Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 08:59 pm GMT

PDB ID	:	5JH7
Title	:	Tubulin-Eribulin complex
Authors	:	Doodhi, H.; Prota, A.E.; Rodriguez-Garcia, R.; Xiao, H.; Custar, D.W.; Bargsten, K.; Katrukha, E.A.; Hilbert, M.; Hua, S.; Jiang, K.; Grigoriev, I.; Yang, C.-P.H.; Cox, D.; Band Horwitz, S.; Kapitein, L.C.; Akhmanova, A.; Steinmetz, M.O.
Deposited on	:	2016-04-20
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:

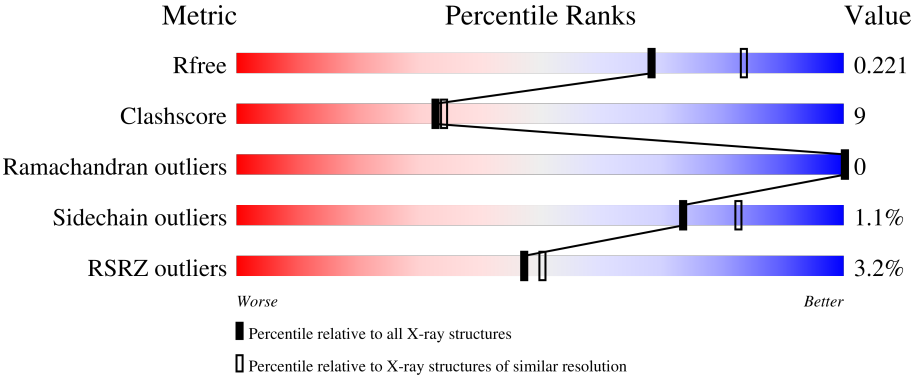
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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	450	.% 83% 14% • •
1	C	450	83% 14% • •
2	B	445	2% 77% 19% •
2	D	445	3% 74% 22% 5%
3	E	143	2% 69% 16% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	11% 70% 18% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	IMD	B	507	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 18483 atoms, of which 118 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	439	3436	2174	583	655	24	0	2	0
1	C	440	3437	2175	584	656	22	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3360	2112	573	648	27	0	1	0
2	D	424	3335	2095	568	644	28	0	1	0

- 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	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

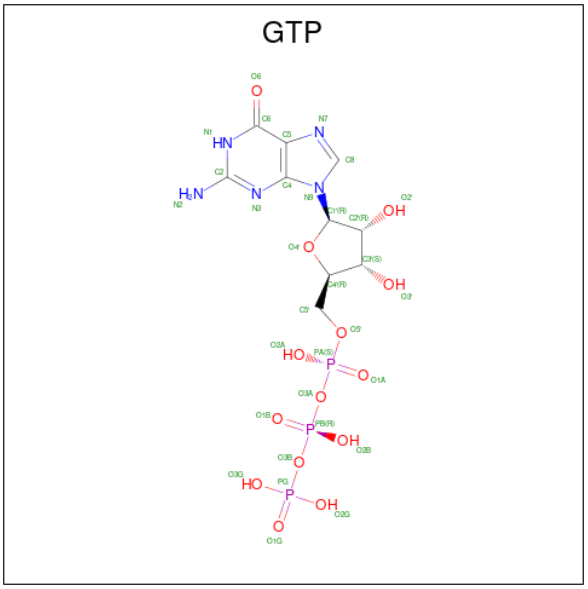
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	342	2800	1797	477	512	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
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

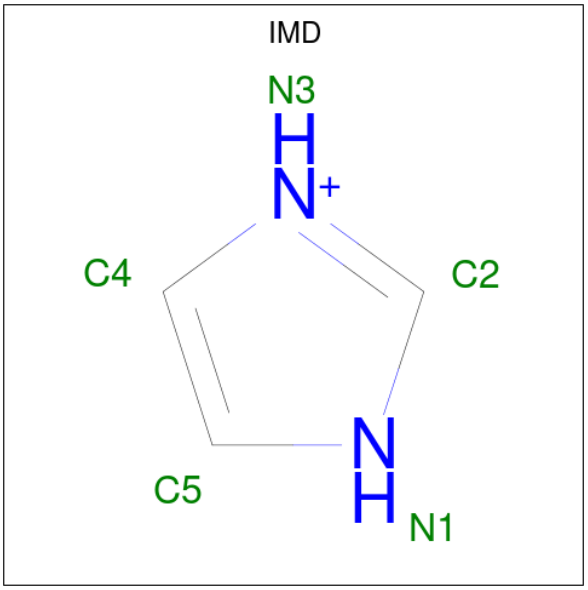
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

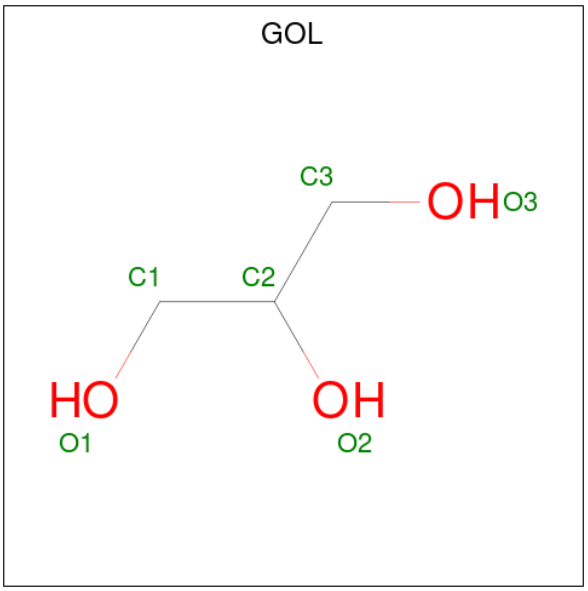
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
7	B	1	1	1	0	0
7	C	2	2	2	0	0
7	E	1	1	1	0	0

- Molecule 8 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



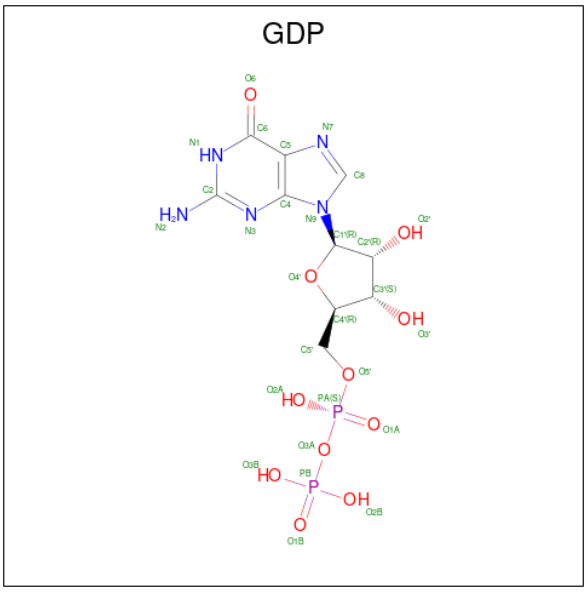
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
8	A	1	5	3	2	0	0
8	B	1	5	3	2	0	0
8	B	1	5	3	2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 10 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		
10	B	1	28	10	5	11	2	0	0

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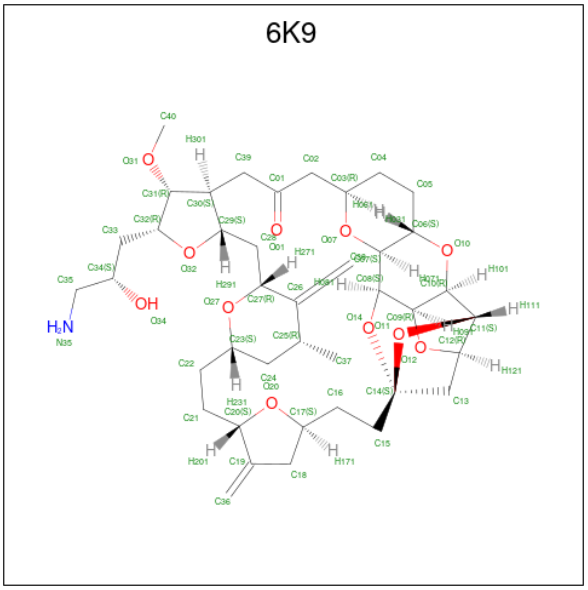
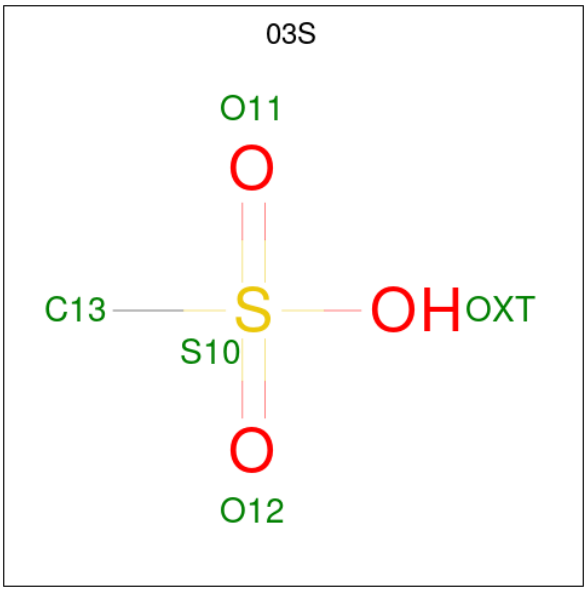
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
10	D	1	28	10	5	11	2	0	0

- Molecule 11 is (1S,3S,6S,9S,12S,14R,16R,18S,20R,21R,22S,26R,29S,31R,32S,33R,35R,36S)-20-[(2S)-3-amino-2-hydroxypropyl]-21-methoxy-14-methyl-8,15-dimethylidene-2,19,30,34,37,39,40,41-octaoxanonacyclo[24.9.2.1 3,32 .1 3,33 .1 6,9 .1 12,16 .0 18,22 .0 29,36 .0 31,35]hen tetracontan-24-one (non-preferred name) (three-letter code: 6K9) (formula: $C_{40}H_{59}NO_{11}$).



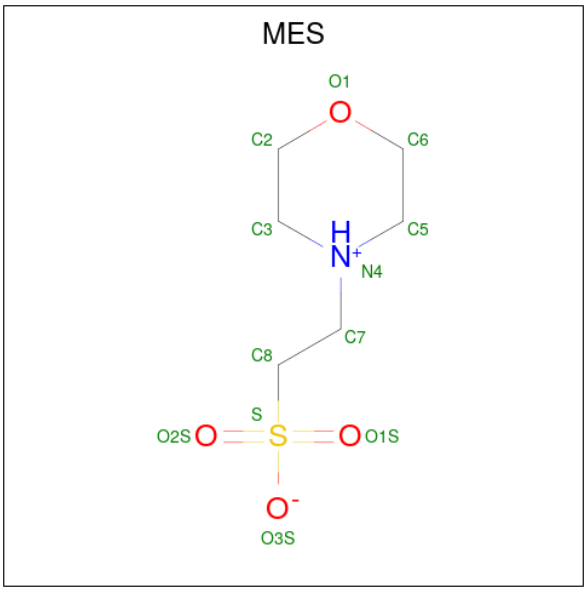
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
11	B	1	111	40	59	1	11	0	0
			Total	C	H	N	O		
11	D	1	111	40	59	1	11	0	0

- Molecule 12 is methanesulfonic acid (three-letter code: 03S) (formula: CH_4O_3S).



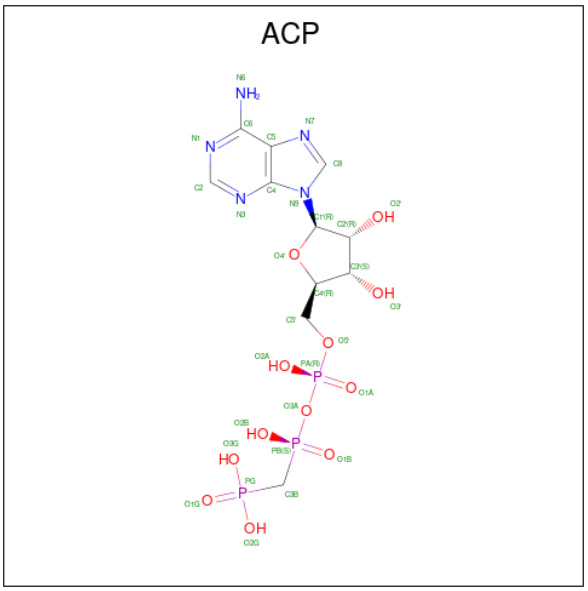
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
12	B	1	5	1	3	1	0	0

- Molecule 13 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		
13	B	1	12	6	1	4	1	0	0

- Molecule 14 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	N	O	P		
14	F	1	31	11	5	12	3	0	0

- Molecule 15 is water.

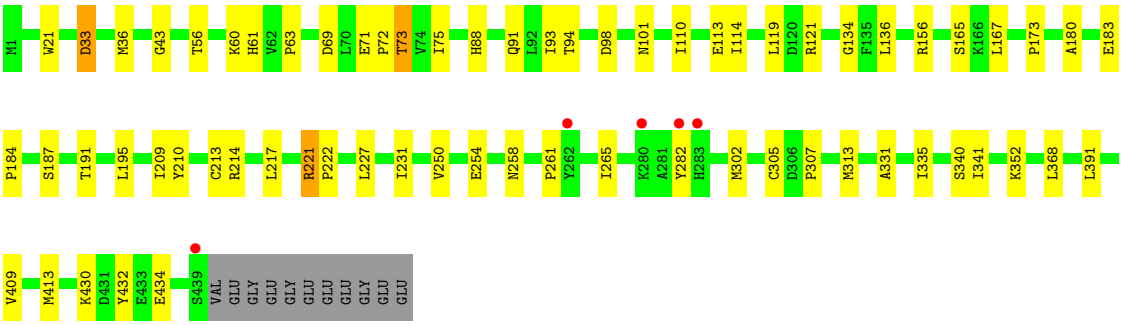
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	150	150	150	0	0
15	B	112	112	112	0	0
15	C	231	231	231	0	0
15	D	99	99	99	0	0
15	E	34	34	34	0	0
15	F	64	64	64	0	0

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.

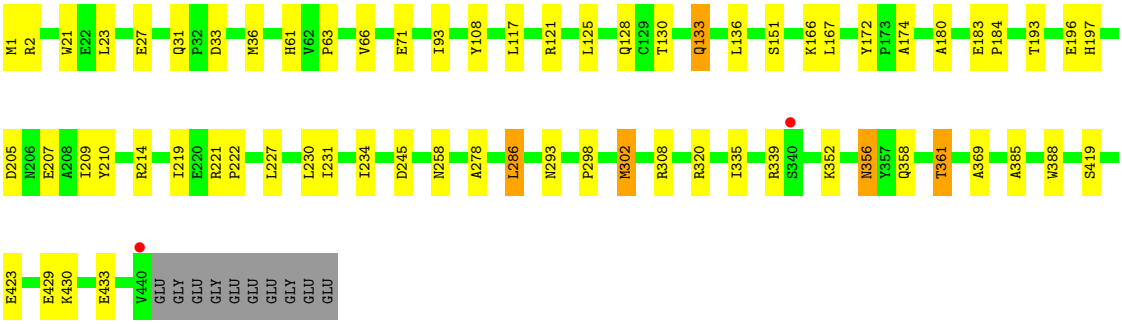
• Molecule 1: Tubulin alpha-1B chain

Chain A:



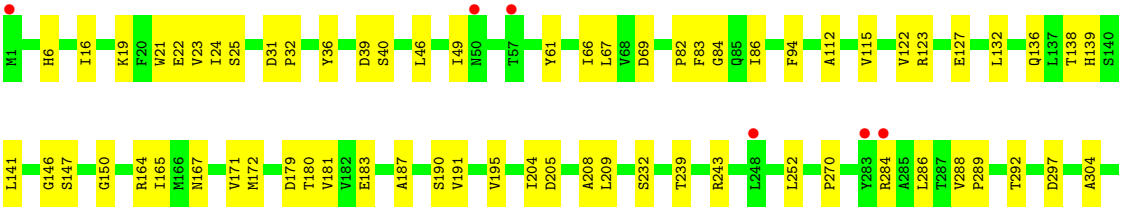
• Molecule 1: Tubulin alpha-1B chain

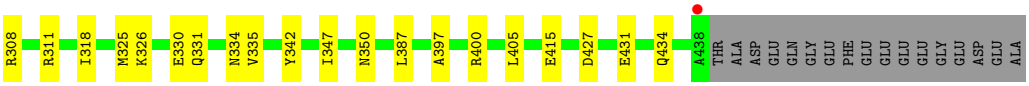
Chain C:



• Molecule 2: Tubulin beta-2B chain

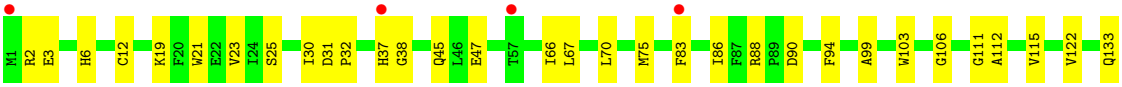
Chain B:

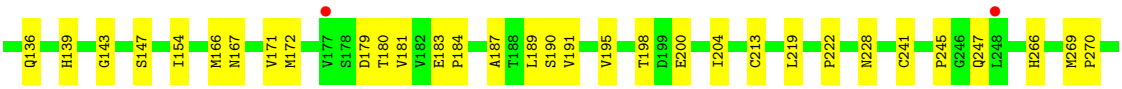


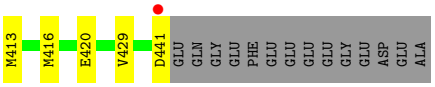


• Molecule 2: Tubulin beta-2B chain

Chain D:

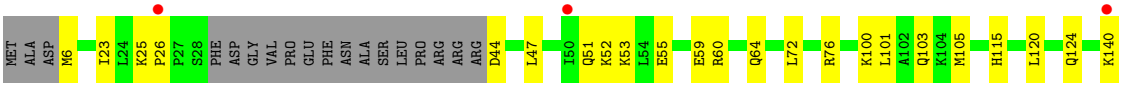






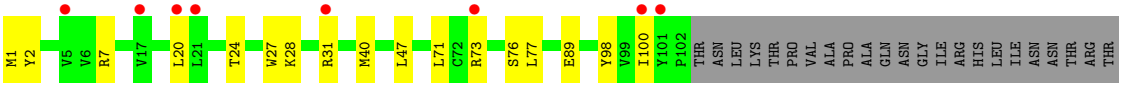
• Molecule 3: Stathmin-4

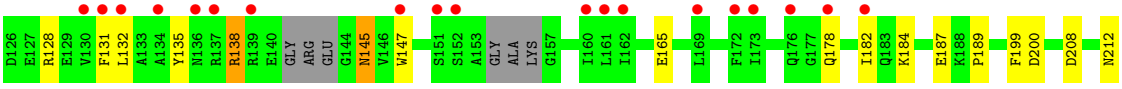
Chain E:

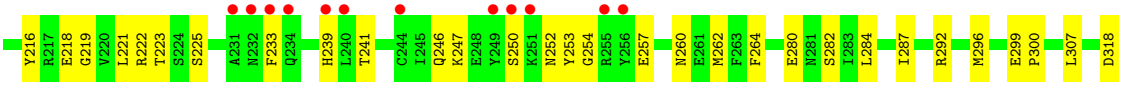


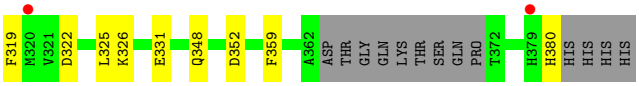
• Molecule 4: Tubulin Tyrosine Ligase

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	105.22Å 157.13Å 182.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.18 – 2.25 78.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.18-2.25) 100.0 (78.87-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.181 , 0.220 0.185 , 0.221	Depositor DCC
R_{free} test set	7166 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18483	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: GOL, ACP, GTP, MES, GDP, 03S, MG, CA, 6K9, IMD

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	0.21	0/3520	0.38	0/4778
1	C	0.22	0/3515	0.39	0/4772
2	B	0.22	0/3438	0.37	0/4658
2	D	0.22	0/3411	0.37	0/4620
3	E	0.20	0/1008	0.30	0/1337
4	F	0.21	0/2863	0.36	0/3866
All	All	0.22	0/17755	0.37	0/24031

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	3436	0	3349	51	0
1	C	3437	0	3348	45	0
2	B	3360	0	3232	72	0
2	D	3335	0	3219	66	0
3	E	1000	0	1018	17	0
4	F	2800	0	2764	53	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	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	2	0	0	0	0
7	E	1	0	0	0	0
8	A	5	0	5	0	0
8	B	10	0	10	4	0
9	A	6	0	8	0	0
9	C	6	0	8	1	0
10	B	28	0	12	1	0
10	D	28	0	12	3	0
11	B	52	59	0	0	0
11	D	52	59	0	0	0
12	B	5	0	4	1	0
13	B	12	0	12	2	0
14	F	31	0	14	3	0
15	A	150	0	0	3	0
15	B	112	0	0	3	0
15	C	231	0	0	2	0
15	D	99	0	0	5	0
15	E	34	0	0	4	0
15	F	64	0	0	0	0
All	All	18365	118	17039	301	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 9.

All (301) 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)
3:E:25:LYS:HD2	3:E:26:PRO:HD2	1.49	0.94
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.53	0.89
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.55	0.88
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.58	0.86
2:D:213:CYS:HB3	2:D:219:LEU:HD11	1.59	0.83
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.61	0.80
2:B:46:LEU:HD12	2:B:49:ILE:HG21	1.64	0.79
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:PRO:HA	2:B:84:GLY:H	1.48	0.78
1:A:110:ILE:O	15:A:601:HOH:O	2.07	0.73
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.36	0.73
1:C:27:GLU:HG2	1:C:361:THR:CG2	2.18	0.73
1:C:128:GLN:NE2	15:C:601:HOH:O	2.23	0.72
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.72	0.71
2:D:241[B]:CYS:SG	15:D:693:HOH:O	2.47	0.71
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.71	0.70
2:D:372:LYS:HE3	2:D:373:MET:HE3	1.73	0.70
2:D:147:SER:OG	2:D:190:SER:OG	2.10	0.70
1:A:114:ILE:N	15:A:601:HOH:O	2.23	0.70
2:B:331:GLN:HA	2:B:334:ASN:ND2	2.08	0.68
3:E:25:LYS:CD	3:E:26:PRO:HD2	2.26	0.65
3:E:120:LEU:O	3:E:124:GLN:HG2	1.96	0.65
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.79	0.65
1:C:27:GLU:HG2	1:C:361:THR:HG23	1.78	0.65
4:F:98:TYR:HB2	4:F:182:ILE:CG2	2.27	0.65
1:C:133:GLN:HG2	9:C:505:GOL:H2	1.79	0.64
4:F:89:GLU:N	4:F:89:GLU:OE1	2.31	0.64
4:F:348:GLN:NE2	4:F:352:ASP:OD2	2.30	0.64
2:B:132:LEU:O	2:B:164:ARG:NH1	2.28	0.63
2:D:136:GLN:HA	2:D:167:ASN:O	1.99	0.63
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.81	0.63
2:B:23:VAL:HG21	2:B:232:SER:OG	1.99	0.62
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.80	0.62
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.35	0.62
1:A:33:ASP:N	1:A:33:ASP:OD1	2.34	0.60
2:B:46:LEU:HD12	2:B:49:ILE:CG2	2.31	0.60
2:D:247:GLN:NE2	15:D:601:HOH:O	2.23	0.60
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.19	0.60
2:D:2:ARG:HB3	2:D:133:GLN:HG3	1.84	0.60
1:C:286:LEU:H	1:C:286:LEU:HD12	1.66	0.60
2:D:25:SER:HB3	2:D:30:ILE:HD11	1.83	0.60
2:D:321:GLY:HA2	2:D:359:PRO:HG3	1.83	0.60
2:B:284:ARG:NH1	15:B:605:HOH:O	2.35	0.60
8:B:506:IMD:H2	8:B:507:IMD:H5	1.84	0.60
3:E:47:LEU:O	3:E:51:GLN:HG2	2.01	0.60
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.38	0.59
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.83	0.59
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.85	0.58
2:B:83:PHE:O	2:B:86:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.38	0.58
1:A:180:ALA:O	1:A:183:GLU:HG3	2.03	0.58
2:B:397:ALA:HA	2:B:400:ARG:NH1	2.18	0.58
2:D:219:LEU:HD12	2:D:219:LEU:O	2.04	0.58
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.86	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.85	0.57
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.87	0.57
2:D:274:PRO:HB3	2:D:286:LEU:CD1	2.33	0.57
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.86	0.57
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.87	0.57
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.86	0.57
1:C:180:ALA:O	1:C:183:GLU:HG3	2.04	0.57
2:D:83:PHE:O	2:D:86:ILE:HG22	2.05	0.57
3:E:6:MET:N	3:E:23:ILE:O	2.38	0.56
2:B:82:PRO:HA	2:B:84:GLY:N	2.18	0.56
4:F:1:MET:CE	4:F:28:LYS:HB2	2.35	0.56
8:B:506:IMD:H2	8:B:507:IMD:C5	2.36	0.56
4:F:178:GLN:N	4:F:178:GLN:OE1	2.39	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.56
4:F:71:LEU:HD12	4:F:77:LEU:HD13	1.88	0.56
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.06	0.55
1:A:110:ILE:O	1:A:113:GLU:HG2	2.06	0.55
2:B:46:LEU:HD11	2:B:61:TYR:OH	2.06	0.55
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.70	0.55
4:F:241:THR:OG1	14:F:400:ACP:O3'	2.19	0.55
2:D:143:GLY:HA3	10:D:501:GDP:O3A	2.07	0.55
2:B:171:VAL:HA	2:B:204:ILE:O	2.06	0.55
4:F:98:TYR:HB2	4:F:182:ILE:HG23	1.88	0.55
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.89	0.55
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.42	0.54
2:D:25:SER:HB3	2:D:30:ILE:CD1	2.36	0.54
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.90	0.54
4:F:318:ASP:OD2	14:F:400:ACP:O3G	2.26	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.07	0.54
2:B:331:GLN:HA	2:B:334:ASN:HD21	1.72	0.54
1:A:71:GLU:OE2	1:A:73:THR:HB	2.07	0.54
2:B:431:GLU:O	2:B:434:GLN:HG2	2.07	0.54
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.18	0.54
4:F:73:ARG:HB2	4:F:76:SER:HB2	1.89	0.54
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.90	0.54
10:B:501:GDP:O1A	12:B:504:03S:H213	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:331:GLU:OE2	14:F:400:ACP:O1G	2.27	0.54
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.91	0.53
4:F:225:SER:HB3	4:F:252:ASN:HB2	1.90	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
3:E:72:LEU:O	3:E:76:ARG:HG2	2.09	0.53
2:B:179:ASP:OD2	15:B:601:HOH:O	2.19	0.53
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.91	0.53
2:B:297:ASP:HA	8:B:507:IMD:C4	2.39	0.53
4:F:184:LYS:NZ	4:F:187:GLU:OE2	2.42	0.53
2:D:409:THR:O	3:E:140:LYS:NZ	2.40	0.53
1:C:234:ILE:HD13	1:C:302:MET:SD	2.48	0.52
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.90	0.52
2:B:181:VAL:HB	1:C:258:ASN:OD1	2.10	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.09	0.52
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.40	0.52
4:F:40:MET:HE2	4:F:47:LEU:HG	1.91	0.52
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.09	0.52
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.92	0.52
4:F:131:PHE:CE1	4:F:182:ILE:HG12	2.45	0.52
2:D:292:THR:O	2:D:295:MET:HG2	2.10	0.51
3:E:44:ASP:N	15:E:304:HOH:O	2.42	0.51
3:E:55:GLU:O	3:E:59:GLU:HG2	2.10	0.51
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.92	0.51
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.92	0.51
1:C:1:MET:HG2	1:C:130:THR:OG1	2.10	0.51
1:A:430:LYS:O	1:A:434:GLU:HG3	2.11	0.51
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.26	0.51
2:B:39:ASP:OD1	2:B:40:SER:N	2.43	0.51
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.51
2:D:274:PRO:HB3	2:D:286:LEU:HD11	1.92	0.51
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.51
2:D:219:LEU:CD1	2:D:222:PRO:HB3	2.41	0.50
3:E:100:LYS:O	3:E:103:GLN:HG3	2.10	0.50
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.35	0.50
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.41	0.50
3:E:100:LYS:NZ	15:E:305:HOH:O	2.43	0.50
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.46	0.50
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.93	0.50
1:C:151:SER:HB3	1:C:193:THR:HG21	1.92	0.50
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.93	0.50
2:D:191:VAL:O	2:D:195:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:247:LYS:HE2	4:F:253:TYR:OH	2.12	0.49
2:D:67:LEU:N	2:D:67:LEU:HD12	2.26	0.49
4:F:299:GLU:N	4:F:300:PRO:HD2	2.27	0.49
2:B:164:ARG:O	13:B:505:MES:H71	2.12	0.49
2:B:67:LEU:N	2:B:67:LEU:HD12	2.27	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.49
2:B:427:ASP:O	2:B:431:GLU:HG3	2.13	0.49
2:D:25:SER:CB	2:D:30:ILE:HD11	2.43	0.49
2:D:180:THR:O	2:D:181:VAL:HB	2.12	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.49
2:D:179:ASP:O	2:D:181:VAL:HG23	2.12	0.49
1:C:286:LEU:HD12	1:C:286:LEU:N	2.28	0.48
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.96	0.48
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.13	0.48
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.43	0.48
1:A:409:VAL:HA	1:A:413:MET:O	2.14	0.48
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.95	0.48
2:D:30:ILE:HD13	2:D:86:ILE:HD11	1.96	0.48
4:F:135:TYR:OH	4:F:165:GLU:HA	2.14	0.48
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.43	0.48
2:B:308:ARG:HG3	2:B:342:TYR:CZ	2.49	0.48
2:D:187:ALA:O	2:D:191:VAL:HG23	2.14	0.48
1:A:210:TYR:CD2	1:A:214:ARG:HD2	2.49	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.49	0.47
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.13	0.47
13:B:505:MES:H51	13:B:505:MES:H81	1.67	0.47
1:A:213:CYS:O	1:A:217:LEU:HB2	2.15	0.47
1:C:27:GLU:HG2	1:C:361:THR:HG21	1.96	0.47
2:D:396:THR:O	2:D:400:ARG:HG2	2.15	0.47
4:F:292:ARG:HG2	4:F:296:MET:SD	2.55	0.47
1:A:341:ILE:N	1:A:341:ILE:HD12	2.29	0.47
2:D:66:ILE:HD12	2:D:122:VAL:HG22	1.95	0.47
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.97	0.47
2:D:213:CYS:O	2:D:219:LEU:HG	2.15	0.47
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.49	0.47
1:A:331:ALA:O	1:A:335:ILE:HG13	2.15	0.47
2:B:123:ARG:O	2:B:127:GLU:HG3	2.14	0.47
4:F:135:TYR:HD1	4:F:145:ASN:HD21	1.63	0.46
2:D:37:HIS:HB2	15:D:692:HOH:O	2.15	0.46
1:A:221:ARG:HG3	2:B:325:MET:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:7:ARG:HD3	4:F:40:MET:CE	2.40	0.46
2:D:441:ASP:HA	15:D:673:HOH:O	2.15	0.46
2:B:36:TYR:OH	2:B:40:SER:O	2.33	0.46
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.98	0.46
1:A:136:LEU:CD2	1:A:167:LEU:HB2	2.46	0.46
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.22	0.46
4:F:138:ARG:NH1	4:F:184:LYS:HE2	2.30	0.46
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.51	0.45
4:F:221:LEU:HD22	4:F:262:MET:CE	2.39	0.45
1:C:419:SER:O	1:C:423:GLU:HG3	2.17	0.45
2:D:213:CYS:HB3	2:D:219:LEU:CD1	2.41	0.45
1:A:227:LEU:O	1:A:231:ILE:HG13	2.17	0.45
1:A:33:ASP:O	1:A:60:LYS:HE2	2.16	0.45
1:A:69:ASP:O	1:A:94:THR:HA	2.17	0.45
1:A:71:GLU:HG2	1:A:72:PRO:N	2.32	0.45
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.46	0.45
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.85	0.45
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.51	0.45
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.98	0.45
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.16	0.45
2:B:318:ILE:N	2:B:318:ILE:HD12	2.32	0.45
1:C:196:GLU:HB2	15:C:685:HOH:O	2.15	0.45
1:C:430:LYS:HB3	1:C:430:LYS:HE2	1.86	0.45
4:F:20:LEU:O	4:F:24:THR:HG23	2.17	0.45
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.45
1:C:352:LYS:HB3	1:C:352:LYS:HE3	1.80	0.45
1:A:43:GLY:HA2	1:A:56:THR:O	2.17	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.45
2:D:19:LYS:O	2:D:23:VAL:HG23	2.16	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.17	0.44
1:A:173:PRO:HB3	1:A:183:GLU:OE2	2.18	0.44
1:A:305:CYS:O	1:A:307:PRO:HD3	2.17	0.44
2:B:187:ALA:O	2:B:191:VAL:HG23	2.18	0.44
2:D:274:PRO:HB3	2:D:286:LEU:HD12	1.98	0.44
2:B:331:GLN:O	2:B:335:VAL:HG23	2.17	0.44
3:E:60:ARG:O	3:E:64:GLN:HG3	2.18	0.44
4:F:246:GLN:O	4:F:250:SER:HB3	2.17	0.44
2:B:83:PHE:HB3	2:B:86:ILE:HD13	1.98	0.44
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.44
1:C:166:LYS:HE2	1:C:197:HIS:O	2.16	0.44
3:E:101:LEU:O	3:E:105:MET:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:GLU:HB2	2:B:83:PHE:CD1	2.53	0.44
3:E:52:LYS:HE3	3:E:52:LYS:HB2	1.86	0.44
2:B:19:LYS:HG3	2:B:232:SER:HB2	1.99	0.44
2:D:198:THR:OG1	2:D:266:HIS:NE2	2.49	0.43
2:D:409:THR:HA	2:D:413:MET:O	2.17	0.43
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.53	0.43
1:A:340:SER:C	1:A:341:ILE:HD12	2.38	0.43
2:B:180:THR:O	2:B:183:GLU:HG3	2.18	0.43
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.54	0.43
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.54	0.43
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.43
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.43
2:D:112:ALA:O	2:D:115:VAL:HG12	2.19	0.43
3:E:115:HIS:HA	15:E:307:HOH:O	2.18	0.43
4:F:128:ARG:O	4:F:132:LEU:HG	2.18	0.43
2:B:22:GLU:HB2	2:B:83:PHE:CE1	2.54	0.43
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.43
2:B:311:ARG:NH1	4:F:31:ARG:HH12	2.17	0.43
2:B:21:TRP:CZ3	2:B:24:ILE:HD11	2.53	0.43
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.43
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.00	0.43
1:C:227:LEU:O	1:C:231:ILE:HG13	2.19	0.43
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.34	0.43
3:E:115:HIS:HB3	15:E:334:HOH:O	2.18	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.42
2:B:325:MET:HE2	15:B:703:HOH:O	2.18	0.42
1:C:31:GLN:HB2	1:C:33:ASP:OD1	2.19	0.42
2:D:75:MET:SD	2:D:94:PHE:HB3	2.59	0.42
2:D:416:MET:O	2:D:420:GLU:HG3	2.19	0.42
2:B:286:LEU:N	2:B:286:LEU:HD12	2.35	0.42
1:A:114:ILE:HG22	15:A:601:HOH:O	2.18	0.42
1:C:108:TYR:CE1	3:E:105:MET:HE1	2.55	0.42
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.49	0.42
4:F:208:ASP:OD2	4:F:212:ASN:HB2	2.20	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.42
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.19	0.42
2:B:239:THR:O	2:B:243:ARG:HG2	2.19	0.42
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.55	0.42
4:F:145:ASN:ND2	4:F:147:TRP:HE1	2.18	0.42
4:F:322:ASP:OD2	4:F:326:LYS:HB3	2.20	0.42
4:F:200:ASP:OD2	4:F:222:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.50	0.42
4:F:199:PHE:HA	4:F:241:THR:HG21	2.01	0.42
2:B:334:ASN:OD1	2:B:335:VAL:N	2.53	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.42
4:F:233:PHE:HD1	4:F:239:HIS:HE2	1.68	0.42
1:A:191:THR:O	1:A:195:LEU:HB2	2.21	0.41
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.02	0.41
2:B:21:TRP:O	2:B:25:SER:OG	2.31	0.41
2:B:179:ASP:OD1	1:C:352:LYS:HD2	2.21	0.41
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.20	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HG3	2.03	0.41
1:A:221:ARG:HG3	2:B:325:MET:HB3	2.02	0.41
1:A:136:LEU:HD23	1:A:167:LEU:HB2	2.02	0.41
2:B:191:VAL:O	2:B:195:VAL:HG23	2.20	0.41
1:C:151:SER:HB3	1:C:193:THR:CG2	2.50	0.41
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.55	0.41
2:B:46:LEU:HD11	2:B:61:TYR:CZ	2.56	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.02	0.41
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.35	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
2:B:326:LYS:O	2:B:330:GLU:HG3	2.20	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.41
2:D:318:ILE:HD13	15:D:606:HOH:O	2.20	0.41
2:B:16:ILE:HD11	2:B:138:THR:HB	2.01	0.41
2:B:405:LEU:HD21	2:B:415:GLU:HG2	2.03	0.41
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.50	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.41
2:B:82:PRO:CA	2:B:84:GLY:H	2.28	0.41
2:D:228:ASN:OD1	10:D:501:GDP:N1	2.32	0.41
4:F:254:GLY:HA2	4:F:257:GLU:O	2.20	0.41
2:B:112:ALA:O	2:B:115:VAL:HG12	2.20	0.41
2:B:146:GLY:O	2:B:150:GLY:HA3	2.20	0.41
2:B:205:ASP:O	2:B:209:LEU:HG	2.20	0.41
4:F:257:GLU:HG2	4:F:260:ASN:HA	2.03	0.41
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.37	0.40
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.03	0.40
1:C:2:ARG:HA	1:C:2:ARG:HD2	1.77	0.40
1:C:429:GLU:O	1:C:433:GLU:HG3	2.21	0.40
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.40	0.40
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.57	0.40
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:C	2:B:387:LEU:HD23	2.42	0.40
2:D:3:GLU:O	2:D:133:GLN:HB2	2.21	0.40
2:D:397:ALA:O	2:D:401:ARG:HD3	2.21	0.40
4:F:189:PRO:HA	4:F:322:ASP:HA	2.03	0.40
4:F:233:PHE:HD1	4:F:239:HIS:NE2	2.19	0.40
2:B:297:ASP:HA	8:B:507:IMD:H4	2.04	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	439/450 (98%)	422 (96%)	17 (4%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
2	D	421/445 (95%)	414 (98%)	7 (2%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	332/384 (86%)	318 (96%)	14 (4%)	0	100	100
All	All	2174/2317 (94%)	2119 (98%)	55 (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	372/378 (98%)	368 (99%)	4 (1%)	73	82
1	C	371/378 (98%)	361 (97%)	10 (3%)	44	54
2	B	367/383 (96%)	365 (100%)	2 (0%)	88	92
2	D	367/383 (96%)	366 (100%)	1 (0%)	92	95
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	86
4	F	307/342 (90%)	304 (99%)	3 (1%)	76	84
All	All	1893/1991 (95%)	1872 (99%)	21 (1%)	73	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	73	THR
1	A	221	ARG
1	A	282	TYR
2	B	139	HIS
2	B	270	PRO
1	C	71	GLU
1	C	133	GLN
1	C	221	ARG
1	C	245	ASP
1	C	286	LEU
1	C	293	ASN
1	C	302	MET
1	C	356	ASN
1	C	358	GLN
1	C	361	THR
2	D	139	HIS
3	E	53	LYS
4	F	138	ARG
4	F	145	ASN
4	F	380	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	342	GLN
2	D	167	ASN
4	F	145	ASN
4	F	242	ASN

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Mol	Chain	Res	Type
4	F	269	GLN

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 22 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.38	5 (15%)
13	MES	B	505	-	12,12,12	2.26	1 (8%)	14,16,16	1.92	5 (35%)
12	03S	B	504	-	4,4,4	1.79	2 (50%)	5,6,6	1.56	1 (20%)
11	6K9	B	503	-	58,60,60	2.21	15 (25%)	60,92,92	1.79	13 (21%)
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.44	5 (15%)
9	GOL	C	505	-	5,5,5	0.35	0	5,5,5	0.34	0
14	ACP	F	400	6	27,33,33	1.99	7 (25%)	32,52,52	1.54	5 (15%)
8	IMD	B	507	-	3,5,5	0.41	0	4,5,5	0.57	0
10	GDP	B	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.16	3 (10%)
8	IMD	B	506	-	3,5,5	0.41	0	4,5,5	0.59	0
10	GDP	D	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.16	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	6K9	D	502	-	58,60,60	2.20	15 (25%)	60,92,92	1.74	15 (25%)
9	GOL	A	505	-	5,5,5	0.38	0	5,5,5	0.26	0
8	IMD	A	504	-	3,5,5	0.42	0	4,5,5	0.59	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
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
13	MES	B	505	-	-	0/6/14/14	0/1/1/1
11	6K9	B	503	-	-	2/31/131/131	-
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
9	GOL	C	505	-	-	1/4/4/4	-
14	ACP	F	400	6	-	10/15/38/38	0/3/3/3
8	IMD	B	507	-	-	-	0/1/1/1
10	GDP	B	501	-	-	4/12/32/32	0/3/3/3
10	GDP	D	501	-	-	4/12/32/32	0/3/3/3
8	IMD	B	506	-	-	-	0/1/1/1
11	6K9	D	502	-	-	3/31/131/131	-
9	GOL	A	505	-	-	2/4/4/4	-
8	IMD	A	504	-	-	-	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	505	MES	C8-S	-7.56	1.66	1.77
11	D	502	6K9	C02-C01	-7.26	1.41	1.51
11	B	503	6K9	C02-C01	-7.02	1.41	1.51
11	D	502	6K9	C18-C19	-6.79	1.40	1.51
11	B	503	6K9	C18-C19	-6.78	1.40	1.51
11	D	502	6K9	C39-C01	-5.64	1.43	1.51
11	B	503	6K9	C39-C01	-5.59	1.43	1.51
14	F	400	ACP	PG-O1G	5.48	1.61	1.50
11	B	503	6K9	O11-C11	4.78	1.50	1.43
11	D	502	6K9	O11-C11	4.51	1.50	1.43
11	B	503	6K9	C38-C26	4.18	1.39	1.32
11	D	502	6K9	C38-C26	4.05	1.39	1.32
5	C	501	GTP	C5-C6	-3.94	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C5-C6	-3.91	1.39	1.47
14	F	400	ACP	C6-N6	3.85	1.48	1.34
14	F	400	ACP	C2'-C1'	-3.62	1.48	1.53
11	B	503	6K9	C33-C32	3.53	1.58	1.52
11	D	502	6K9	C33-C32	3.48	1.58	1.52
11	B	503	6K9	C20-C19	-3.33	1.43	1.51
11	D	502	6K9	C20-C19	-3.30	1.43	1.51
11	B	503	6K9	C30-C29	3.24	1.59	1.53
11	D	502	6K9	C30-C29	3.14	1.59	1.53
14	F	400	ACP	C2'-C3'	-3.03	1.45	1.53
11	B	503	6K9	C08-C07	-2.88	1.46	1.52
11	D	502	6K9	C27-C26	-2.84	1.43	1.52
11	D	502	6K9	C08-C07	-2.83	1.46	1.52
11	B	503	6K9	C27-C26	-2.75	1.43	1.52
11	D	502	6K9	C25-C26	-2.68	1.44	1.52
11	D	502	6K9	C24-C25	2.68	1.57	1.53
11	B	503	6K9	C25-C26	-2.64	1.44	1.52
11	B	503	6K9	C24-C25	2.54	1.57	1.53
10	B	501	GDP	C6-N1	-2.43	1.34	1.37
11	B	503	6K9	C33-C34	2.42	1.58	1.52
11	D	502	6K9	C33-C34	2.40	1.58	1.52
12	B	504	03S	O11-S10	2.37	1.53	1.43
12	B	504	03S	O12-S10	2.36	1.53	1.43
14	F	400	ACP	O5'-C5'	-2.33	1.35	1.44
14	F	400	ACP	PG-O3G	2.33	1.60	1.54
10	D	501	GDP	C6-N1	-2.32	1.34	1.37
11	D	502	6K9	O07-C03	2.29	1.48	1.44
14	F	400	ACP	O3'-C3'	-2.27	1.37	1.43
11	B	503	6K9	O07-C03	2.25	1.48	1.44
5	A	501	GTP	C2-N3	2.15	1.38	1.33
5	C	501	GTP	C2-N3	2.05	1.38	1.33
11	B	503	6K9	C05-C04	2.04	1.58	1.52
11	D	502	6K9	C05-C04	2.02	1.57	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	503	6K9	C16-C15-C14	-4.68	107.94	114.43
14	F	400	ACP	N3-C2-N1	-4.35	121.89	128.68
13	B	505	MES	C5-N4-C3	4.16	118.20	108.83
11	D	502	6K9	C16-C15-C14	-3.93	108.98	114.43
14	F	400	ACP	PB-O3A-PA	-3.91	120.16	132.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	503	6K9	C33-C34-C35	3.86	115.24	111.92
11	B	503	6K9	O27-C23-C24	-3.65	104.22	110.04
11	D	502	6K9	C04-C03-C02	-3.51	106.65	113.21
11	B	503	6K9	C04-C03-C02	-3.48	106.70	113.21
14	F	400	ACP	C3'-C2'-C1'	3.42	106.13	100.98
11	D	502	6K9	C10-O10-C06	3.41	121.68	113.63
11	D	502	6K9	C33-C34-C35	3.40	114.85	111.92
11	B	503	6K9	C10-O10-C06	3.39	121.63	113.63
11	D	502	6K9	O27-C23-C24	-3.32	104.74	110.04
11	D	502	6K9	C18-C19-C36	-3.23	120.19	126.33
12	B	504	03S	O12-S10-O11	-3.23	109.31	118.02
11	B	503	6K9	C23-O27-C27	3.21	117.55	112.42
11	B	503	6K9	C18-C19-C36	-3.15	120.36	126.33
5	A	501	GTP	PA-O3A-PB	-3.13	122.07	132.83
5	A	501	GTP	C8-N7-C5	3.13	108.95	102.99
5	A	501	GTP	C5-C6-N1	3.09	119.40	113.95
10	B	501	GDP	PA-O3A-PB	-3.08	122.25	132.83
5	C	501	GTP	C8-N7-C5	3.08	108.86	102.99
5	C	501	GTP	C5-C6-N1	3.05	119.34	113.95
11	D	502	6K9	C23-O27-C27	3.04	117.27	112.42
10	D	501	GDP	PA-O3A-PB	-2.92	122.80	132.83
5	C	501	GTP	PA-O3A-PB	-2.87	122.99	132.83
11	B	503	6K9	C37-C25-C24	-2.85	106.84	111.40
5	A	501	GTP	C2-N1-C6	-2.76	120.01	125.10
14	F	400	ACP	O5'-C5'-C4'	2.76	118.48	108.99
5	A	501	GTP	PB-O3B-PG	-2.63	123.79	132.83
11	B	503	6K9	C32-C33-C34	-2.61	108.75	114.61
5	C	501	GTP	C2-N1-C6	-2.61	120.29	125.10
11	D	502	6K9	C37-C25-C24	-2.56	107.30	111.40
13	B	505	MES	C6-C5-N4	-2.56	106.23	110.10
11	B	503	6K9	O12-C12-C11	-2.51	99.49	104.87
5	C	501	GTP	PB-O3B-PG	-2.50	124.26	132.83
10	B	501	GDP	C8-N7-C5	2.48	107.72	102.99
11	D	502	6K9	O12-C12-C11	-2.41	99.71	104.87
11	B	503	6K9	C10-C11-C12	2.41	109.44	103.72
10	B	501	GDP	C5-C6-N1	2.37	118.14	113.95
13	B	505	MES	O3S-S-C8	2.35	109.58	105.77
11	B	503	6K9	O01-C01-C02	-2.35	118.20	121.55
10	D	501	GDP	C3'-C2'-C1'	2.32	104.47	100.98
11	D	502	6K9	O01-C01-C02	-2.32	118.24	121.55
10	D	501	GDP	C8-N7-C5	2.31	107.40	102.99
11	B	503	6K9	C40-O31-C31	-2.29	108.52	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	502	6K9	C10-C11-C12	2.28	109.14	103.72
11	D	502	6K9	C32-C33-C34	-2.27	109.51	114.61
13	B	505	MES	O1S-S-C8	2.21	109.58	106.92
11	D	502	6K9	O07-C03-C04	2.20	112.22	109.86
11	D	502	6K9	C40-O31-C31	-2.18	108.80	114.52
10	D	501	GDP	C5-C6-N1	2.17	117.78	113.95
14	F	400	ACP	C5'-C4'-C3'	-2.05	107.50	115.18
13	B	505	MES	C7-N4-C5	2.03	116.44	111.23
11	D	502	6K9	C05-C06-C07	-2.03	106.75	110.89

There are no chirality outliers.

All (43) 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	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	A	505	GOL	O1-C1-C2-O2
9	A	505	GOL	O1-C1-C2-C3
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
11	B	503	6K9	C33-C34-C35-N35
11	B	503	6K9	O34-C34-C35-N35
11	D	502	6K9	C33-C34-C35-N35
11	D	502	6K9	O34-C34-C35-N35
14	F	400	ACP	PB-C3B-PG-O2G
14	F	400	ACP	PG-C3B-PB-O1B
14	F	400	ACP	PG-C3B-PB-O2B
14	F	400	ACP	PG-C3B-PB-O3A
14	F	400	ACP	C5'-O5'-PA-O1A
14	F	400	ACP	C5'-O5'-PA-O2A
14	F	400	ACP	C5'-O5'-PA-O3A
9	C	505	GOL	O1-C1-C2-C3
5	C	501	GTP	PB-O3B-PG-O1G
14	F	400	ACP	PB-C3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O2A
14	F	400	ACP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
11	D	502	6K9	C20-C21-C22-C23
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
14	F	400	ACP	PB-O3A-PA-O2A
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
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
10	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G

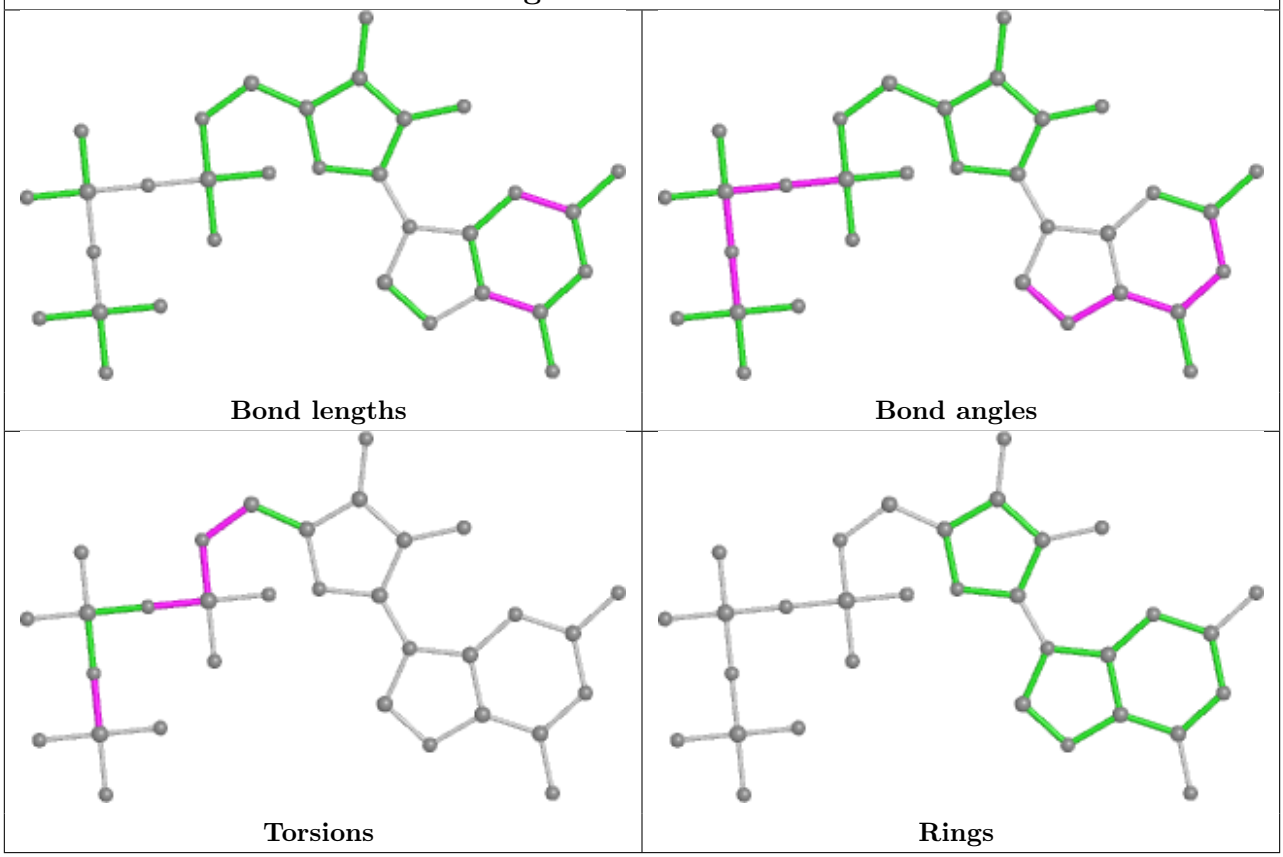
There are no ring outliers.

9 monomers are involved in 15 short contacts:

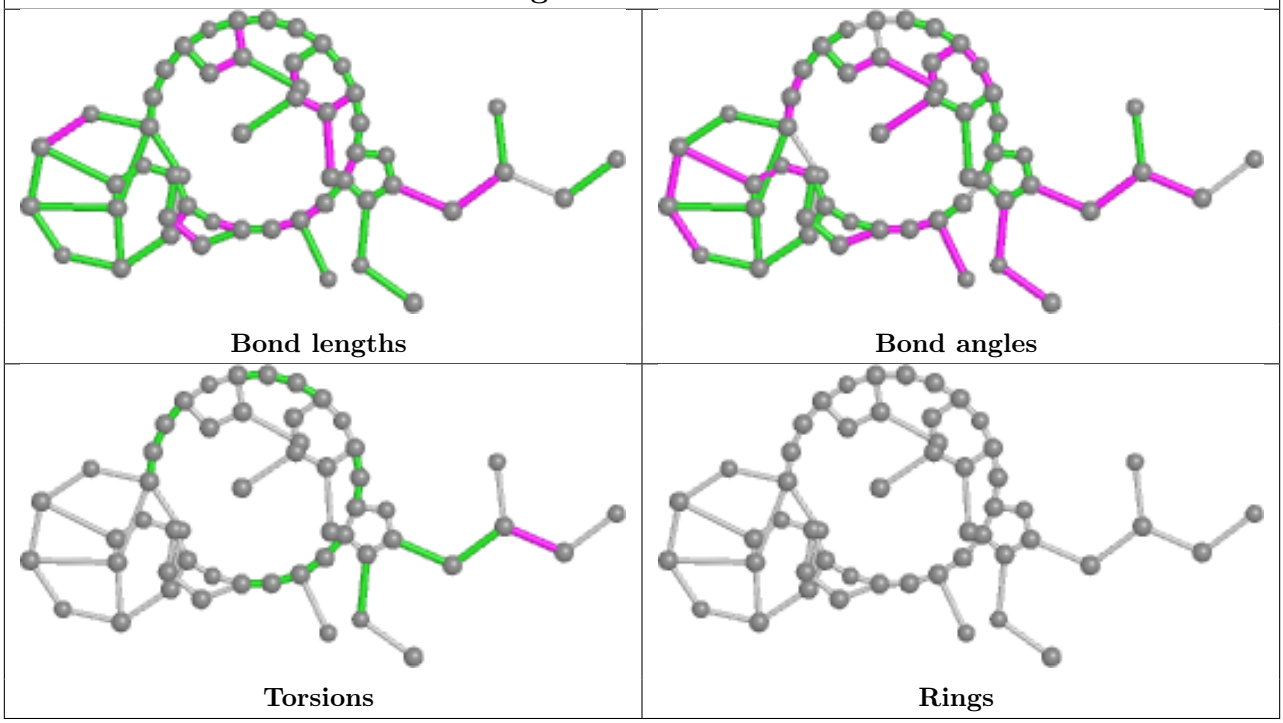
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	505	MES	2	0
12	B	504	03S	1	0
5	A	501	GTP	1	0
9	C	505	GOL	1	0
14	F	400	ACP	3	0
8	B	507	IMD	4	0
10	B	501	GDP	1	0
8	B	506	IMD	2	0
10	D	501	GDP	3	0

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.

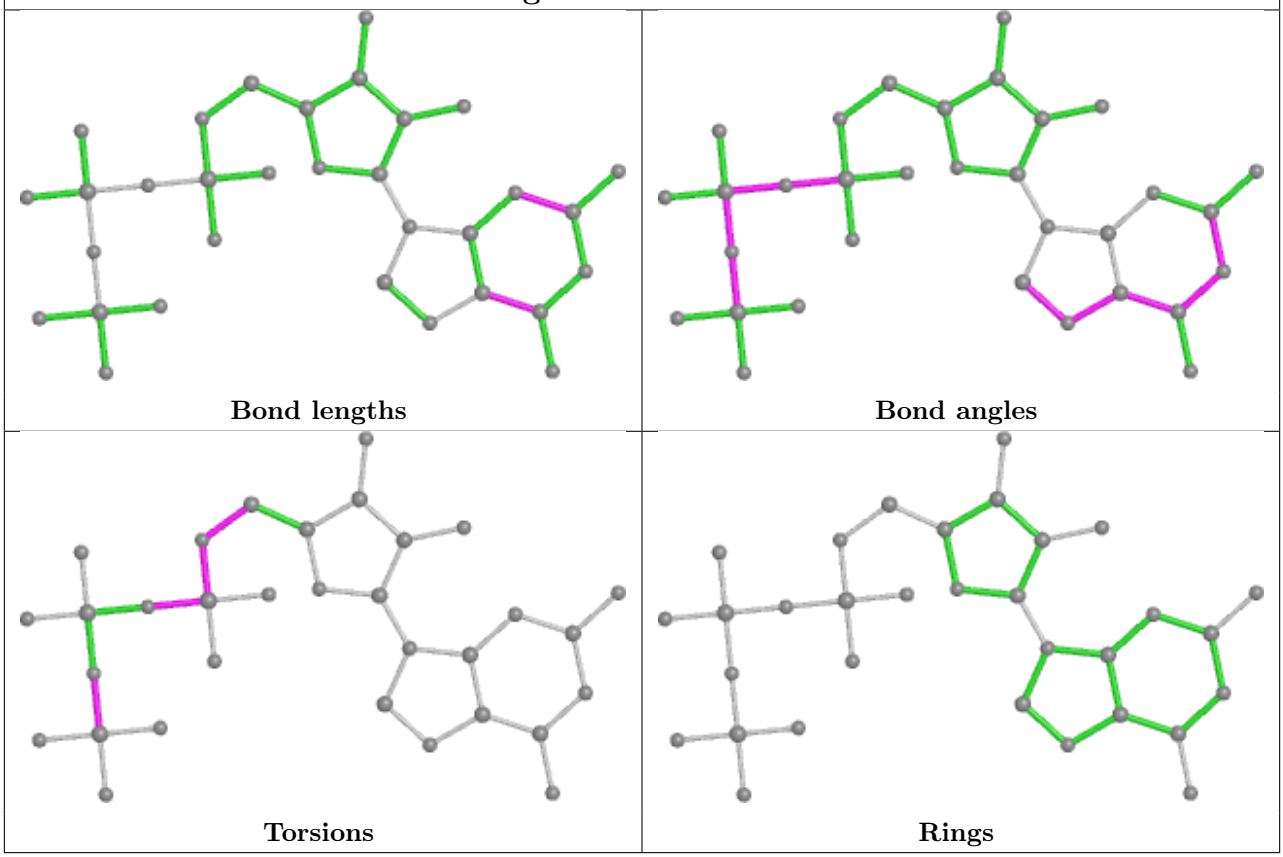
Ligand GTP C 501



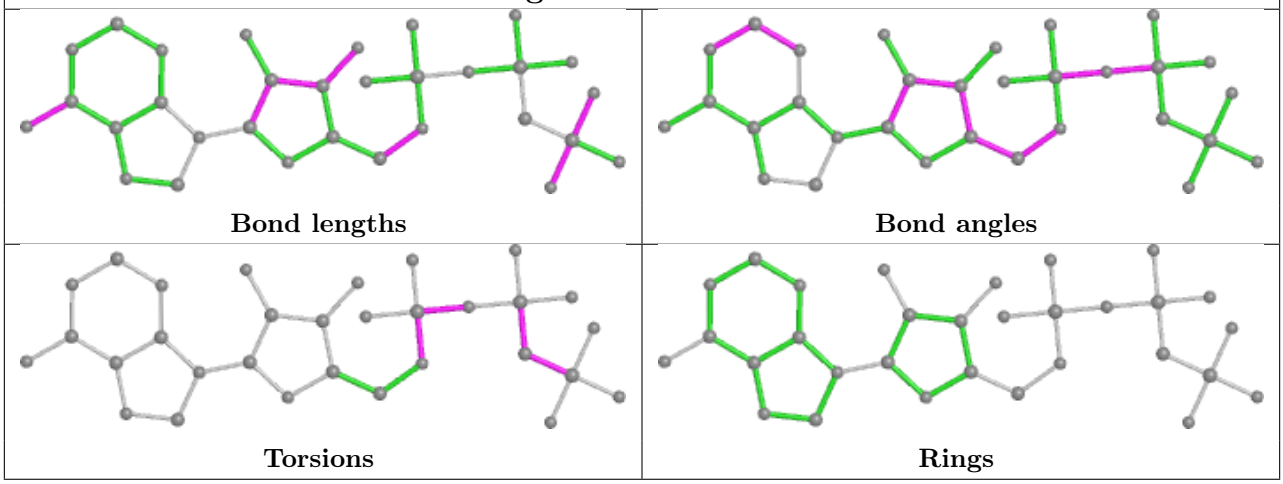
Ligand 6K9 B 503



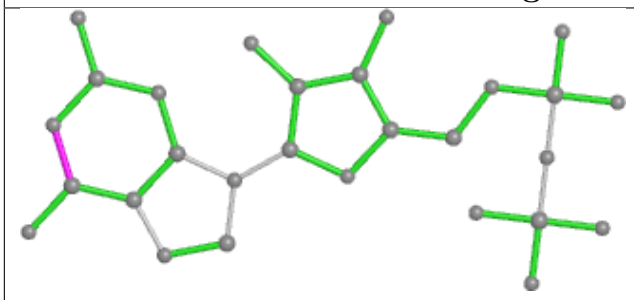
Ligand GTP A 501



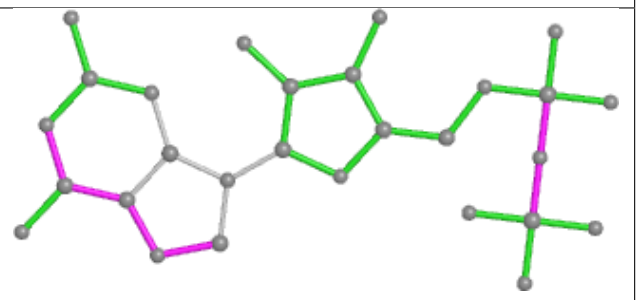
Ligand ACP F 400



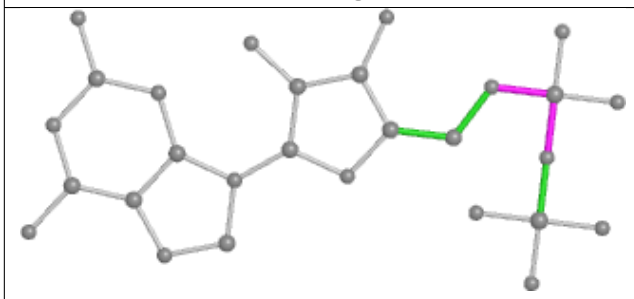
Ligand GDP B 501



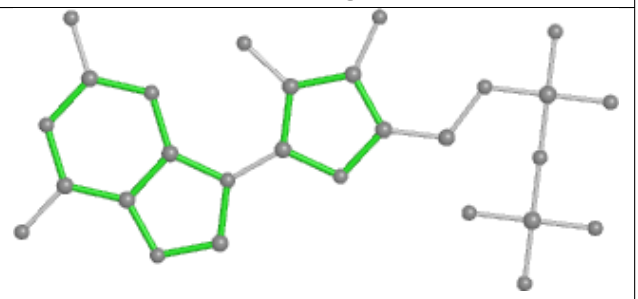
Bond lengths



Bond angles

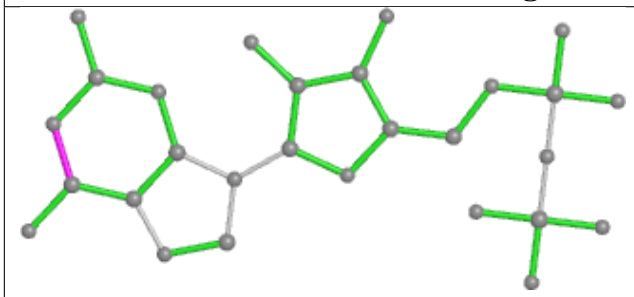


Torsions

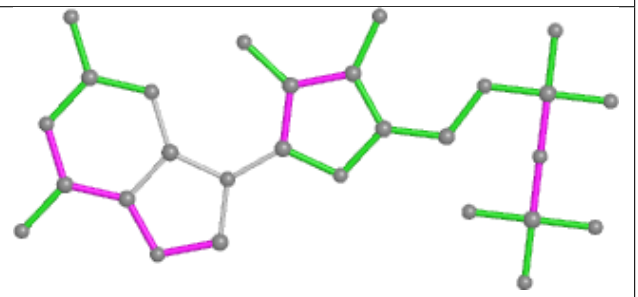


Rings

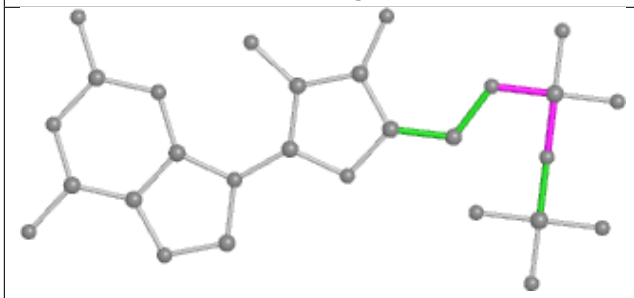
Ligand GDP D 501



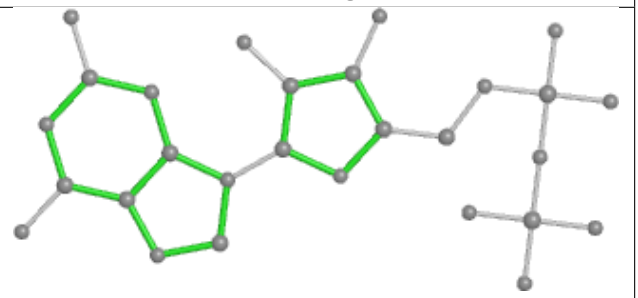
Bond lengths



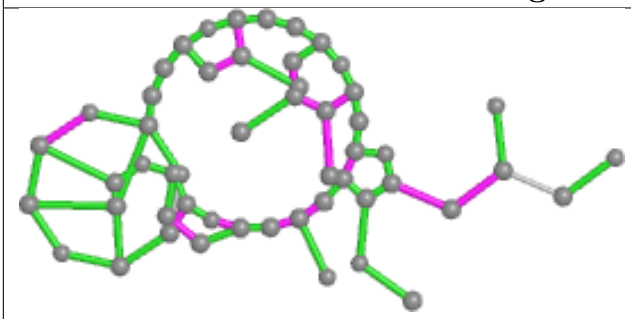
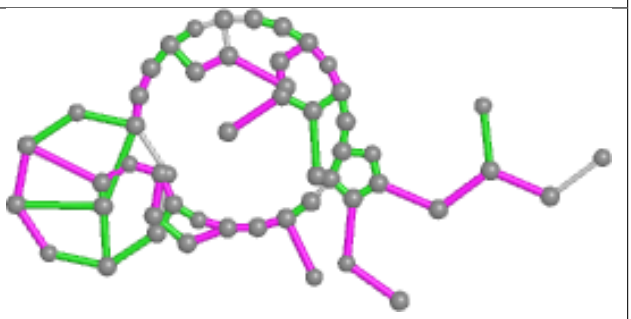
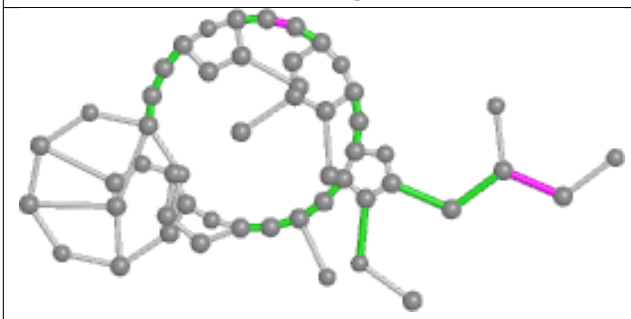
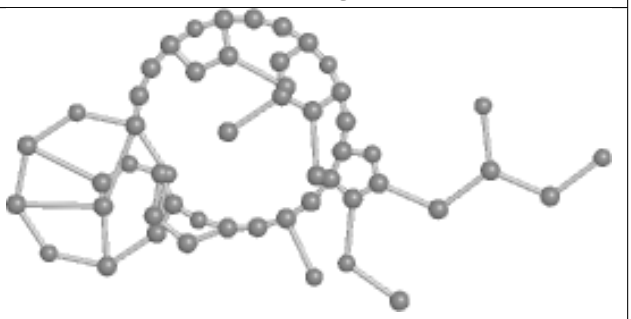
Bond angles



Torsions



Rings

Ligand 6K9 D 502	
 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	439/450 (97%)	-0.05	5 (1%)	80	82	41, 66, 99, 145	0
1	C	440/450 (97%)	0.18	2 (0%)	91	91	37, 53, 79, 100	0
2	B	428/445 (96%)	0.25	7 (1%)	72	74	40, 65, 113, 155	2 (0%)
2	D	424/445 (95%)	0.07	12 (2%)	53	55	43, 71, 105, 136	6 (1%)
3	E	121/143 (84%)	0.37	3 (2%)	57	60	49, 83, 106, 119	0
4	F	342/384 (89%)	0.68	41 (11%)	4	3	48, 86, 145, 172	0
All	All	2194/2317 (94%)	0.22	70 (3%)	47	50	37, 68, 115, 172	8 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	6.3
4	F	173	ILE	6.1
1	A	439	SER	5.8
4	F	132	LEU	5.4
2	D	285	ALA	5.3
4	F	233	PHE	4.8
4	F	182	ILE	4.5
4	F	251	LYS	4.5
4	F	17	VAL	4.2
4	F	162	ILE	4.1
4	F	161	LEU	3.9
2	D	401	ARG	3.9
2	B	1	MET	3.9
4	F	152	SER	3.8
4	F	20	LEU	3.7
4	F	131	PHE	3.7
1	C	440	VAL	3.6
2	D	83	PHE	3.6
4	F	320	MET	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	441	ASP	3.6
4	F	100	ILE	3.5
2	D	284	ARG	3.5
4	F	239	HIS	3.5
2	D	1	MET	3.4
4	F	101	TYR	3.4
2	B	57	THR	3.4
2	D	404	PHE	3.3
4	F	234	GLN	3.3
4	F	130	VAL	3.3
2	B	438	ALA	3.2
2	D	57	THR	3.2
1	A	283	HIS	3.2
4	F	172	PHE	3.1
2	D	400	ARG	3.0
4	F	379	HIS	3.0
4	F	31	ARG	3.0
2	B	284	ARG	3.0
4	F	244	CYS	2.9
4	F	147	TRP	2.9
2	B	50	ASN	2.8
3	E	140	LYS	2.8
4	F	240	LEU	2.8
1	A	262	TYR	2.7
4	F	5	VAL	2.7
4	F	137	ARG	2.6
4	F	136	ASN	2.6
4	F	249	TYR	2.6
2	D	177	VAL	2.6
4	F	139	ARG	2.5
2	D	248	LEU	2.5
1	C	340	SER	2.4
2	B	283	TYR	2.4
4	F	151	SER	2.4
4	F	160	ILE	2.3
3	E	26	PRO	2.3
4	F	21	LEU	2.3
4	F	256	TYR	2.3
1	A	280	LYS	2.3
2	D	37	HIS	2.3
3	E	50	ILE	2.2
4	F	178	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	232	ASN	2.2
4	F	255	ARG	2.1
4	F	250	SER	2.1
4	F	73	ARG	2.0
2	B	248	LEU	2.0
4	F	169	LEU	2.0
4	F	134	ALA	2.0
4	F	231	ALA	2.0
4	F	176	GLN	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
7	CA	A	503	1/1	0.67	0.40	219,219,219,219	0
12	03S	B	504	5/5	0.81	0.16	51,102,113,114	0
9	GOL	A	505	6/6	0.85	0.18	69,85,88,89	0
6	MG	A	502	1/1	0.89	0.16	48,48,48,48	0
8	IMD	B	506	5/5	0.89	0.13	94,96,102,103	0
7	CA	C	504	1/1	0.91	0.15	117,117,117,117	0
8	IMD	A	504	5/5	0.92	0.10	85,87,90,90	0
14	ACP	F	400	31/31	0.92	0.10	71,84,123,146	0
7	CA	E	200	1/1	0.93	0.07	98,98,98,98	0
8	IMD	B	507	5/5	0.94	0.12	107,109,111,113	0
13	MES	B	505	12/12	0.94	0.13	57,78,100,112	0
11	6K9	D	502	52/52	0.94	0.17	63,92,111,115	0
9	GOL	C	505	6/6	0.95	0.15	69,88,89,91	0
7	CA	C	503	1/1	0.96	0.19	69,69,69,69	0

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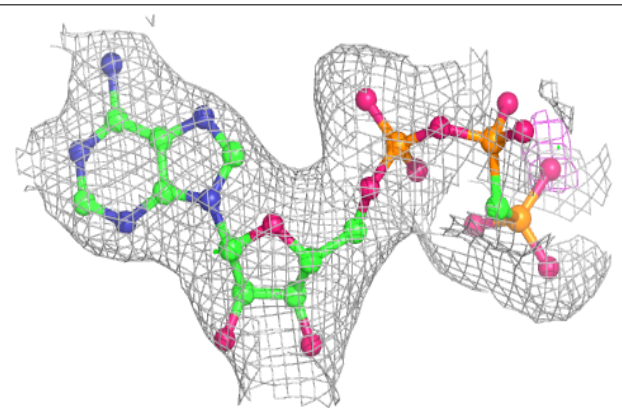
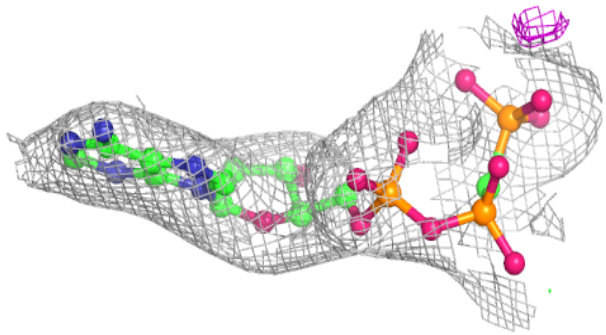
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	F	401	1/1	0.96	0.04	88,88,88,88	0
10	GDP	D	501	28/28	0.96	0.12	45,61,81,86	0
11	6K9	B	503	52/52	0.96	0.11	42,60,74,79	0
6	MG	C	502	1/1	0.97	0.11	40,40,40,40	0
10	GDP	B	501	28/28	0.97	0.19	40,51,57,60	0
5	GTP	C	501	32/32	0.98	0.16	35,40,51,53	0
5	GTP	A	501	32/32	0.98	0.13	38,49,57,84	0
7	CA	B	502	1/1	0.99	0.26	96,96,96,96	0

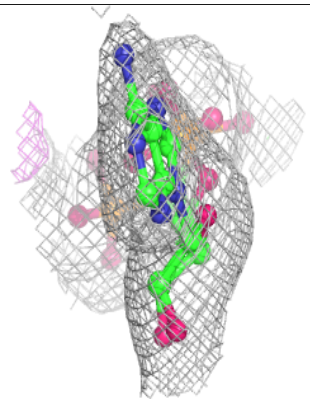
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 400:

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

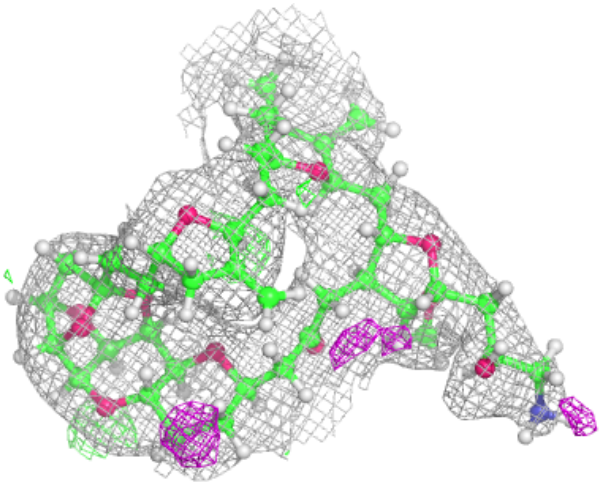


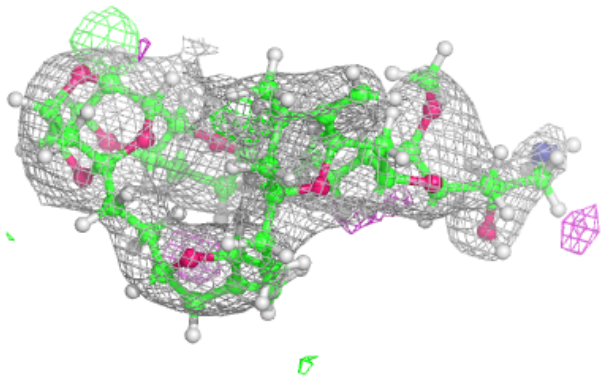


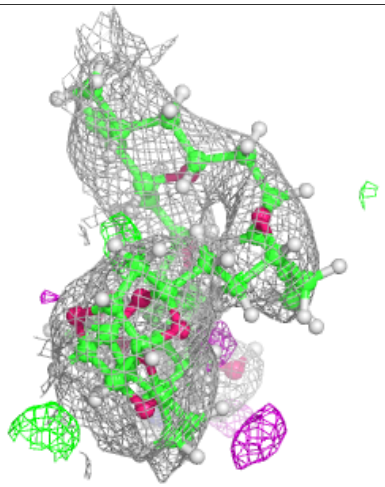


Electron density around 6K9 D 502:

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

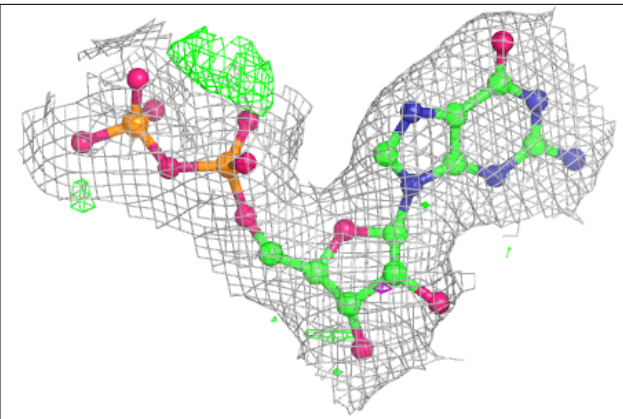


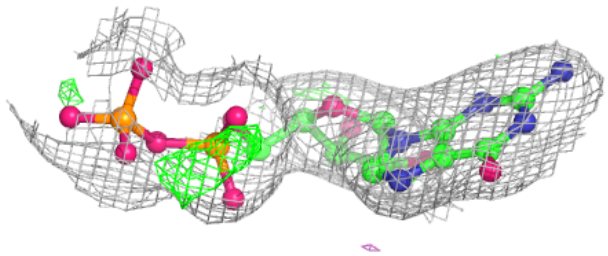




Electron density around GDP D 501:

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





Electron density around 6K9 B 503:

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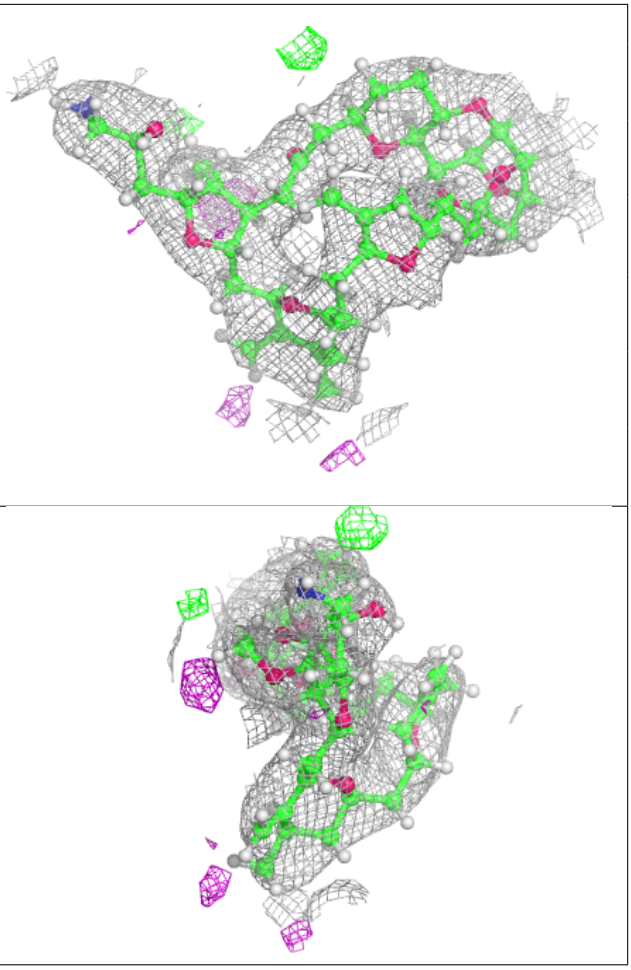
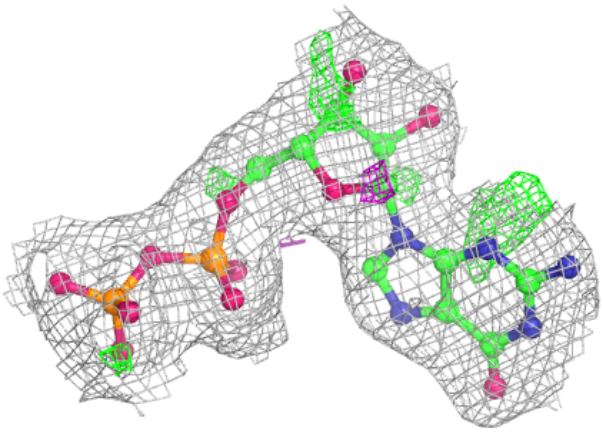
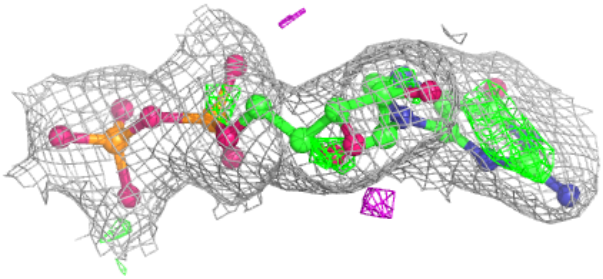
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

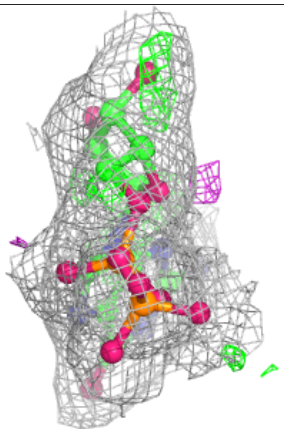


Electron density around GDP B 501:

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

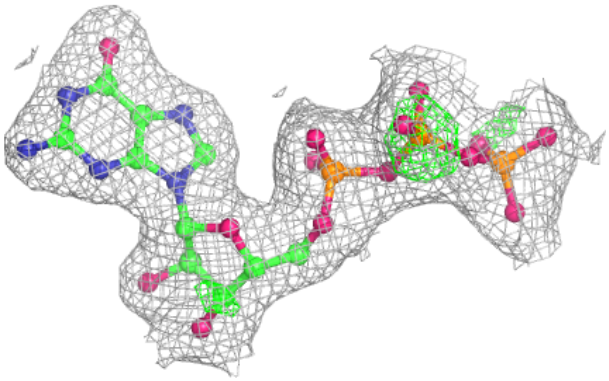


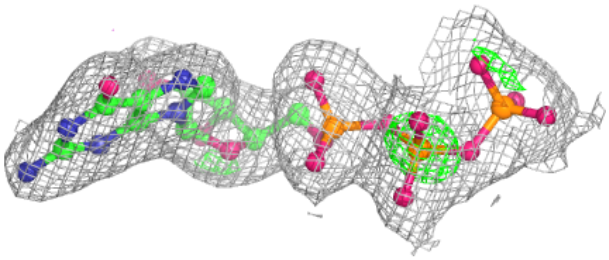


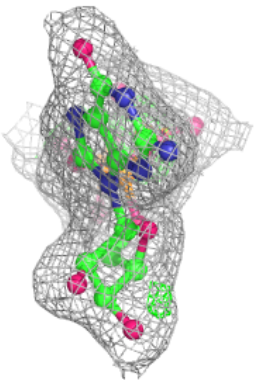


Electron density around GTP C 501:

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

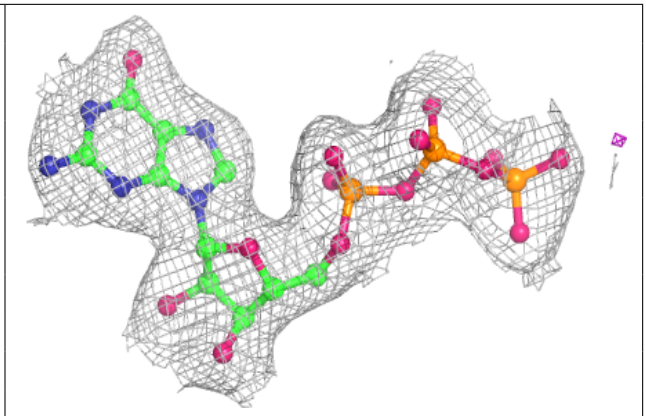


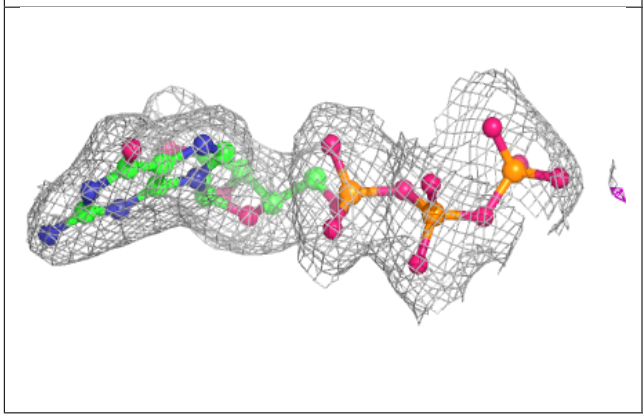


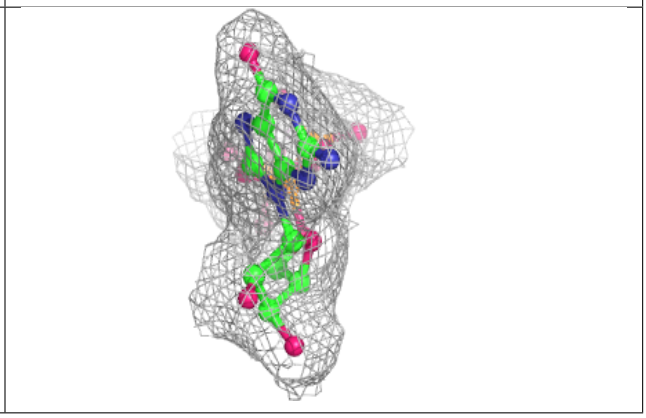


Electron density around GTP A 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.