Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 10:39 AM JST

PDB ID	:	5XI7
Title	:	Crystal structure of T2R-TTL bound with PO-7
Authors	:	Chu, Y.; Wang, Y.; Yang, J.; Li, W.
Deposited on	:	2017-04-26
Resolution	:	2.99 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:

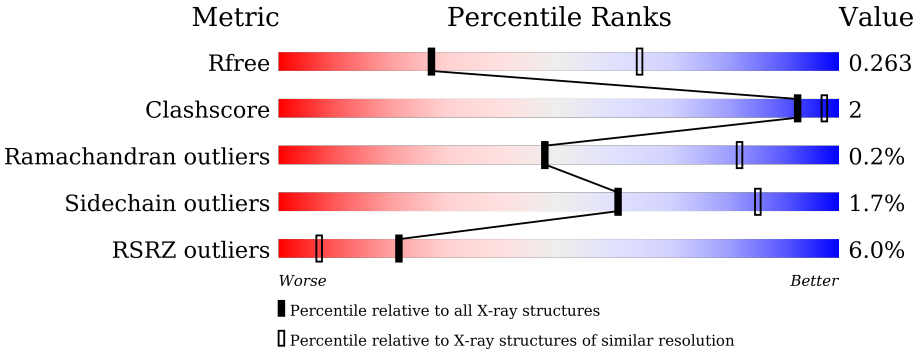
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	450	2%, 92%, • •
1	C	450	93%, 5% •
2	B	445	3%, 89%, 6% 5%
2	D	445	10%, 91%, • 5%
3	E	184	5%, 64%, • 35%
4	F	384	13%, 76%, 5% 20%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17449 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3441	2179	586	652	24	0	4	0
1	C	440	3482	2200	589	668	25	0	9	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	424	3353	2107	574	645	27	0	2	0
2	D	421	3306	2079	562	638	27	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	120	1004	621	181	196	6	0	2	0

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	309	2553	1645	438	455	15	0	3	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

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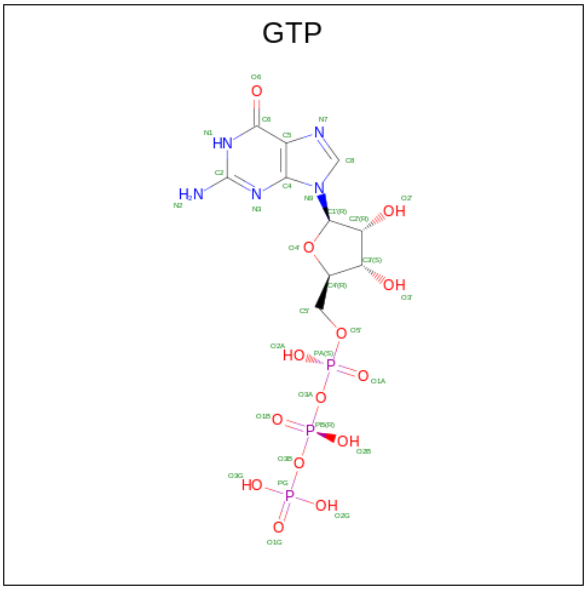
Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- 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		

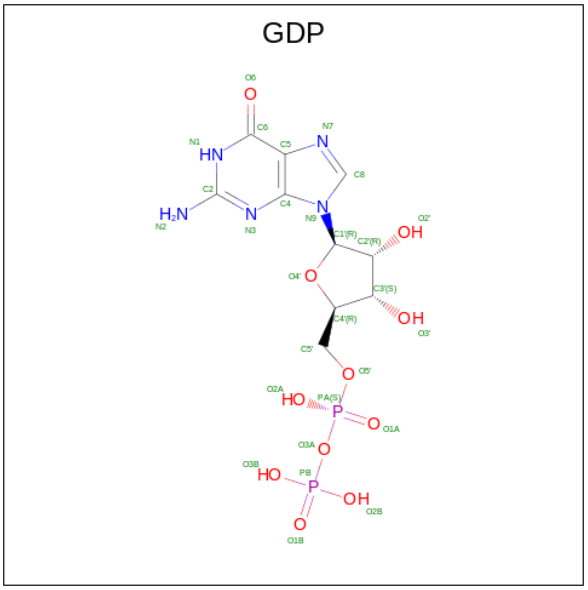
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		
6	D	1	Total	Mg	0	0
			1	1		

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

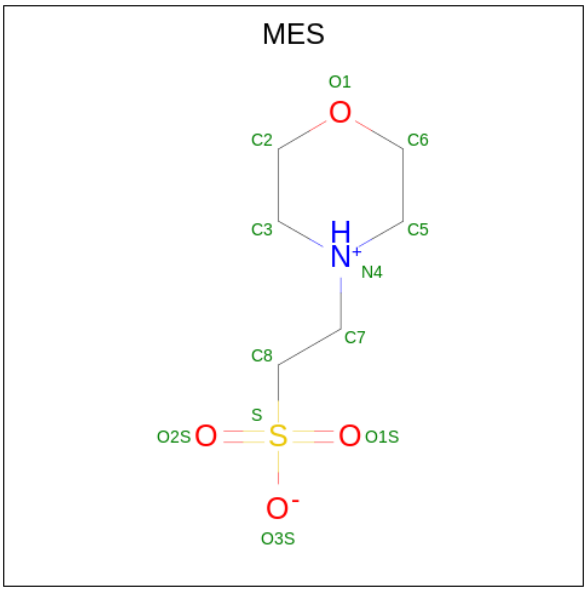
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
7	B	1	1	1	0	0
7	C	1	1	1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



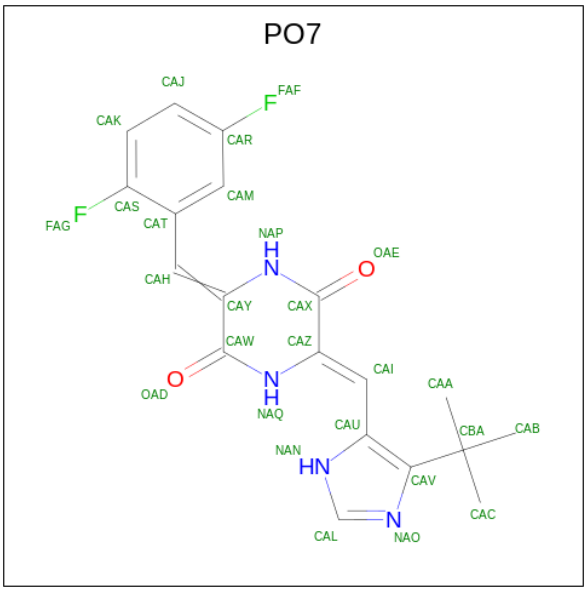
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0

- Molecule 9 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		
9	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is (6Z)-3-[[2,5-bis(fluoranyl)phenyl]methylidene]-6-[(4-tert-butyl-1H-imidazol-5-yl)methylidene]piperazine-2,5-dione (three-letter code: PO7) (formula: $C_{19}H_{18}F_2N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
10	B	1	27	19	2	4	2	0	0

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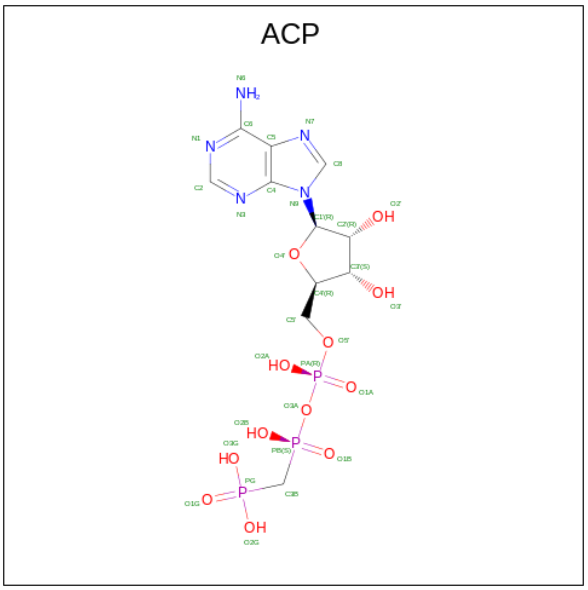
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
10	D	1	27	19	2	4	2	0	0

- Molecule 11 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		
11	F	1	31	11	5	12	3	0	0

- Molecule 12 is water.

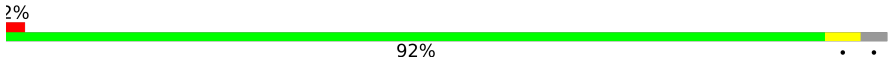
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	16	16	16	0	0
12	B	15	15	15	0	0
12	C	33	33	33	0	0
12	E	2	2	2	0	0
12	F	4	4	4	0	0

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.

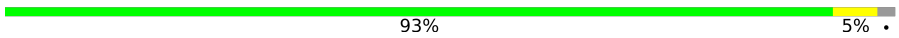
• Molecule 1: Tubulin alpha chain

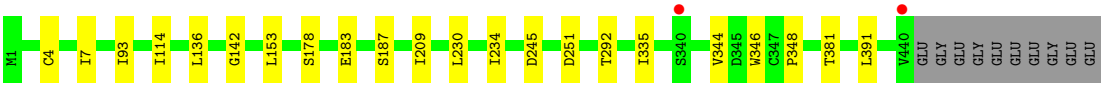
Chain A:



• Molecule 1: Tubulin alpha chain

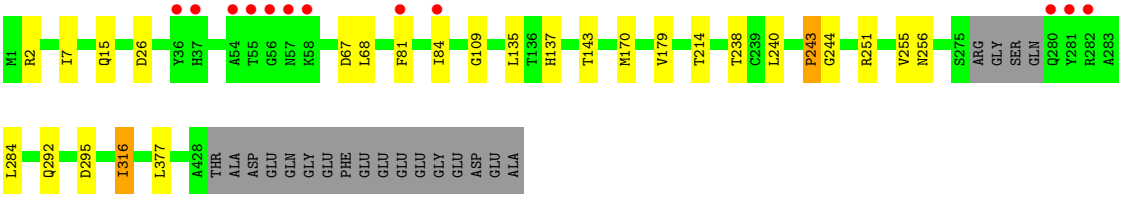
Chain C:





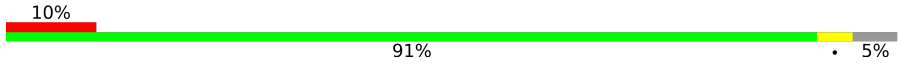
• Molecule 2: Tubulin beta chain

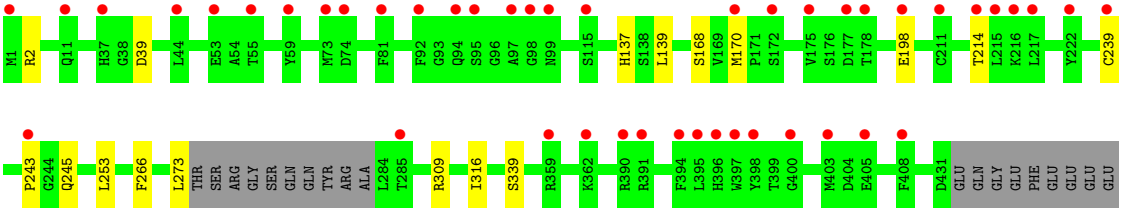
Chain B:

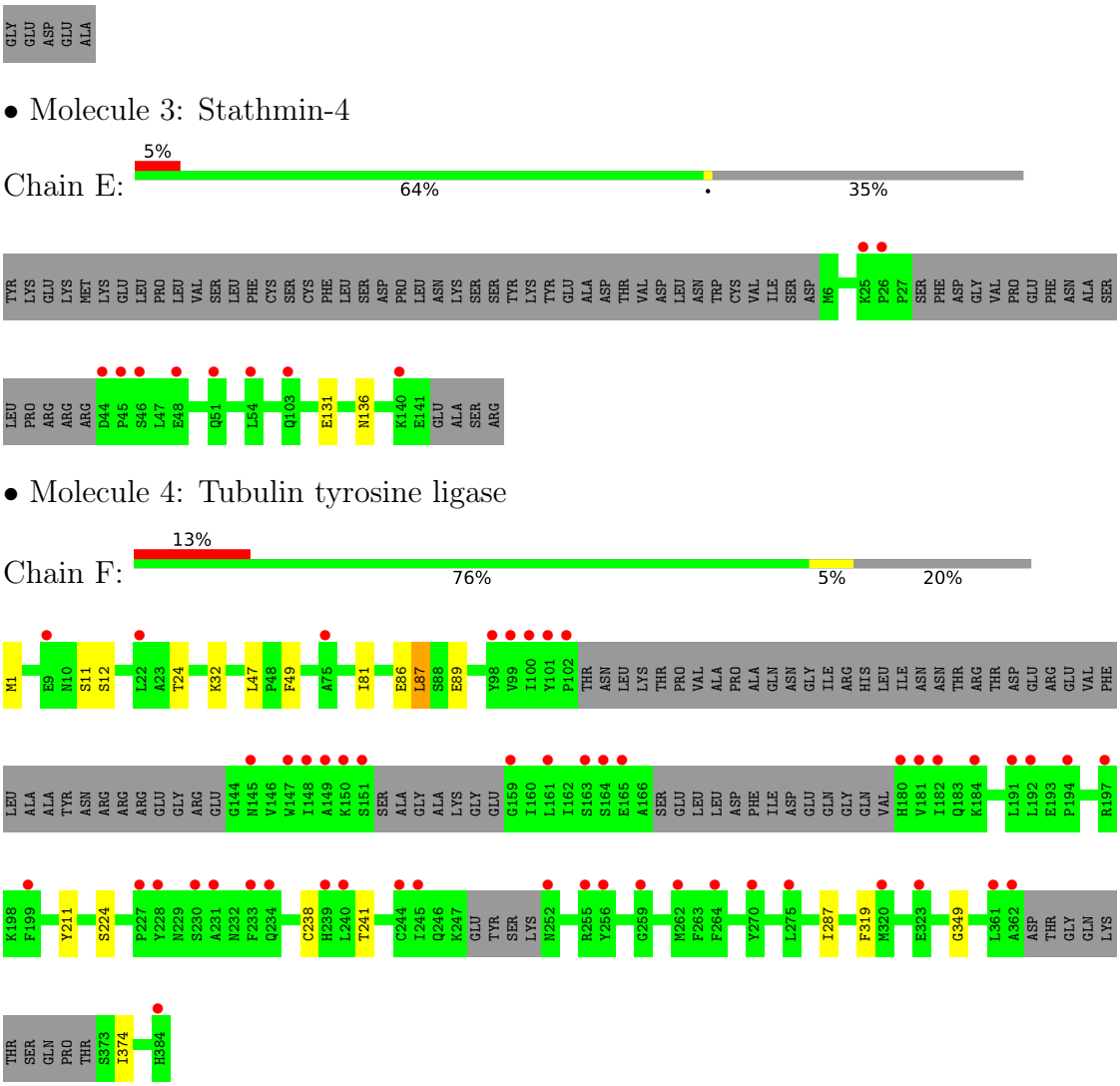


• Molecule 2: Tubulin beta chain

Chain D:






GLY GLU ASP GLU ALA
• Molecule 3: Stathmin-4
Chain E:
5%
64%
35%
TYR LYS GLU LYS MET LYS GLU LEU PRO LEU VAL SER LEU PHE CYS SER CYS PHE LEU SER ASP PRO LEU ASN LYS SER SER TYR LYS TYR GLU ALA ASP THR VAL ASP LEU ASN TRP CYS VAL ILE SER ASP M6 K25 P26 P27 SER PHE ASP GLY VAL PRO GLU PHE ASN ALA SER
LEU PRO ARG ARG ARG D44 P45 S46 L47 E48 Q51 L54 Q103 E131 N136 K140 E141 GLU ALA SER ARG
• Molecule 4: Tubulin tyrosine ligase
Chain F:
13%
76%
5%
20%
M1 E9 N10 S11 S12 L22 A23 T24 K32 L47 P48 F49 A75 I81 E86 L87 S88 E89 Y98 V99 I100 Y101 P102 THR ASN LEU LYS THR PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG THR ASP GLU ARG GLU VAL PHE
LEU ALA ALA TYR ASN ARG ARG ARG GLU GLY ARG GLU G144 N145 V146 W147 I148 A149 K150 S151 SER ALA GLY ALA LYS GLY GLU G159 I160 L161 I162 S163 S164 E165 A166 SER GLU LEU LEU ASP PHE ILE ASP GLU GLN GLY GLN VAL H180 V181 I182 Q183 K184 L191 L192 E193 P194 R197
K198 F199 Y211 S224 P227 Y228 N229 S230 A231 N232 F233 Q234 C238 H239 L240 T241 C244 I245 Q246 K247 GLU TYR SER LYS N252 R255 Y256 G259 M262 F263 F264 Y270 L275 I287 F319 M320 E323 G349 L361 A362 ASP THR GLY GLN LYS
THR SER GLN PRO THR S373 I374 H384

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.25Å 157.38Å 182.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.17 – 2.99 48.12 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (119.17-2.99) 97.3 (48.12-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.222 , 0.266 0.221 , 0.263	Depositor DCC
R_{free} test set	3119 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17449	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: CA, ACP, PO7, GTP, GDP, MG, MES

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	0.38	0/3525	0.61	0/4784
1	C	0.38	0/3572	0.61	0/4850
2	B	0.39	0/3427	0.60	0/4640
2	D	0.41	0/3379	0.59	0/4577
3	E	0.40	0/1018	0.55	0/1350
4	F	0.40	0/2618	0.56	0/3537
All	All	0.39	0/17539	0.59	0/23738

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	3441	0	3363	15	0
1	C	3482	0	3384	11	0
2	B	3353	0	3228	16	0
2	D	3306	0	3181	6	0
3	E	1004	0	1028	0	0
4	F	2553	0	2519	5	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	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	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	2	0
10	B	27	0	0	1	0
10	D	27	0	0	2	0
11	F	31	0	14	0	0
12	A	16	0	0	0	0
12	B	15	0	0	0	0
12	C	33	0	0	0	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17449	0	16791	52	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 (52) 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:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.09	1.08
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.67	1.07
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.85	0.81
1:C:178:SER:OG	1:C:183:GLU:OE2	2.02	0.75
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.19	0.73
2:B:295:ASP:HA	9:B:505:MES:O2S	1.95	0.66
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.80	0.63
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:N	2.15	0.61
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.40	0.61
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:H	1.66	0.59
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.52	0.56
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.87	0.55
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.88	0.54
2:B:251:ARG:NH1	9:B:503:MES:O2S	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:THR:HB	2:B:316:ILE:HD11	1.90	0.52
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.45	0.51
1:A:187:SER:CB	1:A:391:LEU:HD21	2.41	0.50
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.94	0.48
4:F:224:SER:HB2	4:F:241:THR:HG22	1.94	0.48
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.94	0.48
2:D:309:ARG:NH1	2:D:339:SER:O	2.48	0.46
4:F:81:ILE:O	4:F:87:LEU:O	2.33	0.46
2:B:7:ILE:HB	2:B:135:LEU:HD12	1.98	0.45
2:D:139:LEU:HD12	2:D:170:MET:SD	2.57	0.45
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.17	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.52	0.44
2:B:251:ARG:O	2:B:255:VAL:HG23	2.17	0.44
2:B:284:LEU:HD21	2:B:292:GLN:HE22	1.83	0.44
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.44
10:D:503:PO7:NAN	10:D:503:PO7:NAQ	2.66	0.43
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:HG3	1.70	0.43
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.59	0.43
2:D:139:LEU:HD11	2:D:168:SER:HB3	2.00	0.43
2:B:68:LEU:HD21	2:B:109:GLY:HA2	2.01	0.42
2:B:240:LEU:HD12	10:B:506:PO7:FAF	2.10	0.42
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.84	0.42
4:F:47:LEU:HD22	4:F:49:PHE:CE1	2.54	0.42
2:B:67:ASP:HA	2:B:143:THR:HG21	2.01	0.42
2:B:170:MET:HG3	2:B:377:LEU:HD21	2.02	0.42
1:C:230:LEU:O	1:C:234:ILE:HD12	2.19	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.54	0.42
2:B:243:PRO:HB3	2:B:244:GLY:HA2	1.99	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41
2:D:239:CYS:SG	10:D:503:PO7:OAE	2.77	0.41
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.56	0.41
2:D:214:THR:HG21	2:D:273:LEU:HD12	2.03	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.20	0.40
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.03	0.40
2:D:198:GLU:HB2	2:D:266:PHE:CE2	2.56	0.40
2:B:81:PHE:O	2:B:84:ILE:HG22	2.22	0.40
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.03	0.40
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.04	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	439/450 (98%)	427 (97%)	12 (3%)	0	100	100
1	C	446/450 (99%)	437 (98%)	9 (2%)	0	100	100
2	B	422/445 (95%)	404 (96%)	17 (4%)	1 (0%)	47	82
2	D	417/445 (94%)	396 (95%)	19 (5%)	2 (0%)	29	68
3	E	118/184 (64%)	114 (97%)	4 (3%)	0	100	100
4	F	300/384 (78%)	286 (95%)	13 (4%)	1 (0%)	41	76
All	All	2142/2358 (91%)	2064 (96%)	74 (4%)	4 (0%)	47	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	D	243	PRO
4	F	11	SER
2	D	39	ASP

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	372/378 (98%)	363 (98%)	9 (2%)	49	79
1	C	379/378 (100%)	375 (99%)	4 (1%)	73	90
2	B	367/383 (96%)	361 (98%)	6 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	362/383 (94%)	357 (99%)	5 (1%)	67	88
3	E	110/168 (66%)	108 (98%)	2 (2%)	59	85
4	F	281/342 (82%)	272 (97%)	9 (3%)	39	74
All	All	1871/2032 (92%)	1836 (98%)	35 (2%)	60	84

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	237	SER
1	A	316[A]	CYS
1	A	316[B]	CYS
1	A	320	ARG
1	A	326	LYS
1	A	402	ARG
2	B	2	ARG
2	B	15	GLN
2	B	26	ASP
2	B	137	HIS
2	B	214	THR
2	B	316	ILE
1	C	245	ASP
1	C	251[A]	ASP
1	C	251[B]	ASP
1	C	381	THR
2	D	2	ARG
2	D	137	HIS
2	D	245	GLN
2	D	253	LEU
2	D	316	ILE
3	E	131	GLU
3	E	136	ASN
4	F	1	MET
4	F	12	SER
4	F	24	THR
4	F	32	LYS
4	F	86	GLU
4	F	87	LEU
4	F	89	GLU

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Mol	Chain	Res	Type
4	F	211	TYR
4	F	238	CYS

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	35	GLN
1	A	101	ASN
2	B	292	GLN
1	C	249	ASN
1	C	356	ASN
3	E	136	ASN
4	F	242	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 16 ligands modelled in this entry, 7 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	A	501	6	26,34,34	0.98	1 (3%)	32,54,54	1.08	2 (6%)
8	GDP	B	501	6	24,30,30	1.01	1 (4%)	30,47,47	1.08	3 (10%)
5	GTP	C	501	6	26,34,34	0.90	1 (3%)	32,54,54	1.14	1 (3%)
9	MES	B	503	-	12,12,12	1.98	1 (8%)	14,16,16	7.23	9 (64%)
10	PO7	B	506	-	25,29,29	2.08	7 (28%)	32,43,43	1.73	6 (18%)
10	PO7	D	503	-	25,29,29	2.29	6 (24%)	32,43,43	1.81	7 (21%)
11	ACP	F	401	-	27,33,33	2.00	8 (29%)	32,52,52	1.39	3 (9%)
9	MES	B	505	-	12,12,12	2.04	2 (16%)	14,16,16	6.16	7 (50%)
5	GTP	D	501	6	26,34,34	0.92	0	32,54,54	1.26	4 (12%)

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	A	501	6	-	3/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
10	PO7	B	506	-	-	4/14/14/14	0/3/3/3
10	PO7	D	503	-	-	4/14/14/14	0/3/3/3
11	ACP	F	401	-	-	6/15/38/38	0/3/3/3
9	MES	B	505	-	-	2/6/14/14	0/1/1/1
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	PO7	FAF-CAR	-6.30	1.21	1.36
9	B	503	MES	C8-S	-6.28	1.68	1.77
9	B	505	MES	C8-S	-6.28	1.68	1.77
11	F	401	ACP	PG-O1G	5.44	1.61	1.50
10	B	506	PO7	CAY-CAW	-4.15	1.40	1.48
10	D	503	PO7	CAY-CAW	-4.12	1.40	1.48
11	F	401	ACP	PB-O1B	4.04	1.61	1.51
10	D	503	PO7	CAI-CAZ	3.92	1.42	1.34
10	B	506	PO7	CAZ-CAX	-3.90	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	506	PO7	CAT-CAH	-3.85	1.40	1.46
10	D	503	PO7	CAH-CAY	3.66	1.42	1.34
10	D	503	PO7	CAZ-CAX	-3.51	1.41	1.48
11	F	401	ACP	PB-O3A	3.48	1.62	1.58
10	B	506	PO7	CAI-CAZ	3.47	1.41	1.34
10	B	506	PO7	FAF-CAR	-3.46	1.28	1.36
10	B	506	PO7	CAH-CAY	3.34	1.41	1.34
11	F	401	ACP	PB-O2B	-3.24	1.48	1.56
10	D	503	PO7	CAT-CAH	-3.18	1.41	1.46
11	F	401	ACP	PG-O2G	2.94	1.61	1.54
11	F	401	ACP	PG-O3G	-2.81	1.48	1.54
11	F	401	ACP	C5-C4	2.58	1.47	1.40
5	A	501	GTP	C6-N1	-2.37	1.34	1.37
9	B	505	MES	O2S-S	2.19	1.51	1.45
5	C	501	GTP	C6-N1	-2.19	1.34	1.37
8	B	501	GDP	C6-N1	-2.10	1.34	1.37
10	B	506	PO7	CAT-CAS	2.03	1.42	1.39
11	F	401	ACP	C2-N3	2.01	1.35	1.32

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	503	MES	O1S-S-C8	-17.46	85.89	106.92
9	B	505	MES	O3S-S-O1S	-13.78	77.59	111.27
9	B	503	MES	O2S-S-C8	11.46	120.71	106.92
9	B	505	MES	O3S-S-C8	11.05	123.64	105.77
9	B	503	MES	O3S-S-O1S	-10.92	84.60	111.27
9	B	505	MES	O1S-S-C8	-9.44	95.54	106.92
9	B	503	MES	O2S-S-O1S	-9.29	81.79	113.95
9	B	505	MES	O2S-S-O1S	-8.38	84.94	113.95
9	B	503	MES	O3S-S-C8	7.12	117.28	105.77
9	B	505	MES	O3S-S-O2S	6.14	126.28	111.27
10	D	503	PO7	CAZ-CAX-NAP	5.13	121.06	116.02
10	D	503	PO7	CAY-CAW-NAQ	4.58	120.52	116.02
10	B	506	PO7	CAZ-CAX-NAP	4.32	120.27	116.02
10	B	506	PO7	CAY-CAW-NAQ	4.11	120.06	116.02
9	B	503	MES	C2-C3-N4	3.88	115.98	110.10
11	F	401	ACP	N3-C2-N1	-3.82	122.71	128.68
10	B	506	PO7	FAG-CAS-CAT	3.48	122.97	118.10
11	F	401	ACP	C3'-C2'-C1'	3.29	105.94	100.98
9	B	503	MES	O3S-S-O2S	3.10	118.86	111.27
10	D	503	PO7	FAG-CAS-CAT	3.08	122.41	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	503	PO7	CAY-NAP-CAX	-2.96	122.03	125.53
11	F	401	ACP	C4-C5-N7	-2.80	106.48	109.40
10	B	506	PO7	CBA-CAV-NAO	2.77	123.95	120.50
5	D	501	GTP	PA-O3A-PB	-2.75	123.41	132.83
8	B	501	GDP	PA-O3A-PB	-2.60	123.90	132.83
10	B	506	PO7	CAY-NAP-CAX	-2.53	122.53	125.53
9	B	503	MES	C6-C5-N4	2.52	113.93	110.10
9	B	505	MES	C6-C5-N4	2.47	113.85	110.10
5	D	501	GTP	C5-C6-N1	2.46	118.29	113.95
8	B	501	GDP	C8-N7-C5	2.36	107.48	102.99
10	D	503	PO7	CAZ-NAQ-CAW	-2.34	122.76	125.53
10	B	506	PO7	CAZ-NAQ-CAW	-2.31	122.80	125.53
8	B	501	GDP	C5-C6-N1	2.28	117.97	113.95
5	D	501	GTP	C8-N7-C5	2.27	107.32	102.99
5	C	501	GTP	PA-O3A-PB	-2.23	125.16	132.83
5	A	501	GTP	C8-N7-C5	2.20	107.17	102.99
9	B	503	MES	C5-N4-C3	2.16	113.69	108.83
10	D	503	PO7	CAI-CAZ-NAQ	-2.13	120.95	125.02
5	A	501	GTP	PA-O3A-PB	-2.12	125.55	132.83
9	B	505	MES	C7-N4-C5	-2.10	105.88	111.23
5	D	501	GTP	PB-O3B-PG	-2.03	125.84	132.83
10	D	503	PO7	OAE-CAX-NAP	-2.01	116.26	120.12

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	N4-C7-C8-S
10	B	506	PO7	CAT-CAH-CAY-CAW
10	B	506	PO7	CAT-CAH-CAY-NAP
10	B	506	PO7	CAZ-CAI-CAU-NAN
10	B	506	PO7	CAZ-CAI-CAU-CAV
10	D	503	PO7	CAT-CAH-CAY-CAW

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Mol	Chain	Res	Type	Atoms
10	D	503	PO7	CAT-CAH-CAY-NAP
10	D	503	PO7	CAZ-CAI-CAU-NAN
10	D	503	PO7	CAZ-CAI-CAU-CAV
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	503	MES	C7-C8-S-O3S
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	505	MES	C7-C8-S-O3S
5	C	501	GTP	C4'-C5'-O5'-PA
9	B	503	MES	C7-C8-S-O2S
9	B	505	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
5	D	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PB-C3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

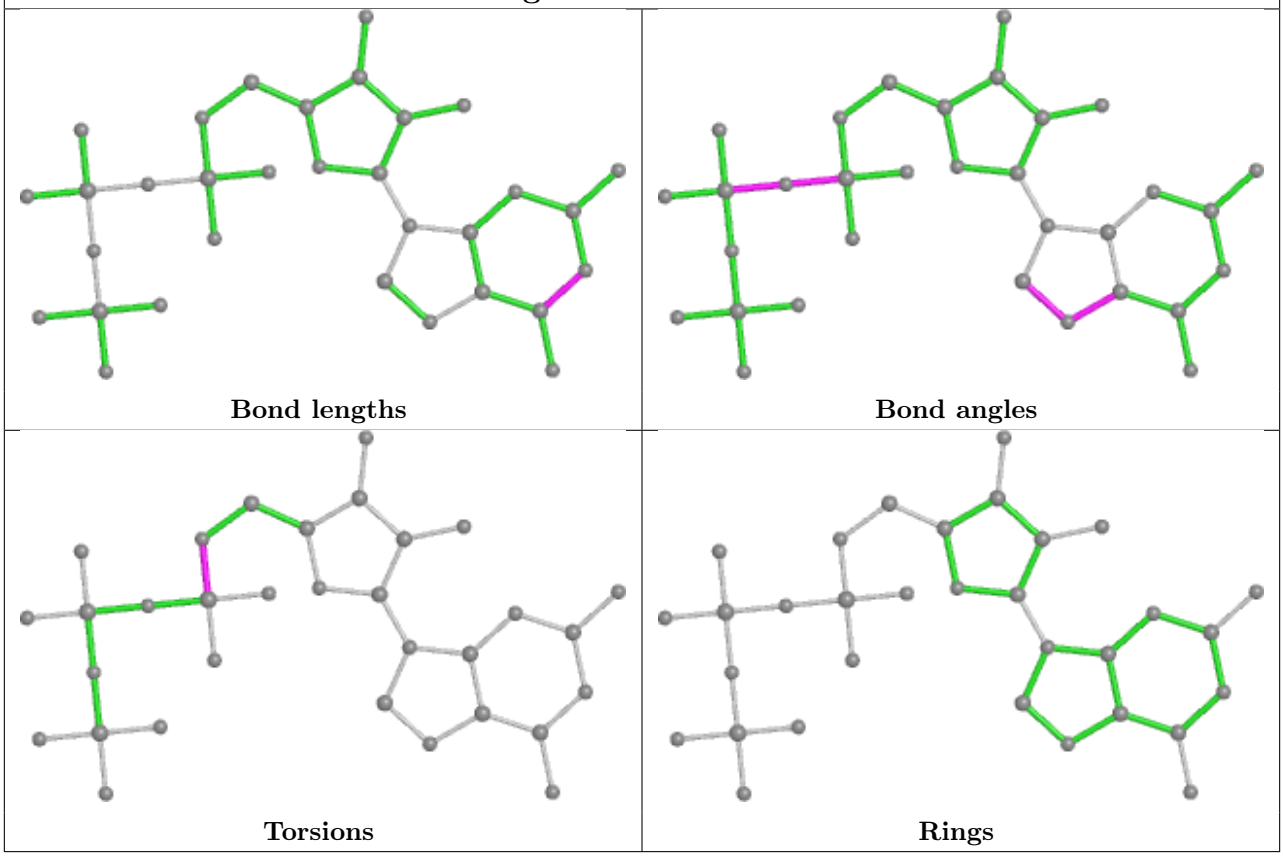
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	1	0
10	B	506	PO7	1	0
10	D	503	PO7	2	0
9	B	505	MES	1	0

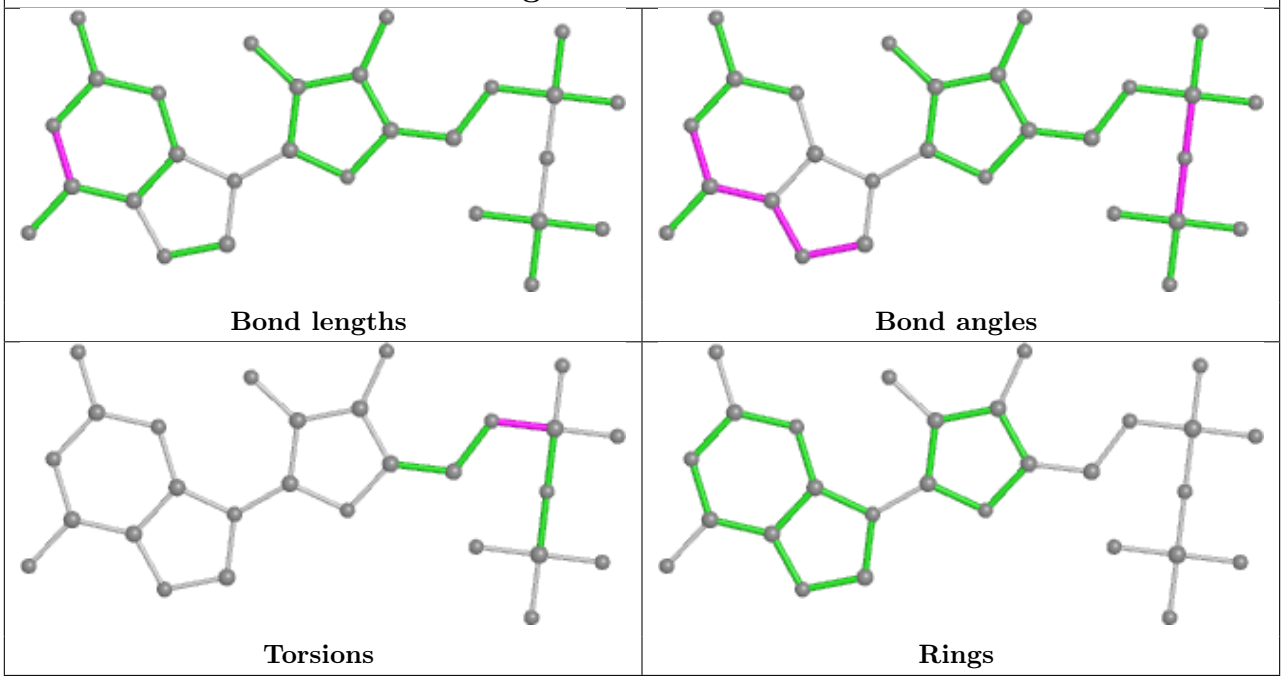
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

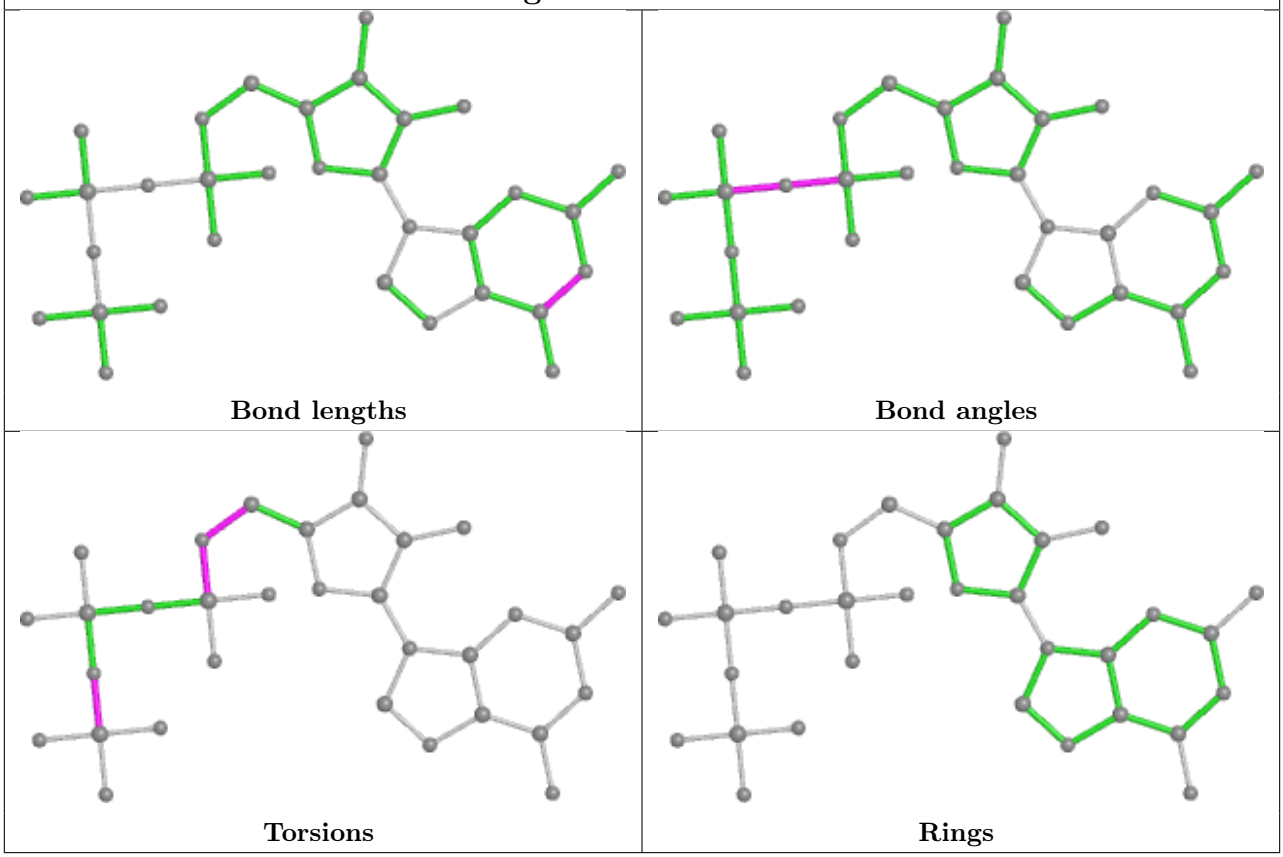
Ligand GTP A 501



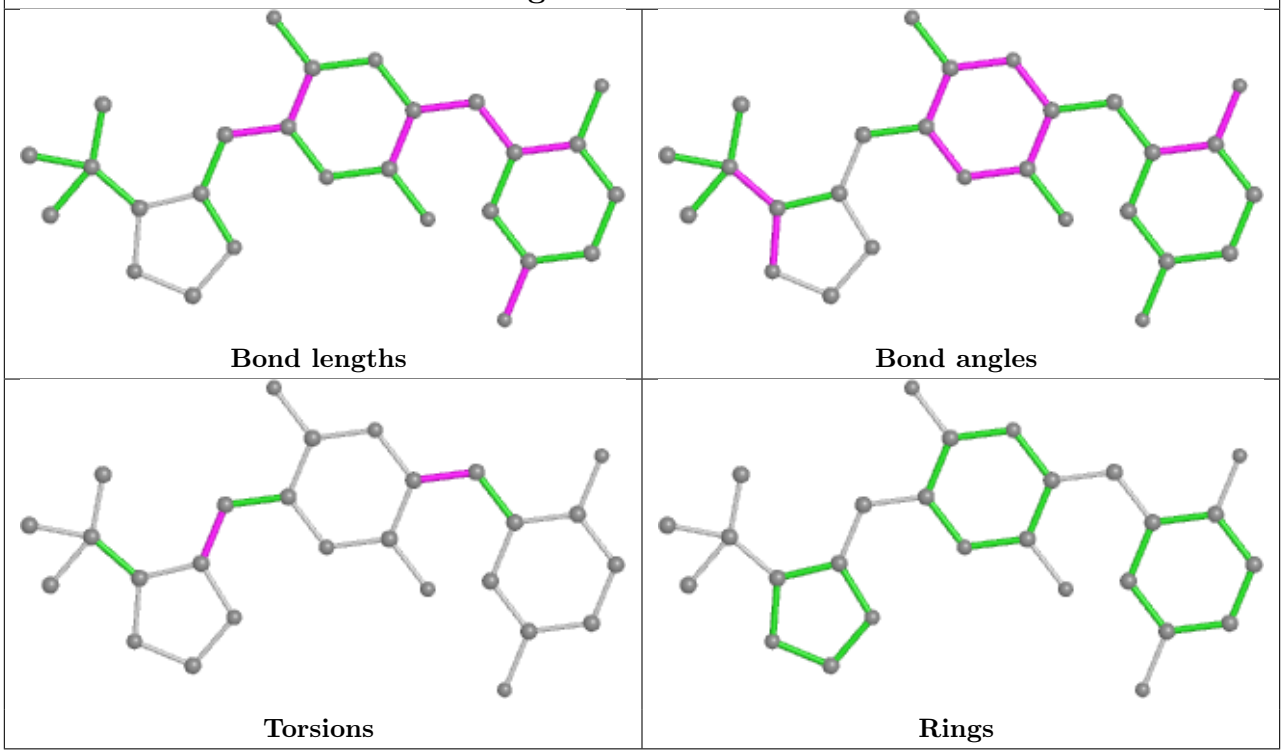
Ligand GDP B 501



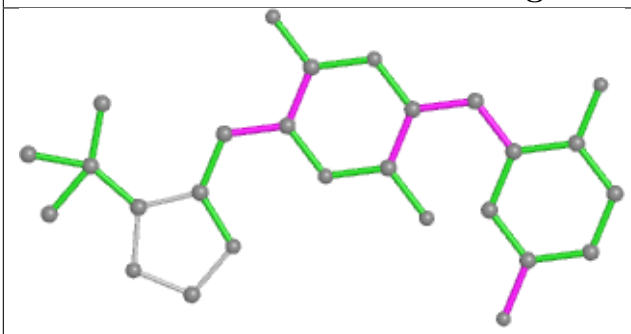
Ligand GTP C 501



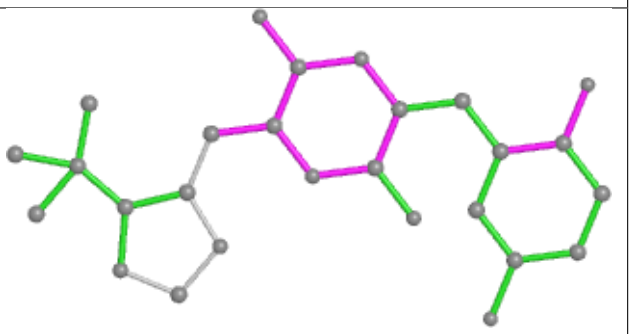
Ligand PO7 B 506



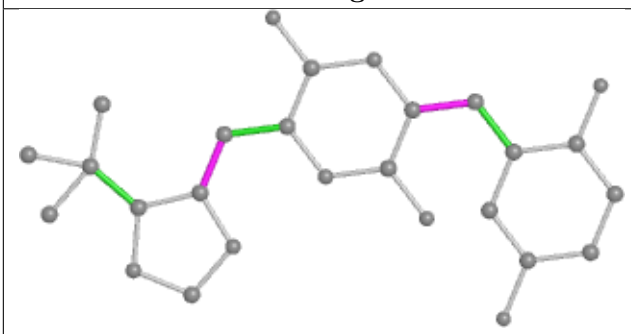
Ligand PO7 D 503



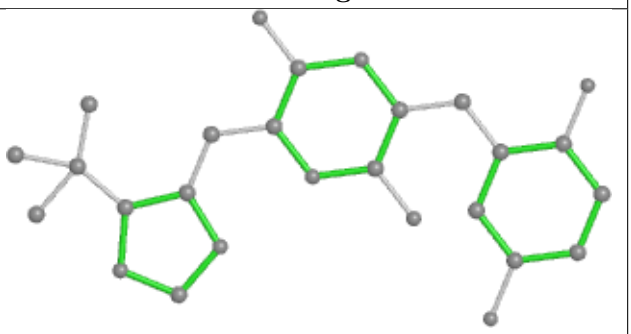
Bond lengths



Bond angles

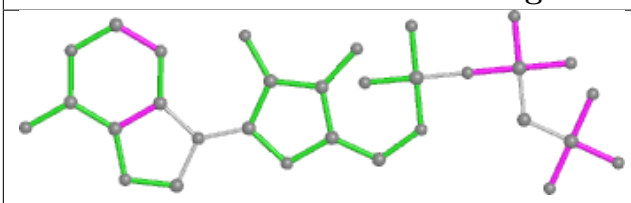


Torsions

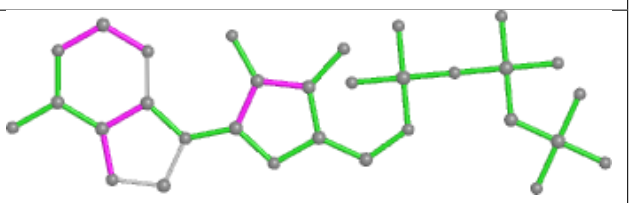


Rings

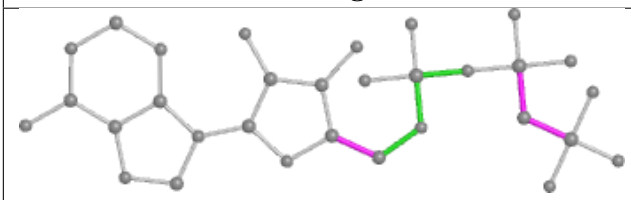
Ligand ACP F 401



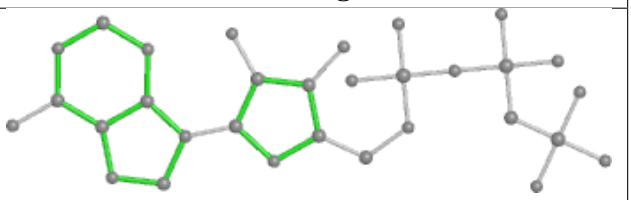
Bond lengths



Bond angles

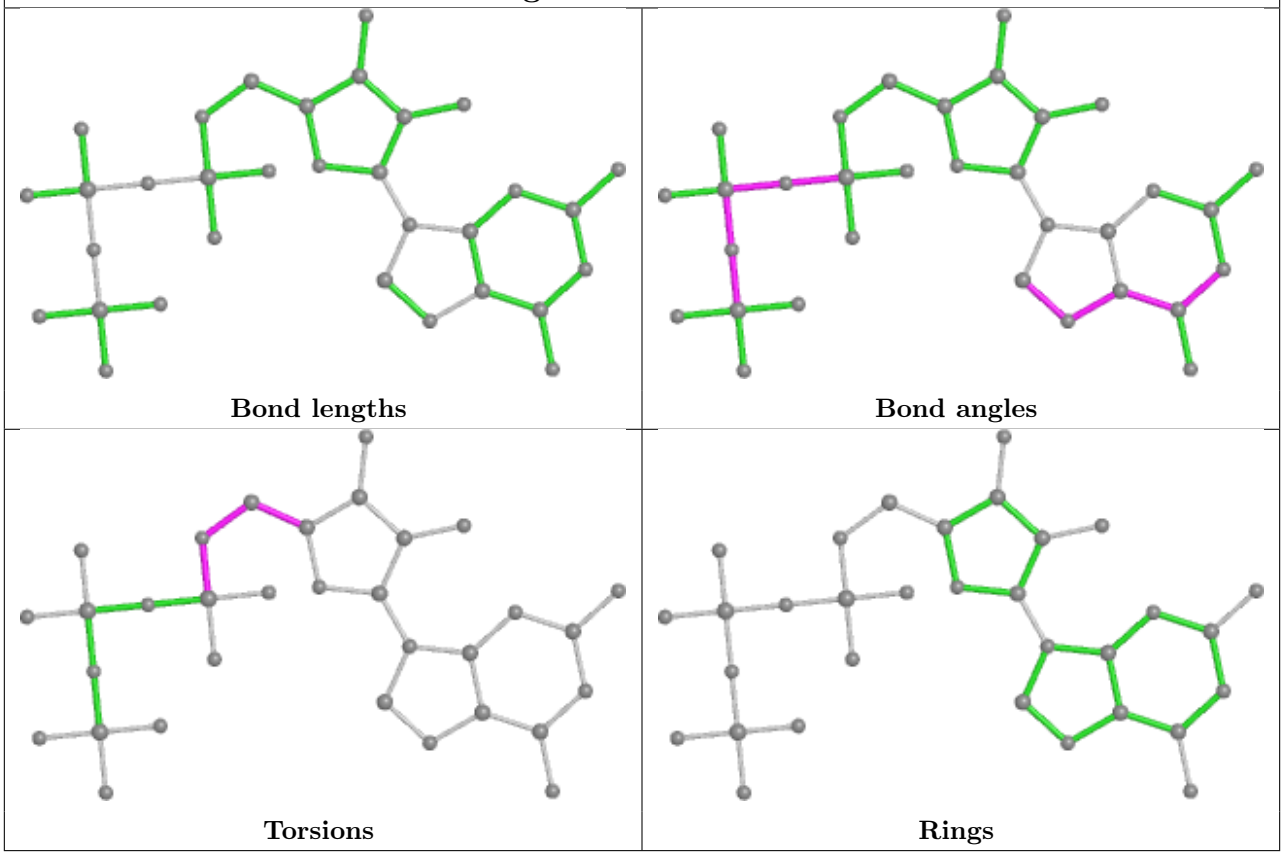


Torsions



Rings

Ligand GTP D 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	437/450 (97%)	0.05	8 (1%) 68 40	30, 49, 78, 98	0
1	C	440/450 (97%)	-0.17	2 (0%) 91 75	23, 39, 66, 81	1 (0%)
2	B	424/445 (95%)	0.02	12 (2%) 53 25	27, 48, 78, 114	1 (0%)
2	D	421/445 (94%)	0.67	45 (10%) 6 2	37, 75, 111, 149	4 (0%)
3	E	120/184 (65%)	0.53	10 (8%) 11 3	39, 71, 104, 116	0
4	F	309/384 (80%)	0.78	51 (16%) 1 0	40, 77, 120, 147	0
All	All	2151/2358 (91%)	0.25	128 (5%) 21 7	23, 55, 104, 149	6 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	8.4
4	F	182	ILE	7.6
2	D	55	THR	5.4
2	D	396	HIS	5.3
4	F	149	ALA	5.0
2	D	215	LEU	4.4
4	F	100	ILE	4.4
2	D	394	PHE	4.2
4	F	147	TRP	4.1
4	F	233	PHE	4.0
4	F	245	ILE	4.0
4	F	362	ALA	4.0
4	F	150	LYS	3.9
2	D	403	MET	3.8
4	F	101	TYR	3.8
4	F	192	LEU	3.8
4	F	180	HIS	3.6
4	F	228	TYR	3.6
2	B	280	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	3.5
4	F	184	LYS	3.5
1	A	346	TRP	3.5
2	B	56	GLY	3.5
2	B	55	THR	3.4
4	F	256	TYR	3.4
2	D	97	ALA	3.4
4	F	191	LEU	3.4
4	F	240	LEU	3.4
2	B	57	ASN	3.4
2	D	397	TRP	3.4
4	F	264	PHE	3.3
2	B	37	HIS	3.3
4	F	98	TYR	3.3
2	D	92	PHE	3.3
2	D	1	MET	3.2
2	D	37	HIS	3.2
2	B	281	TYR	3.2
2	D	391	ARG	3.2
4	F	262	MET	3.2
4	F	197	ARG	3.2
2	D	98	GLY	3.2
2	B	282	ARG	3.1
1	A	163	LYS	3.1
4	F	159	GLY	3.1
4	F	255	ARG	3.1
2	D	211	CYS	3.1
3	E	26	PRO	3.0
1	C	440	VAL	3.0
4	F	165	GLU	2.9
4	F	151	SER	2.9
4	F	199	PHE	2.9
2	D	405	GLU	2.9
2	D	44	LEU	2.9
2	D	214	THR	2.9
4	F	234	GLN	2.9
4	F	320	MET	2.9
2	D	285	THR	2.8
4	F	227	PRO	2.8
2	D	359	ARG	2.8
4	F	361	LEU	2.8
2	D	408	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	398	TYR	2.7
1	A	88	HIS	2.7
4	F	164	SER	2.7
2	D	177	ASP	2.7
2	B	81	PHE	2.7
4	F	102	PRO	2.7
3	E	48	GLU	2.6
2	B	36	TYR	2.6
4	F	231	ALA	2.6
2	B	54	ALA	2.6
2	D	395	LEU	2.6
4	F	239	HIS	2.6
4	F	270	TYR	2.6
4	F	194	PRO	2.6
2	D	73	MET	2.5
2	D	53	GLU	2.5
4	F	22	LEU	2.5
2	D	59	TYR	2.5
1	A	42	ILE	2.5
3	E	45	PRO	2.5
4	F	259	GLY	2.5
2	D	400	GLY	2.5
4	F	275	LEU	2.5
2	D	175	VAL	2.5
2	D	390	ARG	2.4
4	F	230	SER	2.4
2	D	170	MET	2.4
2	D	216	LYS	2.4
3	E	25	LYS	2.4
3	E	46	SER	2.4
2	D	81	PHE	2.4
3	E	51	GLN	2.4
2	D	95	SER	2.4
2	D	74	ASP	2.3
4	F	75	ALA	2.3
4	F	163	SER	2.3
2	D	99	ASN	2.3
2	D	115	SER	2.3
1	C	340	SER	2.3
4	F	145	ASN	2.3
4	F	252	ASN	2.3
2	D	11	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	178	THR	2.2
2	D	94	GLN	2.2
2	D	172	SER	2.2
4	F	384	HIS	2.2
2	B	58	LYS	2.2
4	F	244	CYS	2.2
4	F	9	GLU	2.1
4	F	181	VAL	2.1
1	A	262	TYR	2.1
2	B	84	ILE	2.1
2	D	243	PRO	2.1
1	A	282	TYR	2.1
1	A	196	GLU	2.1
3	E	44	ASP	2.1
2	D	222	TYR	2.1
4	F	323	GLU	2.1
2	D	362	LYS	2.1
2	D	198	GLU	2.0
3	E	140	LYS	2.0
2	D	217	LEU	2.0
3	E	103	GLN	2.0
4	F	99	VAL	2.0
2	D	239	CYS	2.0
3	E	54	LEU	2.0
4	F	148	ILE	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)

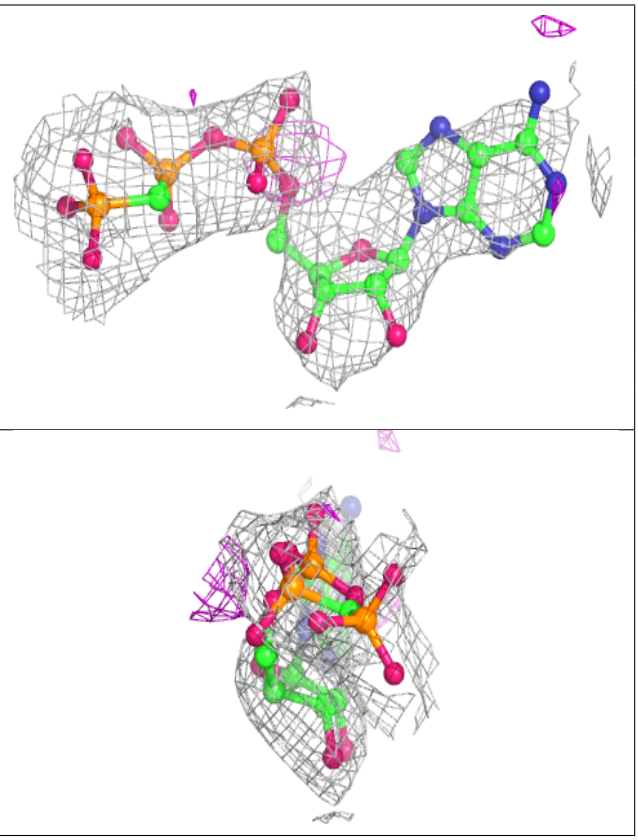
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	ACP	F	401	31/31	0.79	0.36	91,103,119,121	0
6	MG	D	502	1/1	0.85	0.19	60,60,60,60	0
9	MES	B	505	12/12	0.89	0.35	91,93,97,97	0
9	MES	B	503	12/12	0.89	0.23	77,83,87,90	0
7	CA	A	503	1/1	0.90	0.07	76,76,76,76	0
7	CA	B	504	1/1	0.91	0.11	65,65,65,65	0
5	GTP	D	501	32/32	0.91	0.17	55,62,76,82	0
10	PO7	B	506	27/27	0.94	0.22	33,41,59,66	0
10	PO7	D	503	27/27	0.94	0.21	48,57,67,68	0
7	CA	C	503	1/1	0.94	0.12	56,56,56,56	0
6	MG	B	502	1/1	0.96	0.11	40,40,40,40	0
5	GTP	C	501	32/32	0.97	0.17	26,30,31,32	0
8	GDP	B	501	28/28	0.98	0.19	28,30,32,33	0
5	GTP	A	501	32/32	0.98	0.20	29,32,35,36	0
6	MG	C	502	1/1	0.98	0.16	31,31,31,31	0
6	MG	A	502	1/1	0.99	0.23	25,25,25,25	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.

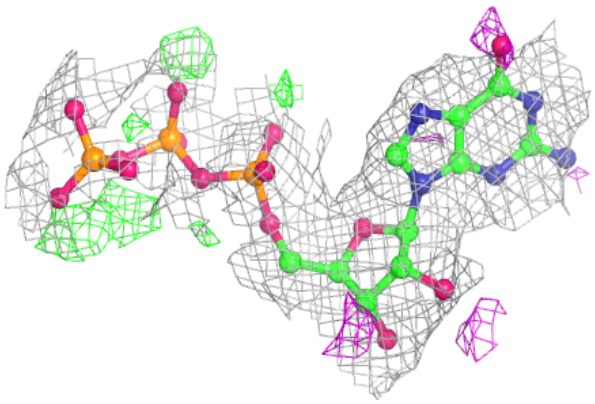
Electron density around ACP F 401:

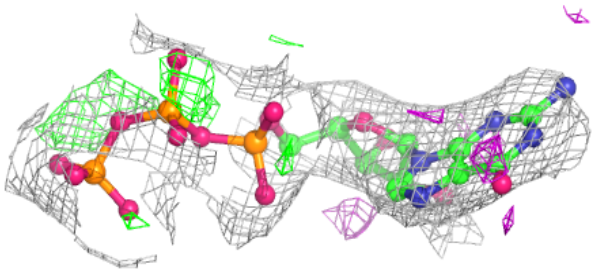
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP D 501:

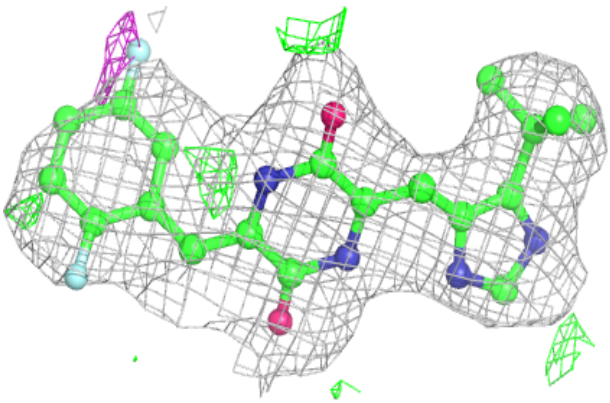
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

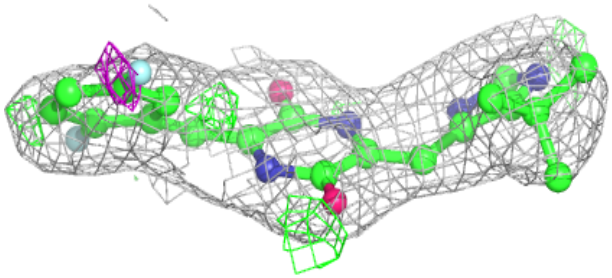


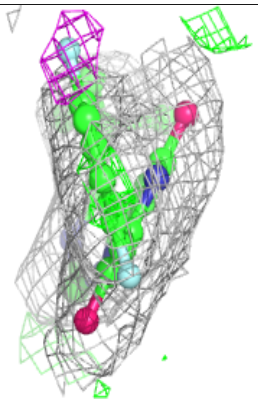


Electron density around PO7 B 506:

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

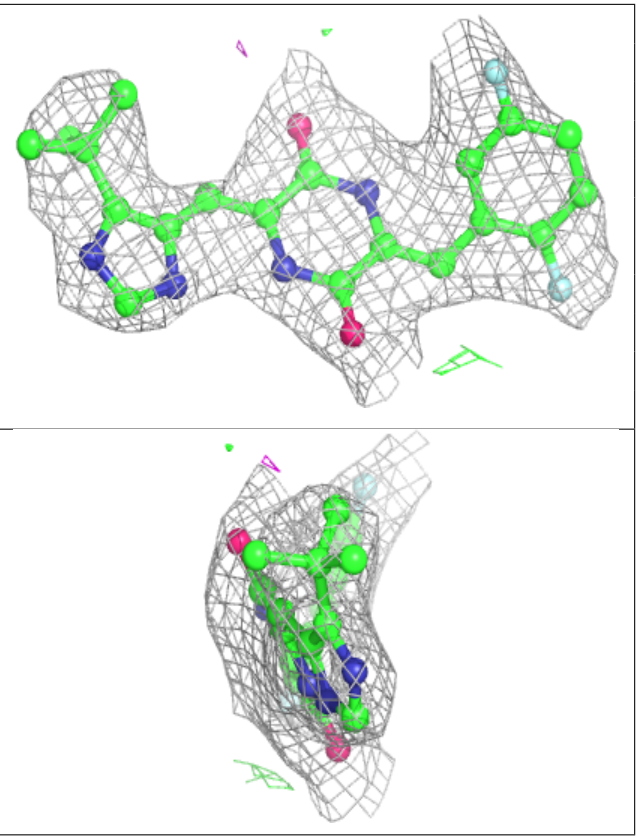






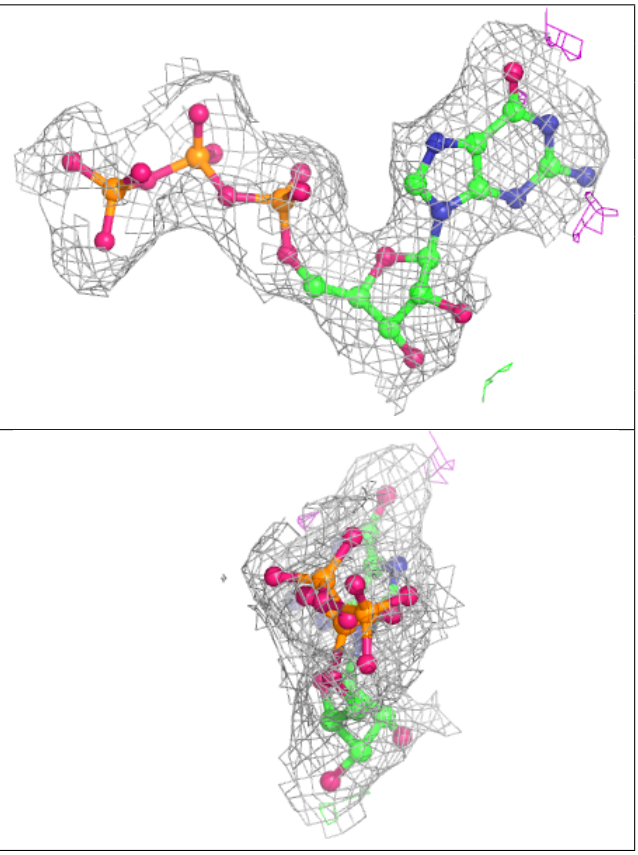
Electron density around PO7 D 503:

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



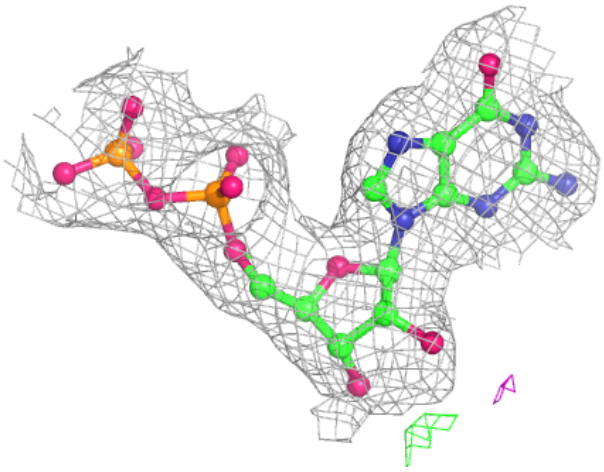
Electron density around GTP C 501:

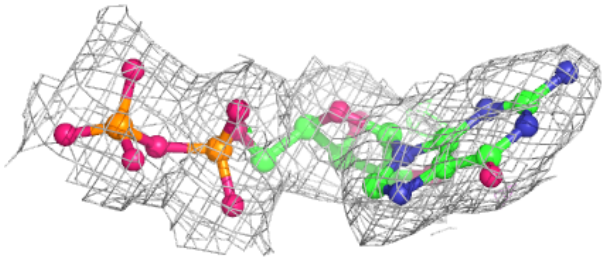
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

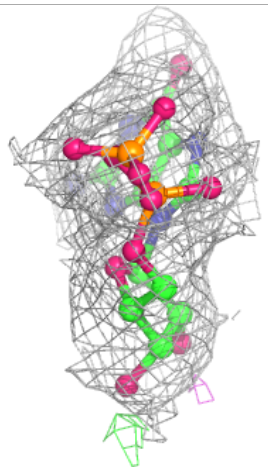


Electron density around GDP B 501:

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

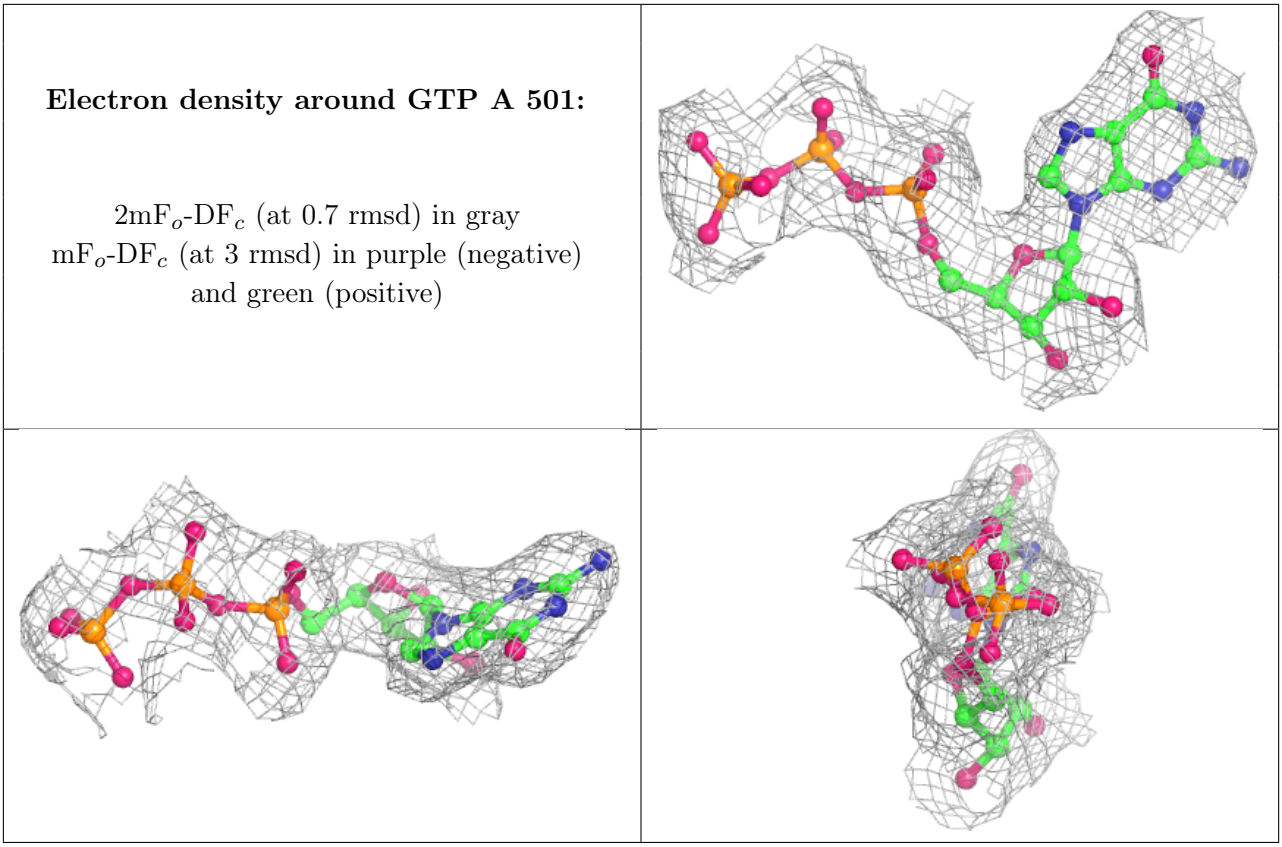






Electron density around GTP A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.