



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:05 AM UTC

PDB ID : 7CDA / pdb_00007cda
Title : Crystal structure of T2R-TTL-PAC complex
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Deposited on : 2020-06-19
Resolution : 2.66 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

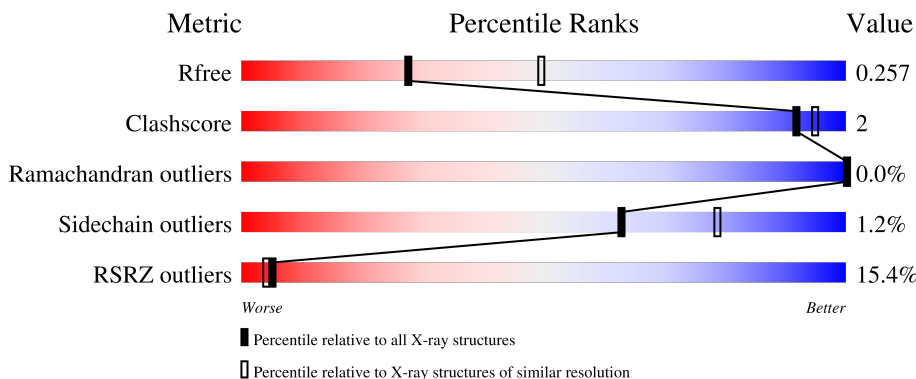
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	 2% 96%
2	B	445	 8% 91% 5%
2	D	445	 35% 86% 8% 5%
3	E	143	 10% 83% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '29%', a large green segment labeled '83%', a small yellow segment labeled '5%', and a grey segment on the far right labeled '12%'.</p>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 34882 atoms, of which 16913 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	
			Total	C	H	N	O				S
1	A	437	Total	C	H	N	O	S	0	3	0
			6772	2174	3335	585	654	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	
			Total	C	H	N	O				S
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
			6486	2080	3177	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	E	121	Total	C	H	N	O	S	0	2	0
			2043	627	1025	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	
			Total	C	H	N	O				S
4	F	338	Total	C	H	N	O	S	0	0	0
			5494	1785	2709	482	504	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: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
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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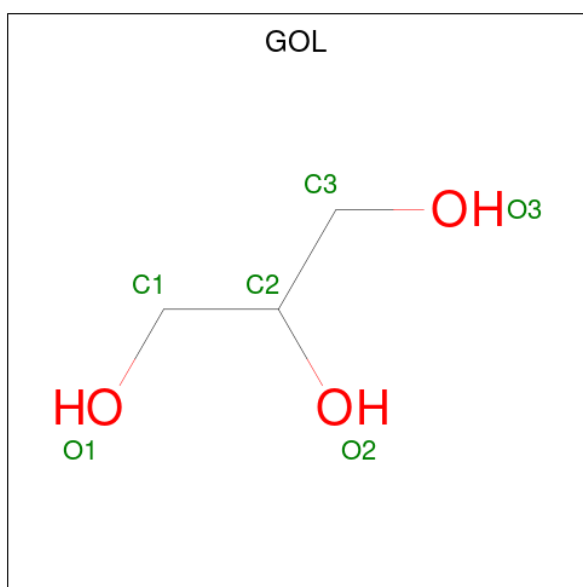
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

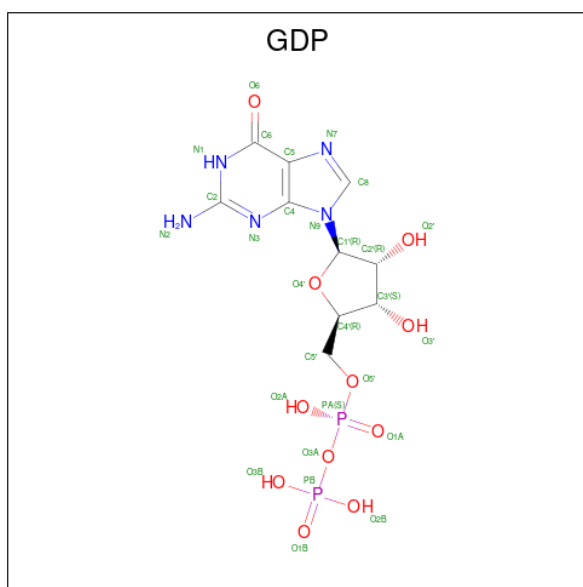
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



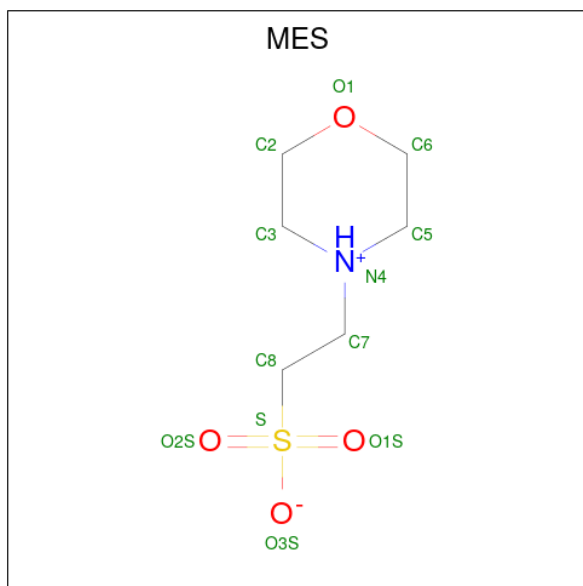
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

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



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

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

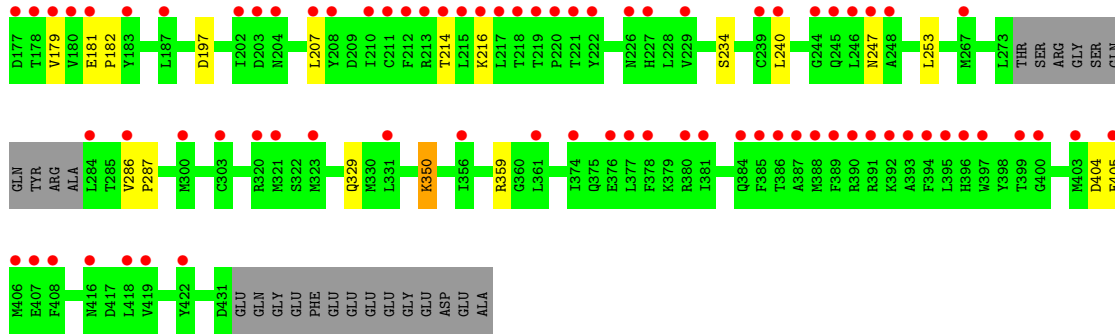


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
10	B	1	25	6	13	1	4	1	0	0

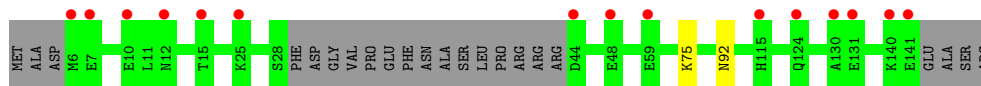
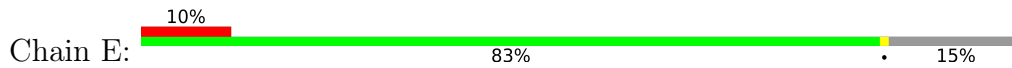
- Molecule 11 is N-[(3-phenoxyphenyl)methyl]-9H-beta-carboline-3-amine (CCD ID: AEU) (formula: C₂₄H₁₉N₃O) (labeled as "Ligand of Interest" by depositor).

- Molecule 13 is water.

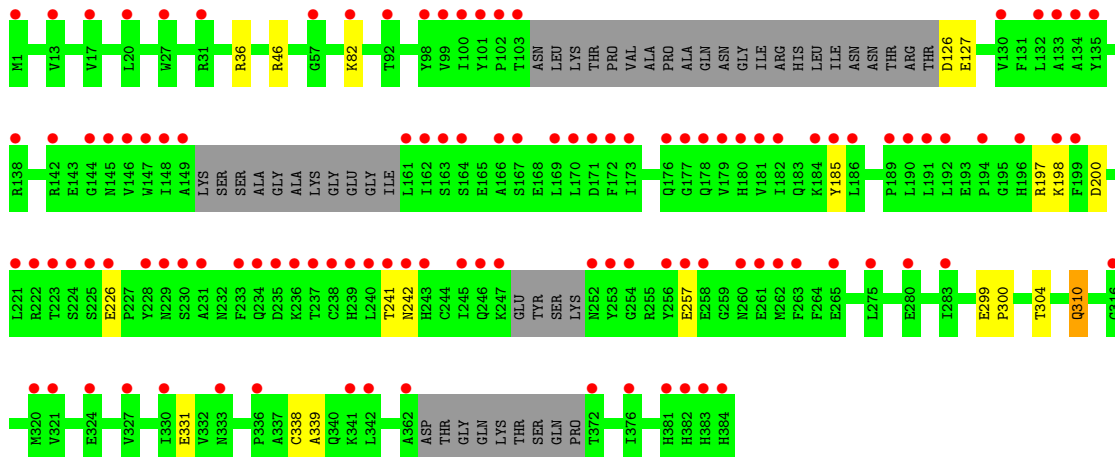
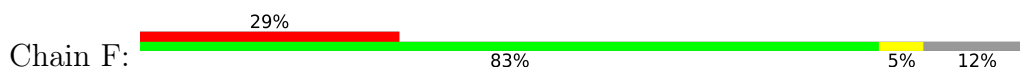
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	104	Total O 104 104	0	0
13	B	69	Total O 69 69	0	0
13	C	120	Total O 120 120	0	0
13	D	35	Total O 35 35	0	0
13	E	13	Total O 13 13	0	0
13	F	40	Total O 40 40	0	0



• 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	105.09Å 156.83Å 182.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 2.66 39.76 – 2.66	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.76-2.66) 98.2 (39.76-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.222 , 0.257 0.225 , 0.257	Depositor DCC
R_{free} test set	4282 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34882	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: MES, GOL, AEU, ACP, GTP, 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	0.31	0/3515	0.63	0/4771
1	C	0.31	0/3521	0.61	0/4781
2	B	0.31	0/3436	0.61	0/4654
2	D	0.30	0/3382	0.62	0/4581
3	E	0.27	0/1027	0.59	0/1363
4	F	0.26	0/2851	0.59	0/3851
All	All	0.30	0/17732	0.61	0/24001

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

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	3437	3335	3346	6	0
1	C	3443	3340	3353	5	0
2	B	3361	3228	3238	10	0
2	D	3309	3177	3189	18	0
3	E	1018	1025	1029	1	0
4	F	2785	2709	2737	15	0
5	A	32	10	12	1	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	1	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	13	12	0	0
11	B	28	19	0	0	0
11	D	28	19	0	1	0
12	F	31	0	14	6	0
13	A	104	0	0	1	0
13	B	69	0	0	1	0
13	C	120	0	0	3	0
13	D	35	0	0	3	0
13	E	13	0	0	1	0
13	F	40	0	0	2	0
All	All	17969	16913	16974	56	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 (56) 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:242:ASN:OD1	12:F:401:ACP:H5'1	1.62	0.98
4:F:331:GLU:OE2	12:F:401:ACP:O2G	1.93	0.87
12:F:401:ACP:O2G	12:F:401:ACP:O1B	2.05	0.74
2:D:207:LEU:O	13:D:601:HOH:O	2.09	0.70
2:D:214:THR:N	13:D:604:HOH:O	2.28	0.66
1:A:433:GLU:OE2	4:F:46:ARG:NH1	2.29	0.66
4:F:241:THR:OG1	12:F:401:ACP:O3'	2.05	0.66
12:F:401:ACP:O1A	12:F:401:ACP:H3B2	1.99	0.63
4:F:82:LYS:NZ	13:F:503:HOH:O	2.32	0.62
2:D:26:ASP:OD1	2:D:359:ARG:NH2	2.33	0.61
4:F:304:THR:O	4:F:310:GLN:NE2	2.34	0.61
3:E:92:ASN:ND2	13:E:202:HOH:O	2.33	0.60
4:F:36:ARG:NH2	13:F:501:HOH:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:NZ	13:A:605:HOH:O	2.36	0.59
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.22	0.58
2:B:301:ALA:O	2:B:303:CYS:N	2.36	0.57
4:F:242:ASN:OD1	12:F:401:ACP:C5'	2.45	0.56
2:B:26:ASP:OD1	2:B:359:ARG:NH1	2.39	0.56
2:D:107:THR:OG1	2:D:108:GLU:N	2.38	0.56
4:F:338:CYS:SG	4:F:339:ALA:N	2.79	0.56
2:B:94:GLN:NE2	13:B:608:HOH:O	2.42	0.53
2:D:216:LYS:N	13:D:604:HOH:O	2.31	0.53
2:D:404:ASP:OD1	2:D:405:GLU:N	2.41	0.53
1:C:1:MET:N	13:C:612:HOH:O	2.39	0.52
2:B:137:HIS:ND1	2:B:144:GLY:O	2.32	0.52
4:F:126:ASP:OD1	4:F:127:GLU:N	2.44	0.51
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.44	0.49
2:D:94:GLN:OE1	2:D:94:GLN:N	2.46	0.49
2:D:27:GLU:OE1	2:D:234:SER:OG	2.29	0.49
2:B:161:ASP:O	2:B:251:ARG:NH2	2.47	0.48
1:C:279:GLU:N	1:C:279:GLU:OE1	2.47	0.48
1:C:366:GLY:N	13:C:619:HOH:O	2.48	0.47
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.48	0.47
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.48	0.46
1:A:90:GLU:OE1	1:A:90:GLU:N	2.48	0.46
2:B:25:SER:OG	2:B:51:TYR:OH	2.33	0.44
1:A:183:GLU:OE2	5:A:501:GTP:O3'	2.30	0.44
2:B:39:ASP:OD1	2:B:40:SER:N	2.50	0.43
4:F:226:GLU:OE1	4:F:226:GLU:N	2.50	0.43
2:D:181:GLU:N	2:D:182:PRO:HD2	2.33	0.43
2:D:350:LYS:HE3	2:D:350:LYS:HA	2.00	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.43
2:D:287:PRO:HA	2:D:329:GLN:HG2	2.01	0.42
2:D:73:MET:HE3	2:D:90:PHE:HD2	1.84	0.42
2:D:142:GLY:N	5:D:501:GTP:O2B	2.49	0.42
1:C:124:LYS:NZ	13:C:621:HOH:O	2.51	0.42
2:D:3:GLU:N	2:D:3:GLU:OE2	2.53	0.42
2:D:67:ASP:OD1	2:D:68:LEU:N	2.53	0.41
2:B:55:THR:O	2:B:55:THR:OG1	2.34	0.41
1:C:71:GLU:OE2	1:C:73:THR:N	2.51	0.41
2:D:286:VAL:N	2:D:287:PRO:CD	2.83	0.41
2:B:145:SER:OG	2:B:188:SER:OG	2.35	0.41
2:B:21:TRP:O	2:B:25:SER:OG	2.34	0.40
1:A:71:GLU:HB2	1:A:98:ASP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:LEU:HB3	11:D:502:AEU:C10	2.51	0.40
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	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%)	424 (97%)	14 (3%)	0	100	100
1	C	439/450 (98%)	427 (97%)	12 (3%)	0	100	100
2	B	425/445 (96%)	411 (97%)	13 (3%)	1 (0%)	43	60
2	D	417/445 (94%)	403 (97%)	14 (3%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	328/384 (85%)	309 (94%)	19 (6%)	0	100	100
All	All	2166/2317 (94%)	2091 (96%)	74 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/378 (98%)	366 (99%)	5 (1%)	61	77
1	C	372/378 (98%)	370 (100%)	2 (0%)	81	91
2	B	369/383 (96%)	365 (99%)	4 (1%)	65	80
2	D	364/383 (95%)	353 (97%)	11 (3%)	36	57
3	E	111/127 (87%)	110 (99%)	1 (1%)	70	82
4	F	305/342 (89%)	304 (100%)	1 (0%)	86	94
All	All	1892/1991 (95%)	1868 (99%)	24 (1%)	63	77

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	124	LYS
1	A	176[A]	GLN
1	A	176[B]	GLN
1	A	221	ARG
2	B	58	LYS
2	B	215	LEU
2	B	245	GLN
2	B	320	ARG
1	C	2	ARG
1	C	284	GLU
2	D	11	GLN
2	D	19	LYS
2	D	30	ILE
2	D	35	SER
2	D	39	ASP
2	D	41	ASP
2	D	167	PHE
2	D	179	VAL
2	D	240	LEU
2	D	247	ASN
2	D	350	LYS
3	E	75	LYS
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN

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Mol	Chain	Res	Type
1	A	342	GLN
1	A	393	HIS
2	B	8	GLN
2	B	134	GLN
2	B	190	HIS
2	B	245	GLN
2	B	375	GLN
2	B	423	GLN
1	C	15	GLN
1	C	101	ASN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	48	ASN
2	D	134	GLN
3	E	78	HIS
3	E	136	ASN
4	F	180	HIS
4	F	252	ASN
4	F	269	GLN
4	F	310	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, 6 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	501	6	33,34,34	1.02	3 (9%)	50,54,54	1.55	9 (18%)
11	AEU	B	504	-	32,32,32	1.65	11 (34%)	43,44,44	1.11	3 (6%)
9	GDP	B	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
8	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.27	0
11	AEU	D	502	-	32,32,32	1.71	12 (37%)	43,44,44	1.11	3 (6%)
5	GTP	A	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.54	8 (16%)
10	MES	B	503	-	12,12,12	2.26	1 (8%)	15,16,16	1.56	2 (13%)
12	ACP	F	401	-	31,33,33	1.59	6 (19%)	47,52,52	2.03	14 (29%)
5	GTP	D	501	6	33,34,34	1.03	3 (9%)	50,54,54	1.60	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
11	AEU	B	504	-	-	0/9/9/9	0/5/5/5
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
11	AEU	D	502	-	-	0/9/9/9	0/5/5/5
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
10	MES	B	503	-	-	3/6/14/14	0/1/1/1
12	ACP	F	401	-	-	10/19/38/38	0/3/3/3
5	GTP	D	501	6	-	5/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.57	1.67	1.77
11	D	502	AEU	C04-C05	3.51	1.45	1.39
11	B	504	AEU	C04-C05	3.31	1.45	1.39
12	F	401	ACP	C5-C4	3.20	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	C5-N7	-3.17	1.33	1.39
9	B	501	GDP	C5-C4	3.04	1.47	1.38
12	F	401	ACP	C8-N9	-2.94	1.32	1.37
11	B	504	AEU	C06-C05	-2.85	1.37	1.41
12	F	401	ACP	PG-O2G	2.83	1.61	1.55
12	F	401	ACP	C4-N9	-2.78	1.31	1.37
9	B	501	GDP	C6-N1	-2.71	1.33	1.38
11	D	502	AEU	C02-C01	2.67	1.43	1.38
11	D	502	AEU	C12-N14	2.66	1.40	1.36
11	D	502	AEU	C06-C05	-2.66	1.37	1.41
11	D	502	AEU	C13-C07	2.64	1.44	1.39
11	D	502	AEU	C21-C20	2.56	1.43	1.39
11	D	502	AEU	C17-C16	2.54	1.43	1.38
11	B	504	AEU	C21-C20	2.52	1.43	1.39
11	B	504	AEU	C17-C16	2.48	1.43	1.38
12	F	401	ACP	PG-O3G	2.46	1.60	1.55
11	B	504	AEU	C02-C01	2.43	1.43	1.38
11	B	504	AEU	C13-C07	2.43	1.43	1.39
5	C	501	GTP	PA-O3A	2.39	1.62	1.59
11	B	504	AEU	C12-N14	2.38	1.39	1.36
5	D	501	GTP	PB-O3A	2.33	1.62	1.59
5	D	501	GTP	C2-N3	2.32	1.38	1.33
11	D	502	AEU	C25-C26	2.30	1.43	1.38
11	B	504	AEU	C25-C26	2.29	1.43	1.38
11	D	502	AEU	C21-C16	-2.27	1.35	1.39
5	A	501	GTP	PA-O3A	2.19	1.61	1.59
11	B	504	AEU	C21-C16	-2.18	1.35	1.39
11	B	504	AEU	C24-C23	2.18	1.42	1.38
5	D	501	GTP	PB-O3B	2.17	1.61	1.59
11	D	502	AEU	C24-C23	2.12	1.42	1.38
5	A	501	GTP	C2-N3	2.11	1.38	1.33
5	A	501	GTP	PB-O3A	2.11	1.61	1.59
5	C	501	GTP	PB-O3A	2.06	1.61	1.59
5	C	501	GTP	C2-N3	2.06	1.38	1.33
11	D	502	AEU	C07-C08	-2.03	1.38	1.41
9	B	501	GDP	C5-N7	-2.02	1.35	1.39
11	B	504	AEU	C25-C24	-2.02	1.35	1.38
11	D	502	AEU	C25-C24	-2.00	1.35	1.38

All (52) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C5-C4-N3	-5.84	119.10	128.39
12	F	401	ACP	C5-C4-N3	-5.69	118.88	126.72
5	D	501	GTP	C5-C4-N3	-5.22	120.08	128.39
9	B	501	GDP	C2-N3-C4	4.89	120.72	112.30
5	C	501	GTP	C5-C4-N3	-4.82	120.72	128.39
5	A	501	GTP	C5-C4-N3	-4.80	120.74	128.39
5	D	501	GTP	C2-N3-C4	4.58	120.19	112.30
9	B	501	GDP	N9-C4-N3	4.53	135.02	125.95
5	C	501	GTP	C2-N3-C4	4.53	120.10	112.30
5	A	501	GTP	C2-N3-C4	4.49	120.04	112.30
12	F	401	ACP	C4-C5-N7	-4.41	105.54	110.58
11	B	504	AEU	C10-N11-C12	4.40	121.95	117.83
11	D	502	AEU	C10-N11-C12	4.30	121.86	117.83
12	F	401	ACP	N3-C2-N1	-4.13	122.33	128.58
10	B	503	MES	C5-N4-C3	4.00	117.45	108.84
12	F	401	ACP	C2-N3-C4	3.99	121.58	111.83
12	F	401	ACP	N3-C4-N9	3.90	133.81	127.17
5	D	501	GTP	N9-C4-N3	3.43	132.81	125.95
9	B	501	GDP	C6-C5-N7	3.30	136.30	130.29
5	A	501	GTP	N9-C4-N3	3.24	132.43	125.95
11	D	502	AEU	C23-O22-C20	-3.19	111.49	118.78
5	C	501	GTP	N9-C4-N3	3.16	132.27	125.95
12	F	401	ACP	PB-O3A-PA	-3.08	122.30	132.37
12	F	401	ACP	C5-N7-C8	3.01	108.19	103.45
5	D	501	GTP	C2-N1-C6	-2.93	119.79	125.11
5	A	501	GTP	C2-N1-C6	-2.85	119.95	125.11
10	B	503	MES	O3S-S-C8	2.84	111.57	106.00
12	F	401	ACP	C2-N1-C6	2.84	123.40	118.73
11	B	504	AEU	C23-O22-C20	-2.84	112.30	118.78
5	C	501	GTP	C2-N1-C6	-2.77	120.09	125.11
5	A	501	GTP	N9-C8-N7	-2.74	108.32	113.40
5	C	501	GTP	N9-C8-N7	-2.73	108.34	113.40
12	F	401	ACP	C6-C5-N7	2.64	137.17	132.09
5	D	501	GTP	N9-C8-N7	-2.62	108.54	113.40
5	A	501	GTP	O6-C6-C5	-2.60	119.67	126.53
5	D	501	GTP	C8-N7-C5	2.57	108.84	104.26
12	F	401	ACP	C4-N9-C8	2.54	108.40	105.74
5	A	501	GTP	C5-C6-N1	2.51	119.63	113.25
5	D	501	GTP	C5-C6-N1	2.50	119.61	113.25
5	C	501	GTP	C8-N7-C5	2.47	108.66	104.26
5	C	501	GTP	C5-C6-N1	2.45	119.48	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	O2'-C2'-C1'	-2.44	101.69	110.10
5	C	501	GTP	O6-C6-C5	-2.44	120.08	126.53
5	D	501	GTP	O6-C6-C5	-2.43	120.12	126.53
9	B	501	GDP	C4-C5-N7	-2.40	106.87	110.67
12	F	401	ACP	C3'-C2'-C1'	2.40	106.00	101.46
5	A	501	GTP	C8-N7-C5	2.40	108.53	104.26
11	D	502	AEU	C13-C12-N11	-2.39	119.78	122.92
12	F	401	ACP	N9-C8-N7	-2.38	110.56	113.94
5	C	501	GTP	O2A-PA-O3A	2.22	113.27	107.27
11	B	504	AEU	C13-C12-N11	-2.15	120.10	122.92
12	F	401	ACP	O2G-PG-O1G	-2.07	107.03	112.39

There are no chirality outliers.

All (38) 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	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
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	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O3S
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
12	F	401	ACP	C3'-C4'-C5'-O5'
8	A	504	GOL	O1-C1-C2-O2
9	B	501	GDP	PA-O3A-PB-O1B
5	D	501	GTP	PA-O3A-PB-O3B
10	B	503	MES	C7-C8-S-O2S
9	B	501	GDP	PA-O3A-PB-O3B
5	D	501	GTP	C4'-C5'-O5'-PA

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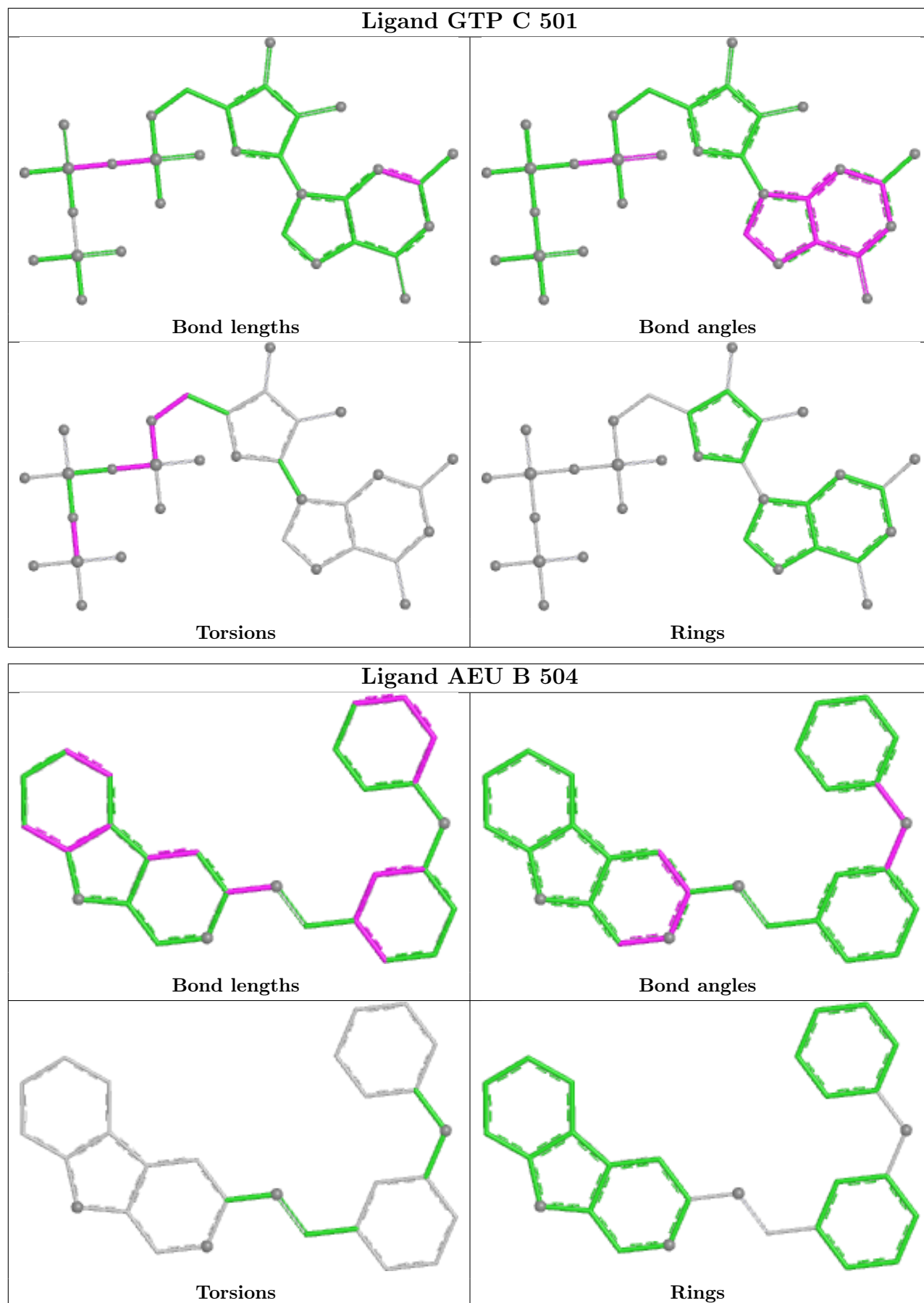
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PG-O3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
12	F	401	ACP	PB-O3A-PA-O1A
12	F	401	ACP	PB-C3B-PG-O1G
5	D	501	GTP	PG-O3B-PB-O2B
5	D	501	GTP	PA-O3A-PB-O2B

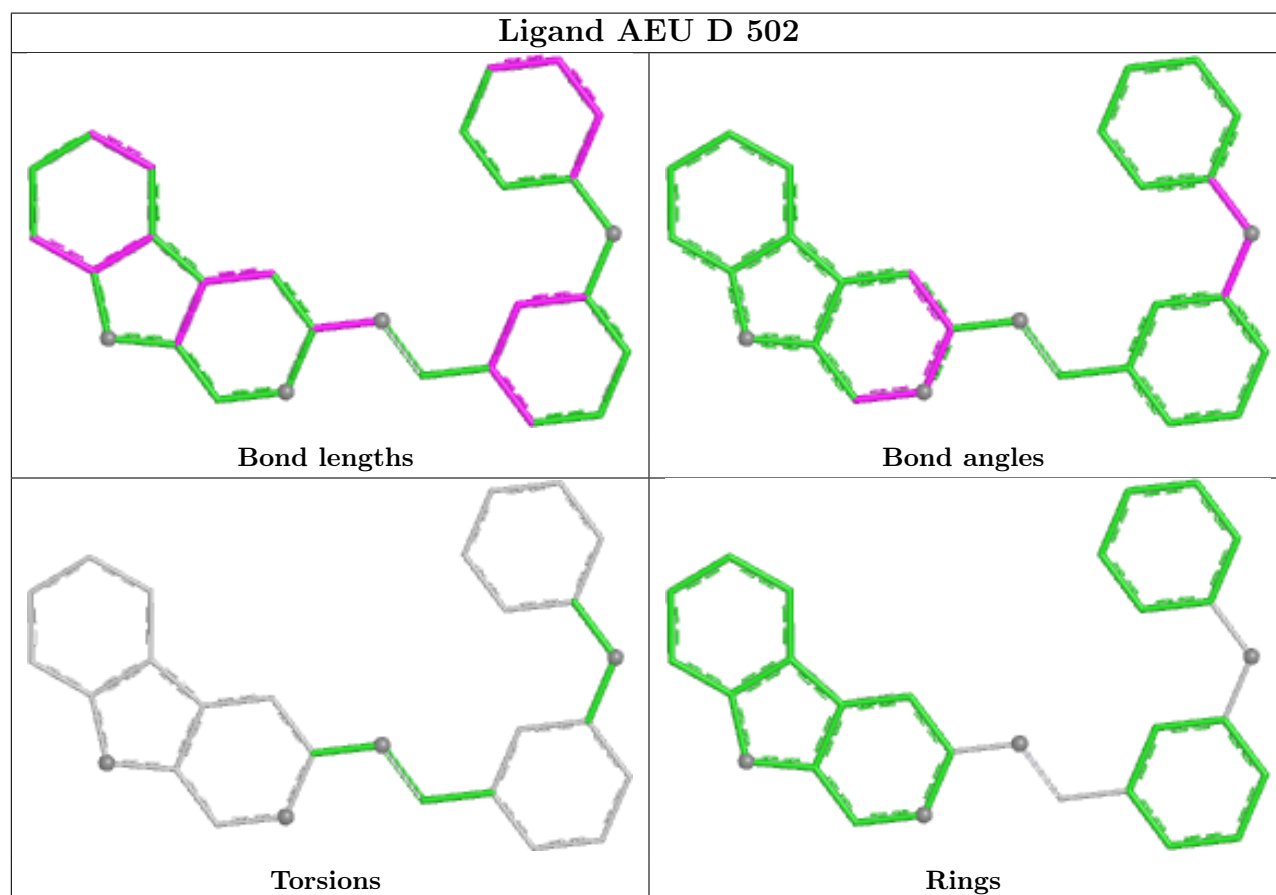
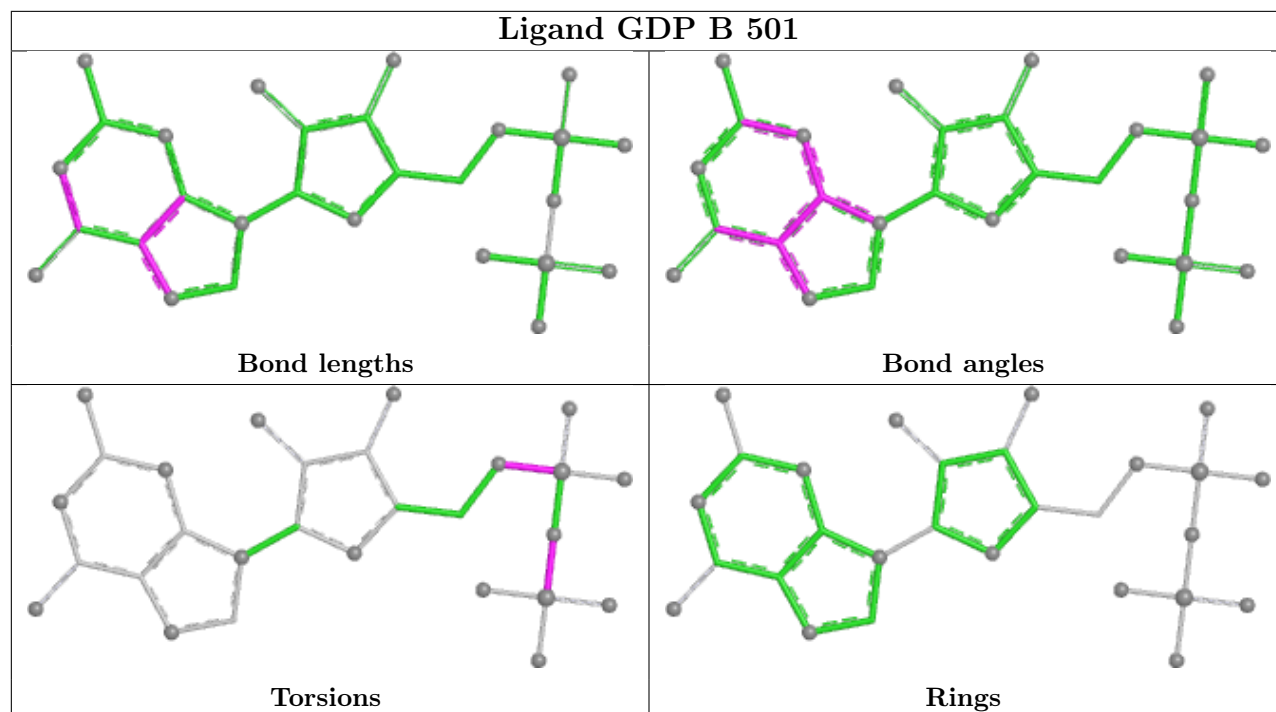
There are no ring outliers.

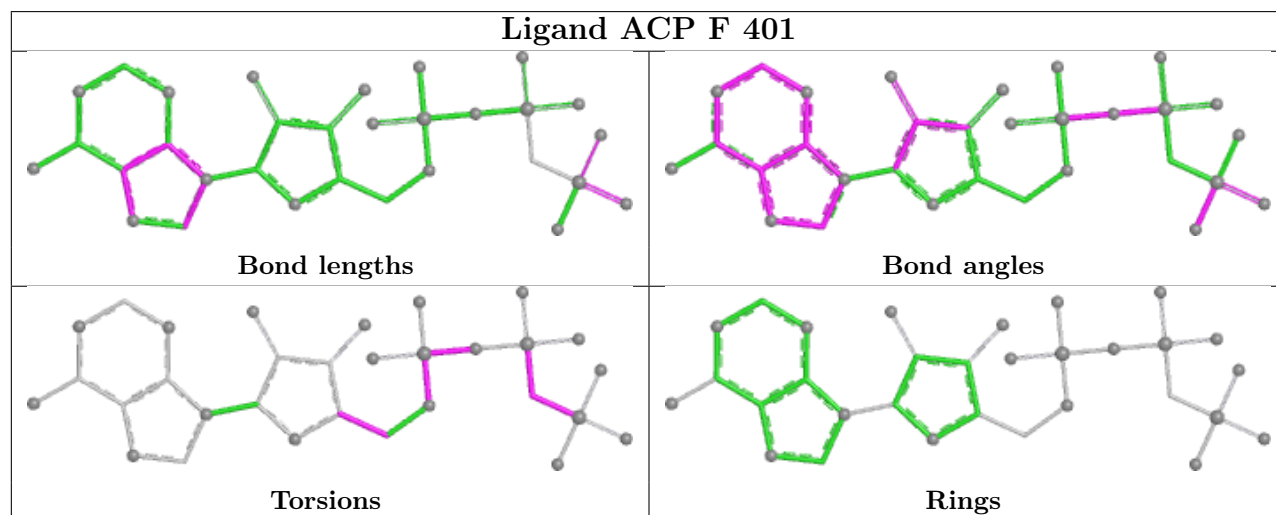
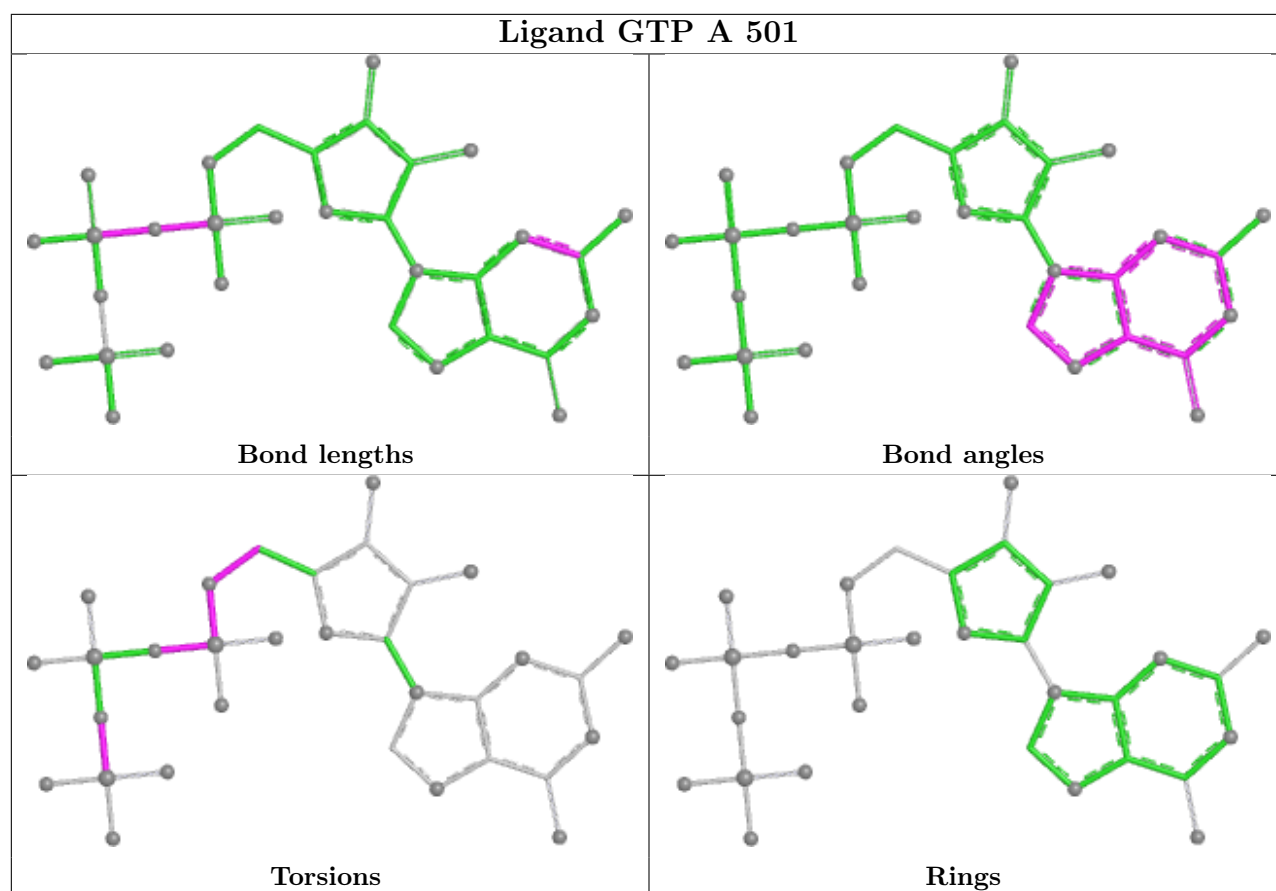
4 monomers are involved in 9 short contacts:

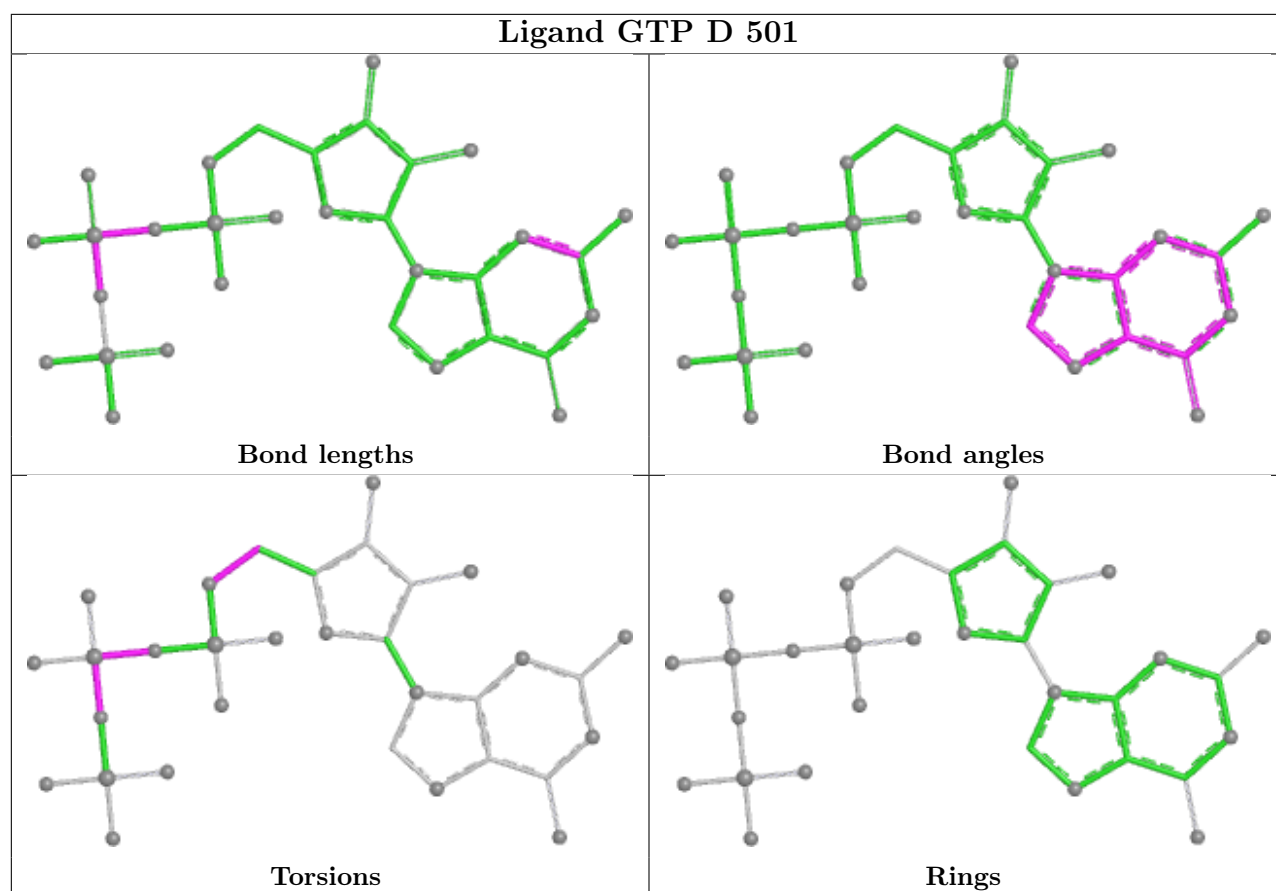
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	502	AEU	1	0
5	A	501	GTP	1	0
12	F	401	ACP	6	0
5	D	501	GTP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	0.23	8 (1%) 67 63	21, 41, 72, 99	3 (0%)
1	C	440/450 (97%)	-0.05	11 (2%) 58 52	15, 32, 66, 127	1 (0%)
2	B	427/445 (95%)	0.44	37 (8%) 16 12	18, 41, 88, 148	0
2	D	421/445 (94%)	1.70	154 (36%) 1 0	36, 74, 120, 157	0
3	E	121/143 (84%)	1.14	15 (12%) 8 7	27, 66, 106, 115	2 (1%)
4	F	338/384 (88%)	1.57	112 (33%) 1 0	36, 79, 143, 165	0
All	All	2184/2317 (94%)	0.75	337 (15%) 5 4	15, 51, 116, 165	6 (0%)

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	115[A]	HIS	14.8
1	C	179	THR	8.4
4	F	161	LEU	7.1
1	A	176[A]	GLN	6.6
2	D	394	PHE	6.0
4	F	240	LEU	5.9
4	F	173	ILE	5.6
4	F	169	LEU	5.6
4	F	320	MET	5.5
4	F	233	PHE	5.4
2	D	245	GLN	5.3
4	F	149	ALA	5.1
4	F	186	LEU	5.0
2	D	393	ALA	4.9
4	F	223	THR	4.9
2	D	217	LEU	4.7
2	D	92	PHE	4.7
1	C	340	SER	4.6
2	D	46	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	84	ILE	4.6
2	D	211	CYS	4.5
2	D	87	PRO	4.4
4	F	178	GLN	4.3
2	D	384	GLN	4.3
2	D	55	THR	4.3
2	D	69	GLU	4.3
4	F	182	ILE	4.3
2	D	59	TYR	4.3
2	D	284	LEU	4.2
2	D	81	PHE	4.2
2	B	276	ARG	4.2
4	F	257	GLU	4.2
4	F	148	ILE	4.2
2	D	396	HIS	4.1
4	F	166	ALA	4.1
4	F	162	ILE	4.1
2	B	275	SER	4.0
2	D	248	ALA	3.9
4	F	236	LYS	3.9
2	D	99	ASN	3.9
2	B	55	THR	3.9
2	D	172	SER	3.9
4	F	172	PHE	3.9
2	D	60	VAL	3.9
2	D	397	TRP	3.9
2	B	279	GLN	3.8
2	D	215	LEU	3.8
2	B	336	LYS	3.8
2	D	170	MET	3.8
4	F	330	ILE	3.8
2	B	278	SER	3.8
2	B	280	GLN	3.7
2	D	1	MET	3.7
1	A	262	TYR	3.7
2	D	389	PHE	3.7
2	D	377	LEU	3.7
2	B	277	GLY	3.7
2	B	246	LEU	3.7
2	B	247	ASN	3.6
2	D	247	ASN	3.6
4	F	253	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	224	SER	3.6
2	D	175	VAL	3.6
3	E	12[A]	ASN	3.5
2	D	49	VAL	3.5
4	F	225	SER	3.5
4	F	228	TYR	3.5
2	D	48	ASN	3.4
2	D	171	PRO	3.4
2	D	246	LEU	3.4
2	D	180	VAL	3.4
4	F	147	TRP	3.4
2	B	274	THR	3.4
2	D	395	LEU	3.4
4	F	243	HIS	3.4
2	B	48	ASN	3.4
4	F	381	HIS	3.4
4	F	237	THR	3.3
4	F	170	LEU	3.3
4	F	199	PHE	3.3
4	F	283	ILE	3.3
2	D	222	TYR	3.3
4	F	100	ILE	3.3
2	D	54	ALA	3.3
3	E	25	LYS	3.3
2	D	408	PHE	3.3
2	D	210	ILE	3.3
2	D	76	VAL	3.2
2	D	80	PRO	3.2
1	A	437	VAL	3.2
2	D	65	LEU	3.2
4	F	221	LEU	3.2
2	D	70	PRO	3.2
1	C	178	SER	3.2
2	D	112	LEU	3.1
4	F	20	LEU	3.1
4	F	241	THR	3.1
2	D	391	ARG	3.1
2	D	30	ILE	3.1
1	A	282	TYR	3.1
4	F	246	GLN	3.1
4	F	103	THR	3.1
2	D	387	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	403	MET	3.1
4	F	238	CYS	3.1
4	F	98	TYR	3.0
4	F	226	GLU	3.0
4	F	133	ALA	3.0
4	F	263	PHE	3.0
3	E	141	GLU	3.0
4	F	101	TYR	3.0
2	D	58	LYS	3.0
2	D	142	GLY	3.0
2	D	381	ILE	3.0
2	D	101	TRP	3.0
2	D	418	LEU	3.0
2	B	58	LYS	3.0
4	F	235	ASP	3.0
2	D	44	LEU	2.9
2	D	405	GLU	2.9
4	F	260	ASN	2.9
2	D	102	ALA	2.9
4	F	181	VAL	2.9
2	D	207	LEU	2.9
4	F	176	GLN	2.9
2	D	67	ASP	2.9
4	F	185	TYR	2.9
2	D	107	THR	2.9
2	D	392	LYS	2.9
3	E	124	GLN	2.9
4	F	372	THR	2.9
2	D	19	LYS	2.9
3	E	6	MET	2.8
2	D	83	GLN	2.8
4	F	163	SER	2.8
2	D	52	ASN	2.8
2	D	177	ASP	2.8
2	D	400	GLY	2.8
1	A	316[A]	CYS	2.8
2	D	97	ALA	2.8
2	B	128	ASP	2.8
2	D	79	GLY	2.8
2	D	72	THR	2.8
2	D	181	GLU	2.8
2	D	2	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	208	TYR	2.8
2	D	176	SER	2.8
4	F	164	SER	2.8
4	F	145	ASN	2.7
2	D	136	THR	2.7
4	F	99	VAL	2.7
4	F	130	VAL	2.7
4	F	189	PRO	2.7
2	D	240	LEU	2.7
2	D	82	GLY	2.7
2	D	321	MET	2.7
4	F	177	GLY	2.7
4	F	262	MET	2.7
4	F	333	ASN	2.7
4	F	231	ALA	2.7
2	D	220	PRO	2.7
4	F	336	PRO	2.7
2	D	356	ILE	2.7
2	D	212	PHE	2.7
4	F	146	VAL	2.7
4	F	132	LEU	2.7
4	F	196	HIS	2.7
4	F	167	SER	2.7
4	F	184	LYS	2.7
4	F	362	ALA	2.7
2	D	320	ARG	2.6
2	D	141	GLY	2.6
3	E	59	GLU	2.6
1	A	96	LYS	2.6
4	F	27	TRP	2.6
4	F	134	ALA	2.6
2	D	300	MET	2.6
2	D	406	MET	2.6
2	B	42	LEU	2.6
2	D	77	ARG	2.6
4	F	31	ARG	2.6
2	D	45	GLU	2.6
4	F	144	GLY	2.6
2	D	179	VAL	2.6
3	E	130	ALA	2.6
4	F	230	SER	2.6
2	D	178	THR	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	1	MET	2.6
2	D	108	GLU	2.6
4	F	102	PRO	2.6
4	F	321	VAL	2.6
2	D	85	PHE	2.6
2	D	218	THR	2.6
2	D	106	TYR	2.6
4	F	280	GLU	2.6
4	F	254	GLY	2.6
2	D	419	VAL	2.6
4	F	17	VAL	2.6
4	F	234	GLN	2.6
2	D	86	ARG	2.5
2	D	32	PRO	2.5
2	D	399	THR	2.5
2	D	130	LEU	2.5
4	F	135	TYR	2.5
4	F	258	GLU	2.5
1	C	342	GLN	2.5
2	D	202	ILE	2.5
3	E	44	ASP	2.5
4	F	192	LEU	2.5
2	B	245	GLN	2.5
2	D	227	HIS	2.5
4	F	384	HIS	2.5
2	D	407	GLU	2.5
4	F	256	TYR	2.5
4	F	341	LYS	2.4
2	D	173	PRO	2.4
2	D	385	PHE	2.4
2	D	219	THR	2.4
4	F	376	ILE	2.4
4	F	180	HIS	2.4
2	B	281	TYR	2.4
2	D	390	ARG	2.4
4	F	242	ASN	2.4
4	F	252	ASN	2.4
4	F	316	GLY	2.4
2	B	54	ALA	2.4
2	B	428	ALA	2.4
2	D	213	ARG	2.4
4	F	342	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	15	THR	2.4
2	D	37	HIS	2.4
2	B	45	GLU	2.4
2	D	73	MET	2.4
2	D	323	MET	2.4
2	D	286	VAL	2.4
4	F	190	LEU	2.3
2	D	386	THR	2.3
2	D	75	SER	2.3
4	F	198	LYS	2.3
4	F	247	LYS	2.3
2	D	96	GLY	2.3
2	D	167	PHE	2.3
4	F	245	ILE	2.3
2	D	376	GLU	2.3
2	D	115	SER	2.3
4	F	171	ASP	2.3
2	D	71	GLY	2.3
2	D	303	CYS	2.3
2	B	333	VAL	2.3
2	B	273	LEU	2.3
2	D	42	LEU	2.3
4	F	191	LEU	2.3
2	B	218	THR	2.3
2	D	216	LYS	2.3
2	D	226	ASN	2.3
2	D	95	SER	2.3
2	B	215	LEU	2.3
2	D	204	ASN	2.3
2	D	94	GLN	2.3
4	F	382	HIS	2.2
2	B	323	MET	2.2
1	A	113	GLU	2.2
3	E	48	GLU	2.2
3	E	131	GLU	2.2
1	C	357	TYR	2.2
2	D	100	ASN	2.2
2	D	165	ASN	2.2
4	F	229	ASN	2.2
4	F	138	ARG	2.2
2	B	291	GLN	2.2
2	D	126	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	174	LYS	2.2
3	E	7	GLU	2.2
1	C	128	GLN	2.2
1	C	440	VAL	2.2
4	F	92	THR	2.2
2	D	380	ARG	2.2
1	C	46	ASP	2.2
2	D	93	GLY	2.2
2	D	151	LEU	2.2
2	D	388	MET	2.2
2	D	221	THR	2.2
1	C	347[A]	CYS	2.2
1	A	88	HIS	2.2
1	C	283	HIS	2.1
2	D	113	VAL	2.1
2	D	378	PHE	2.1
2	B	239	CYS	2.1
2	D	267	MET	2.1
2	B	227	HIS	2.1
2	D	64	ILE	2.1
4	F	383	HIS	2.1
2	D	91	VAL	2.1
2	D	128	ASP	2.1
2	B	338	SER	2.1
4	F	261	GLU	2.1
2	B	320	ARG	2.1
4	F	275	LEU	2.1
2	D	416	ASN	2.1
2	D	51	TYR	2.1
4	F	13	VAL	2.1
1	C	337	THR	2.1
2	D	214	THR	2.1
2	D	187	LEU	2.1
2	D	331	LEU	2.1
2	B	57	ASN	2.1
2	D	57	ASN	2.1
2	D	239	CYS	2.1
2	D	244	GLY	2.1
4	F	57	GLY	2.1
2	D	183	TYR	2.1
2	D	374	ILE	2.1
4	F	327	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	212	PHE	2.1
2	D	18	ALA	2.0
4	F	265	GLU	2.0
2	B	219	THR	2.0
2	D	61	PRO	2.0
4	F	194	PRO	2.0
4	F	239	HIS	2.0
2	B	208	TYR	2.0
2	D	422	TYR	2.0
2	B	46	ARG	2.0
2	B	282	ARG	2.0
4	F	222	ARG	2.0
2	D	53	GLU	2.0
2	D	203	ASP	2.0
3	E	10	GLU	2.0
4	F	324	GLU	2.0
3	E	140	LYS	2.0
4	F	82	LYS	2.0
2	B	126	SER	2.0
2	D	361	LEU	2.0
2	D	16	ILE	2.0
2	D	229	VAL	2.0
4	F	142	ARG	2.0
4	F	179	VAL	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](#)

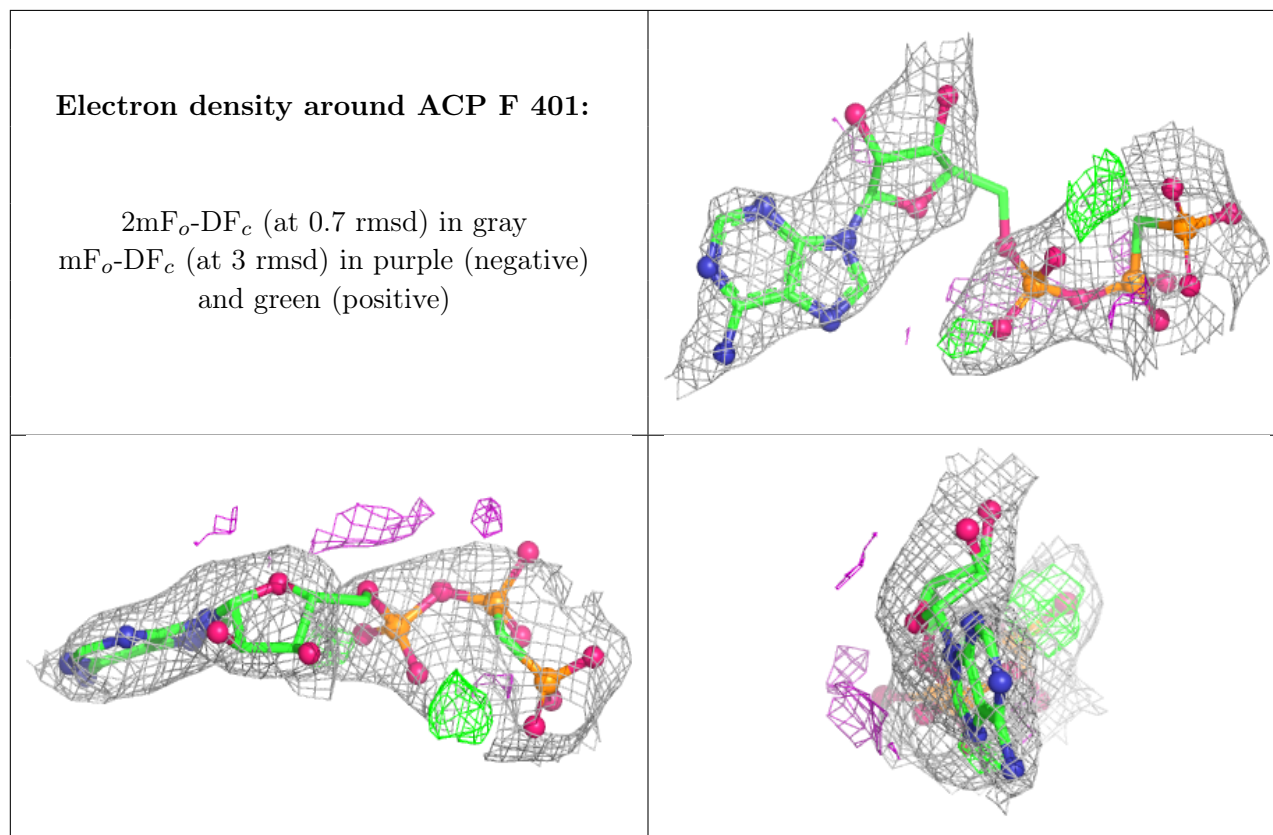
There are no oligosaccharides in this entry.

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.

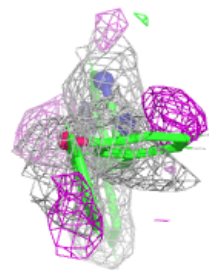
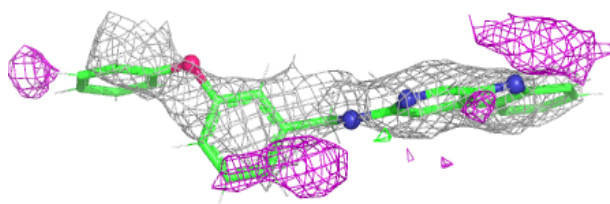
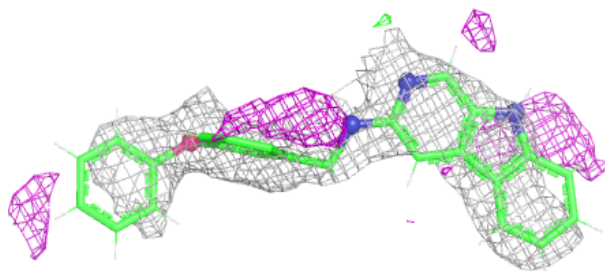
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	503	1/1	0.64	0.19	107,107,107,107	0
12	ACP	F	401	31/31	0.75	0.18	82,103,128,130	0
11	AEU	D	502	28/28	0.81	0.25	59,79,101,112	0
5	GTP	D	501	32/32	0.87	0.17	56,68,95,136	0
8	GOL	A	504	6/6	0.89	0.17	33,50,63,75	0
10	MES	B	503	12/12	0.90	0.13	30,43,61,85	0
11	AEU	B	504	28/28	0.93	0.09	24,31,39,46	0
9	GDP	B	501	28/28	0.95	0.10	12,25,30,36	0
5	GTP	A	501	32/32	0.96	0.08	16,24,30,32	0
5	GTP	C	501	32/32	0.97	0.07	13,21,28,33	0
6	MG	B	502	1/1	0.98	0.06	23,23,23,23	0
7	CA	A	503	1/1	0.99	0.06	53,53,53,53	0
7	CA	C	503	1/1	0.99	0.03	33,33,33,33	0
6	MG	C	502	1/1	0.99	0.04	23,23,23,23	0
6	MG	A	502	1/1	0.99	0.05	21,21,21,21	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.

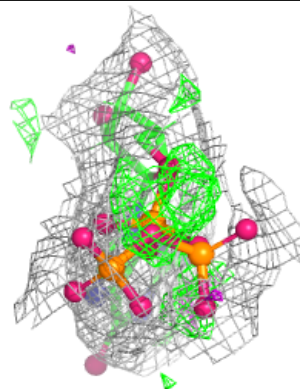
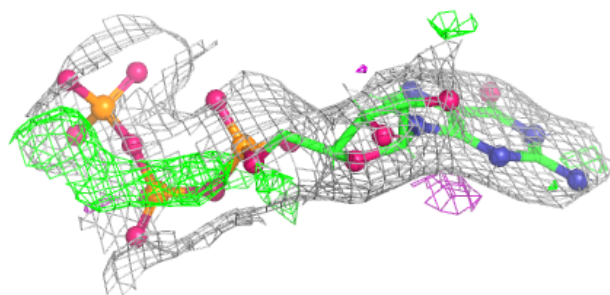
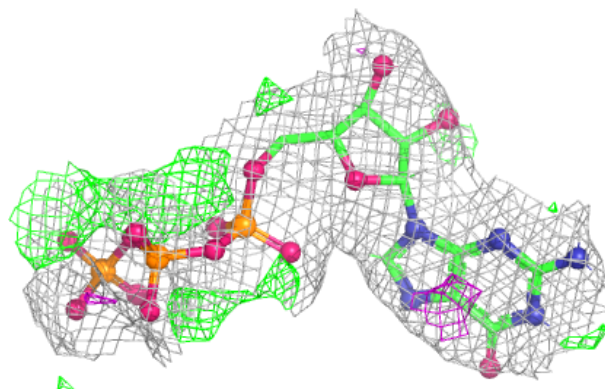


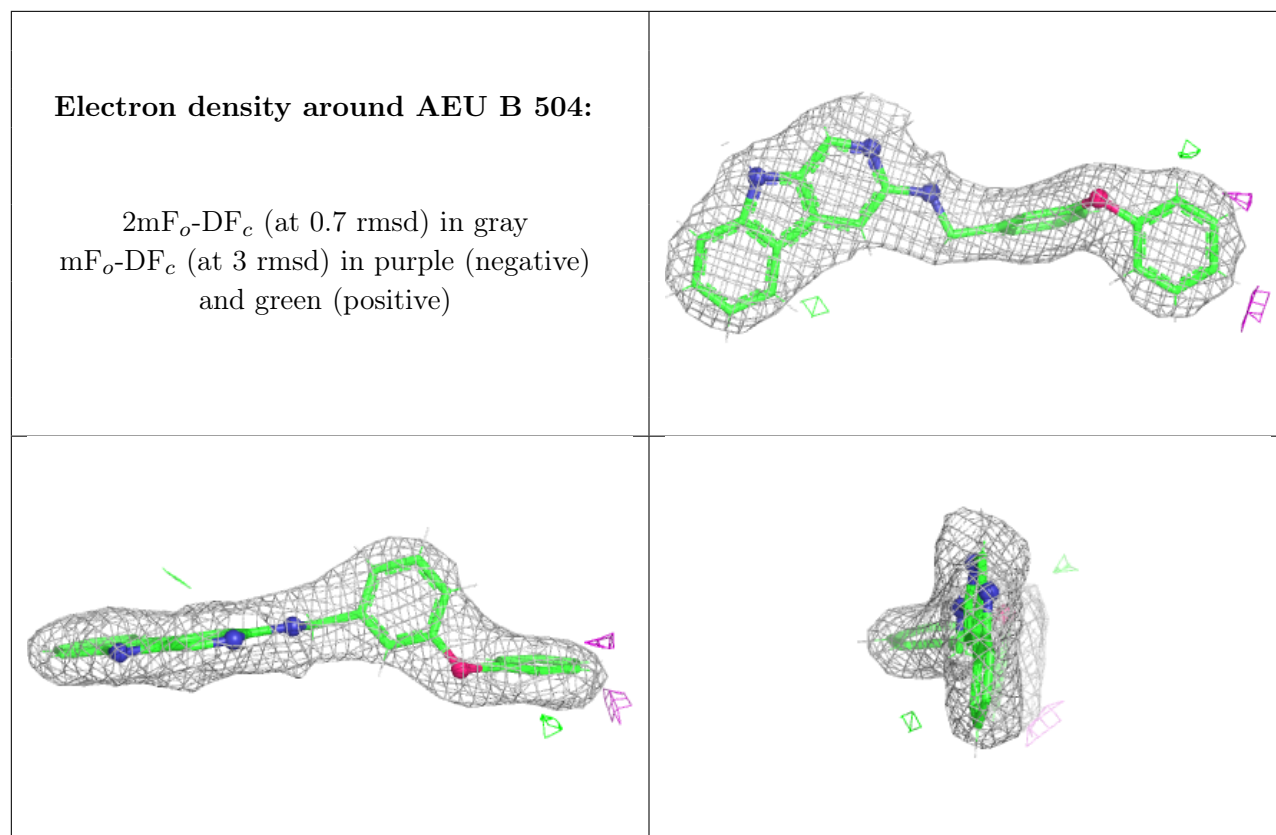
Electron density around AEU D 502:

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

**Electron density around GTP D 501:**

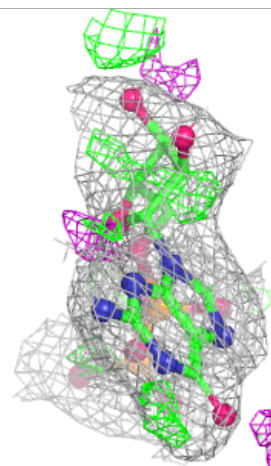
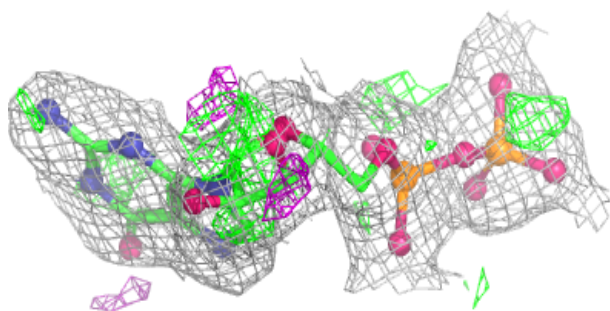
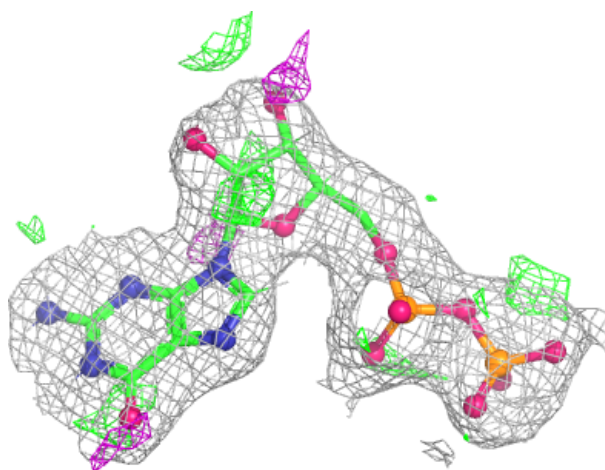
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





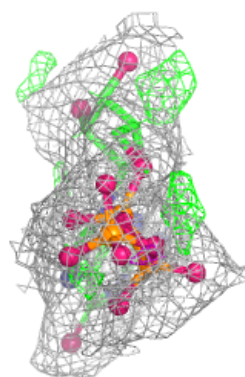
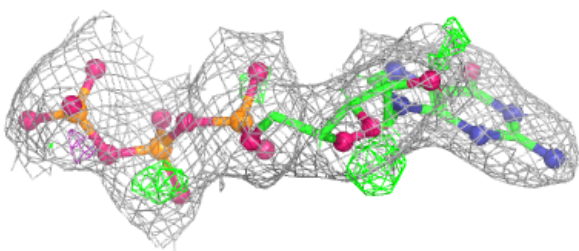
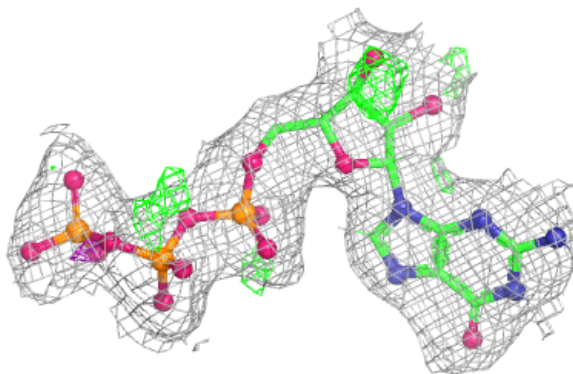
Electron density around GDP B 501:

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

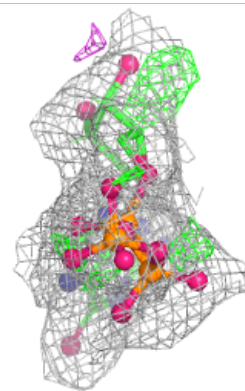
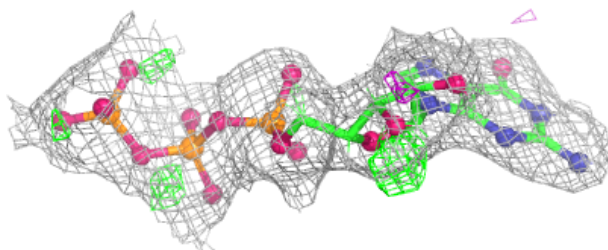
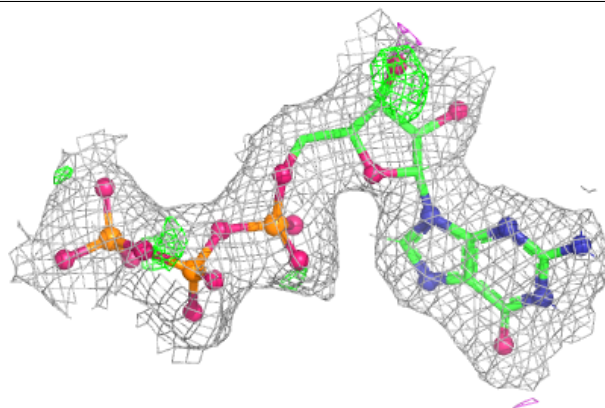


Electron density around GTP A 501:

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

**Electron density around 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.