Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 10:31 AM JST

PDB ID	:	5XKE
Title	:	Crystal structure of T2R-TTL-Demecolcine complex
Authors	:	Wang, Y.; Yang, J.; Wang, T.; Chen, L.
Deposited on	:	2017-05-07
Resolution	:	2.60 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:

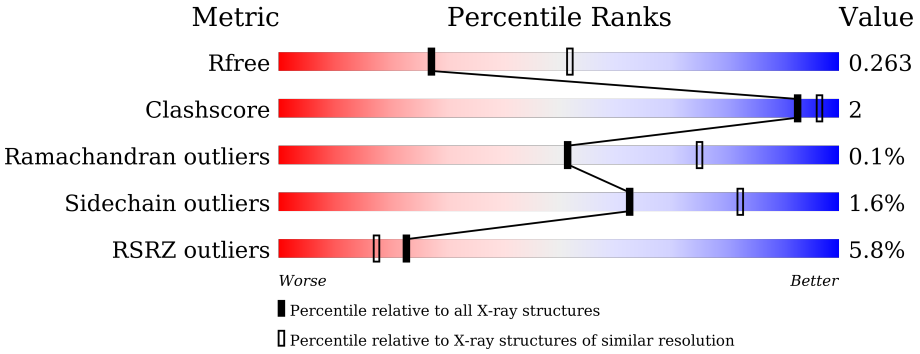
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	451	.% 90% 7% •
1	C	451	.% 94% • •
2	B	445	3% 89% 7% •
2	D	445	9% 89% 5% 5%
3	E	143	7% 83% • 15%
4	F	384	14% 82% 5% 13%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17729 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3416	2163	581	650	22	0	0	0
1	C	440	3437	2175	584	656	22	0	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3369	2115	577	650	27	0	0	0
2	D	421	3309	2080	562	640	27	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLY	GLU	conflict	UNP F2Z5B2
B	441	GLU	GLY	conflict	UNP F2Z5B2
D	440	GLY	GLU	conflict	UNP F2Z5B2
D	441	GLU	GLY	conflict	UNP F2Z5B2

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	1000	617	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

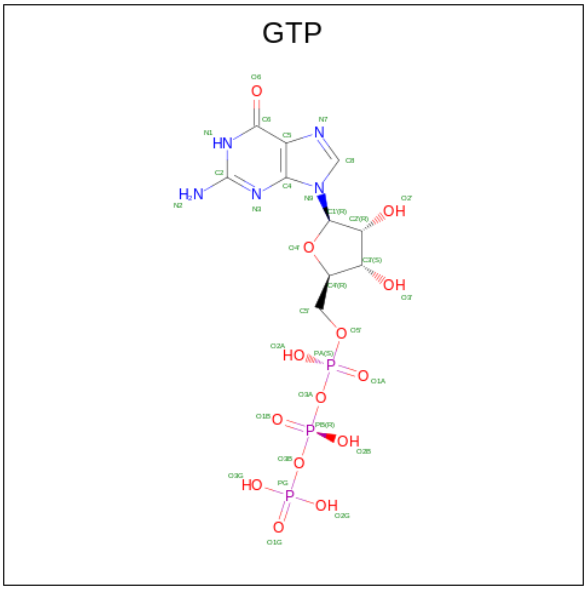
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	334	2744	1761	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	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	D	1	32	10	5	14	3	0	0

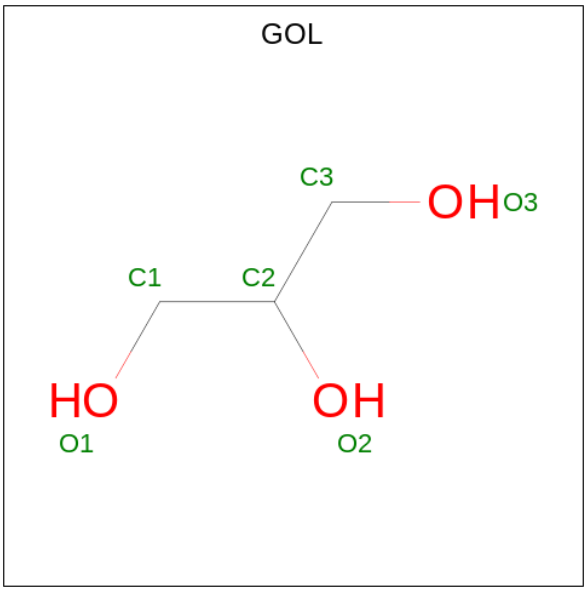
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

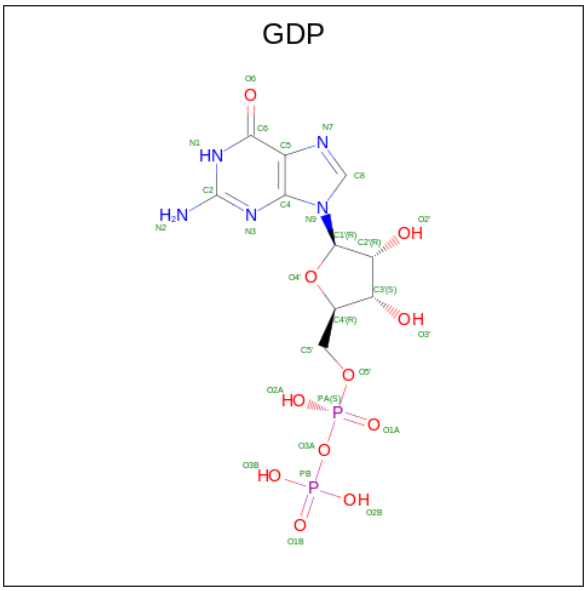
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



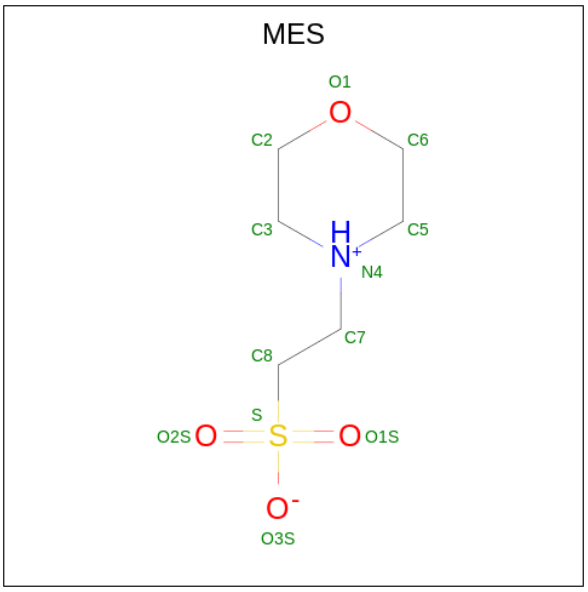
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



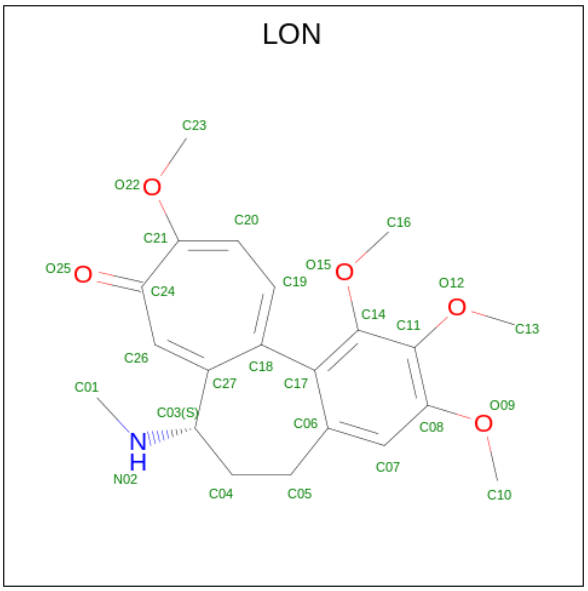
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is (7S)-1,2,3,10-tetramethoxy-7-(methylamino)-6,7-dihydro-5H-benzo[a]heptalen-9-one (three-letter code: LON) (formula: $C_{21}H_{25}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	B	1	27	21	1	5	0	0
			Total	C	N	O		
11	D	1	27	21	1	5	0	0

- Molecule 12 is water.

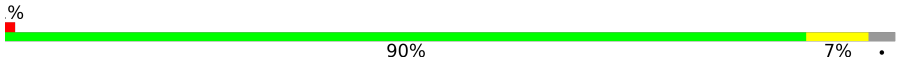
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	53	53	53	0	0
			Total	O		
12	B	55	55	55	0	0
			Total	O		
12	C	98	98	98	0	0
			Total	O		
12	D	11	11	11	0	0
			Total	O		
12	E	13	13	13	0	0
			Total	O		
12	F	22	22	22	0	0

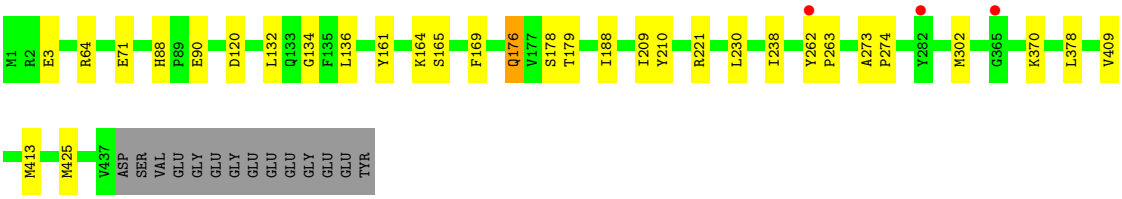
3 Residue-property plots (i)

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

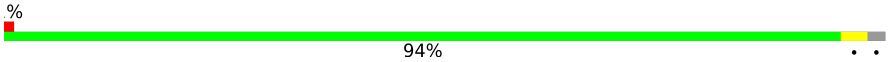
Chain A:





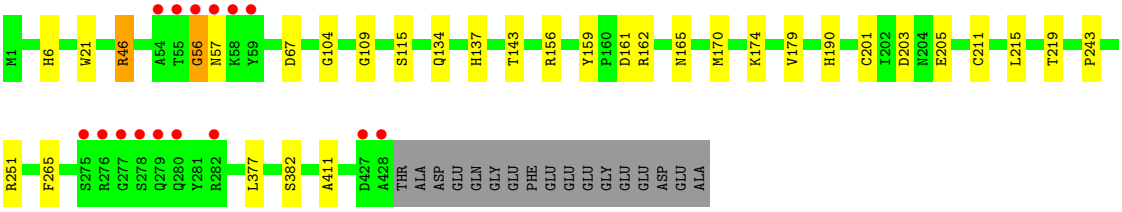
• Molecule 1: Tubulin alpha-1B chain

Chain C:



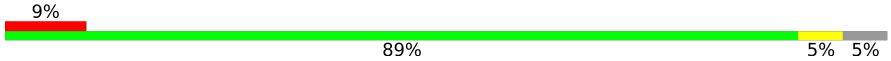
• Molecule 2: Tubulin beta chain

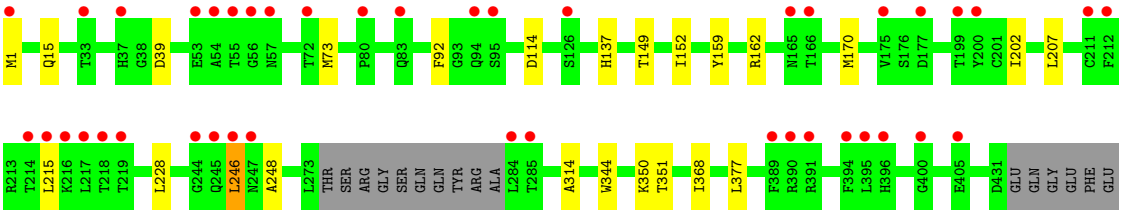
Chain B:

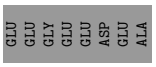


• Molecule 2: Tubulin beta chain

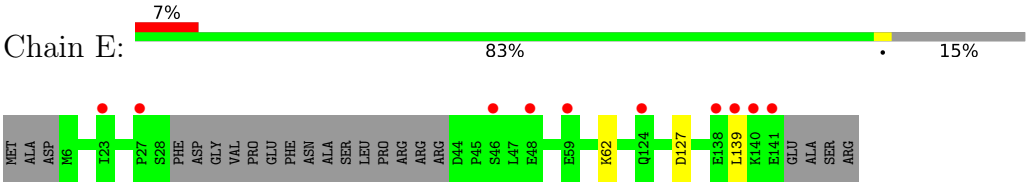
Chain D:



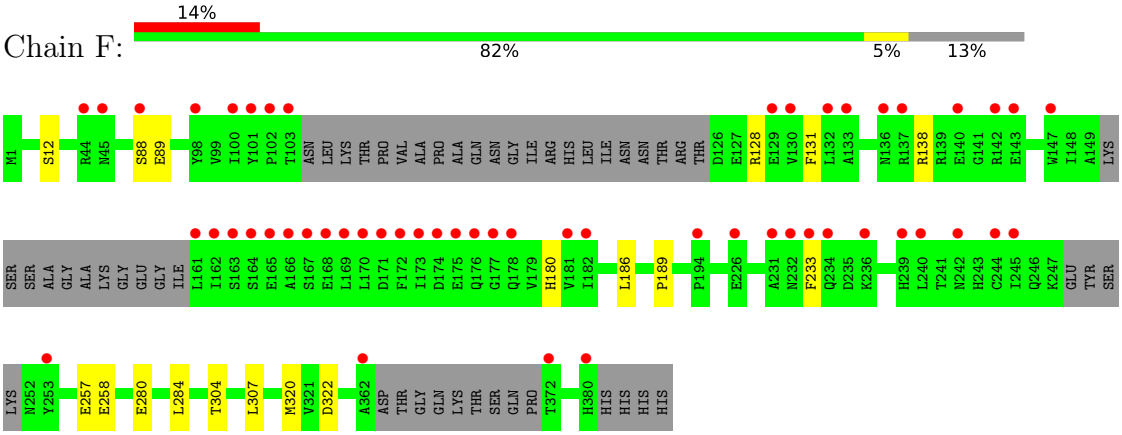




- Molecule 3: Stathmin-4



- Molecule 4: Uncharacterized protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.41Å 158.02Å 182.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 37.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.60) 99.6 (37.26-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.221 , 0.264 0.220 , 0.263	Depositor DCC
R_{free} test set	4629 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.3	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	0.94	EDS
Total number of atoms	17729	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, MES, GTP, CA, MG, GOL, LON

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	0.41	0/3494	0.59	0/4743
1	C	0.40	0/3515	0.61	0/4772
2	B	0.40	0/3444	0.57	0/4664
2	D	0.41	0/3382	0.58	0/4581
3	E	0.35	0/1008	0.54	0/1337
4	F	0.41	0/2806	0.59	0/3791
All	All	0.40	0/17649	0.59	0/23888

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	0	3331	14	0
1	C	3437	0	3348	8	0
2	B	3369	0	3250	18	0
2	D	3309	0	3189	10	0
3	E	1000	0	1018	0	0
4	F	2744	0	2709	6	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	2	0
11	B	27	0	0	0	0
11	D	27	0	0	1	0
12	A	53	0	0	0	0
12	B	55	0	0	0	0
12	C	98	0	0	0	0
12	D	11	0	0	0	0
12	E	13	0	0	0	0
12	F	22	0	0	0	0
All	All	17729	0	16914	53	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 (53) 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:190:HIS:HD2	2:B:411:ALA:HA	1.61	0.63
2:D:246:LEU:HD22	2:D:248:ALA:HB2	1.81	0.62
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.88	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.53
2:B:156:ARG:HG3	10:B:503:MES:H62	1.93	0.51
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.93	0.50
2:B:46:ARG:HH21	2:B:243:PRO:HA	1.75	0.50
2:D:350:LYS:HG3	11:D:503:LON:C24	2.42	0.50
2:B:161:ASP:O	2:B:251:ARG:NH2	2.45	0.49
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.93	0.49
2:D:149:THR:HA	2:D:152:ILE:HD12	1.93	0.49
4:F:189:PRO:HA	4:F:322:ASP:HA	1.94	0.49
2:B:134:GLN:HA	2:B:165:ASN:O	2.12	0.49
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:GLY:N	2:B:57:ASN:HA	2.30	0.47
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.96	0.47
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.97	0.47
1:A:88:HIS:HD2	1:A:90:GLU:H	1.62	0.47
4:F:128:ARG:HA	4:F:131:PHE:HB3	1.96	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.47
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.97	0.47
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.50	0.46
2:D:159:TYR:HB3	2:D:162:ARG:HG3	1.96	0.46
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.97	0.46
2:B:170:MET:HB2	2:B:203:ASP:HA	1.98	0.45
1:A:409:VAL:HA	1:A:413:MET:O	2.17	0.45
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.99	0.44
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.99	0.44
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.00	0.44
2:B:104:GLY:O	2:B:109:GLY:HA3	2.17	0.44
2:B:219:THR:HG21	1:C:326:LYS:HA	2.00	0.44
2:B:211:CYS:HA	2:B:215:LEU:HB2	2.00	0.44
1:A:273:ALA:HA	1:A:274:PRO:HA	1.81	0.44
2:D:314:ALA:HB3	2:D:368:ILE:HB	2.00	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.17	0.43
1:A:176:GLN:HG2	1:A:210:TYR:CE2	2.54	0.43
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.58	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HD3	2.01	0.43
2:B:156:ARG:CZ	10:B:503:MES:H21	2.49	0.43
2:B:159:TYR:HB3	2:B:162:ARG:HG3	2.01	0.43
2:B:67:ASP:HA	2:B:143:THR:HG21	2.02	0.42
1:A:132:LEU:HD23	1:A:164:LYS:HE3	2.02	0.41
2:D:202:ILE:HG22	2:D:207:LEU:HD11	2.02	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.41
4:F:88:SER:HA	4:F:89:GLU:HA	1.72	0.41
1:C:234:ILE:HD13	1:C:302:MET:SD	2.60	0.41
4:F:280:GLU:HA	4:F:284:LEU:HB3	2.03	0.41
4:F:186:LEU:HD13	4:F:320:MET:HG2	2.03	0.40
2:D:215:LEU:HD11	2:D:228:LEU:HD21	2.03	0.40
1:A:136:LEU:HD23	1:A:169:PHE:HE2	1.85	0.40
1:A:209:ILE:HD11	1:A:302:MET:SD	2.62	0.40
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.91	0.40
1:C:140:SER:HA	1:C:171:ILE:HB	2.03	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	435/451 (96%)	427 (98%)	7 (2%)	1 (0%)	47	71
1	C	438/451 (97%)	430 (98%)	8 (2%)	0	100	100
2	B	426/445 (96%)	418 (98%)	7 (2%)	1 (0%)	47	71
2	D	417/445 (94%)	408 (98%)	9 (2%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	324/384 (84%)	318 (98%)	6 (2%)	0	100	100
All	All	2157/2319 (93%)	2118 (98%)	37 (2%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
2	B	56	GLY

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	368/379 (97%)	362 (98%)	6 (2%)	62	82
1	C	371/379 (98%)	367 (99%)	4 (1%)	73	88
2	B	370/383 (97%)	366 (99%)	4 (1%)	73	88
2	D	364/383 (95%)	357 (98%)	7 (2%)	57	79
3	E	109/127 (86%)	106 (97%)	3 (3%)	43	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	301/342 (88%)	295 (98%)	6 (2%)	55	78
All	All	1883/1993 (94%)	1853 (98%)	30 (2%)	62	82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	120	ASP
1	A	176	GLN
1	A	179	THR
1	A	221	ARG
1	A	370	LYS
2	B	46	ARG
2	B	115	SER
2	B	137	HIS
2	B	382	SER
1	C	221	ARG
1	C	251	ASP
1	C	302	MET
1	C	381	THR
2	D	1	MET
2	D	15	GLN
2	D	39	ASP
2	D	114	ASP
2	D	137	HIS
2	D	246	LEU
2	D	351	THR
3	E	62	LYS
3	E	127	ASP
3	E	139	LEU
4	F	12	SER
4	F	138	ARG
4	F	180	HIS
4	F	233	PHE
4	F	257	GLU
4	F	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS

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Mol	Chain	Res	Type
1	A	176	GLN
1	A	329	ASN
2	B	190	HIS
2	B	332	ASN
2	B	375	GLN
1	C	11	GLN
2	D	347	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	LON	D	503	-	29,29,29	3.31	14 (48%)	41,41,41	3.59	12 (29%)
5	GTP	A	501	6	26,34,34	0.90	0	32,54,54	1.16	3 (9%)
9	GDP	B	501	6	24,30,30	0.92	0	30,47,47	1.12	3 (10%)
11	LON	B	504	-	29,29,29	3.34	14 (48%)	41,41,41	3.56	13 (31%)
5	GTP	D	501	6	26,34,34	0.93	0	32,54,54	1.33	5 (15%)
8	GOL	A	504	-	5,5,5	0.23	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	MES	B	503	-	12,12,12	2.26	1 (8%)	14,16,16	1.59	3 (21%)
5	GTP	C	501	6	26,34,34	0.88	0	32,54,54	1.11	3 (9%)

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	LON	D	503	-	-	4/8/23/23	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	LON	B	504	-	-	4/8/23/23	0/3/3/3
5	GTP	D	501	6	-	3/18/38/38	0/3/3/3
8	GOL	A	504	-	-	4/4/4/4	-
10	MES	B	503	-	-	2/6/14/14	0/1/1/1
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.38	1.67	1.77
11	B	504	LON	C17-C06	-7.17	1.26	1.41
11	D	503	LON	C17-C06	-7.04	1.26	1.41
11	D	503	LON	C17-C14	5.62	1.53	1.40
11	B	504	LON	C07-C06	5.52	1.48	1.39
11	B	504	LON	C17-C18	-5.46	1.43	1.50
11	B	504	LON	C17-C14	5.43	1.53	1.40
11	D	503	LON	C07-C06	5.35	1.48	1.39
11	D	503	LON	C17-C18	-5.22	1.43	1.50
11	B	504	LON	C03-C27	4.97	1.62	1.53
11	D	503	LON	C04-C03	4.93	1.61	1.53
11	D	503	LON	C03-C27	4.79	1.61	1.53
11	B	504	LON	C04-C03	4.67	1.61	1.53
11	B	504	LON	C26-C27	4.39	1.44	1.36
11	B	504	LON	O09-C08	4.37	1.44	1.37
11	D	503	LON	C26-C27	4.35	1.44	1.36
11	B	504	LON	C03-N02	-4.30	1.37	1.46
11	D	503	LON	C03-N02	-4.19	1.37	1.46
11	D	503	LON	O09-C08	4.15	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	LON	O22-C21	3.93	1.43	1.35
11	B	504	LON	O22-C21	3.83	1.42	1.35
11	D	503	LON	O15-C14	3.74	1.45	1.38
11	B	504	LON	C18-C27	-3.68	1.39	1.44
11	B	504	LON	O15-C14	3.68	1.45	1.38
11	D	503	LON	C18-C27	-3.57	1.39	1.44
11	D	503	LON	O12-C11	3.16	1.44	1.38
11	B	504	LON	C21-C24	2.84	1.51	1.47
11	B	504	LON	O12-C11	2.81	1.43	1.38
11	D	503	LON	C21-C24	2.50	1.50	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	503	LON	C17-C18-C19	-12.94	93.43	117.12
11	B	504	LON	C17-C18-C19	-12.52	94.19	117.12
11	B	504	LON	C17-C18-C27	10.94	127.31	118.51
11	D	503	LON	C17-C18-C27	10.06	126.60	118.51
11	D	503	LON	C14-C17-C18	-8.52	112.20	121.09
11	B	504	LON	C14-C17-C18	-8.02	112.72	121.09
11	D	503	LON	C06-C17-C18	7.33	128.83	120.25
11	B	504	LON	C06-C17-C18	7.12	128.58	120.25
11	B	504	LON	O22-C21-C20	-5.87	113.06	122.30
11	D	503	LON	O22-C21-C20	-5.39	113.82	122.30
11	D	503	LON	O22-C21-C24	5.24	114.67	109.56
11	B	504	LON	O22-C21-C24	5.17	114.60	109.56
11	D	503	LON	C03-C27-C18	-3.38	111.85	115.27
11	D	503	LON	C03-C27-C26	-3.28	114.02	117.12
10	B	503	MES	O1S-S-C8	3.16	110.72	106.92
5	D	501	GTP	PA-O3A-PB	-3.12	122.14	132.83
5	D	501	GTP	PB-O3B-PG	-3.02	122.46	132.83
11	B	504	LON	C27-C03-N02	-2.97	111.43	114.45
11	D	503	LON	O09-C08-C11	2.92	120.30	115.16
11	B	504	LON	O09-C08-C11	2.91	120.28	115.16
11	D	503	LON	O09-C08-C07	-2.70	119.47	124.12
5	C	501	GTP	PA-O3A-PB	-2.47	124.36	132.83
5	C	501	GTP	C8-N7-C5	2.46	107.67	102.99
11	D	503	LON	C05-C04-C03	2.46	115.36	112.21
10	B	503	MES	C5-N4-C3	2.45	114.34	108.83
9	B	501	GDP	C5-C6-N1	2.45	118.27	113.95
5	A	501	GTP	C8-N7-C5	2.44	107.64	102.99
11	B	504	LON	C05-C04-C03	2.44	115.33	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	GTP	C5-C6-N1	2.40	118.19	113.95
11	B	504	LON	C27-C26-C24	-2.34	129.20	133.89
9	B	501	GDP	PA-O3A-PB	-2.30	124.93	132.83
11	B	504	LON	C03-C27-C18	-2.29	112.95	115.27
11	B	504	LON	O09-C08-C07	-2.28	120.20	124.12
5	D	501	GTP	C8-N7-C5	2.27	107.31	102.99
5	A	501	GTP	PA-O3A-PB	-2.24	125.12	132.83
5	A	501	GTP	C5-C6-N1	2.24	117.90	113.95
9	B	501	GDP	C8-N7-C5	2.21	107.20	102.99
11	B	504	LON	C03-C27-C26	-2.19	115.05	117.12
10	B	503	MES	O3S-S-C8	2.19	109.31	105.77
5	C	501	GTP	C5-C6-N1	2.04	117.55	113.95
5	D	501	GTP	C3'-C2'-C1'	2.02	104.02	100.98
11	D	503	LON	C27-C03-N02	-2.01	112.41	114.45

There are no chirality outliers.

All (34) 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
9	B	501	GDP	C5'-O5'-PA-O1A
10	B	503	MES	C8-C7-N4-C5
11	B	504	LON	C20-C21-O22-C23
11	B	504	LON	C24-C21-O22-C23
11	D	503	LON	C20-C21-O22-C23
11	D	503	LON	C24-C21-O22-C23
11	B	504	LON	C11-C08-O09-C10
11	D	503	LON	C11-C08-O09-C10
11	B	504	LON	C07-C08-O09-C10
11	D	503	LON	C07-C08-O09-C10
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	C1-C2-C3-O3
8	A	504	GOL	O2-C2-C3-O3
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
8	A	504	GOL	O1-C1-C2-O2
9	B	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A

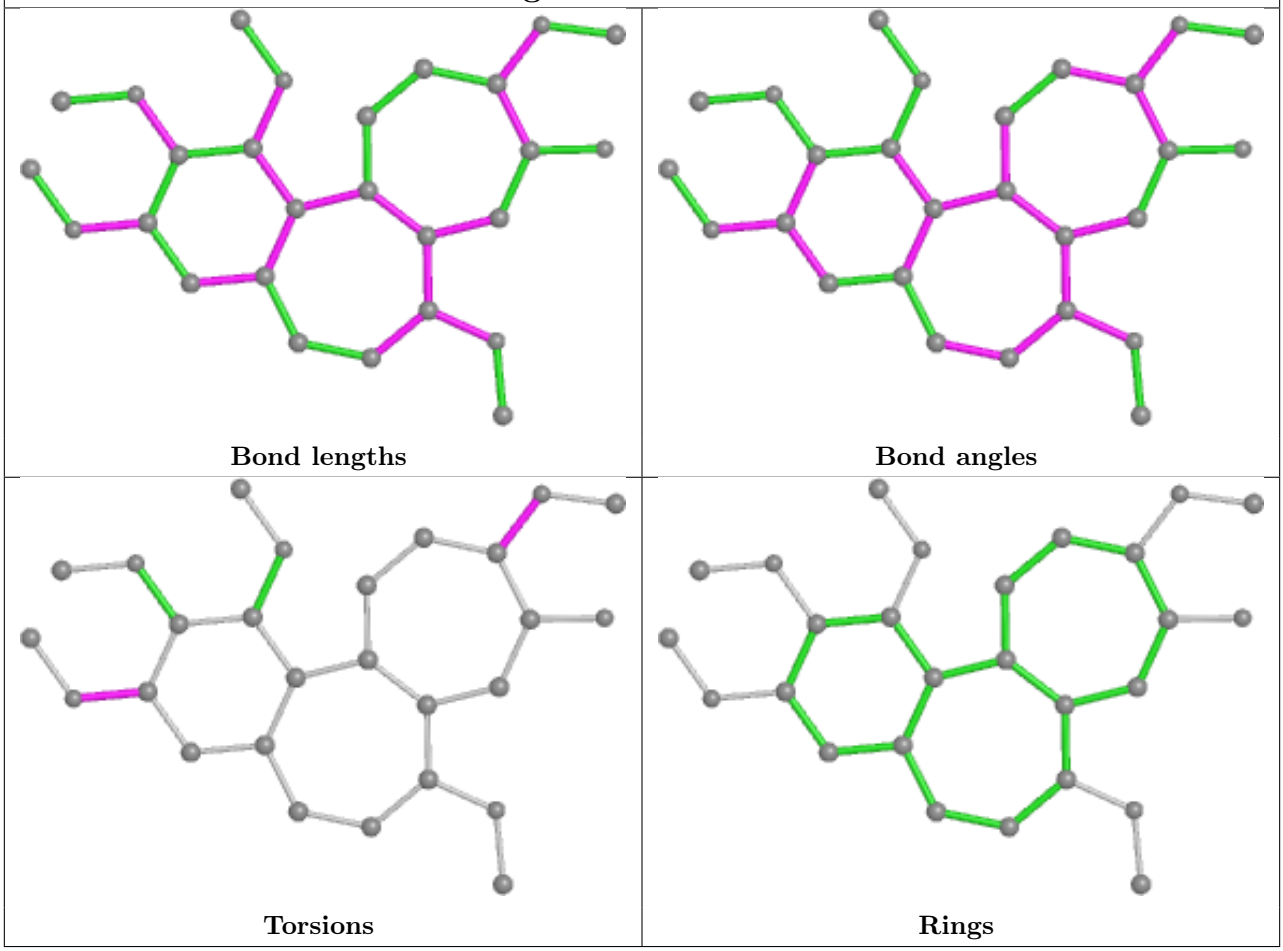
There are no ring outliers.

2 monomers are involved in 3 short contacts:

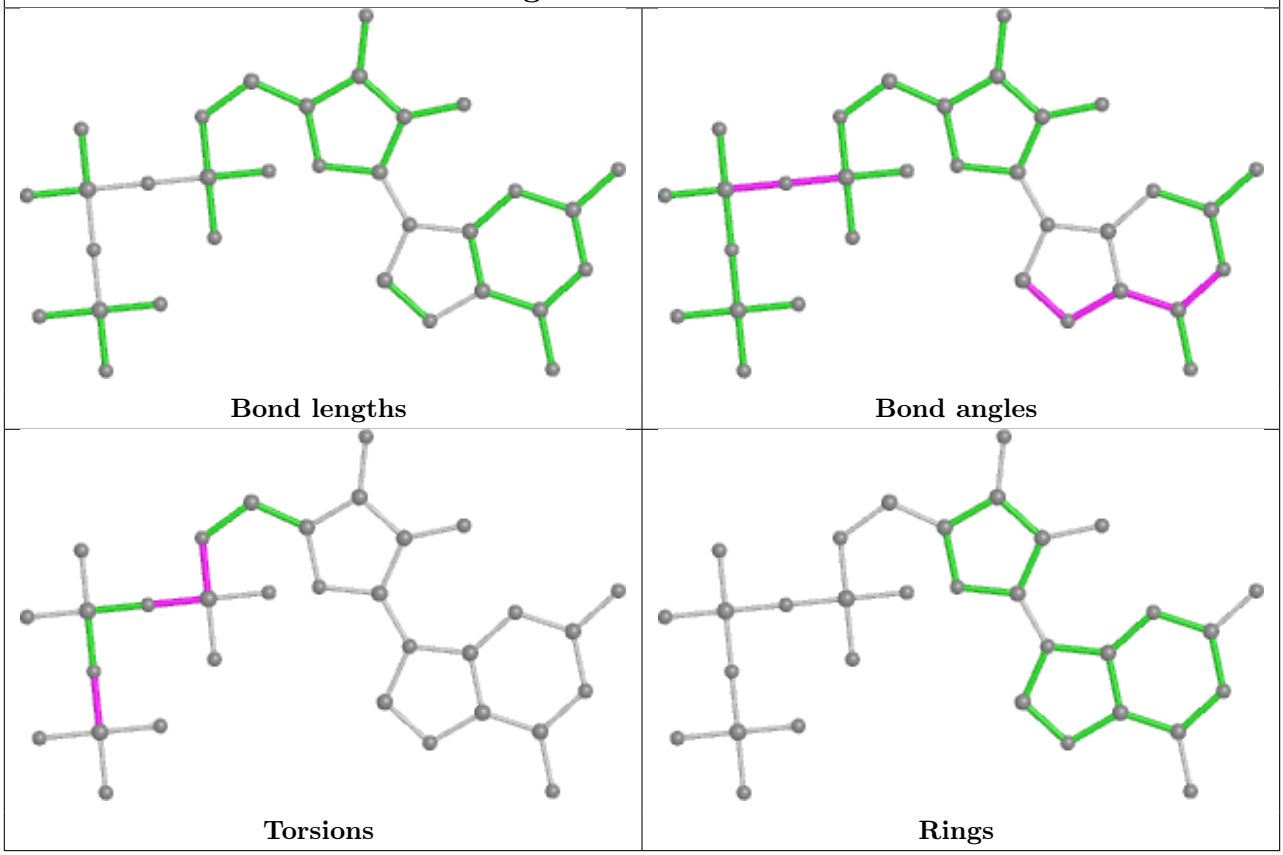
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	503	LON	1	0
10	B	503	MES	2	0

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

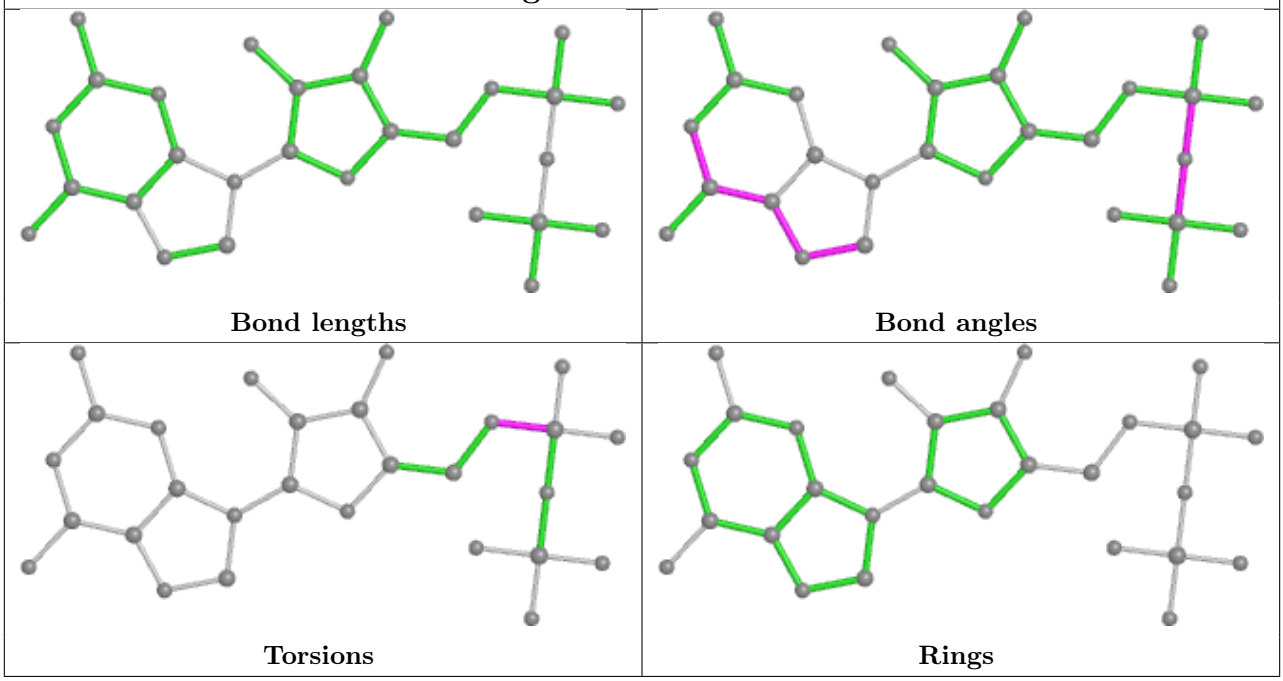
Ligand LON D 503



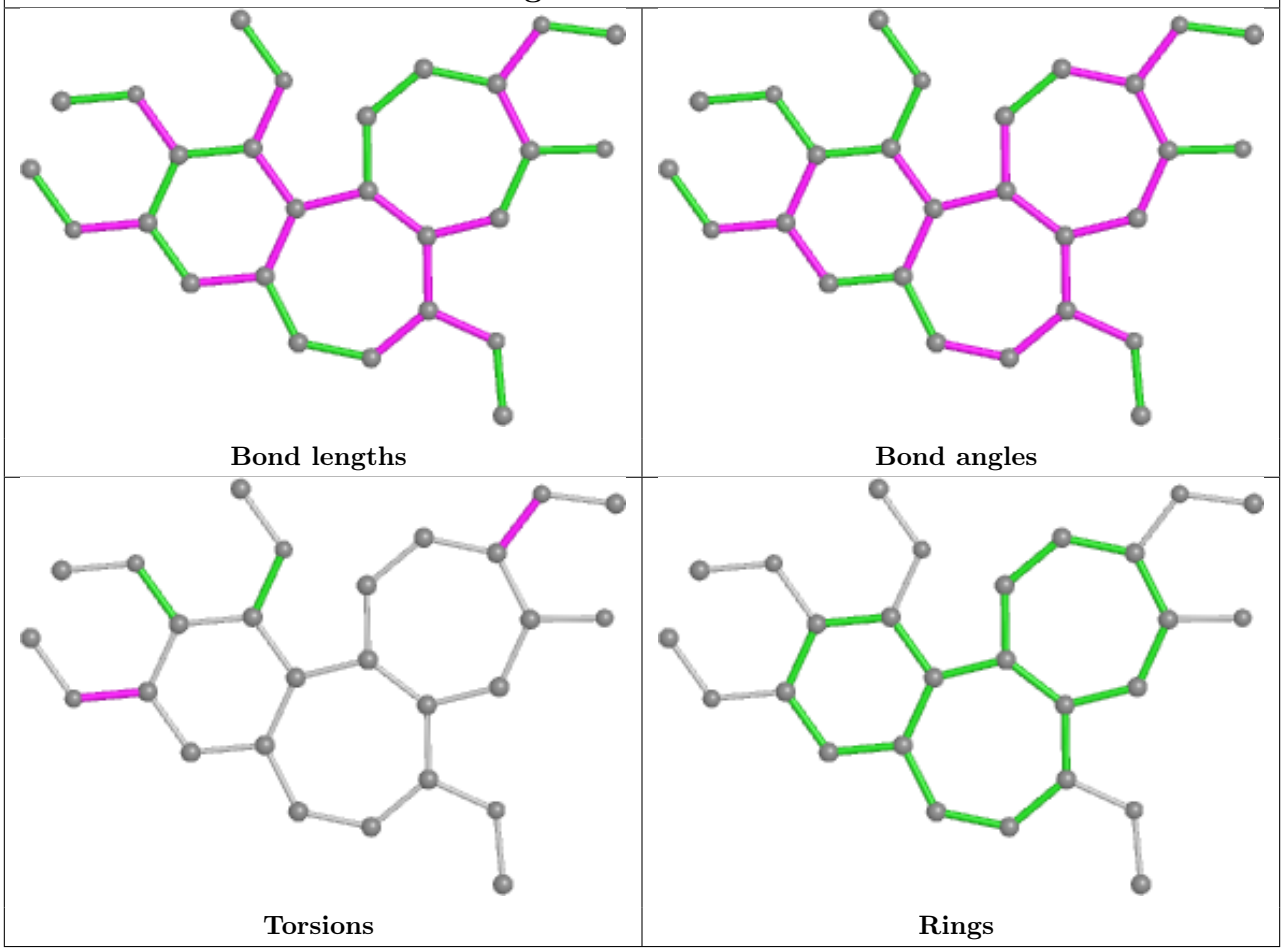
Ligand GTP A 501



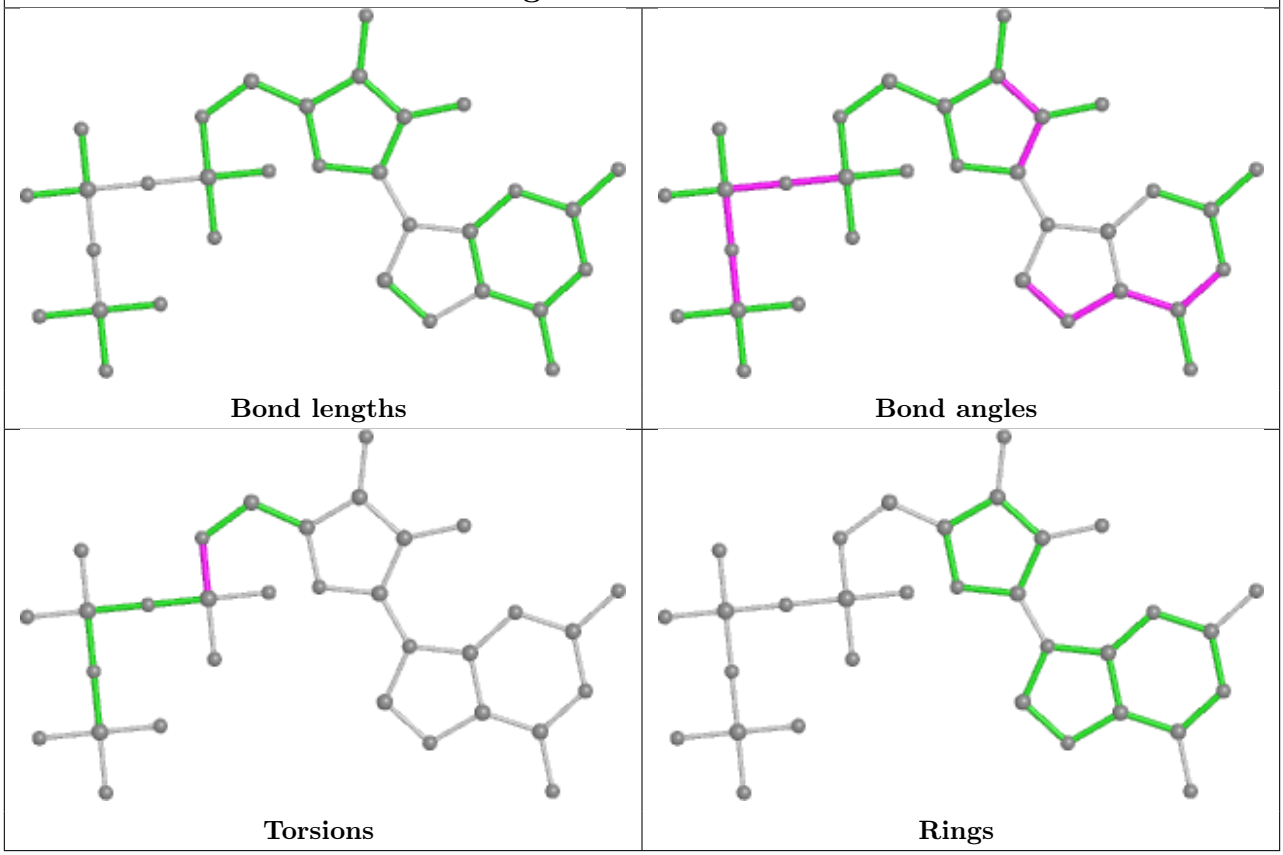
Ligand GDP B 501



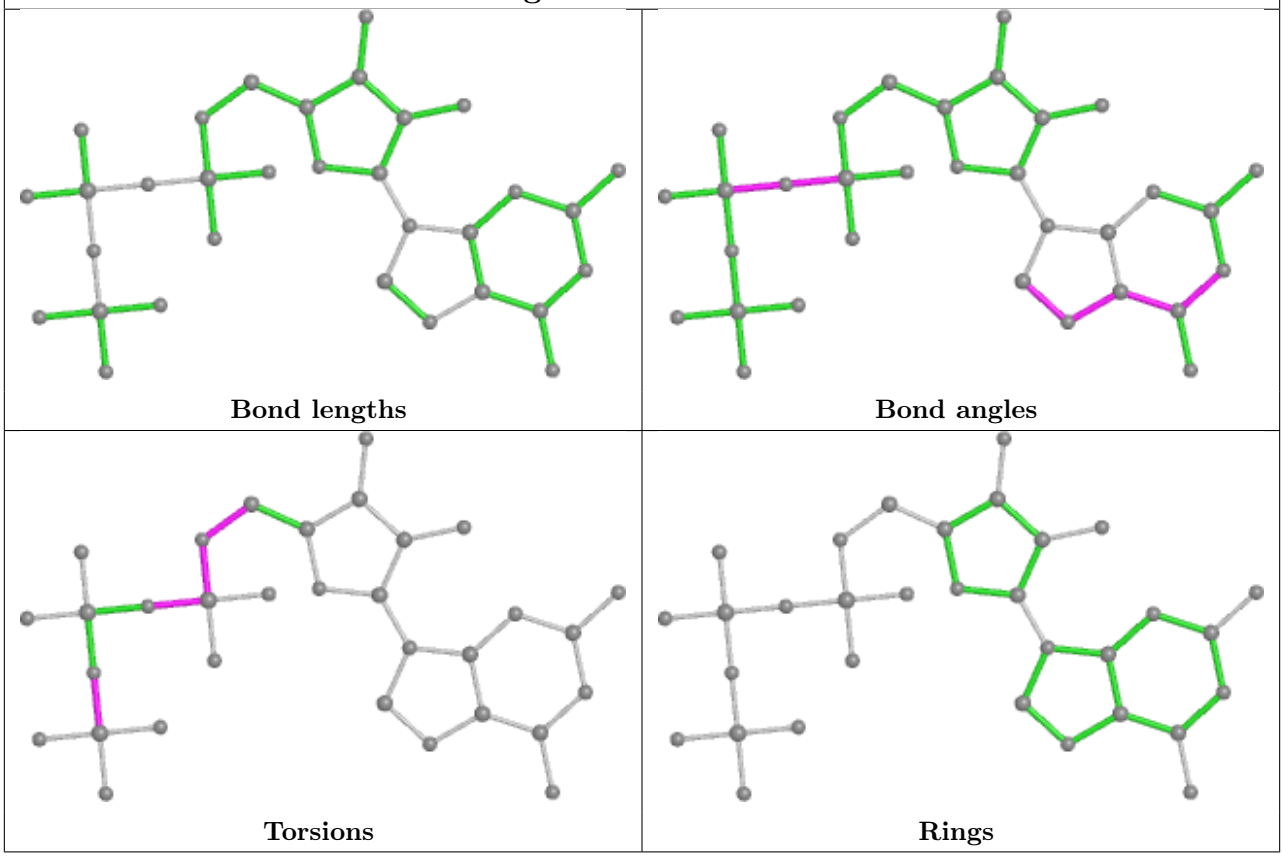
Ligand LON B 504



Ligand GTP D 501



Ligand GTP C 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	437/451 (96%)	-0.05	3 (0%)	87	86	31, 50, 74, 88	0
1	C	440/451 (97%)	-0.24	3 (0%)	87	86	25, 41, 64, 77	0
2	B	428/445 (96%)	0.13	15 (3%)	44	36	29, 49, 89, 121	0
2	D	421/445 (94%)	0.59	42 (9%)	7	4	41, 72, 109, 127	0
3	E	121/143 (84%)	0.57	10 (8%)	11	8	41, 67, 99, 117	0
4	F	334/384 (86%)	0.80	54 (16%)	1	1	40, 75, 138, 151	0
All	All	2181/2319 (94%)	0.23	127 (5%)	23	17	25, 56, 107, 151	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	7.7
2	D	1	MET	6.8
4	F	173	ILE	6.4
4	F	234	GLN	6.2
2	D	245	GLN	5.6
4	F	231	ALA	5.5
4	F	166	ALA	5.5
4	F	132	LEU	5.4
4	F	170	LEU	5.4
4	F	102	PRO	5.1
2	B	57	ASN	5.0
4	F	143	GLU	4.9
2	B	279	GLN	4.9
4	F	163	SER	4.8
2	B	55	THR	4.6
2	B	56	GLY	4.6
4	F	101	TYR	4.5
4	F	171	ASP	4.4
2	D	55	THR	4.4

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Mol	Chain	Res	Type	RSRZ
4	F	167	SER	4.3
4	F	232	ASN	4.3
2	D	72	THR	4.3
4	F	245	ILE	4.3
4	F	175	GLU	4.3
4	F	178	GLN	4.2
2	B	277	GLY	4.1
4	F	226	GLU	4.0
3	E	48	GLU	4.0
2	B	58	LYS	4.0
4	F	177	GLY	4.0
3	E	46	SER	4.0
4	F	182	ILE	3.9
4	F	240	LEU	3.8
4	F	133	ALA	3.8
4	F	130	VAL	3.8
4	F	103	THR	3.8
2	D	53	GLU	3.7
4	F	168	GLU	3.7
2	D	247	ASN	3.7
2	D	391	ARG	3.6
4	F	244	CYS	3.6
2	D	216	LYS	3.6
4	F	136	ASN	3.6
4	F	169	LEU	3.6
4	F	142	ARG	3.5
3	E	139	LEU	3.5
2	D	218	THR	3.5
4	F	88	SER	3.4
2	D	219	THR	3.4
4	F	162	ILE	3.4
2	D	285	THR	3.3
4	F	161	LEU	3.3
2	D	217	LEU	3.3
4	F	137	ARG	3.2
4	F	164	SER	3.2
2	B	275	SER	3.2
2	D	214	THR	3.2
2	D	390	ARG	3.2
4	F	100	ILE	3.2
4	F	129	GLU	3.1
2	B	278	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	244	GLY	3.1
2	D	54	ALA	3.1
4	F	140	GLU	3.0
3	E	27	PRO	3.0
2	D	215	LEU	2.9
2	B	282	ARG	2.9
4	F	239	HIS	2.9
4	F	147	TRP	2.9
4	F	372	THR	2.9
2	B	280	GLN	2.8
2	D	396	HIS	2.8
2	D	284	LEU	2.8
4	F	362	ALA	2.8
4	F	380	HIS	2.8
3	E	141	GLU	2.7
4	F	194	PRO	2.7
4	F	176	GLN	2.7
1	C	340	SER	2.7
4	F	174	ASP	2.7
4	F	165	GLU	2.6
2	D	165	ASN	2.6
2	D	394	PHE	2.6
2	B	276	ARG	2.6
1	A	262	TYR	2.5
2	D	395	LEU	2.5
2	D	95	SER	2.5
2	D	56	GLY	2.5
3	E	140	LYS	2.5
4	F	236	LYS	2.5
4	F	45	ASN	2.5
2	D	246	LEU	2.4
2	B	428	ALA	2.4
3	E	138	GLU	2.4
3	E	23	ILE	2.4
2	D	212	PHE	2.4
4	F	172	PHE	2.4
2	D	37	HIS	2.4
2	B	54	ALA	2.3
2	D	83	GLN	2.3
2	D	166	THR	2.3
2	D	175	VAL	2.3
2	D	57	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	2.3
2	D	199	THR	2.3
2	D	405	GLU	2.2
1	C	440	VAL	2.2
4	F	181	VAL	2.2
3	E	59	GLU	2.2
2	D	211	CYS	2.2
1	C	84	ARG	2.2
2	B	427	ASP	2.2
4	F	98	TYR	2.2
2	D	389	PHE	2.1
4	F	44	ARG	2.1
2	D	177	ASP	2.1
2	D	33	THR	2.1
1	A	365	GLY	2.1
2	D	200	TYR	2.1
2	D	94	GLN	2.1
2	D	126	SER	2.1
2	D	80	PRO	2.1
3	E	124	GLN	2.1
2	B	59	TYR	2.1
4	F	253	TYR	2.1
2	D	400	GLY	2.0
4	F	242	ASN	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)

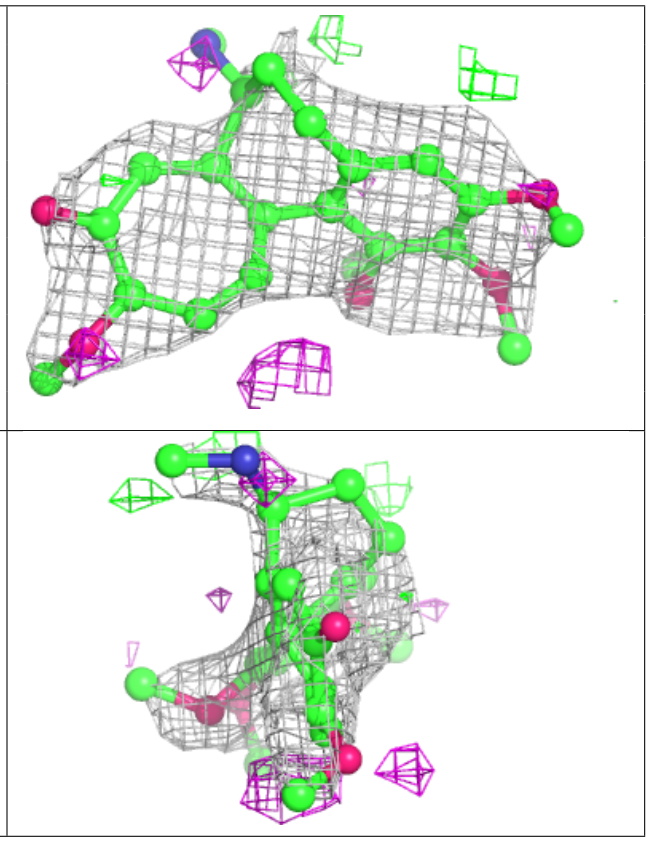
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	LON	D	503	27/27	0.84	0.30	92,97,102,104	0
10	MES	B	503	12/12	0.85	0.23	73,79,86,87	0
7	CA	A	503	1/1	0.85	0.15	72,72,72,72	0
6	MG	D	502	1/1	0.89	0.10	77,77,77,77	0
11	LON	B	504	27/27	0.92	0.26	55,57,60,62	0
8	GOL	A	504	6/6	0.92	0.23	75,77,78,79	0
5	GTP	D	501	32/32	0.93	0.14	61,66,77,79	0
7	CA	C	503	1/1	0.94	0.13	69,69,69,69	0
6	MG	B	502	1/1	0.97	0.13	28,28,28,28	0
6	MG	A	502	1/1	0.97	0.08	33,33,33,33	0
5	GTP	A	501	32/32	0.98	0.14	34,36,37,38	0
6	MG	C	502	1/1	0.98	0.16	34,34,34,34	0
9	GDP	B	501	28/28	0.98	0.15	30,35,36,38	0
5	GTP	C	501	32/32	0.99	0.16	30,32,33,35	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.

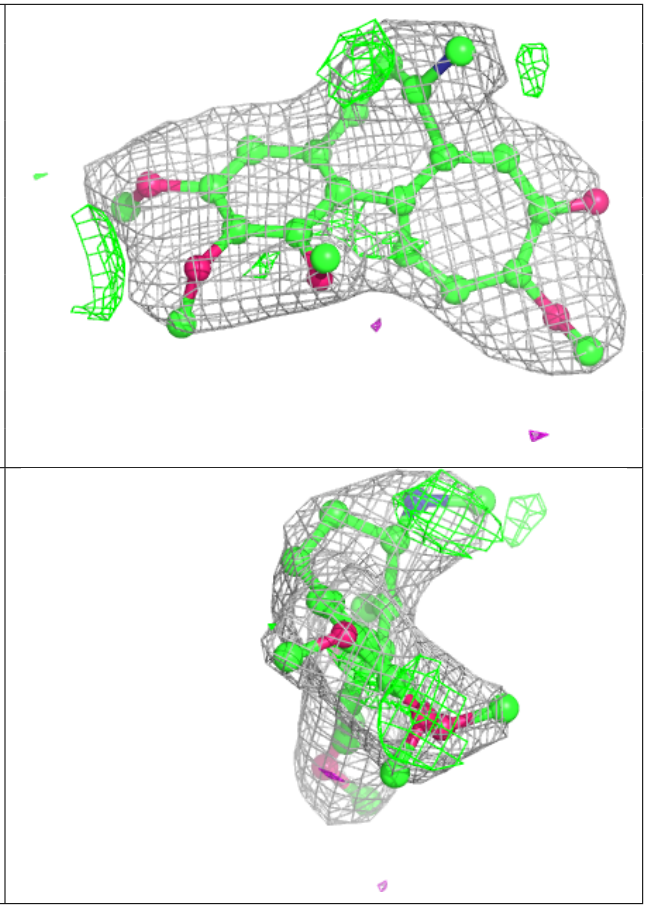
Electron density around LON D 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



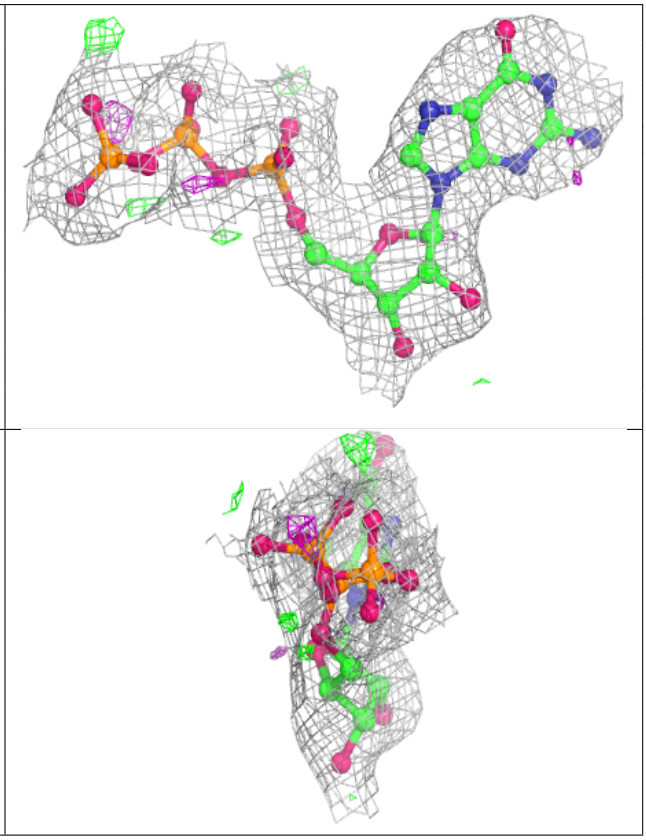
Electron density around LON B 504:

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



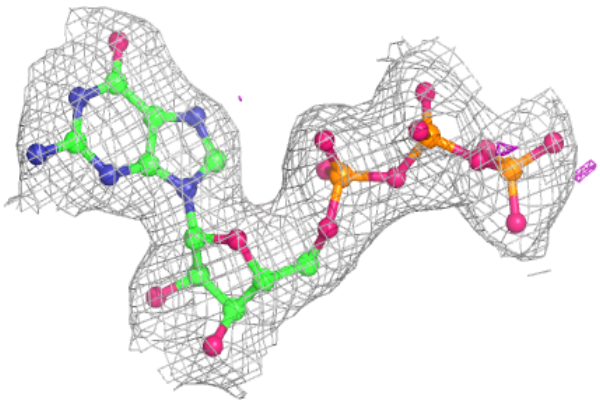
Electron density around GTP D 501:

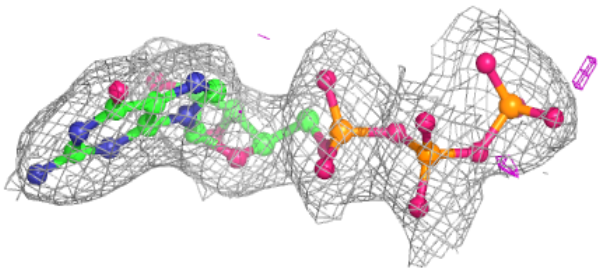
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

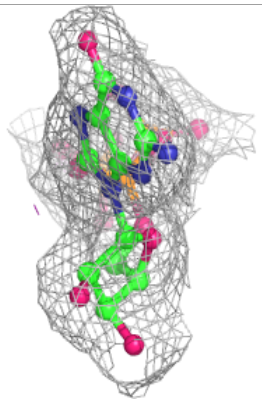


Electron density around GTP A 501:

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

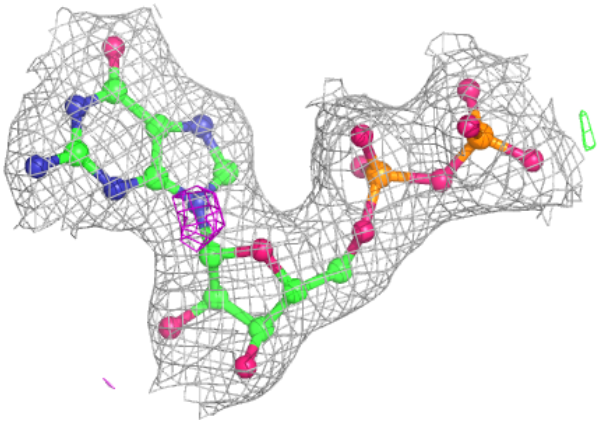


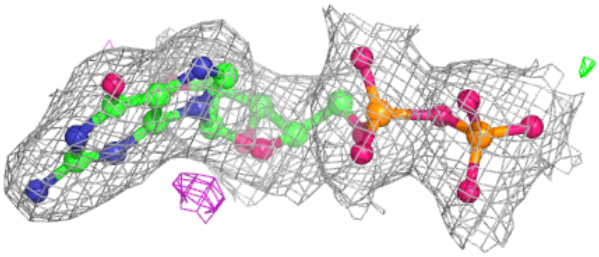


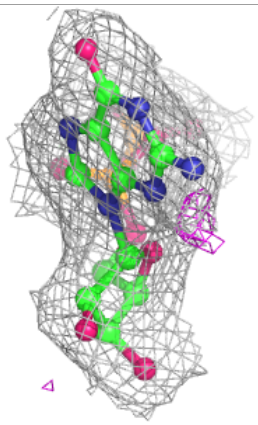


Electron density around GDP B 501:

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

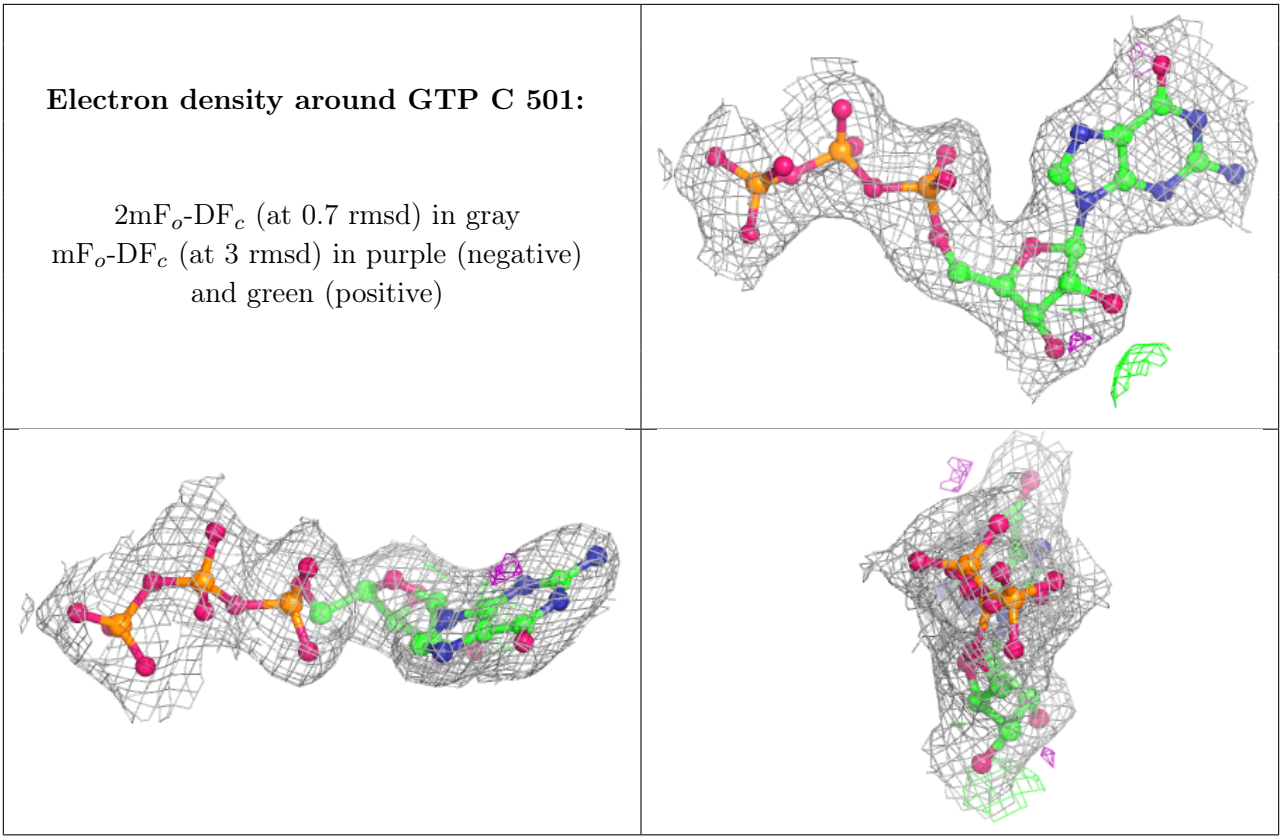






Electron density around GTP C 501:

$2mF_o$-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.