



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:59 AM UTC

PDB ID : 5YL4 / pdb_00005yl4
Title : CRYSTAL STRUCTURE OF T2R-TTL-8WR COMPLEX
Authors : Fu, Z.Y.; Li, W.B.; Chu, Y.Y.; Hou, Y.W.; Ji, C.P.
Deposited on : 2017-10-17
Resolution : 2.64 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

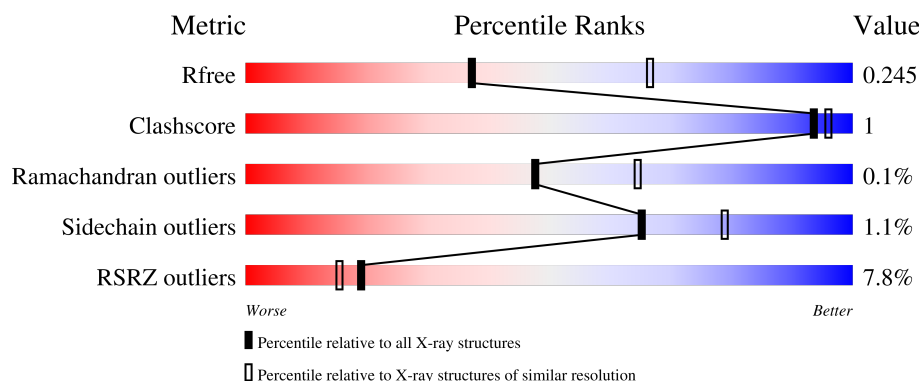
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	0% 94% 0%
1	C	450	2% 92% 5%
2	B	445	5% 90% 5%
2	D	445	12% 91% 5%
3	E	143	11% 82% 16%

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '16%', a green segment in the middle labeled '77%', and a grey segment at the end labeled '20%'. A small yellow dot is located on the green segment, near the end of the bar.

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17466 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	1	0
			3342	2101	570	644	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	0	0
			994	614	180	195	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	2	0
			2544	1640	437	452	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
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 MAGNESIUM ION (CCD ID: 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		

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

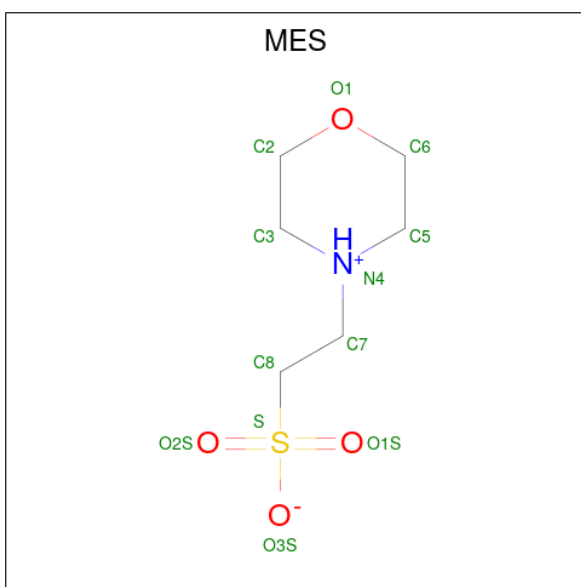
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



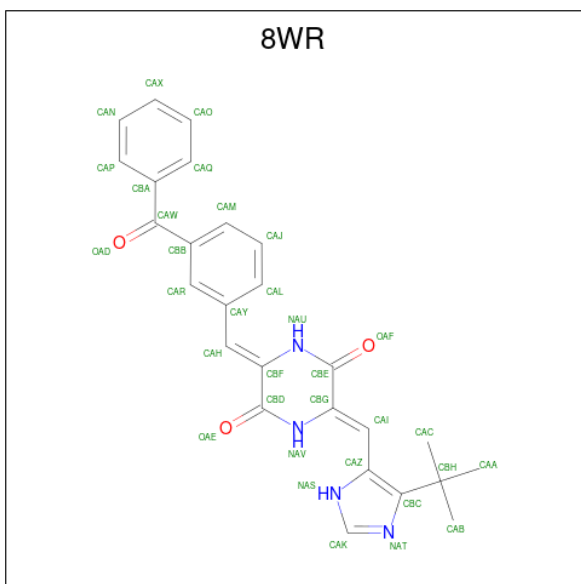
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is (3Z,6Z)-3-[(4-tert-butyl-1H-imidazol-5-yl)methylidene]-6-[[3-(phenylcarbonyl)phenyl]methylidene]piperazine-2,5-dione (CCD ID: 8WR) (formula: C₂₆H₂₄N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			33	26	4	3		

- # ACP

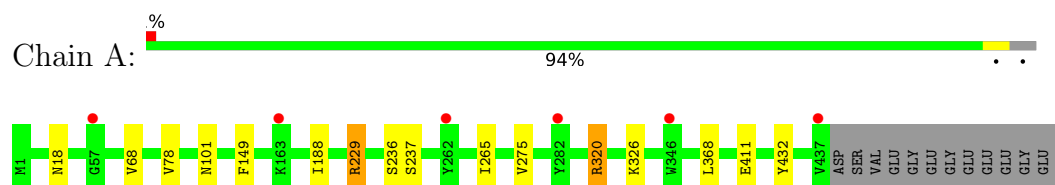
- Molecule 12 is water.



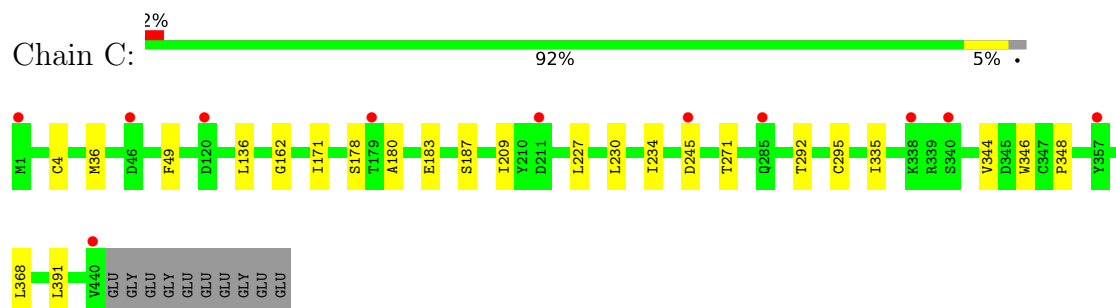
3 Residue-property plots [i](#)

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.

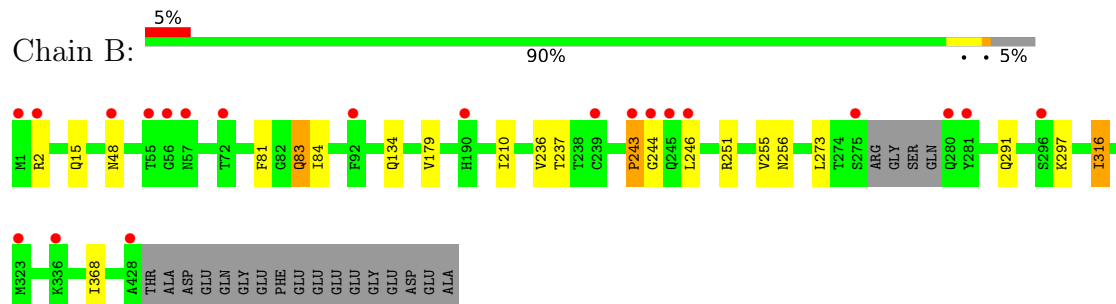
• Molecule 1: Tubulin alpha chain



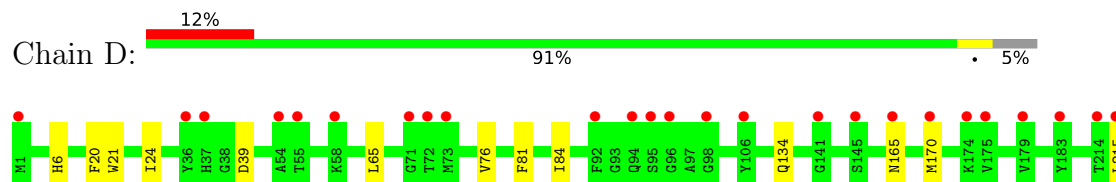
• Molecule 1: Tubulin alpha chain

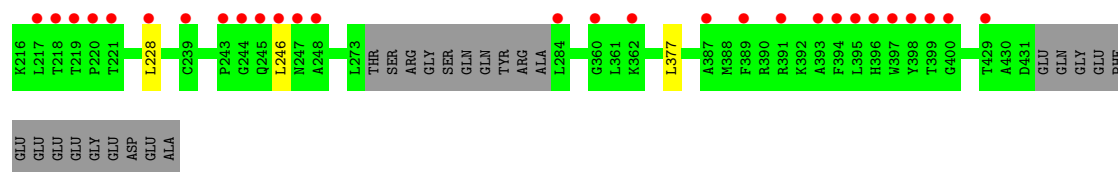


• Molecule 2: Tubulin beta chain

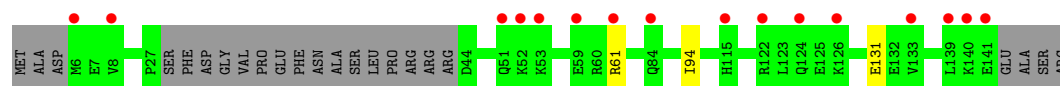
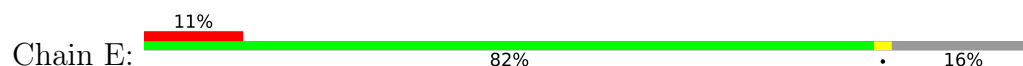


• Molecule 2: Tubulin beta chain

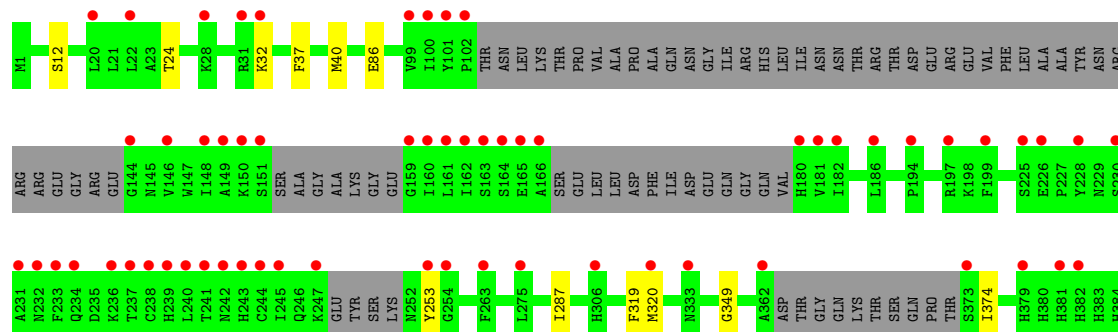
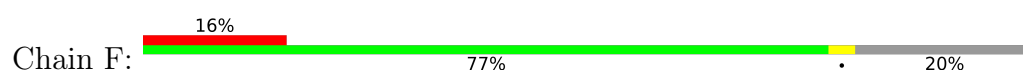




● Molecule 3: Stathmin-4



● 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	105.46Å 157.73Å 182.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.64 48.23 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.23-2.64) 97.4 (48.23-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.218 , 0.256 (Not available) , 0.245	Depositor DCC
R_{free} test set	4341 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.7	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	0.92	EDS
Total number of atoms	17466	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: 8WR, MES, GTP, ACP, CA, GDP, 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	0.59	0/3525	0.84	0/4784
1	C	0.59	0/3572	0.83	0/4850
2	B	0.61	0/3416	0.83	1/4626 (0.0%)
2	D	0.60	0/3379	0.83	0/4577
3	E	0.62	0/1002	0.84	0/1329
4	F	0.59	0/2609	0.74	0/3525
All	All	0.60	0/17503	0.82	1/23691 (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	6.88	118.92	110.73

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	14	0
1	C	3482	0	3384	13	0
2	B	3342	0	3216	11	0
2	D	3306	0	3181	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	994	0	1013	2	0
4	F	2544	0	2514	5	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
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	0	0
10	B	33	0	0	2	0
11	F	31	0	14	2	0
12	A	26	0	0	0	0
12	B	43	0	0	0	0
12	C	62	0	0	0	0
12	E	3	0	0	0	0
12	F	4	0	0	0	0
All	All	17466	0	16759	49	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 (49) 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	1.17
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.76	0.97
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.89	0.80
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.19	0.72
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:H	1.56	0.70
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.77	0.66
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.47	0.65
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:N	2.13	0.63
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.38	0.58
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.86	0.56
2:B:134:GLN:HB2	10:B:506:8WR:CAQ	2.36	0.56
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.56	0.51
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.91	0.51
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.92	0.51
2:B:237:THR:HG22	10:B:506:8WR:CAJ	2.41	0.51
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.92	0.50
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.48	0.49
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.78	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.48	0.48
2:D:134:GLN:HA	2:D:165:ASN:O	2.15	0.47
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.13	0.47
2:D:81:PHE:O	2:D:84:ILE:HG22	2.16	0.46
2:B:236:VAL:HG12	2:B:368:ILE:HD11	1.98	0.46
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.46
4:F:320:MET:HE2	11:F:401:ACP:C2	2.46	0.45
4:F:320:MET:HE2	11:F:401:ACP:H2	1.97	0.45
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.45
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.56	0.45
2:B:81:PHE:O	2:B:84:ILE:HG22	2.17	0.44
2:B:251:ARG:O	2:B:255:VAL:HG23	2.17	0.44
1:C:271:THR:HG21	1:C:295:CYS:O	2.17	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.44
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.01	0.43
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.54	0.43
1:C:171:ILE:N	1:C:171:ILE:HD12	2.34	0.43
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.54	0.43
2:B:210:ILE:HG23	2:B:273:LEU:HD13	2.00	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.42
2:B:83:GLN:HE21	2:B:83:GLN:HA	1.85	0.42
1:A:275:VAL:HG13	1:A:368[A]:LEU:HD21	2.02	0.41
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.50	0.41
2:D:215:LEU:HD11	2:D:228:LEU:HD21	2.02	0.41
1:A:411:GLU:O	3:E:61:ARG:NH1	2.54	0.41
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.56	0.41
1:A:236:SER:OG	1:A:320:ARG:NH1	2.54	0.41
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.02	0.41
1:C:230:LEU:O	1:C:234:ILE:HD12	2.20	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	430 (98%)	9 (2%)	0	100	100
1	C	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
2	B	421/445 (95%)	408 (97%)	12 (3%)	1 (0%)	43	58
2	D	417/445 (94%)	401 (96%)	15 (4%)	1 (0%)	43	58
3	E	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
4	F	299/384 (78%)	289 (97%)	9 (3%)	1 (0%)	36	50
All	All	2138/2317 (92%)	2077 (97%)	58 (3%)	3 (0%)	48	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	D	39	ASP
4	F	253	TYR

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%)	366 (98%)	6 (2%)	55	73
1	C	379/378 (100%)	377 (100%)	2 (0%)	81	89
2	B	366/383 (96%)	358 (98%)	8 (2%)	45	66
2	D	362/383 (94%)	361 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	108/127 (85%)	107 (99%)	1 (1%)	70	82
4	F	280/342 (82%)	276 (99%)	4 (1%)	59	75
All	All	1867/1991 (94%)	1845 (99%)	22 (1%)	65	78

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

Mol	Chain	Res	Type
1	A	188	ILE
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	237	SER
1	A	320	ARG
1	A	326	LYS
2	B	2	ARG
2	B	15	GLN
2	B	48	ASN
2	B	83	GLN
2	B	246	LEU
2	B	291	GLN
2	B	297	LYS
2	B	316	ILE
1	C	245	ASP
1	C	368	LEU
2	D	246	LEU
3	E	131	GLU
4	F	12	SER
4	F	24	THR
4	F	32	LYS
4	F	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	ASN
1	A	101	ASN
1	A	309	HIS
1	A	393	HIS
2	B	57	ASN
2	B	83	GLN

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Mol	Chain	Res	Type
2	B	292	GLN
2	B	375	GLN
2	B	426	GLN
1	C	133	GLN
1	C	249	ASN
1	C	356	ASN
2	D	99	ASN
2	D	165	ASN
2	D	329	GLN
2	D	347	ASN
2	D	375	GLN
2	D	396	HIS
2	D	423	GLN
3	E	90	ASN
3	E	115	HIS
4	F	180	HIS
4	F	333	ASN
4	F	348	GLN

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	1.79	9 (29%)	47,52,52	1.80	10 (21%)
9	MES	B	505	-	12,12,12	2.03	1 (8%)	15,16,16	5.69	9 (60%)
9	MES	B	503	-	12,12,12	2.06	1 (8%)	15,16,16	6.02	9 (60%)
5	GTP	C	501	6	33,34,34	1.27	5 (15%)	50,54,54	1.54	7 (14%)
5	GTP	D	501	6	33,34,34	1.27	3 (9%)	50,54,54	1.60	6 (12%)
5	GTP	A	501	6	33,34,34	1.36	4 (12%)	50,54,54	1.66	7 (14%)
8	GDP	B	501	6	29,30,30	1.34	4 (13%)	45,47,47	1.65	6 (13%)
10	8WR	B	506	-	36,36,36	1.11	2 (5%)	49,52,52	1.62	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	5/19/38/38	0/3/3/3
9	MES	B	505	-	-	2/6/14/14	0/1/1/1
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
5	GTP	D	501	6	-	6/22/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
10	8WR	B	506	-	-	2/22/22/22	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	505	MES	C8-S	-6.46	1.68	1.77
9	B	503	MES	C8-S	-6.42	1.68	1.77
11	F	401	ACP	C5-C4	4.97	1.48	1.39
5	A	501	GTP	PB-O3B	3.77	1.63	1.59
11	F	401	ACP	PB-O3A	3.59	1.62	1.58
10	B	506	8WR	CAK-NAS	-3.47	1.29	1.35
5	D	501	GTP	C5-C4	3.40	1.48	1.38
5	A	501	GTP	C5-C4	3.27	1.47	1.38
5	C	501	GTP	C5-C4	3.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	PA-O3A	3.19	1.62	1.59
8	B	501	GDP	C5-C4	3.05	1.47	1.38
11	F	401	ACP	PG-O2G	2.97	1.61	1.55
11	F	401	ACP	C5-C6	2.96	1.49	1.41
11	F	401	ACP	PG-O3G	2.92	1.61	1.55
5	C	501	GTP	PA-O3A	2.80	1.62	1.59
8	B	501	GDP	C5-N7	-2.63	1.33	1.39
11	F	401	ACP	PA-O3A	2.59	1.62	1.59
5	A	501	GTP	PA-O3A	2.54	1.62	1.59
5	C	501	GTP	PB-O3B	2.53	1.62	1.59
10	B	506	8WR	CAI-CAZ	2.49	1.45	1.40
5	D	501	GTP	PB-O3B	2.48	1.62	1.59
11	F	401	ACP	C8-N7	2.34	1.36	1.31
5	D	501	GTP	C5-N7	-2.31	1.34	1.39
5	C	501	GTP	C5-N7	-2.31	1.34	1.39
5	C	501	GTP	C6-N1	-2.23	1.34	1.38
11	F	401	ACP	C5-N7	-2.21	1.35	1.39
8	B	501	GDP	C6-N1	-2.16	1.34	1.38
5	A	501	GTP	C5-N7	-2.13	1.34	1.39
11	F	401	ACP	PB-O2B	2.11	1.61	1.56

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	505	MES	O3S-S-O1S	-12.10	81.12	111.40
9	B	503	MES	O3S-S-O2S	-11.44	82.77	111.40
9	B	503	MES	O3S-S-C8	-11.21	84.07	106.00
9	B	505	MES	O3S-S-O2S	-10.81	84.34	111.40
9	B	503	MES	O3S-S-O1S	-10.39	85.39	111.40
9	B	503	MES	O2S-S-C8	9.24	120.69	106.73
9	B	505	MES	O2S-S-C8	8.23	119.16	106.73
9	B	505	MES	O3S-S-C8	-8.09	90.17	106.00
9	B	505	MES	O1S-S-C8	7.66	118.31	106.73
9	B	503	MES	O1S-S-C8	7.02	117.34	106.73
5	D	501	GTP	C5-C4-N3	-5.72	119.28	128.39
11	F	401	ACP	C5-C4-N3	-5.64	118.95	126.72
8	B	501	GDP	C5-C4-N3	-5.48	119.67	128.39
5	A	501	GTP	C5-C4-N3	-5.39	119.81	128.39
5	C	501	GTP	C5-C4-N3	-4.92	120.56	128.39
9	B	503	MES	C2-C3-N4	4.76	117.36	110.12
5	D	501	GTP	C2-N3-C4	4.65	120.32	112.30
8	B	501	GDP	C2-N3-C4	4.64	120.30	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	4.63	120.27	112.30
11	F	401	ACP	N3-C4-N9	4.50	134.82	127.17
8	B	501	GDP	N9-C4-N3	4.38	134.71	125.95
5	D	501	GTP	N9-C4-N3	4.37	134.68	125.95
10	B	506	8WR	CAZ-CBC-NAT	-4.35	104.94	110.40
5	C	501	GTP	C2-N3-C4	4.16	119.46	112.30
10	B	506	8WR	CBF-CBD-NAV	4.03	119.99	116.02
5	A	501	GTP	N9-C4-N3	4.02	133.99	125.95
11	F	401	ACP	C2-N3-C4	3.82	121.17	111.83
5	C	501	GTP	N9-C4-N3	3.74	133.44	125.95
10	B	506	8WR	CBG-CBE-NAU	3.73	119.69	116.02
5	A	501	GTP	C6-C5-N7	3.71	137.04	130.29
11	F	401	ACP	N3-C2-N1	-3.67	123.03	128.58
11	F	401	ACP	C4-C5-N7	-3.62	106.44	110.58
10	B	506	8WR	CAK-NAT-CBC	3.47	108.89	104.97
8	B	501	GDP	C6-C5-N7	3.25	136.20	130.29
5	D	501	GTP	C6-C5-N7	3.19	136.09	130.29
5	C	501	GTP	C6-C5-N7	3.12	135.97	130.29
9	B	505	MES	C6-C5-N4	2.98	114.64	110.12
11	F	401	ACP	C4-N9-C8	2.89	108.77	105.74
11	F	401	ACP	C5-N7-C8	2.75	107.77	103.45
9	B	503	MES	O1-C6-C5	-2.75	105.86	111.77
5	A	501	GTP	C4-C5-N7	-2.72	106.36	110.67
5	C	501	GTP	O2A-PA-O3A	2.69	114.55	107.27
9	B	503	MES	C5-N4-C3	2.59	114.42	108.84
10	B	506	8WR	CAI-CBG-CBE	2.58	123.92	119.95
10	B	506	8WR	CBH-CBC-NAT	2.54	121.47	117.42
10	B	506	8WR	CAK-NAS-CAZ	-2.53	106.05	107.57
5	A	501	GTP	O3G-PG-O2G	2.44	116.95	107.80
5	D	501	GTP	C4-C5-N7	-2.39	106.88	110.67
11	F	401	ACP	C6-C5-N7	2.30	136.53	132.09
8	B	501	GDP	C4-C5-N7	-2.29	107.04	110.67
9	B	505	MES	C5-N4-C3	2.27	113.73	108.84
8	B	501	GDP	O6-C6-C5	-2.23	120.65	126.53
11	F	401	ACP	N9-C8-N7	-2.22	110.78	113.94
10	B	506	8WR	CAH-CBF-NAU	-2.21	120.88	124.99
5	C	501	GTP	O6-C6-C5	-2.20	120.73	126.53
5	D	501	GTP	O6-C6-C5	-2.19	120.74	126.53
5	C	501	GTP	C4-C5-N7	-2.19	107.20	110.67
5	A	501	GTP	O6-C6-C5	-2.12	120.93	126.53
9	B	505	MES	C7-N4-C5	-2.08	105.70	111.24
11	F	401	ACP	C2-N1-C6	2.07	122.12	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	505	MES	O2S-S-O1S	2.03	120.43	113.82
9	B	503	MES	C6-C5-N4	2.01	113.18	110.12
10	B	506	8WR	CAY-CAH-CBF	-2.00	126.62	130.66

There are no chirality outliers.

All (35) 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
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
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C7-C8-S-O2S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O3G
9	B	503	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O1G
9	B	503	MES	N4-C7-C8-S
11	F	401	ACP	O4'-C4'-C5'-O5'
5	D	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-C3B-PG-O2G
5	A	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	C4'-C5'-O5'-PA
5	C	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	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O2A
10	B	506	8WR	CBF-CAH-CAY-CAL
10	B	506	8WR	CBF-CAH-CAY-CAR

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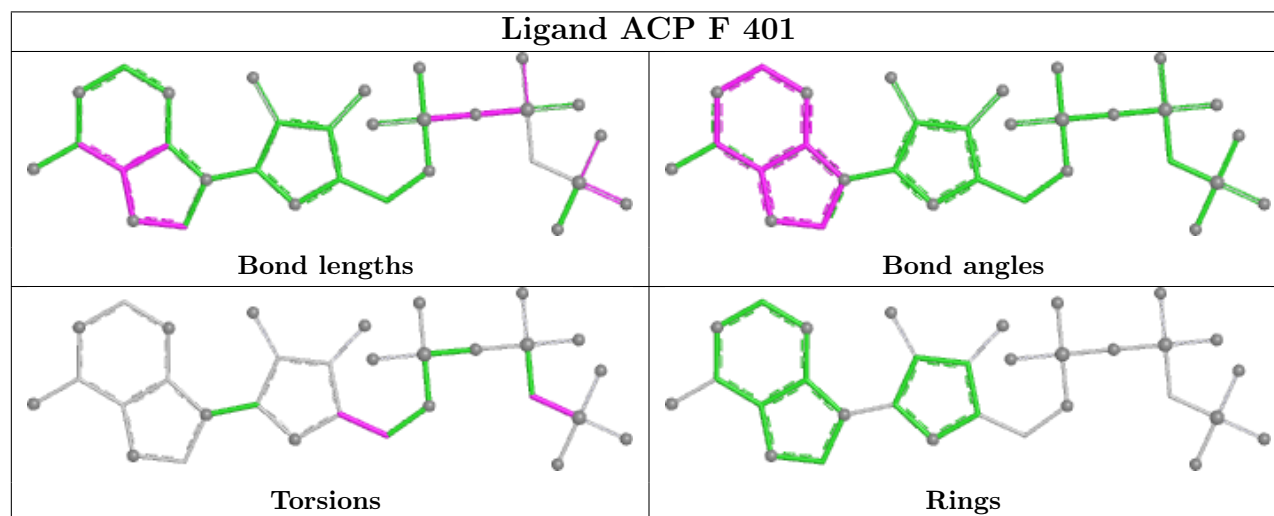
Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C3'-C4'-C5'-O5'

There are no ring outliers.

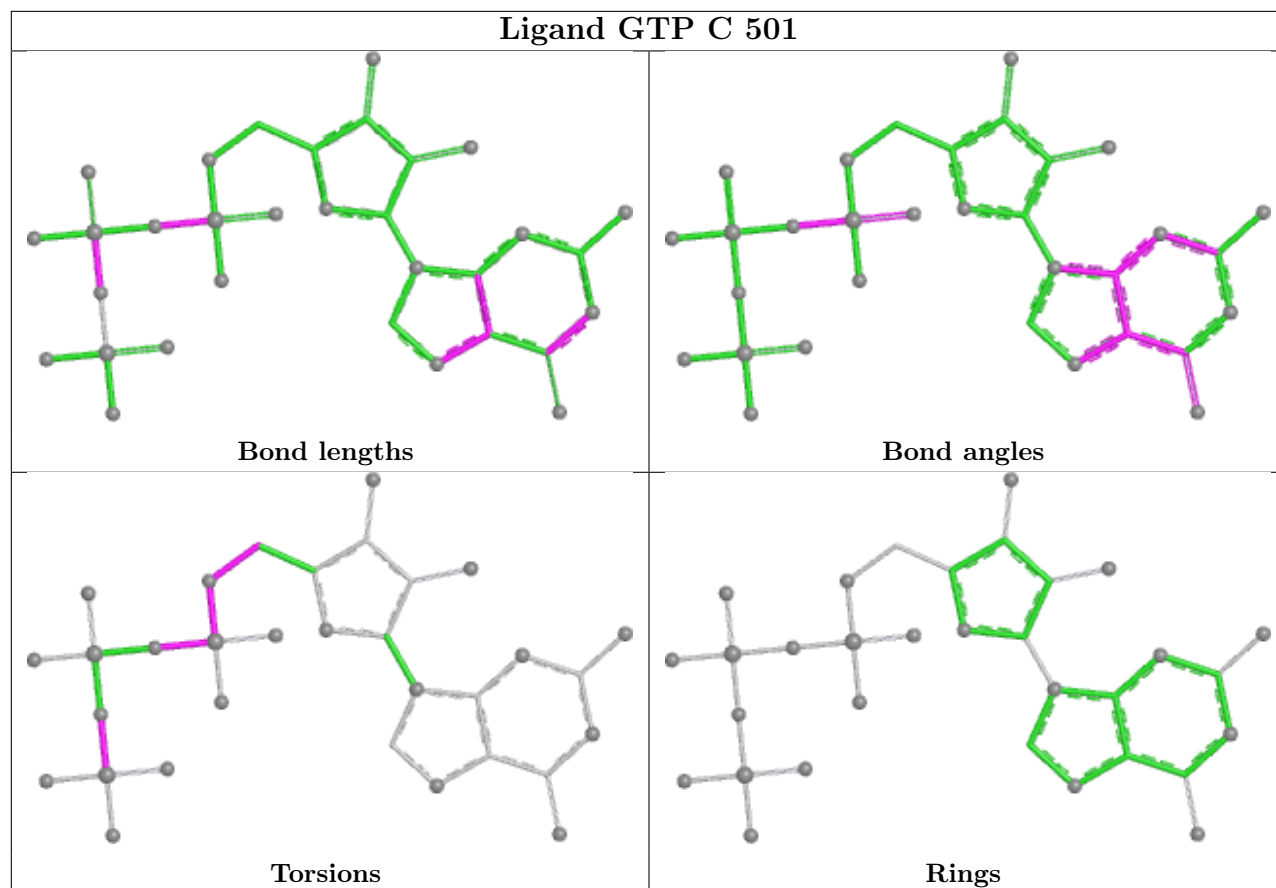
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	2	0
10	B	506	8WR	2	0

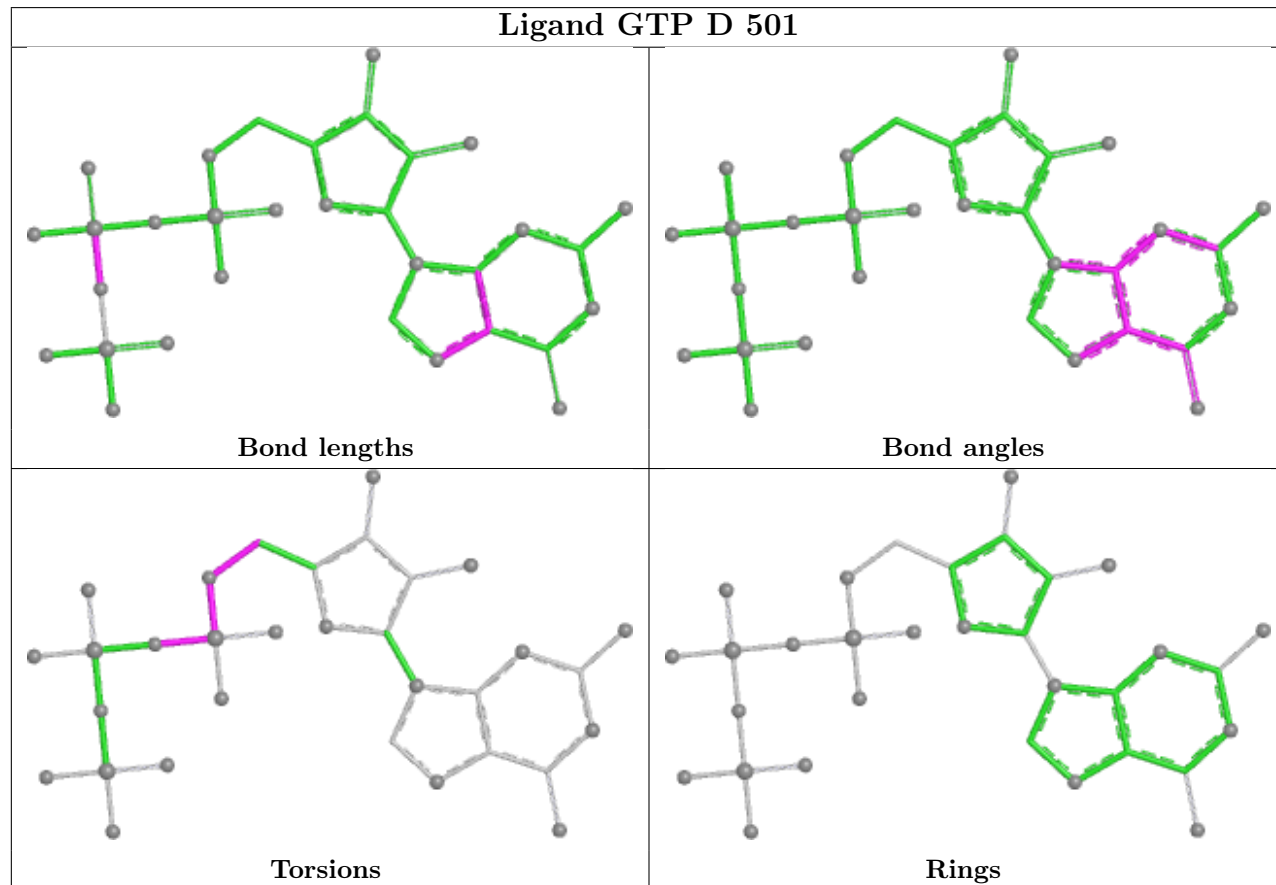
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

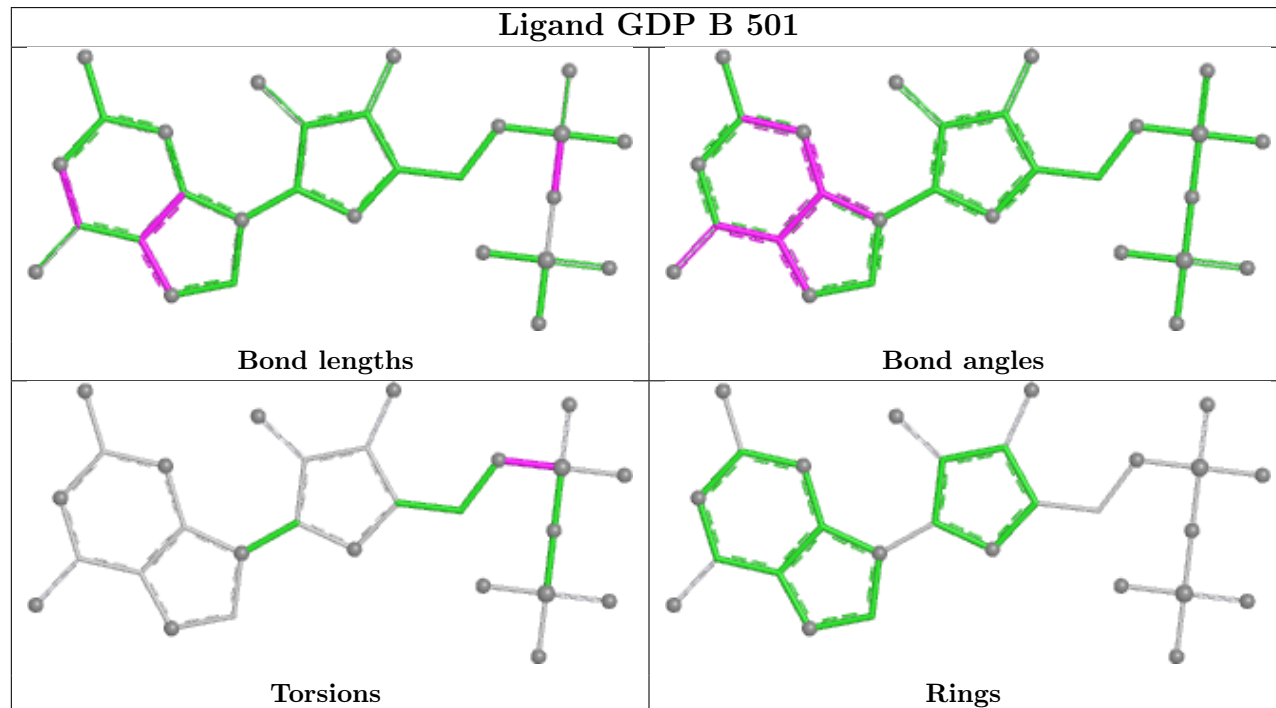
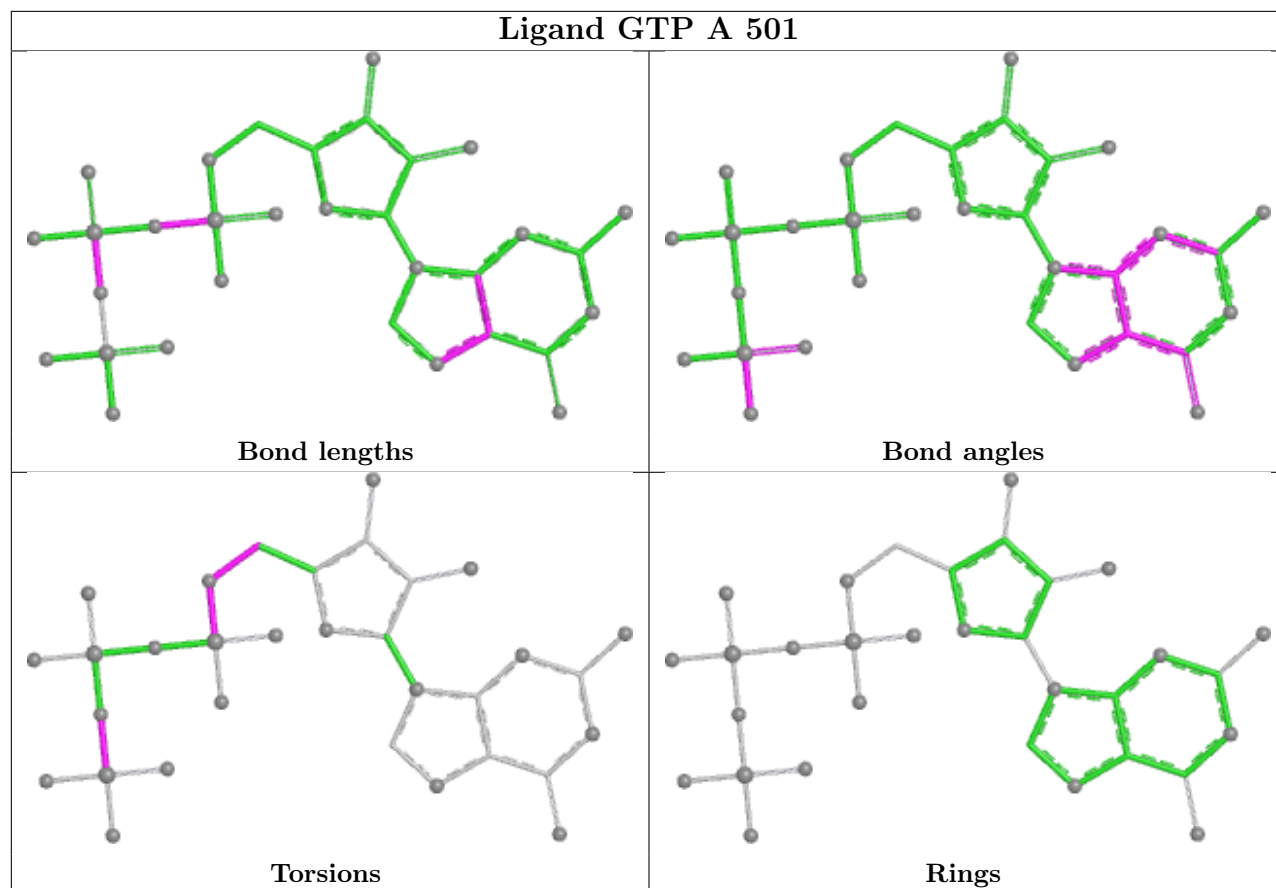


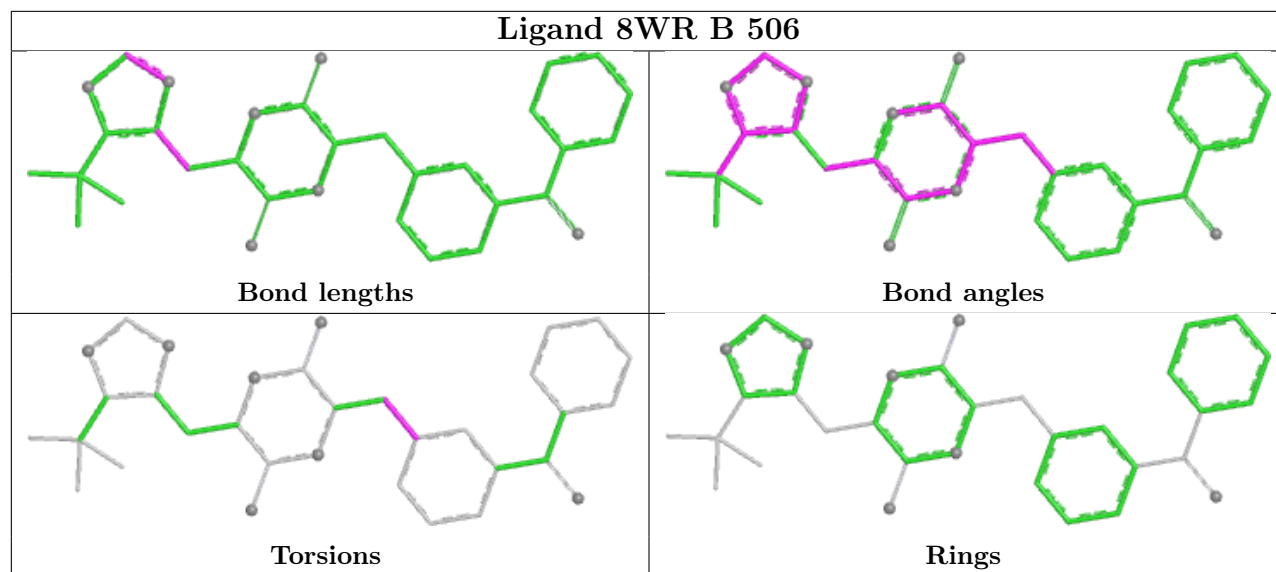
Ligand GTP C 501



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%)	0.19	6 (1%) 73 70	15, 39, 66, 83	4 (0%)
1	C	440/450 (97%)	-0.14	11 (2%) 58 54	11, 30, 52, 73	9 (2%)
2	B	424/445 (95%)	0.23	21 (4%) 34 28	17, 38, 71, 97	2 (0%)
2	D	421/445 (94%)	1.02	53 (12%) 8 6	29, 57, 93, 128	4 (0%)
3	E	120/143 (83%)	0.97	16 (13%) 7 6	30, 57, 89, 102	0
4	F	309/384 (80%)	1.14	61 (19%) 3 2	16, 63, 112, 125	2 (0%)
All	All	2151/2317 (92%)	0.47	168 (7%) 19 15	11, 45, 87, 128	21 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	7.8
4	F	161	LEU	6.4
4	F	102	PRO	5.7
4	F	159	GLY	5.5
4	F	100	ILE	5.3
4	F	182	ILE	5.0
2	D	246	LEU	4.3
4	F	245	ILE	4.3
1	A	262	TYR	4.2
4	F	162	ILE	4.2
2	D	1	MET	4.1
4	F	149	ALA	4.1
2	D	73	MET	4.1
2	D	394	PHE	4.1
4	F	160	ILE	4.0
2	D	247	ASN	4.0
4	F	233	PHE	4.0
2	D	218	THR	3.9
2	B	245	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	219	THR	3.7
3	E	139	LEU	3.7
1	C	179	THR	3.7
4	F	151	SER	3.7
1	A	437	VAL	3.6
2	B	1	MET	3.5
2	D	397	TRP	3.5
4	F	253	TYR	3.5
2	B	55	THR	3.5
4	F	236	LYS	3.5
2	D	72	THR	3.5
2	D	217	LEU	3.4
4	F	164	SER	3.4
4	F	244	CYS	3.4
1	C	245	ASP	3.4
2	D	245	GLN	3.4
4	F	180	HIS	3.4
4	F	237	THR	3.3
2	D	54	ALA	3.3
4	F	240	LEU	3.3
1	C	357	TYR	3.3
4	F	144	GLY	3.3
1	C	211[A]	ASP	3.3
2	D	145[A]	SER	3.2
2	B	244	GLY	3.2
2	D	37	HIS	3.2
2	D	396	HIS	3.2
2	D	215	LEU	3.2
4	F	186	LEU	3.2
1	A	346	TRP	3.2
2	D	360	GLY	3.2
2	D	239	CYS	3.1
4	F	31	ARG	3.1
2	B	243	PRO	3.1
2	D	92	PHE	3.1
4	F	99	VAL	3.1
4	F	225	SER	3.1
2	B	281	TYR	3.0
3	E	51	GLN	3.0
2	D	248	ALA	3.0
4	F	362	ALA	3.0
4	F	150	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	234	GLN	2.9
2	D	393	ALA	2.9
2	D	362	LYS	2.9
4	F	22	LEU	2.9
4	F	247	LYS	2.9
2	B	2	ARG	2.8
1	C	120[A]	ASP	2.8
4	F	381	HIS	2.8
2	B	48	ASN	2.7
2	B	56	GLY	2.7
2	D	170	MET	2.7
4	F	243	HIS	2.7
3	E	141	GLU	2.7
2	B	275	SER	2.7
2	D	94	GLN	2.7
4	F	163	SER	2.7
2	D	175	VAL	2.7
2	D	55	THR	2.6
2	B	280	GLN	2.6
2	D	284	LEU	2.6
3	E	53	LYS	2.6
1	C	340	SER	2.6
2	D	214	THR	2.6
4	F	306	HIS	2.6
4	F	333	ASN	2.6
3	E	115	HIS	2.5
4	F	226	GLU	2.5
2	D	400	GLY	2.5
2	B	57	ASN	2.5
4	F	101	TYR	2.5
2	D	179	VAL	2.5
2	B	428	ALA	2.5
4	F	199	PHE	2.5
2	B	336	LYS	2.5
4	F	263	PHE	2.5
3	E	52	LYS	2.4
4	F	238	CYS	2.4
2	D	71	GLY	2.4
1	C	440	VAL	2.4
2	D	399	THR	2.4
4	F	165	GLU	2.4
1	A	282	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	183	TYR	2.4
2	B	246	LEU	2.4
4	F	320	MET	2.4
3	E	6	MET	2.4
2	D	174	LYS	2.4
1	C	285	GLN	2.4
3	E	124	GLN	2.4
2	D	106	TYR	2.3
2	D	395	LEU	2.3
3	E	126	LYS	2.3
4	F	194	PRO	2.3
3	E	133	VAL	2.3
4	F	379	HIS	2.3
2	B	296	SER	2.3
4	F	181	VAL	2.3
2	D	429	THR	2.3
4	F	230	SER	2.3
1	C	338	LYS	2.2
3	E	59	GLU	2.2
4	F	232	ASN	2.2
2	D	391	ARG	2.2
4	F	239	HIS	2.2
4	F	242	ASN	2.2
2	D	96	GLY	2.2
2	D	387	ALA	2.2
4	F	148	ILE	2.2
3	E	61	ARG	2.2
2	D	243	PRO	2.2
3	E	84	GLN	2.2
1	C	46	ASP	2.2
2	B	323	MET	2.2
4	F	146	VAL	2.2
4	F	241	THR	2.1
2	B	239	CYS	2.1
2	D	95	SER	2.1
2	B	92	PHE	2.1
3	E	140	LYS	2.1
1	C	1	MET	2.1
2	D	165	ASN	2.1
2	D	228	LEU	2.1
4	F	20	LEU	2.1
4	F	32	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	190	HIS	2.1
2	D	244	GLY	2.1
2	D	389	PHE	2.1
4	F	373	SER	2.1
2	B	72	THR	2.1
2	D	220	PRO	2.1
1	A	57	GLY	2.1
2	D	141	GLY	2.1
4	F	228	TYR	2.1
4	F	197	ARG	2.0
1	A	163	LYS	2.0
2	D	58	LYS	2.0
2	D	221	THR	2.0
4	F	275	LEU	2.0
2	D	98	GLY	2.0
4	F	254	GLY	2.0
2	D	398	TYR	2.0
3	E	8	VAL	2.0
3	E	122	ARG	2.0
4	F	28	LYS	2.0
4	F	231	ALA	2.0
4	F	382	HIS	2.0
2	D	36	TYR	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 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.

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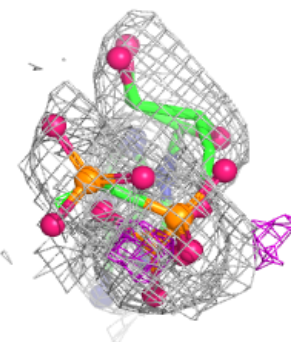
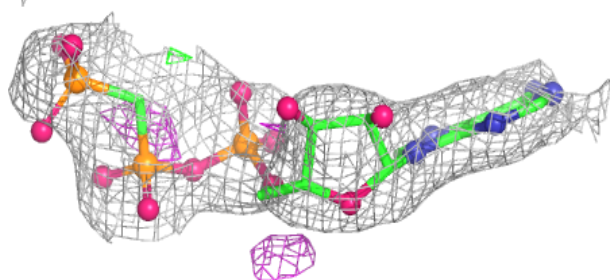
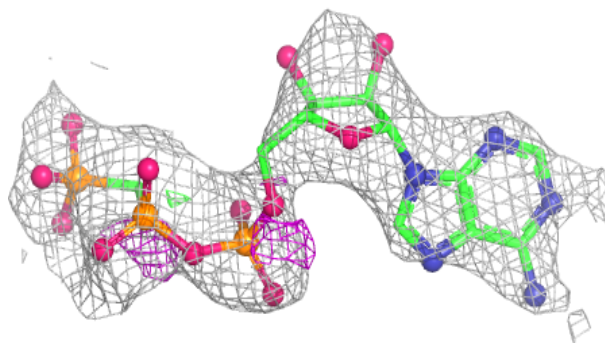
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ACP	F	401	31/31	0.78	0.14	85,92,130,134	0
10	8WR	B	506	33/33	0.81	0.17	35,37,38,39	0
7	CA	B	504	1/1	0.83	0.12	76,76,76,76	0
9	MES	B	503	12/12	0.88	0.17	64,69,75,79	0
9	MES	B	505	12/12	0.91	0.15	78,81,92,93	0
5	GTP	D	501	32/32	0.91	0.10	39,44,57,65	0
6	MG	D	502	1/1	0.91	0.13	50,50,50,50	0
7	CA	A	503	1/1	0.92	0.08	63,63,63,63	0
7	CA	C	503	1/1	0.93	0.06	49,49,49,49	0
5	GTP	C	501	32/32	0.98	0.05	19,20,21,21	0
8	GDP	B	501	28/28	0.98	0.05	19,20,21,23	0
6	MG	B	502	1/1	0.99	0.02	29,29,29,29	0
5	GTP	A	501	32/32	0.99	0.05	20,23,24,24	0
6	MG	C	502	1/1	1.00	0.02	20,20,20,20	0
6	MG	A	502	1/1	1.00	0.01	20,20,20,20	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.

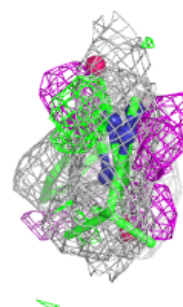
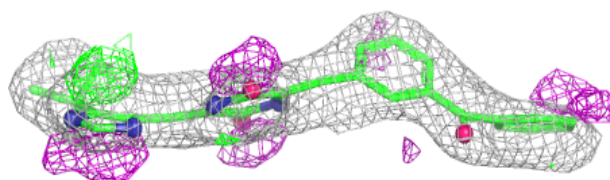
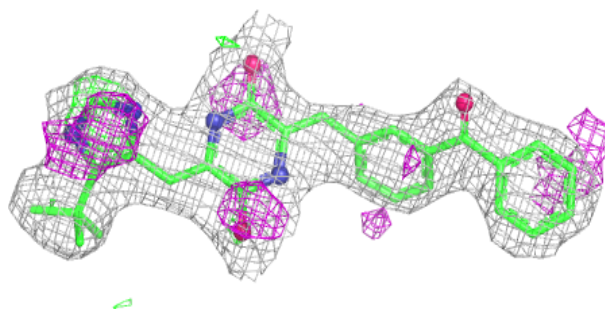
Electron density around ACP F 401:

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

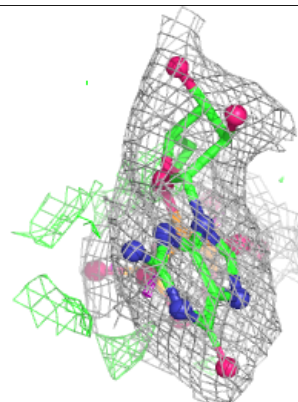
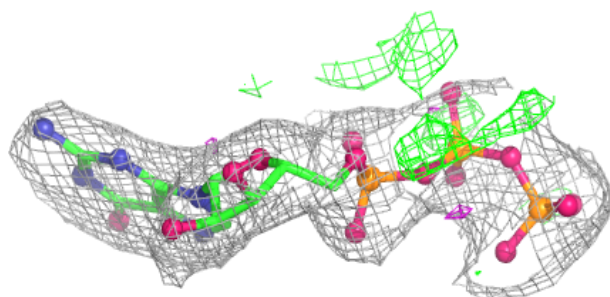
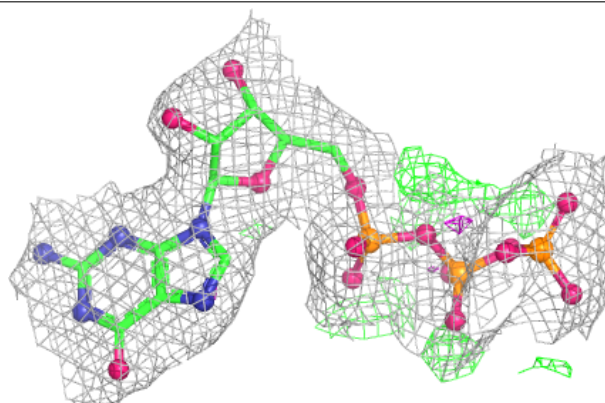


Electron density around 8WR B 506:

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

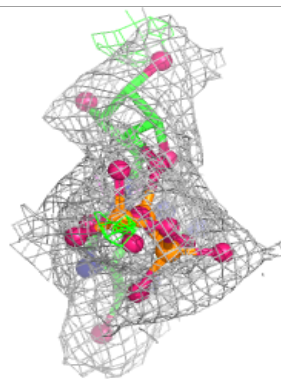
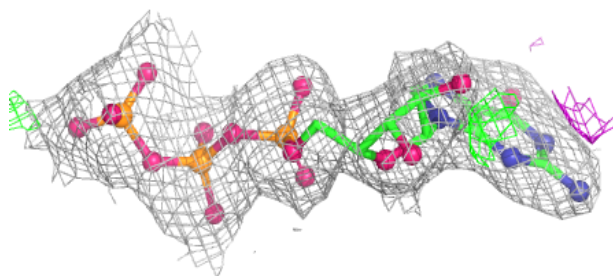
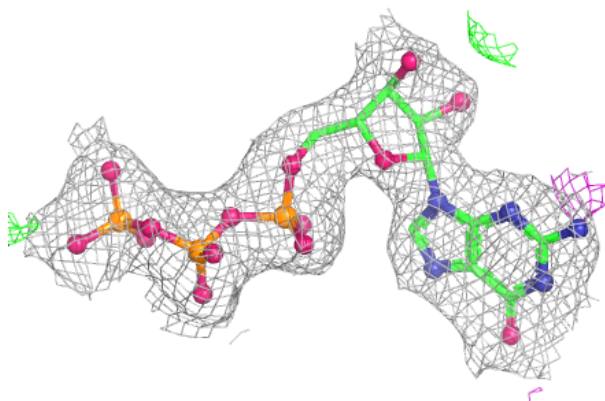
**Electron density around GTP D 501:**

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

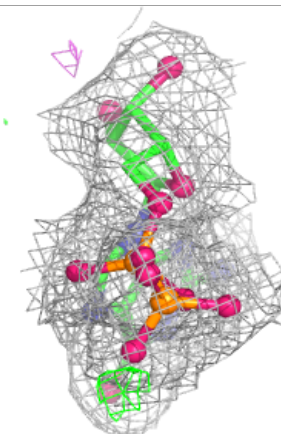
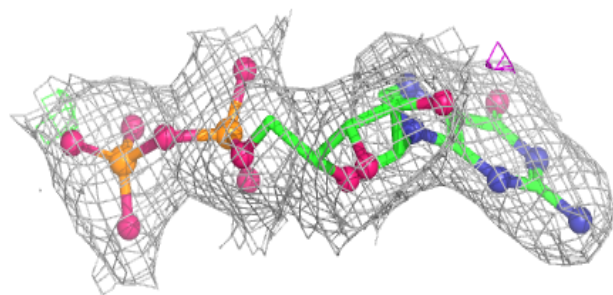
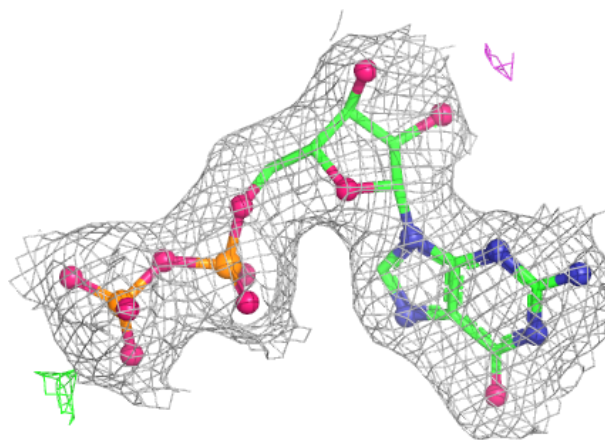


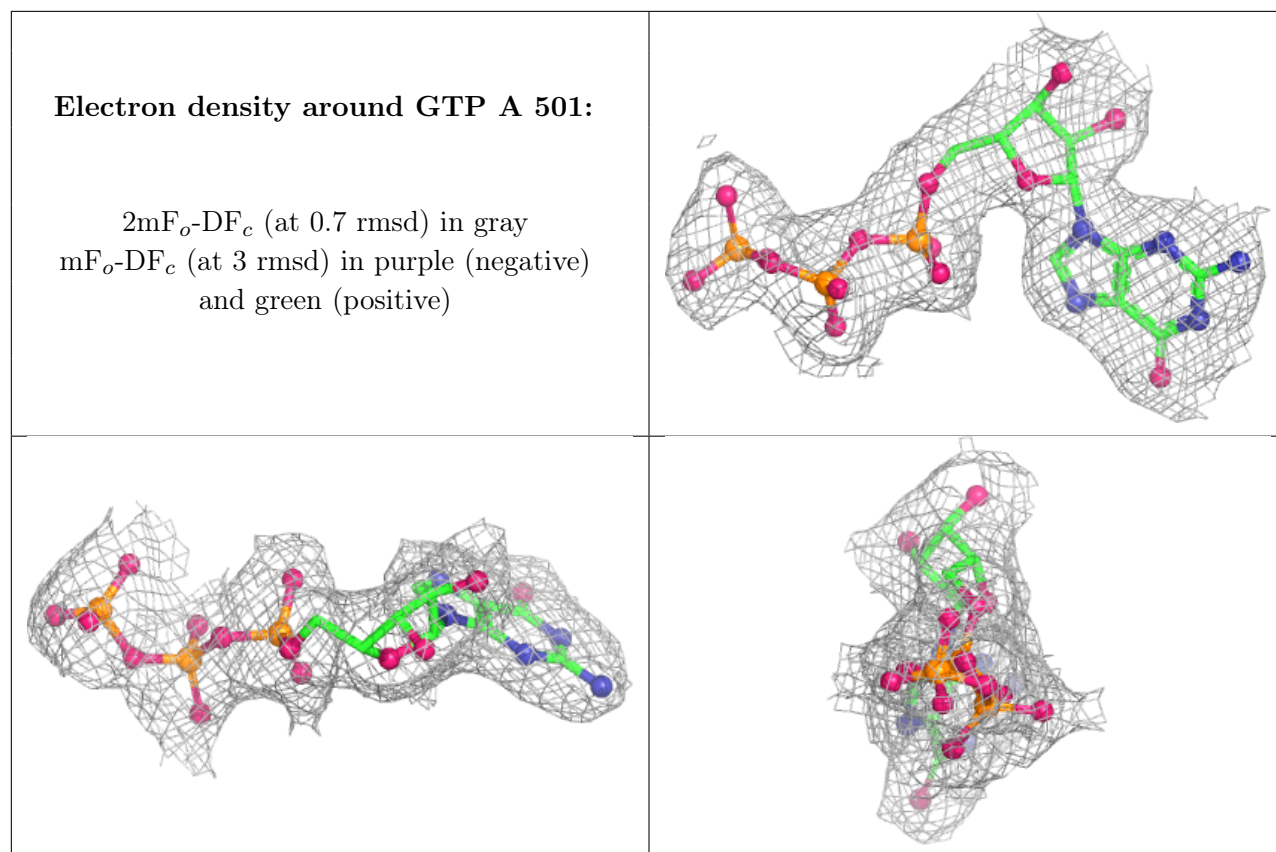
Electron density around GTP C 501:

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

**Electron density around GDP B 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.