



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:57 PM UTC

PDB ID : 7CE8 / pdb_00007ce8
Title : Crystal structure of T2R-TTL-Compound11 complex
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on : 2020-06-22
Resolution : 2.73 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

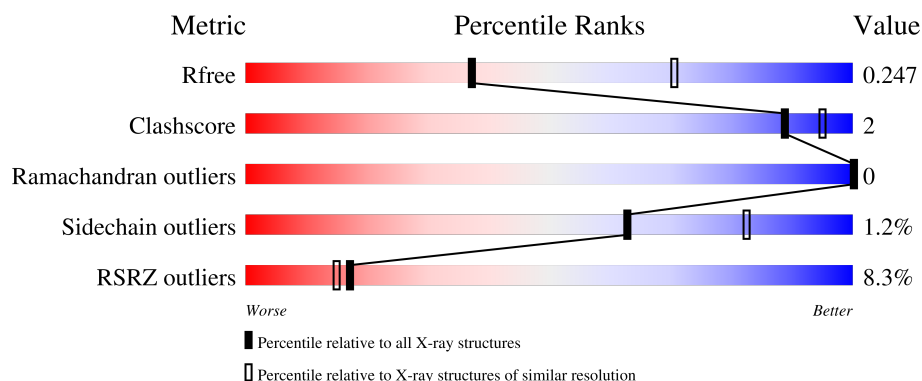
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	2% 95% • •
1	C	450	% 94% • •
2	B	445	5% 91% • •
2	D	445	14% 89% 6% 5%
3	E	143	8% 83% • 15%

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Mol	Chain	Length	Quality of chain
4	F	384	18% 80% 7% 13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34705 atoms, of which 16903 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	437	Total	C	H	N	O	S	0	3	0
			6755	2169	3327	583	652	24			
1	C	440	Total	C	H	N	O	S	0	1	0
			6783	2178	3340	585	657	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6589	2110	3228	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6485	2080	3176	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	4	0
			2046	627	1028	186	200	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	334	Total	C	H	N	O	S	0	0	0
			5441	1761	2697	470	499	14			

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	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	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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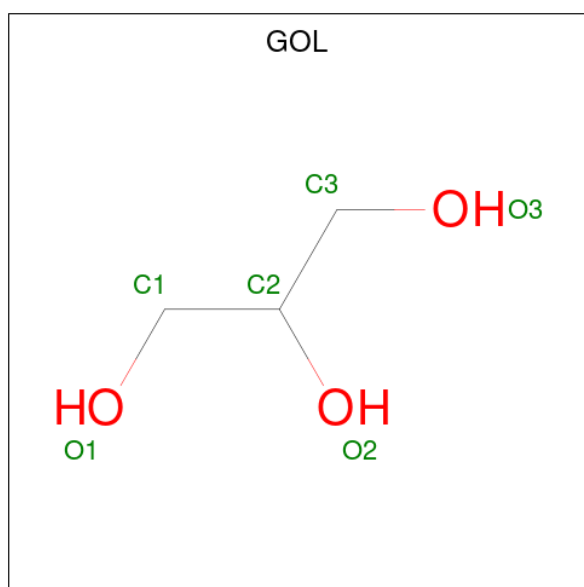
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

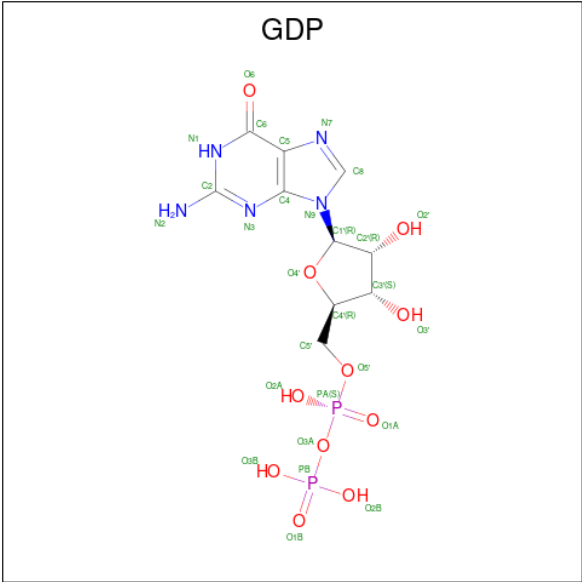
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



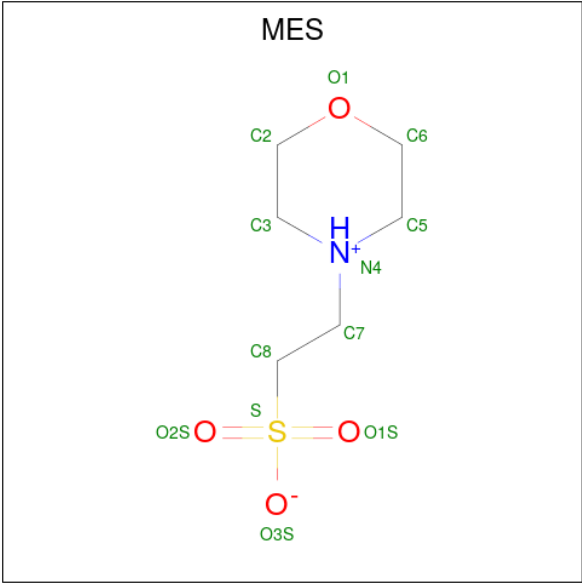
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



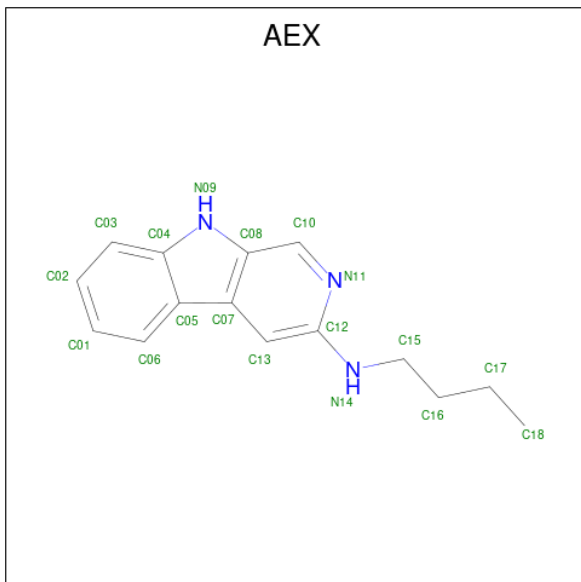
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



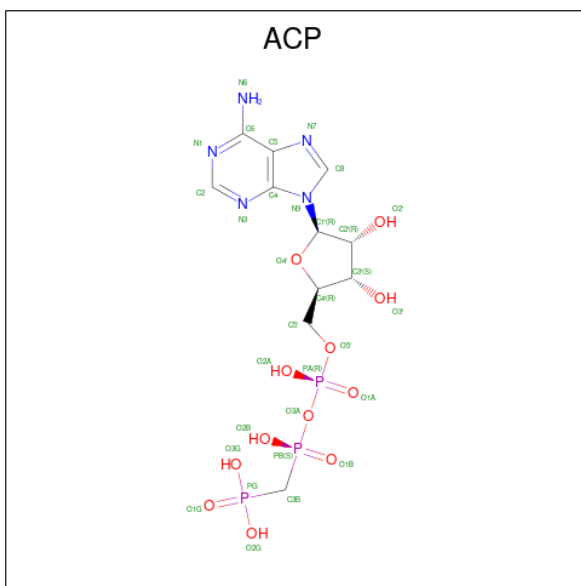
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		
10	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 11 is N-butyl-9H-beta-carbolin-3-amine (CCD ID: AEX) (formula: $C_{15}H_{17}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	N	0	0
			35	15	17	3		
11	D	1	Total	C	H	N	0	0
			35	15	17	3		

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



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

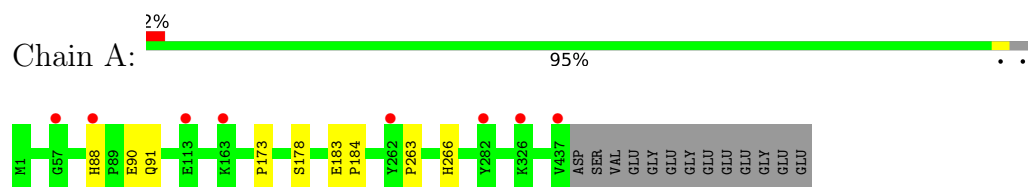
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	58	Total	O	0	0
			58	58		
13	B	58	Total	O	0	0
			58	58		
13	C	89	Total	O	0	0
			89	89		
13	D	13	Total	O	0	0
			13	13		
13	E	17	Total	O	0	0
			17	17		
13	F	37	Total	O	0	0
			37	37		

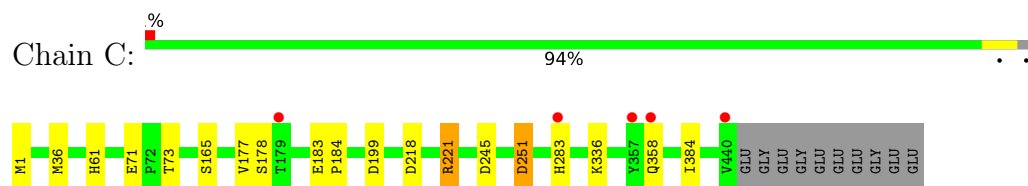
3 Residue-property plots [i](#)

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.

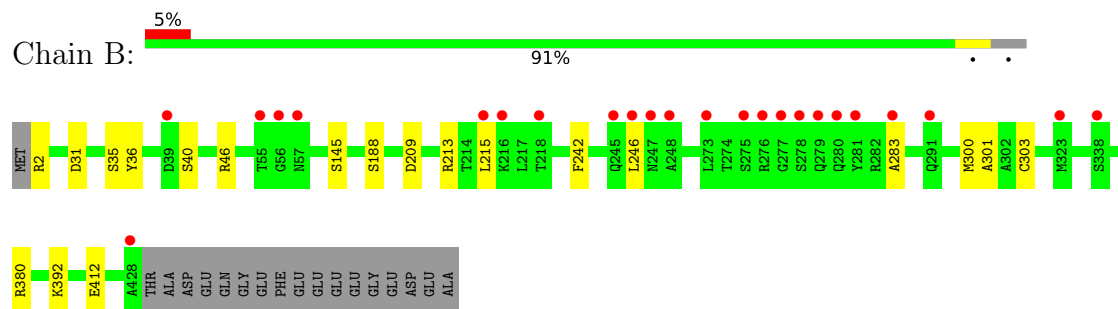
- Molecule 1: Tubulin alpha-1B chain



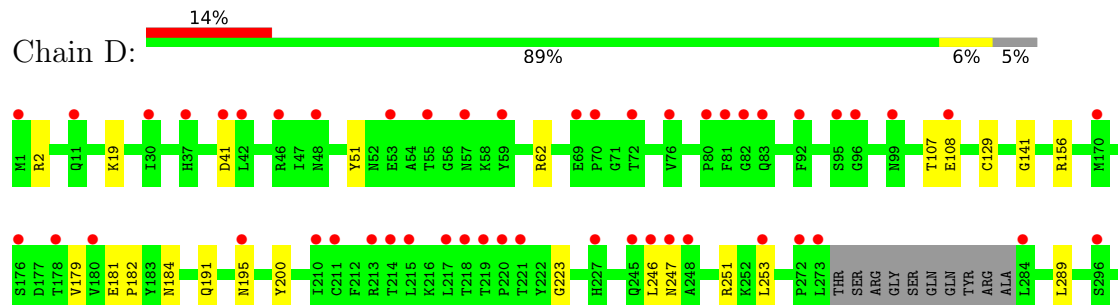
- Molecule 1: Tubulin alpha-1B chain

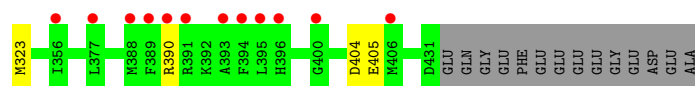


- Molecule 2: Tubulin beta chain

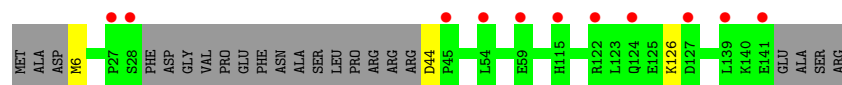
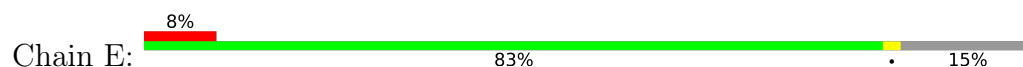


- Molecule 2: Tubulin beta chain

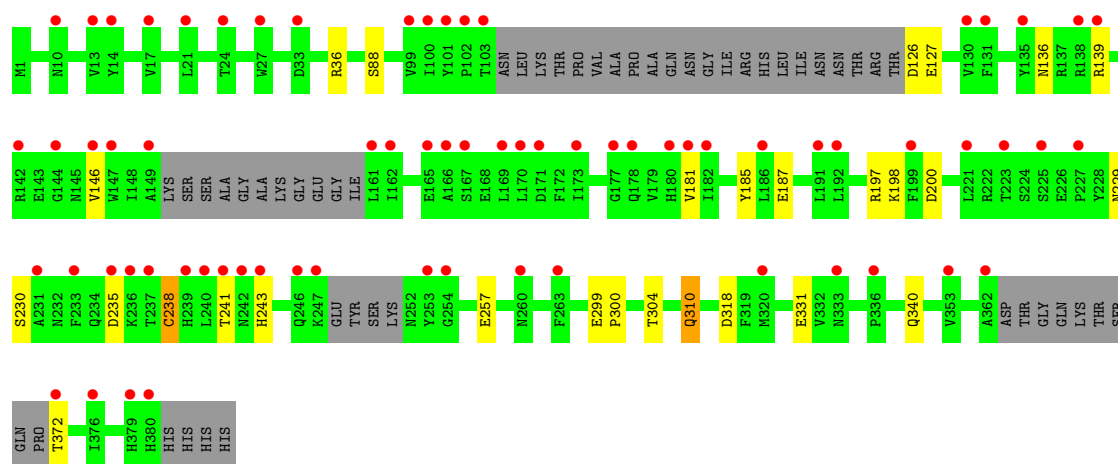
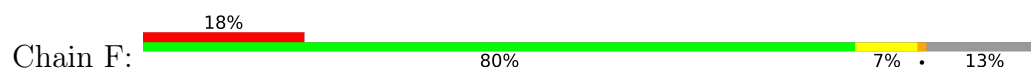




• Molecule 3: Stathmin-4



• 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	105.25Å 157.68Å 181.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 2.73 48.13 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.13-2.73) 98.4 (48.13-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.207 , 0.242 0.213 , 0.247	Depositor DCC
R_{free} test set	1181 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34705	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GOL, GDP, GTP, CA, ACP, AEX, 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	0.33	0/3514	0.63	0/4770
1	C	0.33	0/3521	0.62	0/4781
2	B	0.32	0/3436	0.62	0/4654
2	D	0.30	0/3382	0.62	0/4581
3	E	0.30	0/1044	0.59	0/1385
4	F	0.28	0/2806	0.59	0/3791
All	All	0.31	0/17703	0.62	0/23962

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	3428	3327	3329	6	0
1	C	3443	3340	3353	9	0
2	B	3361	3228	3238	12	0
2	D	3309	3176	3189	16	0
3	E	1018	1028	1007	3	0
4	F	2744	2697	2709	19	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
5	D	32	10	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	C	1	0	0	0	0
8	A	6	8	8	0	0
9	B	28	10	12	0	0
10	B	12	12	12	0	0
10	D	12	13	13	0	0
11	B	18	17	0	0	0
11	D	18	17	0	2	0
12	F	31	0	14	7	0
13	A	58	0	0	0	0
13	B	58	0	0	6	0
13	C	89	0	0	3	0
13	D	13	0	0	3	0
13	E	17	0	0	2	0
13	F	37	0	0	3	0
All	All	17802	16903	16920	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:331:GLU:OE2	12:F:401:ACP:O2G	1.97	0.82
2:B:46:ARG:NH1	2:B:242:PHE:O	2.12	0.80
1:C:251:ASP:OD2	13:C:601:HOH:O	2.02	0.77
12:F:401:ACP:O2G	12:F:401:ACP:O1B	2.05	0.75
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.61	0.74
1:A:88:HIS:ND1	1:A:90:GLU:OE1	2.23	0.71
4:F:229:ASN:N	4:F:238:CYS:SG	2.67	0.67
4:F:241:THR:OG1	12:F:401:ACP:O3'	2.12	0.67
2:D:191:GLN:OE1	3:E:126:LYS:NZ	2.28	0.67
1:C:218:ASP:OD2	13:C:602:HOH:O	2.13	0.67
4:F:126:ASP:N	13:F:501:HOH:O	2.27	0.67
1:A:178:SER:OG	1:A:183:GLU:OE1	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:ARG:NH1	2:D:195:ASN:OD1	2.29	0.64
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.31	0.63
4:F:304:THR:O	4:F:310:GLN:NE2	2.32	0.63
4:F:126:ASP:OD1	4:F:127:GLU:N	2.30	0.63
2:B:36:TYR:OH	2:B:40:SER:O	2.21	0.59
3:E:44:ASP:N	13:E:202:HOH:O	2.38	0.57
4:F:36:ARG:NH2	13:F:504:HOH:O	2.38	0.57
2:B:2:ARG:NH1	13:B:606:HOH:O	2.38	0.56
3:E:6:MET:N	13:E:203:HOH:O	2.40	0.55
4:F:372:THR:N	13:F:508:HOH:O	2.40	0.55
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.28	0.54
4:F:331:GLU:OE2	12:F:401:ACP:O1B	2.26	0.54
4:F:331:GLU:OE2	12:F:401:ACP:PG	2.65	0.54
1:C:178:SER:OG	1:C:183:GLU:OE1	2.24	0.52
2:B:31:ASP:OD1	2:B:35:SER:N	2.37	0.52
2:D:404:ASP:OD1	2:D:405:GLU:N	2.43	0.51
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.26	0.51
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.27	0.51
2:D:390:ARG:NH1	13:D:606:HOH:O	2.44	0.50
2:D:2:ARG:NH2	13:D:605:HOH:O	2.44	0.50
2:B:301:ALA:O	2:B:303:CYS:N	2.44	0.49
2:B:412:GLU:OE2	13:B:601:HOH:O	2.20	0.48
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.32	0.47
2:D:41:ASP:OD1	2:D:41:ASP:N	2.48	0.47
1:A:173:PRO:HB3	1:A:183:GLU:OE2	2.14	0.47
2:D:107:THR:OG1	2:D:108:GLU:N	2.46	0.47
4:F:146:VAL:N	4:F:187:GLU:OE2	2.48	0.47
1:A:263:PRO:O	1:A:266:HIS:ND1	2.34	0.46
2:D:51:TYR:O	2:D:62:ARG:NH2	2.49	0.46
2:D:19:LYS:NZ	2:D:223:GLY:HA2	2.31	0.45
2:B:380:ARG:NH1	13:B:617:HOH:O	2.49	0.45
2:D:141:GLY:O	2:D:184:ASN:ND2	2.50	0.45
1:A:183:GLU:N	1:A:184:PRO:CD	2.81	0.44
2:B:209:ASP:OD2	13:B:602:HOH:O	2.21	0.44
2:B:392:LYS:NZ	13:B:614:HOH:O	2.47	0.44
1:C:221:ARG:NH2	2:D:323:MET:SD	2.91	0.43
4:F:340:GLN:N	4:F:340:GLN:OE1	2.50	0.43
1:A:88:HIS:N	1:A:91:GLN:OE1	2.48	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.43
2:D:200:TYR:OH	11:D:504:AEX:N14	2.52	0.43
4:F:136:ASN:O	4:F:139:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:ALA:N	13:B:613:HOH:O	2.46	0.42
2:D:181:GLU:N	2:D:182:PRO:HD2	2.34	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.82	0.42
1:C:1:MET:N	13:C:613:HOH:O	2.39	0.42
2:D:253:LEU:HB3	11:D:504:AEX:C10	2.50	0.41
4:F:331:GLU:OE2	12:F:401:ACP:O3G	2.38	0.41
2:D:251:ARG:NH1	13:D:607:HOH:O	2.46	0.41
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	0.41
2:B:209:ASP:O	2:B:213:ARG:N	2.54	0.40
2:B:145:SER:HG	2:B:188:SER:HG	1.70	0.40
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.57	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	438/450 (97%)	423 (97%)	15 (3%)	0	100	100
1	C	439/450 (98%)	427 (97%)	12 (3%)	0	100	100
2	B	425/445 (96%)	411 (97%)	14 (3%)	0	100	100
2	D	417/445 (94%)	406 (97%)	11 (3%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	309 (95%)	15 (5%)	0	100	100
All	All	2164/2317 (93%)	2095 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	371/378 (98%)	371 (100%)	0	100	100
1	C	372/378 (98%)	364 (98%)	8 (2%)	45	72
2	B	369/383 (96%)	366 (99%)	3 (1%)	73	87
2	D	364/383 (95%)	360 (99%)	4 (1%)	65	84
3	E	113/127 (89%)	113 (100%)	0	100	100
4	F	301/342 (88%)	294 (98%)	7 (2%)	44	71
All	All	1890/1991 (95%)	1868 (99%)	22 (1%)	63	82

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

Mol	Chain	Res	Type
2	B	215	LEU
2	B	246	LEU
2	B	300	MET
1	C	177	VAL
1	C	221	ARG
1	C	245	ASP
1	C	251	ASP
1	C	283	HIS
1	C	336	LYS
1	C	358	GLN
1	C	384	ILE
2	D	179	VAL
2	D	246	LEU
2	D	247	ASN
2	D	289	LEU
4	F	88	SER
4	F	181	VAL
4	F	230	SER
4	F	235	ASP
4	F	238	CYS
4	F	243	HIS
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	372	GLN
1	A	393	HIS
2	B	165	ASN
2	B	191	GLN
2	B	245	GLN
2	B	298	ASN
2	B	347	ASN
2	B	414	ASN
1	C	101	ASN
1	C	133	GLN
1	C	356	ASN
1	C	393	HIS
2	D	165	ASN
2	D	256	ASN
2	D	347	ASN
4	F	183	GLN
4	F	289	HIS
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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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
10	MES	B	503	-	12,12,12	2.23	1 (8%)	15,16,16	2.07	3 (20%)
12	ACP	F	401	-	31,33,33	1.60	6 (19%)	47,52,52	1.90	12 (25%)
11	AEX	D	504	-	20,20,20	1.20	2 (10%)	26,27,27	0.78	0
8	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.27	0
5	GTP	C	501	6	33,34,34	0.93	0	50,54,54	1.48	9 (18%)
5	GTP	D	501	6	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
10	MES	D	502	-	12,12,12	2.25	1 (8%)	15,16,16	1.57	4 (26%)
9	GDP	B	501	6	29,30,30	1.19	4 (13%)	45,47,47	1.64	5 (11%)
5	GTP	A	501	6	33,34,34	0.96	1 (3%)	50,54,54	1.57	10 (20%)
11	AEX	B	504	-	20,20,20	1.07	2 (10%)	26,27,27	0.79	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
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
12	ACP	F	401	-	-	8/19/38/38	0/3/3/3
11	AEX	D	504	-	-	0/5/5/5	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
5	GTP	D	501	6	-	6/22/38/38	0/3/3/3
10	MES	D	502	-	-	5/6/14/14	0/1/1/1
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
11	AEX	B	504	-	-	0/5/5/5	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	MES	C8-S	-7.50	1.67	1.77
10	B	503	MES	C8-S	-7.47	1.67	1.77
11	D	504	AEX	C12-N14	3.99	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	C5-N7	-3.78	1.32	1.39
11	B	504	AEX	C12-N14	3.52	1.41	1.36
12	F	401	ACP	C5-C4	3.02	1.44	1.39
9	B	501	GDP	C5-C4	2.95	1.46	1.38
9	B	501	GDP	C6-N1	-2.86	1.33	1.38
12	F	401	ACP	C4-N9	-2.71	1.32	1.37
12	F	401	ACP	C8-N9	-2.69	1.33	1.37
12	F	401	ACP	PG-O2G	2.48	1.60	1.55
11	D	504	AEX	C12-N11	2.26	1.38	1.34
5	D	501	GTP	C2-N3	2.22	1.38	1.33
11	B	504	AEX	C12-N11	2.12	1.38	1.34
12	F	401	ACP	O4'-C4'	-2.10	1.40	1.45
9	B	501	GDP	C4-N9	-2.05	1.32	1.38
9	B	501	GDP	C5-N7	-2.04	1.35	1.39
5	A	501	GTP	C2-N3	2.01	1.38	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	C5-C4-N3	-6.20	118.18	126.72
9	B	501	GDP	C5-C4-N3	-5.59	119.49	128.39
10	B	503	MES	C5-N4-C3	5.33	120.33	108.84
5	D	501	GTP	C5-C4-N3	-4.95	120.51	128.39
5	A	501	GTP	C5-C4-N3	-4.93	120.55	128.39
12	F	401	ACP	N3-C4-N9	4.74	135.22	127.17
9	B	501	GDP	C2-N3-C4	4.67	120.34	112.30
5	C	501	GTP	C5-C4-N3	-4.61	121.05	128.39
5	A	501	GTP	C2-N3-C4	4.51	120.07	112.30
5	D	501	GTP	C2-N3-C4	4.50	120.04	112.30
9	B	501	GDP	N9-C4-N3	4.47	134.90	125.95
5	C	501	GTP	C2-N3-C4	4.21	119.55	112.30
12	F	401	ACP	C4-C5-N7	-3.45	106.64	110.58
12	F	401	ACP	C2-N3-C4	3.44	120.24	111.83
5	D	501	GTP	N9-C4-N3	3.28	132.51	125.95
9	B	501	GDP	C6-C5-N7	3.24	136.19	130.29
12	F	401	ACP	PB-O3A-PA	-3.20	121.91	132.37
5	A	501	GTP	N9-C4-N3	3.07	132.09	125.95
5	C	501	GTP	N9-C4-N3	2.94	131.83	125.95
5	A	501	GTP	C2-N1-C6	-2.85	119.94	125.11
5	D	501	GTP	C2-N1-C6	-2.79	120.05	125.11
12	F	401	ACP	C5-N7-C8	2.78	107.82	103.45
5	D	501	GTP	N9-C8-N7	-2.75	108.31	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N9-C8-N7	-2.70	108.39	113.40
10	B	503	MES	C7-N4-C5	2.69	118.40	111.24
12	F	401	ACP	N3-C2-N1	-2.66	124.56	128.58
5	C	501	GTP	C2-N1-C6	-2.64	120.33	125.11
5	A	501	GTP	N9-C8-N7	-2.63	108.52	113.40
12	F	401	ACP	C4-N9-C8	2.63	108.50	105.74
10	B	503	MES	O3S-S-C8	2.56	111.02	106.00
10	D	502	MES	C5-N4-C3	2.53	114.30	108.84
5	D	501	GTP	C8-N7-C5	2.53	108.76	104.26
10	D	502	MES	O2S-S-C8	2.49	110.50	106.73
5	A	501	GTP	C8-N7-C5	2.48	108.69	104.26
12	F	401	ACP	N9-C8-N7	-2.45	110.45	113.94
5	D	501	GTP	C5-C6-N1	2.44	119.47	113.25
5	C	501	GTP	C8-N7-C5	2.43	108.58	104.26
5	D	501	GTP	O6-C6-C5	-2.41	120.17	126.53
12	F	401	ACP	C3'-C2'-C1'	2.41	106.02	101.46
12	F	401	ACP	O3A-PA-O1A	-2.40	103.49	110.70
5	A	501	GTP	C5-C6-N1	2.39	119.34	113.25
5	A	501	GTP	O6-C6-C5	-2.31	120.43	126.53
10	D	502	MES	C2-C3-N4	-2.30	106.63	110.12
9	B	501	GDP	C4-C5-N7	-2.29	107.03	110.67
5	C	501	GTP	C5-C6-N1	2.29	119.09	113.25
5	C	501	GTP	O6-C6-C5	-2.29	120.50	126.53
5	C	501	GTP	O2A-PA-O3A	2.24	113.34	107.27
5	A	501	GTP	O2B-PB-O3A	2.20	113.23	107.27
12	F	401	ACP	O2A-PA-O1A	2.13	122.35	112.44
10	D	502	MES	O1S-S-C8	2.06	109.84	106.73
5	A	501	GTP	O2A-PA-O3A	2.05	112.81	107.27

There are no chirality outliers.

All (42) 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

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Mol	Chain	Res	Type	Atoms
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	D	502	MES	C7-C8-S-O3S
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
10	B	503	MES	C7-C8-S-O3S
12	F	401	ACP	C3'-C4'-C5'-O5'
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	O1-C1-C2-O2
10	D	502	MES	C8-C7-N4-C5
5	D	501	GTP	C3'-C4'-C5'-O5'
12	F	401	ACP	PB-O3A-PA-O1A
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
10	D	502	MES	C7-C8-S-O1S
10	D	502	MES	C7-C8-S-O2S
5	D	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	PB-C3B-PG-O2G
5	D	501	GTP	C4'-C5'-O5'-PA
10	D	502	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3A-PA-O2A
5	A	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
12	F	401	ACP	PB-C3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G

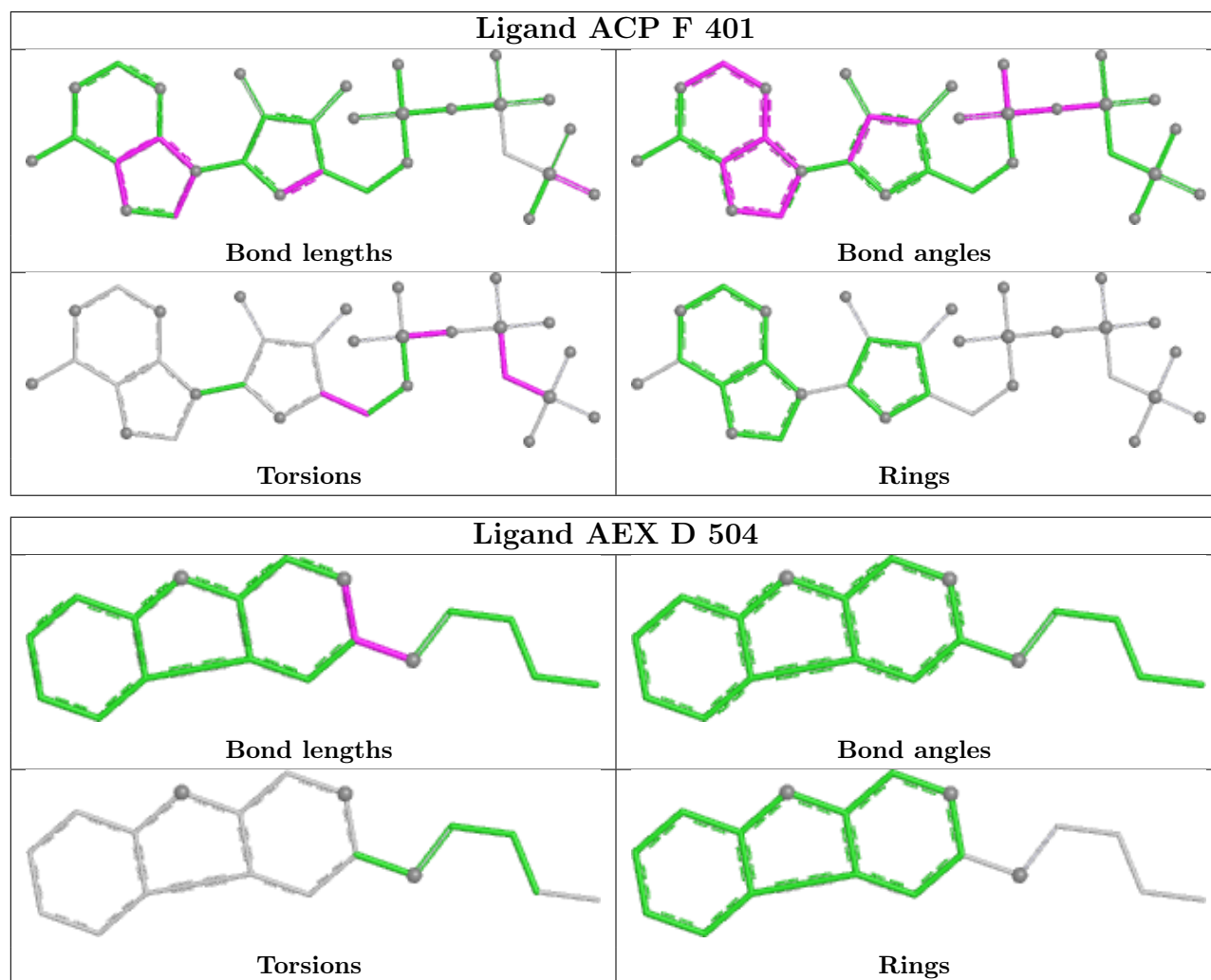
There are no ring outliers.

2 monomers are involved in 9 short contacts:

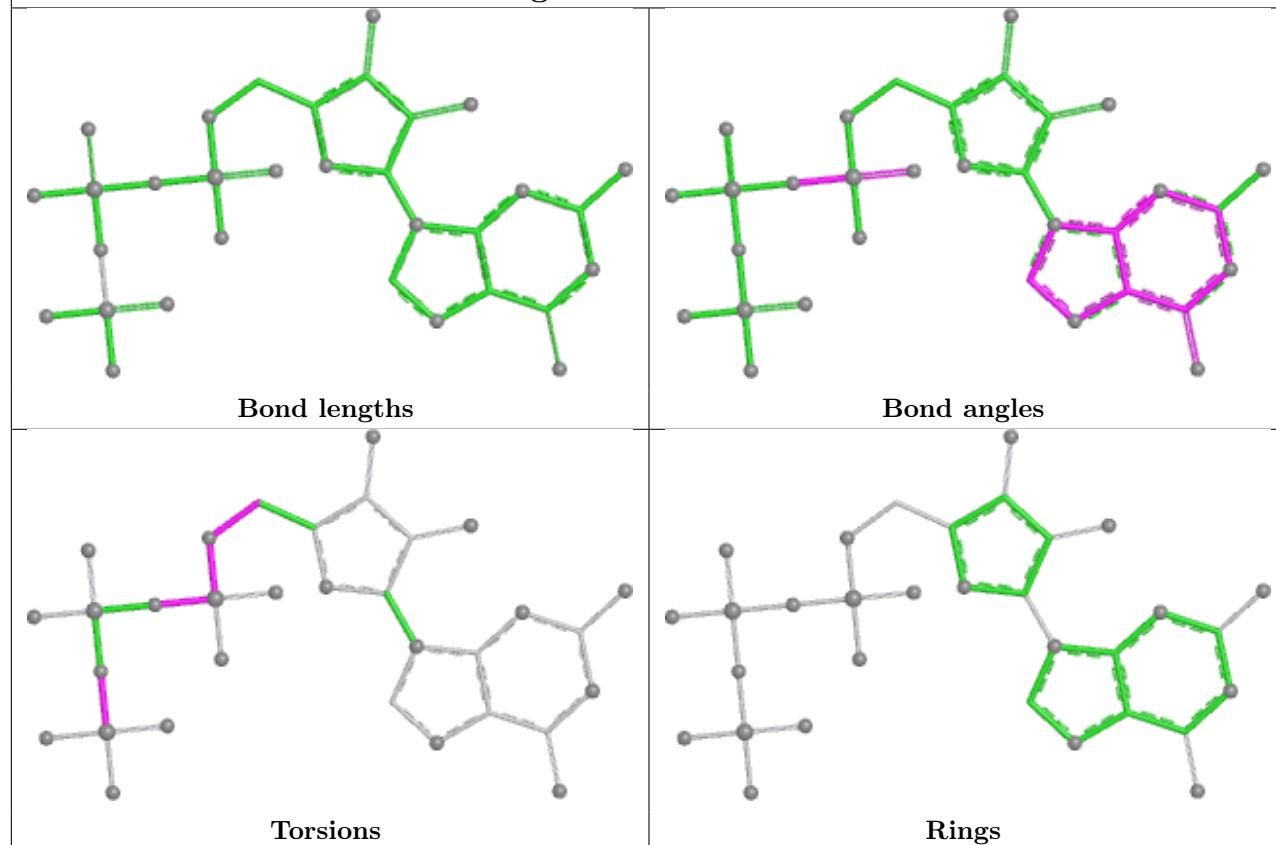
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	7	0
11	D	504	AEX	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

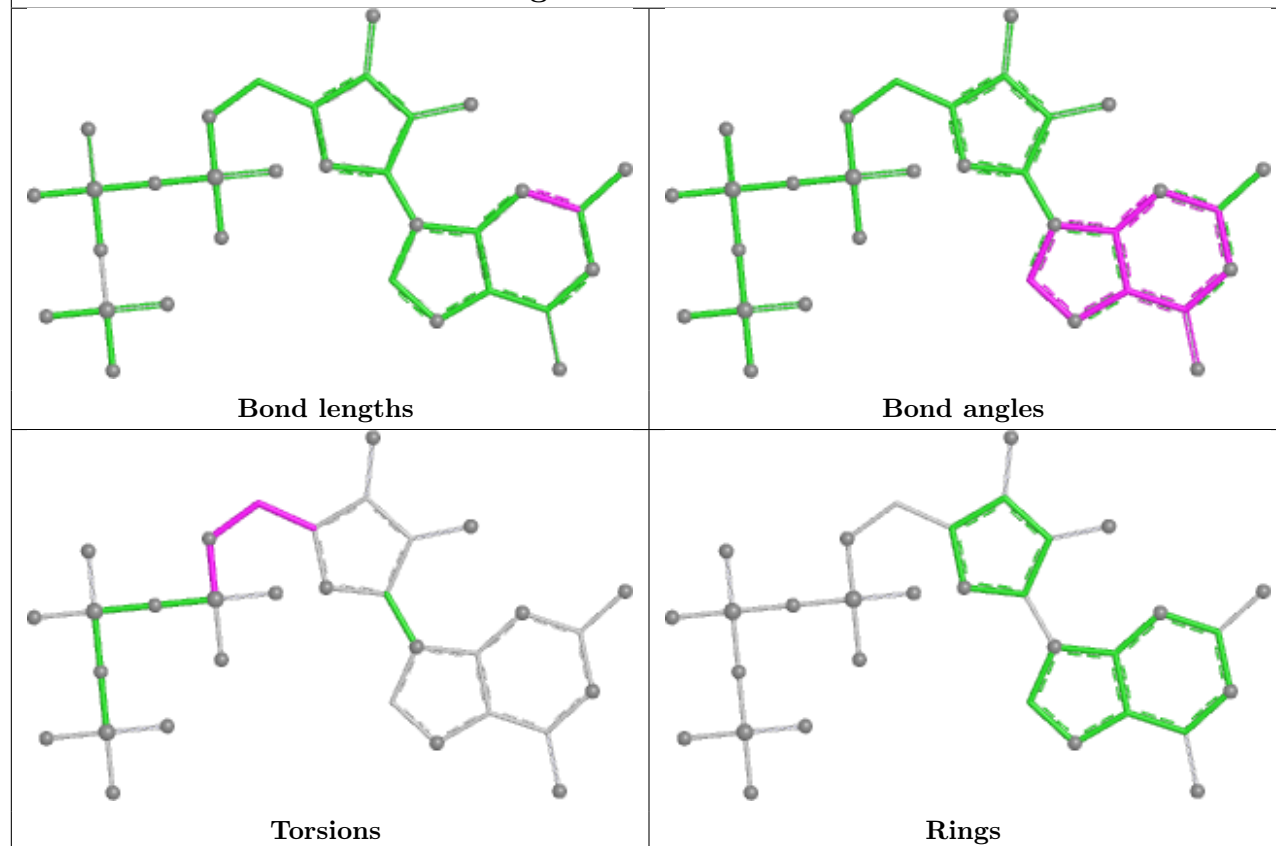
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

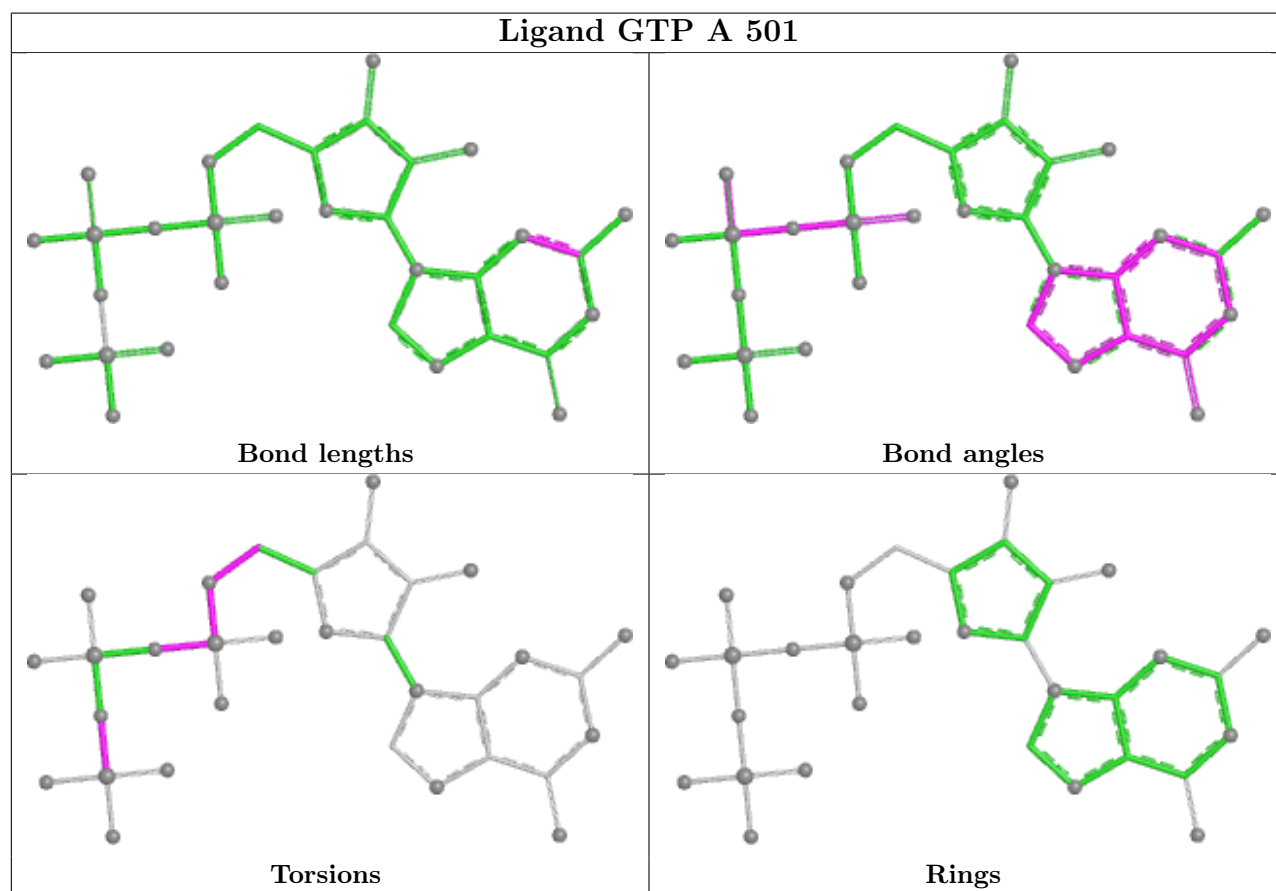
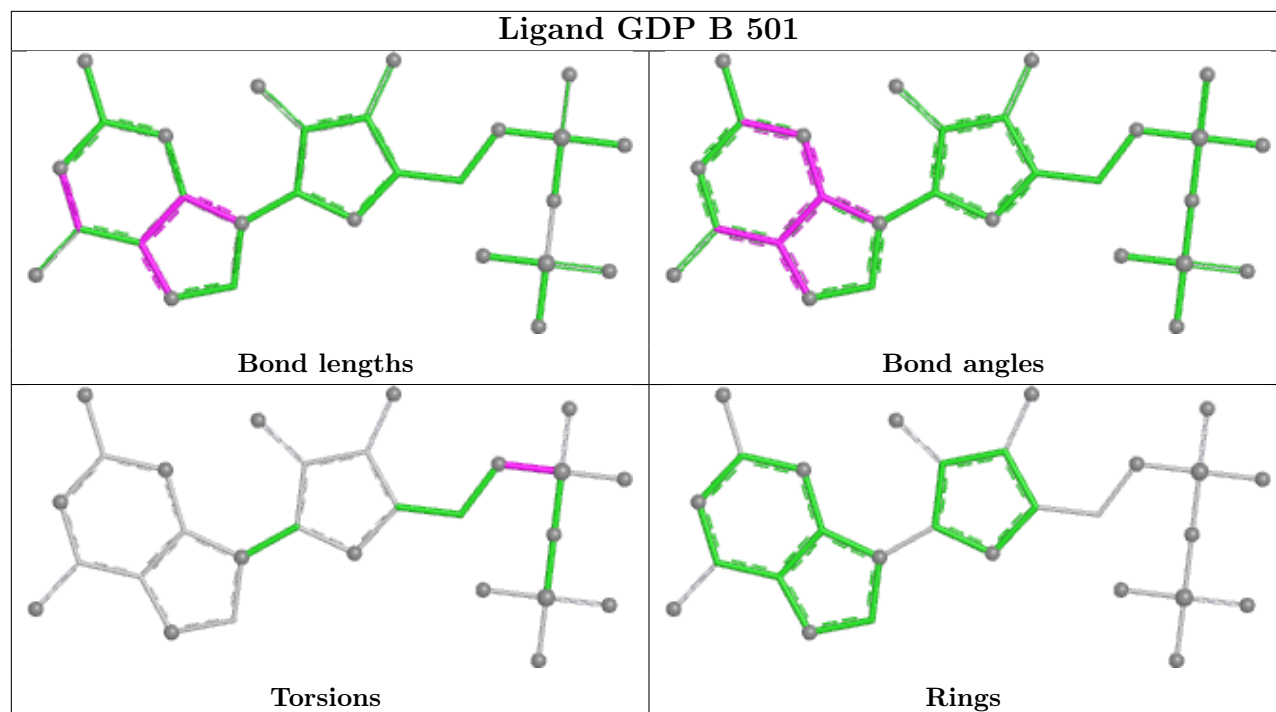


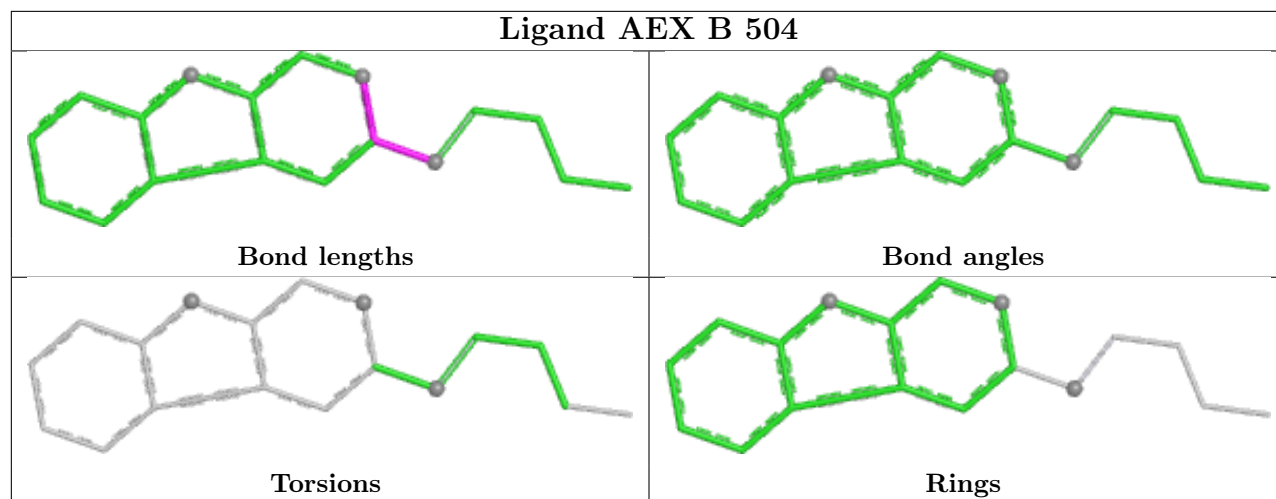
Ligand GTP C 501



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%)	0.07	8 (1%) 67 65	20, 39, 74, 92	2 (0%)
1	C	440/450 (97%)	-0.23	5 (1%) 78 76	15, 29, 63, 115	1 (0%)
2	B	427/445 (95%)	0.15	24 (5%) 30 27	17, 40, 84, 126	0
2	D	421/445 (94%)	0.95	62 (14%) 6 5	27, 62, 103, 127	0
3	E	121/143 (84%)	0.83	11 (9%) 15 13	23, 64, 101, 125	2 (1%)
4	F	334/384 (86%)	1.09	70 (20%) 2 2	32, 71, 132, 155	0
All	All	2180/2317 (94%)	0.39	180 (8%) 17 15	15, 48, 101, 155	5 (0%)

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	245	GLN	7.6
3	E	115[A]	HIS	7.0
1	C	179	THR	6.4
4	F	240	LEU	5.8
4	F	170	LEU	5.7
2	D	394	PHE	5.1
4	F	173	ILE	4.9
4	F	103	THR	4.7
4	F	161	LEU	4.7
2	D	213	ARG	4.3
4	F	253	TYR	4.0
4	F	171	ASP	4.0
2	B	57	ASN	4.0
1	C	357	TYR	3.9
2	D	1	MET	3.9
2	D	92	PHE	3.8
2	D	46	ARG	3.8
2	D	210	ILE	3.8
4	F	101	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	170	MET	3.7
2	D	30	ILE	3.6
4	F	182	ILE	3.6
2	D	214	THR	3.5
4	F	233	PHE	3.5
2	D	69	GLU	3.5
4	F	223	THR	3.4
2	B	280	GLN	3.4
4	F	186	LEU	3.4
3	E	141	GLU	3.3
2	B	279	GLN	3.3
4	F	149	ALA	3.3
4	F	254	GLY	3.3
2	D	217	LEU	3.3
1	A	262	TYR	3.2
4	F	100	ILE	3.2
2	B	247	ASN	3.2
2	D	53	GLU	3.2
2	D	390	ARG	3.2
4	F	372	THR	3.2
2	D	96	GLY	3.2
2	D	393	ALA	3.2
4	F	99	VAL	3.2
4	F	178	GLN	3.1
2	B	39	ASP	3.1
2	D	215	LEU	3.1
2	D	272	PRO	3.0
2	D	180	VAL	3.0
2	D	247	ASN	3.0
2	B	428	ALA	3.0
2	B	245	GLN	3.0
2	D	81	PHE	3.0
4	F	243	HIS	2.9
2	D	284	LEU	2.9
4	F	135	TYR	2.9
2	D	42	LEU	2.9
2	D	83	GLN	2.9
2	D	219	THR	2.9
3	E	139	LEU	2.9
4	F	320	MET	2.8
4	F	144	GLY	2.8
4	F	242	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	56	GLY	2.8
4	F	177	GLY	2.8
4	F	380	HIS	2.8
3	E	122	ARG	2.8
4	F	162	ILE	2.7
1	C	283	HIS	2.7
1	A	437	VAL	2.7
2	D	248	ALA	2.7
4	F	142	ARG	2.7
2	D	70	PRO	2.7
3	E	54	LEU	2.7
4	F	236	LYS	2.7
4	F	169	LEU	2.7
2	D	400	GLY	2.7
2	D	48	ASN	2.7
2	D	176	SER	2.7
2	D	389	PHE	2.7
4	F	247	LYS	2.7
2	D	356	ILE	2.6
2	D	82	GLY	2.6
4	F	263	PHE	2.6
2	B	281	TYR	2.6
2	D	211	CYS	2.6
1	A	113	GLU	2.6
2	B	278	SER	2.6
4	F	13	VAL	2.6
2	D	218	THR	2.6
2	D	76	VAL	2.6
4	F	102	PRO	2.6
2	B	275	SER	2.6
2	B	291	GLN	2.6
2	D	55	THR	2.6
2	D	406	MET	2.6
2	D	59	TYR	2.6
4	F	139	ARG	2.6
3	E	27	PRO	2.6
3	E	28	SER	2.5
4	F	192	LEU	2.5
4	F	14	TYR	2.5
2	D	395	LEU	2.5
2	D	72	THR	2.5
2	D	178	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	358	GLN	2.5
4	F	27	TRP	2.5
4	F	24	THR	2.4
4	F	235	ASP	2.4
4	F	166	ALA	2.4
2	D	246	LEU	2.4
4	F	21	LEU	2.4
4	F	191	LEU	2.4
4	F	227	PRO	2.4
4	F	199	PHE	2.4
4	F	362	ALA	2.4
4	F	180	HIS	2.4
2	D	221	THR	2.4
2	D	396	HIS	2.4
2	B	338	SER	2.4
4	F	225	SER	2.4
4	F	237	THR	2.3
4	F	379	HIS	2.3
4	F	167	SER	2.3
4	F	147	TRP	2.3
3	E	124	GLN	2.3
2	B	215	LEU	2.3
2	B	218	THR	2.3
4	F	165	GLU	2.3
1	A	88	HIS	2.3
1	A	326	LYS	2.3
2	D	391	ARG	2.3
2	D	11	GLN	2.3
1	C	440	VAL	2.3
2	D	37	HIS	2.3
1	A	163	LYS	2.3
3	E	59	GLU	2.3
2	D	195	ASN	2.3
4	F	138	ARG	2.3
2	B	273	LEU	2.3
2	D	227	HIS	2.2
2	D	80	PRO	2.2
2	D	273	LEU	2.2
4	F	221	LEU	2.2
2	B	248	ALA	2.2
4	F	336	PRO	2.2
4	F	246	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	277	GLY	2.2
2	D	41	ASP	2.2
2	D	95	SER	2.2
4	F	376	ILE	2.2
2	B	276	ARG	2.2
2	B	216	LYS	2.2
2	B	246	LEU	2.2
3	E	127	ASP	2.2
2	B	323	MET	2.2
2	D	57	ASN	2.2
4	F	333	ASN	2.1
1	A	282	TYR	2.1
2	D	253	LEU	2.1
4	F	17	VAL	2.1
4	F	131	PHE	2.1
2	B	55	THR	2.1
1	A	57	GLY	2.1
4	F	33	ASP	2.1
4	F	353	VAL	2.1
2	D	388	MET	2.1
2	D	377	LEU	2.1
2	D	99	ASN	2.1
4	F	130	VAL	2.1
4	F	181	VAL	2.1
2	D	108	GLU	2.1
4	F	231	ALA	2.1
3	E	45	PRO	2.1
4	F	241	THR	2.0
2	D	220	PRO	2.0
4	F	260	ASN	2.0
4	F	146	VAL	2.0
2	B	283	ALA	2.0
2	D	296	SER	2.0
4	F	239	HIS	2.0
4	F	10	ASN	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 ⓘ

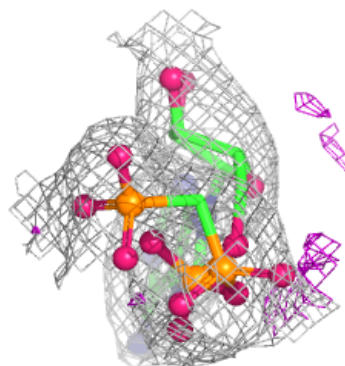
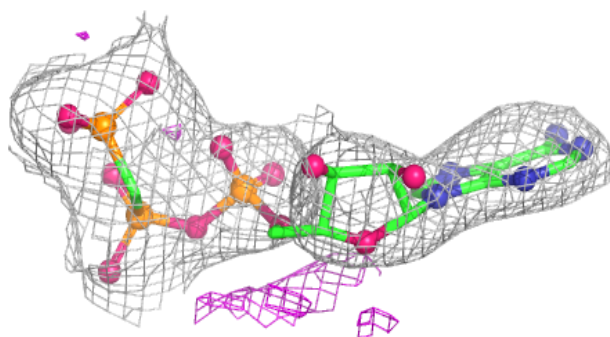
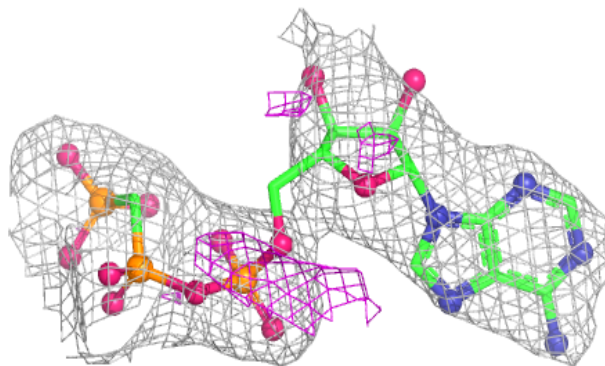
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	MG	D	503	1/1	0.84	0.24	60,60,60,60	0
10	MES	D	502	12/12	0.84	0.21	60,80,113,121	0
12	ACP	F	401	31/31	0.85	0.15	67,92,121,133	0
5	GTP	D	501	32/32	0.89	0.12	37,53,70,76	0
11	AEX	D	504	18/18	0.89	0.20	54,75,96,99	0
8	GOL	A	504	6/6	0.89	0.17	33,57,69,70	0
10	MES	B	503	12/12	0.94	0.10	26,40,47,52	0
11	AEX	B	504	18/18	0.95	0.08	24,32,44,50	0
9	GDP	B	501	28/28	0.97	0.07	15,24,36,44	0
5	GTP	C	501	32/32	0.97	0.07	13,19,25,31	0
5	GTP	A	501	32/32	0.97	0.07	16,26,34,35	0
6	MG	A	502	1/1	0.98	0.03	22,22,22,22	0
7	CA	A	503	1/1	0.98	0.05	58,58,58,58	0
6	MG	B	502	1/1	0.98	0.04	27,27,27,27	0
7	CA	C	503	1/1	0.99	0.02	40,40,40,40	0
6	MG	C	502	1/1	0.99	0.03	26,26,26,26	0

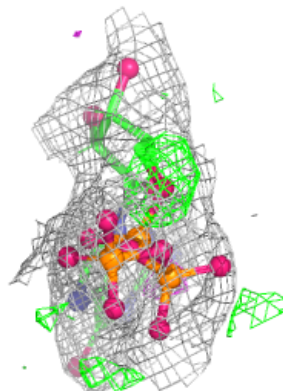
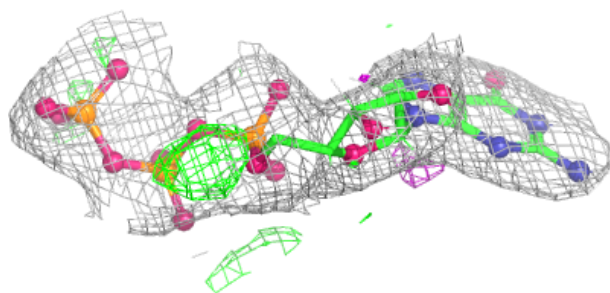
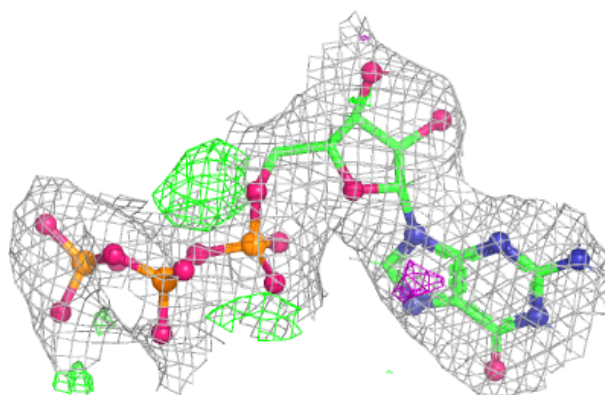
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

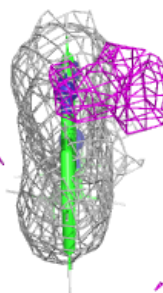
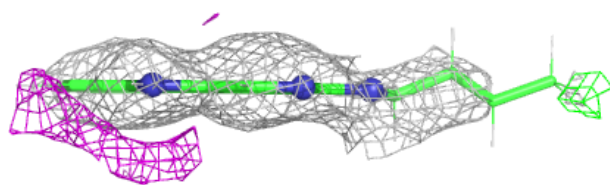
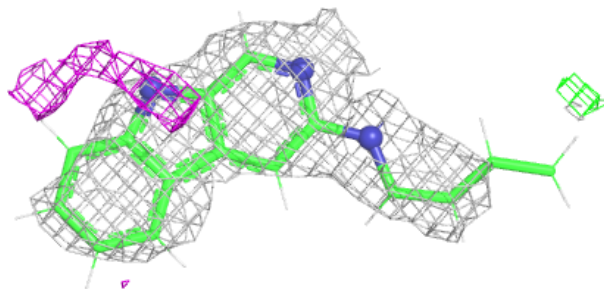
**Electron density around GTP D 501:**

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

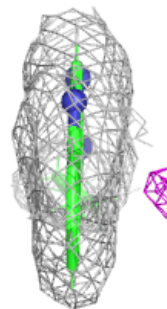
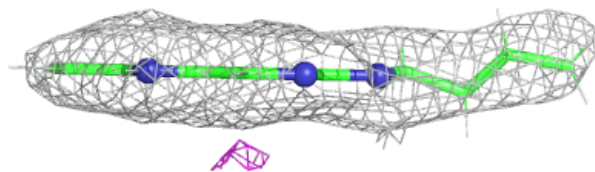


Electron density around AEX D 504:

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

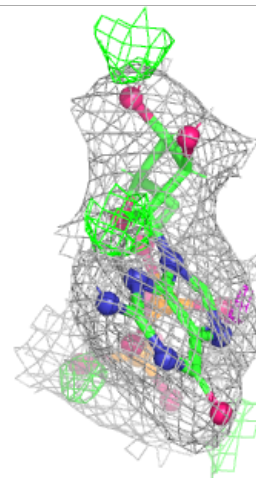
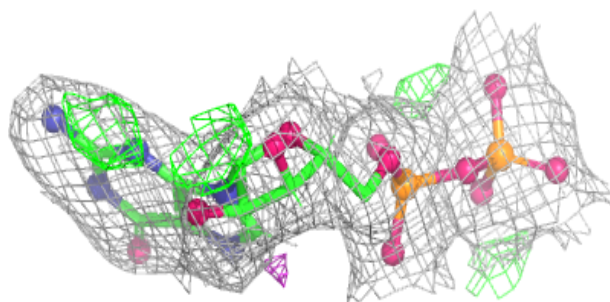
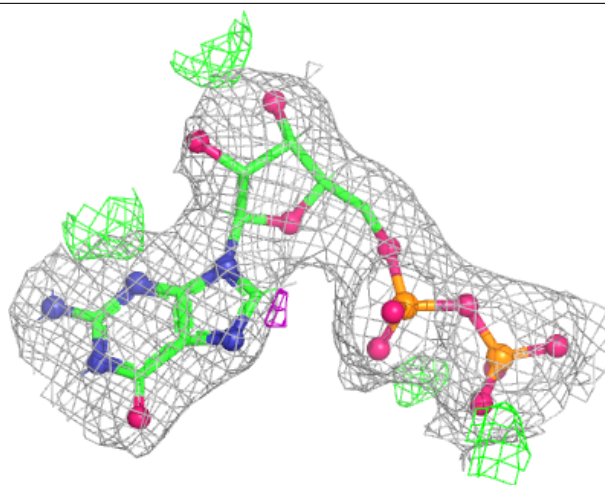
**Electron density around AEX B 504:**

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



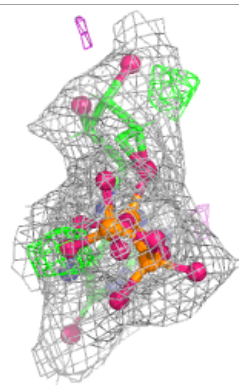
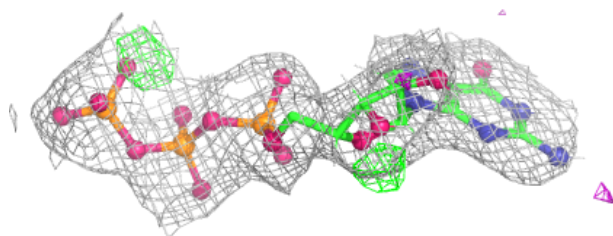
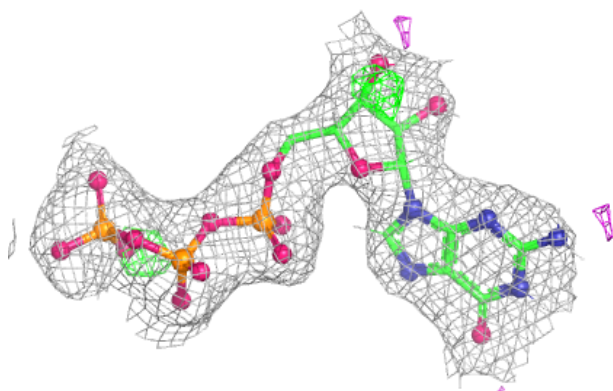
Electron density around GDP B 501:

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

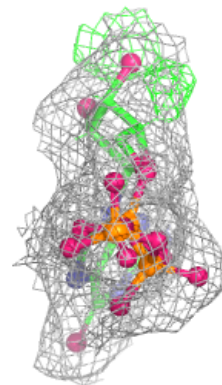
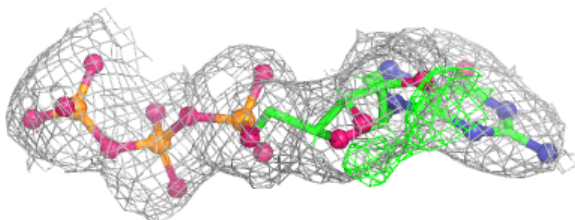
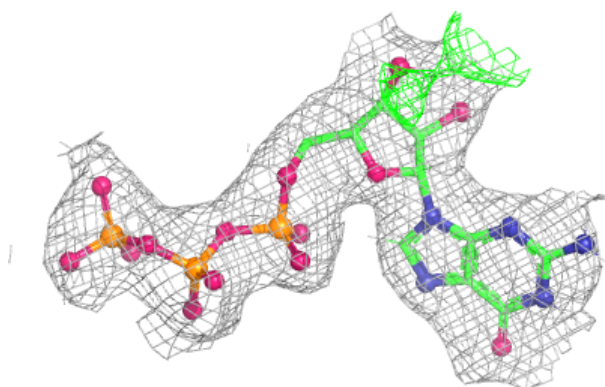


Electron density around GTP C 501:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.