A	32	0	12	5	0
2	B	32	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	0	0	0
5	B	8	0	0	0	0
All	All	6851	0	6987	142	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 (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ALA:HB1	1:B:252:GLU:HG3	1.62	0.79
1:B:456:VAL:HG23	1:B:457:LEU:HD22	1.68	0.74
1:A:237:GLU:HG2	1:A:290:ILE:HA	1.70	0.73
1:B:240:HIS:HB2	1:B:287:LYS:HB2	1.72	0.72
1:A:196:VAL:HG11	1:A:319:MSE:HE3	1.74	0.69
1:A:330:ARG:NH2	1:A:333:GLU:OE2	2.23	0.69
1:B:137:GLN:HE21	1:B:360:ARG:HH21	1.41	0.69
1:B:123:PHE:HD2	1:B:489:MSE:HE3	1.57	0.69
1:A:139:ASN:HB3	1:B:143:ASP:HB3	1.75	0.68
1:B:123:PHE:CD2	1:B:489:MSE:HE3	2.28	0.68
1:B:89:GLN:O	1:B:93:ASN:ND2	2.28	0.67
1:A:213:LEU:HD11	1:A:227:ILE:HD11	1.78	0.66
1:A:101:ARG:HG2	1:A:101:ARG:HH11	1.61	0.66
1:A:206:SER:O	1:A:209:LYS:HD3	1.97	0.65
1:B:213:LEU:HD11	1:B:227:ILE:HD11	1.79	0.64
1:A:240:HIS:HB2	1:A:287:LYS:HB2	1.79	0.64
1:A:110:MSE:HE1	1:A:136:LEU:HD11	1.81	0.63
1:A:200:LYS:HG2	2:A:901:GTP:O1B	1.99	0.63
1:A:409:LYS:HD3	1:A:436:TYR:HE1	1.65	0.62
1:A:200:LYS:NZ	2:A:901:GTP:O1B	2.32	0.61
1:B:373:ASP:OD1	1:B:373:ASP:N	2.24	0.61
1:A:120:ARG:HE	1:A:829:SER:HB3	1.65	0.61
1:B:114:GLN:HB2	1:B:169:ILE:HG21	1.82	0.60
1:A:155:ASN:O	1:B:163:LYS:NZ	2.27	0.59
1:A:295:ARG:HD2	1:A:299:THR:HG23	1.84	0.59
1:A:348:THR:HB	1:B:318:ASN:OD1	2.02	0.59
1:A:373:ASP:N	1:A:373:ASP:OD1	2.34	0.59
1:A:330:ARG:HG2	1:A:330:ARG:HH11	1.69	0.57
1:B:271:LYS:O	1:B:271:LYS:NZ	2.36	0.57
1:A:259:ILE:H	1:A:259:ILE:HD12	1.68	0.57
1:A:837:TYR:O	1:A:841:VAL:HG23	2.04	0.56
1:A:844:LYS:O	1:A:848:GLU:HG3	2.06	0.56
1:B:479:ILE:HG21	1:B:840:THR:HG21	1.88	0.55
1:B:120:ARG:HD2	1:B:829:SER:HB3	1.88	0.54
1:B:844:LYS:O	1:B:848:GLU:HG2	2.08	0.54
1:A:114:GLN:HB2	1:A:169:ILE:HG21	1.90	0.53
1:A:410:ASN:HB3	2:A:901:GTP:C5	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:CE1	1:A:158:LYS:HD2	2.44	0.53
1:A:452:LEU:O	1:A:456:VAL:HG23	2.08	0.53
1:A:182:ARG:NH2	1:A:361:GLU:OE2	2.42	0.52
1:A:488:LYS:O	1:A:491:SER:OG	2.27	0.52
1:A:361:GLU:HG3	1:A:362:LYS:HG3	1.91	0.52
1:A:225:SER:HB2	1:A:313:ASP:HB3	1.92	0.52
1:B:257:TYR:CD2	1:B:287:LYS:HE3	2.45	0.51
1:B:198:THR:HG22	1:B:342:ASN:HB2	1.93	0.51
1:A:300:SER:O	1:A:453:ARG:NH1	2.43	0.51
1:B:231:ARG:NH2	1:B:308:ASP:OD1	2.44	0.51
1:A:224:PHE:CZ	1:A:330:ARG:HG3	2.46	0.50
1:A:324:THR:O	1:A:328:MSE:HG2	2.11	0.50
1:B:182:ARG:HH22	1:B:361:GLU:CD	2.19	0.50
1:A:229:GLU:OE2	1:A:303:ARG:HG3	2.11	0.50
1:A:330:ARG:HG2	1:A:330:ARG:NH1	2.27	0.50
1:A:381:CYS:O	1:A:385:ILE:HG12	2.12	0.50
1:B:123:PHE:CD2	1:B:489:MSE:HB3	2.46	0.50
1:B:352:LYS:HG2	1:B:392:LEU:HD11	1.94	0.49
1:A:105:LYS:HE2	1:A:105:LYS:HA	1.94	0.49
1:A:224:PHE:CE1	1:A:330:ARG:HG3	2.47	0.49
1:B:273:LEU:HD11	1:B:288:ILE:HD13	1.94	0.49
1:B:127:ASN:OD1	1:B:127:ASN:N	2.44	0.49
1:A:364:LEU:HD21	1:A:395:GLU:HG3	1.94	0.49
1:B:405:HIS:CG	1:B:448:LEU:HD23	2.47	0.49
1:B:229:GLU:HG3	1:B:231:ARG:HG2	1.94	0.48
1:B:385:ILE:O	1:B:389:ILE:HG12	2.13	0.48
1:A:110:MSE:HE3	1:A:169:ILE:HD13	1.94	0.48
1:B:192:ILE:HD13	1:B:204:CYS:SG	2.53	0.48
1:A:156:ILE:HD12	1:A:156:ILE:H	1.77	0.48
1:B:123:PHE:CE2	1:B:489:MSE:HB3	2.49	0.47
1:B:157:GLU:HA	1:B:157:GLU:OE1	2.14	0.47
1:A:157:GLU:H	1:B:159:LYS:NZ	2.12	0.47
1:A:233:ASN:O	1:A:236:ILE:HD12	2.15	0.47
1:A:466:LEU:HA	1:A:852:LEU:HD13	1.96	0.47
1:B:211:ARG:NH2	1:B:411:GLY:O	2.48	0.47
1:A:409:LYS:HD3	1:A:436:TYR:CE1	2.49	0.47
1:A:132:LYS:HA	1:A:132:LYS:HD2	1.61	0.46
1:A:320:ASP:OD1	1:A:321:SER:N	2.48	0.46
1:B:199:GLY:HA3	1:B:370:LYS:HD3	1.97	0.46
1:A:390:ARG:HG3	1:A:397:TYR:CD2	2.51	0.46
1:A:270:LEU:HD21	1:A:290:ILE:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:HE2	1:B:184:ASP:OD1	2.15	0.46
1:B:191:PHE:CE1	1:B:314:SER:HB2	2.51	0.46
1:B:461:SER:HB2	1:B:852:LEU:HD12	1.98	0.46
1:A:182:ARG:HD2	1:A:335:ASP:OD1	2.16	0.46
1:A:462:LEU:HD22	1:A:466:LEU:HD22	1.97	0.46
1:A:484:LYS:O	1:A:488:LYS:HG3	2.16	0.46
1:A:220:CYS:N	2:A:901:GTP:O3G	2.37	0.46
1:A:268:HIS:CD2	1:A:276:LEU:HD21	2.51	0.45
1:A:827:LEU:O	1:A:831:LYS:HG2	2.16	0.45
1:A:141:LYS:HD3	1:B:143:ASP:HB2	1.99	0.45
1:A:347:LEU:HB2	1:A:388:GLN:OE1	2.16	0.45
1:B:269:THR:N	1:B:272:GLU:OE2	2.42	0.45
1:A:195:ASP:OD2	1:A:348:THR:OG1	2.23	0.45
1:B:295:ARG:HG3	1:B:296:PRO:HD2	1.99	0.45
1:B:381:CYS:O	1:B:385:ILE:HG13	2.17	0.44
1:A:132:LYS:HE3	1:A:137:GLN:HB3	2.00	0.44
1:A:151:LYS:O	1:A:151:LYS:NZ	2.48	0.44
1:B:200:LYS:HB2	1:B:200:LYS:HE2	1.81	0.44
1:A:361:GLU:O	1:A:467:PRO:HA	2.17	0.44
1:B:452:LEU:O	1:B:456:VAL:HG22	2.16	0.44
1:A:146:TYR:CD1	1:B:328:MSE:HG3	2.53	0.44
1:A:293:ASP:OD1	1:A:303:ARG:NH1	2.36	0.43
1:B:382:LYS:HG3	1:B:406:PHE:CZ	2.53	0.43
1:A:410:ASN:HB3	2:A:901:GTP:C6	2.52	0.43
1:B:187:SER:O	1:B:464:LYS:NZ	2.42	0.43
1:A:105:LYS:HE2	1:A:108:ALA:HB3	1.99	0.43
1:B:179:LEU:O	1:B:183:VAL:HG23	2.18	0.43
1:B:182:ARG:NH2	1:B:361:GLU:OE2	2.44	0.43
1:A:101:ARG:HG2	1:A:101:ARG:NH1	2.33	0.43
1:A:165:PHE:CE2	1:A:169:ILE:HD11	2.54	0.43
1:A:249:THR:OG1	1:A:250:LEU:N	2.51	0.43
1:B:130:ARG:O	1:B:131:GLU:HG2	2.20	0.42
1:B:159:LYS:HE3	1:B:160:ALA:N	2.34	0.42
1:B:277:VAL:HG23	1:B:278:PRO:HD3	2.01	0.42
1:A:257:TYR:CD2	1:A:287:LYS:HE3	2.54	0.42
1:A:272:GLU:OE2	1:A:272:GLU:N	2.45	0.42
1:A:386:LEU:HD21	1:A:404:VAL:HG11	2.01	0.42
1:A:200:LYS:HG2	1:A:200:LYS:H	1.66	0.42
1:A:88:SER:OG	1:A:855:ASP:OD1	2.27	0.42
1:A:152:ASN:O	1:A:154:PHE:N	2.47	0.42
1:B:442:ASP:HB3	1:B:445:PHE:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:HG2	1:B:290:ILE:HA	2.02	0.42
1:A:369:VAL:HB	1:A:406:PHE:CD2	2.54	0.42
1:B:121:PRO:HB3	1:B:162:SER:HB3	2.02	0.41
1:B:370:LYS:HE3	2:B:901:GTP:N7	2.36	0.41
1:A:121:PRO:HG2	1:A:159:LYS:HG3	2.01	0.41
1:A:164:LEU:HD21	1:B:156:ILE:HG13	2.01	0.41
1:A:842:ALA:O	1:A:846:MSE:HG2	2.20	0.41
1:B:96:ARG:HH11	1:B:96:ARG:HG2	1.85	0.41
1:B:328:MSE:HE1	1:B:354:PHE:CD2	2.54	0.41
1:A:152:ASN:CG	1:A:153:GLY:H	2.23	0.41
1:A:192:ILE:HD13	1:A:204:CYS:SG	2.61	0.41
1:A:201:SER:OG	1:A:313:ASP:OD2	2.27	0.41
1:B:342:ASN:OD1	1:B:344:GLU:HG2	2.21	0.41
1:A:137:GLN:H	1:A:137:GLN:HG2	1.62	0.41
1:B:250:LEU:HG	1:B:284:ALA:HB1	2.03	0.41
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.86	0.41
1:B:193:THR:HG21	1:B:354:PHE:CE2	2.56	0.40
1:B:320:ASP:HB3	1:B:323:GLN:HB3	2.02	0.40
1:A:148:THR:OG1	1:A:149:LYS:N	2.55	0.40
1:B:484:LYS:O	1:B:488:LYS:HG3	2.21	0.40
1:A:146:TYR:CG	1:B:328:MSE:HG3	2.57	0.40
1:A:266:GLU:HB2	1:A:268:HIS:CE1	2.55	0.40
1:B:275:ASP:O	1:B:279:GLN:NE2	2.46	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	417/468 (89%)	391 (94%)	25 (6%)	1 (0%)	43	62
1	B	405/468 (86%)	393 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	822/936 (88%)	784 (95%)	37 (4%)	1 (0%)	48 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	ARG

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	395/419 (94%)	391 (99%)	4 (1%)	68 80
1	B	387/419 (92%)	383 (99%)	4 (1%)	68 80
All	All	782/838 (93%)	774 (99%)	8 (1%)	68 80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	SER
1	A	231	ARG
1	A	382	LYS
1	A	410	ASN
1	B	119	ILE
1	B	186	VAL
1	B	271	LYS
1	B	373	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	107	GLN
1	A	268	HIS
1	B	134	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	137	GLN
1	B	260	GLN
1	B	851	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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
2	GTP	A	901	3,4	33,34,34	3.52	14 (42%)	50,54,54	1.53	10 (20%)
2	GTP	B	901	3,4	33,34,34	3.62	14 (42%)	50,54,54	1.53	9 (18%)

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	A	901	3,4	-	4/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	B	901	3,4	-	6/22/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	GTP	O6-C6	9.12	1.40	1.23
2	A	901	GTP	O6-C6	9.04	1.40	1.23
2	B	901	GTP	PB-O3B	8.75	1.68	1.59
2	A	901	GTP	PB-O3B	8.46	1.68	1.59
2	B	901	GTP	PB-O3A	7.85	1.68	1.59
2	A	901	GTP	PB-O3A	7.29	1.67	1.59
2	B	901	GTP	PA-O3A	7.09	1.67	1.59
2	A	901	GTP	PA-O3A	6.75	1.66	1.59
2	B	901	GTP	C5-N7	5.37	1.49	1.39
2	A	901	GTP	C5-N7	5.30	1.49	1.39
2	B	901	GTP	C2-N3	5.13	1.45	1.33
2	A	901	GTP	C2-N3	5.11	1.45	1.33
2	B	901	GTP	C2-N2	4.72	1.45	1.34
2	A	901	GTP	C2-N2	4.66	1.45	1.34
2	B	901	GTP	C2-N1	3.65	1.46	1.37
2	A	901	GTP	C2-N1	3.60	1.46	1.37
2	B	901	GTP	C2'-C3'	-2.74	1.45	1.53
2	B	901	GTP	C4-N3	2.73	1.40	1.34
2	A	901	GTP	C2'-C3'	-2.66	1.46	1.53
2	A	901	GTP	C4-N3	2.66	1.40	1.34
2	A	901	GTP	O4'-C1'	2.62	1.48	1.42
2	B	901	GTP	O4'-C1'	2.62	1.48	1.42
2	A	901	GTP	C8-N9	-2.35	1.32	1.37
2	B	901	GTP	C8-N9	-2.34	1.32	1.37
2	B	901	GTP	PA-O5'	2.23	1.68	1.59
2	A	901	GTP	O4'-C4'	2.21	1.49	1.45
2	B	901	GTP	O4'-C4'	2.18	1.49	1.45
2	A	901	GTP	PA-O5'	2.06	1.67	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	GTP	C8-N9-C4	4.55	114.56	106.03
2	B	901	GTP	C8-N9-C4	4.50	114.46	106.03
2	A	901	GTP	C2-N1-C6	-3.22	119.28	125.11
2	B	901	GTP	C2-N1-C6	-3.16	119.37	125.11
2	B	901	GTP	O3G-PG-O3B	2.82	114.08	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	GTP	O2G-PG-O3B	2.79	114.00	104.64
2	A	901	GTP	O3G-PG-O3B	2.77	113.93	104.64
2	A	901	GTP	O2G-PG-O3B	2.77	113.92	104.64
2	B	901	GTP	C3'-C2'-C1'	2.60	106.38	101.46
2	A	901	GTP	C5-C6-N1	2.49	119.59	113.25
2	A	901	GTP	C3'-C2'-C1'	2.48	106.16	101.46
2	B	901	GTP	C5-C6-N1	2.44	119.45	113.25
2	B	901	GTP	O2A-PA-O1A	-2.43	101.16	112.44
2	A	901	GTP	O2A-PA-O1A	-2.36	101.49	112.44
2	A	901	GTP	O6-C6-C5	-2.32	120.40	126.53
2	B	901	GTP	O6-C6-C5	-2.32	120.41	126.53
2	B	901	GTP	O2B-PB-O1B	-2.29	101.81	112.44
2	A	901	GTP	O2B-PB-O1B	-2.18	102.31	112.44
2	A	901	GTP	C2'-C3'-C4'	2.09	106.64	102.61

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GTP	C5'-O5'-PA-O2A
2	B	901	GTP	C5'-O5'-PA-O3A
2	B	901	GTP	C5'-O5'-PA-O1A
2	B	901	GTP	C5'-O5'-PA-O2A
2	A	901	GTP	C3'-C4'-C5'-O5'
2	A	901	GTP	O4'-C4'-C5'-O5'
2	B	901	GTP	O4'-C4'-C5'-O5'
2	B	901	GTP	C3'-C4'-C5'-O5'
2	A	901	GTP	C5'-O5'-PA-O3A
2	B	901	GTP	PB-O3A-PA-O2A

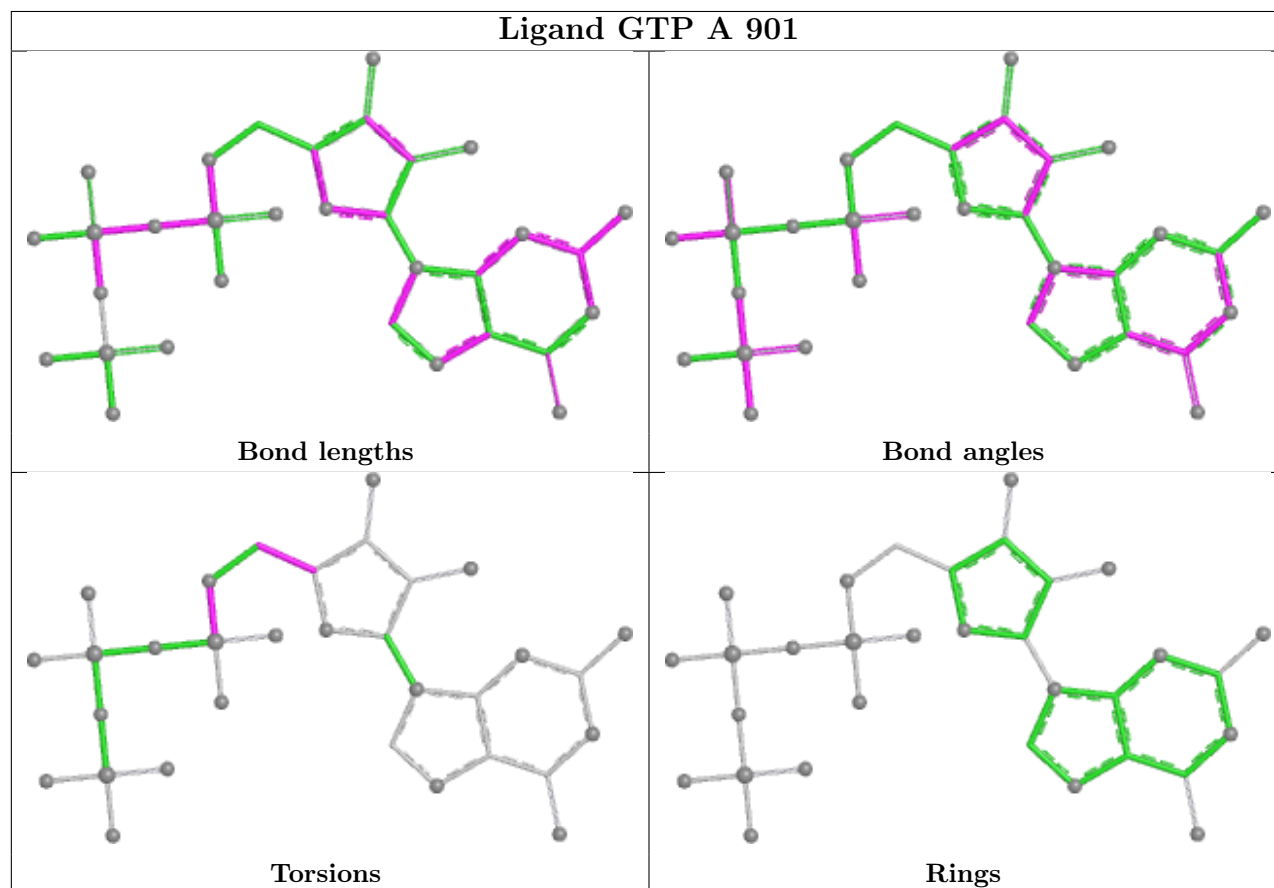
There are no ring outliers.

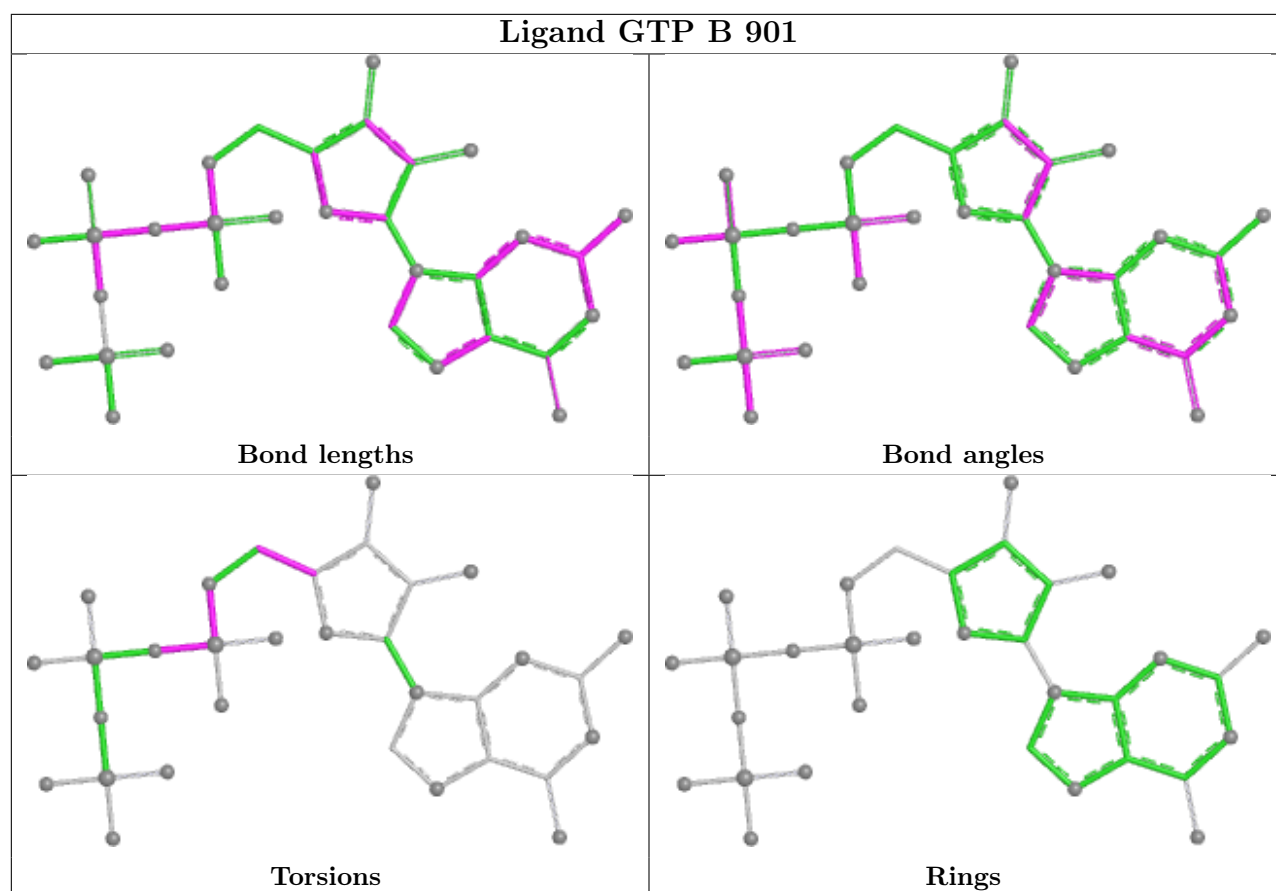
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	GTP	5	0
2	B	901	GTP	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	416/468 (88%)	0.72	43 (10%)	12 12	52, 72, 145, 172	0
1	B	407/468 (86%)	0.78	52 (12%)	7 7	52, 77, 141, 184	0
All	All	823/936 (87%)	0.75	95 (11%)	9 9	52, 74, 143, 184	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	819	LEU	5.3
1	B	819	LEU	4.8
1	B	155	ASN	4.7
1	B	441	PRO	4.7
1	A	151	LYS	4.4
1	A	263	LYS	4.3
1	B	126	ALA	4.2
1	A	149	LYS	4.2
1	B	853	ASP	4.2
1	A	441	PRO	4.1
1	A	152	ASN	4.1
1	A	410	ASN	4.0
1	A	490	TYR	4.0
1	A	125	ALA	4.0
1	A	437	SER	3.9
1	B	437	SER	3.8
1	A	148	THR	3.7
1	A	127	ASN	3.6
1	A	409	LYS	3.6
1	B	145	GLN	3.6
1	B	148	THR	3.6
1	A	492	GLU	3.6
1	B	411	GLY	3.5
1	B	409	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	817	LYS	3.5
1	B	125	ALA	3.5
1	B	85	SER	3.4
1	B	436	TYR	3.4
1	A	126	ALA	3.3
1	A	816	LYS	3.3
1	A	297	ALA	3.2
1	A	382	LYS	3.2
1	A	436	TYR	3.2
1	B	262	PRO	3.2
1	B	815	THR	3.1
1	A	131	GLU	3.0
1	B	263	LYS	3.0
1	B	264	THR	3.0
1	A	154	PHE	3.0
1	B	491	SER	3.0
1	B	259	ILE	3.0
1	B	816	LYS	2.9
1	A	299	THR	2.9
1	A	491	SER	2.9
1	A	411	GLY	2.8
1	A	230	ALA	2.8
1	A	439	SER	2.8
1	A	132	LYS	2.8
1	A	376	ARG	2.8
1	A	259	ILE	2.6
1	B	493	GLU	2.6
1	B	410	ASN	2.6
1	B	131	GLU	2.6
1	B	440	ASP	2.5
1	A	827	LEU	2.5
1	B	321	SER	2.5
1	B	124	ILE	2.5
1	B	86	GLN	2.5
1	B	280	ASN	2.5
1	A	854	ILE	2.5
1	A	153	GLY	2.5
1	A	373	ASP	2.4
1	B	374	LYS	2.4
1	B	132	LYS	2.4
1	A	406	PHE	2.4
1	A	105	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	855	ASP	2.3
1	B	412	ASP	2.3
1	B	814	SER	2.3
1	B	823	LYS	2.3
1	B	186	VAL	2.3
1	A	291	LYS	2.3
1	B	824	GLU	2.3
1	B	296	PRO	2.3
1	A	823	LYS	2.3
1	B	247	ALA	2.2
1	B	142	LEU	2.2
1	B	119	ILE	2.2
1	A	488	LYS	2.2
1	B	144	GLY	2.2
1	B	184	ASP	2.2
1	B	817	LYS	2.2
1	B	820	GLU	2.2
1	B	101	ARG	2.2
1	B	297	ALA	2.1
1	B	299	THR	2.1
1	B	377	ASP	2.1
1	A	85	SER	2.1
1	B	291	LYS	2.1
1	B	137	GLN	2.1
1	B	159	LYS	2.1
1	B	89	GLN	2.1
1	B	156	ILE	2.1
1	A	294	LYS	2.0
1	A	147	ASN	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

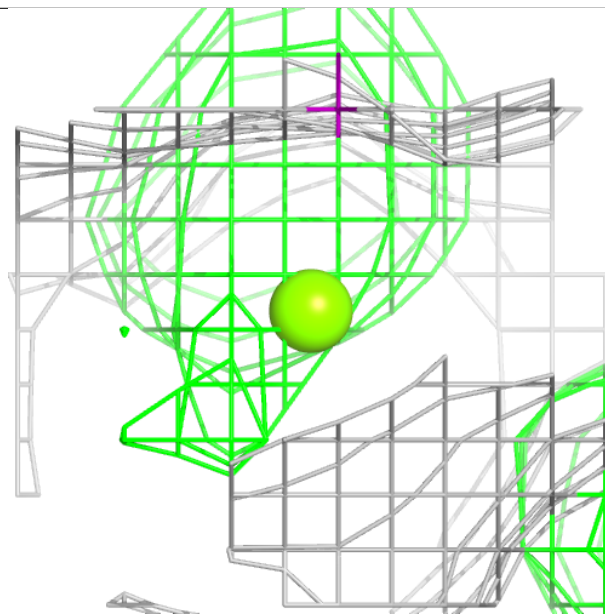
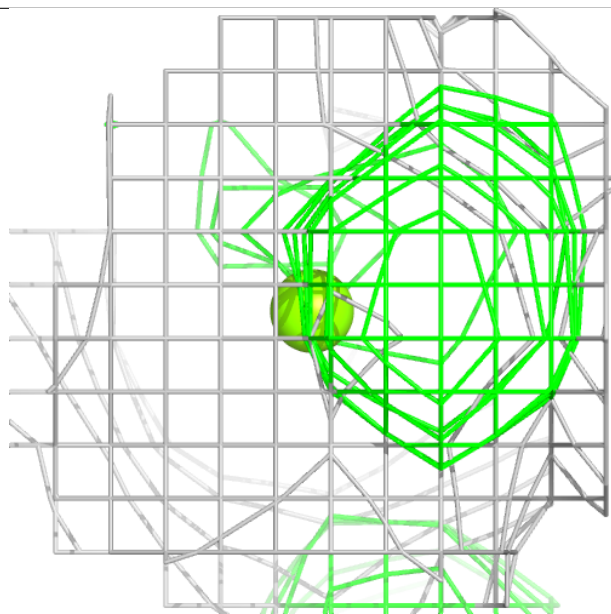
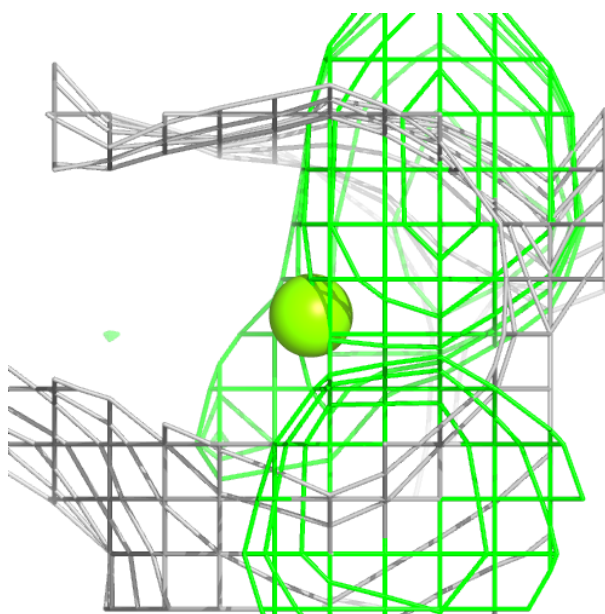
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	902	1/1	0.90	0.16	61,61,61,61	0
4	NA	B	903	1/1	0.91	0.11	67,67,67,67	0
4	NA	A	903	1/1	0.93	0.10	62,62,62,62	0
2	GTP	A	901	32/32	0.95	0.10	59,75,84,88	0
2	GTP	B	901	32/32	0.96	0.10	59,79,96,99	0
3	MG	B	902	1/1	0.98	0.07	65,65,65,65	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.

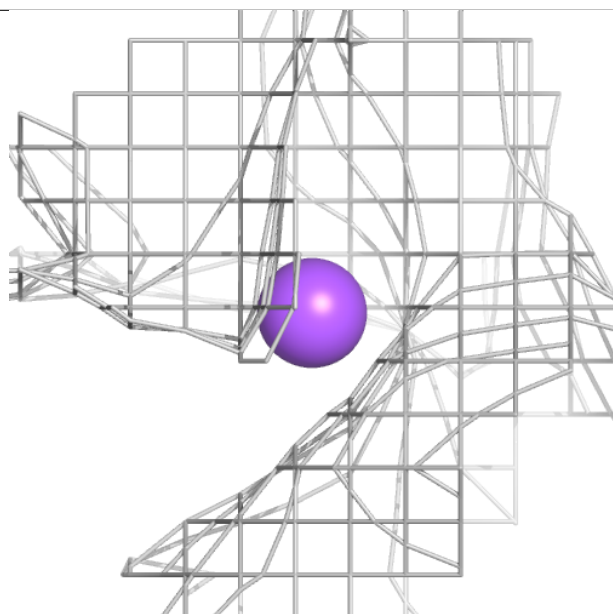
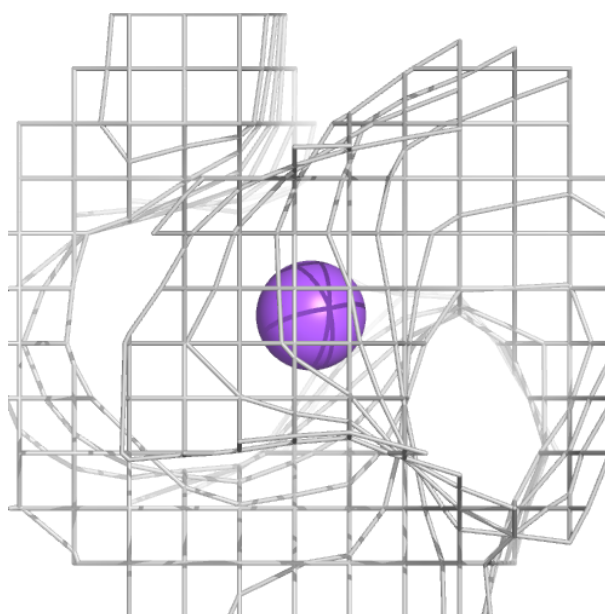
Electron density around MG A 902:

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



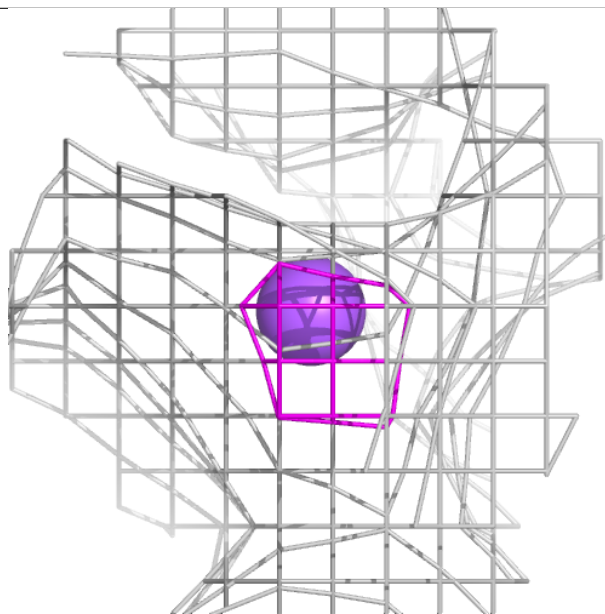
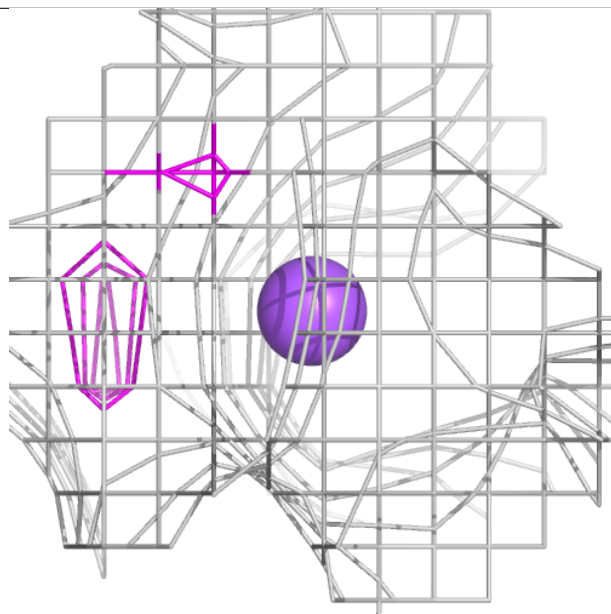
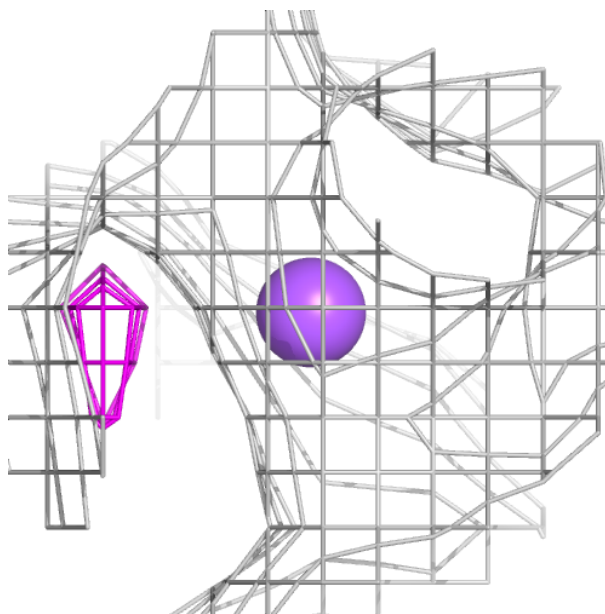
Electron density around NA B 903:

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



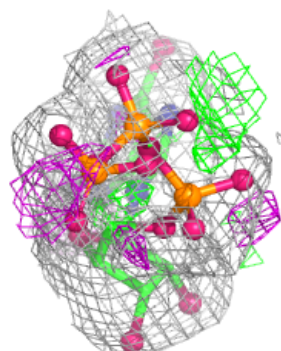
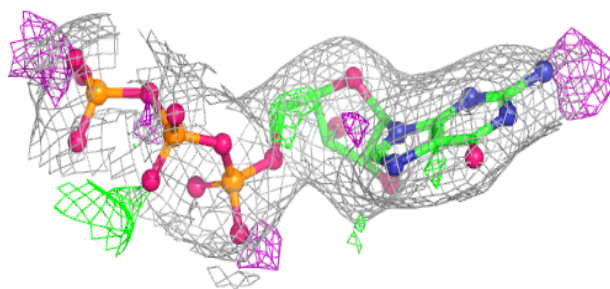
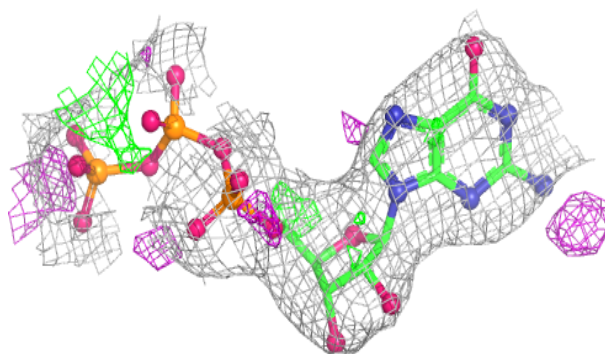
Electron density around NA A 903:

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

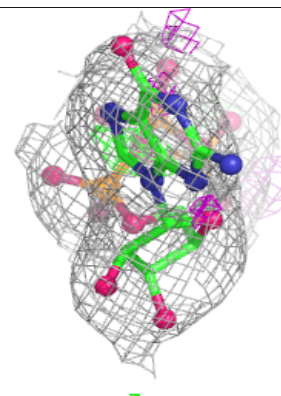
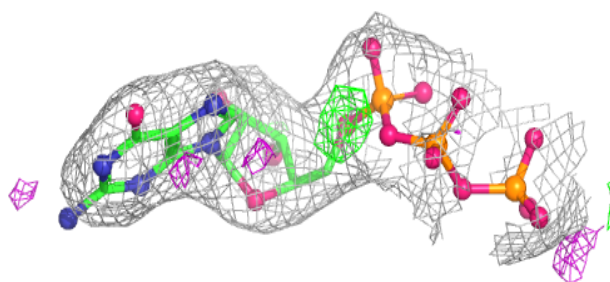
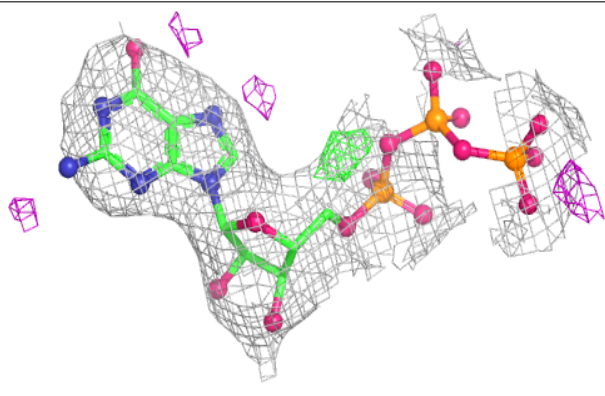


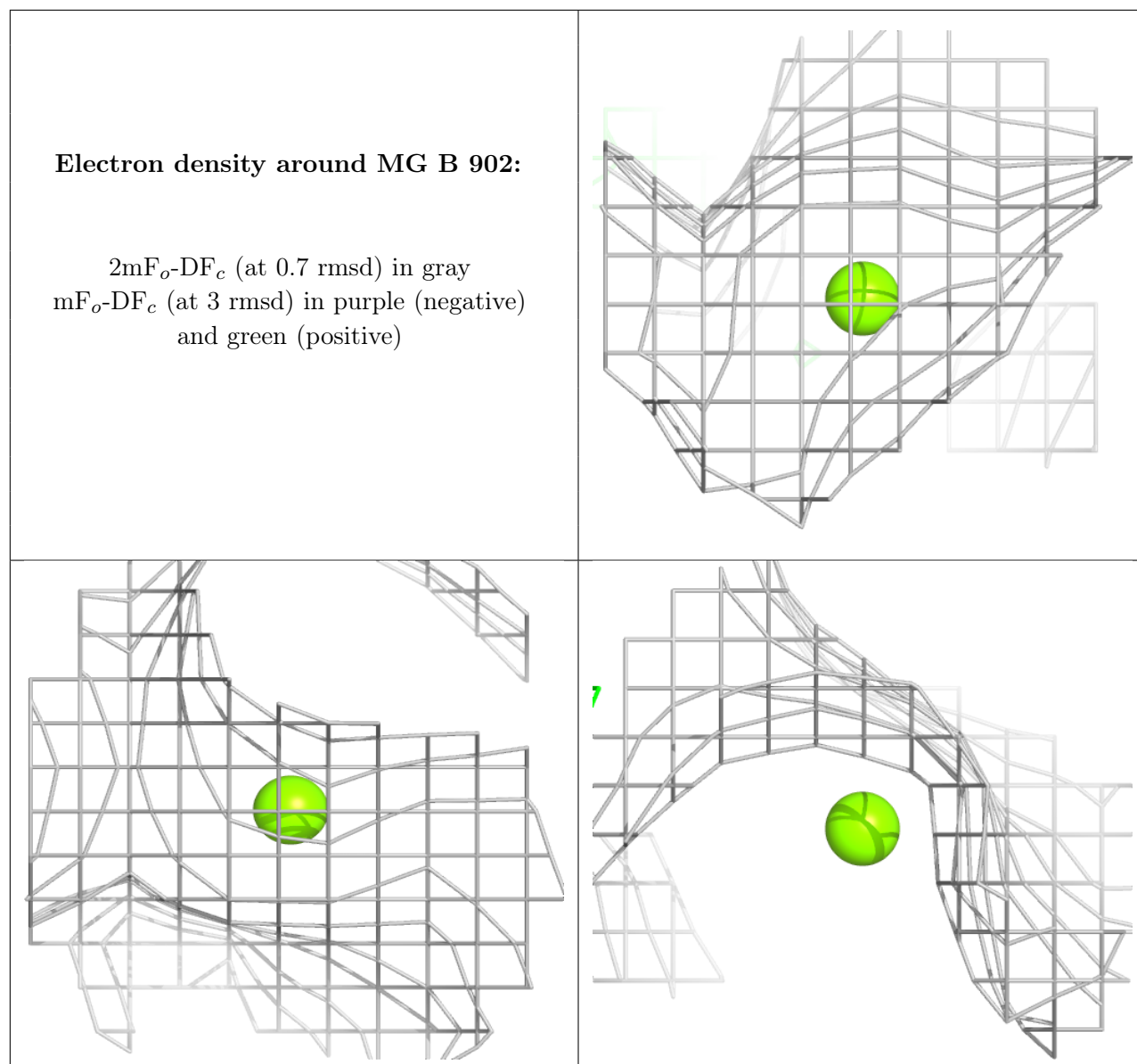
Electron density around GTP A 901:

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

**Electron density around GTP B 901:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.