Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 12:08 AM JST

PDB ID	:	6K9V
Title	:	Crystal structure of tubulin in complex with inhibitor D64
Authors	:	Yu, Y.; Chen, Q.
Deposited on	:	2019-06-18
Resolution	:	2.54 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:

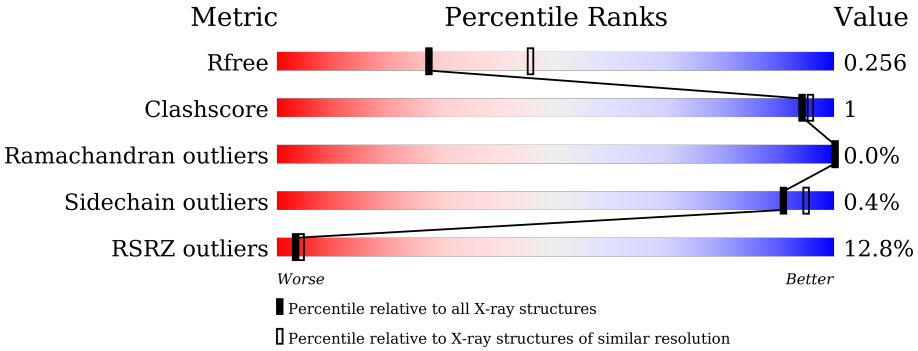
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.54 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	450	4%, 94%, • •
1	C	450	%, 96%, • •
2	B	445	5%, 94%, • •
2	D	445	19%, 91%, • 5%
3	E	143	7%, 85%, 15%
4	F	384	36%, 79%, 8%, 13%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 34786 atoms, of which 16865 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	6734	2163	3318	581	650	22	0	0	0
1	C	440	6783	2178	3340	585	657	23	0	1	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	427	6613	2116	3241	580	650	26	0	1	0
2	D	421	6488	2080	3179	562	640	27	0	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	121	2014	617	1014	181	197	5	0	0	0

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

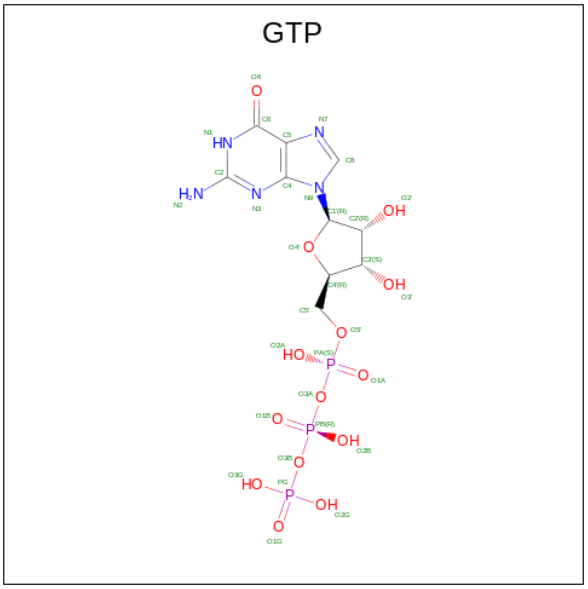
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	334	5435	1761	2691	470	499	14	0	0	0

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 (three-letter code: 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	42	10	10	5	14	3	0	0
5	C	1	42	10	10	5	14	3	0	0
5	D	1	42	10	10	5	14	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0
6	B	1	1	1	0	0
6	C	1	1	1	0	0

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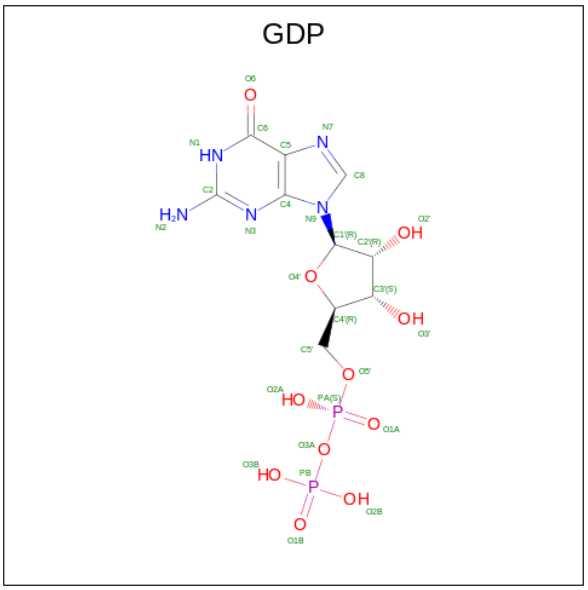
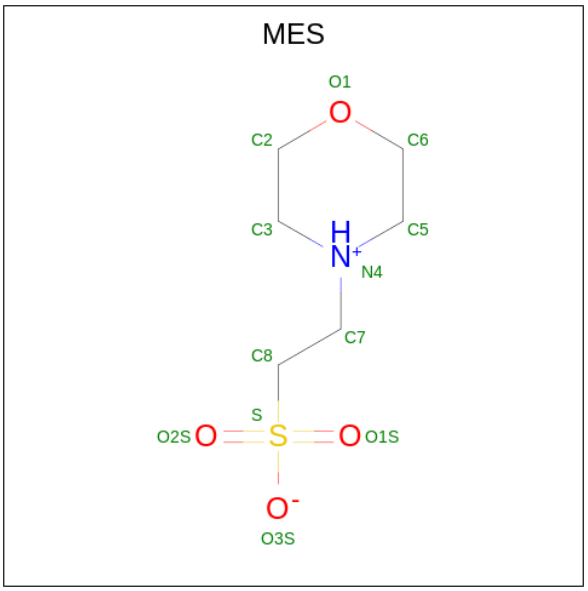
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	D	1	1	1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



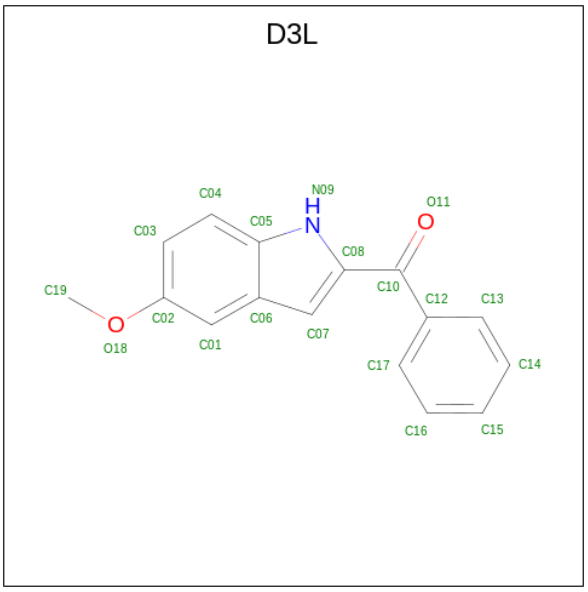
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
7	B	1	38	10	10	5	11	2	0	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
8	B	1	24	6	12	1	4	1	0	0

- Molecule 9 is (5-methoxy-1H-indol-2-yl)-phenyl-methanone (three-letter code: D3L) (formula: $C_{16}H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).

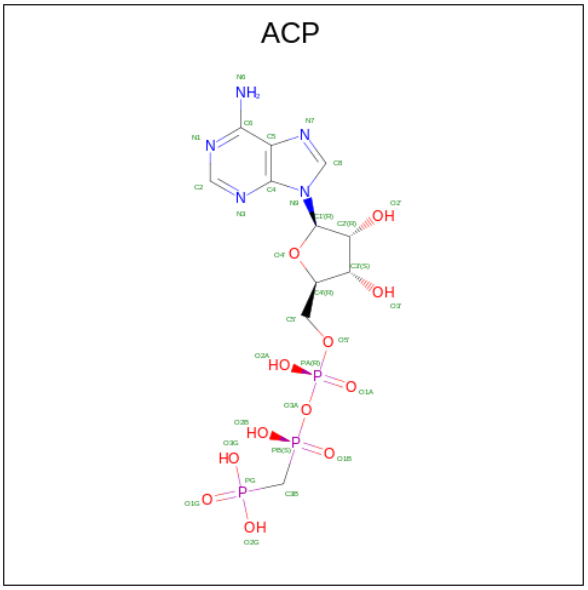


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	B	1	32	16	13	1	2	0	0
9	D	1	32	16	13	1	2	0	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
11	F	1	35	11	4	5	12	3	0	0

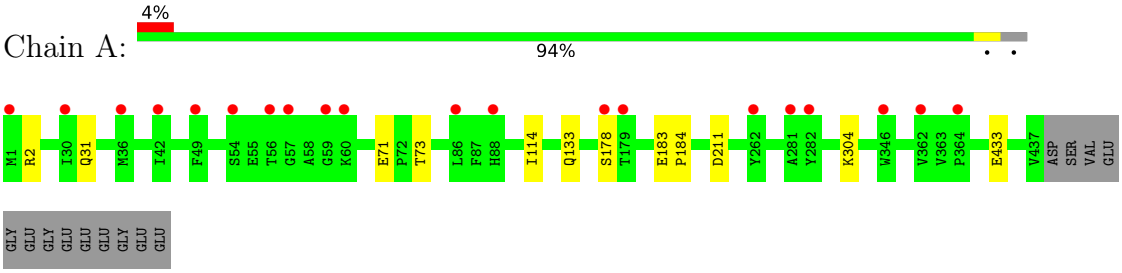
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	97	97	97	0	0
			Total	O		
12	B	83	83	83	0	0
			Total	O		
12	C	156	156	156	0	0
			Total	O		
12	D	35	35	35	0	0
			Total	O		
12	E	14	14	14	0	0
			Total	O		
12	F	41	41	41	0	0

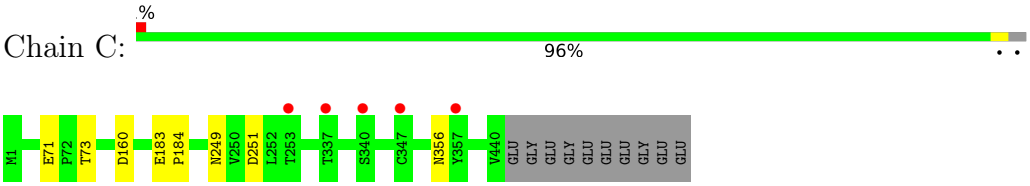
3 Residue-property plots (i)

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.

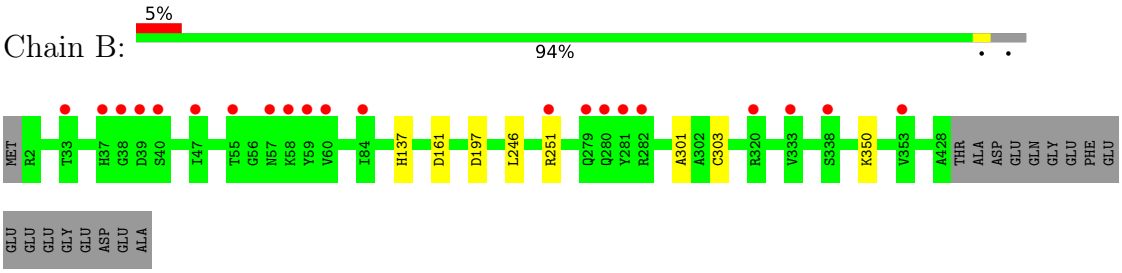
• Molecule 1: Tubulin alpha-1B chain



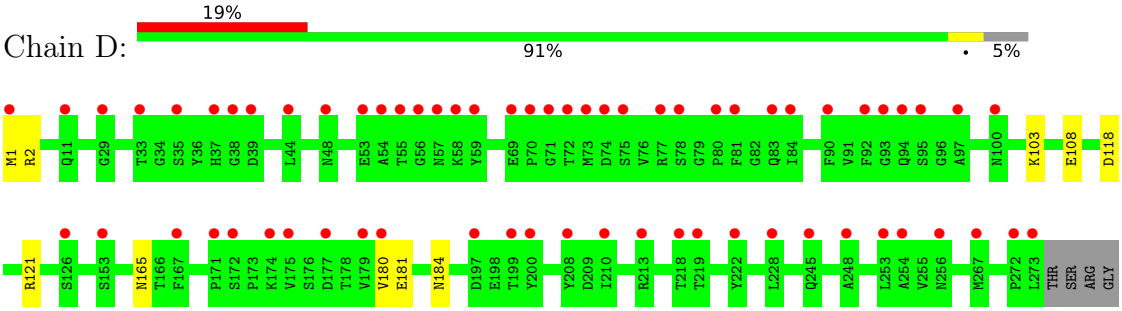
• Molecule 1: Tubulin alpha-1B chain

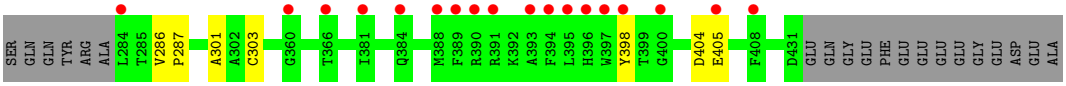


• Molecule 2: Tubulin beta-2B chain



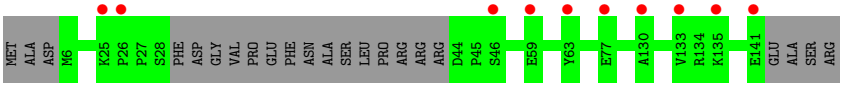
• Molecule 2: Tubulin beta-2B chain





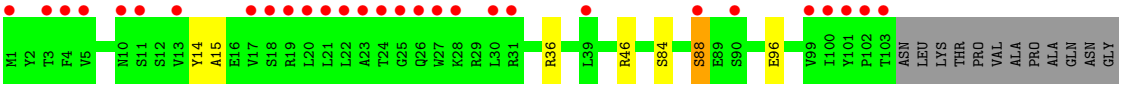
• Molecule 3: Stathmin-4

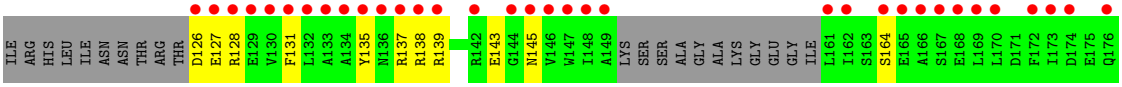
Chain E:

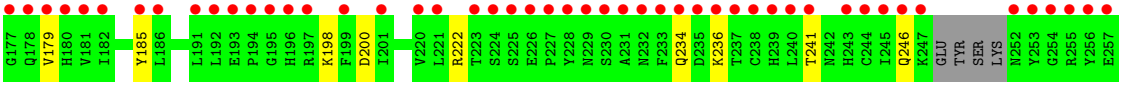


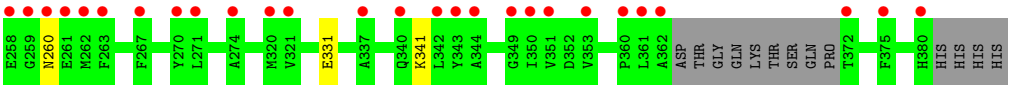
• Molecule 4: Tubulin tyrosine ligase

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	104.22Å 157.44Å 180.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.73 – 2.54 47.73 – 2.54	Depositor EDS
% Data completeness (in resolution range)	96.3 (47.73-2.54) 96.3 (47.73-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.216 , 0.248 0.222 , 0.256	Depositor DCC
R_{free} test set	1025 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.0	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	0.92	EDS
Total number of atoms	34786	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: GDP, ACP, MG, CA, MES, GTP, D3L

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	0.24	0/3494	0.39	0/4743
1	C	0.25	0/3521	0.39	0/4781
2	B	0.25	0/3447	0.39	0/4668
2	D	0.24	0/3382	0.38	0/4581
3	E	0.22	0/1008	0.33	0/1337
4	F	0.24	0/2806	0.39	0/3791
All	All	0.24	0/17658	0.38	0/23901

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	3416	3318	3331	8	0
1	C	3443	3340	3353	4	0
2	B	3372	3241	3250	6	0
2	D	3309	3179	3189	10	0
3	E	1000	1014	1018	0	0
4	F	2744	2691	2709	17	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	1	0
6	A	2	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	B	28	10	12	0	0
8	B	12	12	12	0	0
9	B	19	13	0	0	0
9	D	19	13	0	0	0
10	C	1	0	0	0	0
11	F	31	4	14	3	0
12	A	97	0	0	2	0
12	B	83	0	0	1	1
12	C	156	0	0	1	1
12	D	35	0	0	1	0
12	E	14	0	0	0	0
12	F	41	0	0	5	0
All	All	17921	16865	16924	44	1

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 (44) 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	11:F:401:ACP:O1B	2.00	0.80
2:D:118:ASP:OD1	2:D:121:ARG:NH2	2.25	0.69
11:F:401:ACP:O1B	11:F:401:ACP:O3G	2.13	0.67
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.29	0.65
1:C:160:ASP:OD1	12:C:601:HOH:O	2.14	0.64
4:F:96:GLU:OE2	4:F:138:ARG:NH2	2.33	0.61
4:F:126:ASP:OD1	4:F:127:GLU:N	2.34	0.60
4:F:222:ARG:N	12:F:505:HOH:O	2.35	0.60
4:F:135:TYR:OH	4:F:164:SER:O	2.22	0.57
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.23	0.55
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.41	0.54
2:D:404:ASP:OD1	2:D:405:GLU:N	2.41	0.54
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.23	0.53
4:F:84:SER:O	4:F:88:SER:N	2.42	0.52
4:F:234:GLN:O	4:F:236:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:O	12:A:601:HOH:O	2.19	0.50
1:A:178:SER:O	2:B:350:LYS:NZ	2.40	0.49
2:D:181:GLU:OE2	5:D:501:GTP:O3'	2.15	0.49
4:F:14:TYR:N	12:F:508:HOH:O	2.44	0.49
1:A:433:GLU:OE2	4:F:46:ARG:NH1	2.46	0.48
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.26	0.48
4:F:36:ARG:NH2	12:F:514:HOH:O	2.46	0.47
4:F:241:THR:H	11:F:401:ACP:HO3'	1.61	0.47
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.39	0.47
4:F:15:ALA:N	12:F:508:HOH:O	2.46	0.46
2:D:165:ASN:ND2	12:D:606:HOH:O	2.48	0.45
4:F:128:ARG:O	4:F:131:PHE:N	2.47	0.45
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.45	0.44
2:D:180:VAL:HG12	2:D:180:VAL:O	2.18	0.44
2:D:103:LYS:O	2:D:108:GLU:N	2.51	0.44
4:F:341:LYS:O	12:F:501:HOH:O	2.21	0.44
2:D:301:ALA:O	2:D:303:CYS:N	2.51	0.44
2:B:301:ALA:O	2:B:303:CYS:N	2.52	0.43
2:B:161:ASP:O	2:B:251[B]:ARG:NH2	2.49	0.43
1:A:31:GLN:NE2	12:A:616:HOH:O	2.51	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.42
2:B:197:ASP:OD1	12:B:601:HOH:O	2.21	0.42
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.01	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.42
2:B:246:LEU:HD13	2:B:350:LYS:HE3	2.02	0.41
2:D:1:MET:HG3	2:D:2:ARG:N	2.36	0.41
2:D:184:ASN:OD1	2:D:398:TYR:OH	2.34	0.41
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.03	0.40
2:B:161:ASP:O	2:B:251[A]:ARG:NH2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:649:HOH:O	12:C:747:HOH:O[4_545]	2.18	0.02

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	435/450 (97%)	420 (97%)	14 (3%)	1 (0%)	47	60
1	C	439/450 (98%)	428 (98%)	11 (2%)	0	100	100
2	B	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	406 (97%)	11 (3%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	324/384 (84%)	307 (95%)	17 (5%)	0	100	100
All	All	2158/2317 (93%)	2090 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ILE

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	368/378 (97%)	368 (100%)	0	100	100
1	C	372/378 (98%)	371 (100%)	1 (0%)	92	96
2	B	370/383 (97%)	369 (100%)	1 (0%)	92	96
2	D	364/383 (95%)	364 (100%)	0	100	100
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	301/342 (88%)	295 (98%)	6 (2%)	55	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1884/1991 (95%)	1876 (100%)	8 (0%)	91 95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
1	C	251	ASP
4	F	88	SER
4	F	137	ARG
4	F	139	ARG
4	F	143	GLU
4	F	145	ASN
4	F	179	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
3	E	18	GLN
4	F	246	GLN
4	F	260	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	ACP	F	401	-	27,33,33	1.40	4 (14%)	32,52,52	1.51	5 (15%)
7	GDP	B	501	6	24,30,30	1.03	1 (4%)	30,47,47	1.11	4 (13%)
9	D3L	D	502	-	19,21,21	0.87	0	24,29,29	0.69	1 (4%)
5	GTP	D	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.57	7 (21%)
9	D3L	B	504	-	19,21,21	0.84	0	24,29,29	0.78	1 (4%)
5	GTP	C	501	6	26,34,34	1.15	1 (3%)	32,54,54	1.42	6 (18%)
8	MES	B	503	-	12,12,12	2.32	1 (8%)	14,16,16	2.42	5 (35%)
5	GTP	A	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.48	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	4/15/38/38	0/3/3/3
7	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	D3L	D	502	-	-	2/6/10/10	0/3/3/3
5	GTP	D	501	6	-	8/18/38/38	0/3/3/3
9	D3L	B	504	-	-	2/6/10/10	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
8	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	10/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	503	MES	C8-S	-7.83	1.66	1.77
5	D	501	GTP	C5-C6	-4.15	1.39	1.47
5	C	501	GTP	C5-C6	-4.15	1.39	1.47
5	A	501	GTP	C5-C6	-4.08	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	GDP	C6-N1	-3.29	1.33	1.37
11	F	401	ACP	C2'-C1'	-3.28	1.48	1.53
11	F	401	ACP	PG-O3G	2.45	1.60	1.54
11	F	401	ACP	PG-O2G	2.30	1.60	1.54
5	D	501	GTP	C2-N3	2.15	1.38	1.33
5	A	501	GTP	C2-N3	2.02	1.38	1.33
11	F	401	ACP	PB-O3A	2.01	1.60	1.58

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	503	MES	C5-N4-C3	5.34	120.84	108.83
8	B	503	MES	C7-N4-C5	4.26	122.12	111.23
5	D	501	GTP	PB-O3B-PG	-4.08	118.81	132.83
5	A	501	GTP	C5-C6-N1	3.22	119.64	113.95
5	D	501	GTP	C5-C6-N1	3.14	119.49	113.95
5	D	501	GTP	C8-N7-C5	3.13	108.94	102.99
5	C	501	GTP	C5-C6-N1	3.06	119.35	113.95
5	C	501	GTP	C8-N7-C5	3.04	108.77	102.99
5	C	501	GTP	PA-O3A-PB	-3.00	122.52	132.83
5	D	501	GTP	PA-O3A-PB	-2.99	122.57	132.83
11	F	401	ACP	N3-C2-N1	-2.98	124.01	128.68
5	A	501	GTP	C2-N1-C6	-2.96	119.64	125.10
5	A	501	GTP	C8-N7-C5	2.94	108.60	102.99
11	F	401	ACP	C4-C5-N7	-2.80	106.48	109.40
5	C	501	GTP	PB-O3B-PG	-2.73	123.45	132.83
8	B	503	MES	O2S-S-C8	2.73	110.20	106.92
5	D	501	GTP	C2-N1-C6	-2.72	120.09	125.10
8	B	503	MES	O1S-S-C8	2.72	110.19	106.92
5	A	501	GTP	PB-O3B-PG	-2.71	123.52	132.83
5	C	501	GTP	C2-N1-C6	-2.71	120.11	125.10
11	F	401	ACP	O1G-PG-C3B	2.66	116.98	111.24
8	B	503	MES	C6-C5-N4	-2.56	106.22	110.10
9	B	504	D3L	C08-N09-C05	2.51	109.68	104.45
7	B	501	GDP	O2B-PB-O3A	2.47	112.91	104.64
5	A	501	GTP	PA-O3A-PB	-2.40	124.57	132.83
9	D	502	D3L	C08-N09-C05	2.39	109.44	104.45
7	B	501	GDP	C8-N7-C5	2.30	107.38	102.99
5	A	501	GTP	C3'-C2'-C1'	2.30	104.44	100.98
5	A	501	GTP	O6-C6-C5	-2.26	119.95	124.37
7	B	501	GDP	C5-C6-N1	2.23	117.90	113.95
5	D	501	GTP	C3'-C2'-C1'	2.22	104.32	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	401	ACP	C5'-C4'-C3'	-2.17	107.04	115.18
11	F	401	ACP	O5'-C5'-C4'	2.15	116.39	108.99
7	B	501	GDP	C3'-C2'-C1'	2.14	104.20	100.98
5	C	501	GTP	O6-C6-C5	-2.11	120.25	124.37
5	D	501	GTP	O6-C6-C5	-2.08	120.31	124.37

There are no chirality outliers.

All (39) 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	C	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
8	B	503	MES	C8-C7-N4-C5
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	504	D3L	C03-C02-O18-C19
9	B	504	D3L	C01-C02-O18-C19
5	D	501	GTP	O4'-C4'-C5'-O5'
11	F	401	ACP	O4'-C4'-C5'-O5'
9	D	502	D3L	C03-C02-O18-C19
9	D	502	D3L	C01-C02-O18-C19
5	D	501	GTP	C3'-C4'-C5'-O5'
5	D	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
5	D	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
7	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A

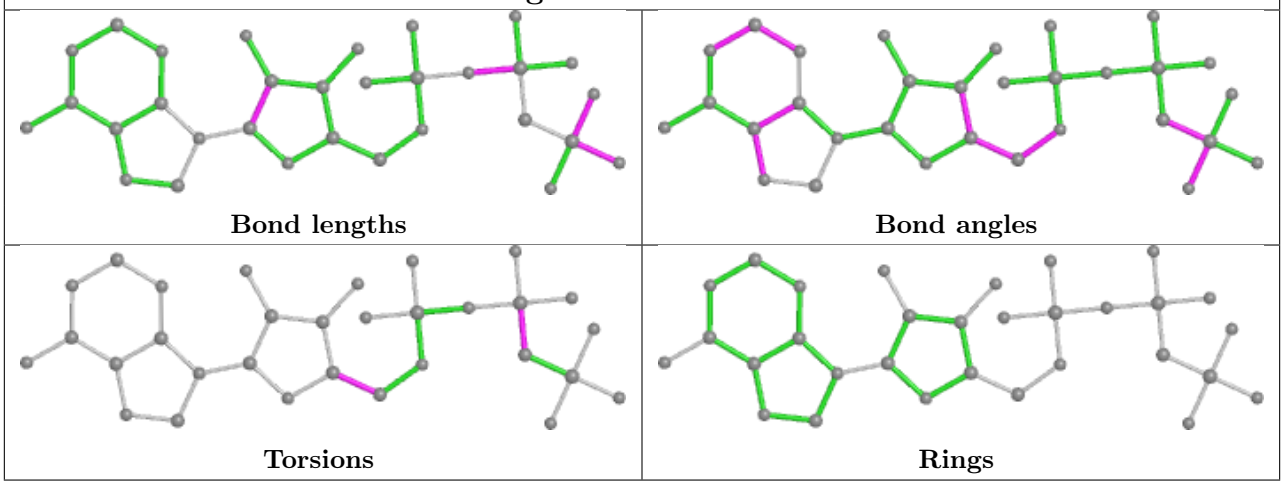
There are no ring outliers.

2 monomers are involved in 4 short contacts:

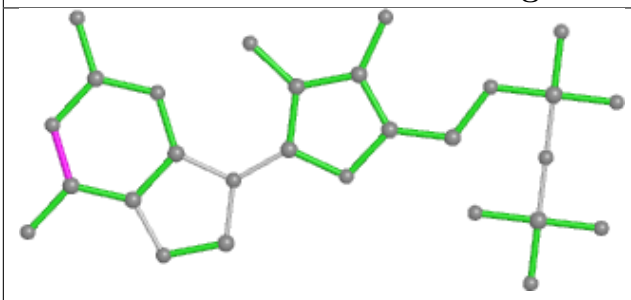
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	3	0
5	D	501	GTP	1	0

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 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.

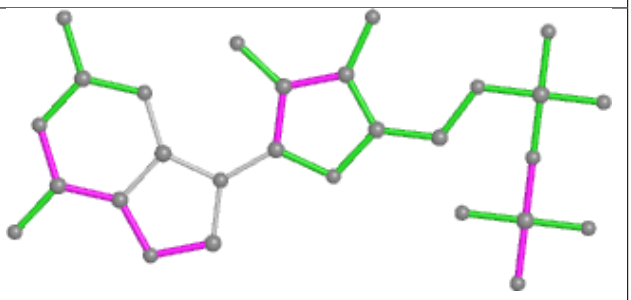
Ligand ACP F 401



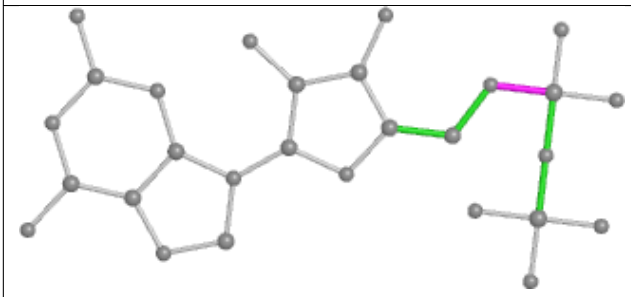
Ligand GDP B 501



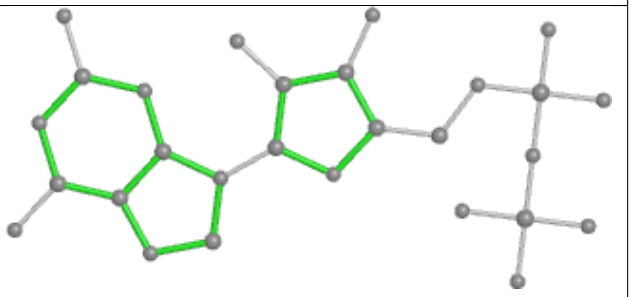
Bond lengths



Bond angles

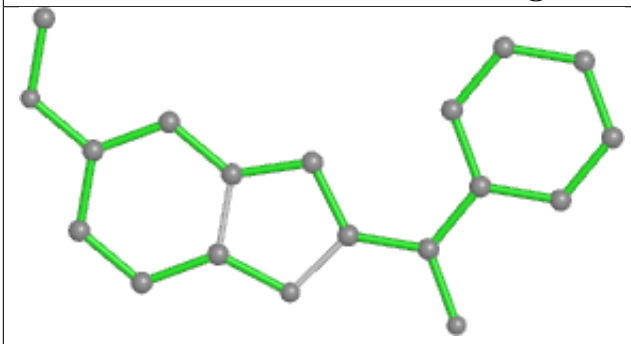


Torsions

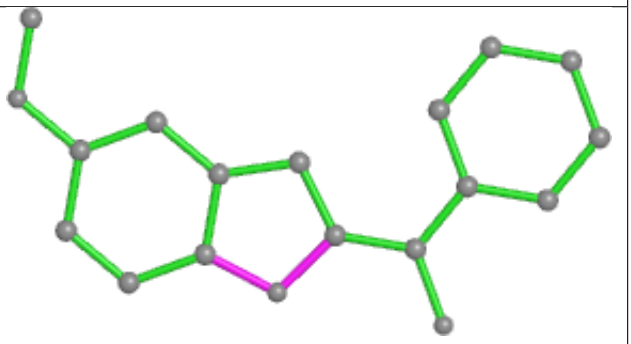


Rings

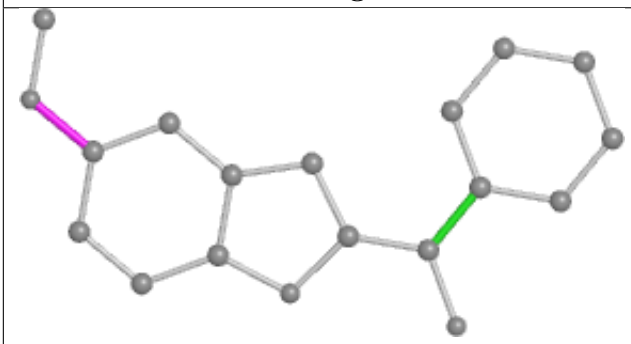
Ligand D3L D 502



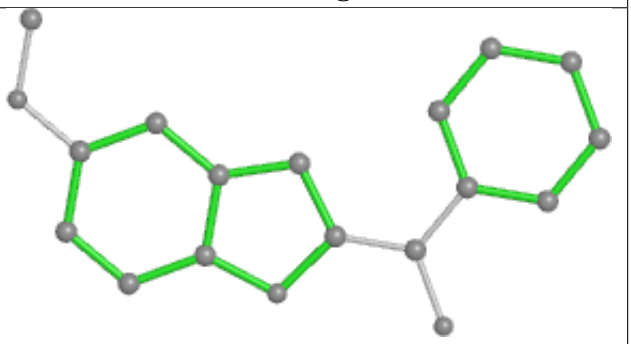
Bond lengths



Bond angles

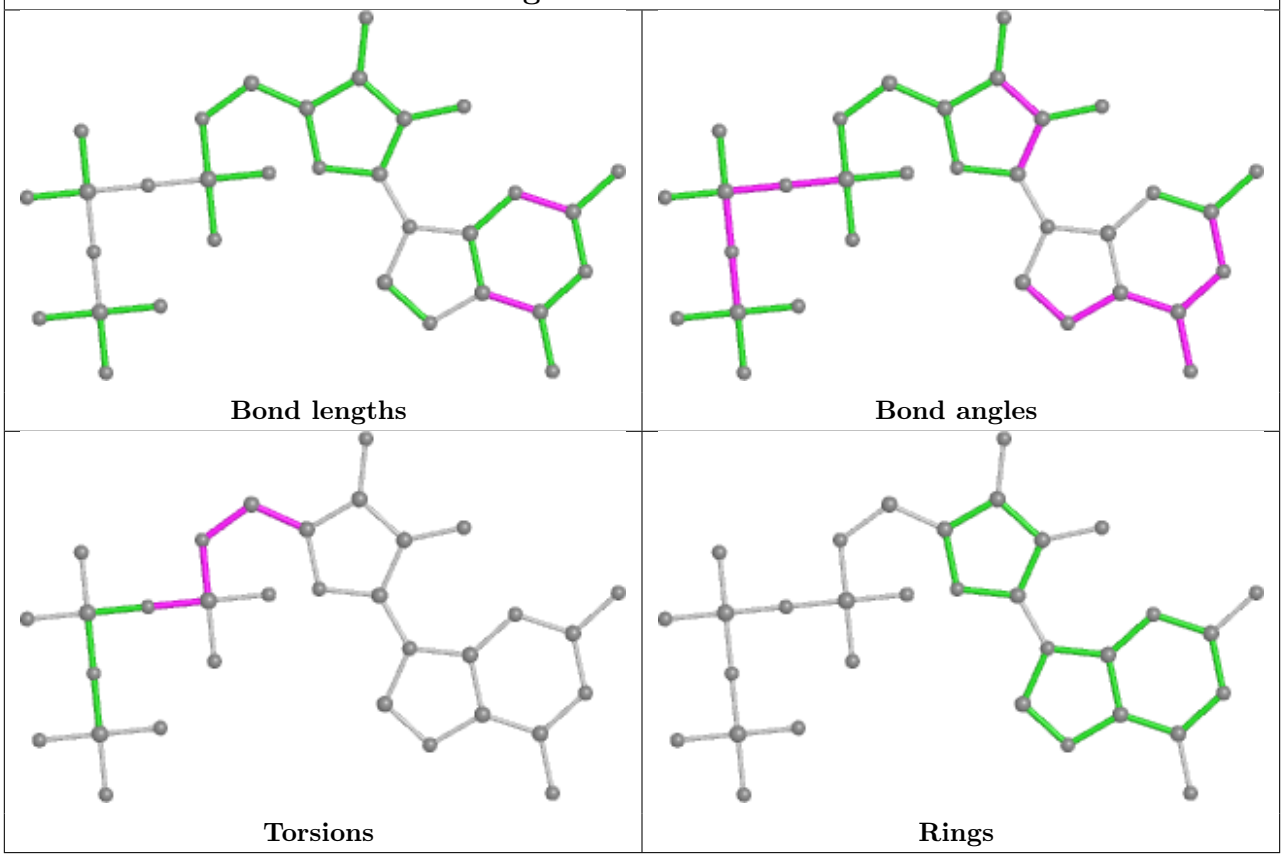


Torsions

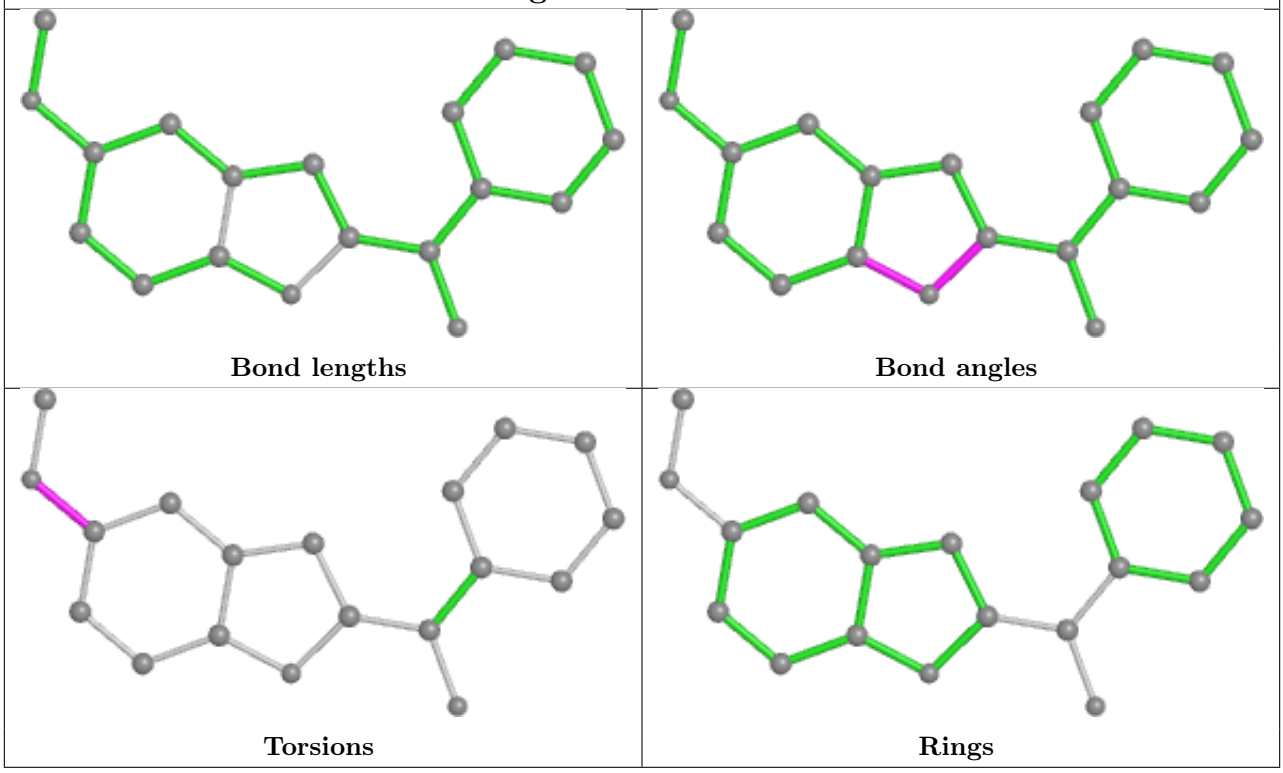


Rings

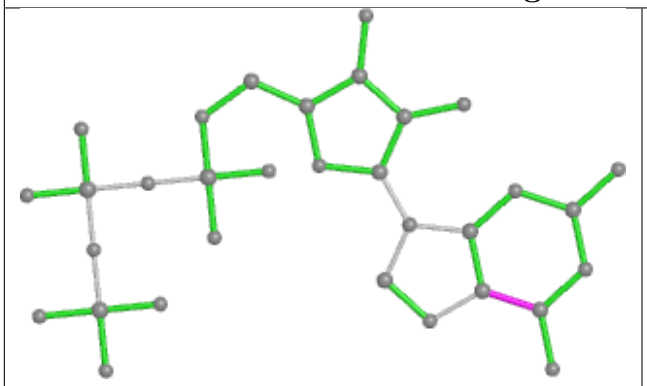
Ligand GTP D 501



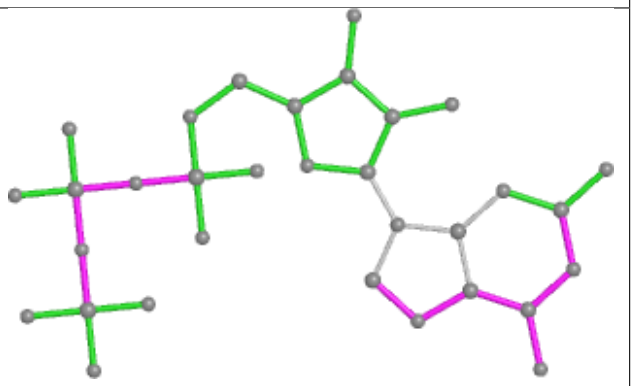
Ligand D3L B 504



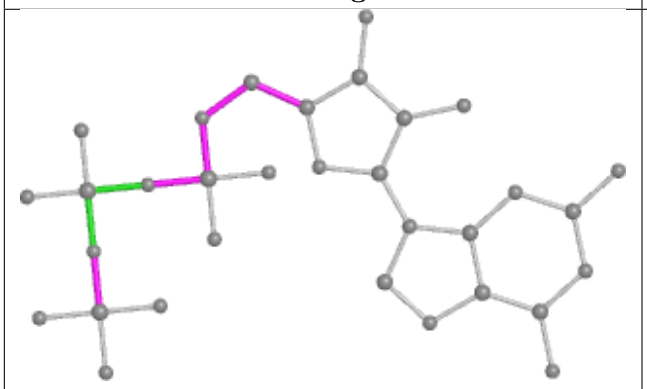
Ligand GTP C 501



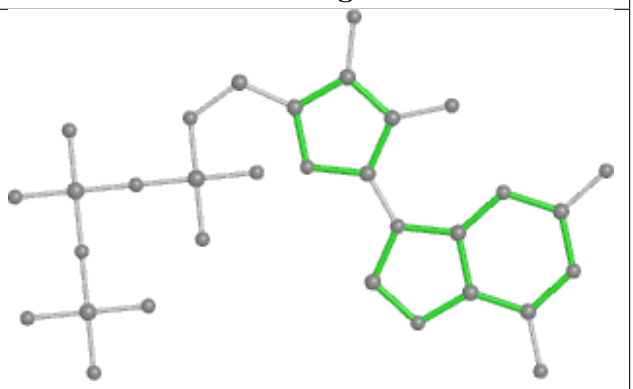
Bond lengths



Bond angles

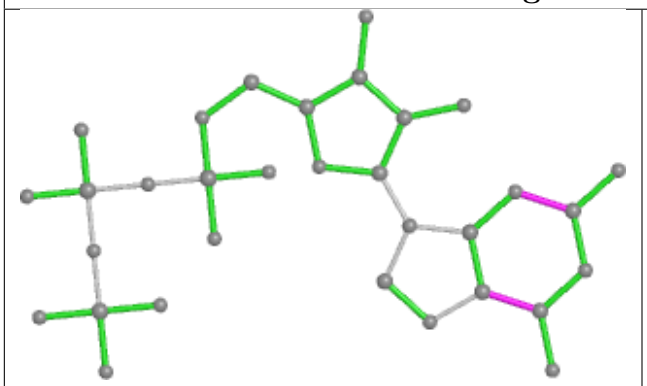


Torsions

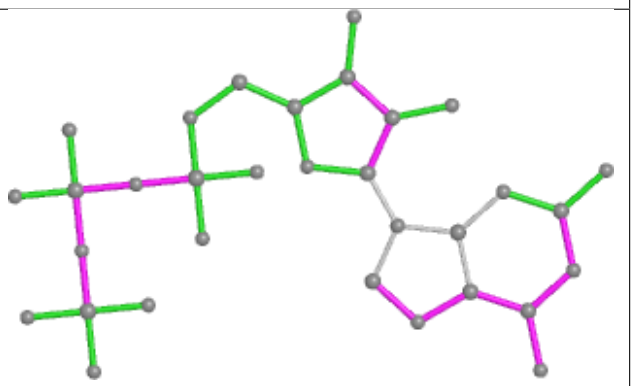


Rings

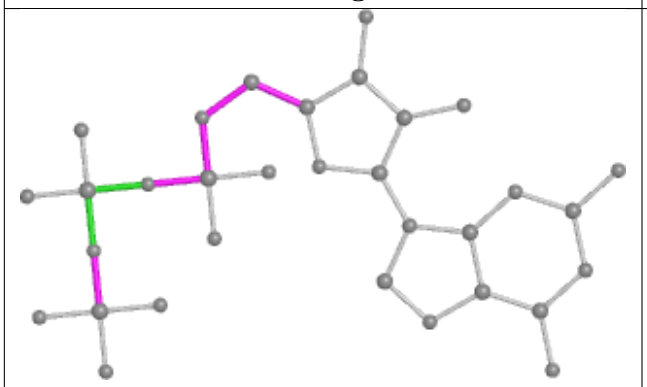
Ligand GTP A 501



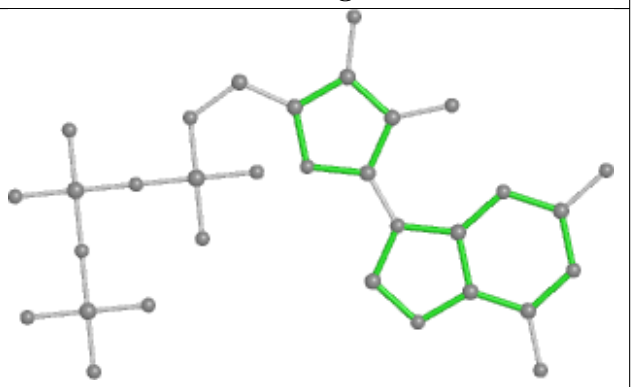
Bond lengths



Bond angles



Torsions



Rings

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%)	0.59	20 (4%) 32 39	26, 42, 65, 85	0
1	C	440/450 (97%)	0.12	5 (1%) 80 85	17, 32, 59, 81	0
2	B	427/445 (95%)	0.47	21 (4%) 29 35	18, 41, 75, 111	0
2	D	421/445 (94%)	1.12	83 (19%) 1 1	28, 61, 89, 107	0
3	E	121/143 (84%)	0.84	10 (8%) 11 13	30, 55, 85, 109	0
4	F	334/384 (86%)	1.90	139 (41%) 0 0	33, 69, 126, 136	0
All	All	2180/2317 (94%)	0.79	278 (12%) 3 4	17, 47, 93, 136	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	9.2
4	F	173	ILE	8.4
4	F	130	VAL	7.7
4	F	103	THR	6.8
4	F	231	ALA	6.8
4	F	170	LEU	6.5
4	F	102	PRO	6.3
4	F	27	TRP	6.1
4	F	21	LEU	6.1
4	F	223	THR	6.1
4	F	1	MET	6.1
4	F	132	LEU	6.0
4	F	253	TYR	6.0
4	F	20	LEU	5.9
4	F	256	TYR	5.8
4	F	240	LEU	5.8
4	F	226	GLU	5.5
4	F	177	GLY	5.5
4	F	100	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
2	D	92	PHE	5.5
4	F	245	ILE	5.4
2	B	57	ASN	5.4
4	F	227	PRO	5.3
4	F	244	CYS	5.3
4	F	167	SER	5.3
2	D	94	GLN	5.3
2	B	55	THR	5.1
4	F	230	SER	5.1
4	F	99	VAL	5.1
4	F	228	TYR	5.1
4	F	255	ARG	5.0
4	F	24	THR	4.9
2	D	394	PHE	4.9
2	D	73	MET	4.9
4	F	25	GLY	4.8
4	F	191	LEU	4.8
2	D	177	ASP	4.8
4	F	236	LYS	4.7
2	D	55	THR	4.7
4	F	166	ALA	4.7
4	F	22	LEU	4.6
4	F	13	VAL	4.6
4	F	101	TYR	4.6
4	F	129	GLU	4.6
4	F	225	SER	4.5
2	D	71	GLY	4.4
4	F	136	ASN	4.4
4	F	361	LEU	4.4
4	F	234	GLN	4.4
4	F	142	ARG	4.3
4	F	149	ALA	4.3
4	F	224	SER	4.3
4	F	186	LEU	4.3
2	D	391	ARG	4.3
4	F	372	THR	4.2
4	F	176	GLN	4.2
2	D	390	ARG	4.1
4	F	194	PRO	4.1
2	D	175	VAL	4.1
2	D	80	PRO	4.1
4	F	247	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	4.0
2	B	37	HIS	4.0
4	F	241	THR	4.0
4	F	126	ASP	4.0
3	E	130	ALA	4.0
2	D	81	PHE	3.9
4	F	252	ASN	4.0
2	D	44	LEU	3.9
2	D	1	MET	3.9
4	F	161	LEU	3.9
4	F	243	HIS	3.9
4	F	178	GLN	3.8
1	A	59	GLY	3.8
4	F	133	ALA	3.8
2	D	37	HIS	3.8
4	F	259	GLY	3.7
4	F	135	TYR	3.7
4	F	138	ARG	3.7
2	B	33	THR	3.7
4	F	182	ILE	3.6
1	C	340	SER	3.6
4	F	164	SER	3.6
4	F	196	HIS	3.6
4	F	199	PHE	3.6
4	F	192	LEU	3.6
4	F	90	SER	3.6
4	F	342	LEU	3.6
3	E	133	VAL	3.5
4	F	195	GLY	3.5
2	D	39	ASP	3.5
2	D	245	GLN	3.5
2	D	84	ILE	3.5
4	F	254	GLY	3.5
2	B	338	SER	3.4
4	F	26	GLN	3.4
4	F	162	ILE	3.4
4	F	137	ARG	3.4
4	F	262	MET	3.4
2	D	405	GLU	3.4
2	D	78	SER	3.4
4	F	232	ASN	3.4
2	B	282	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	58	LYS	3.3
4	F	165	GLU	3.3
4	F	180	HIS	3.3
4	F	267	PHE	3.3
2	D	389	PHE	3.2
2	D	48	ASN	3.2
4	F	221	LEU	3.2
1	A	262	TYR	3.2
4	F	23	ALA	3.2
4	F	17	VAL	3.2
4	F	139	ARG	3.2
4	F	337	ALA	3.1
4	F	320	MET	3.1
1	C	357	TYR	3.1
2	D	126	SER	3.1
4	F	260	ASN	3.1
2	D	54	ALA	3.1
2	B	280	GLN	3.1
4	F	134	ALA	3.1
4	F	144	GLY	3.1
2	D	179	VAL	3.1
1	A	42	ILE	3.1
2	D	74	ASP	3.1
4	F	4	PHE	3.0
4	F	263	PHE	3.0
2	D	59	TYR	3.0
4	F	88	SER	3.0
2	D	29	GLY	3.0
4	F	145	ASN	3.0
2	D	53	GLU	3.0
2	D	83	GLN	3.0
4	F	169	LEU	3.0
4	F	238	CYS	3.0
1	A	1	MET	3.0
1	A	282	TYR	3.0
2	D	95	SER	2.9
4	F	181	VAL	2.9
4	F	353	VAL	2.9
2	D	284	LEU	2.9
4	F	362	ALA	2.9
4	F	28	LYS	2.8
1	A	346	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	254	ALA	2.8
4	F	19	ARG	2.8
4	F	179	VAL	2.8
1	A	86	LEU	2.8
3	E	63	TYR	2.8
1	A	54	SER	2.8
2	B	59	TYR	2.8
2	D	72	THR	2.8
4	F	39	LEU	2.7
2	D	77	ARG	2.7
4	F	229	ASN	2.7
1	A	56	THR	2.7
2	B	58	LYS	2.7
2	D	393	ALA	2.7
2	D	172	SER	2.7
2	D	398	TYR	2.7
4	F	246	GLN	2.7
1	A	57	GLY	2.7
4	F	148	ILE	2.7
4	F	18	SER	2.7
2	B	281	TYR	2.6
1	A	362	VAL	2.6
2	D	97	ALA	2.6
2	D	100	ASN	2.6
4	F	5	VAL	2.6
4	F	168	GLU	2.6
4	F	220	VAL	2.6
2	D	253	LEU	2.6
4	F	197	ARG	2.6
2	D	75	SER	2.6
4	F	349	GLY	2.6
4	F	172	PHE	2.6
2	D	93	GLY	2.5
4	F	147	TRP	2.5
4	F	351	VAL	2.5
2	D	267	MET	2.5
2	B	39	ASP	2.5
4	F	10	ASN	2.5
2	D	210	ILE	2.5
4	F	174	ASP	2.5
4	F	360	PRO	2.5
2	D	69	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	251[A]	ARG	2.4
2	D	213	ARG	2.4
4	F	31	ARG	2.4
1	A	49	PHE	2.4
1	A	281	ALA	2.4
1	C	337	THR	2.4
3	E	25	LYS	2.4
2	D	408	PHE	2.4
3	E	59	GLU	2.4
1	A	178	SER	2.4
2	D	248	ALA	2.4
2	D	180	VAL	2.4
4	F	258	GLU	2.4
2	D	397	TRP	2.4
2	B	333	VAL	2.4
4	F	343	TYR	2.4
3	E	46	SER	2.4
3	E	141	GLU	2.4
2	D	388	MET	2.3
2	D	38	GLY	2.3
2	D	400	GLY	2.3
2	B	84	ILE	2.3
2	B	279	GLN	2.3
4	F	201	ILE	2.3
4	F	340	GLN	2.3
3	E	135	LYS	2.3
2	B	38	GLY	2.3
2	B	47	ILE	2.3
2	D	199	THR	2.3
4	F	193	GLU	2.3
2	D	384	GLN	2.3
2	D	11	GLN	2.3
2	B	353	VAL	2.3
2	D	56	GLY	2.3
4	F	344	ALA	2.3
4	F	11	SER	2.3
2	D	167	PHE	2.3
4	F	239	HIS	2.3
2	D	395	LEU	2.3
4	F	30	LEU	2.3
1	A	364	PRO	2.2
1	A	30	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	208	TYR	2.2
2	D	35	SER	2.2
2	D	90	PHE	2.2
2	D	219	THR	2.2
4	F	128	ARG	2.2
2	D	171	PRO	2.2
2	D	360	GLY	2.2
1	A	88	HIS	2.2
2	D	381	ILE	2.2
4	F	271	LEU	2.2
4	F	274	ALA	2.2
2	B	40	SER	2.2
2	D	153	SER	2.2
4	F	380	HIS	2.2
4	F	3	THR	2.2
4	F	375	PHE	2.2
4	F	127	GLU	2.2
4	F	185	TYR	2.1
4	F	146	VAL	2.1
4	F	235	ASP	2.1
2	D	33	THR	2.1
2	D	228	LEU	2.1
1	A	60	LYS	2.1
2	D	222	TYR	2.1
2	B	60	VAL	2.1
2	B	320	ARG	2.1
4	F	261	GLU	2.1
2	D	218	THR	2.1
2	D	273	LEU	2.1
2	D	396	HIS	2.1
4	F	237	THR	2.1
2	D	200	TYR	2.1
4	F	350	ILE	2.1
2	D	57	ASN	2.1
3	E	26	PRO	2.1
2	D	197	ASP	2.1
3	E	77	GLU	2.1
2	D	70	PRO	2.0
4	F	270	TYR	2.0
2	D	256	ASN	2.0
1	A	179	THR	2.0
2	D	366	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	272	PRO	2.0
4	F	257	GLU	2.0
1	C	253	THR	2.0
1	C	347[A]	CYS	2.0
4	F	321	VAL	2.0
2	D	174	LYS	2.0
1	A	36	MET	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 monosaccharides 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.

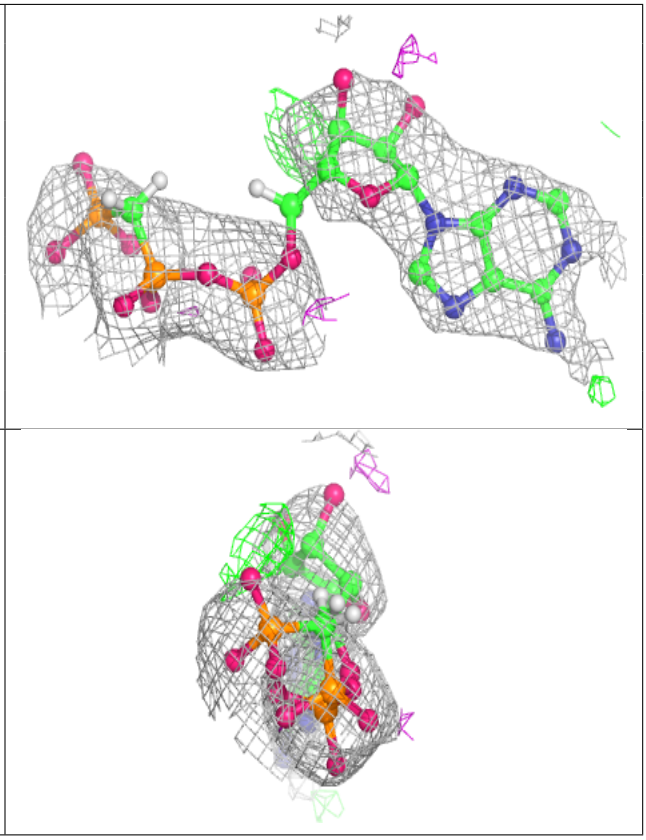
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	503	1/1	0.66	0.13	76,76,76,76	0
11	ACP	F	401	31/31	0.85	0.20	84,96,128,134	0
6	MG	A	502	1/1	0.88	0.20	26,26,26,26	0
9	D3L	D	502	19/19	0.90	0.25	44,55,71,86	0
5	GTP	D	501	32/32	0.90	0.21	51,66,94,175	0
6	MG	A	503	1/1	0.91	0.12	56,56,56,56	0
6	MG	C	502	1/1	0.92	0.22	22,22,22,22	0
8	MES	B	503	12/12	0.94	0.17	40,54,66,75	0
9	D3L	B	504	19/19	0.94	0.20	35,46,56,61	0
6	MG	B	502	1/1	0.97	0.26	28,28,28,28	0
5	GTP	C	501	32/32	0.97	0.18	12,25,39,47	0
5	GTP	A	501	32/32	0.97	0.24	18,32,45,50	0
10	CA	C	503	1/1	0.97	0.07	41,41,41,41	0
7	GDP	B	501	28/28	0.97	0.21	17,30,42,53	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.

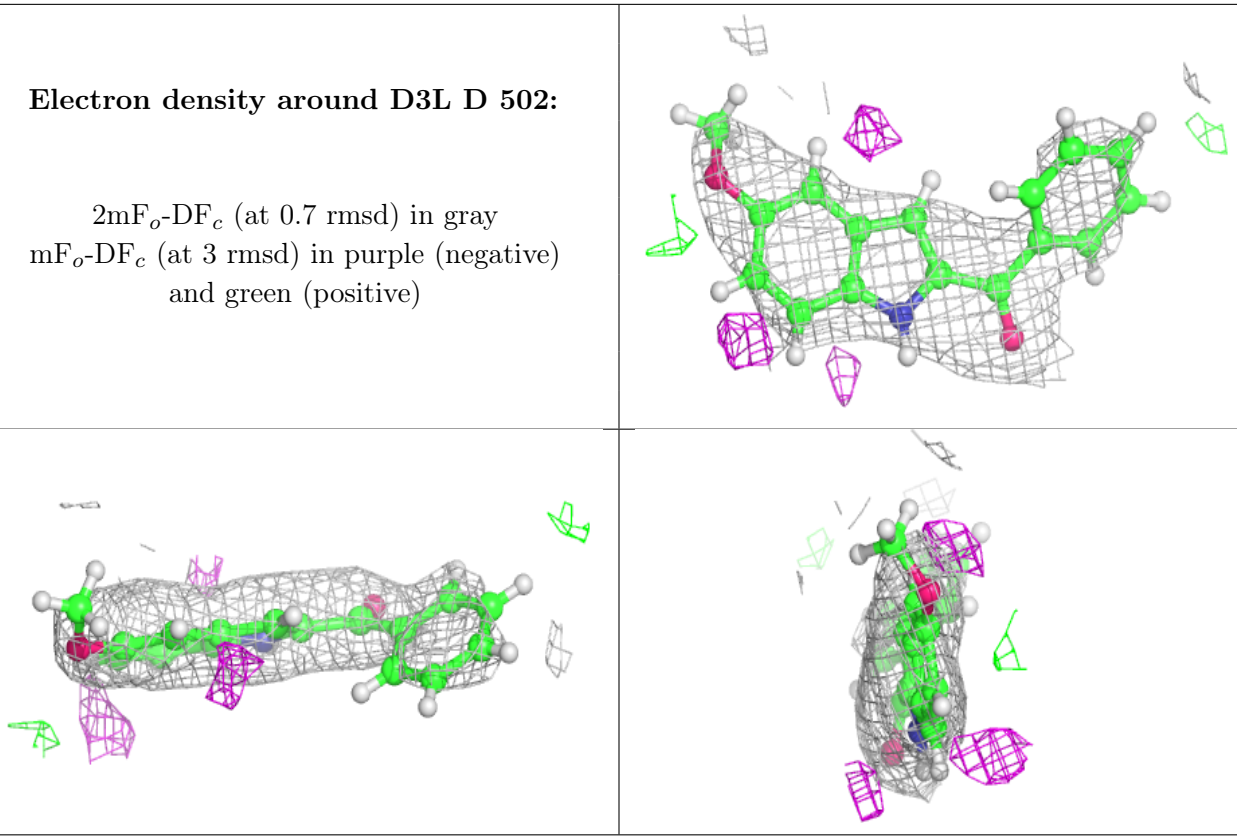
Electron density around ACP F 401:

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



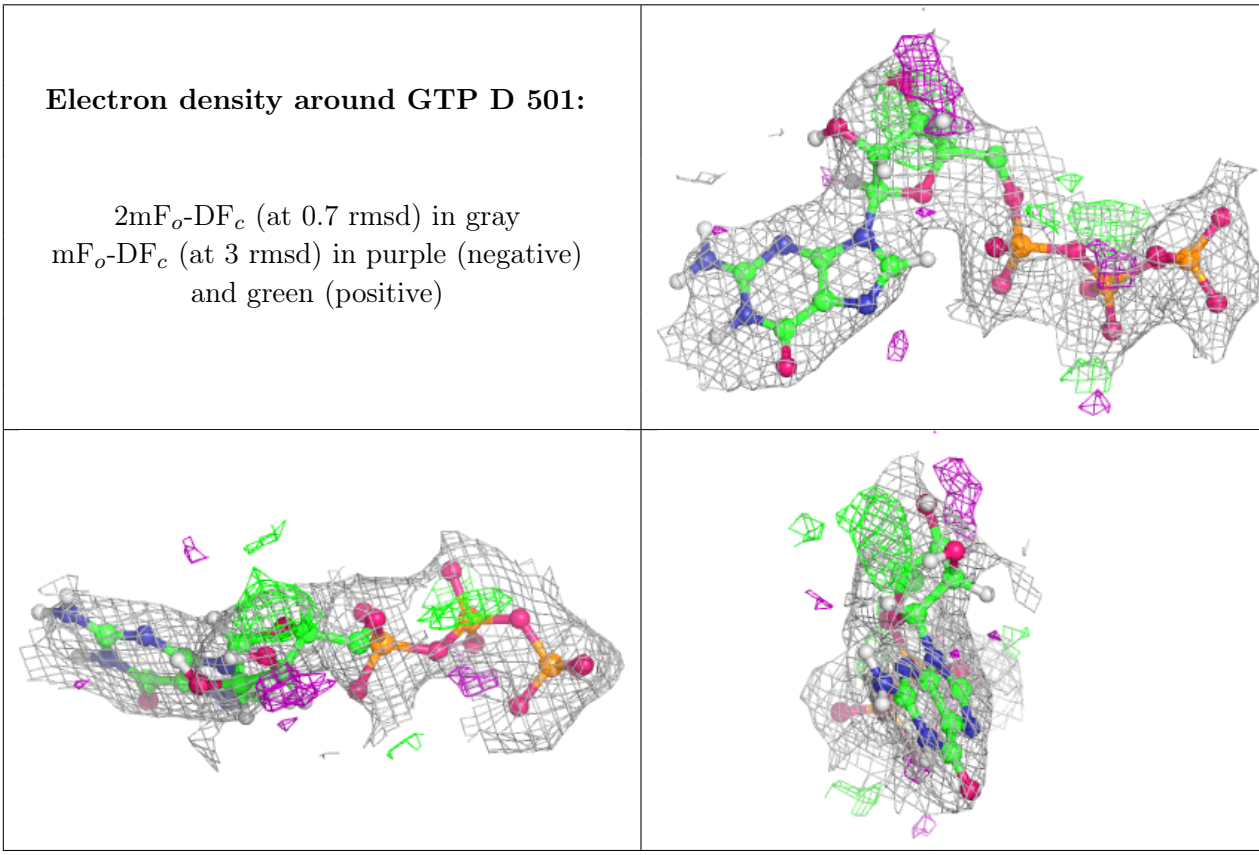
Electron density around D3L D 502:

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



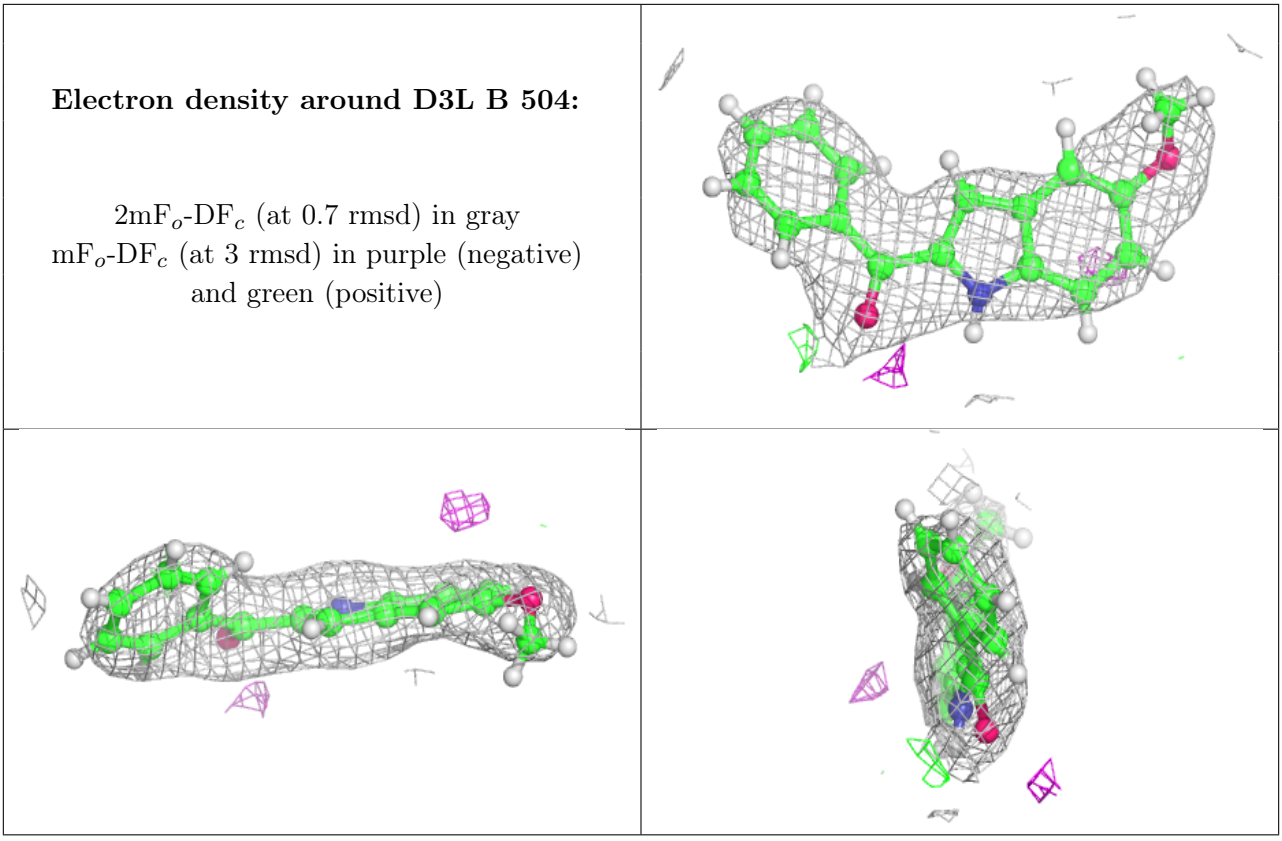
Electron density around GTP D 501:

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



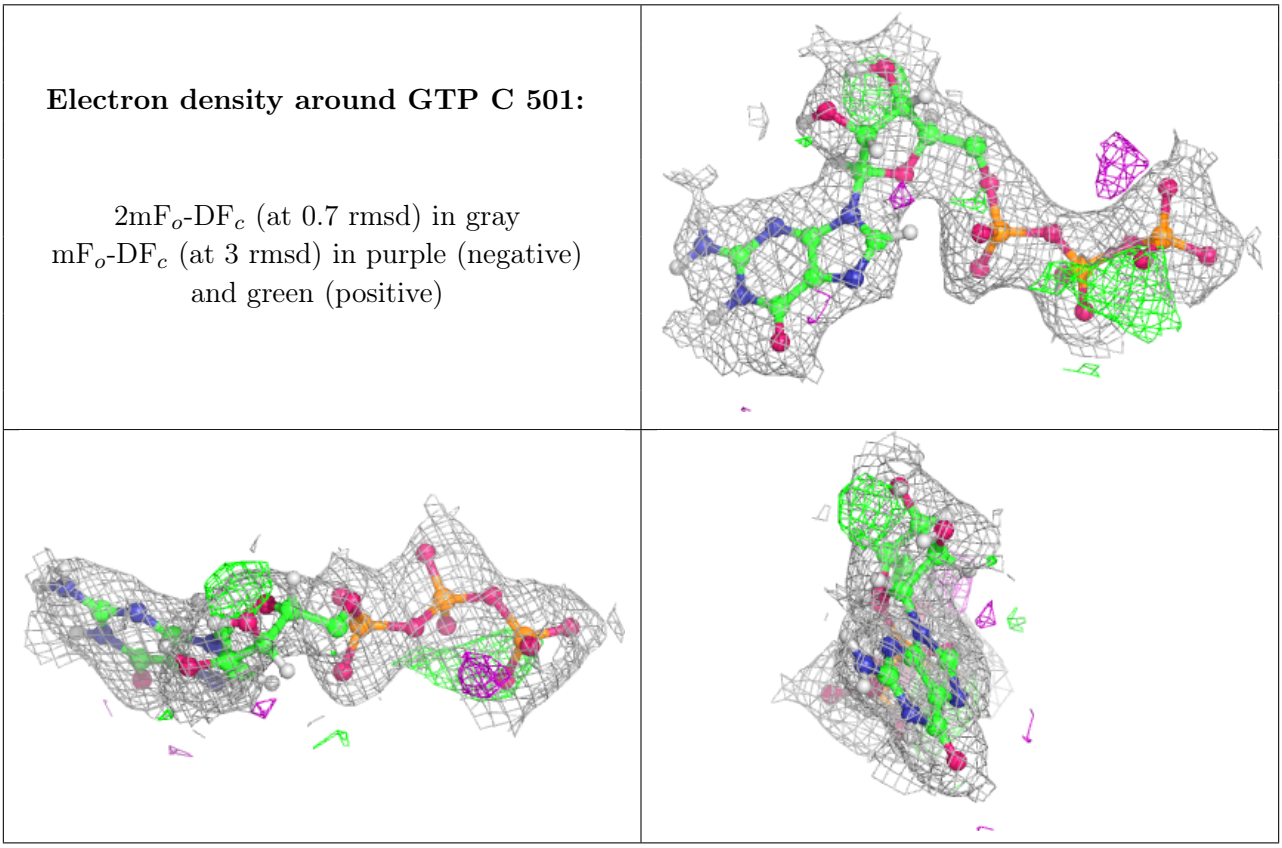
Electron density around D3L B 504:

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



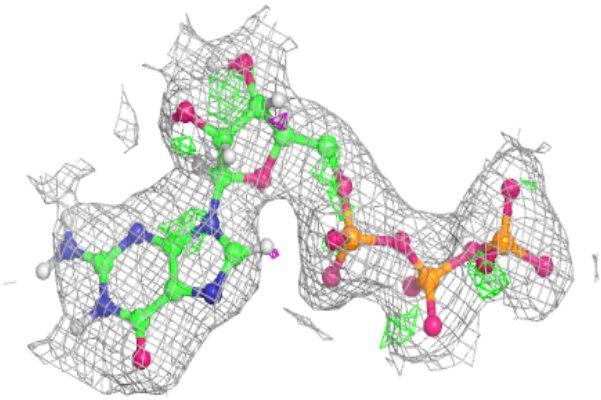
Electron density around GTP C 501:

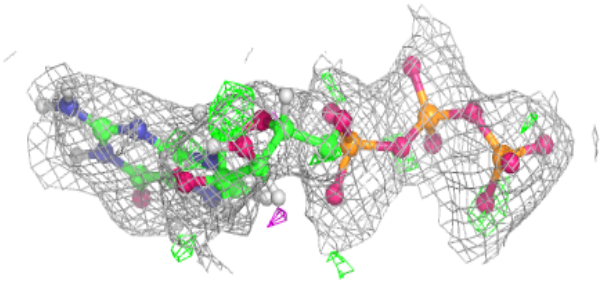
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

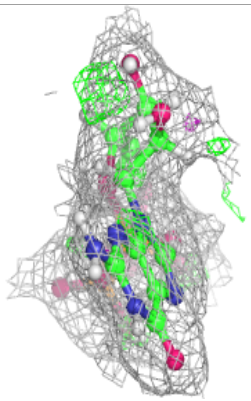


Electron density around GTP A 501:

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

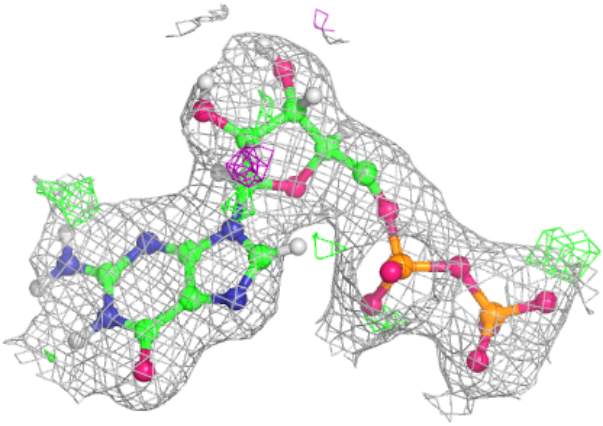


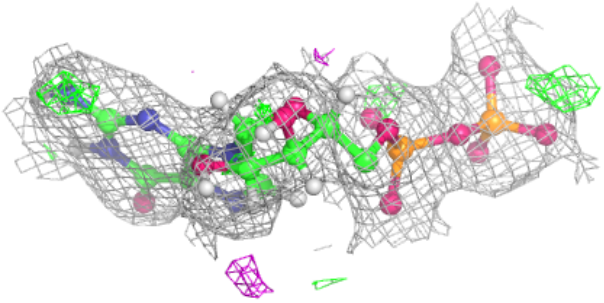


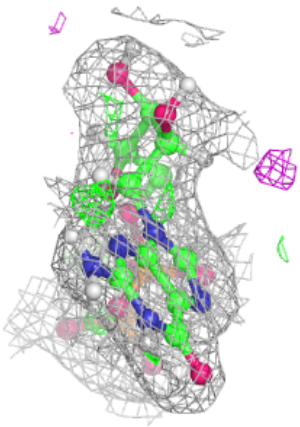


Electron density around GDP B 501:

$2mF_o$-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.