



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:55 PM UTC

PDB ID : 9QFN / pdb\_00009qfn  
Title : Crystal structure of T2R-TTL-Li5 complex  
Authors : Oliva, M.A.; Balaguer, F.A.; Diaz, J.F.  
Deposited on : 2025-03-12  
Resolution : 2.25 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

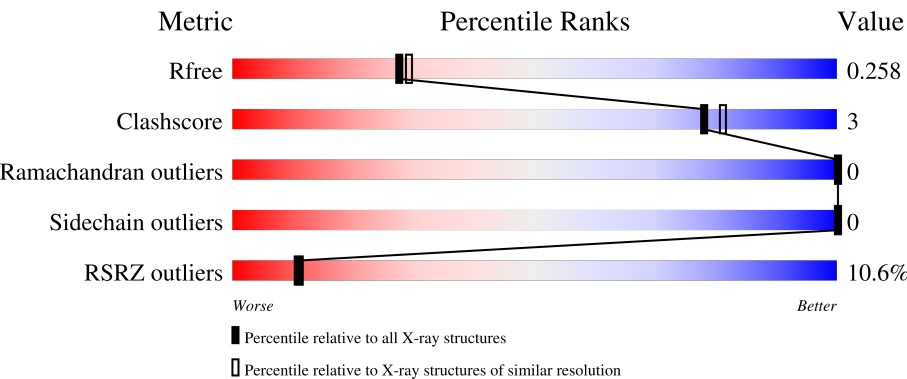
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 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 i

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

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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  $\geq 3$ , 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	451	<div><div>8%</div><div>87%</div><div>9%</div><div>.</div></div>
1	C	451	<div><div>3%</div><div>92%</div><div>5%</div><div>.</div></div>
2	B	445	<div><div>6%</div><div>89%</div><div>6%</div><div>.</div></div>
2	D	445	<div><div>16%</div><div>89%</div><div>5%</div><div>5%</div></div>
3	E	189	<div><div>12%</div><div>58%</div><div>38%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div> <div>14%</div> <div>71%</div> <div>5%</div> <div>24%</div> </div>

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 34216 atoms, of which 16745 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
1	A	435	Total	C	H	N	O	S	0	5	0
			6776	2168	3344	585	655	24			
1	C	439	Total	C	H	N	O	S	0	21	0
			6981	2233	3439	603	681	25			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	418	Total	C	H	N	O	S	0	7	0
			6605	2113	3247	573	646	26			
2	D	422	Total	C	H	N	O	S	0	1	0
			6527	2087	3204	567	643	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	118	Total	C	H	N	O	S	0	3	0
			2029	620	1026	184	193	6			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	290	Total	C	H	N	O	S	0	1	0
			4763	1546	2370	404	429	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	B	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

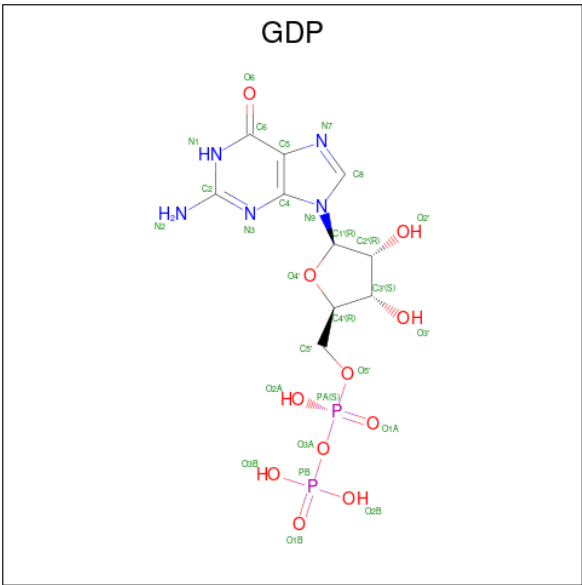
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

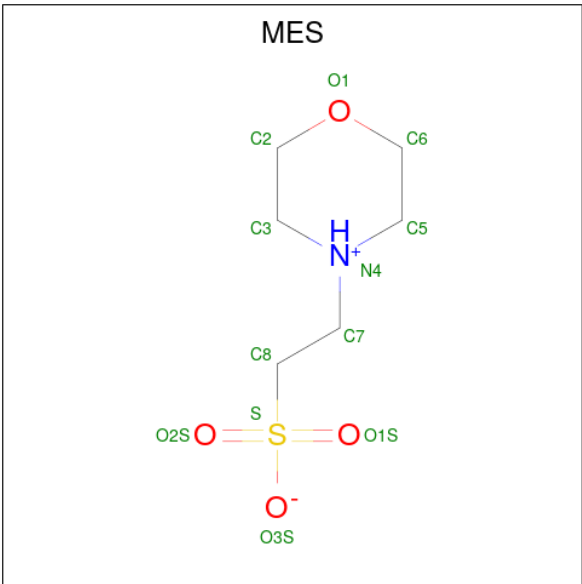
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
10	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

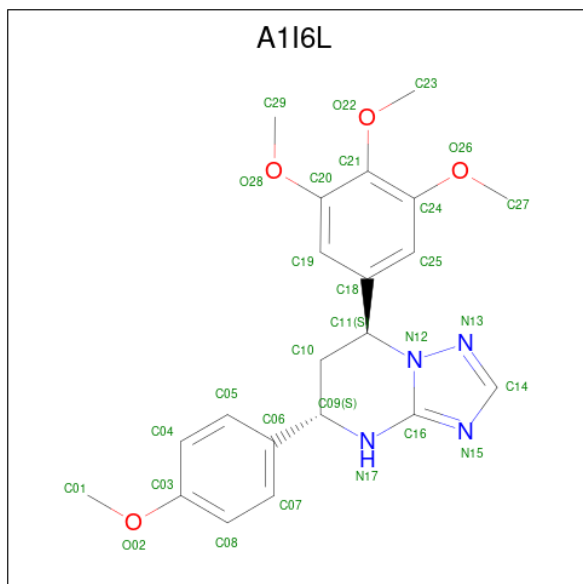
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

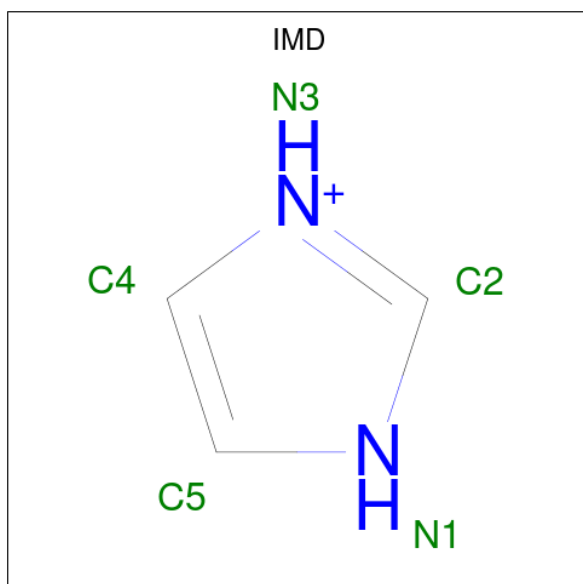


- Molecule 12 is (5 {S},7 {S})-5-(4-methoxyphenyl)-7-(3,4,5-trimethoxyphenyl)-4,5,6,7-tetrahydro-[1,2,4]triazolo[1,5-a]pyrimidine (CCD ID: A1I6L) (formula:  $C_{21}H_{24}N_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	0	0
			51	21	22	4	4		

- Molecule 13 is IMIDAZOLE (CCD ID: IMD) (formula:  $C_3H_5N_2$ ).



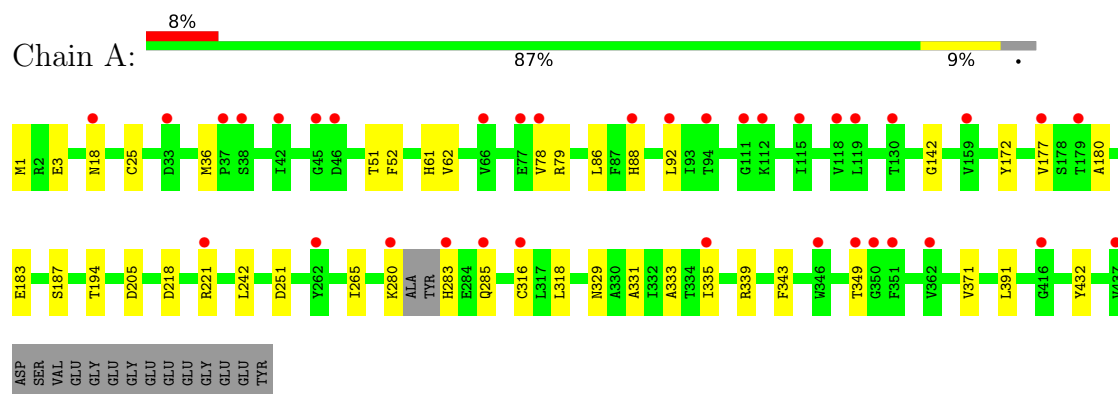
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	H	N	0	0
			10	3	5	2		



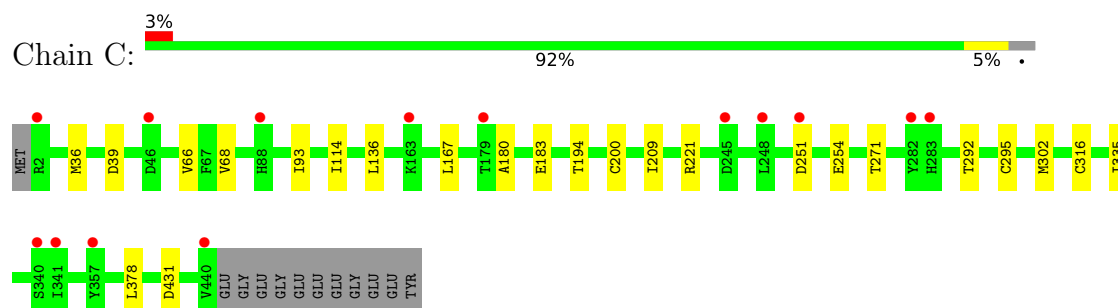
### 3 Residue-property plots [i](#)

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.

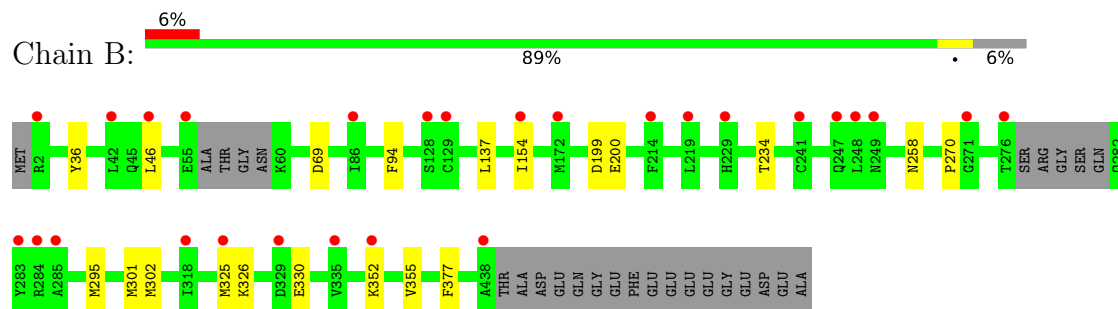
- Molecule 1: Tubulin alpha-1B chain



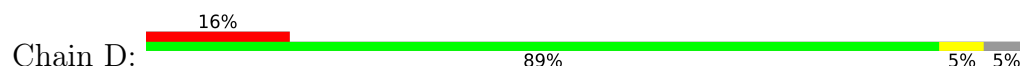
- Molecule 1: Tubulin alpha-1B chain

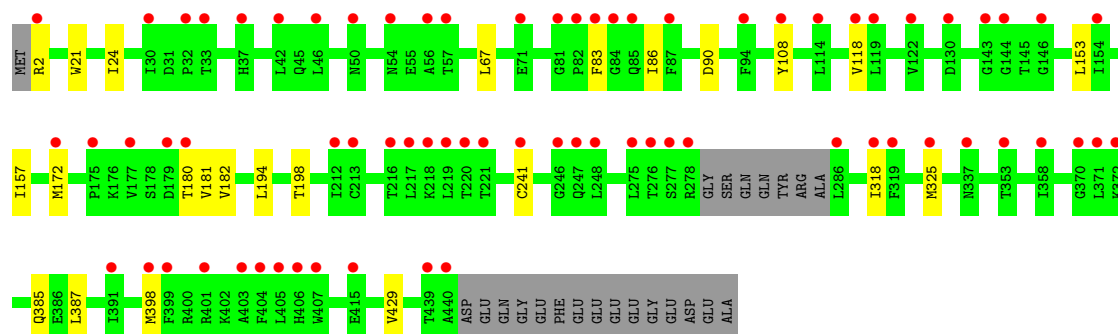


- Molecule 2: Tubulin beta-2B chain

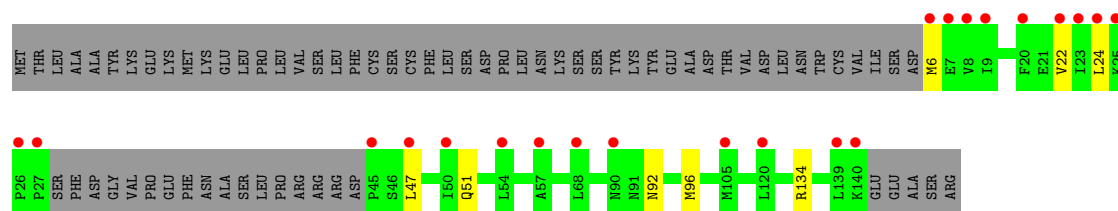


- Molecule 2: Tubulin beta-2B chain





• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.45Å 157.94Å 180.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.25 49.65 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.65-2.25) 99.7 (49.65-2.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.25Å)	Xtriage
Refinement program	PHENIX (dev_5493: ???)	Depositor
R, $R_{free}$	0.217 , 0.258 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	7267 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GTP, GDP, A1I6L, CA, MES, ACP, GOL, IMD, MG

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	0.11	0/3508	0.27	0/4760
1	C	0.12	0/3665	0.27	0/4981
2	B	0.11	0/3431	0.26	0/4644
2	D	0.12	0/3396	0.26	0/4600
3	E	0.13	0/1012	0.25	0/1341
4	F	0.10	0/2447	0.26	0/3303
All	All	0.11	0/17459	0.27	0/23629

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	3432	3344	3339	32	0
1	C	3542	3439	3374	14	0
2	B	3358	3247	3238	14	0
2	D	3323	3204	3202	18	0
3	E	1003	1026	1023	12	0
4	F	2393	2370	2373	11	0
5	A	32	9	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	9	12	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	12	16	16	1	0
7	B	6	8	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
10	B	28	10	12	0	0
10	D	28	10	12	0	0
11	B	12	13	13	0	0
12	B	29	22	0	2	0
13	C	5	5	5	1	0
14	F	31	13	14	0	0
15	A	25	0	0	0	0
15	B	40	0	0	0	0
15	C	109	0	0	0	0
15	D	12	0	0	0	0
15	E	6	0	0	0	0
15	F	2	0	0	0	0
All	All	17471	16745	16653	96	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 3.

All (96) 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)
3:E:47:LEU:HD11	3:E:51:GLN:OE1	1.71	0.90
2:B:36:TYR:CE1	2:B:46:LEU:HD21	2.10	0.85
3:E:47:LEU:HD11	3:E:51:GLN:CD	2.08	0.79
3:E:47:LEU:CD1	3:E:51:GLN:OE1	2.36	0.74
3:E:47:LEU:HD12	3:E:47:LEU:O	1.94	0.67
1:C:209:ILE:HD11	1:C:302:MET:SD	2.34	0.67
1:A:51[B]:THR:HG23	1:A:52:PHE:CD1	2.33	0.64
1:A:51[B]:THR:HG23	1:A:52:PHE:HD1	1.65	0.61
2:B:301:MET:HA	2:B:301:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:79:LYS:O	4:F:83:THR:HG23	2.01	0.61
1:A:333:ALA:N	3:E:6:MET:HE1	2.18	0.59
1:A:187:SER:CB	1:A:391:LEU:HD21	2.33	0.57
2:B:325:MET:SD	2:B:355:VAL:HG11	2.44	0.57
2:D:180:THR:HG22	2:D:181:VAL:H	1.71	0.56
2:D:153:LEU:O	2:D:157:ILE:HG13	2.05	0.55
4:F:1:MET:HE2	4:F:28:LYS:HB2	1.89	0.55
4:F:131:PHE:C	4:F:131:PHE:CD2	2.85	0.54
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.54
2:B:234[A]:THR:OG1	2:B:302:MET:HE2	2.07	0.54
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.48	0.54
4:F:305:LYS:HD3	4:F:306:HIS:CE1	2.43	0.53
1:A:221:ARG:HD3	2:B:325:MET:HB2	1.90	0.52
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.45	0.52
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.92	0.51
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.45	0.51
3:E:92[A]:ASN:OD1	3:E:96:MET:HE3	2.09	0.51
1:A:51[B]:THR:HG21	1:A:242:LEU:O	2.10	0.51
3:E:47:LEU:HD12	3:E:47:LEU:C	2.36	0.51
1:A:329:ASN:ND2	3:E:22:VAL:HG21	2.26	0.51
3:E:47:LEU:HD11	3:E:51:GLN:NE2	2.26	0.51
2:D:67:LEU:N	2:D:67:LEU:HD12	2.26	0.51
2:D:180:THR:HG22	2:D:181:VAL:N	2.27	0.50
1:C:221:ARG:NE	2:D:325:MET:SD	2.85	0.50
2:D:2:ARG:HG2	2:D:2:ARG:HH11	1.78	0.49
4:F:31:ARG:H	4:F:31:ARG:HD3	1.79	0.48
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.94	0.48
3:E:47:LEU:CD1	3:E:51:GLN:CD	2.83	0.48
1:A:194:THR:HG22	1:A:194:THR:O	2.14	0.47
1:C:180:ALA:O	1:C:183:GLU:HG3	2.15	0.47
3:E:6:MET:HE2	3:E:24:LEU:HD21	1.96	0.46
1:A:285:GLN:HA	1:A:285:GLN:OE1	2.16	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.45	0.46
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.16	0.46
1:A:285:GLN:HE22	1:A:371:VAL:HA	1.80	0.46
2:D:387:LEU:C	2:D:387:LEU:HD23	2.41	0.46
1:A:1:MET:C	1:A:1:MET:SD	2.99	0.46
1:A:285:GLN:NE2	1:A:371:VAL:HA	2.31	0.46
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.52	0.45
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.57	0.45
2:D:83:PHE:O	2:D:86:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:LYS:O	2:B:330:GLU:HG3	2.17	0.44
4:F:31:ARG:NH1	4:F:34:ASN:ND2	2.65	0.44
1:C:431:ASP:HB3	13:C:503:IMD:H5	2.00	0.44
1:A:280:LYS:NZ	1:A:283:HIS:ND1	2.60	0.44
4:F:32:LYS:HG3	4:F:33:ASP:N	2.33	0.44
1:A:177:VAL:O	1:A:177:VAL:HG12	2.18	0.44
1:C:251[B]:ASP:OD1	1:C:254:GLU:HB2	2.17	0.44
1:C:316[B]:CYS:SG	1:C:378:LEU:HB2	2.58	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.52	0.44
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.50	0.44
1:C:36:MET:SD	1:C:39:ASP:HB2	2.57	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.43
1:A:88:HIS:CD2	1:A:88:HIS:H	2.36	0.43
2:D:90:ASP:O	2:D:90:ASP:OD1	2.36	0.43
1:A:331:ALA:O	1:A:335:ILE:HD13	2.19	0.43
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.00	0.43
2:D:182:VAL:HA	2:D:398:MET:HE1	2.01	0.43
1:A:79:ARG:HG2	1:A:92:LEU:HD12	2.00	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.00	0.43
1:A:218:ASP:OD2	7:A:507:GOL:H2	2.19	0.43
2:D:180:THR:HG22	2:D:182:VAL:H	1.84	0.43
1:A:1:MET:HE1	1:A:3:GLU:OE2	2.19	0.42
2:B:234[A]:THR:HG21	2:B:270:PRO:HB2	2.02	0.42
1:C:66:VAL:HG12	1:C:68[B]:VAL:HG23	2.01	0.42
4:F:131:PHE:CE1	4:F:182:ILE:HD12	2.54	0.42
2:B:199:ASP:C	2:B:200:GLU:HG3	2.45	0.42
2:B:352[B]:LYS:HG3	12:B:507:A1I6L:C04	2.49	0.42
1:C:194[A]:THR:HG22	1:C:194[A]:THR:O	2.19	0.42
1:A:251:ASP:OD1	1:A:251:ASP:C	2.62	0.42
4:F:3:THR:HB	4:F:30:LEU:HD11	2.02	0.42
2:D:385:GLN:HB2	2:D:429:VAL:HG13	2.02	0.41
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.03	0.41
4:F:268:ASN:O	4:F:272:MET:HG3	2.21	0.41
2:B:137:LEU:HD23	2:B:154:ILE:HD11	2.02	0.41
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.01	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.20	0.41
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.60	0.41
1:A:180:ALA:O	1:A:183:GLU:HG3	2.20	0.41
2:D:108:TYR:O	3:E:134:ARG:HD3	2.21	0.41
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:ASN:HB3	12:B:507:A1I6L:C04	2.51	0.40
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.56	0.40
2:D:194:LEU:HA	2:D:198:THR:HG23	2.03	0.40
2:B:69:ASP:O	2:B:94:PHE:HA	2.20	0.40
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.02	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	436/451 (97%)	427 (98%)	9 (2%)	0	100	100
1	C	458/451 (102%)	449 (98%)	9 (2%)	0	100	100
2	B	419/445 (94%)	406 (97%)	13 (3%)	0	100	100
2	D	419/445 (94%)	409 (98%)	10 (2%)	0	100	100
3	E	117/189 (62%)	115 (98%)	2 (2%)	0	100	100
4	F	277/384 (72%)	269 (97%)	8 (3%)	0	100	100
All	All	2126/2365 (90%)	2075 (98%)	51 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/379 (98%)	372 (100%)	0	100	100
1	C	389/379 (103%)	389 (100%)	0	100	100
2	B	370/383 (97%)	370 (100%)	0	100	100
2	D	366/383 (96%)	366 (100%)	0	100	100
3	E	109/171 (64%)	109 (100%)	0	100	100
4	F	263/342 (77%)	263 (100%)	0	100	100
All	All	1869/2037 (92%)	1869 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	35	GLN
1	A	256	GLN
1	A	266	HIS
1	A	329	ASN
2	B	8	GLN
2	B	192	HIS
2	B	229	HIS
2	B	249	ASN
2	B	436	GLN
1	C	15	GLN
1	C	342	GLN
1	C	372	GLN
1	C	393	HIS
2	D	37	HIS
2	D	331	GLN
4	F	306	HIS
4	F	333	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 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	33,34,34	0.88	0	50,54,54	1.52	8 (16%)
11	MES	B	504	-	12,12,12	1.16	1 (8%)	15,16,16	0.84	0
7	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.45	0
7	GOL	B	503	-	5,5,5	0.33	0	5,5,5	0.36	0
12	A1I6L	B	507	-	32,32,32	3.33	5 (15%)	42,45,45	3.47	16 (38%)
14	ACP	F	401	6	31,33,33	2.12	3 (9%)	47,52,52	0.97	3 (6%)
7	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.40	0
10	GDP	D	501	6	29,30,30	1.15	3 (10%)	45,47,47	1.73	5 (11%)
5	GTP	C	501	6	33,34,34	0.97	2 (6%)	50,54,54	1.49	7 (14%)
10	GDP	B	501	6	29,30,30	1.15	3 (10%)	45,47,47	1.67	5 (11%)
13	IMD	C	503	-	5,5,5	0.31	0	5,5,5	0.81	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	A	501	6	-	9/22/38/38	0/3/3/3
11	MES	B	504	-	-	0/6/14/14	0/1/1/1
7	GOL	A	503	-	-	0/4/4/4	-
7	GOL	B	503	-	-	0/4/4/4	-
12	A1I6L	B	507	-	-	8/16/28/28	0/4/4/4
14	ACP	F	401	6	-	3/19/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	507	-	-	0/4/4/4	-
10	GDP	D	501	6	-	4/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
10	GDP	B	501	6	-	3/16/32/32	0/3/3/3
13	IMD	C	503	-	-	-	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	507	A1I6L	C16-N17	15.31	1.48	1.35
14	F	401	ACP	PB-O3A	10.62	1.70	1.58
12	B	507	A1I6L	C11-N12	7.04	1.54	1.46
12	B	507	A1I6L	C09-N17	-4.89	1.42	1.47
12	B	507	A1I6L	C10-C09	-3.34	1.48	1.53
11	B	504	MES	C8-S	3.11	1.82	1.77
10	D	501	GDP	C5-C4	3.04	1.47	1.38
10	B	501	GDP	C5-C4	3.01	1.47	1.38
12	B	507	A1I6L	C16-N15	2.51	1.36	1.33
10	B	501	GDP	C6-N1	-2.51	1.34	1.38
10	D	501	GDP	C6-N1	-2.45	1.34	1.38
14	F	401	ACP	PA-O3A	2.43	1.62	1.59
5	C	501	GTP	PB-O3B	2.24	1.61	1.59
14	F	401	ACP	PB-O2B	-2.13	1.51	1.56
10	B	501	GDP	C5-N7	-2.08	1.34	1.39
5	C	501	GTP	C2-N3	2.03	1.38	1.33
10	D	501	GDP	C5-N7	-2.03	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	507	A1I6L	N12-C16-N15	-11.72	106.62	111.03
12	B	507	A1I6L	C14-N15-C16	10.10	108.24	101.80
12	B	507	A1I6L	C14-N13-N12	7.09	106.68	101.28
12	B	507	A1I6L	C10-C09-N17	6.43	117.79	108.20
12	B	507	A1I6L	N17-C16-N15	6.38	132.66	128.29
10	D	501	GDP	C5-C4-N3	-5.81	119.14	128.39
10	B	501	GDP	C5-C4-N3	-5.58	119.51	128.39
12	B	507	A1I6L	C06-C09-N17	5.48	120.67	110.76
12	B	507	A1I6L	N13-C14-N15	-5.40	108.22	116.78
10	D	501	GDP	C2-N3-C4	4.78	120.53	112.30
10	B	501	GDP	C2-N3-C4	4.75	120.49	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C5-C4-N3	-4.70	120.91	128.39
5	A	501	GTP	C5-C4-N3	-4.67	120.95	128.39
5	A	501	GTP	C2-N3-C4	4.53	120.10	112.30
10	D	501	GDP	N9-C4-N3	4.40	134.74	125.95
5	C	501	GTP	C2-N3-C4	4.38	119.84	112.30
10	B	501	GDP	N9-C4-N3	4.23	134.42	125.95
10	B	501	GDP	C6-C5-N7	3.61	136.87	130.29
10	D	501	GDP	C6-C5-N7	3.42	136.52	130.29
5	C	501	GTP	N9-C4-N3	2.94	131.83	125.95
5	C	501	GTP	N9-C8-N7	-2.90	108.03	113.40
5	A	501	GTP	N9-C4-N3	2.85	131.64	125.95
14	F	401	ACP	O2B-PB-O1B	2.84	119.20	109.95
5	A	501	GTP	C2-N1-C6	-2.81	120.01	125.11
5	A	501	GTP	N9-C8-N7	-2.79	108.23	113.40
5	C	501	GTP	C2-N1-C6	-2.78	120.07	125.11
12	B	507	A1I6L	O26-C24-C21	2.71	119.78	115.14
12	B	507	A1I6L	O28-C20-C21	2.67	119.72	115.14
12	B	507	A1I6L	C27-O26-C24	-2.65	113.63	117.51
5	C	501	GTP	C8-N7-C5	2.64	108.95	104.26
12	B	507	A1I6L	C09-N17-C16	2.61	119.69	115.89
10	D	501	GDP	C4-C5-N7	-2.60	106.54	110.67
14	F	401	ACP	O1G-PG-C3B	-2.59	105.72	111.37
5	A	501	GTP	C8-N7-C5	2.56	108.81	104.26
12	B	507	A1I6L	C11-N12-N13	2.55	126.07	122.23
10	B	501	GDP	C4-C5-N7	-2.55	106.63	110.67
5	A	501	GTP	C5-C6-N1	2.48	119.56	113.25
5	C	501	GTP	C5-C6-N1	2.47	119.53	113.25
12	B	507	A1I6L	C10-C09-C06	2.41	117.89	112.52
12	B	507	A1I6L	C29-O28-C20	-2.38	114.03	117.51
14	F	401	ACP	PB-O3A-PA	-2.29	124.89	132.37
12	B	507	A1I6L	O26-C24-C25	-2.25	120.20	124.08
5	A	501	GTP	O6-C6-C5	-2.22	120.68	126.53
12	B	507	A1I6L	O28-C20-C19	-2.12	120.43	124.08

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
10	B	501	GDP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O2A
14	F	401	ACP	C5'-O5'-PA-O1A
14	F	401	ACP	C5'-O5'-PA-O3A
12	B	507	A1I6L	C21-C20-O28-C29
12	B	507	A1I6L	C19-C20-O28-C29
12	B	507	A1I6L	C21-C24-O26-C27
12	B	507	A1I6L	C04-C03-O02-C01
12	B	507	A1I6L	C08-C03-O02-C01
12	B	507	A1I6L	C25-C24-O26-C27
5	A	501	GTP	PB-O3A-PA-O1A
14	F	401	ACP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
12	B	507	A1I6L	C10-C11-C18-C25
12	B	507	A1I6L	C10-C11-C18-C19
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
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	PB-O3B-PG-O1G
10	D	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A

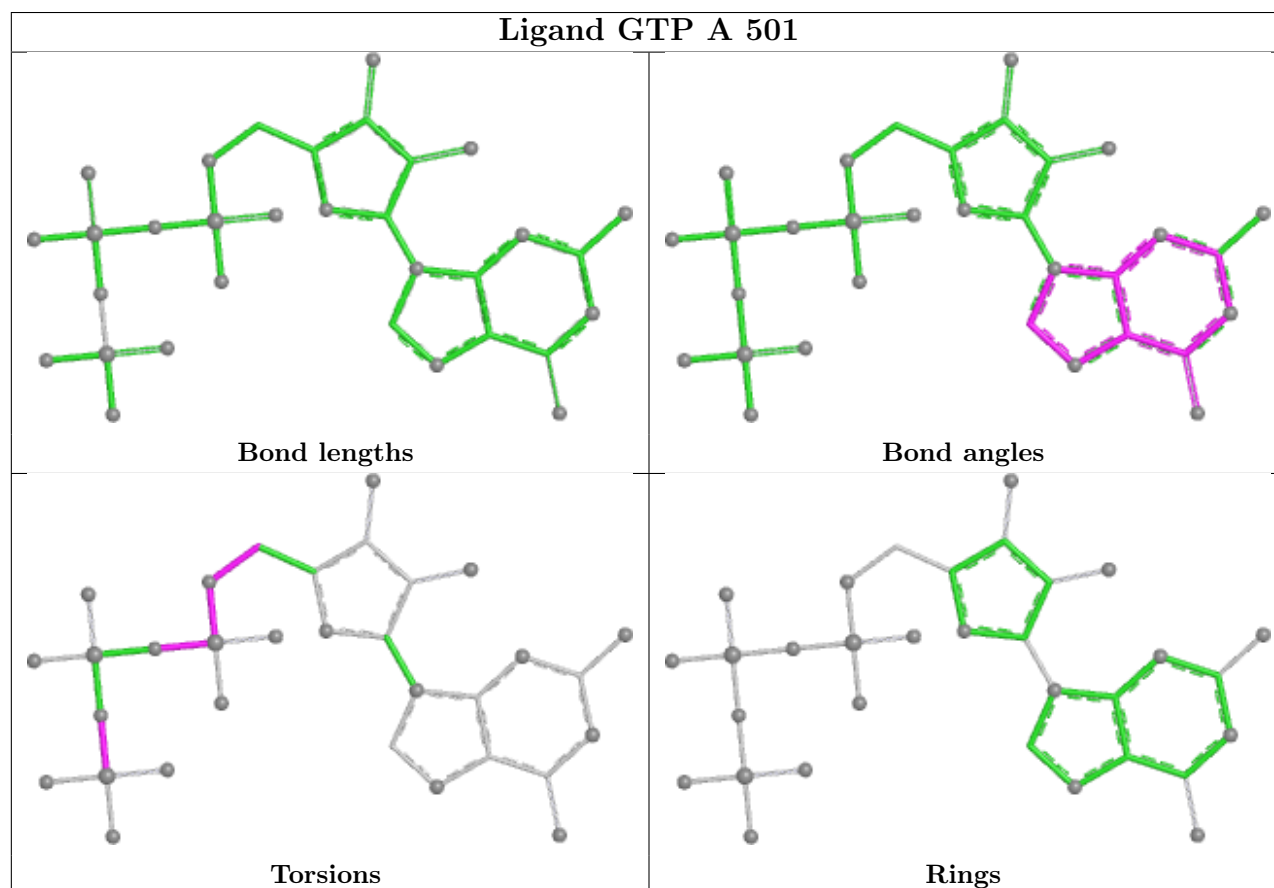
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	507	A1I6L	2	0
7	A	507	GOL	1	0
13	C	503	IMD	1	0

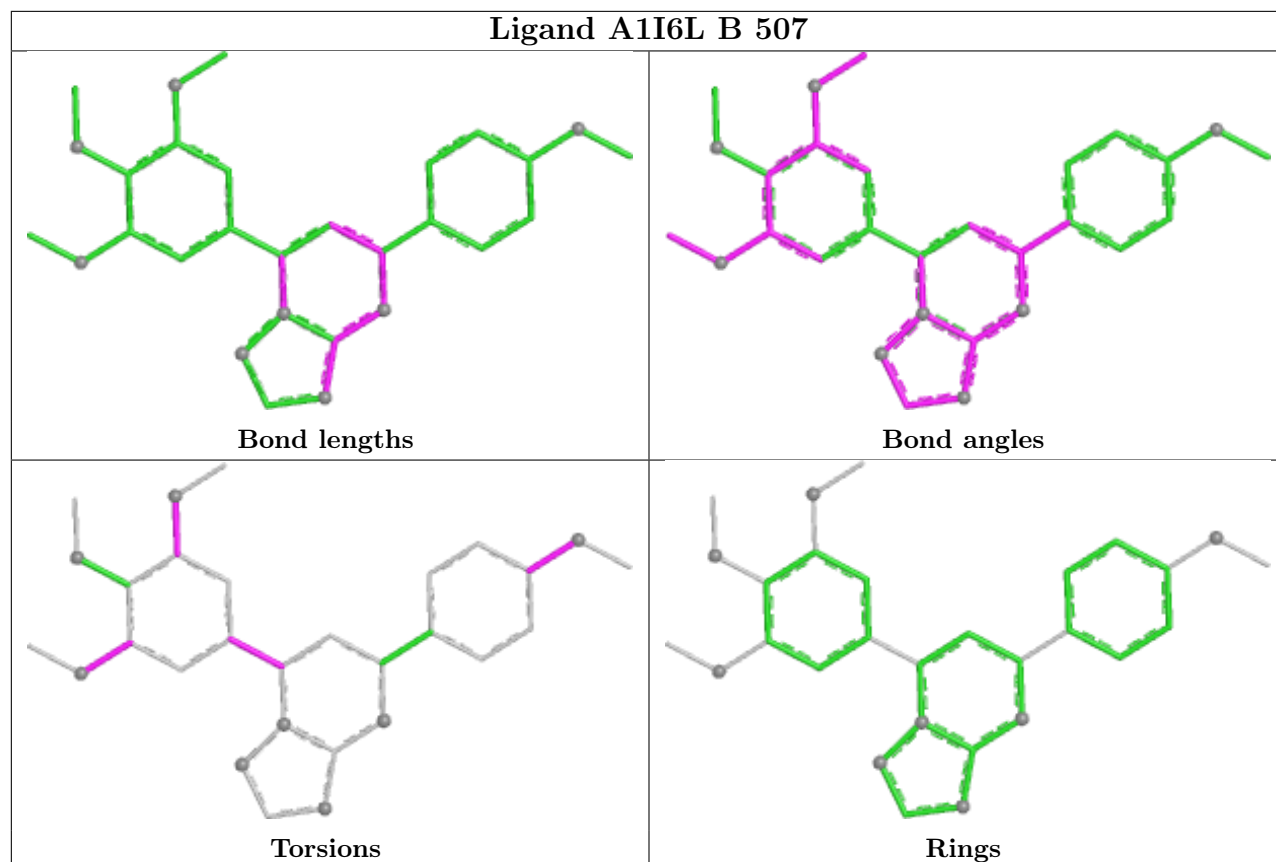
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

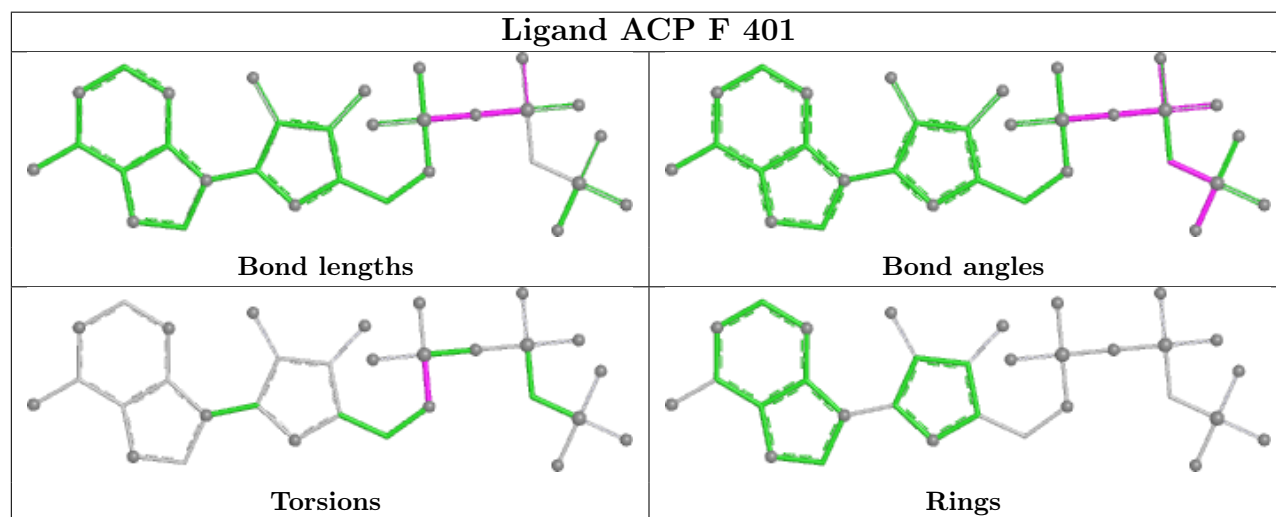


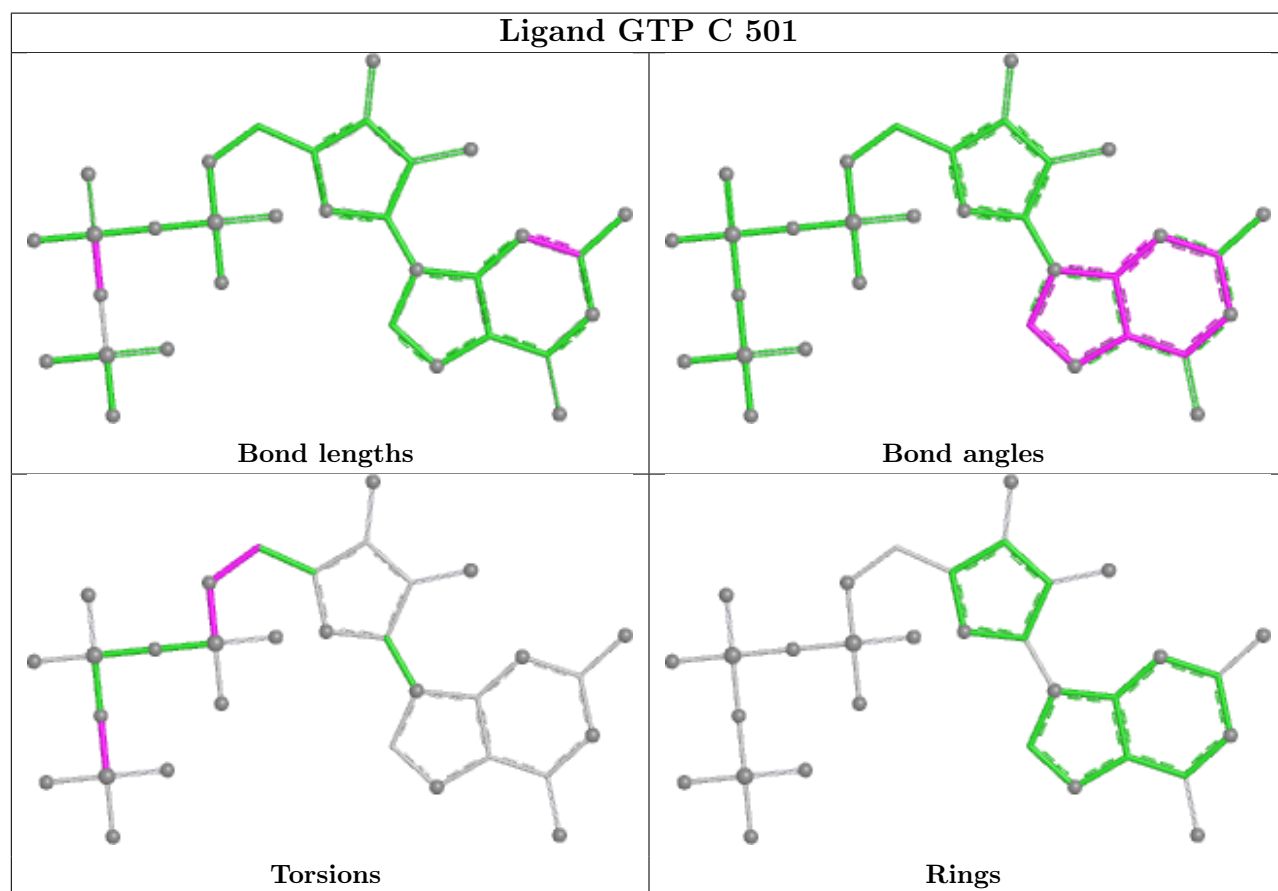
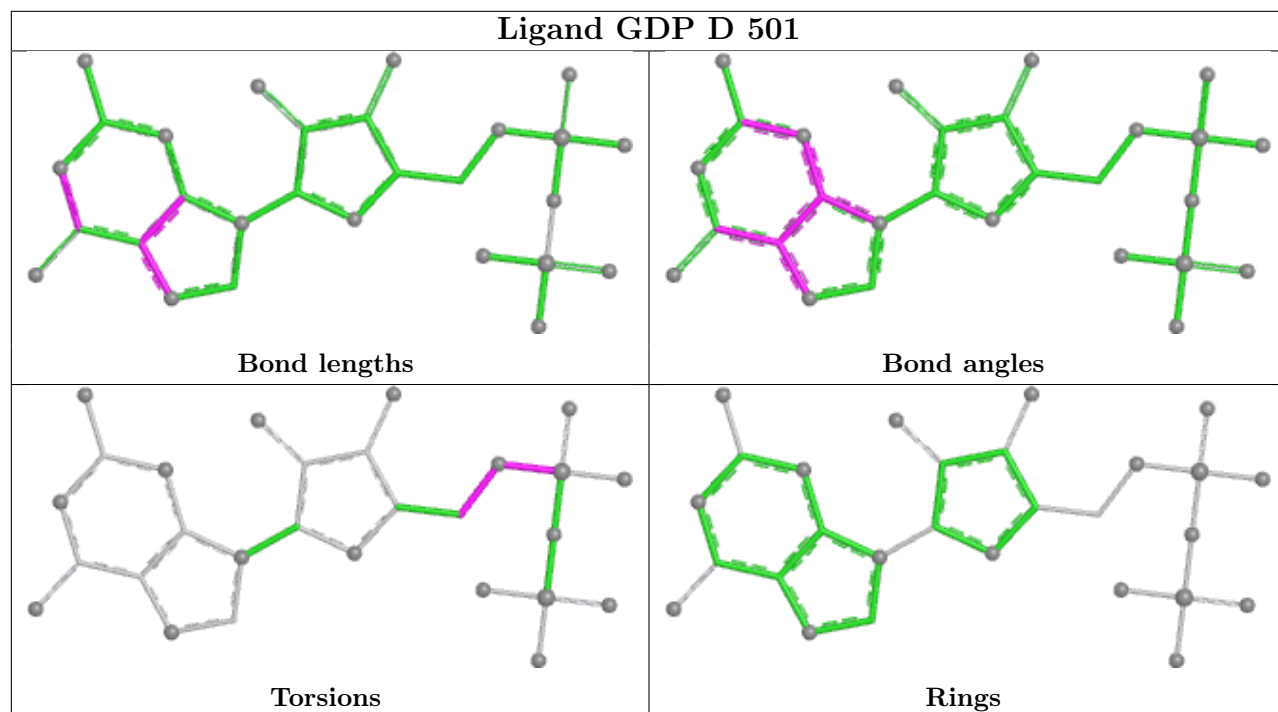


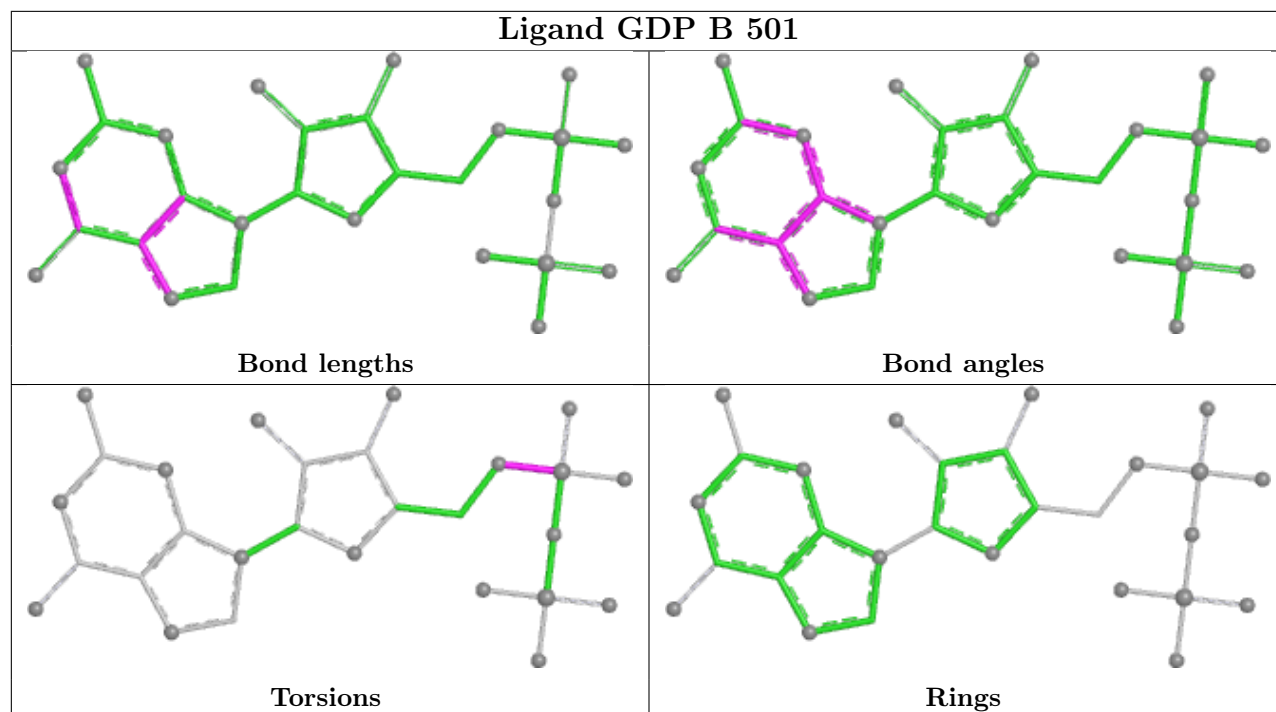
## Ligand A1I6L B 507



## Ligand ACP F 401







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	435/451 (96%)	0.81	36 (8%)	17 16	25, 61, 87, 101	5 (1%)
1	C	439/451 (97%)	0.24	14 (3%)	50 50	19, 45, 70, 94	15 (3%)
2	B	418/445 (93%)	0.61	27 (6%)	25 23	22, 56, 88, 107	7 (1%)
2	D	422/445 (94%)	1.24	72 (17%)	4 3	31, 73, 103, 117	1 (0%)
3	E	118/189 (62%)	1.22	22 (18%)	3 3	24, 72, 103, 119	3 (2%)
4	F	290/384 (75%)	1.25	53 (18%)	3 3	29, 79, 112, 122	1 (0%)
All	All	2122/2365 (89%)	0.82	224 (10%)	11 11	19, 62, 98, 122	32 (1%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	240	LEU	7.5
1	C	440	VAL	5.5
2	D	248	LEU	5.2
4	F	131	PHE	5.2
4	F	134	ALA	4.9
2	B	438	ALA	4.9
3	E	27	PRO	4.8
1	A	437	VAL	4.8
1	A	283	HIS	4.7
3	E	45	PRO	4.6
4	F	130	VAL	4.5
4	F	181	VAL	4.4
2	D	407	TRP	4.3
4	F	151	SER	4.2
1	A	262	TYR	4.1
2	D	82	PRO	4.1
2	D	57	THR	4.1
4	F	182	ILE	4.1
1	A	115	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	180	THR	4.0
4	F	237	THR	4.0
4	F	241	THR	3.9
2	D	276	THR	3.9
4	F	145	ASN	3.9
2	B	248	LEU	3.8
4	F	379	HIS	3.8
2	D	286	LEU	3.7
4	F	135	TYR	3.7
2	D	404	PHE	3.7
1	A	179	THR	3.7
4	F	98	TYR	3.7
1	C	88[A]	HIS	3.7
1	C	357	TYR	3.7
4	F	132	LEU	3.6
2	B	249	ASN	3.6
3	E	8	VAL	3.6
4	F	136	ASN	3.6
2	D	32	PRO	3.6
4	F	253	TYR	3.6
2	B	352[A]	LYS	3.6
1	C	163	LYS	3.5
4	F	150	LYS	3.5
4	F	239	HIS	3.5
1	A	92	LEU	3.5
3	E	47	LEU	3.5
2	B	284	ARG	3.5
2	B	247	GLN	3.5
2	D	275	LEU	3.4
3	E	105[A]	MET	3.4
2	D	278	ARG	3.4
4	F	238	CYS	3.3
2	D	84	GLY	3.3
4	F	31	ARG	3.2
3	E	54	LEU	3.2
2	D	83	PHE	3.2
2	D	277	SER	3.2
2	D	212	ILE	3.2
4	F	133	ALA	3.1
2	D	217	LEU	3.1
1	A	346	TRP	3.1
4	F	330	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	172	MET	3.1
2	D	220	THR	3.1
4	F	362	ALA	3.1
3	E	50	ILE	3.1
2	D	221	THR	3.1
2	D	337	ASN	3.1
1	A	42	ILE	3.0
2	B	285	ALA	3.0
2	D	440	ALA	3.0
3	E	120	LEU	3.0
4	F	230	SER	3.0
2	D	81	GLY	3.0
3	E	139	LEU	3.0
1	C	341	ILE	3.0
2	D	246	GLY	3.0
2	B	42	LEU	2.9
2	D	46	LEU	2.9
2	D	318	ILE	2.9
2	D	216	THR	2.9
2	D	219	LEU	2.9
1	A	177	VAL	2.9
1	C	340	SER	2.9
2	D	179	ASP	2.9
2	D	353	THR	2.9
4	F	320	MET	2.9
1	A	350	GLY	2.8
4	F	186	LEU	2.8
3	E	22	VAL	2.8
1	C	179	THR	2.8
2	D	213	CYS	2.8
1	C	251[A]	ASP	2.8
4	F	149	ALA	2.8
2	D	177	VAL	2.8
2	D	2	ARG	2.8
1	C	283	HIS	2.8
4	F	22	LEU	2.8
1	C	2	ARG	2.8
2	B	128	SER	2.7
2	D	143	GLY	2.7
2	D	241	CYS	2.7
2	D	42	LEU	2.7
2	B	2	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	256	TYR	2.7
4	F	228	TYR	2.7
2	B	283	TYR	2.7
1	C	245	ASP	2.7
3	E	140	LYS	2.7
2	D	358	ILE	2.7
4	F	335	ALA	2.6
2	B	229	HIS	2.6
3	E	24	LEU	2.6
2	D	372	LYS	2.6
2	B	241	CYS	2.6
4	F	252	ASN	2.6
2	D	154	ILE	2.6
1	A	280	LYS	2.6
4	F	194	PRO	2.5
1	A	78	VAL	2.5
4	F	224	SER	2.5
2	D	94	PHE	2.5
4	F	147	TRP	2.5
1	A	118	VAL	2.5
3	E	23	ILE	2.5
2	D	50	ASN	2.5
4	F	306	HIS	2.5
1	A	66	VAL	2.5
3	E	9	ILE	2.5
4	F	27	TRP	2.5
2	D	218	LYS	2.5
1	A	18	ASN	2.5
4	F	57	GLY	2.5
2	B	276	THR	2.4
4	F	191	LEU	2.4
2	D	56	ALA	2.4
1	A	45	GLY	2.4
2	D	87	PHE	2.4
2	B	329	ASP	2.4
4	F	373	SER	2.4
2	D	114	LEU	2.4
2	D	37	HIS	2.4
2	D	247	GLN	2.4
3	E	7	GLU	2.4
4	F	126	ASP	2.4
1	A	37	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	259	GLY	2.4
2	B	318	ILE	2.4
1	A	88	HIS	2.4
1	A	33	ASP	2.3
1	A	335	ILE	2.3
1	A	111	GLY	2.3
4	F	380	HIS	2.3
2	B	214	PHE	2.3
1	C	46	ASP	2.3
3	E	26	PRO	2.3
1	A	351	PHE	2.3
3	E	20	PHE	2.3
4	F	263	PHE	2.3
1	A	112	LYS	2.3
4	F	25	GLY	2.3
2	D	406	HIS	2.3
1	A	159	VAL	2.3
1	A	46	ASP	2.2
1	A	221	ARG	2.2
2	D	71	GLU	2.2
2	D	108	TYR	2.2
1	A	285	GLN	2.2
4	F	336	PRO	2.2
2	D	403	ALA	2.2
2	D	391	ILE	2.2
2	D	175	PRO	2.2
3	E	6	MET	2.2
3	E	25	LYS	2.2
4	F	344	ALA	2.2
2	B	219	LEU	2.2
3	E	90	ASN	2.2
1	A	77	GLU	2.2
2	B	55	GLU	2.2
2	D	85	GLN	2.2
2	D	144	GLY	2.2
1	A	38	SER	2.2
1	C	248	LEU	2.1
2	D	119	LEU	2.1
2	D	405	LEU	2.1
2	B	172	MET	2.1
2	D	130	ASP	2.1
1	A	416	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	94	THR	2.1
4	F	12	SER	2.1
1	A	119	LEU	2.1
2	D	399	PHE	2.1
2	D	370	GLY	2.1
2	D	33	THR	2.1
2	B	325	MET	2.1
2	D	415	GLU	2.1
1	C	282	TYR	2.1
2	B	86	ILE	2.1
2	D	54	ASN	2.1
2	B	335	VAL	2.1
4	F	146	VAL	2.1
2	D	319	PHE	2.1
4	F	199	PHE	2.1
1	A	130	THR	2.1
3	E	57	ALA	2.1
2	D	325	MET	2.1
2	D	398	MET	2.1
4	F	361	LEU	2.1
2	B	154	ILE	2.1
1	A	362	VAL	2.1
2	D	122	VAL	2.1
2	D	401	ARG	2.1
1	A	349	THR	2.0
4	F	225	SER	2.0
1	A	316[A]	CYS	2.0
2	B	46	LEU	2.0
2	D	371	LEU	2.0
3	E	68	LEU	2.0
2	D	118	VAL	2.0
2	B	271	GLY	2.0
2	D	146	GLY	2.0
2	D	439	THR	2.0
2	B	129	CYS	2.0
4	F	20	LEU	2.0
2	D	30	ILE	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 ⓘ

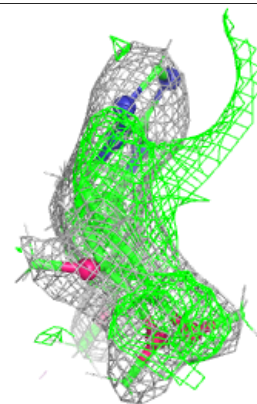
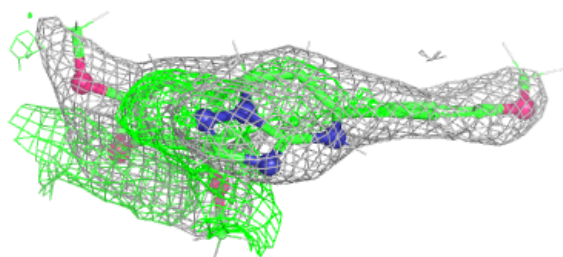
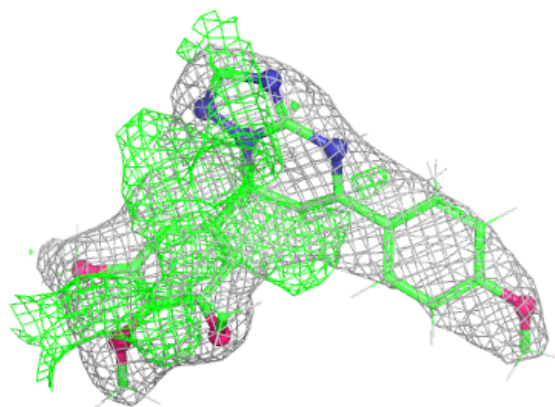
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	F	402	1/1	0.59	0.21	92,92,92,92	0
7	GOL	A	507	6/6	0.69	0.14	76,92,100,108	0
13	IMD	C	503	5/5	0.82	0.21	55,66,78,83	0
7	GOL	A	503	6/6	0.83	0.16	57,73,88,96	0
7	GOL	B	503	6/6	0.84	0.19	69,83,86,97	0
9	CL	A	506	1/1	0.85	0.13	82,82,82,82	0
12	A1I6L	B	507	29/29	0.87	0.29	37,51,65,68	51
6	MG	B	506	1/1	0.87	0.11	79,79,79,79	0
14	ACP	F	401	31/31	0.87	0.12	85,97,117,121	0
11	MES	B	504	12/12	0.88	0.14	50,66,83,84	0
8	CA	B	505	1/1	0.89	0.10	93,93,93,93	0
10	GDP	D	501	28/28	0.89	0.14	54,67,85,97	0
6	MG	A	505	1/1	0.94	0.49	80,80,80,80	0
6	MG	D	502	1/1	0.96	0.07	65,65,65,65	0
10	GDP	B	501	28/28	0.97	0.08	30,37,53,69	0
5	GTP	C	501	32/32	0.97	0.07	27,35,42,58	0
5	GTP	A	501	32/32	0.97	0.08	30,41,49,56	0
6	MG	B	502	1/1	0.98	0.04	30,30,30,30	0
8	CA	A	504	1/1	0.98	0.05	74,74,74,74	0
6	MG	A	502	1/1	0.99	0.03	37,37,37,37	0
8	CA	C	504	1/1	0.99	0.03	54,54,54,54	0
6	MG	C	502	1/1	0.99	0.06	32,32,32,32	0

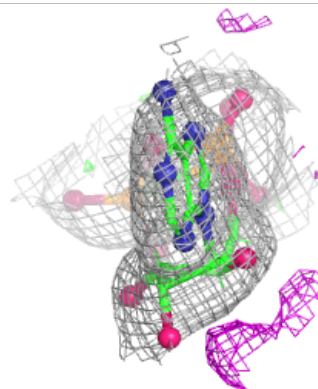
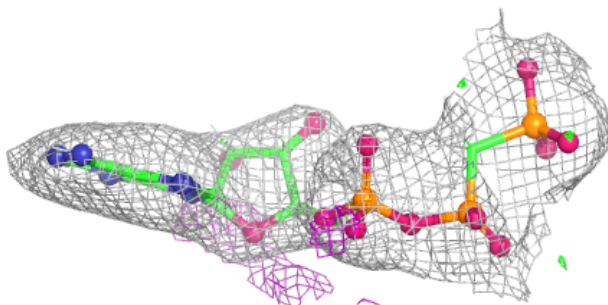
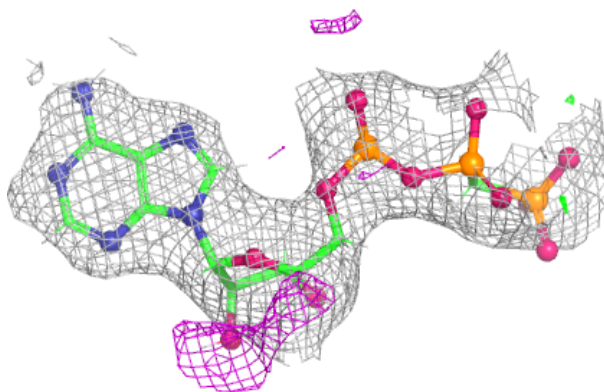
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1I6L B 507:**

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

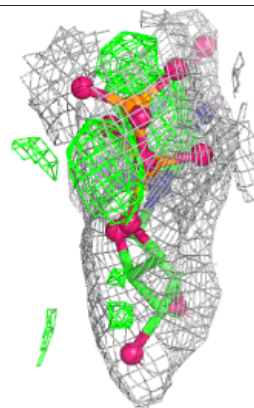
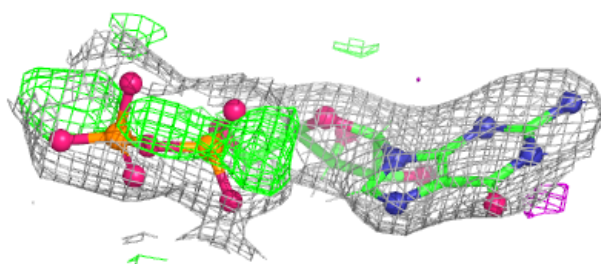
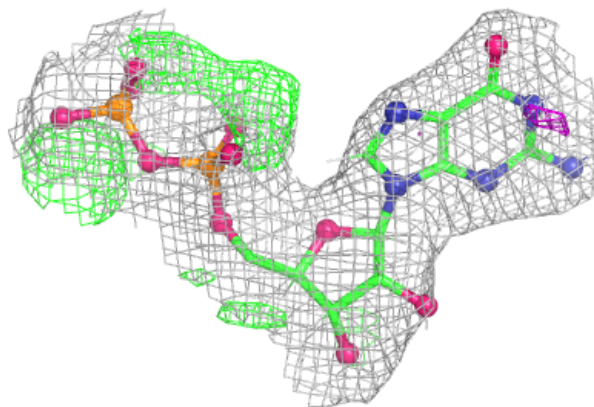
**Electron density around ACP F 401:**

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



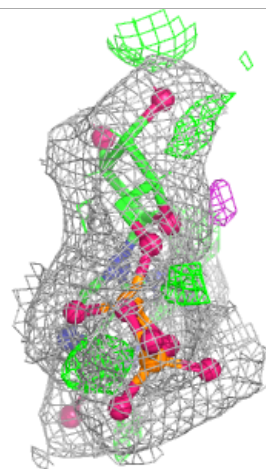
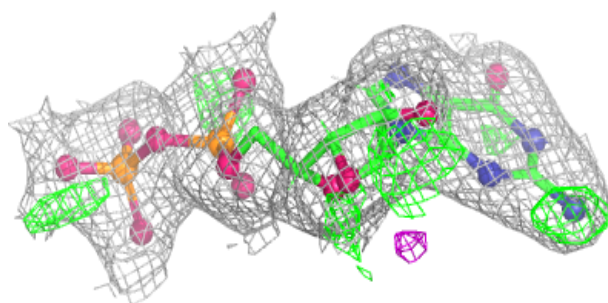
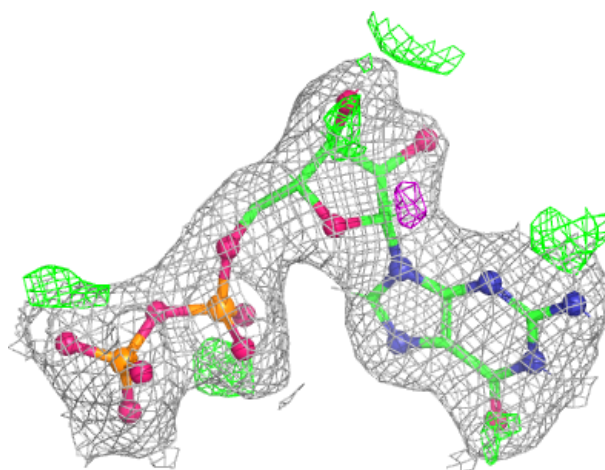
**Electron density around GDP D 501:**

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



**Electron density around GDP B 501:**

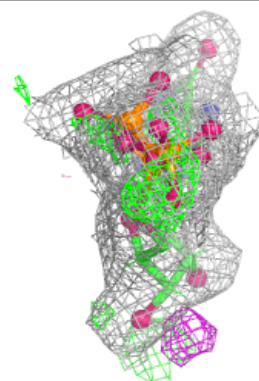
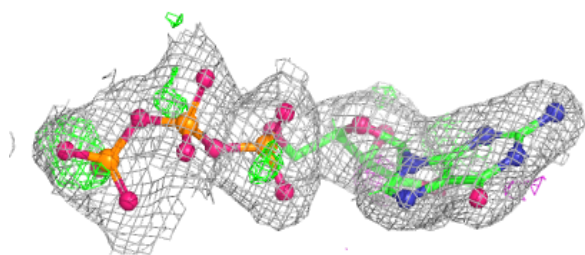
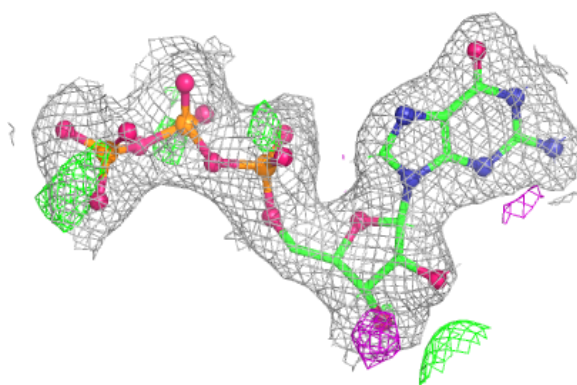
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



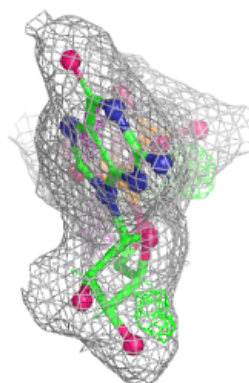
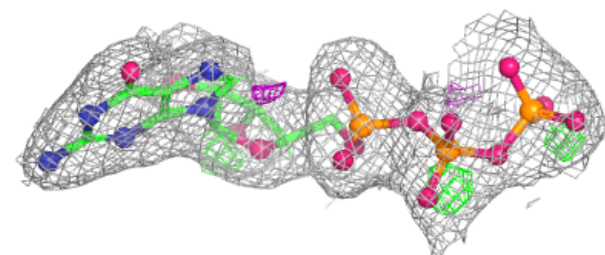
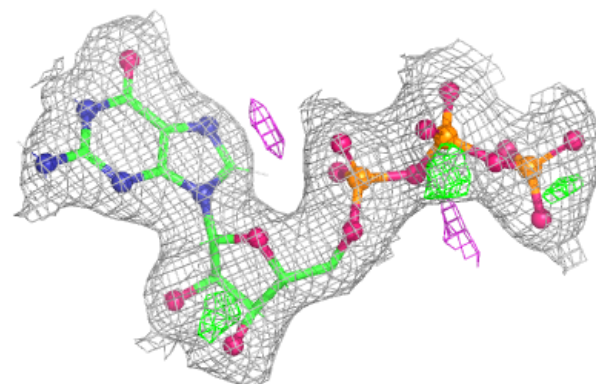


**Electron density around GTP C 501:**

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

**Electron density around 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.