Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 04:46 am BST

PDB ID	:	6S9E / pdb_00006s9e
Title	:	Tubulin-GDP.AlF complex
Authors	:	Oliva, M.A.; Estevez-Gallego, J.; Diaz, J.F.; Prota, A.E.; Steinmetz, M.O.; Balaguer, F.A.; Lucena-Agell, D.
Deposited on	:	2019-07-12
Resolution	:	2.25 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

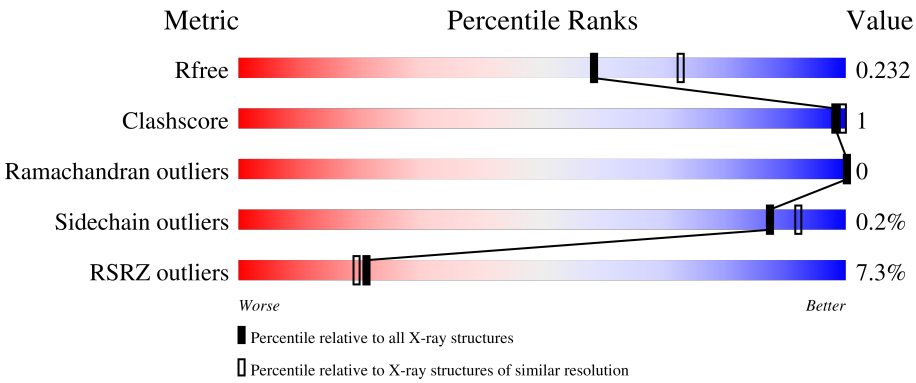
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	440	4% 97%
1	C	440	5% 97%
2	B	445	5% 93% 5%
2	D	445	8% 94% 5%
3	E	189	7% 63% 37%

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Mol	Chain	Length	Quality of chain
4	F	378	12% 84% 16%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 34744 atoms, of which 17043 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	435	6789	2172	3361	580	651	25	0	7	0
1	C	440	6926	2216	3430	589	665	26	0	13	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	423	6627	2119	3258	573	651	26	0	8	0
2	D	423	6591	2107	3238	567	651	28	0	6	0

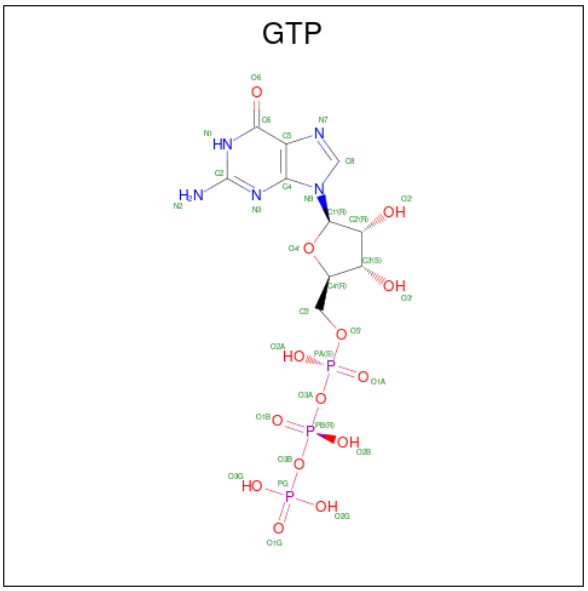
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	120	2064	631	1044	184	199	6	0	5	0

- Molecule 4 is a protein called Tubulin Tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	319	5207	1686	2594	437	475	15	0	1	0

- 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
			Total	C	H	N	O	P		
5	A	1	41	10	9	5	14	3	0	0
5	C	1	41	10	9	5	14	3	0	0

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

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

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

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

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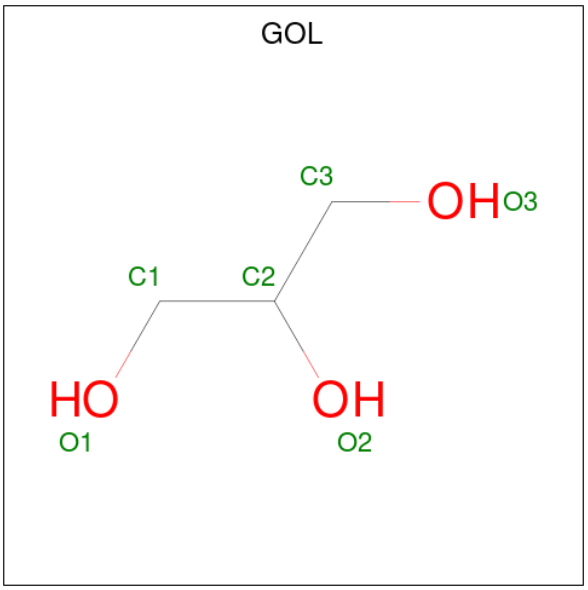
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	C	1	1	1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

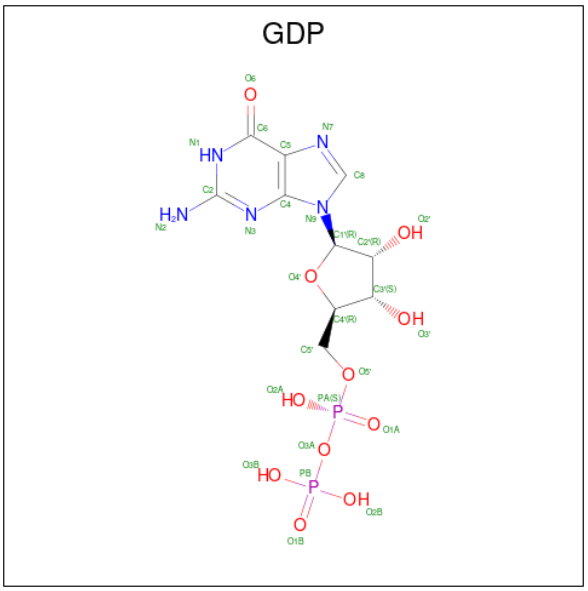
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	1	1	1	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



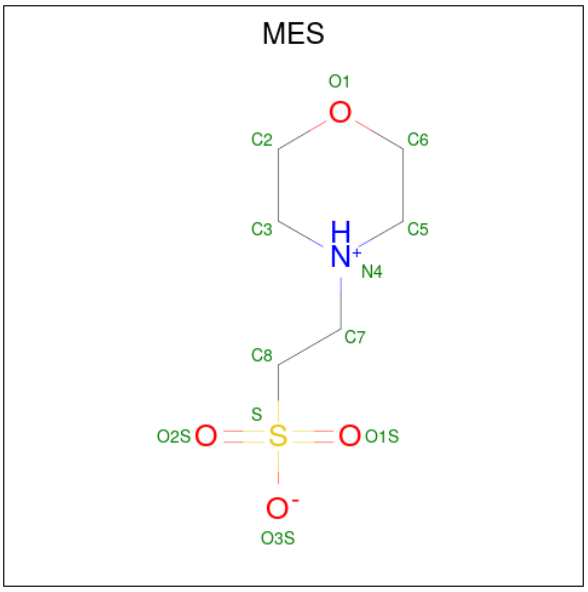
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	A	1	14	3	8	3	0	0
			Total	C	H	O		
9	A	1	14	3	8	3	0	0
			Total	C	H	O		
9	A	1	14	3	8	3	0	0
			Total	C	H	O		
9	B	1	12	3	6	3	0	0
			Total	C	H	O		
9	B	1	13	3	7	3	0	0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
10	B	1	37	10	9	5	11	2	0	0
			Total	C	H	N	O	P		
10	D	1	37	10	9	5	11	2	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

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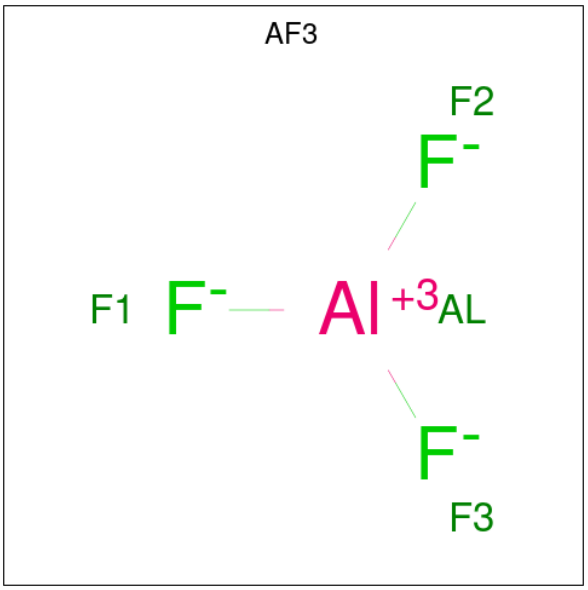
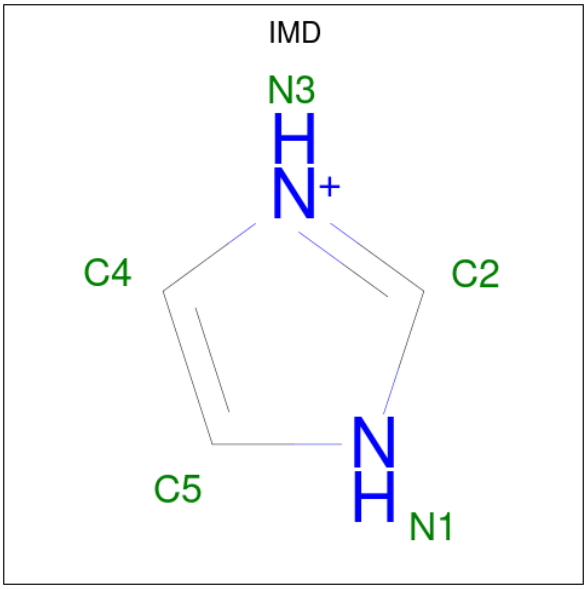
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
11	B	1	25	6	13	1	4	1	0	0

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



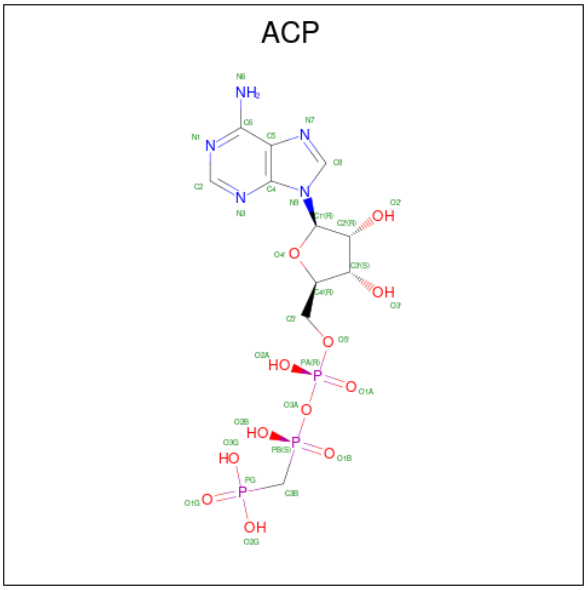
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
12	B	1	4	1	3	0	0

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



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

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
14	F	1	45	11	14	5	12	3	0	0

- Molecule 15 is water.

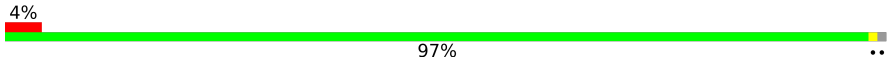
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	39	39	39	0	0
15	B	40	40	40	0	0
15	C	99	99	99	0	0
15	D	14	14	14	0	0
15	E	4	4	4	0	0
15	F	3	3	3	0	0

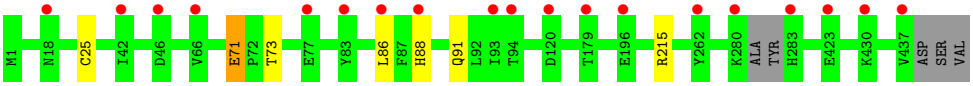
3 Residue-property plots (i)

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

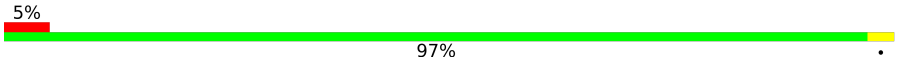
Chain A:

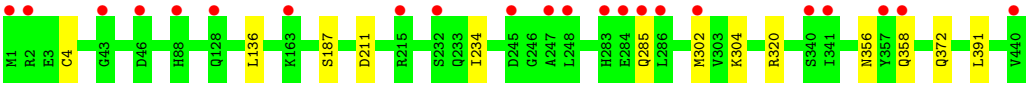




- Molecule 1: Tubulin alpha-1B chain

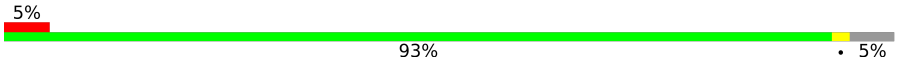
Chain C:

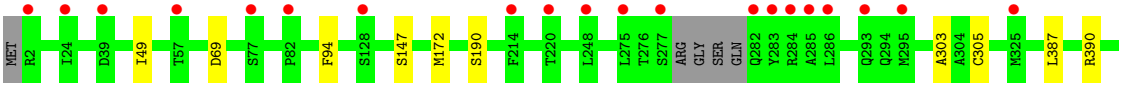


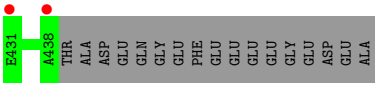


- Molecule 2: Tubulin beta-2B chain

Chain B:

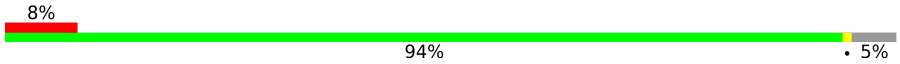


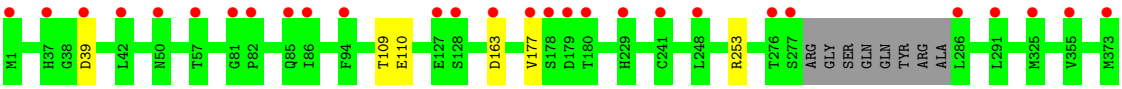


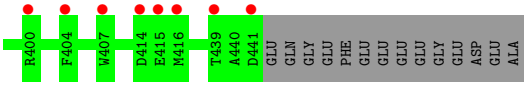


- Molecule 2: Tubulin beta-2B chain

Chain D:

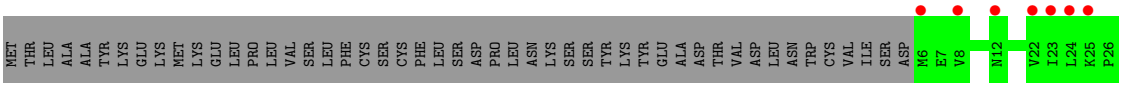


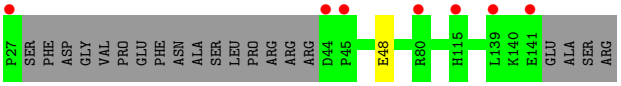




- Molecule 3: Stathmin-4

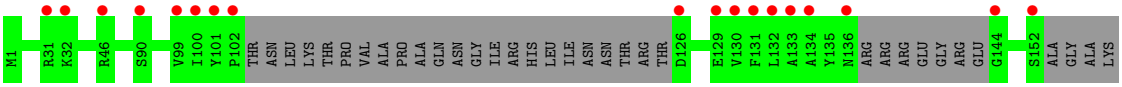
Chain E:

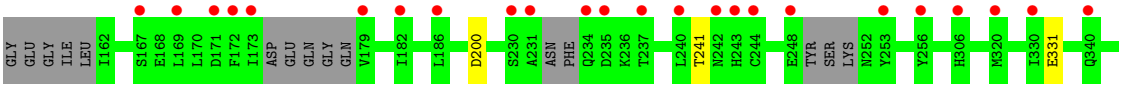


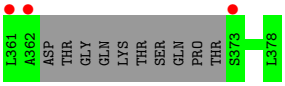


- Molecule 4: Tubulin Tyrosine ligase

Chain F:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.00Å 157.36Å 180.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.25 48.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.00-2.25) 98.8 (48.00-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.203 , 0.228 0.207 , 0.232	Depositor DCC
R_{free} test set	6925 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34744	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ACP, IMD, AF3, GDP, MES, CA, CL, GOL, MG, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.11	0/3525	0.27	0/4783
1	C	0.12	0/3614	0.29	0/4909
2	B	0.11	0/3474	0.27	0/4705
2	D	0.10	0/3439	0.26	0/4660
3	E	0.10	0/1043	0.20	0/1384
4	F	0.10	0/2672	0.26	0/3606
All	All	0.11	0/17767	0.27	0/24047

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	3361	3360	3	0
1	C	3496	3430	3430	7	0
2	B	3369	3258	3249	5	0
2	D	3353	3238	3228	4	0
3	E	1020	1044	1048	1	0
4	F	2613	2594	2594	1	0
5	A	32	9	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	9	12	0	0
6	A	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
6	F	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	A	1	0	0	0	0
9	A	18	24	24	0	0
9	B	12	13	16	0	0
10	B	28	9	12	0	0
10	D	28	9	12	0	0
11	B	24	26	26	0	0
12	B	4	0	0	0	0
13	C	5	5	5	0	0
14	F	31	14	13	0	0
15	A	39	0	0	0	0
15	B	40	0	0	1	0
15	C	99	0	0	0	0
15	D	14	0	0	0	0
15	E	4	0	0	0	0
15	F	3	0	0	0	0
All	All	17701	17043	17041	21	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 (21) 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)
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.42	0.65
1:A:88:HIS:N	1:A:91:GLN:OE1	2.35	0.58
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.24	0.52
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.43	0.51
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.52	0.49
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.39	0.49
3:E:48:GLU:OE1	3:E:48:GLU:N	2.46	0.49
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.33	0.47
2:D:163:ASP:O	2:D:253:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.56	0.45
2:B:390:ARG:NH1	15:B:609:HOH:O	2.48	0.44
2:D:39:ASP:OD1	2:D:39:ASP:N	2.51	0.43
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.43
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.01	0.43
1:C:234:ILE:HD13	1:C:302[B]:MET:SD	2.60	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.20	0.42
2:B:303:ALA:O	2:B:305:CYS:N	2.49	0.42
2:B:172:MET:HG3	2:B:387:LEU:HD21	2.03	0.41
2:D:177:VAL:HG12	2:D:177:VAL:O	2.21	0.41
1:C:356[B]:ASN:ND2	1:C:358[B]:GLN:OE1	2.55	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	438/440 (100%)	431 (98%)	7 (2%)	0	100	100
1	C	451/440 (102%)	441 (98%)	10 (2%)	0	100	100
2	B	427/445 (96%)	417 (98%)	10 (2%)	0	100	100
2	D	425/445 (96%)	415 (98%)	10 (2%)	0	100	100
3	E	121/189 (64%)	120 (99%)	1 (1%)	0	100	100
4	F	304/378 (80%)	295 (97%)	9 (3%)	0	100	100
All	All	2166/2337 (93%)	2119 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/371 (101%)	372 (100%)	2 (0%)	81	87
1	C	384/371 (104%)	384 (100%)	0	100	100
2	B	374/383 (98%)	373 (100%)	1 (0%)	86	90
2	D	372/383 (97%)	372 (100%)	0	100	100
3	E	113/171 (66%)	113 (100%)	0	100	100
4	F	289/336 (86%)	288 (100%)	1 (0%)	86	90
All	All	1906/2015 (95%)	1902 (100%)	4 (0%)	87	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	215	ARG
2	B	49	ILE
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	HIS
2	B	331	GLN
2	B	339	ASN
2	B	349	ASN
2	B	385	GLN
2	B	436	GLN
1	C	393	HIS
2	D	101	ASN
2	D	331	GLN
3	E	64	GLN
3	E	136	ASN
4	F	239	HIS
4	F	243	HIS

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 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 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	MES	B	505	-	12,12,12	2.29	1 (8%)	14,16,16	1.44	3 (21%)
9	GOL	A	505	-	5,5,5	0.90	0	5,5,5	0.99	0
10	GDP	D	501	6	28,30,30	1.15	3 (10%)	44,47,47	1.74	6 (13%)
14	ACP	F	501	6	30,33,33	3.02	10 (33%)	45,52,52	1.94	13 (28%)
5	GTP	C	501	6	30,34,34	0.82	1 (3%)	46,54,54	1.61	10 (21%)
5	GTP	A	501	6	30,34,34	0.82	1 (3%)	46,54,54	1.65	10 (21%)
12	AF3	B	507	-	0,3,3	-	-	-		
9	GOL	B	508	-	5,5,5	0.92	0	5,5,5	0.93	0
11	MES	B	504	-	12,12,12	2.23	1 (8%)	14,16,16	1.46	4 (28%)
10	GDP	B	501	6	28,30,30	1.18	3 (10%)	44,47,47	1.61	6 (13%)
13	IMD	C	504	-	5,5,5	0.67	0	5,5,5	0.41	0
9	GOL	B	506	-	5,5,5	0.93	0	5,5,5	0.94	0
9	GOL	A	506	-	5,5,5	0.89	0	5,5,5	0.99	0
9	GOL	A	507	-	5,5,5	0.91	0	5,5,5	1.00	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
11	MES	B	505	-	-	1/6/14/14	0/1/1/1
9	GOL	A	505	-	-	0/4/4/4	-
10	GDP	D	501	6	-	4/16/32/32	0/3/3/3
14	ACP	F	501	6	-	3/19/38/38	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
9	GOL	B	508	-	-	0/4/4/4	-
11	MES	B	504	-	-	3/6/14/14	0/1/1/1
10	GDP	B	501	6	-	4/16/32/32	0/3/3/3
13	IMD	C	504	-	-	-	0/1/1/1
9	GOL	B	506	-	-	1/4/4/4	-
9	GOL	A	506	-	-	0/4/4/4	-
9	GOL	A	507	-	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	501	ACP	O4'-C1'	8.61	1.62	1.42
11	B	505	MES	C8-S	-7.67	1.66	1.77
11	B	504	MES	C8-S	-7.46	1.66	1.77
14	F	501	ACP	C6-N6	6.35	1.50	1.34
14	F	501	ACP	C2'-C1'	-6.14	1.33	1.53
14	F	501	ACP	O4'-C4'	-5.69	1.32	1.45
14	F	501	ACP	PB-O2B	-4.27	1.46	1.56
14	F	501	ACP	O3'-C3'	-3.50	1.34	1.43
14	F	501	ACP	PB-O3A	3.45	1.62	1.58
10	D	501	GDP	C5-C4	3.07	1.47	1.38
10	B	501	GDP	C6-N1	-2.98	1.33	1.38
14	F	501	ACP	PA-O5'	2.96	1.71	1.59
10	B	501	GDP	C5-C4	2.95	1.46	1.38
10	D	501	GDP	C6-N1	-2.66	1.33	1.38
14	F	501	ACP	C8-N7	2.33	1.36	1.31
10	B	501	GDP	C5-N7	-2.27	1.34	1.39
14	F	501	ACP	PG-O2G	-2.26	1.49	1.54
10	D	501	GDP	C5-N7	-2.22	1.34	1.39
5	C	501	GTP	C2-N3	2.20	1.38	1.33
5	A	501	GTP	C2-N3	2.09	1.38	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	501	GDP	C5-C4-N3	-5.66	119.28	128.46
14	F	501	ACP	N3-C2-N1	-5.54	119.93	128.60
10	B	501	GDP	C5-C4-N3	-5.02	120.31	128.46
14	F	501	ACP	C5-C4-N3	-5.01	120.22	126.75
5	A	501	GTP	C5-C4-N3	-4.71	120.82	128.46
5	C	501	GTP	C5-C4-N3	-4.70	120.84	128.46
10	D	501	GDP	C2-N3-C4	4.64	120.56	112.30
5	A	501	GTP	C2-N3-C4	4.45	120.23	112.30
10	D	501	GDP	N9-C4-N3	4.43	134.84	125.94
10	B	501	GDP	C2-N3-C4	4.34	120.03	112.30
14	F	501	ACP	N9-C8-N7	-4.33	107.99	113.91
5	C	501	GTP	C2-N3-C4	4.30	119.95	112.30
10	B	501	GDP	N9-C4-N3	3.95	133.87	125.94
10	B	501	GDP	C6-C5-N7	3.49	136.74	130.25
14	F	501	ACP	C2-N3-C4	3.41	119.82	111.75
5	C	501	GTP	PB-O3B-PG	-3.31	121.45	132.83
14	F	501	ACP	N6-C6-N1	-3.29	111.14	118.35
10	D	501	GDP	C6-C5-N7	3.25	136.30	130.25
14	F	501	ACP	C5-N7-C8	3.19	108.04	103.51
5	A	501	GTP	PA-O3A-PB	-3.13	122.07	132.83
5	A	501	GTP	PB-O3B-PG	-3.12	122.11	132.83
10	D	501	GDP	PA-O3A-PB	-3.10	122.20	132.83
5	C	501	GTP	N9-C4-N3	3.06	132.09	125.94
5	A	501	GTP	N9-C4-N3	2.87	131.70	125.94
14	F	501	ACP	N3-C4-N9	2.83	131.74	127.08
11	B	504	MES	C5-N4-C3	2.80	115.12	108.83
10	B	501	GDP	PA-O3A-PB	-2.72	123.49	132.83
11	B	505	MES	C5-N4-C3	2.71	114.92	108.83
14	F	501	ACP	C5-C6-N6	2.68	129.25	123.43
5	A	501	GTP	N9-C8-N7	-2.61	108.47	113.39
14	F	501	ACP	PB-O3A-PA	-2.61	124.30	132.56
5	C	501	GTP	N9-C8-N7	-2.59	108.51	113.39
5	A	501	GTP	C2-N1-C6	-2.58	120.39	125.10
5	C	501	GTP	C2-N1-C6	-2.49	120.55	125.10
5	A	501	GTP	C8-N7-C5	2.40	108.58	104.24
10	D	501	GDP	C4-C5-N7	-2.39	106.94	110.72
11	B	504	MES	O1S-S-C8	2.38	109.78	106.92
5	A	501	GTP	C5-C6-N1	2.37	119.22	113.19
5	C	501	GTP	C5-C6-N1	2.37	119.22	113.19
5	C	501	GTP	C8-N7-C5	2.37	108.53	104.24
5	C	501	GTP	PA-O3A-PB	-2.33	124.84	132.83
5	C	501	GTP	O6-C6-C5	-2.29	120.52	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	GTP	O6-C6-C5	-2.25	120.63	126.60
14	F	501	ACP	C4-C5-N7	-2.23	107.91	110.62
11	B	505	MES	O3S-S-C8	2.21	109.34	105.77
10	B	501	GDP	C4-C5-N7	-2.20	107.24	110.72
11	B	504	MES	O3S-S-C8	2.16	109.27	105.77
14	F	501	ACP	C3'-C2'-C1'	2.14	105.49	101.43
14	F	501	ACP	C4-N9-C8	2.12	108.02	105.73
11	B	505	MES	O1S-S-C8	2.09	109.43	106.92
11	B	504	MES	O2S-S-C8	2.05	109.38	106.92
14	F	501	ACP	C6-C5-C4	2.04	119.92	117.18

There are no chirality outliers.

All (30) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O2A
14	F	501	ACP	C5'-O5'-PA-O1A
14	F	501	ACP	O4'-C4'-C5'-O5'
9	B	506	GOL	O1-C1-C2-C3
11	B	504	MES	C8-C7-N4-C3
11	B	504	MES	C8-C7-N4-C5
10	B	501	GDP	PB-O3A-PA-O2A
11	B	505	MES	C8-C7-N4-C5
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O3A
14	F	501	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C4'-C5'-O5'-PA

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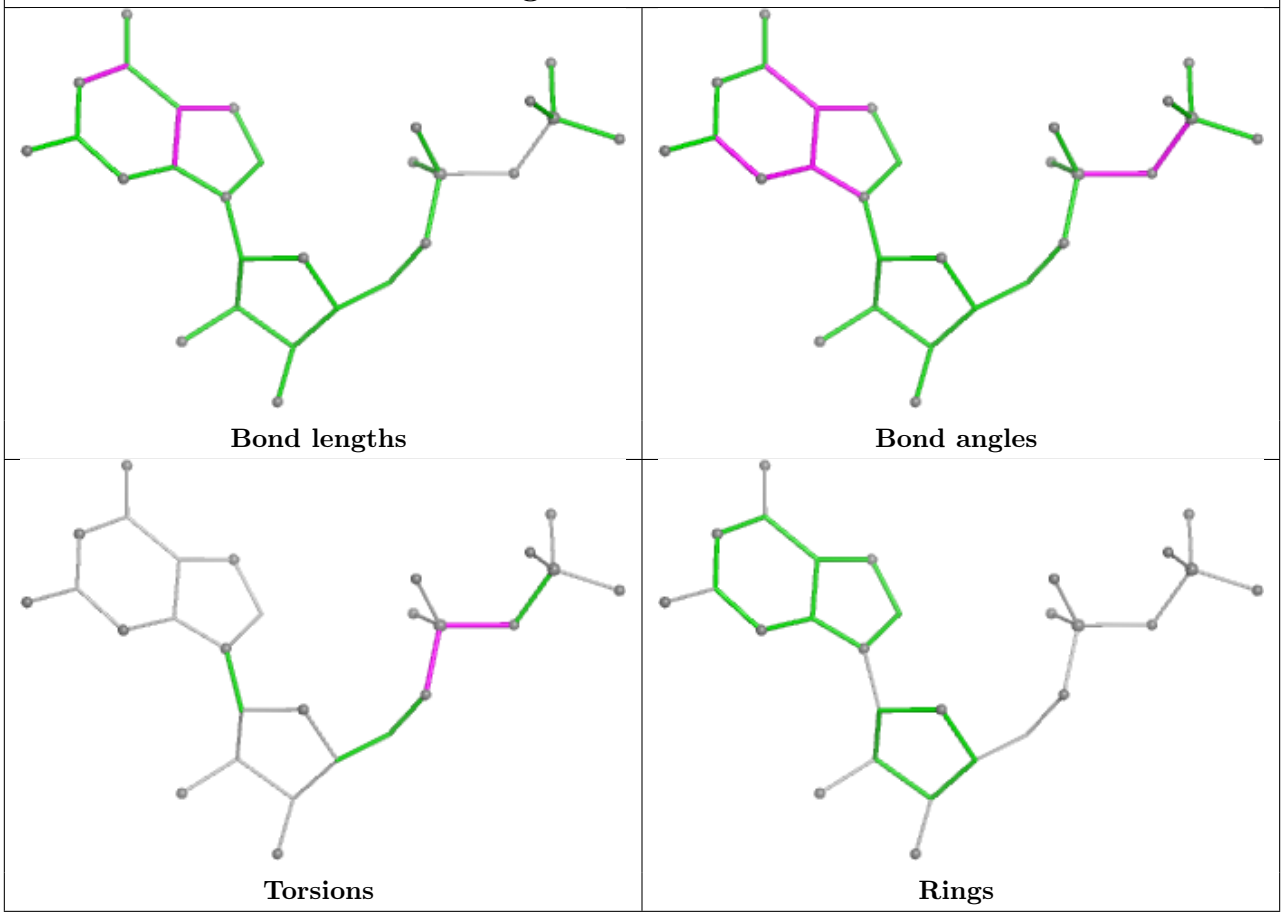
Mol	Chain	Res	Type	Atoms
10	D	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
11	B	504	MES	C7-C8-S-O1S

There are no ring outliers.

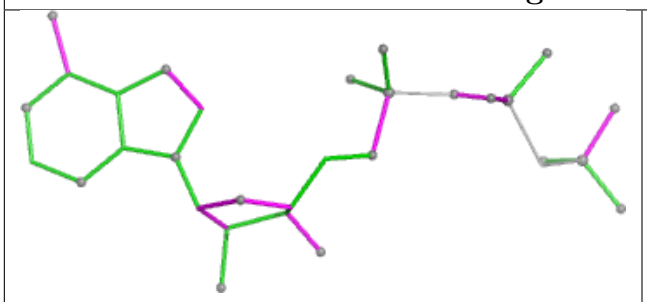
No monomer is involved in short contacts.

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 then 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.

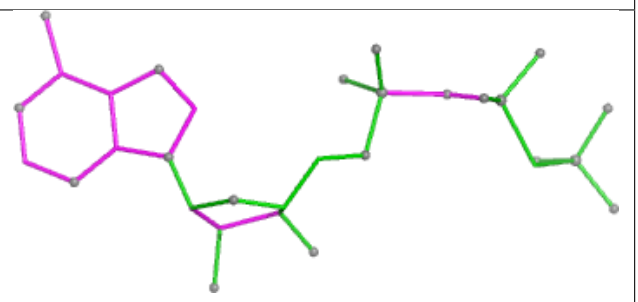
Ligand GDP D 501



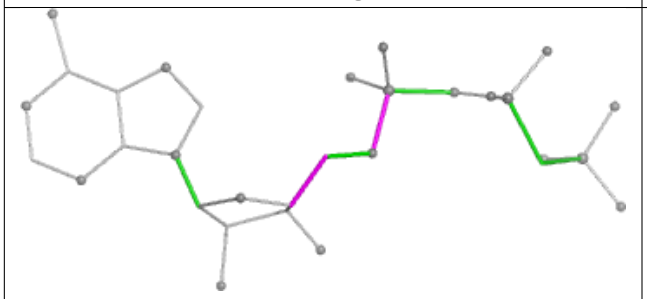
Ligand ACP F 501



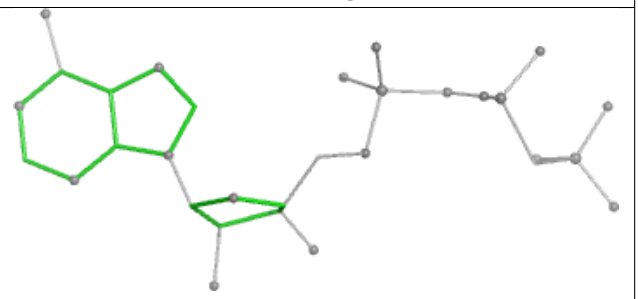
Bond lengths



Bond angles

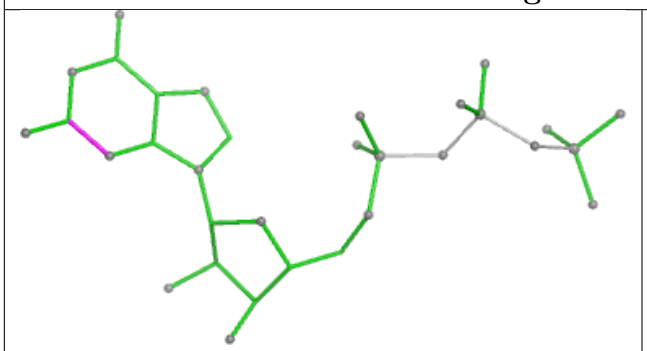


Torsions



Rings

Ligand GTP C 501



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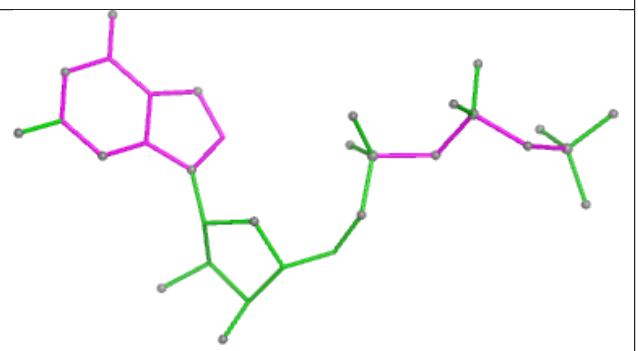
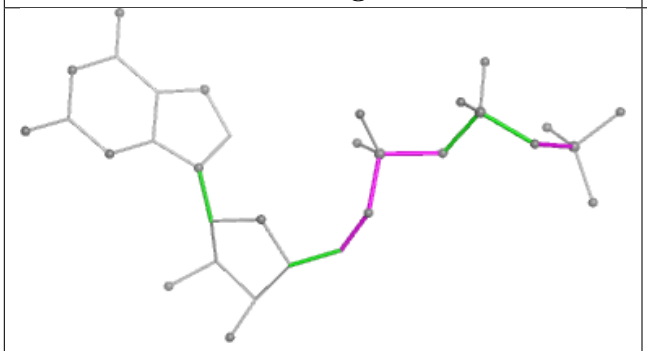
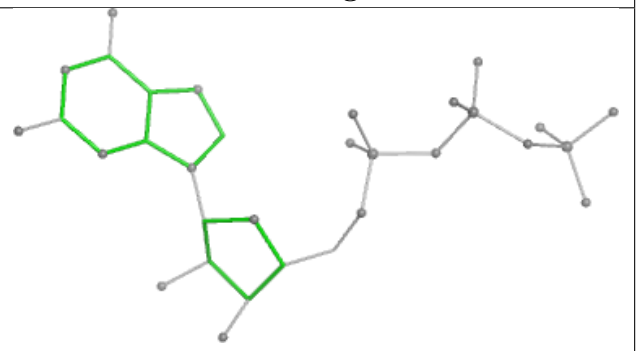


Bond angles

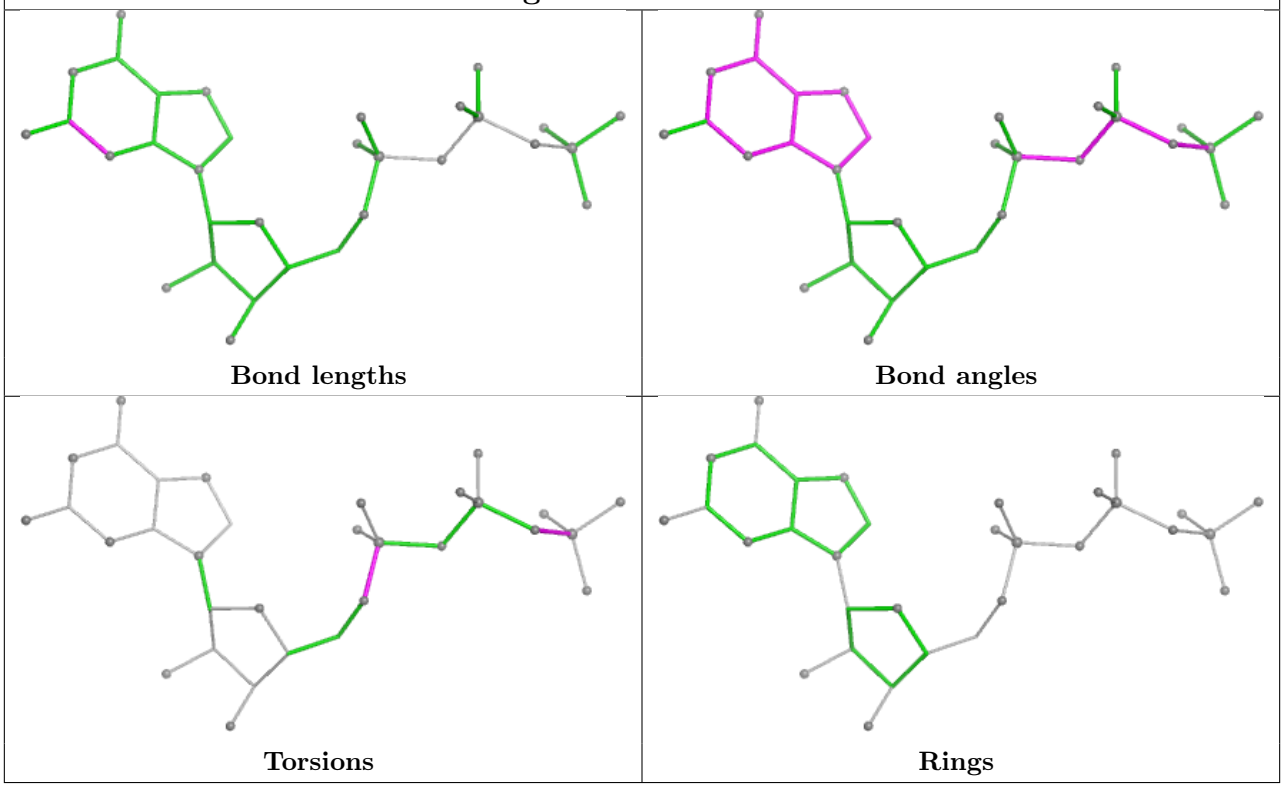


Torsions

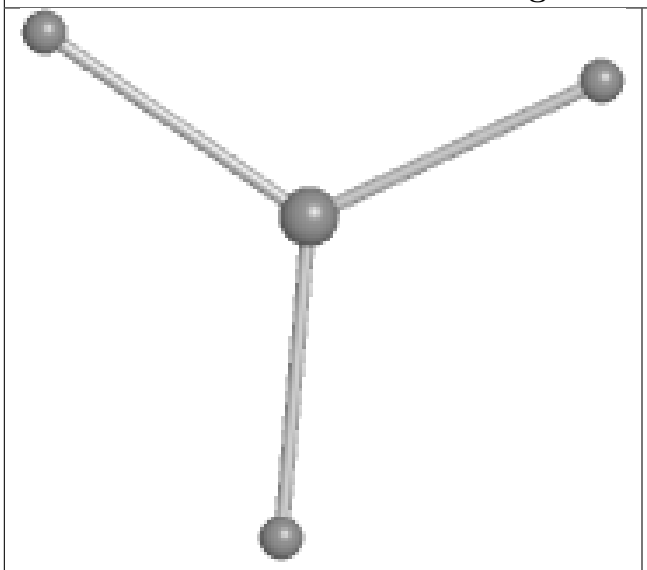


Rings

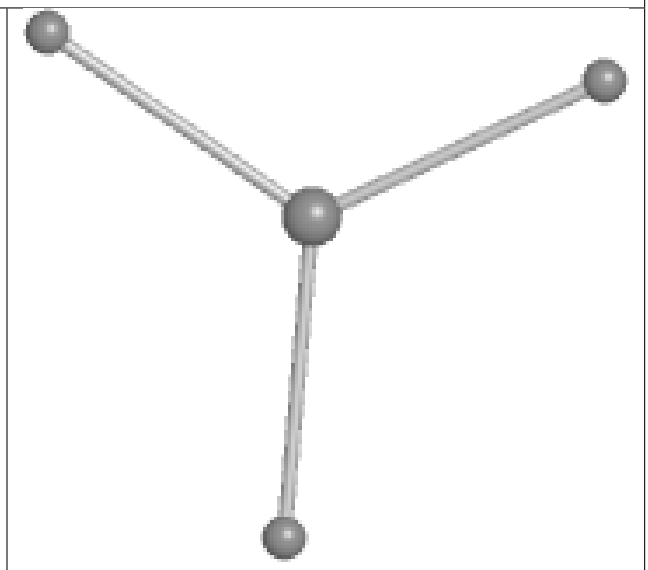
Ligand GTP A 501



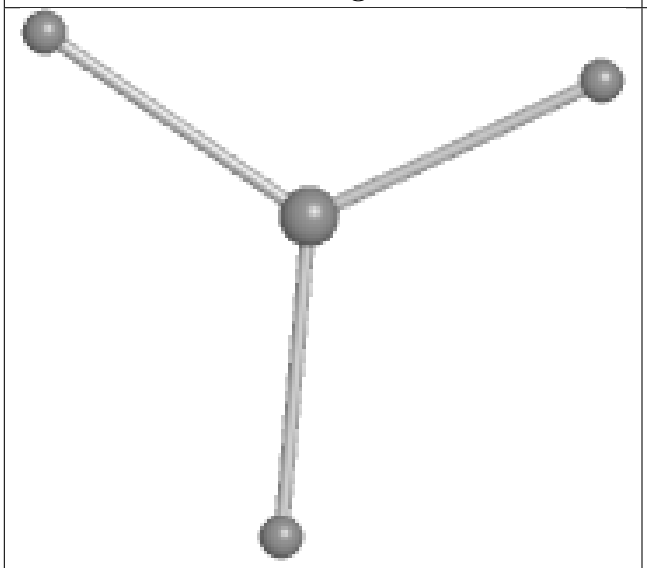
Ligand AF3 B 507



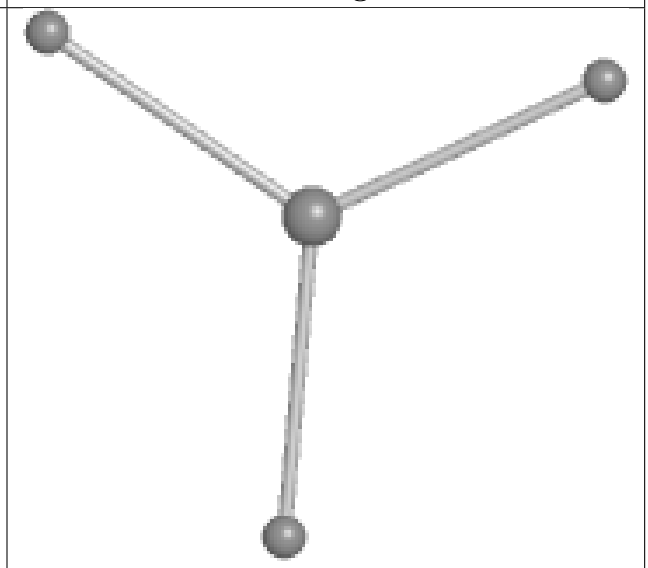
Bond lengths



Bond angles

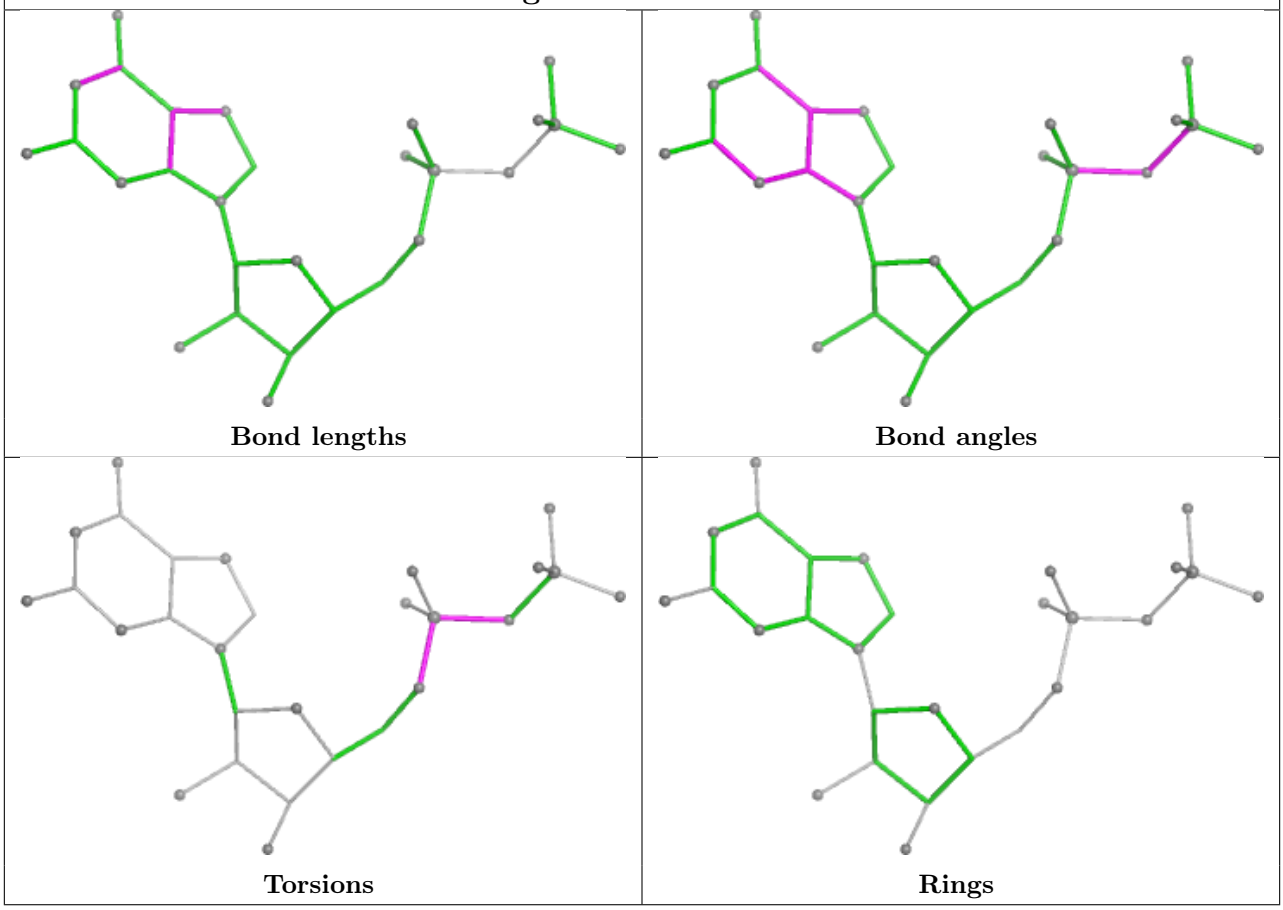


Torsions



Rings

Ligand GDP B 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 (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	435/440 (98%)	0.49	19 (4%)	39	38	26, 62, 92, 112	7 (1%)
1	C	440/440 (100%)	0.33	22 (5%)	34	33	23, 49, 78, 106	13 (2%)
2	B	423/445 (95%)	0.50	22 (5%)	33	31	23, 58, 95, 139	9 (2%)
2	D	423/445 (95%)	0.74	36 (8%)	16	15	32, 68, 102, 139	10 (2%)
3	E	120/189 (63%)	0.91	14 (11%)	9	9	31, 75, 109, 119	5 (4%)
4	F	319/378 (84%)	0.96	45 (14%)	6	5	36, 82, 131, 152	1 (0%)
All	All	2160/2337 (92%)	0.60	158 (7%)	21	19	23, 63, 105, 152	45 (2%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	6.2
4	F	152	SER	5.3
2	B	277	SER	5.2
1	C	340	SER	5.1
2	D	179[A]	ASP	4.9
4	F	179	VAL	4.8
4	F	130	VAL	4.7
1	C	1	MET	4.7
1	A	262	TYR	4.6
4	F	173	ILE	4.6
1	C	440	VAL	4.5
2	B	438	ALA	4.5
4	F	362	ALA	4.5
2	D	1	MET	4.4
4	F	102	PRO	4.4
4	F	240	LEU	4.4
1	A	283	HIS	4.3
4	F	231	ALA	4.3
1	C	357	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	284	GLU	4.2
4	F	172	PHE	4.2
2	D	286	LEU	4.1
4	F	136	ASN	3.8
4	F	129	GLU	3.7
2	D	81	GLY	3.7
1	C	285	GLN	3.6
4	F	248	GLU	3.6
1	C	245	ASP	3.5
4	F	131	PHE	3.5
4	F	132	LEU	3.5
2	D	178[A]	SER	3.4
2	D	407	TRP	3.4
4	F	171	ASP	3.4
1	A	88	HIS	3.4
2	B	284	ARG	3.4
2	D	277	SER	3.4
4	F	373	SER	3.4
3	E	27	PRO	3.3
4	F	306	HIS	3.3
3	E	23	ILE	3.3
4	F	134	ALA	3.3
2	B	57	THR	3.3
3	E	12[A]	ASN	3.3
2	B	285	ALA	3.2
1	C	341	ILE	3.2
4	F	101	TYR	3.2
1	C	286	LEU	3.2
4	F	90	SER	3.2
2	D	82	PRO	3.2
2	D	276	THR	3.2
3	E	141	GLU	3.1
1	A	120[A]	ASP	3.1
4	F	126	ASP	3.1
2	D	248	LEU	3.1
1	A	280	LYS	3.1
1	A	94	THR	3.1
2	D	416	MET	3.1
2	D	57	THR	3.0
4	F	100	ILE	3.0
2	D	325	MET	3.0
2	B	283	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	293	GLN	2.9
2	D	85	GLN	2.9
4	F	320	MET	2.9
2	D	404	PHE	2.9
1	C	283	HIS	2.8
2	B	431[A]	GLU	2.8
1	C	358[A]	GLN	2.8
4	F	167	SER	2.8
1	A	179	THR	2.7
1	A	18	ASN	2.7
2	B	128	SER	2.7
1	A	86	LEU	2.7
2	B	2	ARG	2.7
4	F	133	ALA	2.7
3	E	44	ASP	2.7
1	A	77	GLU	2.7
4	F	46	ARG	2.7
2	D	177	VAL	2.7
2	D	355	VAL	2.7
3	E	25	LYS	2.7
2	D	241	CYS	2.7
1	C	247	ALA	2.6
1	C	163	LYS	2.6
3	E	8	VAL	2.6
3	E	80	ARG	2.6
2	B	82	PRO	2.6
4	F	244	CYS	2.6
4	F	256	TYR	2.6
1	A	430	LYS	2.6
4	F	169	LEU	2.6
2	B	39	ASP	2.6
2	D	180[A]	THR	2.6
3	E	22	VAL	2.5
4	F	99	VAL	2.5
1	A	83	TYR	2.5
2	B	282	GLN	2.5
4	F	186	LEU	2.5
2	B	325	MET	2.5
4	F	234	GLN	2.5
2	D	439	THR	2.4
3	E	6	MET	2.4
2	D	441	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	253	TYR	2.4
1	A	46	ASP	2.4
2	D	414	ASP	2.4
4	F	235	ASP	2.4
2	D	229	HIS	2.4
4	F	340	GLN	2.4
2	B	275	LEU	2.4
3	E	115	HIS	2.4
2	B	214	PHE	2.3
4	F	182	ILE	2.3
2	D	400	ARG	2.3
2	B	248	LEU	2.3
2	D	415	GLU	2.3
2	D	50	ASN	2.3
4	F	242	ASN	2.3
4	F	144	GLY	2.3
4	F	237	THR	2.3
2	D	128	SER	2.3
3	E	45	PRO	2.3
2	D	37	HIS	2.3
2	D	127	GLU	2.3
1	C	46	ASP	2.2
1	C	215	ARG	2.2
1	A	423	GLU	2.2
2	B	220	THR	2.2
1	C	248	LEU	2.2
2	B	286	LEU	2.2
2	D	42	LEU	2.2
3	E	139	LEU	2.2
1	C	128	GLN	2.2
2	B	295	MET	2.2
2	D	86	ILE	2.2
3	E	24	LEU	2.2
4	F	31	ARG	2.2
1	A	66	VAL	2.2
2	D	373	MET	2.2
1	C	88[A]	HIS	2.2
2	D	94	PHE	2.1
4	F	32	LYS	2.1
4	F	230	SER	2.1
1	A	93	ILE	2.1
2	B	24	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	361	LEU	2.1
2	D	39	ASP	2.1
4	F	243	HIS	2.1
1	C	2	ARG	2.1
1	C	232	SER	2.1
2	B	77	SER	2.1
1	C	43	GLY	2.1
1	C	302[A]	MET	2.0
1	A	196	GLU	2.0
2	D	291	LEU	2.0
4	F	330	ILE	2.0
2	D	163	ASP	2.0
1	A	42	ILE	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(Å^2)	Q<0.9
6	MG	F	502	1/1	0.78	0.15	91,91,91,91	0
9	GOL	B	506	6/6	0.80	0.19	83,100,117,117	0
9	GOL	A	505	6/6	0.81	0.19	68,86,103,103	0
13	IMD	C	504	5/5	0.81	0.20	54,66,80,87	0
9	GOL	B	508	6/6	0.83	0.18	64,76,88,93	0
12	AF3	B	507	4/4	0.84	0.21	63,71,78,95	4
11	MES	B	505	12/12	0.86	0.14	80,99,118,118	0
6	MG	D	502	1/1	0.86	0.12	62,62,62,62	0
9	GOL	A	507	6/6	0.86	0.17	55,70,84,84	14
9	GOL	A	506	6/6	0.87	0.13	59,80,99,107	0

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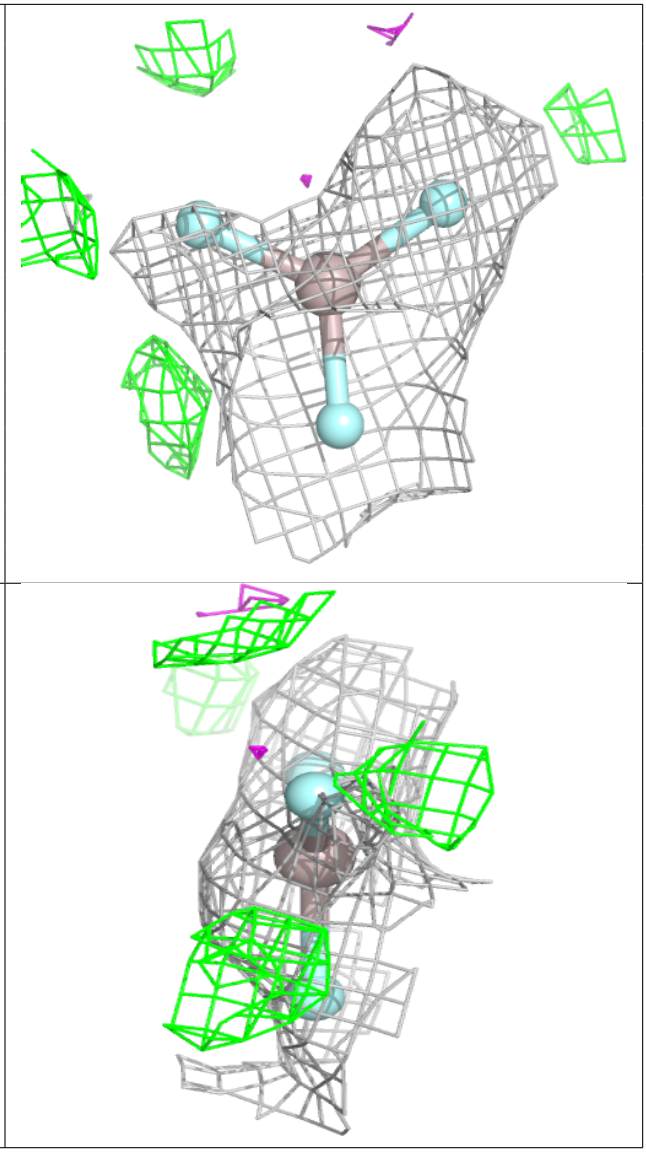
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ACP	F	501	31/31	0.87	0.12	72,92,118,138	0
8	CL	A	504	1/1	0.89	0.13	67,67,67,67	0
10	GDP	D	501	28/28	0.90	0.12	46,59,75,81	0
11	MES	B	504	12/12	0.93	0.13	46,62,70,76	25
7	CA	B	503	1/1	0.94	0.06	79,79,79,79	0
7	CA	A	503	1/1	0.96	0.06	71,71,71,71	0
5	GTP	A	501	32/32	0.97	0.07	31,42,53,56	0
5	GTP	C	501	32/32	0.97	0.07	29,36,45,48	0
10	GDP	B	501	28/28	0.97	0.07	28,39,54,55	0
6	MG	C	502	1/1	0.98	0.03	32,32,32,32	0
7	CA	C	503	1/1	0.98	0.05	58,58,58,58	0
6	MG	A	502	1/1	0.98	0.04	38,38,38,38	0
6	MG	B	502	1/1	0.99	0.02	34,34,34,34	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.

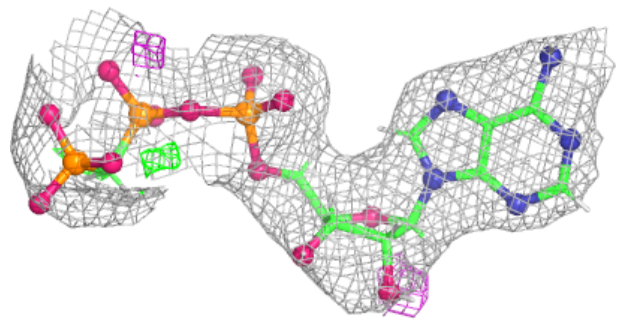
Electron density around AF3 B 507:

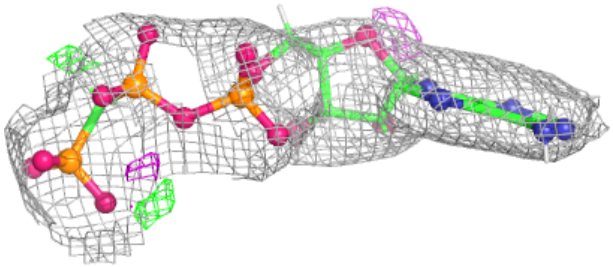
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ACP F 501:

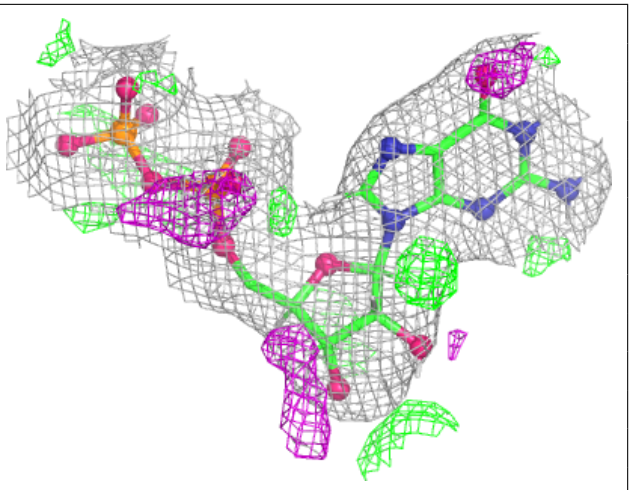
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

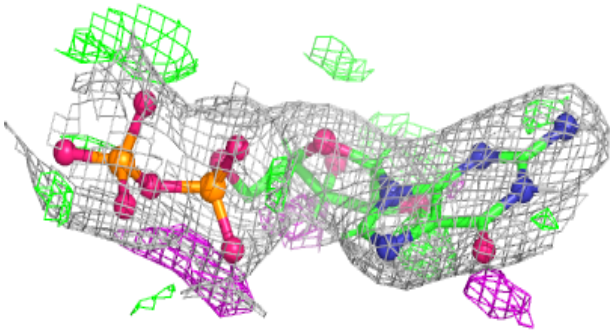


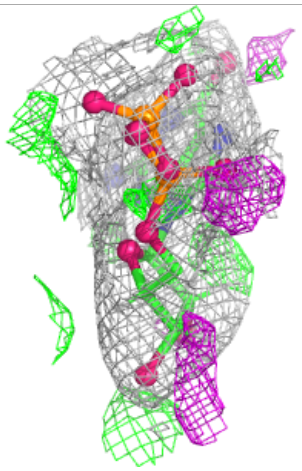


Electron density around GDP D 501:

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

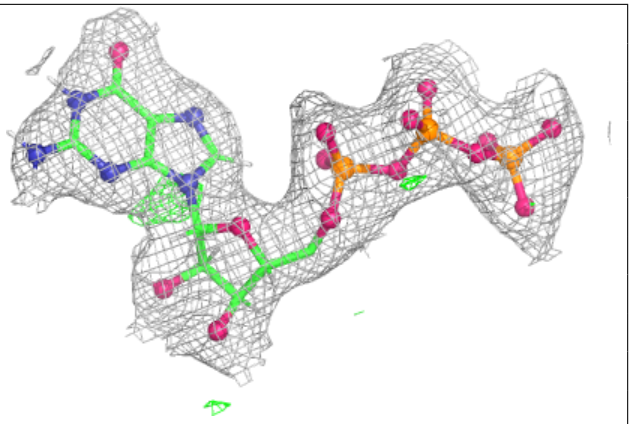


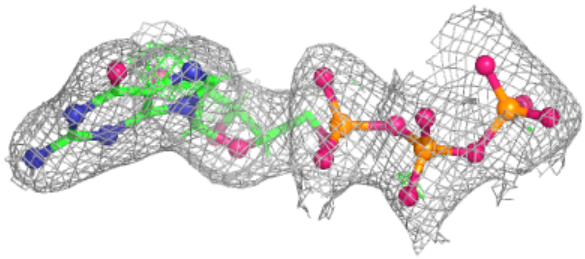


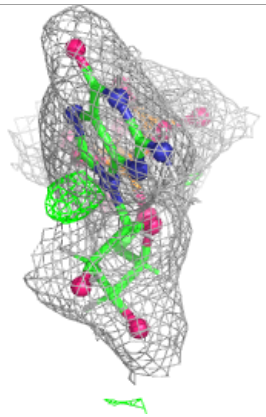


Electron density around GTP A 501:

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

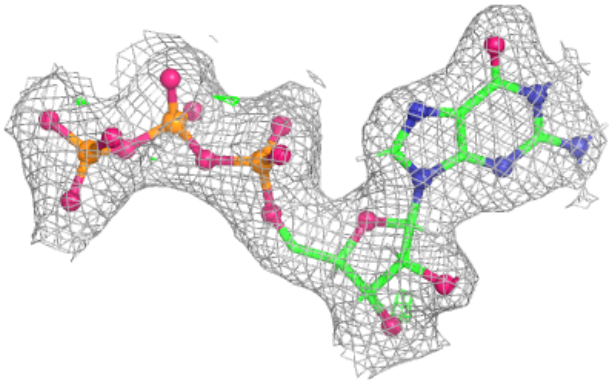


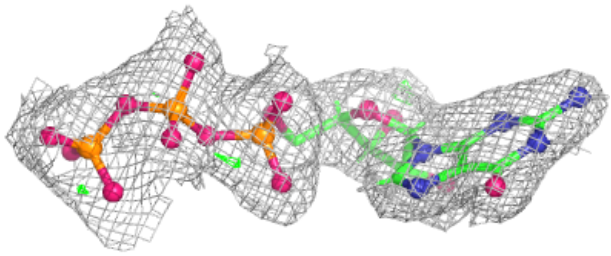


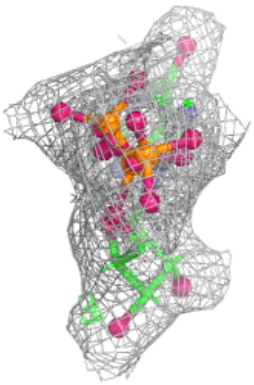


Electron density around GTP C 501:

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

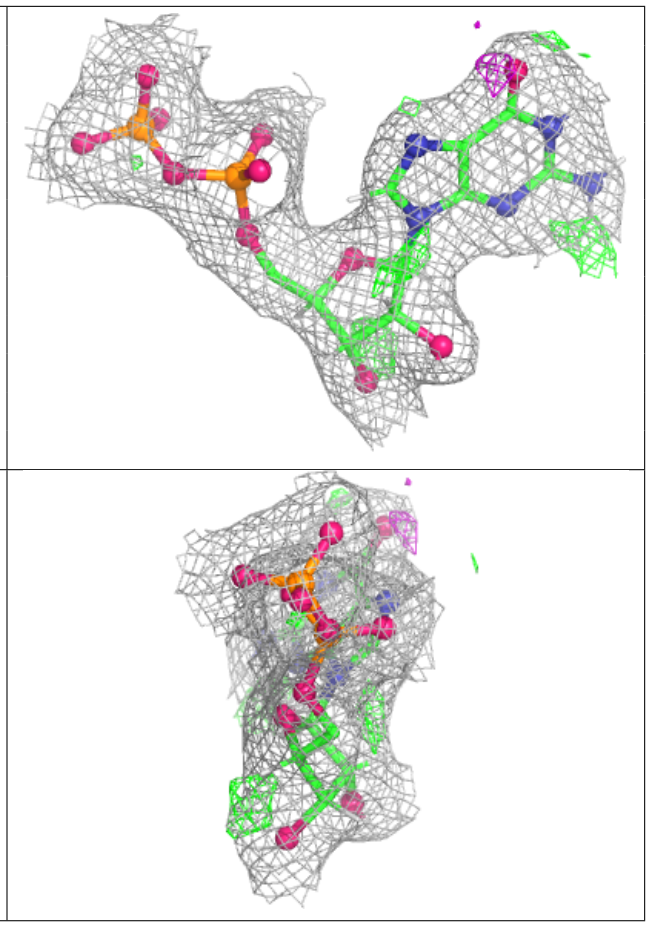






Electron density around GDP B 501:

$2mF_o$-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.