Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 11:51 AM JST

PDB ID	:	5YL2
Title	:	Crystal structure of T2R-TTL-Y28 complex
Authors	:	Yang, J.H.; Yang, T.; Wen, J.L.; Chen, L.J.
Deposited on	:	2017-10-16
Resolution	:	2.09 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 (i) 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 (i)) were used in the production of this report:

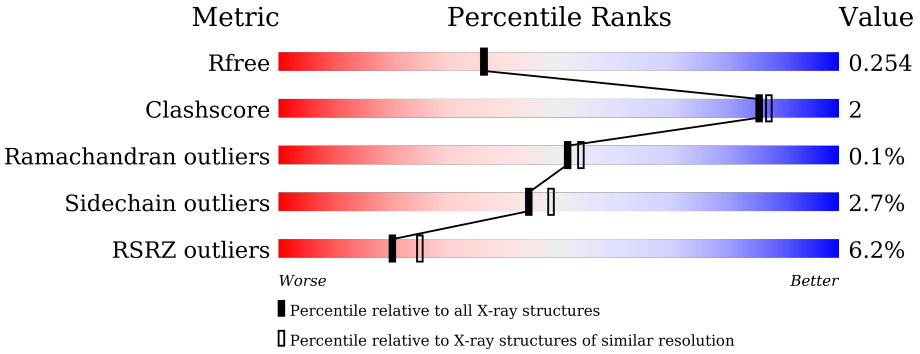
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	451	.%, 89%, 7%, •
1	C	451	89%, 8%, • •
2	B	445	3%, 89%, 7%, •
2	D	445	8%, 86%, 8%, 5%
3	E	143	9%, 80%, • •, 15%
4	F	384	16%, 80%, 6%, •, 13%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18366 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3416	2163	581	650	22	0	0	0
1	C	440	3437	2175	584	656	22	0	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3369	2115	577	650	27	0	0	0
2	D	421	3309	2080	562	640	27	0	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	1000	617	181	197	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

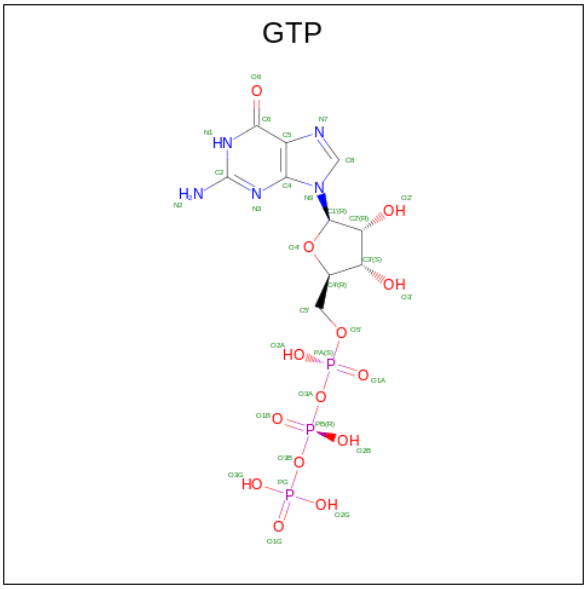
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	334	2744	1761	470	499	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

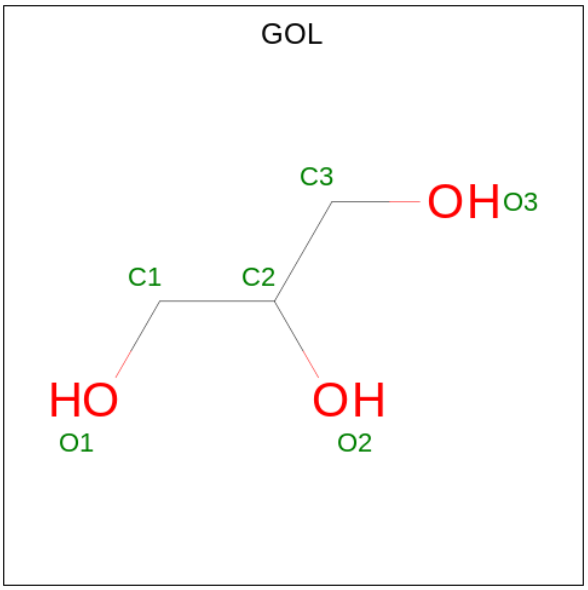
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	D	1	1	1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

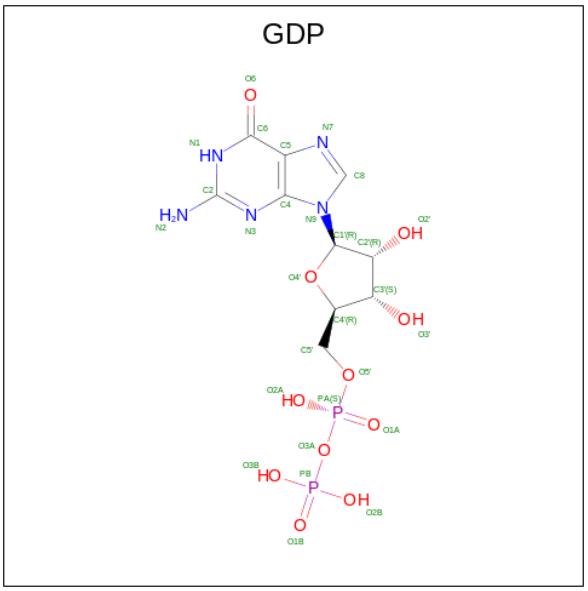
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



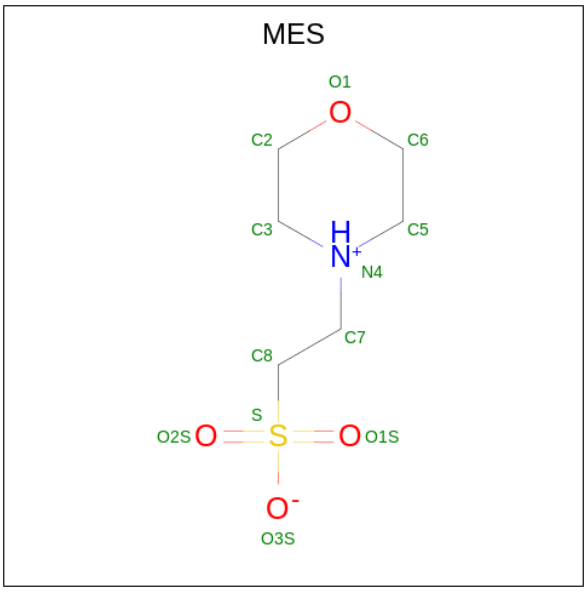
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



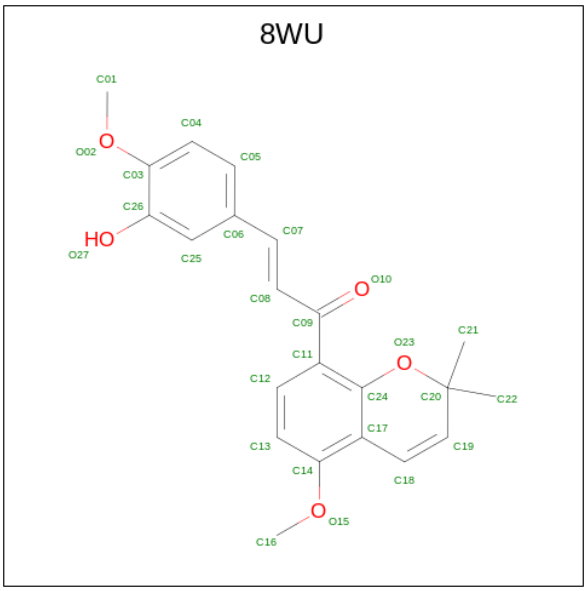
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



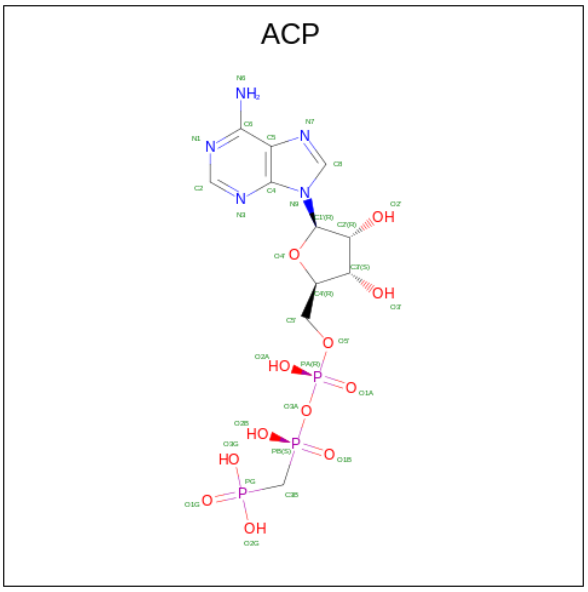
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is (E)-1-(5-methoxy-2,2-dimethyl-chromen-8-yl)-3-(4-methoxy-3-oxidanyl-phenyl)prop-2-en-1-one (three-letter code: 8WU) (formula: $C_{22}H_{22}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	B	1	27	22	5	0	0
			Total	C	O		
11	D	1	27	22	5	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	F	1	31	11	5	12	3	0	0

- Molecule 13 is water.

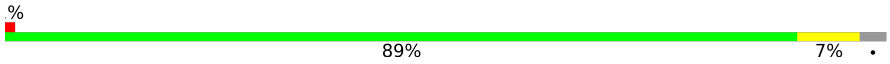
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	204	204	204	0	0
			Total	O		
13	B	145	145	145	0	0
			Total	O		
13	C	292	292	292	0	0
			Total	O		
13	D	81	81	81	0	0
			Total	O		
13	E	37	37	37	0	0
			Total	O		
13	F	99	99	99	0	0

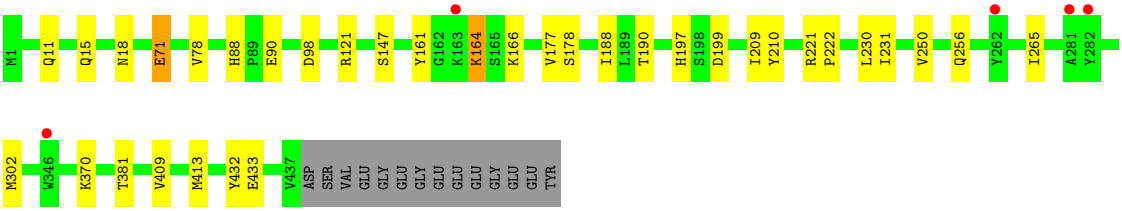
3 Residue-property plots (i)

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: Tubulin alpha-1B chain

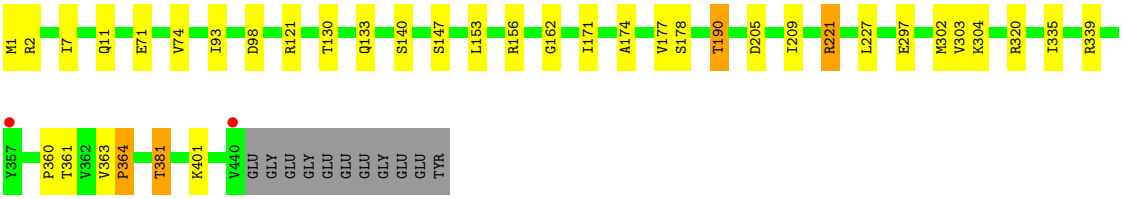
Chain A:





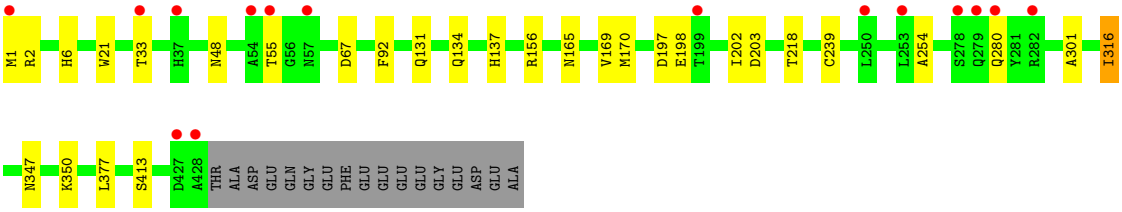
• Molecule 1: Tubulin alpha-1B chain

Chain C:



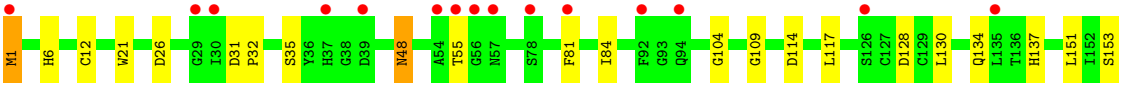
• Molecule 2: Tubulin beta chain

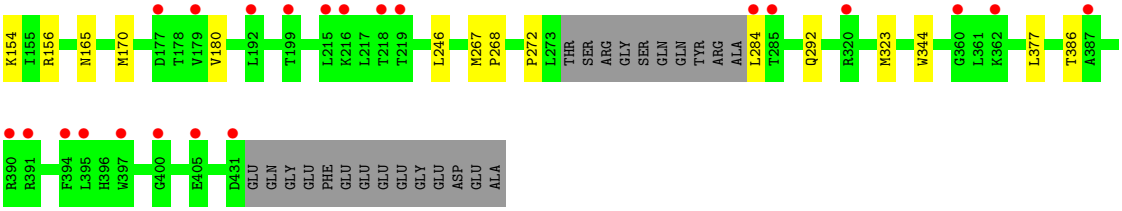
Chain B:



• Molecule 2: Tubulin beta chain

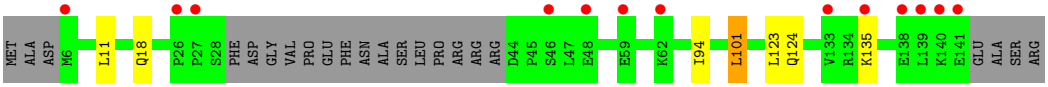
Chain D:





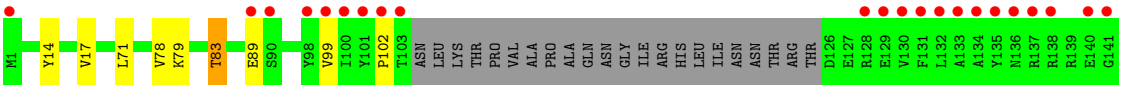
- Molecule 3: Stathmin-4

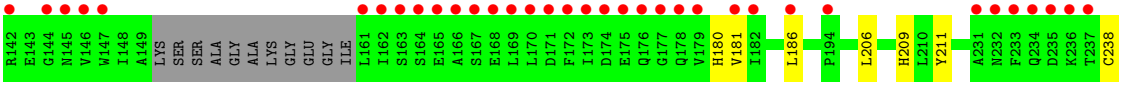
Chain E:



- Molecule 4: Tubulin tyrosine ligase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.54Å 158.20Å 181.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.09 41.74 – 2.09	Depositor EDS
% Data completeness (in resolution range)	57.7 (50.01-2.09) 57.7 (41.74-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.209 , 0.254 0.208 , 0.254	Depositor DCC
R_{free} test set	5217 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18366	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MG, 8WU, MES, GTP, GDP, CA, ACP

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	0.43	0/3494	0.62	0/4743
1	C	0.44	0/3515	0.66	0/4772
2	B	0.46	0/3444	0.62	0/4664
2	D	0.42	0/3382	0.62	0/4581
3	E	0.36	0/1008	0.59	1/1337 (0.1%)
4	F	0.50	0/2806	0.65	0/3791
All	All	0.45	0/17649	0.63	1/23888 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	101	LEU	CA-CB-CG	6.01	129.13	115.30

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	3416	0	3331	17	0
1	C	3437	0	3348	22	0
2	B	3369	0	3250	13	0
2	D	3309	0	3189	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1000	0	1018	5	0
4	F	2744	0	2709	10	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	2	0
11	B	27	0	0	0	0
11	D	27	0	0	0	0
12	F	31	0	14	0	0
13	A	204	0	0	2	0
13	B	145	0	0	0	0
13	C	292	0	0	3	0
13	D	81	0	0	1	0
13	E	37	0	0	0	0
13	F	99	0	0	0	0
All	All	18366	0	16928	76	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 2.

All (76) 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)
4:F:79:LYS:O	4:F:83:THR:OG1	1.72	1.07
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.60	0.84
1:A:209:ILE:HD11	1:A:302:MET:SD	2.27	0.75
2:B:1:MET:HB2	2:B:131:GLN:HB3	1.76	0.66
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.79	0.65
1:C:381:THR:CG2	13:C:615:HOH:O	2.47	0.61
1:C:297:GLU:HG2	1:C:339:ARG:HH22	1.68	0.58
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.86	0.58
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.86	0.57
2:D:1:MET:HG3	2:D:48:ASN:HB2	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HH11	2:D:323:MET:HB3	1.70	0.56
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.86	0.56
1:C:381:THR:HG23	13:C:615:HOH:O	2.05	0.56
1:C:147:SER:O	1:C:190:THR:HG23	2.09	0.53
1:C:1:MET:HB3	1:C:130:THR:OG1	2.09	0.53
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.92	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
2:B:197:ASP:OD1	10:B:503:MES:H32	2.11	0.51
2:B:156:ARG:HG3	10:B:503:MES:H62	1.93	0.50
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.94	0.50
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.93	0.50
1:C:320:ARG:HG3	1:C:360:PRO:HD3	1.94	0.49
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.77	0.49
1:A:231:ILE:HD11	13:A:672:HOH:O	2.13	0.49
1:C:156:ARG:HD2	3:E:101:LEU:HD21	1.95	0.48
4:F:296:MET:HE3	4:F:296:MET:HA	1.95	0.48
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.96	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.48
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.15	0.47
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.97	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.47
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.97	0.47
1:A:178:SER:O	2:B:350:LYS:HE2	2.15	0.47
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.98	0.46
4:F:14:TYR:HA	4:F:17:VAL:HB	1.98	0.46
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.96	0.45
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.99	0.45
2:D:267:MET:HA	2:D:268:PRO:HD3	1.85	0.45
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.99	0.44
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.98	0.44
2:D:117:LEU:HD21	2:D:154:LYS:HB3	1.99	0.44
4:F:99:VAL:HA	4:F:181:VAL:HG22	2.00	0.44
1:A:88:HIS:HD2	1:A:90:GLU:HB2	1.83	0.44
1:C:156:ARG:CD	3:E:101:LEU:HD21	2.48	0.44
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.43
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.01	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.43
2:B:239:CYS:SG	2:B:316:ILE:HD13	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:272:PRO:HB3	2:D:284:LEU:HD12	2.00	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
1:A:88:HIS:HE1	13:A:666:HOH:O	2.00	0.43
1:C:174:ALA:O	1:C:178:SER:HB3	2.19	0.42
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.84	0.42
2:B:170:MET:HG3	2:B:377:LEU:HD11	2.01	0.42
1:C:360:PRO:HB2	13:C:758:HOH:O	2.19	0.42
2:D:31:ASP:HB2	2:D:35:SER:H	1.83	0.42
2:D:12:CYS:HB2	5:D:501:GTP:C8	2.55	0.42
2:D:284:LEU:HD13	2:D:292:GLN:HE22	1.84	0.42
1:C:363:VAL:HA	1:C:364:PRO:HD2	1.80	0.42
2:B:198:GLU:OE2	2:B:254:ALA:HB2	2.20	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.41
1:A:11:GLN:O	1:A:15:GLN:HG3	2.21	0.41
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.56	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.20	0.41
2:B:55:THR:O	2:B:55:THR:OG1	2.39	0.41
2:B:203:ASP:HB2	2:B:301:ALA:HA	2.02	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.21	0.40
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.03	0.40
2:D:32:PRO:HB3	13:D:605:HOH:O	2.20	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.22	0.40
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.57	0.40
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.40
2:D:104:GLY:O	2:D:109:GLY:HA3	2.21	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	435/451 (96%)	424 (98%)	11 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	438/451 (97%)	428 (98%)	9 (2%)	1 (0%)	47	49
2	B	426/445 (96%)	409 (96%)	17 (4%)	0	100	100
2	D	417/445 (94%)	406 (97%)	11 (3%)	0	100	100
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	308 (95%)	15 (5%)	1 (0%)	41	41
All	All	2157/2319 (93%)	2090 (97%)	65 (3%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	102	PRO
1	C	364	PRO

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	368/379 (97%)	359 (98%)	9 (2%)	49	53
1	C	371/379 (98%)	362 (98%)	9 (2%)	49	53
2	B	370/383 (97%)	361 (98%)	9 (2%)	49	53
2	D	364/383 (95%)	351 (96%)	13 (4%)	35	36
3	E	109/127 (86%)	107 (98%)	2 (2%)	59	65
4	F	301/342 (88%)	292 (97%)	9 (3%)	41	44
All	All	1883/1993 (94%)	1832 (97%)	51 (3%)	44	48

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	164	LYS
1	A	177	VAL
1	A	188	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	221	ARG
1	A	250	VAL
1	A	370	LYS
1	A	381	THR
1	A	433	GLU
2	B	2	ARG
2	B	33	THR
2	B	48	ASN
2	B	137	HIS
2	B	218	THR
2	B	280	GLN
2	B	316	ILE
2	B	347	ASN
2	B	413	SER
1	C	2	ARG
1	C	133	GLN
1	C	177	VAL
1	C	190	THR
1	C	221	ARG
1	C	302	MET
1	C	304	LYS
1	C	361	THR
1	C	381	THR
2	D	1	MET
2	D	26	ASP
2	D	48	ASN
2	D	55	THR
2	D	114	ASP
2	D	128	ASP
2	D	130	LEU
2	D	137	HIS
2	D	151	LEU
2	D	153	SER
2	D	180	VAL
2	D	246	LEU
2	D	386	THR
3	E	124	GLN
3	E	135	LYS
4	F	83	THR
4	F	89	GLU
4	F	180	HIS
4	F	211	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	238	CYS
4	F	296	MET
4	F	310	GLN
4	F	326	LYS
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	329	ASN
1	A	358	GLN
2	B	48	ASN
2	B	165	ASN
2	B	245	GLN
2	B	375	GLN
1	C	11	GLN
2	D	292	GLN
3	E	18	GLN
4	F	252	ASN
4	F	260	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	GTP	D	501	6	26,34,34	0.90	0	32,54,54	1.12	4 (12%)
11	8WU	B	504	-	29,29,29	2.81	13 (44%)	41,42,42	1.54	7 (17%)
12	ACP	F	401	-	27,33,33	1.80	7 (25%)	32,52,52	1.32	4 (12%)
10	MES	B	503	-	12,12,12	2.05	2 (16%)	14,16,16	7.40	8 (57%)
5	GTP	A	501	6	26,34,34	0.94	1 (3%)	32,54,54	1.13	4 (12%)
11	8WU	D	503	-	29,29,29	2.89	14 (48%)	41,42,42	1.48	7 (17%)
5	GTP	C	501	6	26,34,34	0.89	0	32,54,54	1.05	2 (6%)
9	GDP	B	501	6	24,30,30	0.90	1 (4%)	30,47,47	1.08	2 (6%)
8	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.20	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
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3
11	8WU	B	504	-	-	5/13/24/24	0/3/3/3
12	ACP	F	401	-	-	3/15/38/38	0/3/3/3
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
11	8WU	D	503	-	-	7/13/24/24	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	8WU	C18-C19	8.38	1.44	1.33
11	B	504	8WU	C18-C19	8.00	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	8WU	O23-C24	7.30	1.49	1.37
11	B	504	8WU	O23-C24	7.28	1.49	1.37
10	B	503	MES	C8-S	-6.23	1.68	1.77
12	F	401	ACP	PG-O1G	5.46	1.61	1.50
11	D	503	8WU	C11-C09	4.12	1.56	1.48
11	B	504	8WU	C11-C09	4.00	1.56	1.48
11	D	503	8WU	O15-C14	3.68	1.43	1.37
11	D	503	8WU	C11-C24	3.65	1.48	1.40
11	B	504	8WU	C11-C24	3.61	1.47	1.40
11	D	503	8WU	C13-C12	3.39	1.44	1.38
11	B	504	8WU	C08-C09	3.22	1.53	1.47
11	B	504	8WU	C13-C12	3.14	1.44	1.38
12	F	401	ACP	PB-O3A	3.14	1.61	1.58
11	D	503	8WU	C08-C09	3.01	1.52	1.47
11	B	504	8WU	C05-C04	2.87	1.44	1.38
11	B	504	8WU	O15-C14	2.82	1.41	1.37
12	F	401	ACP	PG-O3G	2.80	1.61	1.54
12	F	401	ACP	PG-O2G	-2.78	1.48	1.54
12	F	401	ACP	C5-C4	2.76	1.48	1.40
11	D	503	8WU	C17-C14	2.72	1.45	1.41
11	B	504	8WU	C17-C14	2.54	1.45	1.41
11	D	503	8WU	C06-C07	2.48	1.54	1.47
11	B	504	8WU	C06-C07	2.38	1.54	1.47
11	B	504	8WU	C08-C07	2.36	1.39	1.33
11	D	503	8WU	C05-C04	2.32	1.43	1.38
9	B	501	GDP	C6-N1	-2.31	1.34	1.37
11	D	503	8WU	C08-C07	2.30	1.39	1.33
10	B	503	MES	O2S-S	2.25	1.51	1.45
11	D	503	8WU	C20-C19	2.23	1.54	1.50
11	D	503	8WU	O10-C09	-2.21	1.19	1.24
11	B	504	8WU	C20-C19	2.21	1.54	1.50
12	F	401	ACP	C2-N3	2.20	1.35	1.32
5	A	501	GTP	C6-N1	-2.16	1.34	1.37
12	F	401	ACP	PB-O2B	2.15	1.61	1.56
11	D	503	8WU	C21-C20	2.13	1.57	1.52
11	B	504	8WU	C21-C20	2.10	1.57	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	503	MES	O1S-S-C8	-18.92	84.14	106.92
10	B	503	MES	O2S-S-C8	11.07	120.25	106.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	503	MES	O3S-S-O1S	-10.86	84.75	111.27
10	B	503	MES	O2S-S-O1S	-8.65	84.01	113.95
10	B	503	MES	O3S-S-C8	8.01	118.72	105.77
11	B	504	8WU	C22-C20-C21	-4.26	99.16	111.29
11	B	504	8WU	C16-O15-C14	-4.00	111.49	117.53
11	D	503	8WU	C22-C20-C21	-3.61	101.02	111.29
12	F	401	ACP	N3-C2-N1	-3.45	123.29	128.68
11	D	503	8WU	C16-O15-C14	-3.27	112.59	117.53
11	D	503	8WU	O02-C03-C26	3.27	119.31	114.57
12	F	401	ACP	C3'-C2'-C1'	3.18	105.76	100.98
11	B	504	8WU	O15-C14-C13	-3.06	119.13	124.37
10	B	503	MES	C5-N4-C3	2.94	115.45	108.83
10	B	503	MES	O3S-S-O2S	2.80	118.11	111.27
11	D	503	8WU	O15-C14-C17	2.77	120.61	115.26
12	F	401	ACP	C4-C5-N7	-2.71	106.57	109.40
11	B	504	8WU	O02-C03-C26	2.63	118.38	114.57
11	D	503	8WU	O15-C14-C13	-2.61	119.89	124.37
11	B	504	8WU	O15-C14-C17	2.58	120.24	115.26
9	B	501	GDP	C8-N7-C5	2.54	107.83	102.99
5	C	501	GTP	C8-N7-C5	2.50	107.75	102.99
9	B	501	GDP	C5-C6-N1	2.44	118.25	113.95
11	D	503	8WU	C06-C25-C26	-2.40	119.04	120.76
5	D	501	GTP	C8-N7-C5	2.33	107.44	102.99
5	D	501	GTP	PA-O3A-PB	-2.33	124.84	132.83
5	A	501	GTP	PB-O3B-PG	-2.32	124.88	132.83
11	B	504	8WU	C20-O23-C24	-2.30	114.07	118.04
5	A	501	GTP	C5-C6-N1	2.18	117.81	113.95
10	B	503	MES	C6-C5-N4	2.15	113.36	110.10
11	B	504	8WU	C20-C19-C18	-2.15	118.57	121.49
5	A	501	GTP	O3G-PG-O2G	2.15	115.84	107.64
11	D	503	8WU	C07-C08-C09	-2.13	118.17	121.64
12	F	401	ACP	PB-O3A-PA	-2.12	125.85	132.56
5	D	501	GTP	C5-C6-N1	2.07	117.61	113.95
5	A	501	GTP	C8-N7-C5	2.06	106.92	102.99
5	D	501	GTP	PB-O3B-PG	-2.03	125.86	132.83
5	C	501	GTP	C5-C6-N1	2.02	117.51	113.95

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	C7-C8-S-O2S
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O3A
11	D	503	8WU	C13-C14-O15-C16
11	B	504	8WU	C13-C14-O15-C16
11	D	503	8WU	C07-C08-C09-O10
11	D	503	8WU	C07-C08-C09-C11
11	D	503	8WU	C17-C14-O15-C16
11	B	504	8WU	C17-C14-O15-C16
11	D	503	8WU	C26-C03-O02-C01
11	B	504	8WU	C07-C08-C09-C11
11	B	504	8WU	C07-C08-C09-O10
11	D	503	8WU	C04-C03-O02-C01
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	C5'-O5'-PA-O3A
11	D	503	8WU	O10-C09-C11-C24
5	D	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O1S
11	B	504	8WU	O10-C09-C11-C24
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	501	GTP	PB-O3A-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	O1-C1-C2-O2

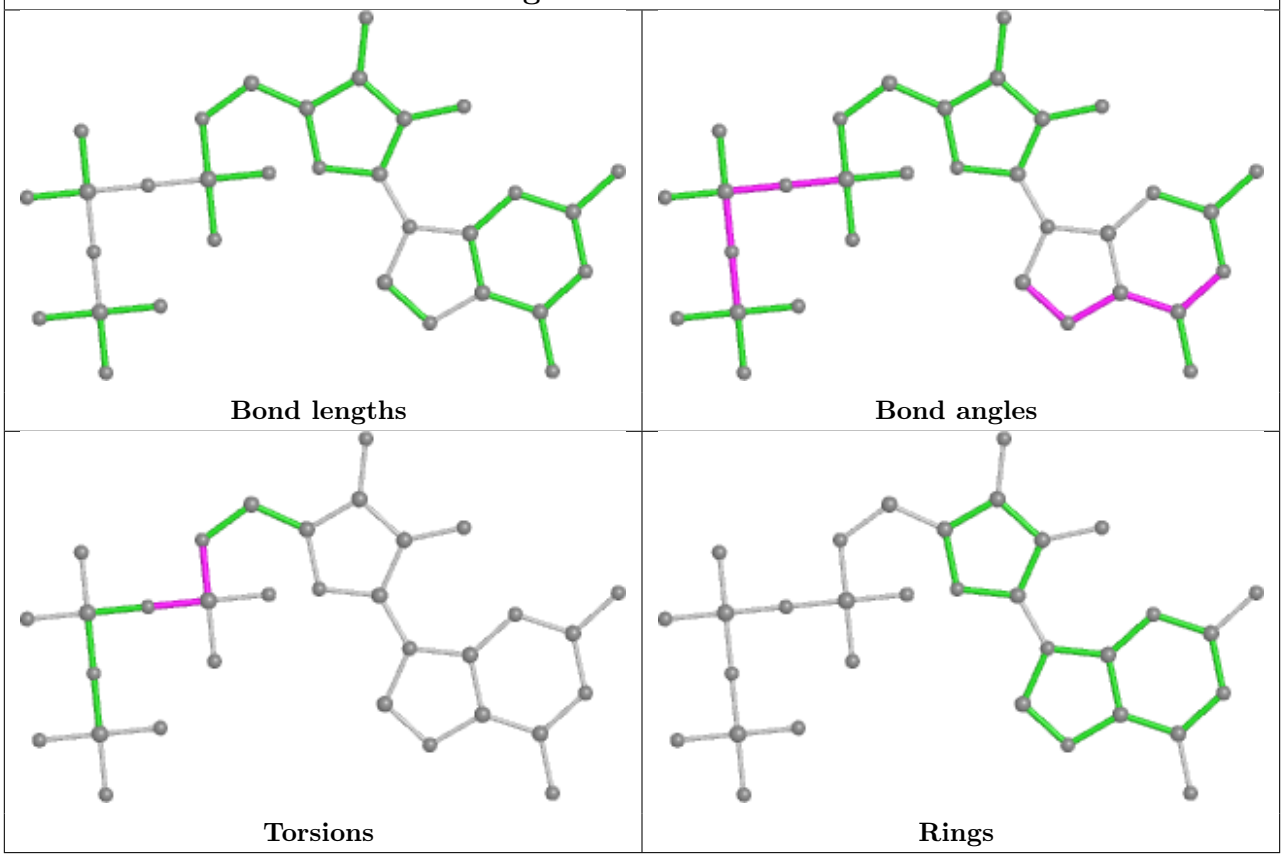
There are no ring outliers.

2 monomers are involved in 3 short contacts:

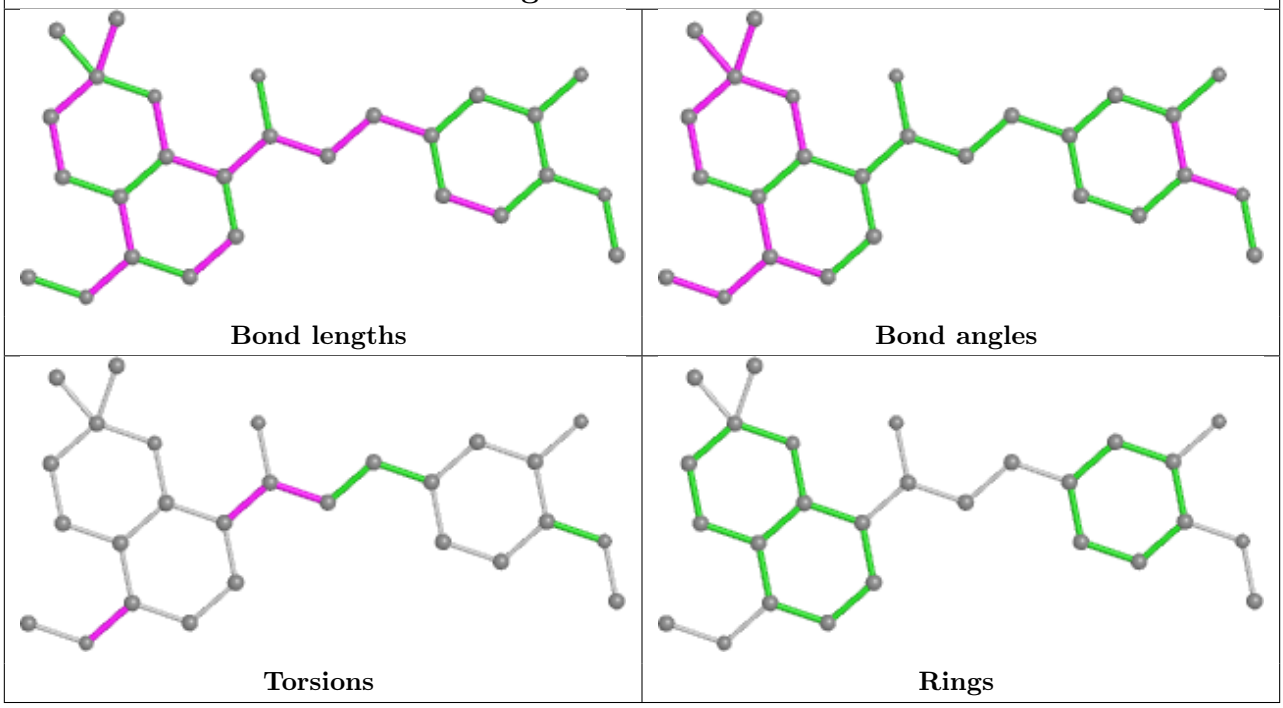
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	GTP	1	0
10	B	503	MES	2	0

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 then 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.

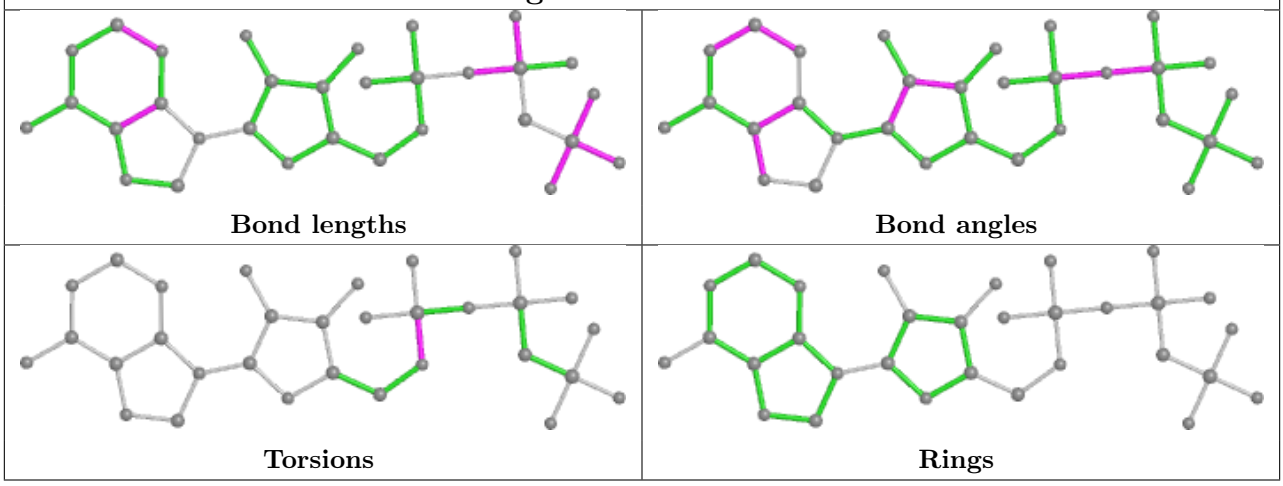
Ligand GTP D 501



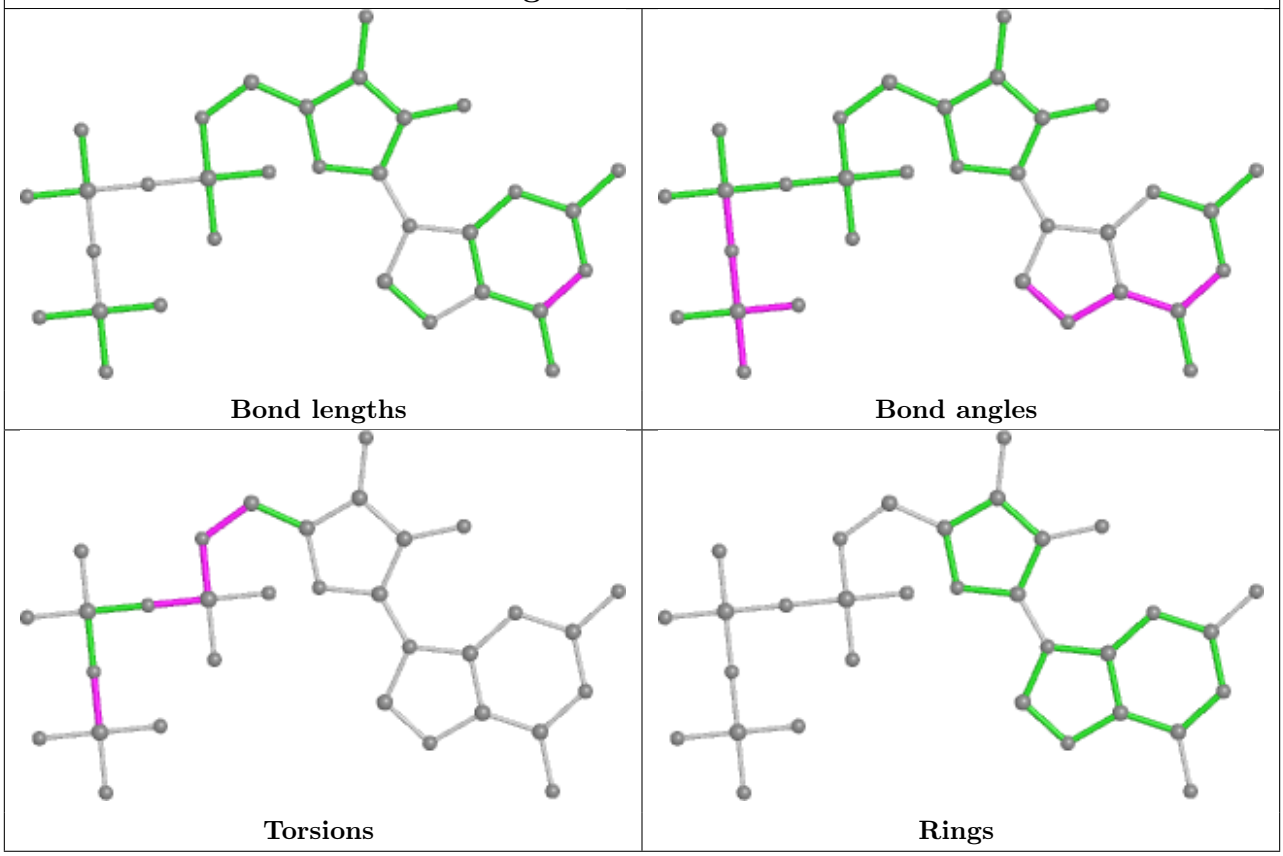
Ligand 8WU B 504



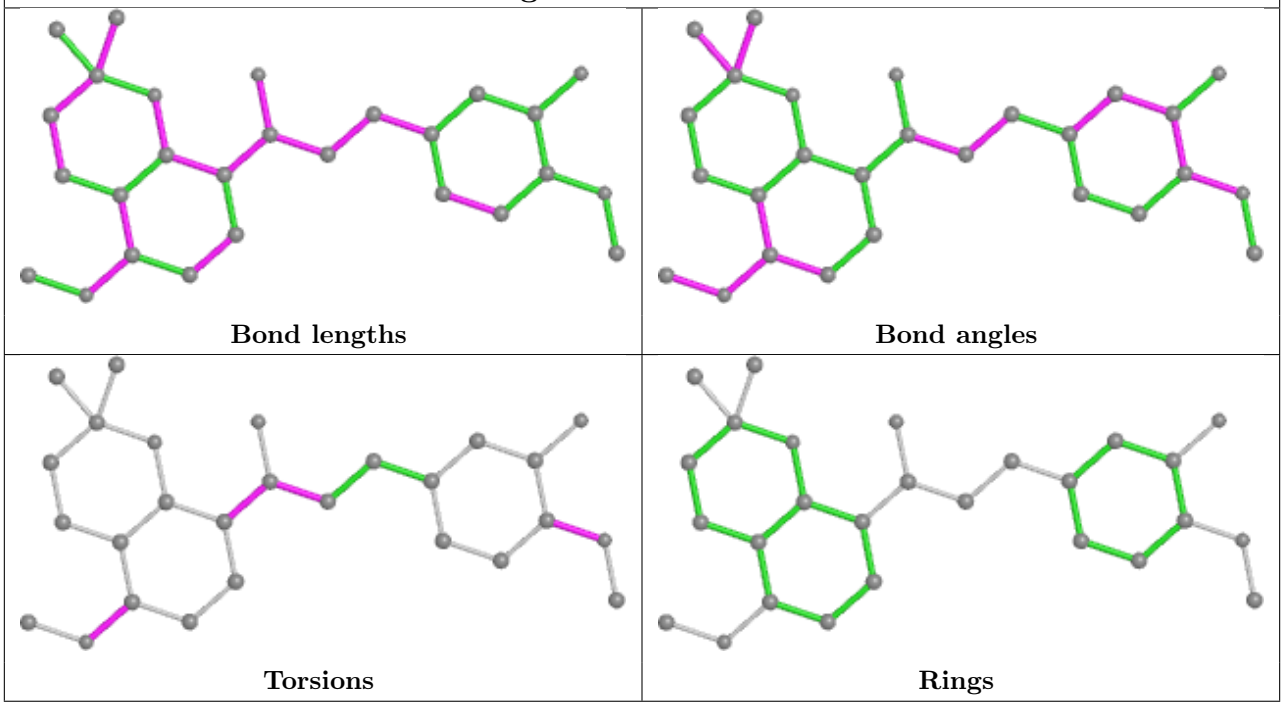
Ligand ACP F 401



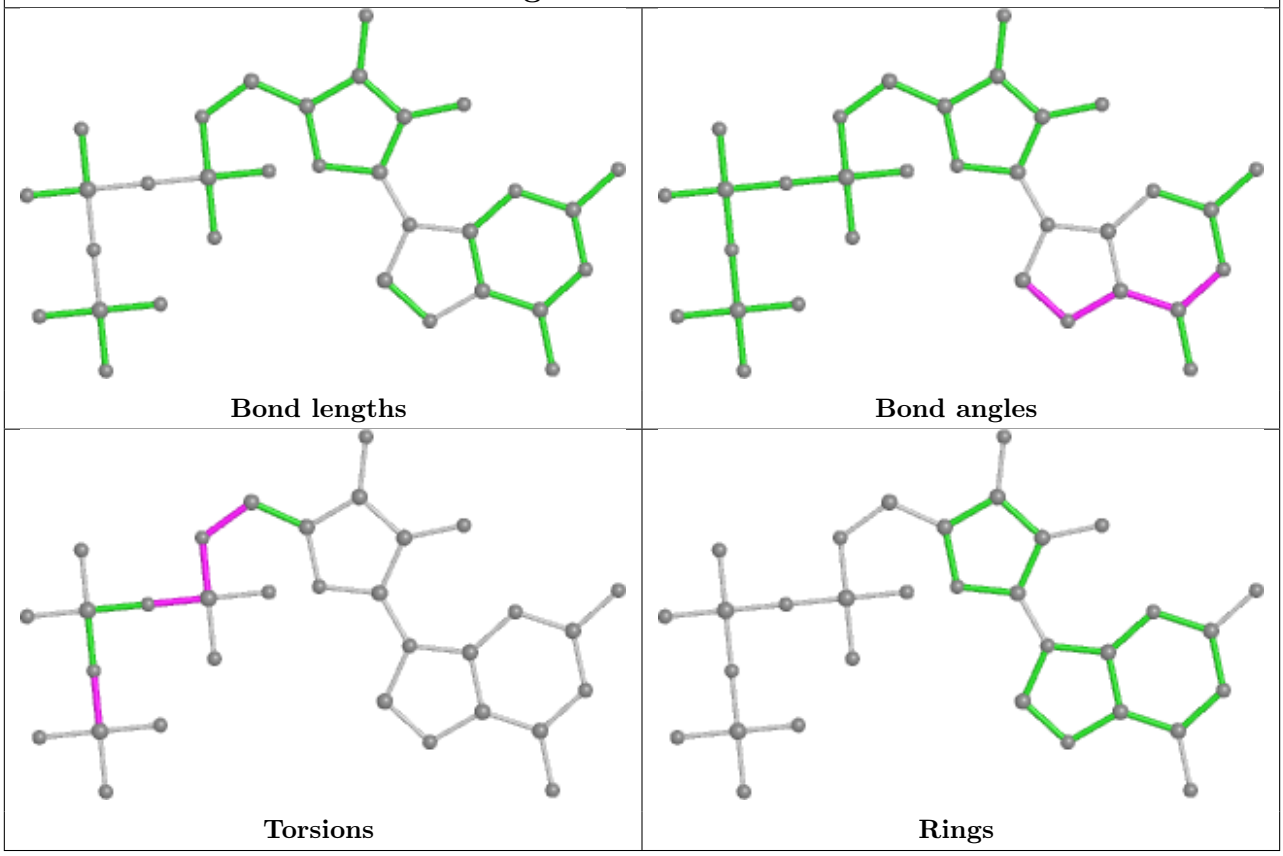
Ligand GTP A 501



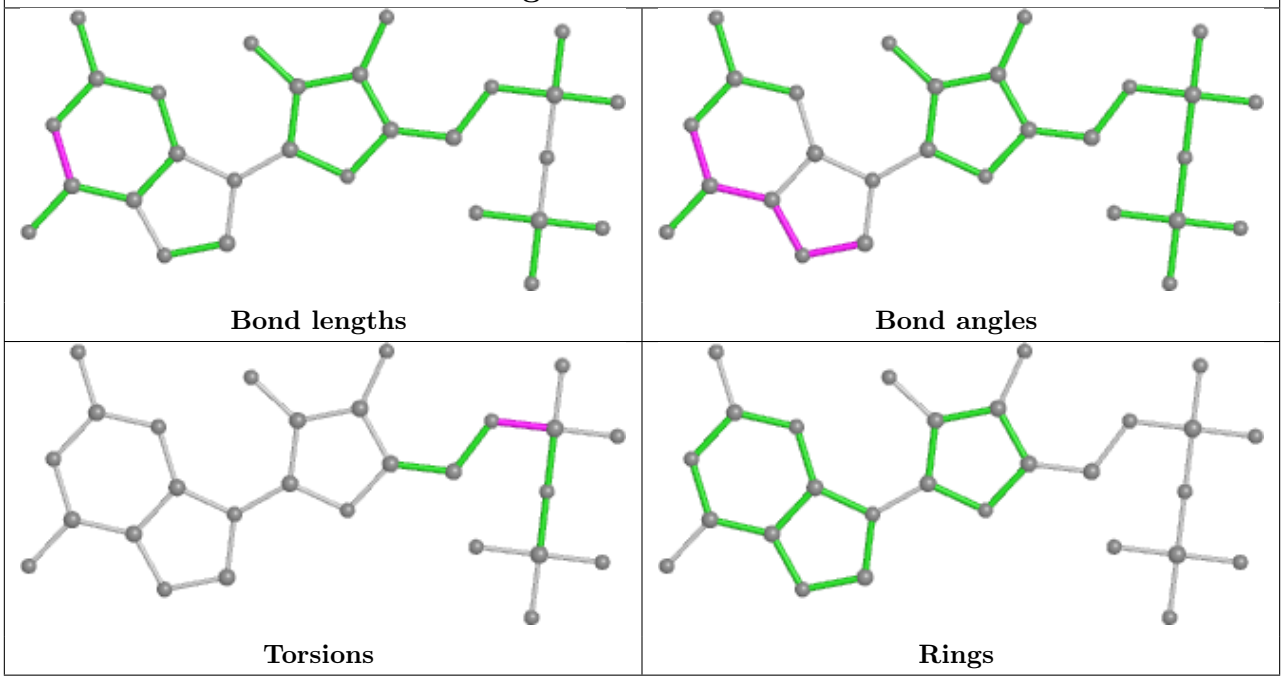
Ligand 8WU D 503



Ligand GTP C 501



Ligand GDP B 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	437/451 (96%)	-0.22	5 (1%) 80 84	13, 26, 45, 65	0
1	C	440/451 (97%)	-0.37	2 (0%) 91 92	8, 20, 39, 50	0
2	B	428/445 (96%)	-0.08	15 (3%) 44 50	11, 27, 51, 87	0
2	D	421/445 (94%)	0.45	37 (8%) 10 12	14, 42, 69, 84	0
3	E	121/143 (84%)	0.37	13 (10%) 6 7	23, 44, 72, 92	0
4	F	334/384 (86%)	0.69	63 (18%) 1 1	19, 46, 108, 123	0
All	All	2181/2319 (94%)	0.08	135 (6%) 20 25	8, 30, 71, 123	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.6
4	F	132	LEU	6.8
4	F	166	ALA	6.7
2	B	55	THR	6.4
4	F	172	PHE	6.4
4	F	133	ALA	6.3
2	D	55	THR	6.3
4	F	162	ILE	6.3
4	F	169	LEU	6.3
4	F	102	PRO	5.8
4	F	130	VAL	5.7
4	F	372	THR	5.6
4	F	182	ILE	5.5
2	B	57	ASN	5.2
4	F	176	GLN	5.1
4	F	137	ARG	5.0
4	F	245	ILE	4.8
4	F	161	LEU	4.7
4	F	103	THR	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	219	THR	4.4
2	B	278	SER	4.4
4	F	170	LEU	4.4
2	D	284	LEU	4.3
4	F	101	TYR	4.3
2	D	394	PHE	4.3
4	F	100	ILE	4.2
4	F	177	GLY	4.2
4	F	171	ASP	4.0
4	F	175	GLU	4.0
3	E	135	LYS	4.0
4	F	181	VAL	3.9
2	D	29	GLY	3.9
2	D	54	ALA	3.9
4	F	129	GLU	3.9
4	F	167	SER	3.9
1	A	282	TYR	3.9
3	E	140	LYS	3.9
4	F	362	ALA	3.8
3	E	139	LEU	3.8
4	F	233	PHE	3.8
4	F	135	TYR	3.8
4	F	136	ASN	3.6
4	F	231	ALA	3.6
4	F	234	GLN	3.6
4	F	141	GLY	3.5
2	D	390	ARG	3.5
2	D	360	GLY	3.5
4	F	168	GLU	3.4
4	F	178	GLN	3.4
4	F	179	VAL	3.4
4	F	131	PHE	3.4
2	D	57	ASN	3.4
4	F	236	LYS	3.3
4	F	140	GLU	3.3
2	B	1	MET	3.3
4	F	134	ALA	3.3
2	D	1	MET	3.3
3	E	141	GLU	3.3
4	F	90	SER	3.2
4	F	142	ARG	3.2
2	B	280	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	237	THR	3.1
1	A	281	ALA	3.1
2	D	391	ARG	3.1
4	F	232	ASN	3.1
4	F	145	ASN	3.1
4	F	165	GLU	3.1
2	B	279	GLN	3.1
2	D	37	HIS	3.1
4	F	174	ASP	3.0
1	A	163	LYS	3.0
2	D	218	THR	2.9
4	F	194	PRO	2.9
3	E	59	GLU	2.9
3	E	138	GLU	2.9
2	D	179	VAL	2.9
2	D	216	LYS	2.8
2	D	320	ARG	2.8
2	D	431	ASP	2.8
4	F	128	ARG	2.8
2	D	362	LYS	2.8
2	D	94	GLN	2.8
1	C	357	TYR	2.8
2	D	30	ILE	2.7
4	F	164	SER	2.7
3	E	26	PRO	2.7
2	D	81	PHE	2.7
4	F	144	GLY	2.7
2	D	285	THR	2.6
2	D	177	ASP	2.6
4	F	235	ASP	2.6
2	D	400	GLY	2.6
2	D	92	PHE	2.6
3	E	6	MET	2.6
4	F	244	CYS	2.6
2	B	282	ARG	2.5
1	C	440	VAL	2.5
4	F	138	ARG	2.5
2	D	395	LEU	2.5
2	D	126	SER	2.5
4	F	373	SER	2.5
4	F	163	SER	2.5
2	D	192	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	2.4
4	F	146	VAL	2.4
3	E	46	SER	2.4
1	A	346	TRP	2.4
2	B	428	ALA	2.4
4	F	89	GLU	2.3
1	A	262	TYR	2.3
2	D	397	TRP	2.3
2	D	215	LEU	2.3
2	B	54	ALA	2.3
2	B	33	THR	2.3
2	D	199	THR	2.3
2	D	387	ALA	2.3
4	F	1	MET	2.3
2	B	253	LEU	2.3
2	D	135	LEU	2.2
3	E	62	LYS	2.2
2	D	405	GLU	2.2
4	F	99	VAL	2.2
4	F	98	TYR	2.2
3	E	133	VAL	2.2
2	B	427	ASP	2.2
2	D	56	GLY	2.2
4	F	186	LEU	2.1
2	D	78	SER	2.1
4	F	255	ARG	2.1
2	B	199	THR	2.1
2	B	250	LEU	2.1
2	B	37	HIS	2.1
3	E	48	GLU	2.0
2	D	39	ASP	2.0
4	F	147	TRP	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)

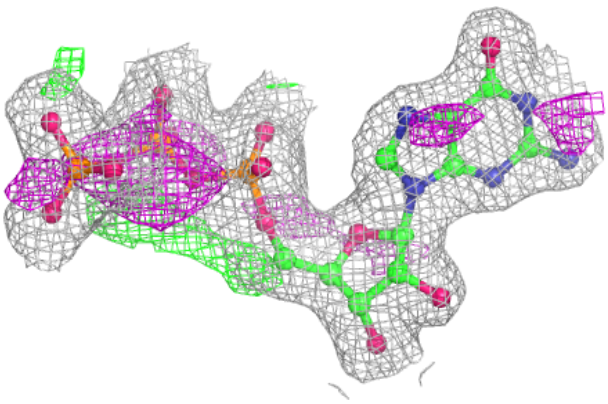
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

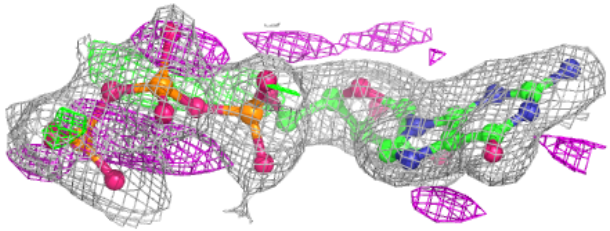
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GTP	D	501	32/32	0.93	0.10	29,34,39,41	0
8	GOL	A	504	6/6	0.93	0.13	35,36,38,39	0
10	MES	B	503	12/12	0.93	0.13	58,59,61,61	0
12	ACP	F	401	31/31	0.93	0.12	66,68,74,75	0
11	8WU	D	503	27/27	0.95	0.11	24,31,36,37	0
11	8WU	B	504	27/27	0.96	0.17	24,26,27,28	0
5	GTP	A	501	32/32	0.98	0.12	12,13,14,14	0
6	MG	A	502	1/1	0.98	0.12	17,17,17,17	0
6	MG	B	502	1/1	0.98	0.09	12,12,12,12	0
6	MG	D	502	1/1	0.98	0.05	22,22,22,22	0
7	CA	C	503	1/1	0.98	0.03	24,24,24,24	0
7	CA	A	503	1/1	0.99	0.04	28,28,28,28	0
6	MG	C	502	1/1	0.99	0.09	10,10,10,10	0
5	GTP	C	501	32/32	0.99	0.11	10,12,13,13	0
9	GDP	B	501	28/28	0.99	0.08	14,16,17,17	0

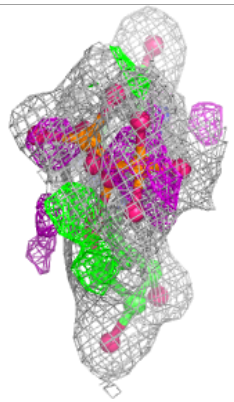
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP D 501:

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

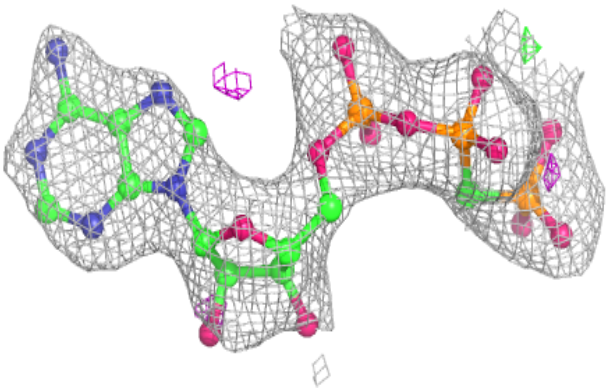


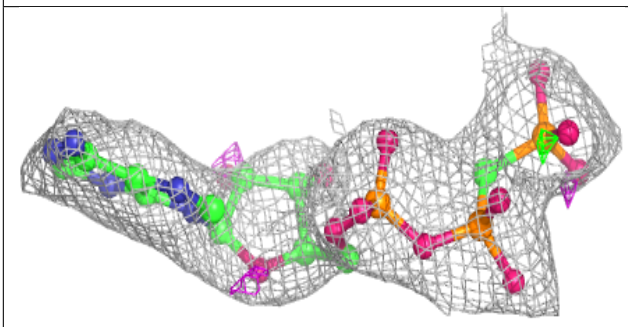


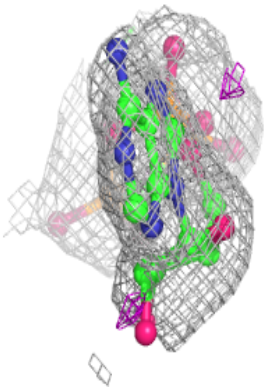


Electron density around ACP F 401:

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

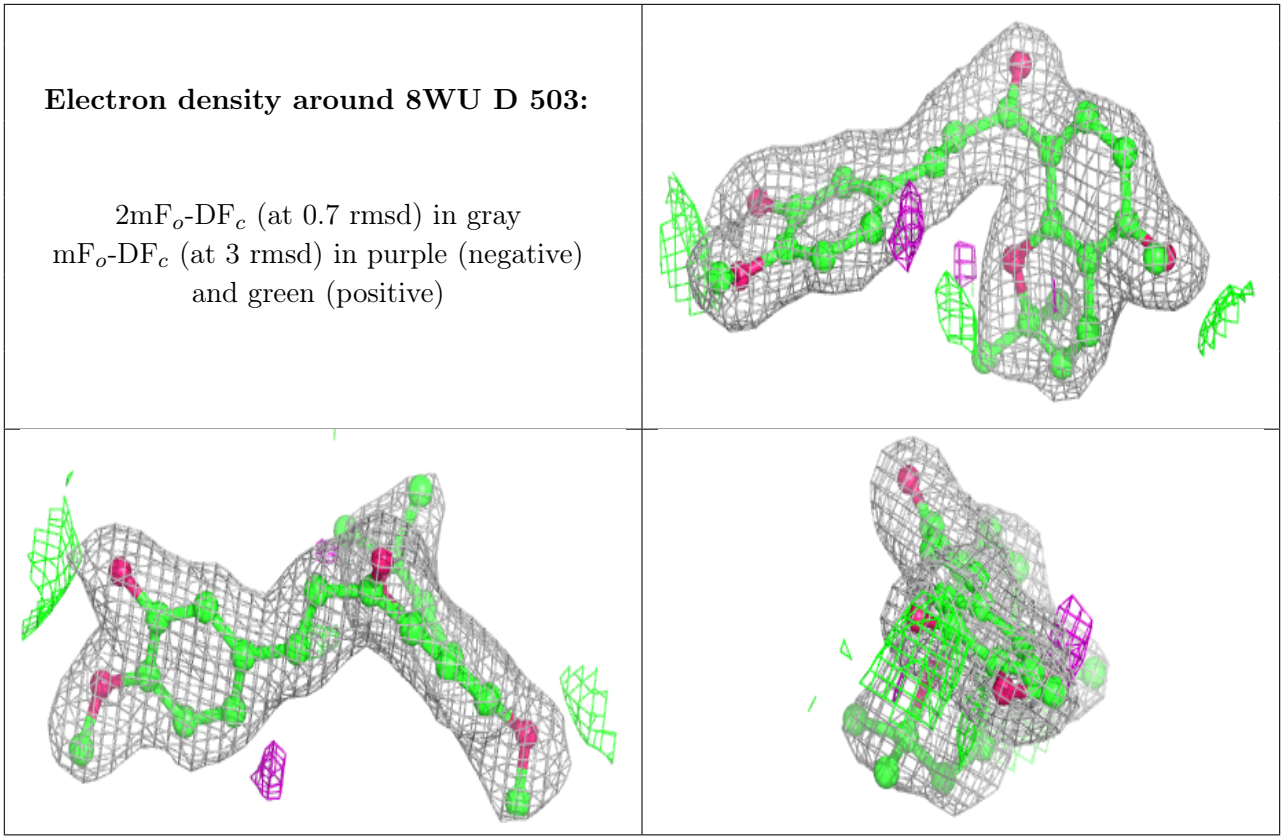






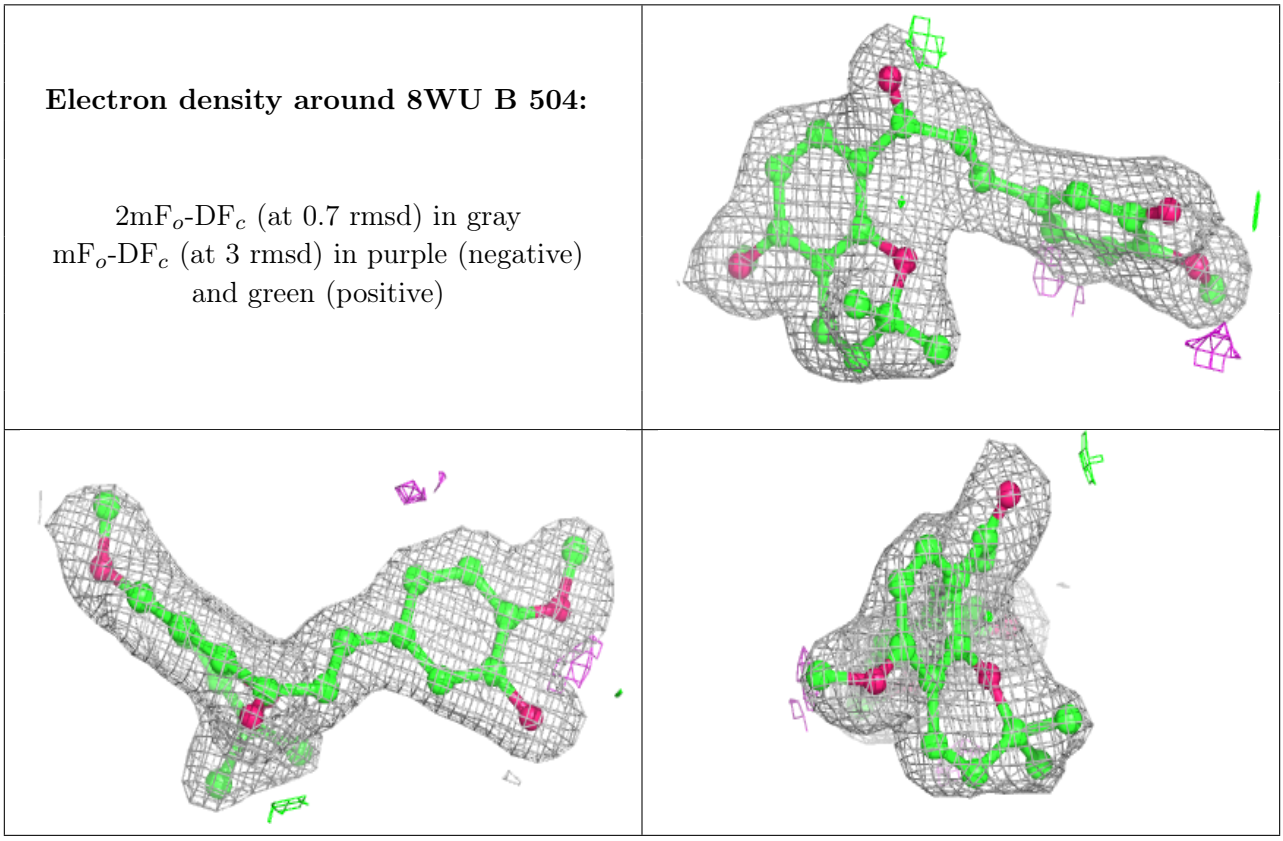
Electron density around 8WU D 503:

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



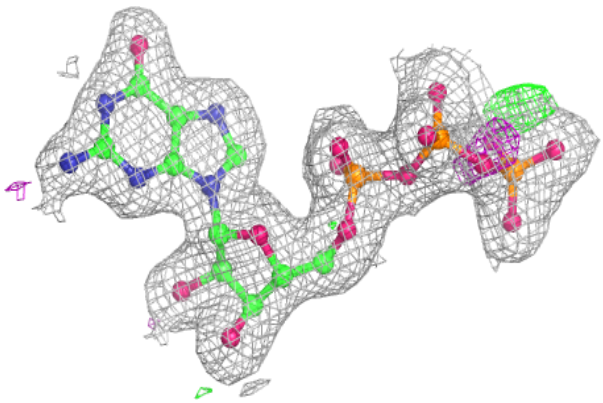
Electron density around 8WU B 504:

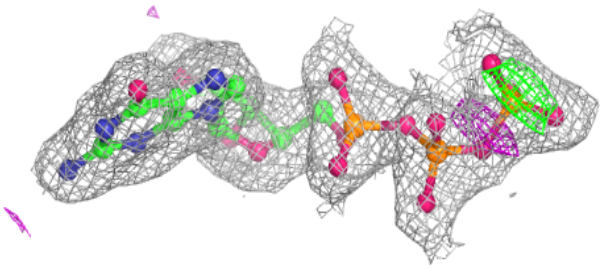
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

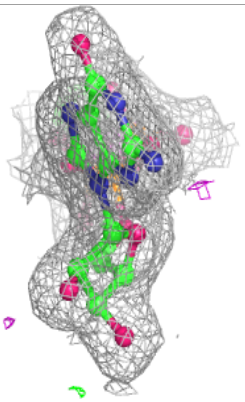


Electron density around GTP A 501:

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

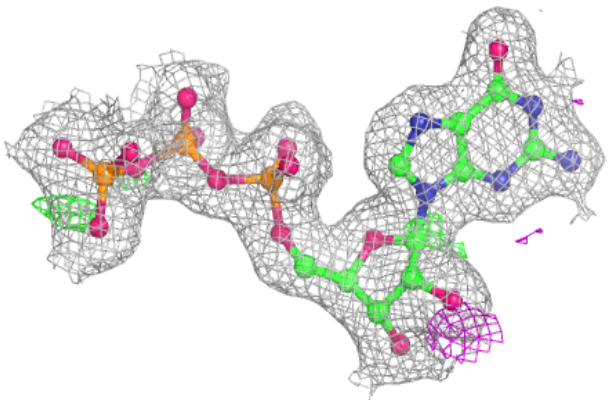


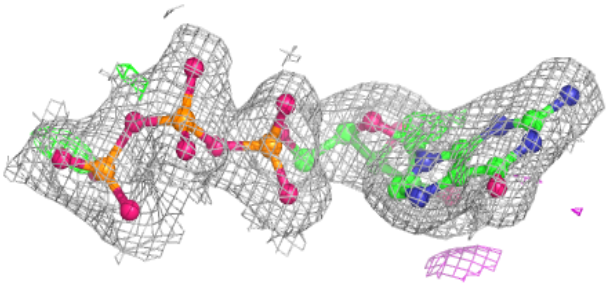


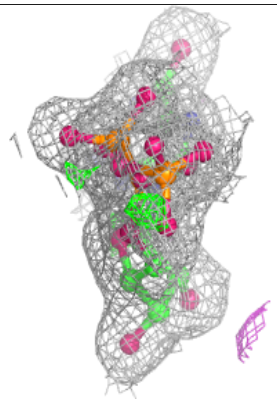


Electron density around GTP C 501:

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

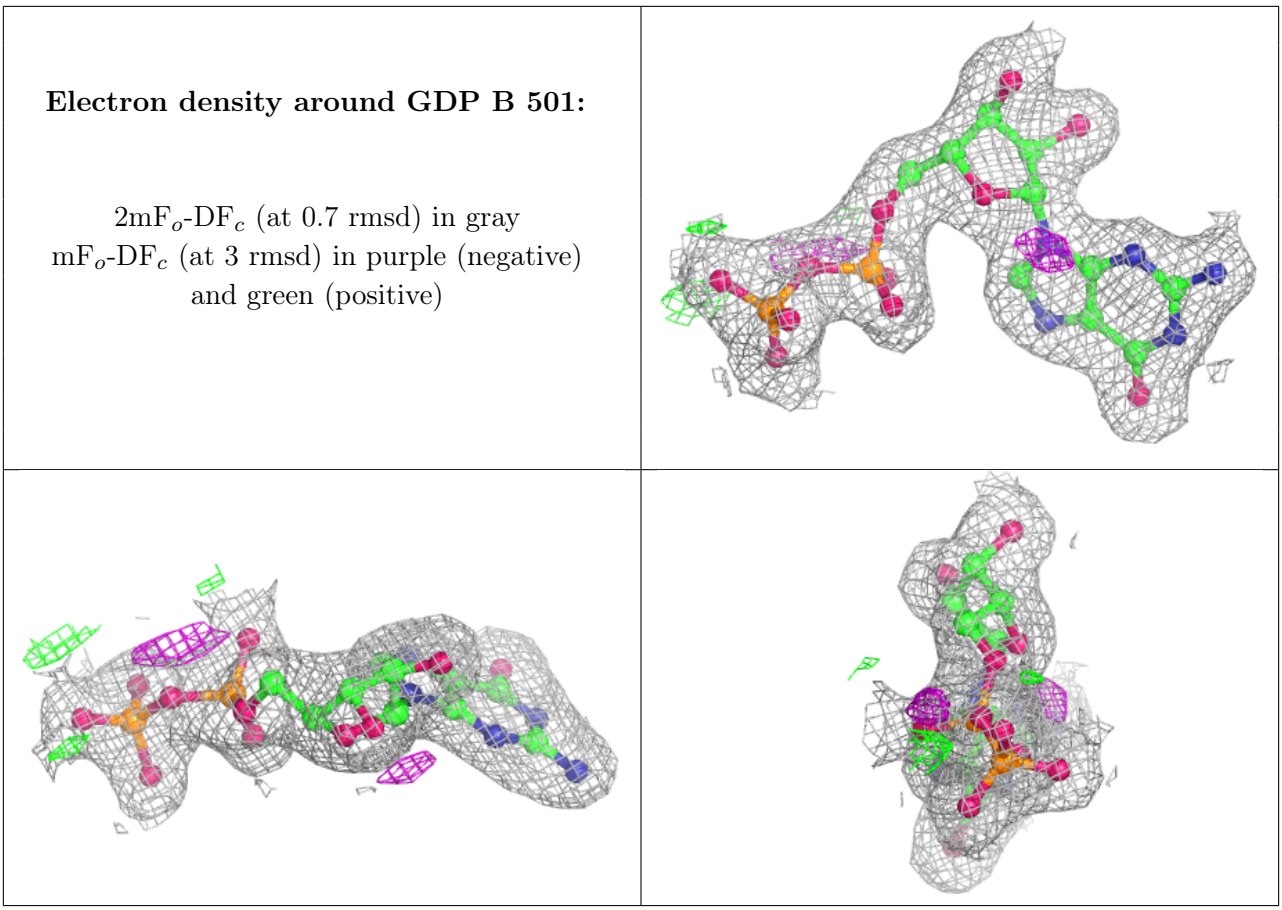






Electron density around GDP B 501:

$2mF_o$-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.