



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:38 PM UTC

PDB ID : 5XHC / pdb_00005xhc
Title : Crystal structure of T2R-TTL-PO10 complex
Authors : Chu, Y.; Wang, Y.; Yang, J.; Li, W.
Deposited on : 2017-04-20
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

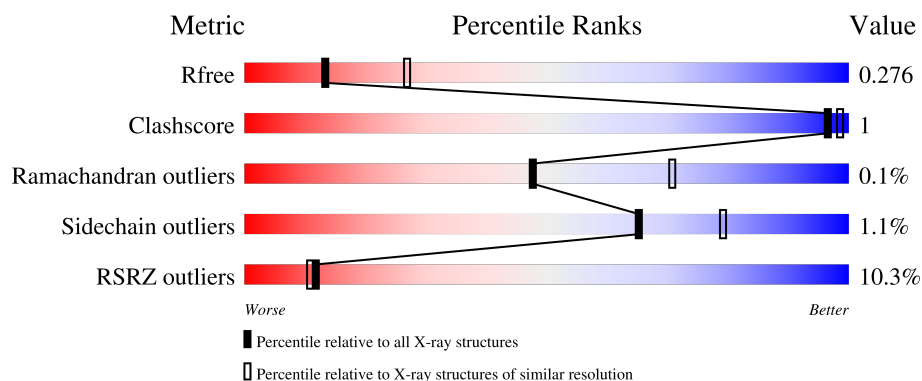
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

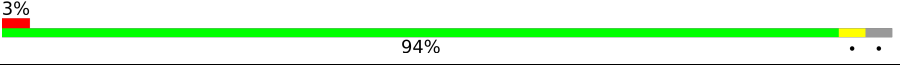
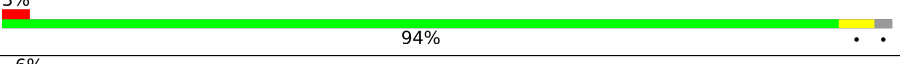
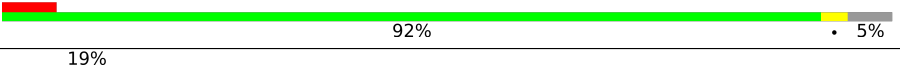
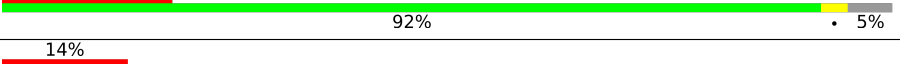
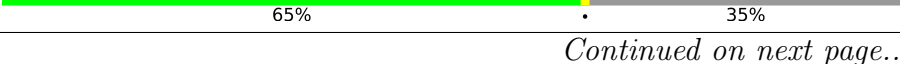
The reported resolution of this entry is 2.75 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	
1	C	450	
2	B	445	
2	D	445	
3	E	184	

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Mol	Chain	Length	Quality of chain
4	F	384	16% 77% 20%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17462 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
1	A	437	Total	C	N	O	S	0	4	0
			3441	2179	586	652	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- Molecule 2 is a protein called Tubulin beta chain.

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

- Molecule 3 is a protein called Stathmin-4.

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

- Molecule 4 is a protein called TUBULIN TYROSINE LIGASE.

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

There are 6 discrepancies between the modelled and reference sequences:

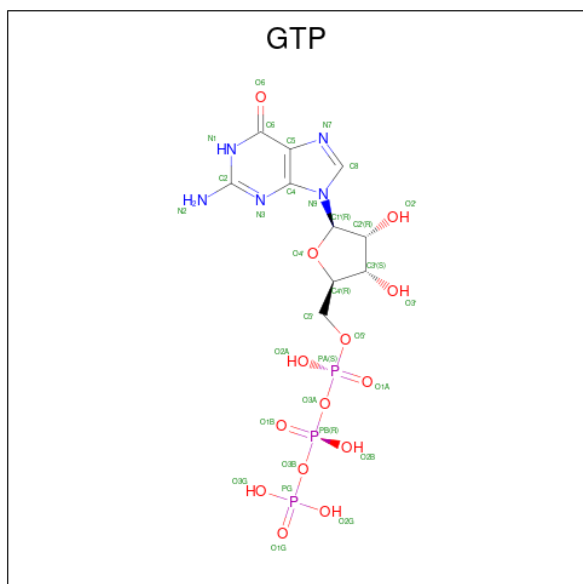
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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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 (CCD ID: 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		

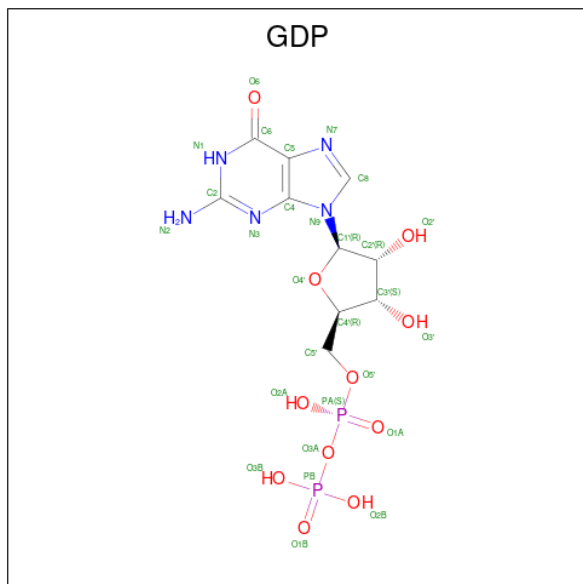
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

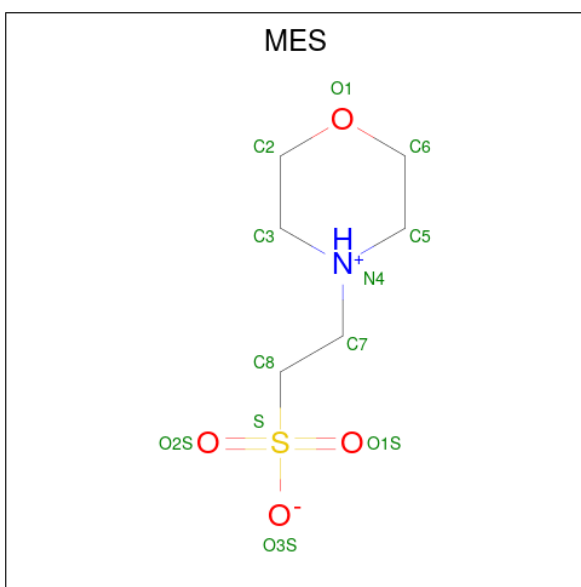
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mg	0	0
			2	2		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

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



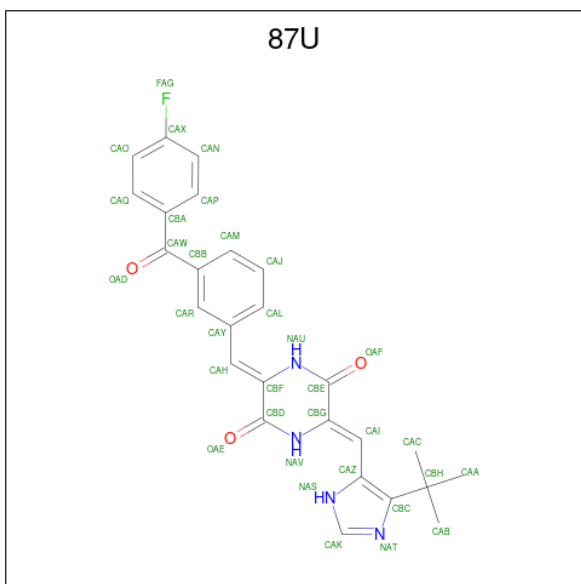
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



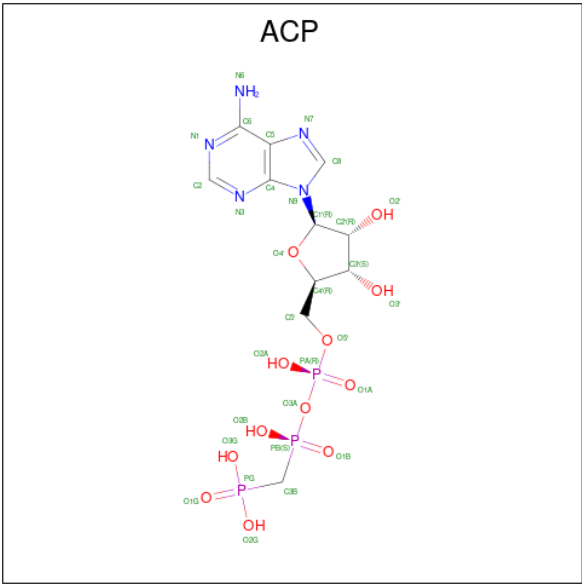
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (3Z,6Z)-3-[(4-tert-butyl-1H-imidazol-5-yl)methylidene]-6-[[3-(4-fluorophenyl)carbonylphenyl]methylidene]piperazine-2,5-dione (CCD ID: 87U) (formula: C₂₆H₂₃FN₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	F	N	O	0	0
			34	26	1	4	3		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

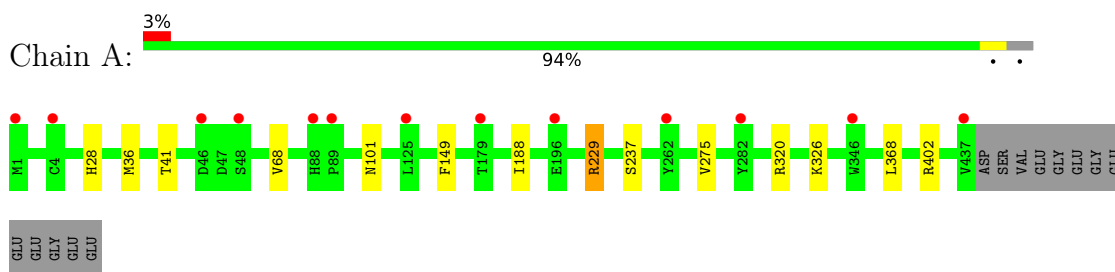
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	20	Total	O	0	0
			20	20		
12	B	22	Total	O	0	0
			22	22		
12	C	55	Total	O	0	0
			55	55		
12	E	2	Total	O	0	0
			2	2		
12	F	4	Total	O	0	0
			4	4		

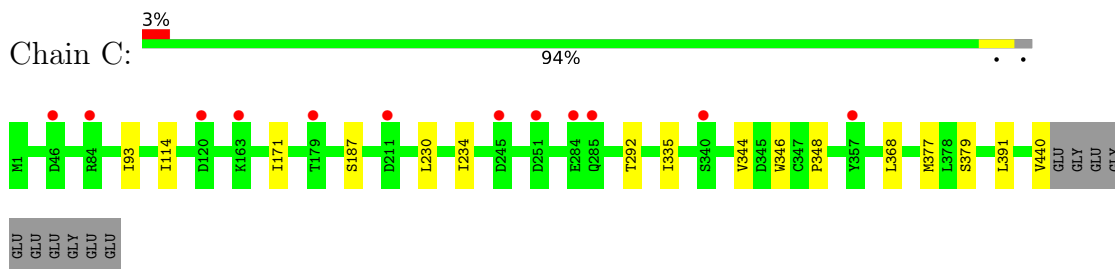
3 Residue-property plots [i](#)

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.

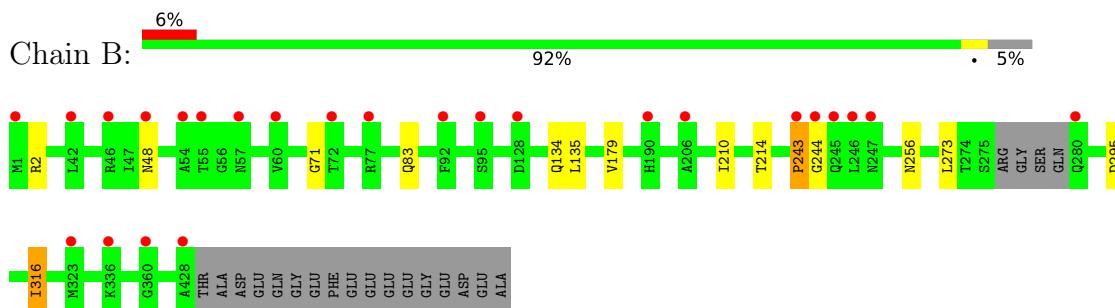
- Molecule 1: Tubulin alpha chain



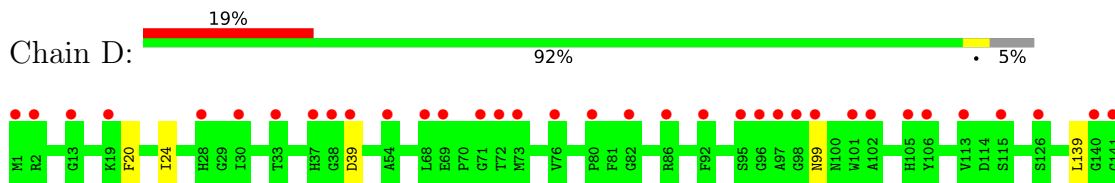
- Molecule 1: Tubulin alpha chain

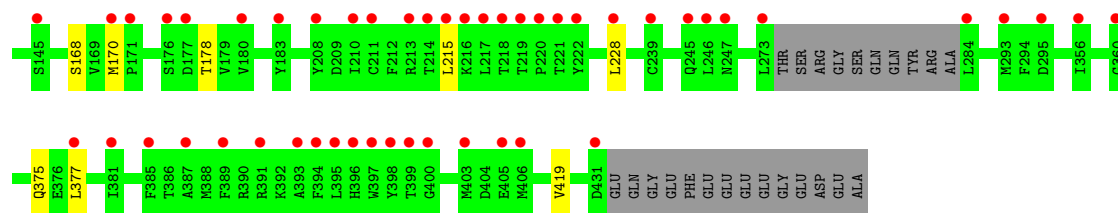


- Molecule 2: Tubulin beta chain

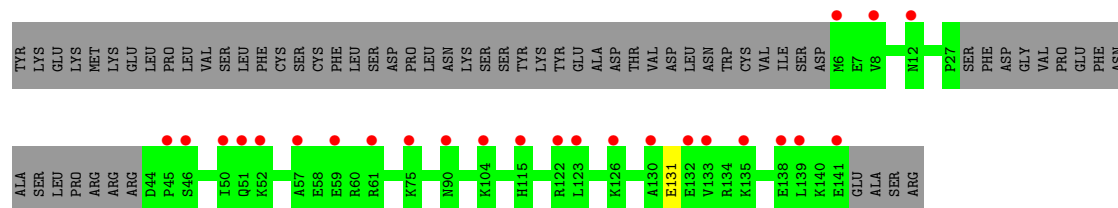


- Molecule 2: Tubulin beta chain

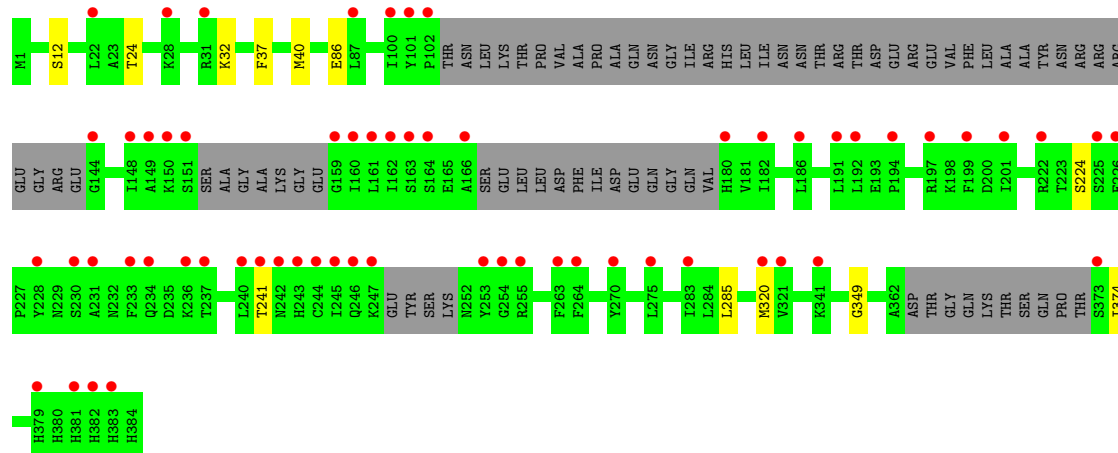
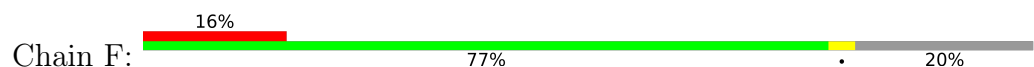




● Molecule 3: Stathmin-4



● 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, α , β , γ	105.26Å 157.88Å 182.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.38 – 2.75 119.38 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (119.38-2.75) 98.5 (119.38-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.227 , 0.277 0.228 , 0.276	Depositor DCC
R_{free} test set	3932 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17462	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 87U, MES, GDP, GTP, ACP, MG, CA

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	0.57	0/3525	0.82	0/4784
1	C	0.55	0/3572	0.82	0/4850
2	B	0.57	0/3427	0.81	1/4640 (0.0%)
2	D	0.56	0/3379	0.80	0/4577
3	E	0.57	0/1018	0.80	0/1350
4	F	0.54	0/2618	0.71	0/3537
All	All	0.56	0/17539	0.80	1/23738 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	316	ILE	CB-CA-C	5.49	118.12	110.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3441	0	3363	10	0
1	C	3482	0	3384	8	0
2	B	3353	0	3228	7	0
2	D	3306	0	3181	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1004	0	1028	0	0
4	F	2553	0	2519	4	0
5	A	32	0	12	0	0
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
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	1	0
10	B	34	0	0	2	0
11	F	31	0	14	1	0
12	A	20	0	0	0	0
12	B	22	0	0	0	0
12	C	55	0	0	0	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17462	0	16791	35	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 1.

All (35) 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	1.07	1.20
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.75	0.98
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.87	0.84
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.67	0.75
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.22	0.69
2:B:295:ASP:HA	9:B:507:MES:O2S	1.96	0.64
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.46	0.63
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:N	2.13	0.63
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:H	1.62	0.62
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.91	0.53
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.50	0.47
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.96	0.47
4:F:320:MET:HE2	11:F:401:ACP:C2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.61	0.47
2:B:210:ILE:HG23	2:B:273:LEU:HD13	1.97	0.47
2:D:139:LEU:HD12	2:D:170:MET:SD	2.54	0.47
1:A:28:HIS:O	1:A:36:MET:HE3	2.15	0.46
10:B:505:87U:NAS	10:B:505:87U:NAV	2.62	0.46
1:C:230:LEU:O	1:C:234:ILE:HD12	2.15	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.45
2:D:139:LEU:HD11	2:D:168:SER:HB3	1.98	0.44
4:F:224:SER:HB2	4:F:241:THR:HG22	2.00	0.43
1:A:275:VAL:HG13	1:A:368[A]:LEU:HD21	2.01	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
1:C:377:MET:HE3	1:C:379:SER:HB3	2.01	0.43
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.00	0.42
2:D:375:GLN:HB2	2:D:419:VAL:HG13	2.01	0.42
2:D:170:MET:HE2	2:D:377:LEU:HD21	2.03	0.41
1:C:171:ILE:N	1:C:171:ILE:HD12	2.35	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.55	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.41
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.56	0.41
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.86	0.41
2:B:134:GLN:HB2	10:B:505:87U:CAP	2.51	0.41
2:D:215:LEU:HD11	2:D:228:LEU:HD21	2.03	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%)	426 (97%)	13 (3%)	0	100	100
1	C	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
2	B	422/445 (95%)	407 (96%)	13 (3%)	2 (0%)	24	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	417/445 (94%)	404 (97%)	12 (3%)	1 (0%)	43	64
3	E	118/184 (64%)	116 (98%)	2 (2%)	0	100	100
4	F	300/384 (78%)	286 (95%)	14 (5%)	0	100	100
All	All	2142/2358 (91%)	2074 (97%)	65 (3%)	3 (0%)	48	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	B	71	GLY
2	D	39	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/378 (98%)	364 (98%)	8 (2%)	45	67
1	C	379/378 (100%)	377 (100%)	2 (0%)	81	89
2	B	367/383 (96%)	361 (98%)	6 (2%)	55	73
2	D	362/383 (94%)	362 (100%)	0	100	100
3	E	110/168 (66%)	109 (99%)	1 (1%)	70	82
4	F	281/342 (82%)	276 (98%)	5 (2%)	51	71
All	All	1871/2032 (92%)	1849 (99%)	22 (1%)	65	78

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

Mol	Chain	Res	Type
1	A	41	THR
1	A	188	ILE
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	237	SER

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Mol	Chain	Res	Type
1	A	320	ARG
1	A	326	LYS
1	A	402	ARG
2	B	2	ARG
2	B	48	ASN
2	B	83	GLN
2	B	135	LEU
2	B	214	THR
2	B	316	ILE
1	C	368	LEU
1	C	440	VAL
3	E	131	GLU
4	F	12	SER
4	F	24	THR
4	F	32	LYS
4	F	86	GLU
4	F	285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	101	ASN
1	A	216	ASN
1	A	233	GLN
1	A	393	HIS
2	B	37	HIS
2	B	83	GLN
2	B	94	GLN
2	B	375	GLN
2	B	426	GLN
1	C	31	GLN
1	C	133	GLN
1	C	249	ASN
1	C	283	HIS
1	C	356	ASN
1	C	358	GLN
1	C	372	GLN
1	C	393	HIS
1	C	406	HIS
2	D	37	HIS
2	D	99	ASN

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Mol	Chain	Res	Type
2	D	329	GLN
2	D	335	ASN
2	D	347	ASN
2	D	375	GLN
2	D	396	HIS
3	E	90	ASN
3	E	124	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\# Z > 2$
11	ACP	F	401	-	31,33,33	2.20	11 (35%)	47,52,52	1.84	11 (23%)
5	GTP	C	501	7	33,34,34	1.27	5 (15%)	50,54,54	1.56	7 (14%)
5	GTP	D	501	7	33,34,34	1.23	3 (9%)	50,54,54	1.65	6 (12%)
9	MES	B	507	-	12,12,12	2.10	2 (16%)	15,16,16	5.48	6 (40%)
9	MES	B	504	-	12,12,12	2.08	1 (8%)	15,16,16	6.23	10 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	B	502	7	29,30,30	1.26	4 (13%)	45,47,47	1.67	6 (13%)
5	GTP	A	501	7	33,34,34	1.28	5 (15%)	50,54,54	1.63	9 (18%)
10	87U	B	505	-	37,37,37	2.18	11 (29%)	51,54,54	1.95	15 (29%)

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
11	ACP	F	401	-	-	4/19/38/38	0/3/3/3
5	GTP	C	501	7	-	7/22/38/38	0/3/3/3
5	GTP	D	501	7	-	4/22/38/38	0/3/3/3
9	MES	B	507	-	-	2/6/14/14	0/1/1/1
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
8	GDP	B	502	7	-	3/16/32/32	0/3/3/3
5	GTP	A	501	7	-	3/22/38/38	0/3/3/3
10	87U	B	505	-	-	2/22/22/22	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-6.56	1.68	1.77
9	B	507	MES	C8-S	-6.51	1.68	1.77
11	F	401	ACP	PG-O1G	5.65	1.61	1.50
10	B	505	87U	FAG-CAX	-5.48	1.23	1.36
10	B	505	87U	CBA-CAW	-5.05	1.41	1.49
11	F	401	ACP	C5-C4	4.92	1.47	1.39
10	B	505	87U	CBB-CAW	-4.29	1.42	1.49
11	F	401	ACP	PB-O1B	4.12	1.61	1.51
10	B	505	87U	CAY-CAH	-3.89	1.39	1.46
10	B	505	87U	CBF-CBD	-3.83	1.41	1.48
10	B	505	87U	CBG-CBE	-3.62	1.41	1.48
11	F	401	ACP	PB-O3A	3.41	1.62	1.58
5	D	501	GTP	C5-C4	3.37	1.48	1.38
5	C	501	GTP	C5-C4	3.29	1.47	1.38
10	B	505	87U	CAZ-CBC	-3.24	1.34	1.38
8	B	502	GDP	C5-C4	3.23	1.47	1.38
5	A	501	GTP	C5-C4	3.18	1.47	1.38
10	B	505	87U	CAZ-NAS	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O2B	-3.17	1.48	1.56
11	F	401	ACP	PG-O2G	3.01	1.61	1.55
11	F	401	ACP	C5-C6	2.87	1.49	1.41
10	B	505	87U	CAH-CBF	2.86	1.40	1.34
11	F	401	ACP	PG-O3G	-2.81	1.48	1.55
5	A	501	GTP	PB-O3B	2.62	1.62	1.59
5	D	501	GTP	PB-O3B	2.56	1.62	1.59
8	B	502	GDP	PA-O3A	2.51	1.62	1.59
5	C	501	GTP	PA-O3A	2.49	1.62	1.59
5	C	501	GTP	C6-N1	-2.43	1.34	1.38
11	F	401	ACP	C5-N7	-2.43	1.34	1.39
11	F	401	ACP	C8-N7	2.42	1.36	1.31
11	F	401	ACP	PA-O3A	2.41	1.62	1.59
5	A	501	GTP	PA-O3A	2.32	1.62	1.59
8	B	502	GDP	C5-N7	-2.30	1.34	1.39
5	A	501	GTP	C5-N7	-2.27	1.34	1.39
8	B	502	GDP	C6-N1	-2.27	1.34	1.38
9	B	507	MES	O2S-S	2.15	1.51	1.45
5	D	501	GTP	C5-N7	-2.12	1.34	1.39
5	A	501	GTP	C4-N9	-2.06	1.32	1.38
5	C	501	GTP	C5-N7	-2.04	1.35	1.39
10	B	505	87U	CBE-NAU	2.02	1.42	1.38
5	C	501	GTP	PB-O3B	2.02	1.61	1.59
10	B	505	87U	CAI-CAZ	-2.01	1.35	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	O1S-S-C8	-14.83	84.32	106.73
9	B	507	MES	O3S-S-O1S	-13.11	78.60	111.40
9	B	504	MES	O3S-S-O1S	-10.44	85.27	111.40
9	B	504	MES	O2S-S-O1S	-9.33	83.47	113.82
9	B	507	MES	O2S-S-O1S	-9.30	83.57	113.82
9	B	504	MES	O2S-S-C8	9.21	120.65	106.73
9	B	507	MES	O3S-S-C8	8.58	122.79	106.00
9	B	507	MES	O1S-S-C8	-7.99	94.65	106.73
9	B	504	MES	O3S-S-C8	6.19	118.12	106.00
11	F	401	ACP	C5-C4-N3	-5.87	118.63	126.72
9	B	507	MES	O3S-S-O2S	5.82	125.96	111.40
5	D	501	GTP	C5-C4-N3	-5.71	119.30	128.39
8	B	502	GDP	C5-C4-N3	-5.41	119.77	128.39
5	A	501	GTP	C5-C4-N3	-5.15	120.19	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C5-C4-N3	-5.12	120.24	128.39
5	D	501	GTP	C2-N3-C4	4.83	120.62	112.30
8	B	502	GDP	C2-N3-C4	4.68	120.36	112.30
11	F	401	ACP	N3-C4-N9	4.66	135.10	127.17
5	C	501	GTP	C2-N3-C4	4.48	120.02	112.30
5	A	501	GTP	C2-N3-C4	4.48	120.01	112.30
5	D	501	GTP	N9-C4-N3	4.38	134.71	125.95
10	B	505	87U	CBG-CBE-NAU	4.37	120.32	116.02
10	B	505	87U	CBF-CBD-NAV	4.36	120.30	116.02
8	B	502	GDP	N9-C4-N3	4.30	134.56	125.95
10	B	505	87U	NAS-CAK-NAT	-4.24	108.06	112.98
9	B	504	MES	C2-C3-N4	4.20	116.50	110.12
10	B	505	87U	CBH-CBC-NAT	3.99	123.77	117.42
5	A	501	GTP	N9-C4-N3	3.95	133.85	125.95
11	F	401	ACP	C2-N3-C4	3.94	121.44	111.83
11	F	401	ACP	N3-C2-N1	-3.81	122.82	128.58
5	C	501	GTP	N9-C4-N3	3.76	133.47	125.95
5	A	501	GTP	C6-C5-N7	3.54	136.73	130.29
10	B	505	87U	CBF-NAU-CBE	-3.53	121.51	125.51
11	F	401	ACP	C4-C5-N7	-3.51	106.57	110.58
5	C	501	GTP	C6-C5-N7	3.51	136.68	130.29
8	B	502	GDP	C6-C5-N7	3.48	136.62	130.29
10	B	505	87U	CAY-CAR-CBB	3.41	124.04	121.10
5	D	501	GTP	C6-C5-N7	3.29	136.28	130.29
10	B	505	87U	CAZ-CAI-CBG	-3.11	121.88	130.82
10	B	505	87U	CAM-CBB-CAR	-2.83	115.97	119.25
9	B	504	MES	O3S-S-O2S	2.78	118.35	111.40
10	B	505	87U	CBG-NAV-CBD	-2.77	122.37	125.51
11	F	401	ACP	C5-N7-C8	2.73	107.74	103.45
10	B	505	87U	CAK-NAT-CBC	2.69	108.00	104.97
9	B	504	MES	C5-N4-C3	2.64	114.53	108.84
11	F	401	ACP	C4-N9-C8	2.60	108.47	105.74
5	A	501	GTP	O3B-PG-O1G	-2.48	97.99	111.04
5	A	501	GTP	C4-C5-N7	-2.42	106.83	110.67
5	D	501	GTP	C4-C5-N7	-2.41	106.85	110.67
5	C	501	GTP	O3G-PG-O2G	2.38	116.73	107.80
8	B	502	GDP	C4-C5-N7	-2.34	106.96	110.67
9	B	504	MES	C6-C5-N4	2.30	113.61	110.12
5	C	501	GTP	C4-C5-N7	-2.27	107.07	110.67
11	F	401	ACP	C3'-C2'-C1'	2.24	105.70	101.46
5	A	501	GTP	O3B-PB-O1B	-2.21	104.05	110.70
5	A	501	GTP	O6-C6-C5	-2.21	120.70	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	O1-C6-C5	-2.20	107.03	111.77
10	B	505	87U	CBH-CBC-CAZ	-2.19	128.18	131.26
5	D	501	GTP	O6-C6-C5	-2.19	120.76	126.53
10	B	505	87U	CAJ-CAL-CAY	-2.15	118.12	120.64
5	A	501	GTP	O2B-PB-O3B	2.15	113.09	107.27
11	F	401	ACP	C6-C5-N7	2.15	136.23	132.09
10	B	505	87U	CAM-CBB-CAW	2.15	125.27	120.55
11	F	401	ACP	N9-C8-N7	-2.10	110.95	113.94
9	B	507	MES	C6-C5-N4	2.10	113.31	110.12
8	B	502	GDP	O6-C6-C5	-2.08	121.04	126.53
10	B	505	87U	CAK-NAS-CAZ	2.07	108.81	107.57
10	B	505	87U	CAI-CBG-NAV	-2.04	119.89	122.75
11	F	401	ACP	C2-N1-C6	2.04	122.07	118.73
5	C	501	GTP	O2B-PB-O3B	2.02	112.74	107.27

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
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-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	502	GDP	C5'-O5'-PA-O3A
8	B	502	GDP	C5'-O5'-PA-O1A
8	B	502	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O2S
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O3S
9	B	507	MES	C7-C8-S-O3S
9	B	504	MES	N4-C7-C8-S
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	507	MES	C7-C8-S-O1S
10	B	505	87U	CBG-CAI-CAZ-NAS
5	C	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PG-C3B-PB-O1B

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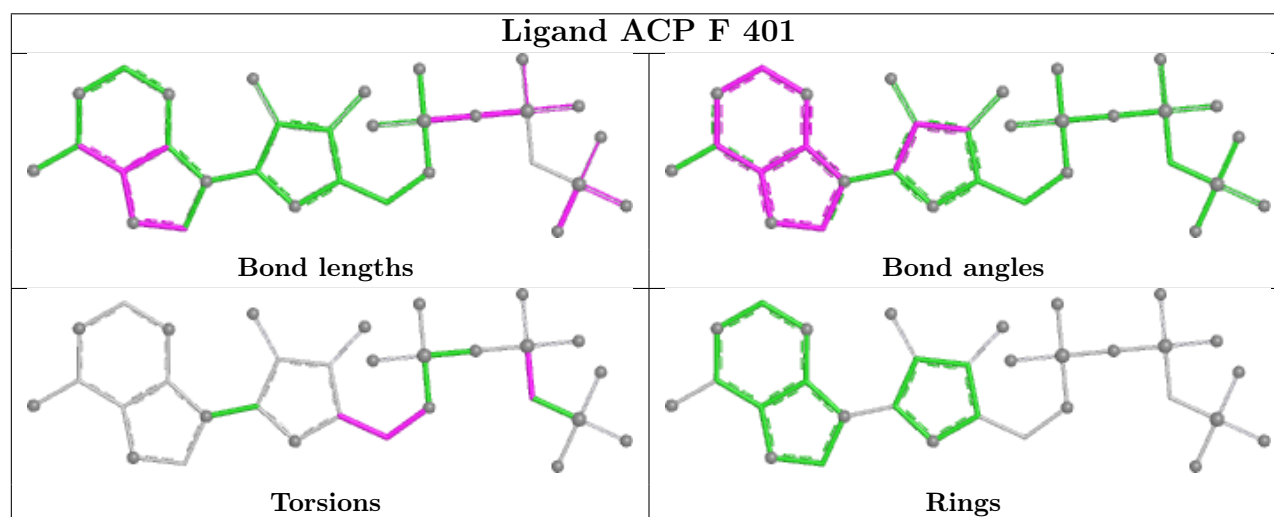
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	C4'-C5'-O5'-PA
10	B	505	87U	CBG-CAI-CAZ-CBC
11	F	401	ACP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

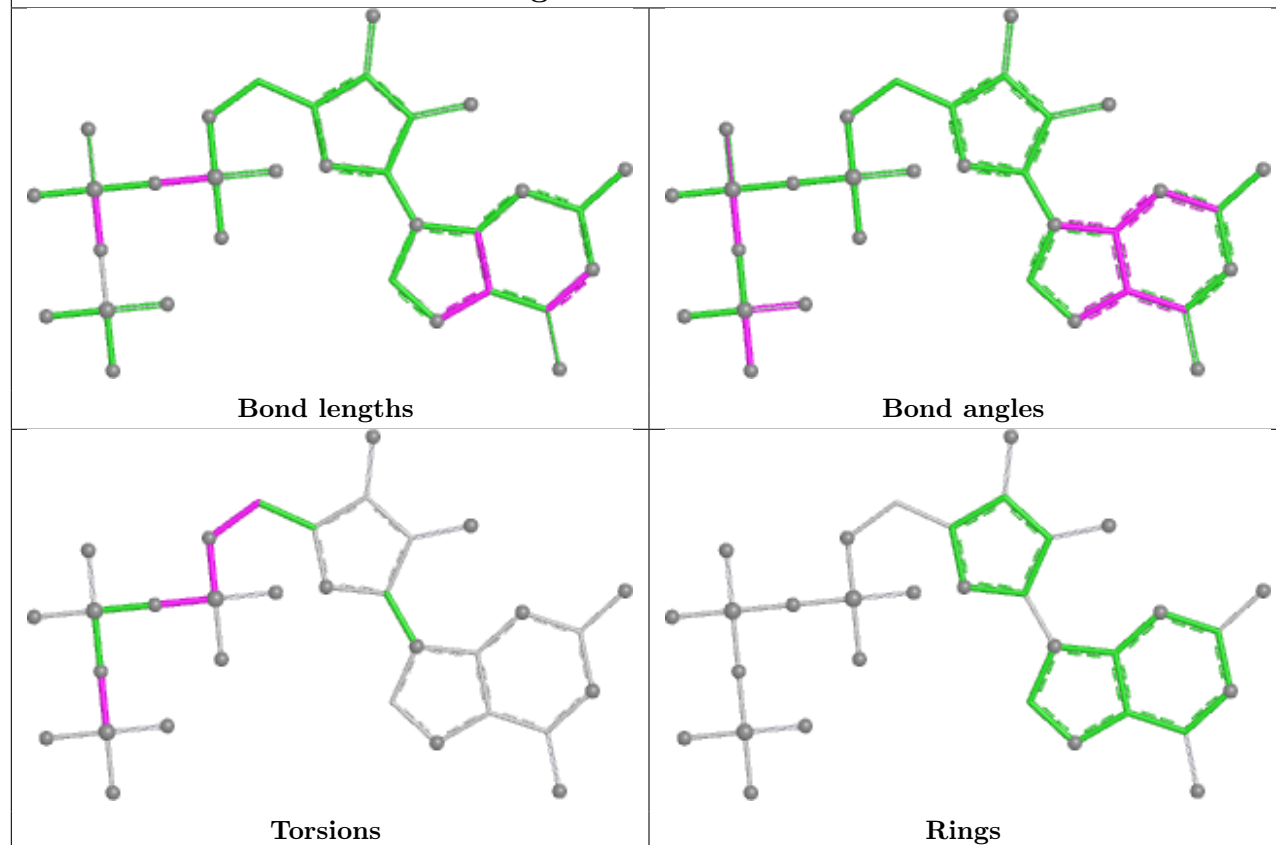
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	1	0
9	B	507	MES	1	0
10	B	505	87U	2	0

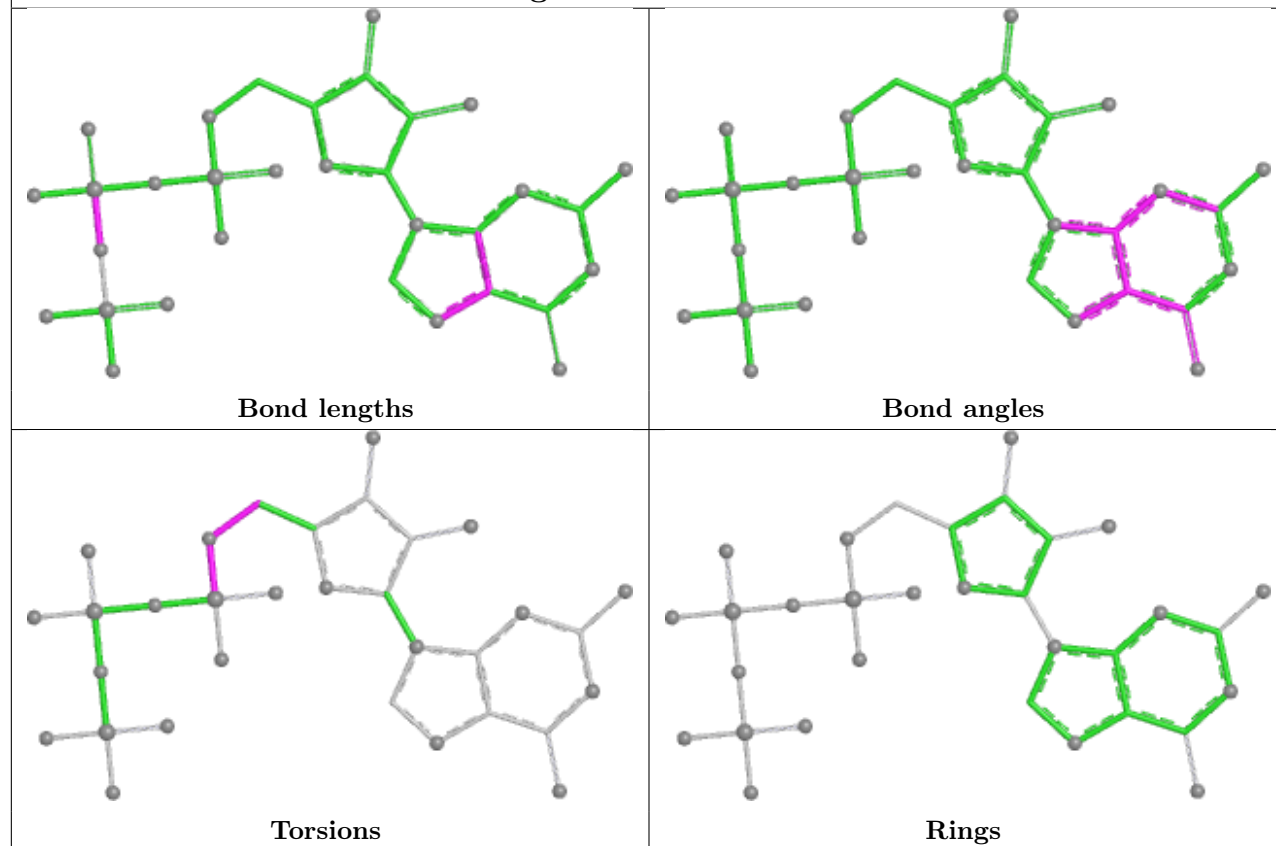
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

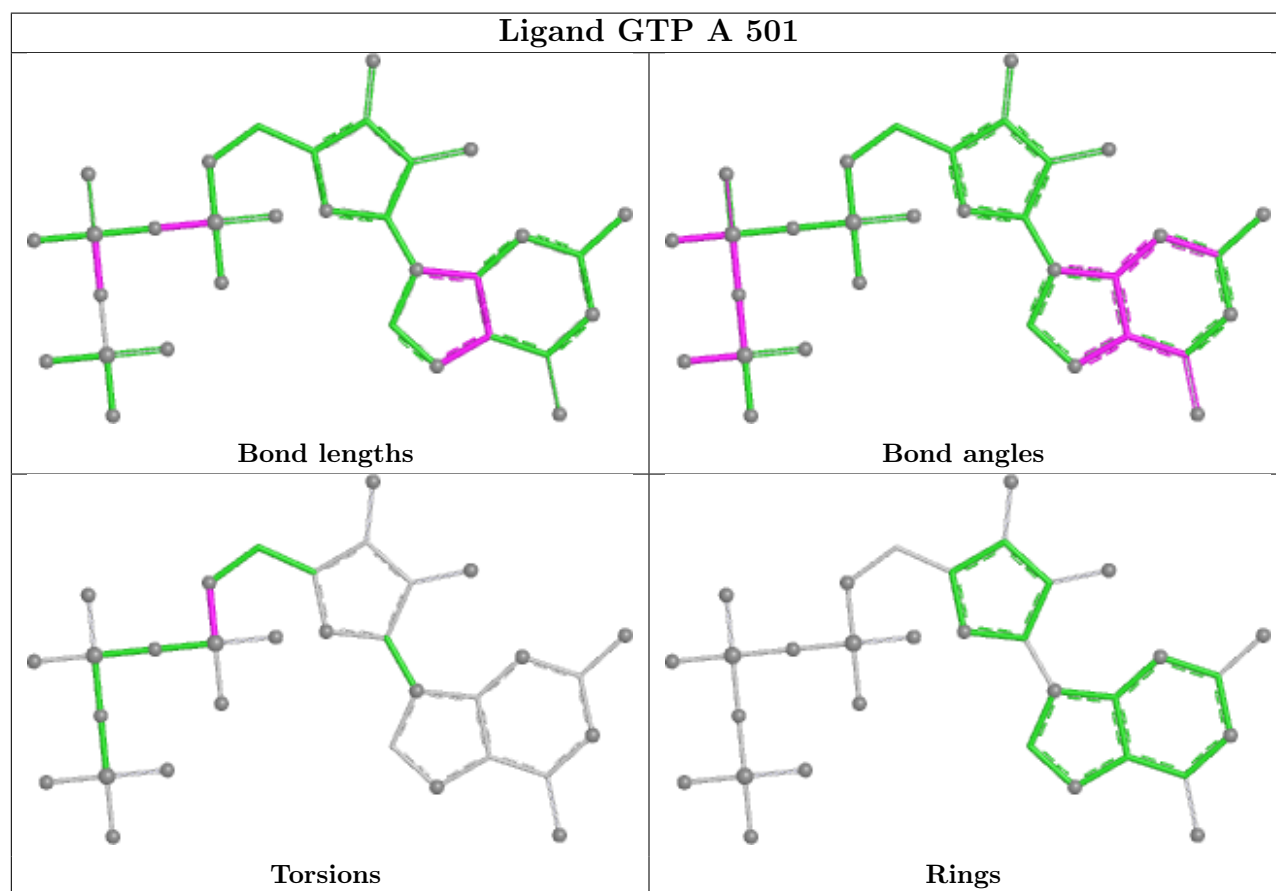
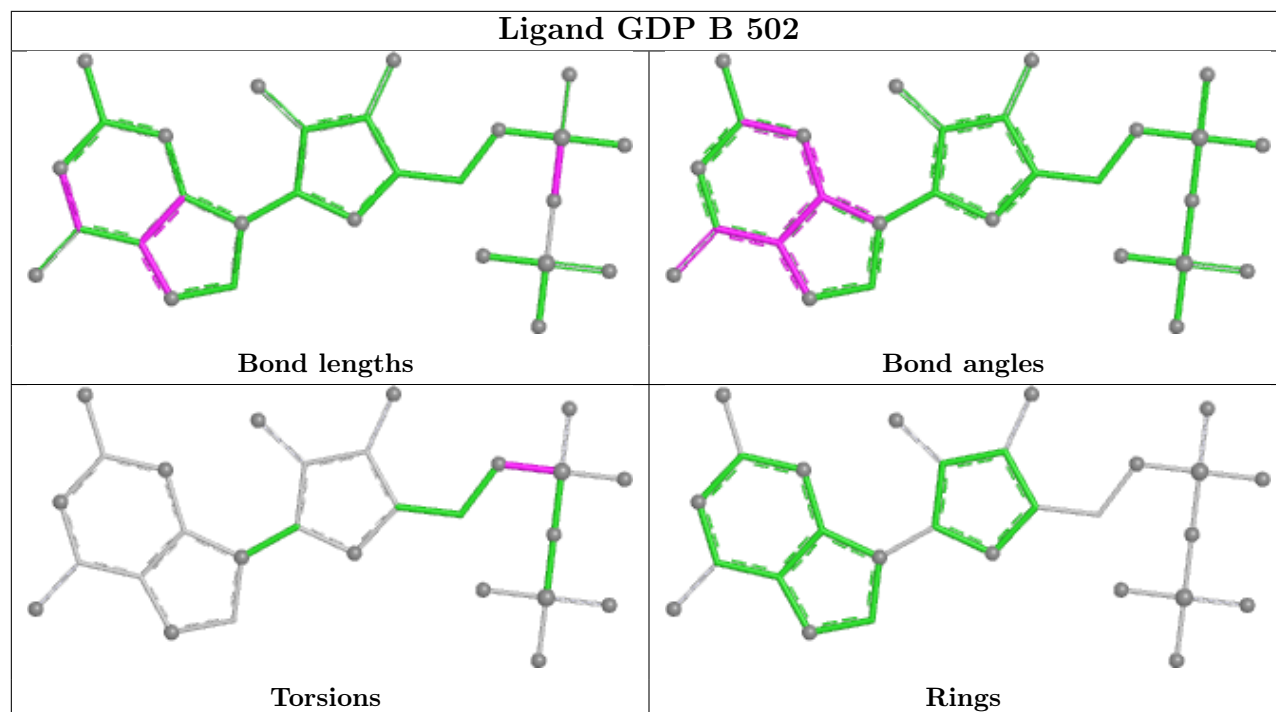


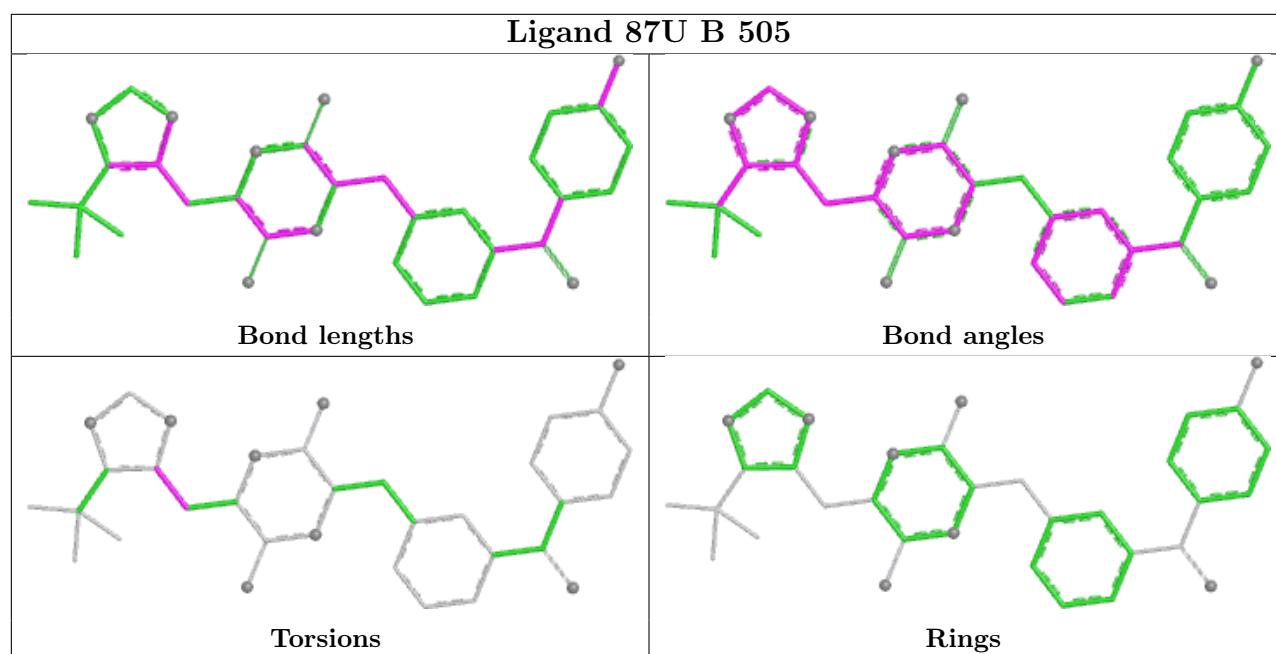
Ligand GTP C 501



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	437/450 (97%)	0.48	13 (2%)	52	50	18, 45, 71, 91	4 (0%)
1	C	440/450 (97%)	0.20	12 (2%)	56	54	14, 36, 58, 80	9 (2%)
2	B	424/445 (95%)	0.62	25 (5%)	28	28	17, 45, 75, 102	3 (0%)
2	D	421/445 (94%)	1.29	84 (19%)	3	2	35, 64, 96, 126	4 (0%)
3	E	120/184 (65%)	1.26	25 (20%)	2	2	34, 64, 95, 106	2 (1%)
4	F	309/384 (80%)	1.27	62 (20%)	3	2	18, 68, 107, 122	3 (0%)
All	All	2151/2358 (91%)	0.77	221 (10%)	12	11	14, 50, 92, 126	25 (1%)

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	6.8
4	F	182	ILE	5.8
4	F	161	LEU	5.6
4	F	102	PRO	5.4
4	F	100	ILE	5.3
4	F	233	PHE	5.0
2	D	210	ILE	4.8
3	E	12[A]	ASN	4.7
3	E	51	GLN	4.7
2	D	98	GLY	4.7
2	D	92	PHE	4.7
2	B	246	LEU	4.6
2	D	97	ALA	4.4
4	F	159	GLY	4.2
1	A	262	TYR	4.2
1	C	211[A]	ASP	4.2
2	D	73	MET	4.1
4	F	245	ILE	4.1
2	D	214	THR	3.9

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Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	3.9
2	D	217	LEU	3.9
2	D	1	MET	3.6
2	D	219	THR	3.6
2	D	396	HIS	3.6
2	D	106	TYR	3.6
2	B	336	LYS	3.5
2	D	220	PRO	3.5
2	D	215	LEU	3.5
1	C	340	SER	3.5
4	F	225	SER	3.5
4	F	237	THR	3.5
4	F	186	LEU	3.4
4	F	240	LEU	3.4
2	D	96	GLY	3.4
2	D	394	PHE	3.3
2	B	244	GLY	3.3
2	D	170	MET	3.3
4	F	226	GLU	3.2
2	D	395	LEU	3.1
3	E	50	ILE	3.1
4	F	162	ILE	3.1
1	C	120[A]	ASP	3.1
3	E	139	LEU	3.1
2	D	101	TRP	3.1
3	E	52	LYS	3.1
1	C	245	ASP	3.0
4	F	263	PHE	3.0
2	D	72	THR	3.0
2	B	1	MET	3.0
3	E	6	MET	3.0
4	F	180	HIS	3.0
4	F	194	PRO	3.0
4	F	247	LYS	3.0
1	C	251[A]	ASP	3.0
2	D	54	ALA	3.0
2	D	180	VAL	3.0
2	D	228	LEU	2.9
4	F	87	LEU	2.9
4	F	192	LEU	2.9
1	C	285	GLN	2.9
2	B	245	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	247	ASN	2.9
4	F	144	GLY	2.9
2	D	218	THR	2.9
3	E	45	PRO	2.9
1	A	282	TYR	2.9
2	D	431	ASP	2.9
4	F	381	HIS	2.9
2	D	381	ILE	2.9
4	F	31	ARG	2.8
2	D	360	GLY	2.8
2	D	400	GLY	2.8
4	F	199	PHE	2.8
4	F	383	HIS	2.8
2	B	280	GLN	2.8
2	D	38	GLY	2.8
1	A	179	THR	2.8
2	D	398	TYR	2.8
2	D	397	TRP	2.8
2	D	99	ASN	2.8
3	E	133	VAL	2.8
3	E	61	ARG	2.8
2	B	128	ASP	2.7
2	D	356	ILE	2.7
2	D	211	CYS	2.7
4	F	160	ILE	2.7
2	D	377	LEU	2.7
2	D	37	HIS	2.7
2	D	140	GLY	2.7
1	A	437	VAL	2.7
2	D	39	ASP	2.7
2	D	295	ASP	2.7
4	F	197	ARG	2.7
3	E	59	GLU	2.6
4	F	254	GLY	2.6
2	B	95	SER	2.6
2	D	176	SER	2.6
4	F	191	LEU	2.6
2	D	95	SER	2.6
2	D	399	THR	2.6
1	A	1	MET	2.6
2	D	183	TYR	2.6
1	A	346	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	55	THR	2.6
2	D	71	GLY	2.5
2	B	247	ASN	2.5
2	D	115	SER	2.5
2	D	145[A]	SER	2.5
4	F	230	SER	2.5
4	F	373	SER	2.5
4	F	148	ILE	2.5
3	E	75	LYS	2.5
2	B	92	PHE	2.5
3	E	123	LEU	2.5
4	F	234	GLN	2.5
2	D	239	CYS	2.5
2	D	245	GLN	2.5
3	E	135	LYS	2.4
1	A	46	ASP	2.4
1	C	357	TYR	2.4
3	E	126	LYS	2.4
4	F	264	PHE	2.4
2	B	46	ARG	2.4
2	B	72	THR	2.4
2	D	213	ARG	2.4
2	D	30	ILE	2.4
4	F	151	SER	2.4
4	F	163	SER	2.4
4	F	382	HIS	2.4
2	D	69	GLU	2.4
4	F	341	LYS	2.4
1	C	84	ARG	2.4
2	D	273	LEU	2.4
2	B	48	ASN	2.4
2	D	13	GLY	2.4
2	D	113	VAL	2.4
2	D	86	ARG	2.4
2	D	389	PHE	2.4
2	D	246	LEU	2.4
3	E	115	HIS	2.4
2	D	293	MET	2.4
2	B	243	PRO	2.4
2	D	393	ALA	2.4
4	F	228	TYR	2.3
4	F	246	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	243	HIS	2.3
3	E	104	LYS	2.3
2	D	82	GLY	2.3
2	D	284	LEU	2.3
3	E	57	ALA	2.3
2	D	406	MET	2.3
3	E	141	GLU	2.3
4	F	379	HIS	2.3
4	F	236	LYS	2.3
4	F	253	TYR	2.3
3	E	90	ASN	2.3
3	E	46	SER	2.3
2	B	360	GLY	2.3
2	D	141	GLY	2.3
1	C	179	THR	2.2
2	D	221	THR	2.2
2	D	208	TYR	2.2
2	B	57	ASN	2.2
2	D	126	SER	2.2
4	F	22	LEU	2.2
4	F	321	VAL	2.2
2	B	428	ALA	2.2
4	F	244	CYS	2.2
3	E	122	ARG	2.2
1	C	46	ASP	2.2
2	B	42	LEU	2.2
3	E	8	VAL	2.2
4	F	28	LYS	2.2
2	B	323	MET	2.2
2	D	105	HIS	2.2
4	F	201	ILE	2.2
4	F	320	MET	2.2
2	D	68	LEU	2.2
4	F	150	LYS	2.2
2	D	403	MET	2.2
1	A	88	HIS	2.2
2	B	77	ARG	2.2
1	A	89	PRO	2.2
1	C	163	LYS	2.2
4	F	275	LEU	2.2
3	E	130	ALA	2.1
3	E	138	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	2	ARG	2.1
2	D	171	PRO	2.1
2	D	216	LYS	2.1
4	F	164	SER	2.1
2	D	19	LYS	2.1
1	A	48	SER	2.1
2	D	385	PHE	2.1
2	D	33	THR	2.1
4	F	241	THR	2.1
1	A	4	CYS	2.1
4	F	242	ASN	2.1
4	F	270	TYR	2.1
2	B	60	VAL	2.1
4	F	283	ILE	2.1
1	C	284	GLU	2.1
2	B	206	ALA	2.1
3	E	132	GLU	2.1
4	F	222	ARG	2.1
4	F	231	ALA	2.1
2	D	80	PRO	2.1
1	A	125	LEU	2.1
1	A	196	GLU	2.0
2	D	387	ALA	2.0
2	D	405	GLU	2.0
2	B	190	HIS	2.0
2	D	222	TYR	2.0
4	F	101	TYR	2.0
4	F	255	ARG	2.0
2	B	54	ALA	2.0
2	D	102	ALA	2.0
2	D	177	ASP	2.0
2	D	28	HIS	2.0
2	D	76	VAL	2.0
2	D	391	ARG	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

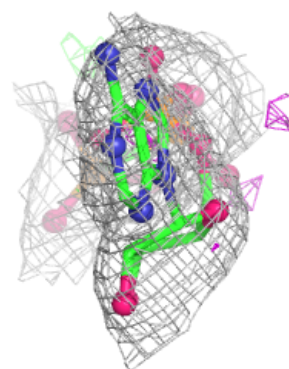
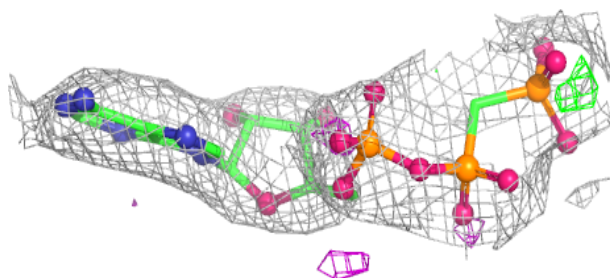
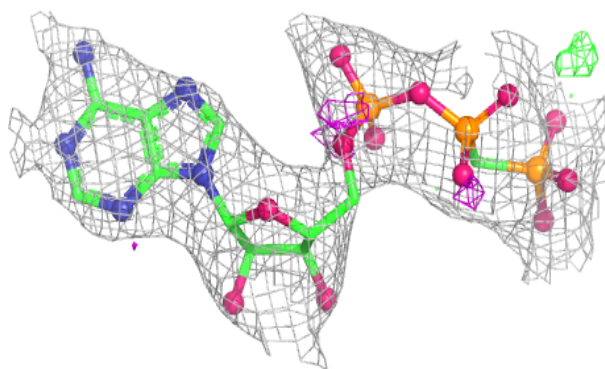
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ACP	F	401	31/31	0.77	0.14	79,83,112,115	0
9	MES	B	507	12/12	0.84	0.22	95,97,101,104	0
9	MES	B	504	12/12	0.85	0.18	70,74,76,78	0
6	CA	B	506	1/1	0.87	0.10	78,78,78,78	0
5	GTP	D	501	32/32	0.87	0.12	45,49,67,70	0
7	MG	D	502	1/1	0.89	0.09	52,52,52,52	0
10	87U	B	505	34/34	0.91	0.12	48,54,55,55	0
6	CA	A	502	1/1	0.92	0.07	67,67,67,67	0
6	CA	C	503	1/1	0.94	0.06	56,56,56,56	0
5	GTP	A	501	32/32	0.97	0.06	26,28,30,30	0
8	GDP	B	502	28/28	0.97	0.06	22,25,26,28	0
5	GTP	C	501	32/32	0.97	0.06	24,26,28,30	0
7	MG	B	501	1/1	0.98	0.04	22,22,22,22	0
7	MG	B	503	1/1	0.98	0.03	24,24,24,24	0
7	MG	C	502	1/1	1.00	0.01	24,24,24,24	0

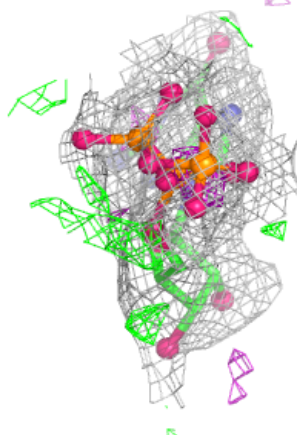
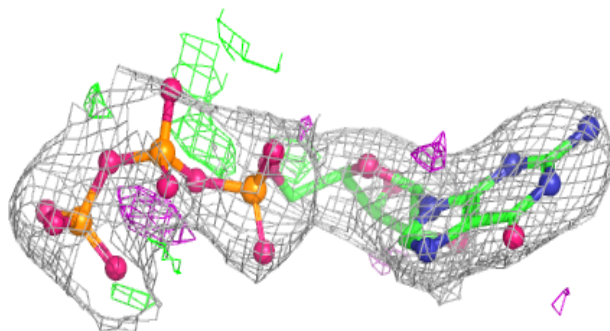
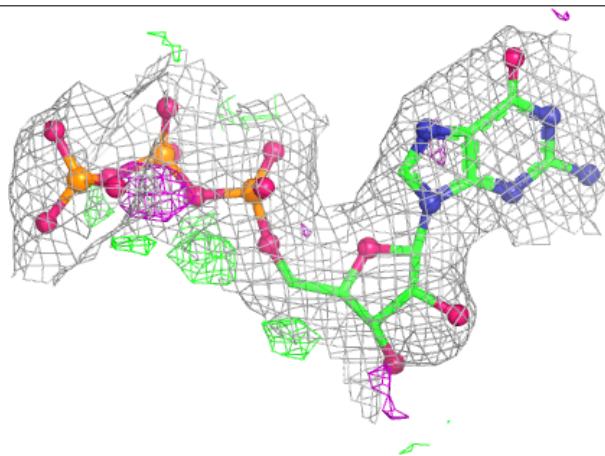
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

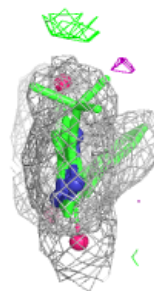
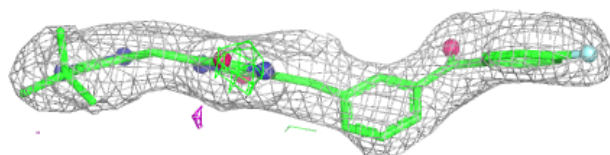
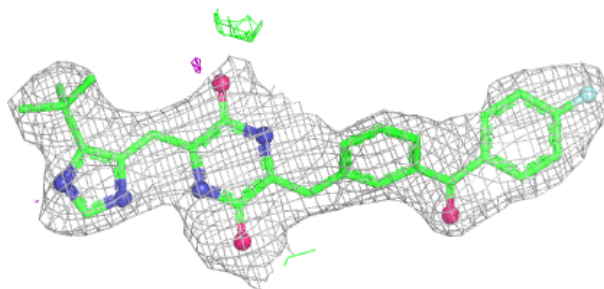
**Electron density around GTP D 501:**

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

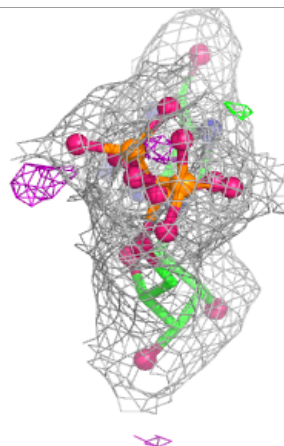
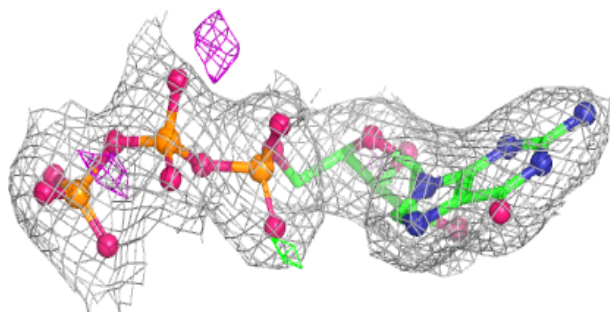
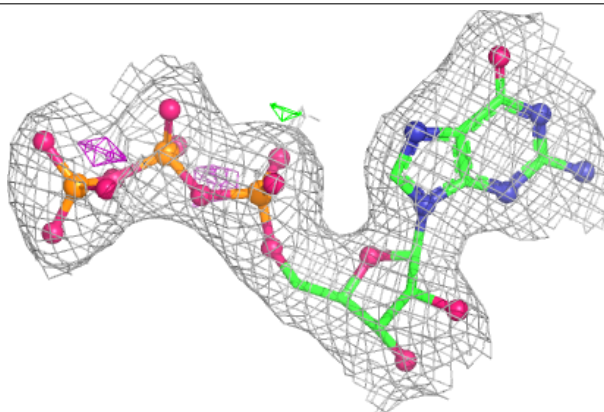


Electron density around 87U B 505:

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

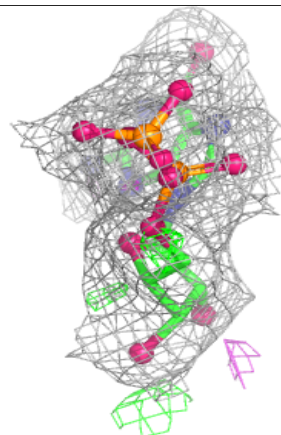
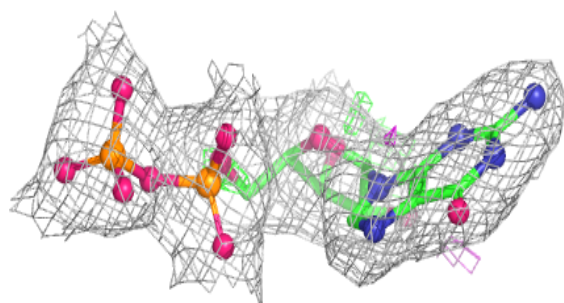
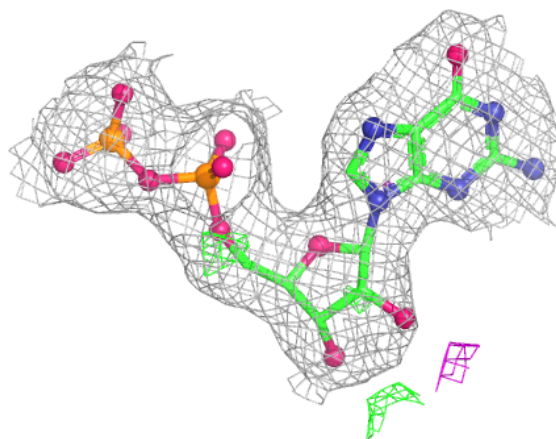
**Electron density around GTP A 501:**

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

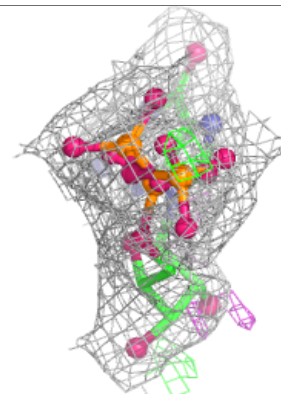
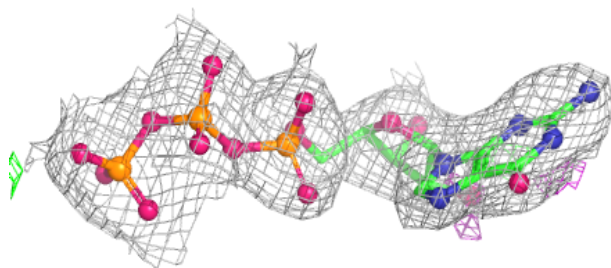
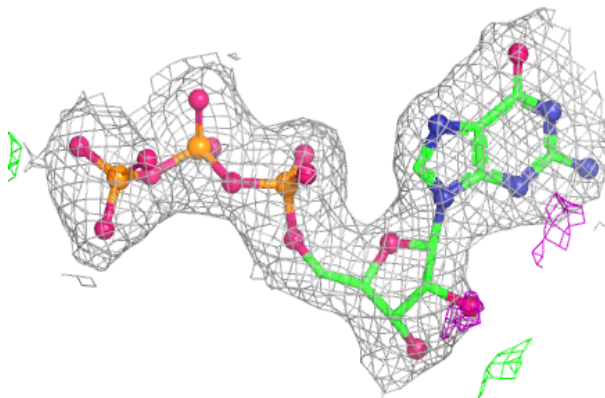


Electron density around GDP B 502:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.