Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 10:19 PM JST

PDB ID	:	7DP8
Title	:	Crystal structure of T2R-TTL-Cevipabulin-eribulin complex
Authors	:	Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on	:	2020-12-18
Resolution	:	2.45 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:

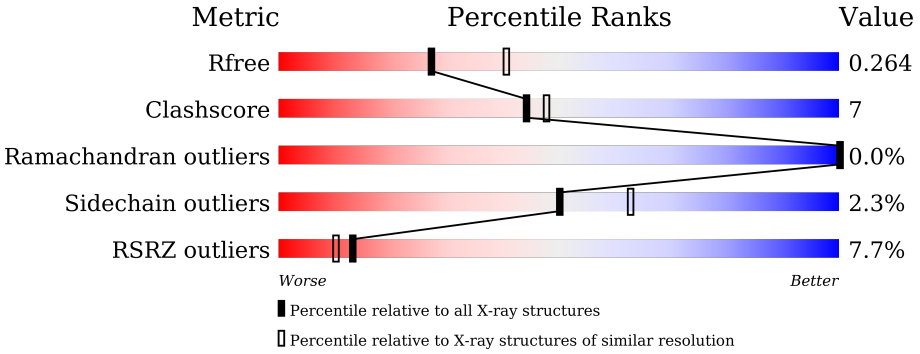
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.45 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	2%, 83%, 14%, •
1	C	450	2%, 88%, 9%, •
2	B	445	2%, 79%, 14%, • 6%
2	D	445	9%, 81%, 14%, •
3	E	143	11%, 69%, 15%, • • 14%
4	F	384	23%, 67%, 23%, 9%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 35012 atoms, of which 17101 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	438	6802	2182	3351	588	657	24	0	4	0
1	C	440	6844	2201	3369	589	662	23	0	8	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	418	6498	2080	3185	565	639	29	0	4	0
2	D	426	6563	2100	3217	570	649	27	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	123	2069	635	1037	188	204	5	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

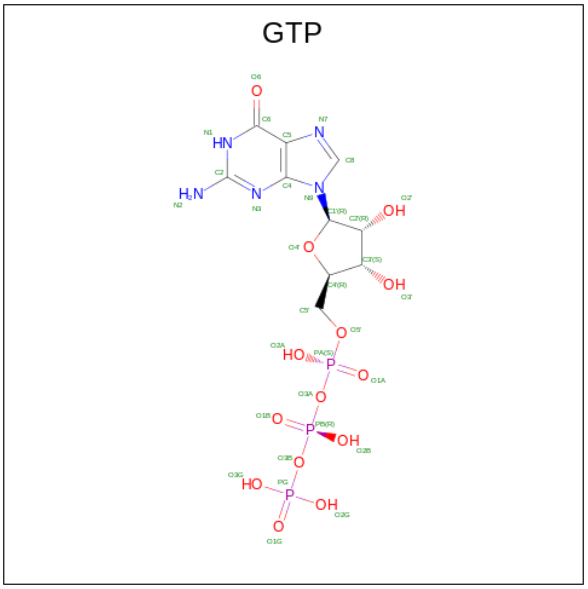
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	351	5696	1838	2824	491	528	15	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
5	A	1	42	10	10	5	14	3	0	0
5	C	1	42	10	10	5	14	3	0	0
5	D	1	42	10	10	5	14	3	0	0

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

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

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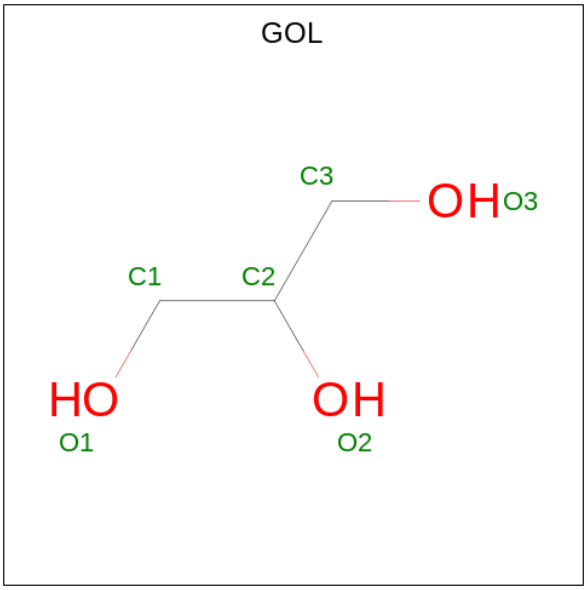
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

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

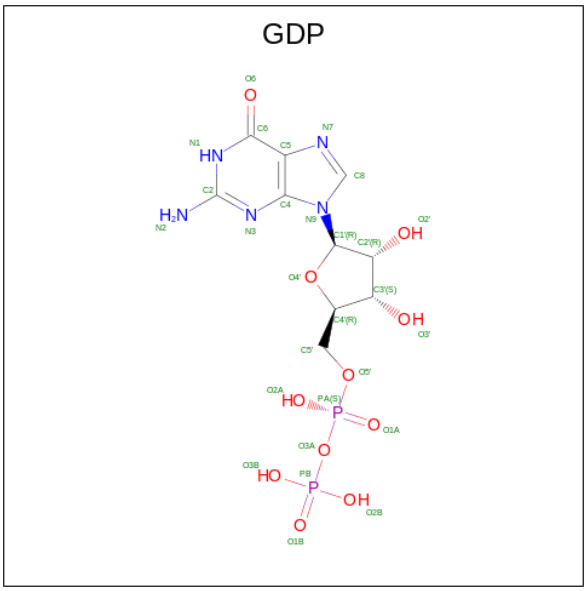
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0
7	B	2	Total Ca 2 2	0	0
7	C	2	Total Ca 2 2	0	0

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



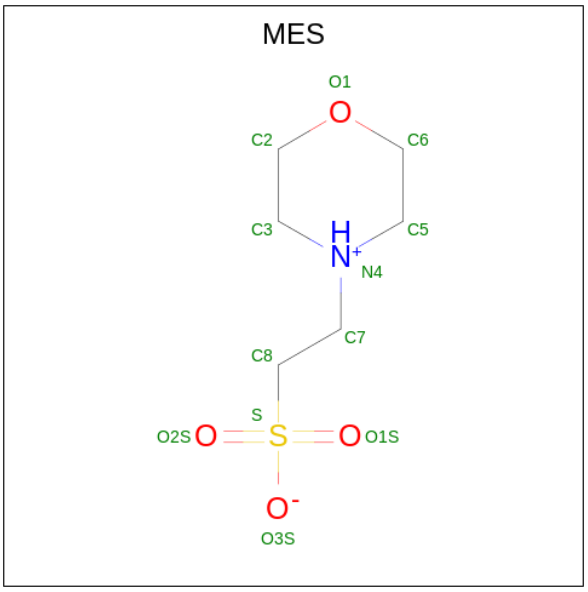
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 14 3 8 3	0	0
8	A	1	Total C H O 14 3 8 3	0	0

- 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	H	N	O	P		
9	B	1	38	10	10	5	11	2	0	0

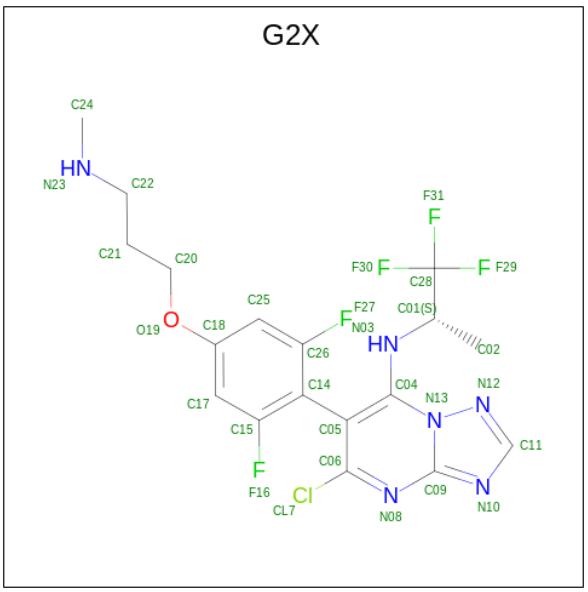
- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

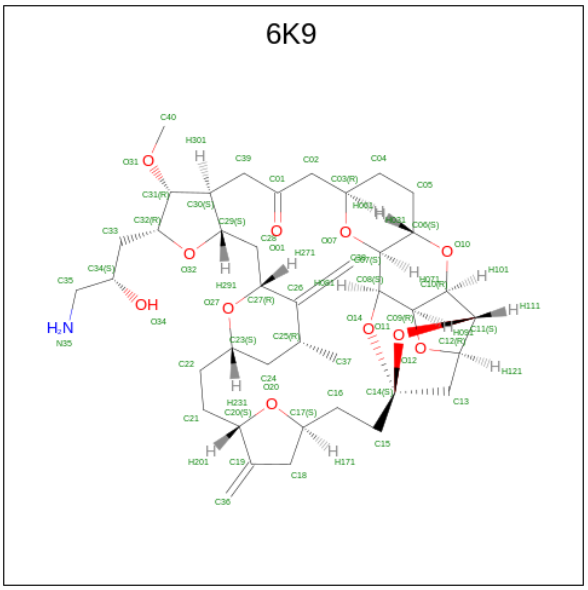
- Molecule 11 is 6-[2,6-bis(fluoranyl)-4-[3-(methylamino)propoxy]phenyl]-5-chloranyl-N-[(2S)-1,1,1-tris(fluoranyl)propan-2-yl]-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (three-letter code:

G2X) (formula: $C_{18}H_{18}ClF_5N_6O$) (labeled as "Ligand of Interest" by depositor).



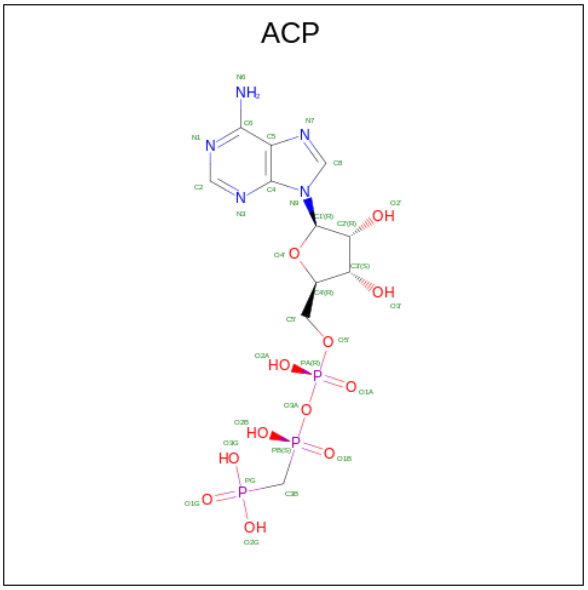
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	H	N	O		
11	C	1	49	18	1	5	18	6	1	0	0
			Total	C	Cl	F	H	N	O		
11	C	1	49	18	1	5	18	6	1	0	0

- Molecule 12 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	N	O		
12	D	1	52	40	1	11	0	0

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

- Molecule 14 is water.

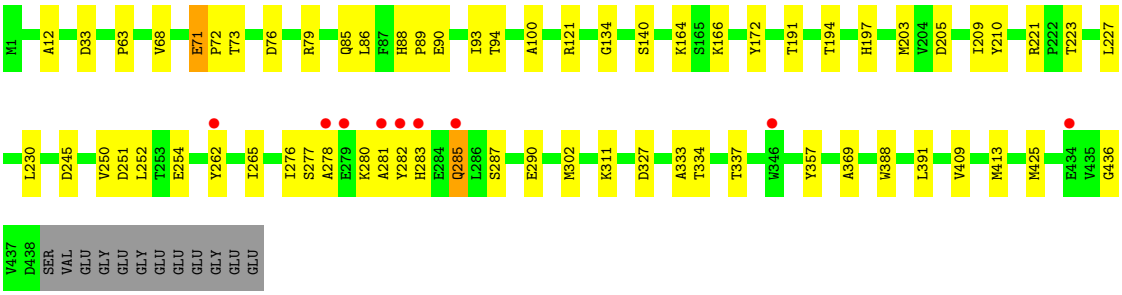
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	18	18	18	0	0
14	B	29	29	29	0	0
14	C	57	57	57	0	0
14	D	7	7	7	0	0
14	E	4	4	4	0	0
14	F	3	3	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

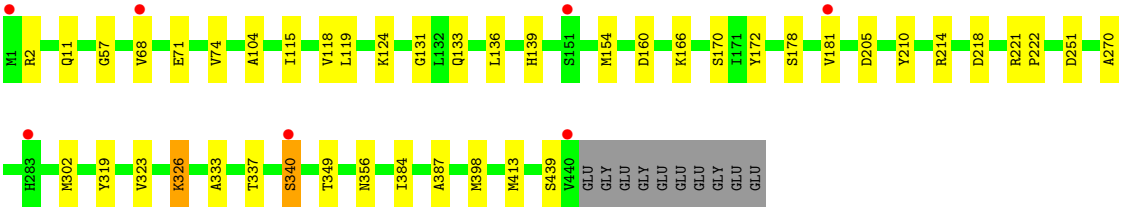
• Molecule 1: Tubulin alpha-1B chain

Chain A:



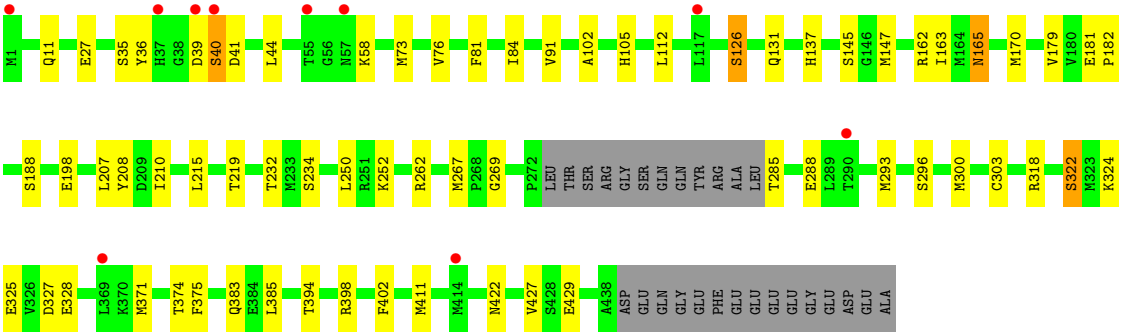
• Molecule 1: Tubulin alpha-1B chain

Chain C:



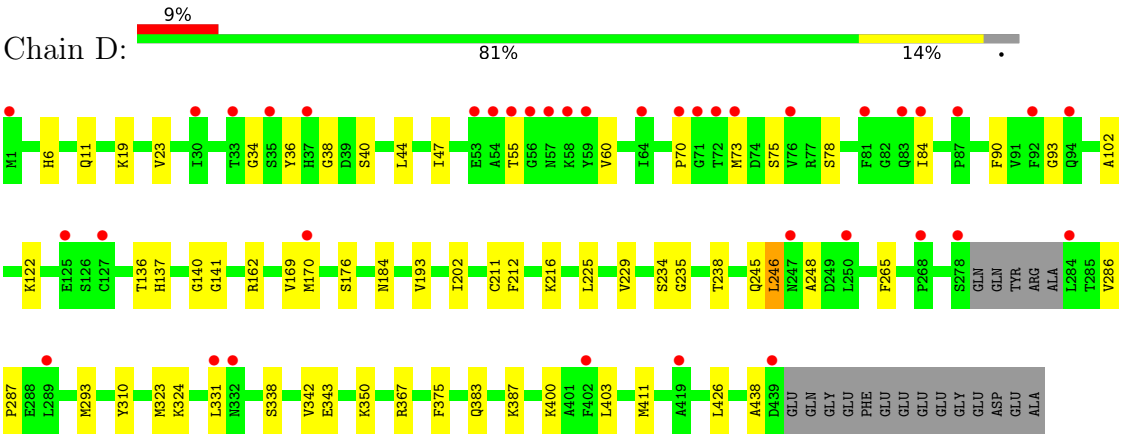
• Molecule 2: Tubulin beta chain

Chain B:



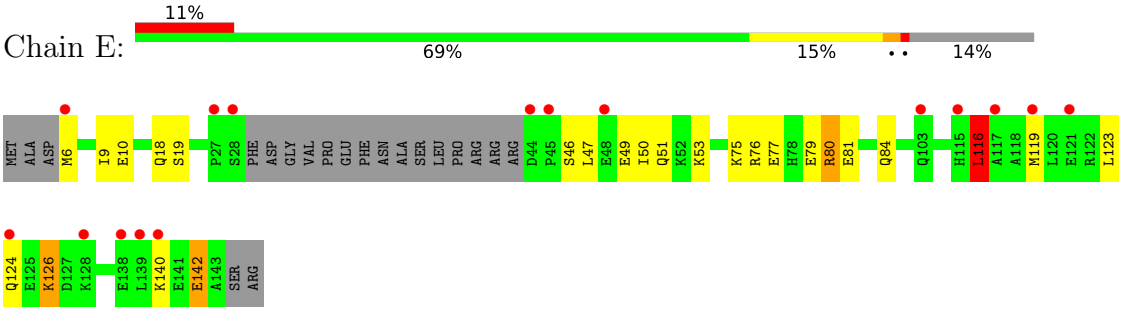
- Molecule 2: Tubulin beta chain

Chain D:



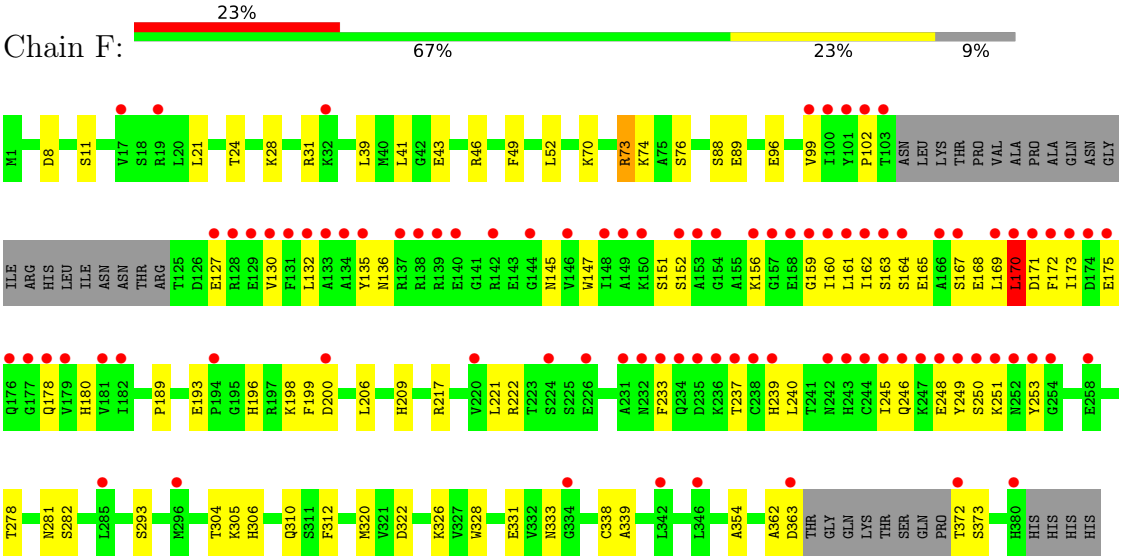
- Molecule 3: Stathmin-4

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	103.94Å 159.07Å 176.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.46 – 2.45 59.46 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.0 (59.46-2.45) 95.0 (59.46-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.227 , 0.264 0.227 , 0.264	Depositor DCC
R_{free} test set	5151 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	35012	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: CA, MG, GDP, 6K9, MES, GTP, ACP, GOL, G2X

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	0.36	1/3532 (0.0%)	0.51	2/4794 (0.0%)
1	C	0.34	1/3577 (0.0%)	0.56	3/4859 (0.1%)
2	B	0.30	0/3389	0.48	0/4588
2	D	0.29	0/3422	0.48	0/4634
3	E	0.32	0/1041	0.56	2/1382 (0.1%)
4	F	0.29	0/2937	0.51	1/3967 (0.0%)
All	All	0.32	2/17898 (0.0%)	0.51	8/24224 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	D	0	1
3	E	0	1
4	F	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	340	SER	CB-OG	8.83	1.53	1.42
1	A	285	GLN	CB-CG	-7.39	1.32	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	340	SER	CA-CB-OG	14.11	149.30	111.20
3	E	116	LEU	CA-CB-CG	9.04	136.10	115.30
1	C	340	SER	CB-CA-C	-7.62	95.61	110.10
3	E	116	LEU	CB-CG-CD1	-7.41	98.41	111.00
1	C	340	SER	N-CA-CB	6.93	120.90	110.50
1	A	285	GLN	CG-CD-OE1	-6.78	108.04	121.60
1	A	285	GLN	CB-CG-CD	-5.99	96.02	111.60
4	F	170	LEU	CA-CB-CG	5.69	128.40	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	GLN	Sidechain
1	C	340	SER	Mainchain
2	D	55	THR	Peptide
3	E	116	LEU	Peptide
4	F	170	LEU	Peptide

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	3451	3351	3362	43	1
1	C	3475	3369	3384	26	1
2	B	3313	3185	3192	47	0
2	D	3346	3217	3227	37	0
3	E	1032	1037	1040	23	0
4	F	2872	2824	2835	62	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	2	0	0	0	0
7	C	2	0	0	0	0
8	A	12	16	16	1	0
9	B	28	10	12	2	0
10	B	12	12	12	0	0
11	C	62	36	0	0	0
12	D	52	0	0	2	0
13	F	31	14	14	1	0
14	A	18	0	0	1	0
14	B	29	0	0	4	0
14	C	57	0	0	3	0
14	D	7	0	0	0	0
14	E	4	0	0	2	0
14	F	3	0	0	0	0
All	All	17911	17101	17130	232	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (232) 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:162:ARG:NH1	14:B:601:HOH:O	1.93	1.00
3:E:116:LEU:HA	3:E:119:MET:H	1.47	0.80
2:D:75:SER:O	2:D:78:SER:OG	1.99	0.79
1:A:276:ILE:HG21	1:A:283:HIS:CE1	2.19	0.77
4:F:168:GLU:HA	4:F:171:ASP:HB3	1.68	0.76
1:C:439:SER:O	14:C:701:HOH:O	2.05	0.74
1:C:218:ASP:OD2	14:C:702:HOH:O	2.10	0.69
2:D:73:MET:HG3	2:D:90:PHE:HD2	1.59	0.68
2:D:60:VAL:HG23	2:D:84:ILE:O	1.93	0.68
2:B:145[A]:SER:HG	2:B:188:SER:HG	1.34	0.67
4:F:168:GLU:HA	4:F:171:ASP:CB	2.24	0.67
4:F:304:THR:OG1	4:F:310:GLN:OE1	2.11	0.67
1:A:250:VAL:HG22	1:A:254:GLU:OE2	1.96	0.66
2:B:262:ARG:NH1	2:B:429:GLU:OE2	2.28	0.66
2:B:11:GLN:NE2	14:B:605:HOH:O	2.29	0.65
3:E:75:LYS:HD3	3:E:76:ARG:NH2	2.10	0.65
9:B:501:GDP:O1A	14:B:602:HOH:O	2.14	0.65
2:D:44:LEU:HD22	2:D:47:ILE:HD13	1.80	0.64
2:B:422:ASN:OD1	14:B:603:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:SER:HG	2:B:325:GLU:HB2	1.63	0.64
8:A:504:GOL:O1	8:A:504:GOL:O3	2.13	0.63
4:F:217:ARG:NH2	4:F:373:SER:O	2.32	0.63
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.81	0.62
2:D:343:GLU:HG3	2:D:438:ALA:HB2	1.81	0.62
1:A:276:ILE:HG21	1:A:283:HIS:ND1	2.18	0.59
2:D:245:GLN:HA	2:D:248:ALA:HB2	1.85	0.58
2:B:322:SER:OG	2:B:325:GLU:HB2	2.03	0.58
1:A:265:ILE:O	1:A:265:ILE:HG22	2.02	0.58
1:C:178:SER:OG	2:D:350:LYS:NZ	2.37	0.58
4:F:170:LEU:HA	4:F:173:ILE:HG12	1.86	0.58
1:A:327:ASP:OD2	14:A:601:HOH:O	2.17	0.57
4:F:278:THR:OG1	4:F:281:ASN:N	2.36	0.57
2:D:36:TYR:OH	2:D:40:SER:O	2.21	0.57
4:F:278:THR:O	4:F:282:SER:OG	2.16	0.57
3:E:53:LYS:O	14:E:201:HOH:O	2.18	0.56
1:A:221:ARG:NH1	2:B:327:ASP:OD2	2.39	0.55
2:D:141:GLY:O	2:D:184:ASN:ND2	2.39	0.55
2:B:215:LEU:HD12	2:B:215:LEU:H	1.71	0.55
3:E:116:LEU:HB2	3:E:119:MET:HB3	1.88	0.55
2:B:126:SER:O	2:B:126:SER:OG	2.25	0.54
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.89	0.54
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.42	0.54
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.88	0.54
2:B:131:GLN:OE1	2:B:250:LEU:N	2.37	0.53
3:E:140:LYS:NZ	14:E:202:HOH:O	2.32	0.53
3:E:116:LEU:CB	3:E:119:MET:HB3	2.39	0.53
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.90	0.53
4:F:151:SER:HB3	4:F:180:HIS:CG	2.44	0.53
4:F:246:GLN:O	4:F:250:SER:HB3	2.08	0.53
1:A:71:GLU:OE1	1:A:73:THR:HG23	2.08	0.53
1:A:281:ALA:O	1:A:282:TYR:HB2	2.09	0.53
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.38	0.53
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.91	0.52
2:B:262:ARG:NH2	2:B:422:ASN:OD1	2.43	0.52
1:C:160:ASP:OD2	14:C:703:HOH:O	2.19	0.52
2:D:293:MET:HG2	2:D:375:PHE:HB2	1.92	0.52
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.92	0.52
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.93	0.51
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.44	0.51
1:A:276:ILE:CG2	1:A:283:HIS:CE1	2.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.46	0.51
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.46	0.51
1:A:209:ILE:HD11	1:A:302:MET:SD	2.50	0.51
2:D:212:PHE:O	2:D:216:LYS:HA	2.10	0.51
3:E:116:LEU:HB3	3:E:119:MET:HB2	1.93	0.50
4:F:200:ASP:OD2	4:F:222:ARG:HB2	2.11	0.50
2:D:34:GLY:HA2	2:D:84:ILE:HD11	1.94	0.50
4:F:46:ARG:NH1	4:F:46:ARG:HG2	2.27	0.50
4:F:193:GLU:OE1	4:F:196:HIS:ND1	2.35	0.50
2:D:193:VAL:HG22	2:D:265:PHE:HE2	1.77	0.49
4:F:233:PHE:HA	4:F:239:HIS:NE2	2.27	0.49
1:A:251:ASP:OD1	1:A:252:LEU:N	2.45	0.49
4:F:178:GLN:HA	4:F:178:GLN:OE1	2.13	0.49
2:B:35:SER:OG	2:B:58:LYS:HE3	2.12	0.49
2:D:193:VAL:HG22	2:D:265:PHE:CE2	2.48	0.49
4:F:73:ARG:HE	4:F:152:SER:HB3	1.77	0.49
4:F:46:ARG:HG2	4:F:46:ARG:HH11	1.78	0.48
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.46	0.48
4:F:170:LEU:HA	4:F:173:ILE:CG1	2.43	0.48
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.48	0.48
1:A:287:SER:OG	1:A:290:GLU:N	2.42	0.48
1:C:181[A]:VAL:HG12	1:C:398:MET:HE3	1.95	0.48
3:E:116:LEU:HB3	3:E:119:MET:CB	2.44	0.48
4:F:8:ASP:HB2	4:F:43:GLU:HA	1.95	0.48
2:D:19:LYS:O	2:D:23:VAL:HG23	2.14	0.48
4:F:127:GLU:HA	4:F:130:VAL:HG23	1.95	0.48
3:E:123:LEU:HD22	3:E:126:LYS:HD3	1.94	0.48
4:F:96:GLU:HG2	4:F:147:TRP:CH2	2.49	0.48
4:F:135:TYR:HD1	4:F:136:ASN:OD1	1.97	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.31	0.48
4:F:127:GLU:HB3	4:F:130:VAL:HB	1.95	0.48
4:F:163:SER:OG	4:F:164:SER:N	2.46	0.48
2:D:235:GLY:O	2:D:238:THR:HG22	2.14	0.47
4:F:233:PHE:HA	4:F:239:HIS:CE1	2.50	0.47
4:F:372:THR:OG1	4:F:373:SER:N	2.47	0.47
2:D:140:GLY:O	2:D:184:ASN:ND2	2.42	0.47
2:D:202:ILE:HG21	2:D:229:VAL:HG22	1.96	0.47
1:A:265:ILE:HD12	1:A:265:ILE:N	2.28	0.47
4:F:70:LYS:HA	4:F:76:SER:HB3	1.97	0.47
1:A:203:MET:HE1	1:A:388:TRP:CH2	2.49	0.47
1:C:2:ARG:HA	1:C:131:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:189:PRO:HA	4:F:322:ASP:HA	1.96	0.47
2:B:40:SER:OG	2:B:41:ASP:N	2.47	0.47
2:D:169:VAL:HA	2:D:202:ILE:O	2.15	0.47
4:F:89:GLU:CD	4:F:89:GLU:H	2.19	0.47
4:F:161:LEU:HD23	4:F:169:LEU:HD13	1.97	0.46
2:B:383:GLN:HG3	2:B:427:VAL:HG13	1.97	0.46
1:A:79:ARG:NH2	1:A:94:THR:HG23	2.31	0.46
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.98	0.46
2:D:193:VAL:CG2	2:D:426:LEU:HD22	2.46	0.46
4:F:338:CYS:SG	4:F:339:ALA:N	2.89	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.46
4:F:362:ALA:O	4:F:363:ASP:HB2	2.16	0.46
2:B:210:ILE:HG22	2:B:215:LEU:CD1	2.46	0.46
2:B:285:THR:N	2:B:288:GLU:OE1	2.48	0.46
4:F:237:THR:O	4:F:246:GLN:NE2	2.49	0.46
2:B:318:ARG:O	2:B:371:MET:HA	2.16	0.46
1:C:133:GLN:OE1	1:C:251:ASP:HB2	2.16	0.45
3:E:116:LEU:HA	3:E:119:MET:N	2.23	0.45
1:C:115:ILE:O	1:C:119:LEU:HD23	2.17	0.45
4:F:246:GLN:O	4:F:253:TYR:HB2	2.17	0.45
2:B:105:HIS:HE1	3:E:75:LYS:NZ	2.14	0.45
2:B:170:MET:SD	2:B:385:LEU:HD21	2.55	0.45
3:E:116:LEU:CA	3:E:119:MET:H	2.23	0.45
2:B:39:ASP:OD1	2:B:39:ASP:N	2.44	0.45
2:D:176:SER:HA	12:D:503:6K9:O01	2.16	0.45
1:A:68:VAL:HG12	1:A:93:ILE:HD12	1.99	0.45
1:A:71:GLU:CD	1:A:73:THR:HG1	2.21	0.45
2:D:193:VAL:HG21	2:D:426:LEU:HD22	1.98	0.45
3:E:50:ILE:O	3:E:53:LYS:HB3	2.17	0.45
4:F:99:VAL:HG12	4:F:127:GLU:OE1	2.16	0.45
1:A:191:THR:HG21	1:A:425:MET:HE1	1.97	0.45
1:A:210:TYR:OH	1:A:221:ARG:CD	2.65	0.44
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.44
2:B:162:ARG:HG2	2:B:162:ARG:HH11	1.81	0.44
2:B:207:LEU:HD21	2:B:300:MET:HB3	1.98	0.44
4:F:333:ASN:ND2	13:F:402:ACP:O3G	2.51	0.44
2:D:70:PRO:HG3	2:D:93:GLY:O	2.18	0.44
4:F:239:HIS:C	4:F:240:LEU:HD23	2.38	0.44
1:A:90:GLU:HG2	1:A:121:ARG:HD2	1.99	0.44
2:B:267:MET:HE1	2:B:303:CYS:O	2.17	0.44
4:F:161:LEU:HD23	4:F:169:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.44
4:F:305:LYS:HD3	4:F:306:HIS:NE2	2.33	0.44
3:E:116:LEU:CB	3:E:119:MET:CB	2.95	0.44
2:B:91:VAL:HG12	2:B:112:LEU:HD11	2.00	0.44
2:B:383:GLN:CG	2:B:427:VAL:HG13	2.48	0.44
2:B:219:THR:HG22	1:C:326:LYS:HE3	1.99	0.43
4:F:326:LYS:HE3	4:F:328:TRP:CZ2	2.53	0.43
2:B:394:THR:O	2:B:398:ARG:HG3	2.18	0.43
2:B:36:TYR:CE1	2:B:44:LEU:HD11	2.53	0.43
2:D:383:GLN:O	2:D:387:LYS:HG3	2.18	0.43
1:A:88:HIS:NE2	1:A:90:GLU:HB2	2.33	0.43
1:A:280:LYS:HZ2	1:A:280:LYS:HB3	1.84	0.43
9:B:501:GDP:H8	9:B:501:GDP:H5"	1.83	0.43
1:C:270:ALA:O	1:C:302:MET:HB2	2.19	0.43
2:B:165:ASN:ND2	2:B:198:GLU:HB2	2.34	0.43
2:B:293[B]:MET:CG	2:B:375:PHE:HB2	2.48	0.43
4:F:209:HIS:H	4:F:209:HIS:CD2	2.37	0.43
2:B:269:GLY:O	2:B:374:THR:HG23	2.19	0.43
4:F:167:SER:CB	4:F:168:GLU:OE1	2.67	0.43
1:A:33:ASP:HA	1:A:85:GLN:HG3	2.00	0.43
4:F:172:PHE:O	4:F:175:GLU:HB3	2.18	0.43
1:A:223:THR:O	1:A:227:LEU:HG	2.18	0.43
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	2.01	0.43
1:C:11:GLN:HG3	1:C:74:VAL:HG21	2.01	0.42
2:D:11:GLN:OE1	12:D:503:6K9:C13	2.67	0.42
2:D:44:LEU:HA	2:D:47:ILE:HB	2.00	0.42
2:B:112:LEU:HB3	2:B:147:MET:HE3	2.02	0.42
2:B:208:TYR:OH	1:C:326:LYS:HG3	2.20	0.42
2:B:324:LYS:C	2:B:324:LYS:HE2	2.40	0.42
1:C:384:ILE:HG12	1:C:384:ILE:O	2.19	0.42
3:E:80:ARG:O	3:E:84:GLN:HG3	2.20	0.42
4:F:156:LYS:C	4:F:245:ILE:HD11	2.39	0.42
2:B:73:MET:HA	2:B:76:VAL:HG22	2.00	0.42
1:C:154:MET:HE3	1:C:166:LYS:HE2	2.00	0.42
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.01	0.42
1:A:333:ALA:O	1:A:337:THR:HG23	2.19	0.42
2:D:6:HIS:HE1	2:D:136:THR:HG21	1.83	0.42
2:D:102:ALA:HB2	2:D:411:MET:SD	2.60	0.42
3:E:9:ILE:HB	3:E:10:GLU:OE1	2.19	0.42
4:F:198:LYS:HE2	4:F:320:MET:CE	2.49	0.42
2:B:27:GLU:OE2	2:B:234:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:77:GLU:O	3:E:81:GLU:HG3	2.20	0.42
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.01	0.42
1:A:334:THR:O	1:A:337:THR:OG1	2.27	0.42
2:D:343:GLU:CG	2:D:438:ALA:HB2	2.47	0.42
4:F:135:TYR:OH	4:F:165:GLU:HA	2.20	0.42
4:F:278:THR:OG1	4:F:281:ASN:HB2	2.20	0.42
2:D:6:HIS:CE1	2:D:136:THR:HG21	2.55	0.42
1:A:63:PRO:HG2	1:A:86:LEU:HD23	2.02	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.03	0.41
1:A:134:GLY:HA2	1:A:164:LYS:HB3	2.01	0.41
1:A:333:ALA:HB2	3:E:6:MET:SD	2.60	0.41
2:B:102:ALA:HB2	2:B:411:MET:SD	2.60	0.41
2:B:232:THR:HG21	2:B:300:MET:SD	2.60	0.41
1:A:100:ALA:HA	2:B:252:LYS:HG3	2.02	0.41
1:A:357:TYR:OH	3:E:18:GLN:HG3	2.20	0.41
2:B:181:GLU:CG	2:B:182:PRO:HD3	2.50	0.41
4:F:198:LYS:NZ	4:F:239:HIS:O	2.45	0.41
2:B:179:VAL:HG11	2:B:402:PHE:CZ	2.55	0.41
1:C:172:TYR:CE2	1:C:387:ALA:HB1	2.56	0.41
2:D:400:LYS:HB3	2:D:403:LEU:HD12	2.02	0.41
1:A:88:HIS:ND1	1:A:89:PRO:HD2	2.35	0.41
2:B:81:PHE:O	2:B:84:ILE:HG22	2.20	0.41
2:D:44:LEU:CD2	2:D:47:ILE:HD13	2.49	0.41
4:F:250:SER:OG	4:F:253:TYR:HB2	2.20	0.41
1:A:172:TYR:OH	1:A:391:LEU:HG	2.21	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.03	0.41
1:C:154:MET:HE1	1:C:166:LYS:HB3	2.02	0.41
2:D:211:CYS:SG	2:D:225:LEU:HD23	2.60	0.41
2:B:179:VAL:O	1:C:349:THR:OG1	2.39	0.41
2:B:324:LYS:HE3	2:B:328:GLU:OE1	2.20	0.41
1:A:72:PRO:HB2	1:A:76:ASP:OD2	2.20	0.41
2:D:310:TYR:O	2:D:342:VAL:HG22	2.21	0.41
4:F:163:SER:HA	4:F:233:PHE:CD1	2.56	0.41
2:D:246:LEU:HD21	2:D:350:LYS:HB3	2.02	0.41
3:E:75:LYS:CE	3:E:79:GLU:OE2	2.69	0.41
1:C:349:THR:OG1	1:C:349:THR:O	2.34	0.40
3:E:46:SER:HB3	3:E:49:GLU:HG3	2.02	0.40
3:E:142:GLU:CA	3:E:142:GLU:OE2	2.69	0.40
4:F:159:GLY:O	4:F:160:ILE:HG12	2.21	0.40
4:F:162:ILE:HD11	4:F:240:LEU:HD21	2.03	0.40
1:A:166:LYS:HE2	1:A:197:HIS:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181[B]:VAL:HG22	1:C:398:MET:HE3	2.01	0.40
1:C:333:ALA:O	1:C:337:THR:HG23	2.21	0.40
1:A:194:THR:O	1:A:194:THR:HG22	2.21	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.22	0.40
4:F:312:PHE:CG	4:F:354:ALA:HB1	2.57	0.40
1:C:139:HIS:O	1:C:170:SER:HA	2.21	0.40
4:F:102:PRO:HB3	4:F:173:ILE:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:OD1	1:C:57:GLY:H[2_565]	1.50	0.10

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	440/450 (98%)	426 (97%)	14 (3%)	0	100	100
1	C	446/450 (99%)	431 (97%)	15 (3%)	0	100	100
2	B	418/445 (94%)	402 (96%)	16 (4%)	0	100	100
2	D	423/445 (95%)	409 (97%)	14 (3%)	0	100	100
3	E	121/143 (85%)	118 (98%)	3 (2%)	0	100	100
4	F	346/384 (90%)	329 (95%)	16 (5%)	1 (0%)	41	49
All	All	2194/2317 (95%)	2115 (96%)	78 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	88	SER

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	373/378 (99%)	370 (99%)	3 (1%)	81	88
1	C	379/378 (100%)	372 (98%)	7 (2%)	59	71
2	B	365/383 (95%)	359 (98%)	6 (2%)	62	74
2	D	369/383 (96%)	358 (97%)	11 (3%)	41	53
3	E	112/127 (88%)	105 (94%)	7 (6%)	18	23
4	F	314/342 (92%)	304 (97%)	10 (3%)	39	50
All	All	1912/1991 (96%)	1868 (98%)	44 (2%)	50	63

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	262	TYR
1	A	277	SER
2	B	40	SER
2	B	126	SER
2	B	137	HIS
2	B	165	ASN
2	B	296	SER
2	B	322	SER
1	C	71	GLU
1	C	136	LEU
1	C	205	ASP
1	C	214	ARG
1	C	221	ARG
1	C	326	LYS
1	C	356	ASN
2	D	122	LYS
2	D	137	HIS
2	D	162	ARG
2	D	170	MET
2	D	234	SER
2	D	246	LEU

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Mol	Chain	Res	Type
2	D	323	MET
2	D	324	LYS
2	D	331	LEU
2	D	338	SER
2	D	367	ARG
3	E	19	SER
3	E	47	LEU
3	E	51	GLN
3	E	80	ARG
3	E	124	GLN
3	E	126	LYS
3	E	142	GLU
4	F	11	SER
4	F	28	LYS
4	F	31	ARG
4	F	73	ARG
4	F	145	ASN
4	F	170	LEU
4	F	248	GLU
4	F	249	TYR
4	F	251	LYS
4	F	293	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	107	HIS
1	A	226	ASN
1	A	329	ASN
2	B	105	HIS
1	C	11	GLN
1	C	18	ASN
1	C	31	GLN
1	C	61	HIS
1	C	128	GLN
1	C	197	HIS
2	D	37	HIS
2	D	245	GLN
2	D	292	GLN
3	E	18	GLN
3	E	78	HIS

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Mol	Chain	Res	Type
3	E	136	ASN
4	F	180	HIS
4	F	242	ASN
4	F	243	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
10	MES	B	503	-	12,12,12	2.03	1 (8%)	14,16,16	1.82	5 (35%)
11	G2X	C	601	-	28,33,33	2.76	10 (35%)	30,48,48	1.34	5 (16%)
13	ACP	F	402	6	27,33,33	2.56	8 (29%)	32,52,52	1.92	8 (25%)
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.40	6 (18%)
8	GOL	A	505	-	5,5,5	0.53	0	5,5,5	0.74	0
9	GDP	B	501	-	24,30,30	1.02	2 (8%)	30,47,47	1.26	6 (20%)
11	G2X	C	605	-	28,33,33	2.91	12 (42%)	30,48,48	1.61	5 (16%)
12	6K9	D	503	-	58,60,60	2.20	15 (25%)	60,92,92	1.74	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	C	602	6	26,34,34	1.15	2 (7%)	32,54,54	1.52	6 (18%)
8	GOL	A	504	-	5,5,5	0.80	0	5,5,5	0.76	0
5	GTP	D	502	6	26,34,34	1.13	2 (7%)	32,54,54	1.59	6 (18%)

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
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
11	G2X	C	601	-	-	3/20/20/20	0/3/3/3
13	ACP	F	402	6	-	2/15/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
8	GOL	A	505	-	-	4/4/4/4	-
9	GDP	B	501	-	-	3/12/32/32	0/3/3/3
11	G2X	C	605	-	-	6/20/20/20	0/3/3/3
12	6K9	D	503	-	-	3/31/131/131	-
5	GTP	C	602	6	-	7/18/38/38	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	D	502	6	-	5/18/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	601	G2X	C28-C01	9.07	1.62	1.51
11	C	605	G2X	C28-C01	8.61	1.61	1.51
13	F	402	ACP	O4'-C1'	7.80	1.52	1.41
12	D	503	6K9	C02-C01	-7.23	1.41	1.51
12	D	503	6K9	C18-C19	-6.79	1.40	1.51
10	B	503	MES	C8-S	-6.71	1.68	1.77
11	C	605	G2X	C06-N08	6.32	1.36	1.30
11	C	601	G2X	C06-N08	6.27	1.36	1.30
13	F	402	ACP	PB-O3A	5.75	1.64	1.58
12	D	503	6K9	C39-C01	-5.67	1.43	1.51
12	D	503	6K9	O11-C11	4.53	1.50	1.43
5	C	602	GTP	C5-C6	-4.15	1.39	1.47
12	D	503	6K9	C38-C26	4.01	1.39	1.32
11	C	605	G2X	C14-C15	3.88	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	GTP	C5-C6	-3.87	1.39	1.47
11	C	605	G2X	C25-C26	3.86	1.44	1.37
5	A	501	GTP	C5-C6	-3.81	1.39	1.47
11	C	605	G2X	C06-C05	3.79	1.43	1.39
13	F	402	ACP	C2'-C1'	-3.52	1.48	1.53
11	C	601	G2X	C06-C05	3.48	1.43	1.39
12	D	503	6K9	C33-C32	3.48	1.58	1.52
11	C	601	G2X	C17-C15	3.38	1.43	1.37
12	D	503	6K9	C20-C19	-3.34	1.43	1.51
11	C	601	G2X	C25-C26	3.25	1.43	1.37
11	C	605	G2X	C14-C26	3.13	1.43	1.39
12	D	503	6K9	C30-C29	3.13	1.59	1.53
13	F	402	ACP	C6-N6	3.08	1.45	1.34
11	C	605	G2X	C09-N10	3.04	1.40	1.35
13	F	402	ACP	C4-N3	-3.03	1.31	1.35
11	C	605	G2X	C11-N12	3.02	1.38	1.33
11	C	605	G2X	C17-C15	3.02	1.42	1.37
13	F	402	ACP	O4'-C4'	3.02	1.51	1.45
11	C	601	G2X	C14-C15	2.87	1.43	1.39
13	F	402	ACP	C2'-C3'	-2.86	1.45	1.53
12	D	503	6K9	C08-C07	-2.84	1.46	1.52
12	D	503	6K9	C27-C26	-2.82	1.43	1.52
9	B	501	GDP	O4'-C1'	2.71	1.44	1.41
11	C	601	G2X	C11-N12	2.70	1.37	1.33
12	D	503	6K9	C25-C26	-2.67	1.44	1.52
12	D	503	6K9	C24-C25	2.63	1.57	1.53
11	C	605	G2X	C05-C04	2.62	1.45	1.42
9	B	501	GDP	C6-N1	-2.54	1.34	1.37
11	C	601	G2X	C06-CL7	2.53	1.78	1.74
11	C	601	G2X	C09-N10	2.46	1.39	1.35
11	C	605	G2X	C06-CL7	2.45	1.78	1.74
12	D	503	6K9	C33-C34	2.42	1.58	1.52
12	D	503	6K9	O07-C03	2.29	1.48	1.44
11	C	605	G2X	C21-C22	2.14	1.60	1.51
5	D	502	GTP	C2-N3	2.14	1.38	1.33
5	A	501	GTP	C2-N3	2.12	1.38	1.33
11	C	601	G2X	C21-C22	2.06	1.59	1.51
12	D	503	6K9	C05-C04	2.04	1.58	1.52
13	F	402	ACP	PB-O2B	-2.03	1.51	1.56
5	C	602	GTP	C2-N3	2.01	1.38	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	605	G2X	C14-C05-C04	4.92	128.45	121.41
13	F	402	ACP	C3'-C2'-C1'	4.57	107.85	100.98
13	F	402	ACP	N3-C2-N1	-4.54	121.59	128.68
13	F	402	ACP	C4-C5-N7	-3.98	105.25	109.40
12	D	503	6K9	C16-C15-C14	-3.94	108.98	114.43
5	C	602	GTP	PA-O3A-PB	-3.91	119.43	132.83
10	B	503	MES	C5-N4-C3	3.89	117.59	108.83
5	D	502	GTP	PA-O3A-PB	-3.51	120.78	132.83
12	D	503	6K9	C04-C03-C02	-3.51	106.65	113.21
12	D	503	6K9	C33-C34-C35	3.42	114.86	111.92
12	D	503	6K9	C10-O10-C06	3.42	121.70	113.63
5	D	502	GTP	PB-O3B-PG	-3.32	121.42	132.83
12	D	503	6K9	O27-C23-C24	-3.32	104.74	110.04
5	C	602	GTP	C5-C6-N1	3.31	119.80	113.95
13	F	402	ACP	C1'-N9-C4	-3.30	120.84	126.64
5	D	502	GTP	C8-N7-C5	3.27	109.23	102.99
12	D	503	6K9	C18-C19-C36	-3.25	120.16	126.33
5	C	602	GTP	C8-N7-C5	3.22	109.13	102.99
13	F	402	ACP	PB-O3A-PA	-3.22	122.34	132.56
11	C	605	G2X	C06-C05-C14	-3.21	117.67	123.88
5	D	502	GTP	C5-C6-N1	3.21	119.62	113.95
11	C	601	G2X	C05-C04-N03	-3.17	117.68	121.93
5	A	501	GTP	C8-N7-C5	3.15	109.00	102.99
5	A	501	GTP	C5-C6-N1	3.05	119.33	113.95
12	D	503	6K9	C23-O27-C27	3.03	117.26	112.42
5	D	502	GTP	C2-N1-C6	-2.75	120.04	125.10
5	C	602	GTP	C2-N1-C6	-2.73	120.07	125.10
5	A	501	GTP	C2-N1-C6	-2.71	120.11	125.10
5	C	602	GTP	PB-O3B-PG	-2.70	123.57	132.83
9	B	501	GDP	C3'-C2'-C1'	2.65	104.97	100.98
13	F	402	ACP	C2'-C3'-C4'	2.65	107.79	102.64
13	F	402	ACP	C2-N1-C6	2.64	123.27	118.75
10	B	503	MES	C7-N4-C5	2.62	117.94	111.23
9	B	501	GDP	C8-N7-C5	2.62	107.97	102.99
5	A	501	GTP	PA-O3A-PB	-2.61	123.86	132.83
10	B	503	MES	O3S-S-C8	2.57	109.93	105.77
12	D	503	6K9	C37-C25-C24	-2.54	107.33	111.40
9	B	501	GDP	C5-C6-N1	2.49	118.35	113.95
12	D	503	6K9	O12-C12-C11	-2.42	99.68	104.87
10	B	503	MES	O2S-S-C8	2.34	109.74	106.92
10	B	503	MES	O1S-S-C8	2.34	109.74	106.92
12	D	503	6K9	O01-C01-C02	-2.34	118.22	121.55
13	F	402	ACP	O2A-PA-O1A	-2.32	100.79	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	601	G2X	C25-C18-C17	-2.31	117.30	120.98
5	A	501	GTP	O2G-PG-O3B	2.30	112.33	104.64
12	D	503	6K9	C10-C11-C12	2.29	109.16	103.72
12	D	503	6K9	C32-C33-C34	-2.27	109.52	114.61
12	D	503	6K9	O07-C03-C04	2.24	112.27	109.86
12	D	503	6K9	C40-O31-C31	-2.19	108.79	114.52
11	C	605	G2X	C25-C18-C17	-2.17	117.53	120.98
5	C	602	GTP	O6-C6-C5	-2.16	120.16	124.37
11	C	605	G2X	C05-C06-CL7	-2.14	117.85	119.27
9	B	501	GDP	PA-O3A-PB	-2.14	125.48	132.83
11	C	605	G2X	C25-C26-C14	-2.12	121.03	123.45
5	D	502	GTP	C2'-C3'-C4'	2.10	106.73	102.64
9	B	501	GDP	C2'-C3'-C4'	2.04	106.60	102.64
5	A	501	GTP	PB-O3B-PG	-2.03	125.86	132.83
9	B	501	GDP	C2-N1-C6	-2.02	121.38	125.10
11	C	601	G2X	C14-C05-C04	2.02	124.30	121.41
11	C	601	G2X	C26-C14-C15	2.02	116.54	114.56
12	D	503	6K9	C05-C06-C07	-2.01	106.81	110.89
11	C	601	G2X	C05-C06-CL7	-2.00	117.94	119.27

There are no chirality outliers.

All (41) 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	602	GTP	PB-O3B-PG-O2G
5	C	602	GTP	C5'-O5'-PA-O1A
5	C	602	GTP	C5'-O5'-PA-O2A
5	D	502	GTP	C5'-O5'-PA-O1A
5	D	502	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
8	A	505	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
11	C	605	G2X	C02-C01-C28-F31
11	C	605	G2X	C05-C04-N03-C01
12	D	503	6K9	C33-C34-C35-N35
12	D	503	6K9	O34-C34-C35-N35
13	F	402	ACP	C5'-O5'-PA-O1A
8	A	505	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
11	C	601	G2X	C21-C22-N23-C24
8	A	505	GOL	C1-C2-C3-O3
8	A	504	GOL	O1-C1-C2-O2
8	A	505	GOL	O2-C2-C3-O3
11	C	605	G2X	N13-C04-N03-C01
5	D	502	GTP	PB-O3B-PG-O1G
5	D	502	GTP	PB-O3B-PG-O2G
5	C	602	GTP	C5'-O5'-PA-O3A
13	F	402	ACP	C5'-O5'-PA-O3A
11	C	601	G2X	O19-C20-C21-C22
11	C	601	G2X	C02-C01-N03-C04
11	C	605	G2X	C02-C01-N03-C04
5	A	501	GTP	PB-O3A-PA-O2A
5	C	602	GTP	PB-O3A-PA-O1A
12	D	503	6K9	C20-C21-C22-C23
11	C	605	G2X	C02-C01-C28-F30
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	502	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
11	C	605	G2X	N03-C01-C28-F31
5	C	602	GTP	PB-O3A-PA-O2A
5	C	602	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

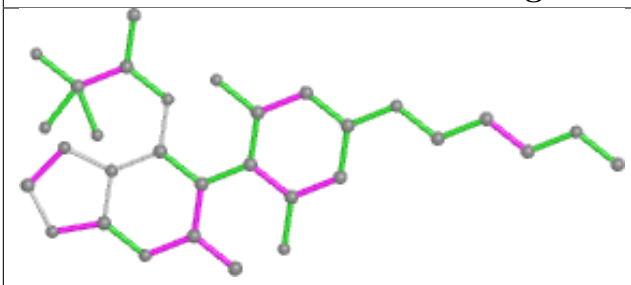
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	402	ACP	1	0
9	B	501	GDP	2	0
12	D	503	6K9	2	0
8	A	504	GOL	1	0

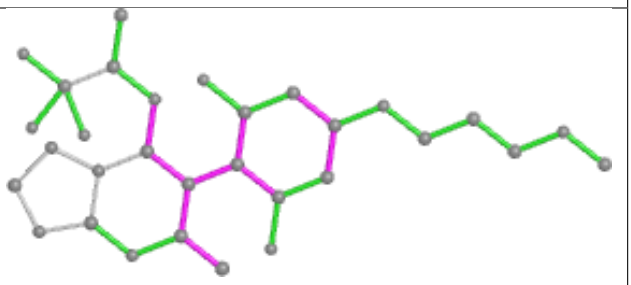
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

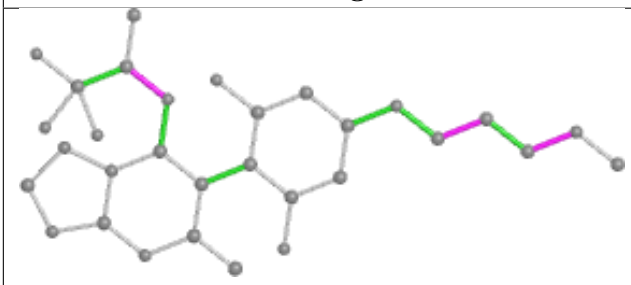
Ligand G2X C 601



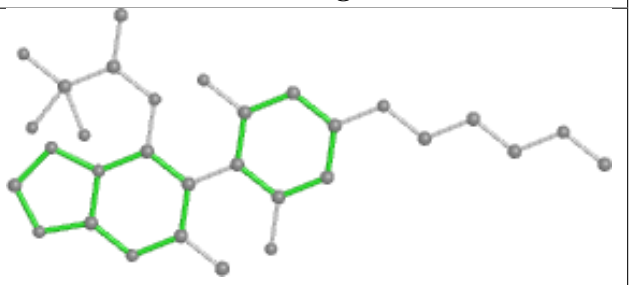
Bond lengths



Bond angles

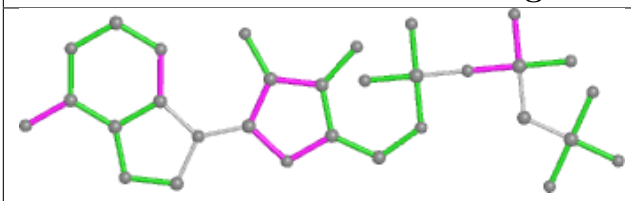


Torsions

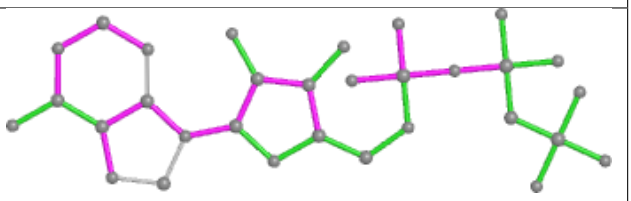


Rings

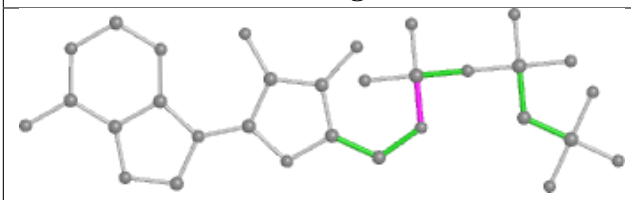
Ligand ACP F 402



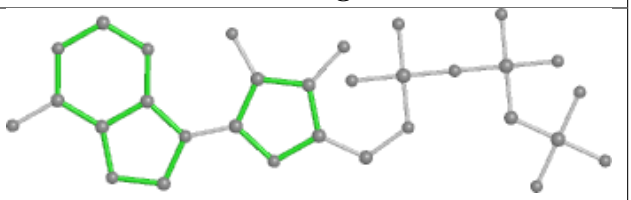
Bond lengths



Bond angles

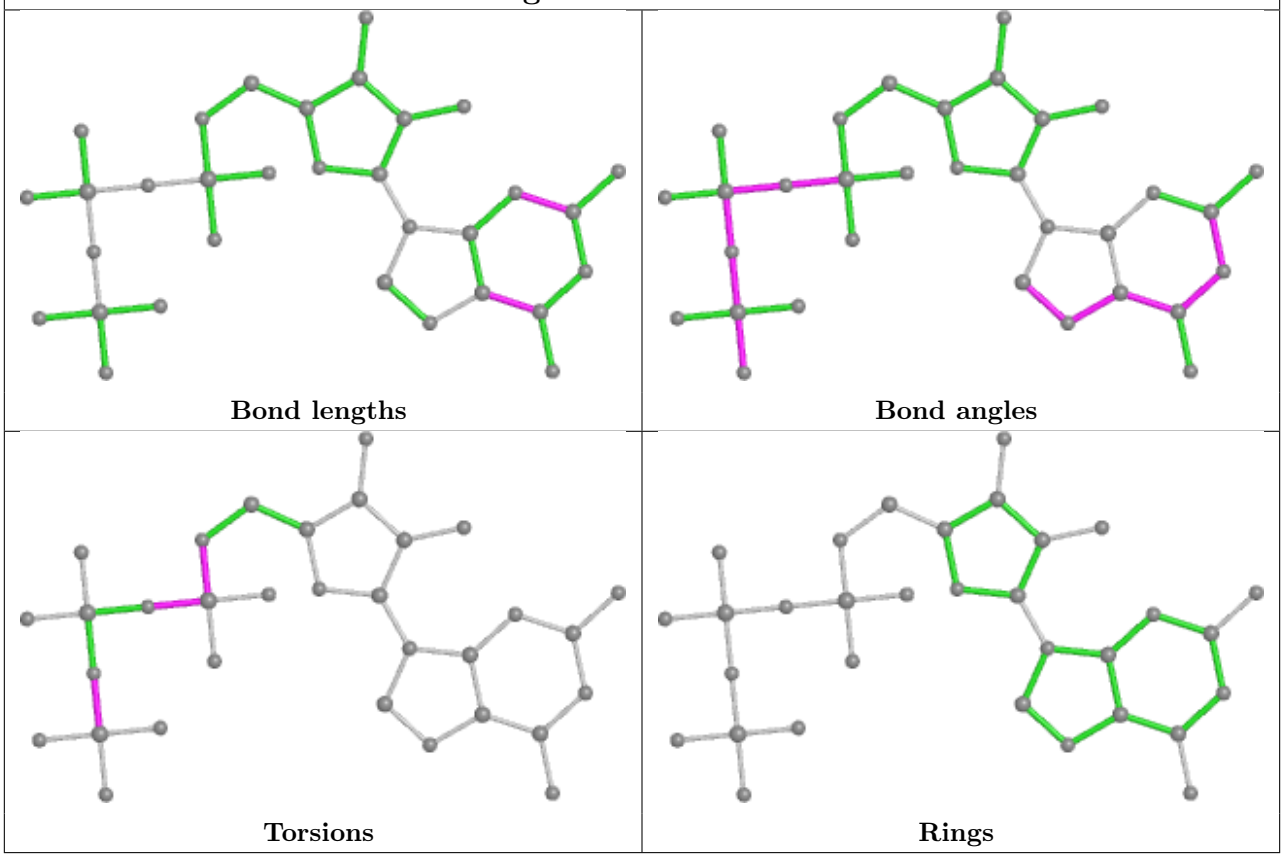


Torsions

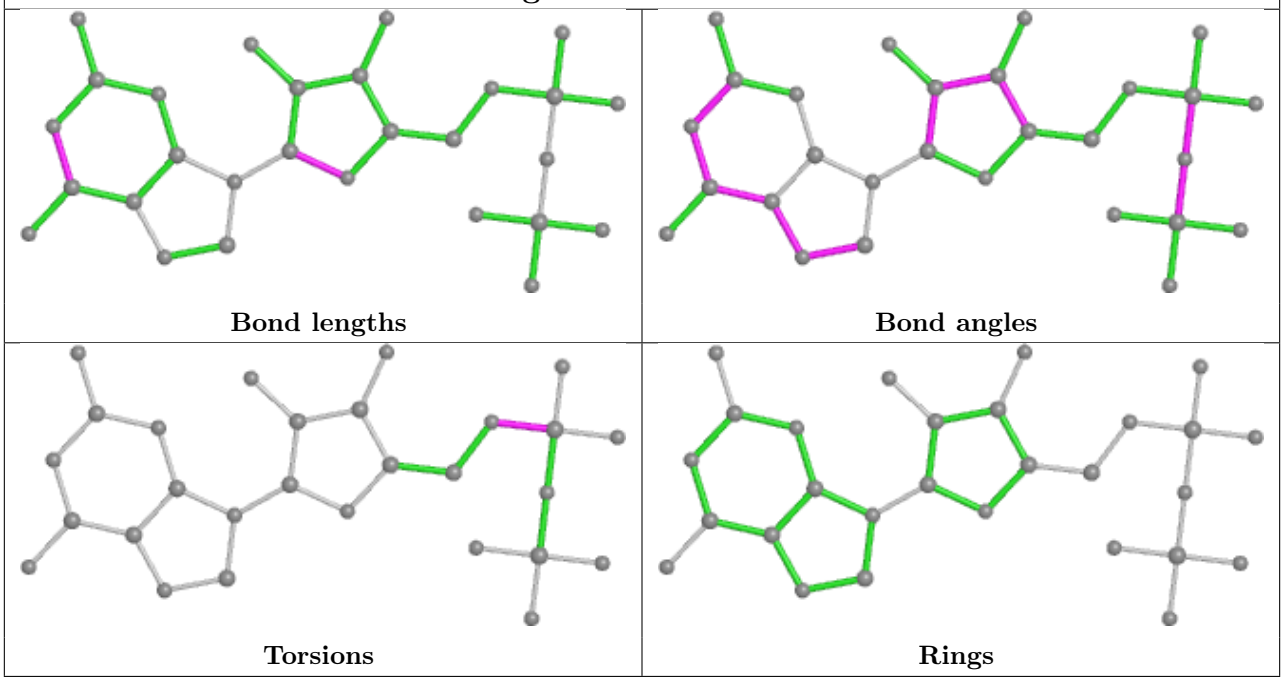


Rings

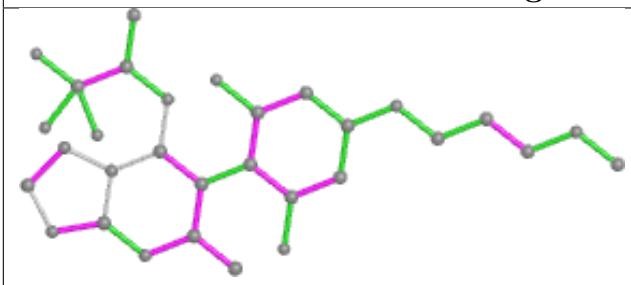
Ligand GTP A 501



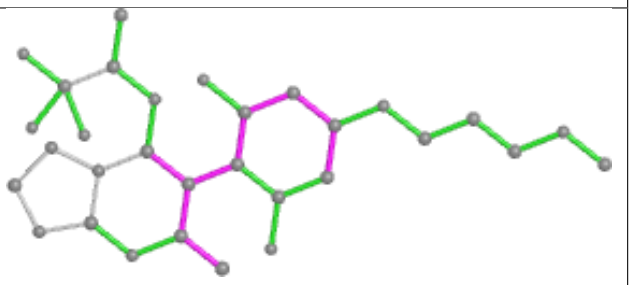
Ligand GDP B 501



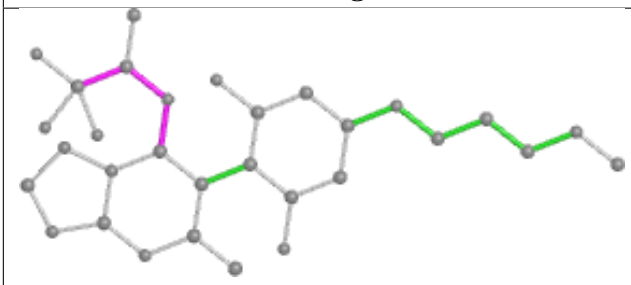
Ligand G2X C 605



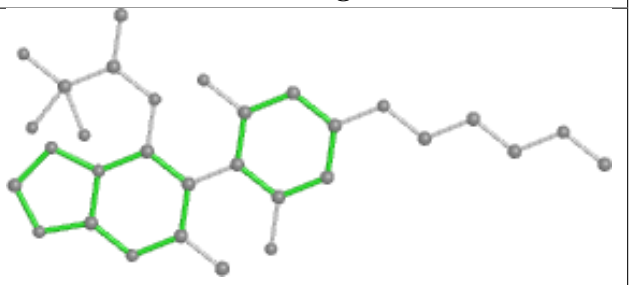
Bond lengths



Bond angles

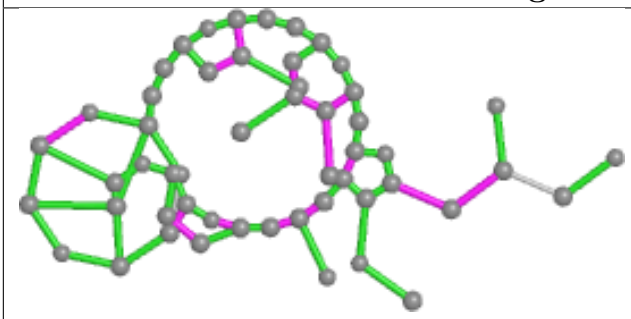


Torsions

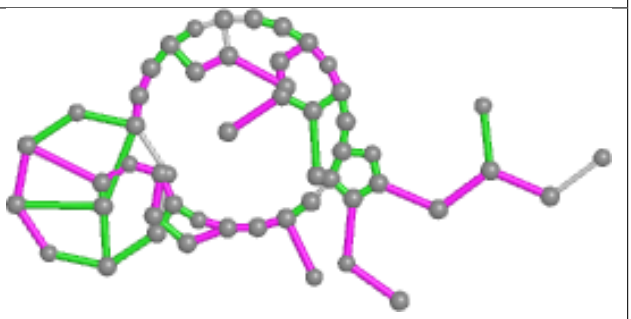


Rings

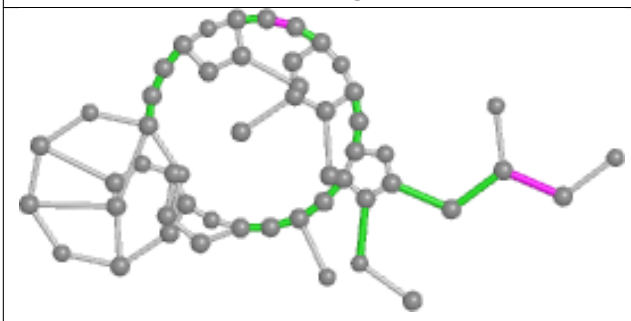
Ligand 6K9 D 503



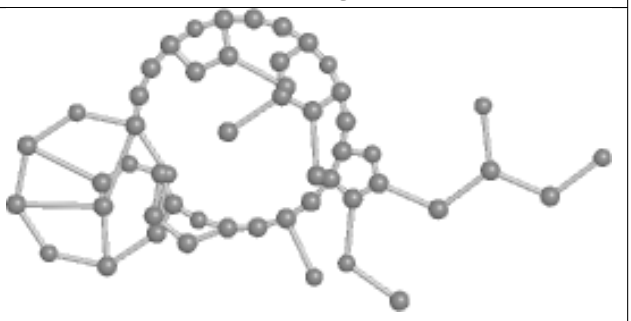
Bond lengths



Bond angles

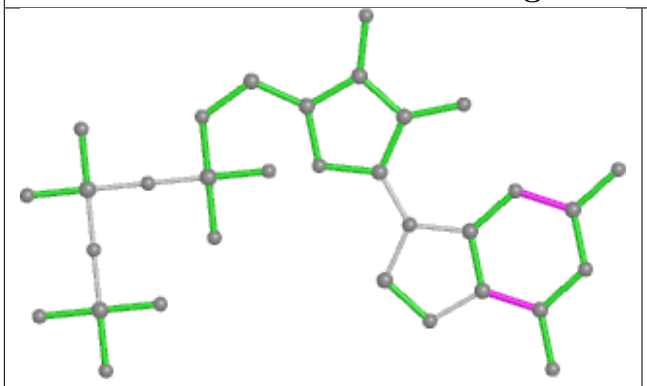


Torsions

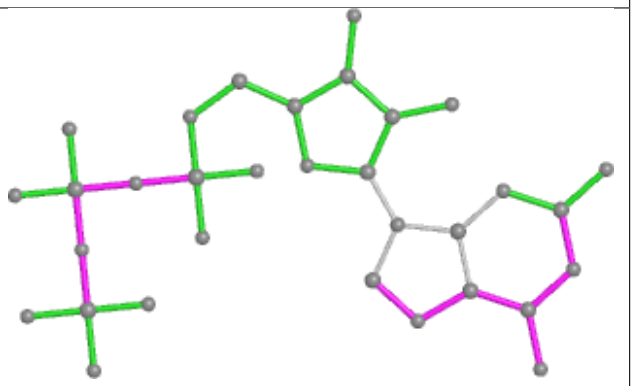


Rings

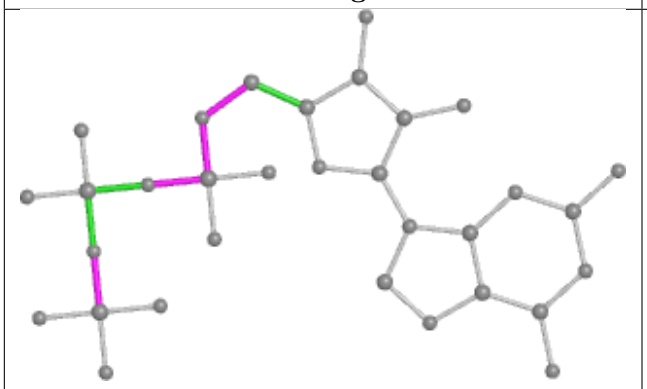
Ligand GTP C 602



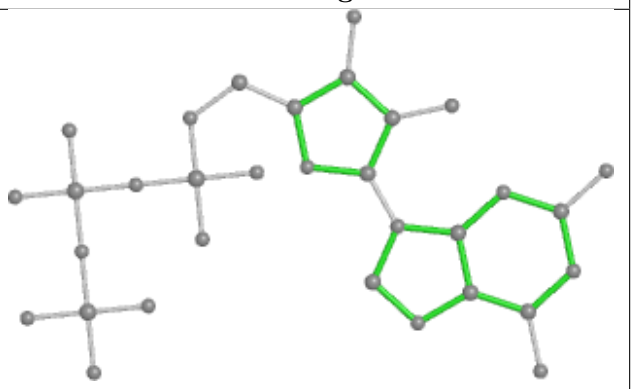
Bond lengths



Bond angles

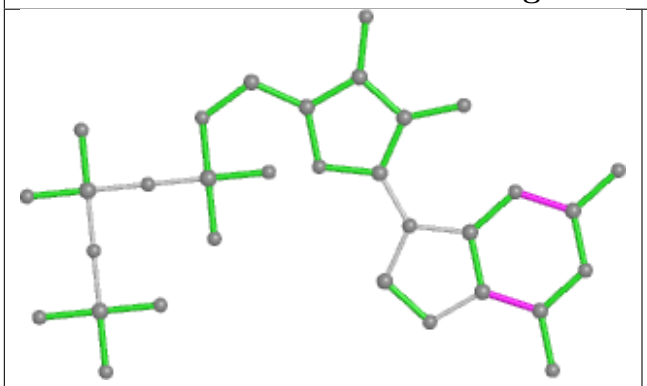


Torsions

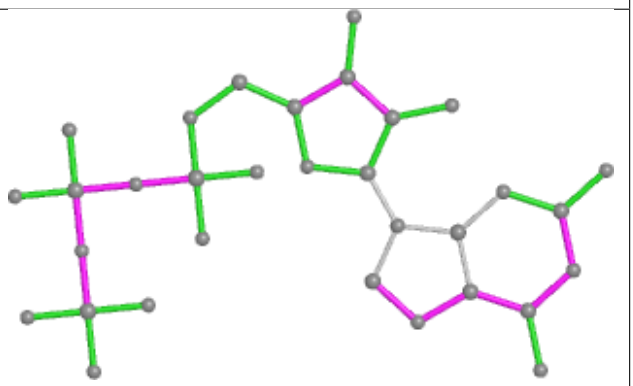


Rings

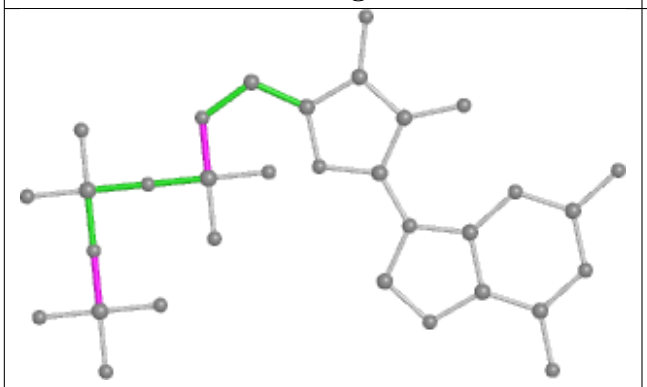
Ligand GTP D 502



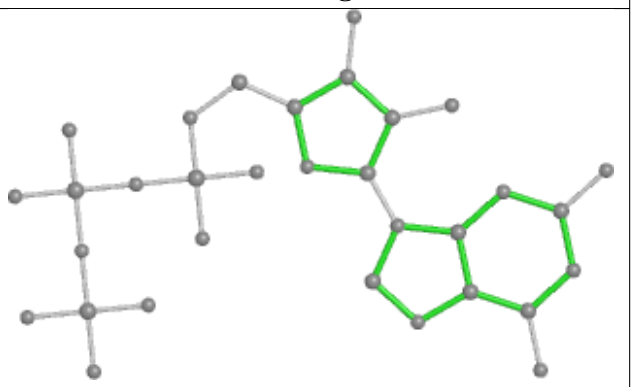
Bond lengths



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	438/450 (97%)	0.44	9 (2%) 63 60	41, 60, 79, 107	0
1	C	440/450 (97%)	0.35	7 (1%) 72 69	35, 50, 65, 108	0
2	B	418/445 (93%)	0.48	10 (2%) 59 54	37, 56, 77, 91	0
2	D	426/445 (95%)	0.80	38 (8%) 9 7	46, 64, 82, 100	0
3	E	123/143 (86%)	0.85	16 (13%) 3 2	46, 66, 91, 96	0
4	F	351/384 (91%)	1.38	90 (25%) 0 0	53, 74, 109, 113	0
All	All	2196/2317 (94%)	0.67	170 (7%) 13 10	35, 60, 91, 113	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	8.9
4	F	245	ILE	8.1
4	F	249	TYR	7.9
4	F	166	ALA	7.7
1	A	281	ALA	7.5
4	F	173	ILE	7.1
1	A	282	TYR	6.9
4	F	159	GLY	6.6
4	F	233	PHE	6.3
1	A	283	HIS	6.3
4	F	167	SER	6.2
2	D	56	GLY	6.1
4	F	177	GLY	6.1
1	A	346	TRP	6.1
2	D	57	ASN	5.9
4	F	153	ALA	5.8
4	F	250	SER	5.5
2	D	55	THR	5.4
4	F	234	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
4	F	154	GLY	5.1
4	F	236	LYS	5.1
2	D	1	MET	5.0
2	B	414	MET	5.0
4	F	157	GLY	4.9
4	F	170	LEU	4.9
4	F	176	GLN	4.6
1	C	440	VAL	4.6
4	F	182	ILE	4.4
4	F	156	LYS	4.4
2	D	73	MET	4.4
4	F	178	GLN	4.4
1	A	262	TYR	4.4
2	D	54	ALA	4.3
2	D	71	GLY	4.2
2	D	92	PHE	4.2
2	D	37	HIS	4.1
4	F	161	LEU	4.1
3	E	45	PRO	4.1
4	F	171	ASP	4.0
4	F	246	GLN	4.0
4	F	251	LYS	4.0
2	B	1	MET	4.0
4	F	130	VAL	4.0
4	F	162	ILE	3.9
2	B	57	ASN	3.9
2	D	59	TYR	3.8
1	C	151[A]	SER	3.7
4	F	253	TYR	3.7
4	F	138	ARG	3.7
3	E	128	LYS	3.6
2	B	55	THR	3.6
4	F	134	ALA	3.6
4	F	252	ASN	3.6
4	F	158	GLU	3.6
2	D	70	PRO	3.5
3	E	6	MET	3.5
4	F	372	THR	3.5
4	F	242	ASN	3.5
4	F	224	SER	3.5
3	E	124	GLN	3.4
4	F	244	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	137	ARG	3.4
4	F	132	LEU	3.3
2	D	81	PHE	3.3
4	F	243	HIS	3.3
4	F	129	GLU	3.3
4	F	152	SER	3.3
2	D	58	LYS	3.2
4	F	175	GLU	3.2
4	F	100	ILE	3.2
2	D	72	THR	3.2
4	F	248	GLU	3.2
4	F	172	PHE	3.1
4	F	232	ASN	3.1
1	C	283	HIS	3.1
1	C	68[A]	VAL	3.1
4	F	235	ASP	3.0
4	F	103	THR	3.0
1	A	278	ALA	3.0
4	F	231	ALA	2.9
2	D	53	GLU	2.9
2	D	76	VAL	2.9
4	F	342	LEU	2.9
4	F	160	ILE	2.8
4	F	149	ALA	2.8
4	F	150	LYS	2.8
4	F	163	SER	2.8
1	A	279	GLU	2.8
4	F	247	LYS	2.8
2	B	369	LEU	2.8
1	A	285	GLN	2.8
3	E	44	ASP	2.8
2	D	278	SER	2.8
4	F	101	TYR	2.7
4	F	32	LYS	2.7
4	F	139	ARG	2.7
3	E	48	GLU	2.7
4	F	226	GLU	2.7
2	D	332	ASN	2.7
2	B	37	HIS	2.7
2	D	402	PHE	2.7
2	D	127	CYS	2.6
1	C	340	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	238	CYS	2.6
4	F	296[A]	MET	2.6
4	F	179	VAL	2.6
4	F	237	THR	2.5
4	F	194	PRO	2.5
1	C	181[A]	VAL	2.5
3	E	27	PRO	2.5
4	F	131	PHE	2.5
4	F	102	PRO	2.5
4	F	99	VAL	2.5
3	E	119	MET	2.5
4	F	127	GLU	2.5
4	F	239	HIS	2.4
4	F	164	SER	2.4
2	D	33	THR	2.4
4	F	135	TYR	2.4
2	D	331	LEU	2.4
4	F	380	HIS	2.4
1	C	1	MET	2.4
3	E	140	LYS	2.3
4	F	346	LEU	2.3
2	D	268	PRO	2.3
2	D	84	ILE	2.3
2	B	39	ASP	2.3
2	D	125	GLU	2.3
2	D	30	ILE	2.3
4	F	133	ALA	2.3
2	D	439	ASP	2.3
4	F	19	ARG	2.3
3	E	103	GLN	2.3
2	B	40	SER	2.3
4	F	285	LEU	2.3
4	F	140	GLU	2.3
4	F	142	ARG	2.3
4	F	254	GLY	2.2
3	E	138	GLU	2.2
3	E	117	ALA	2.2
2	D	83	GLN	2.2
2	B	117	LEU	2.2
4	F	146	VAL	2.2
4	F	258	GLU	2.2
2	D	247	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	289	LEU	2.2
3	E	139	LEU	2.2
4	F	144	GLY	2.2
2	D	94	GLN	2.2
2	D	284	LEU	2.2
2	D	64	ILE	2.1
2	D	35	SER	2.1
1	A	434	GLU	2.1
4	F	334	GLY	2.1
4	F	220	VAL	2.1
2	D	250	LEU	2.1
2	D	170	MET	2.1
2	B	290	THR	2.1
4	F	148	ILE	2.1
4	F	174	ASP	2.1
3	E	121	GLU	2.1
4	F	128	ARG	2.1
4	F	363	ASP	2.1
2	D	419	ALA	2.0
4	F	200	ASP	2.0
4	F	181	VAL	2.0
3	E	115	HIS	2.0
3	E	28	SER	2.0
4	F	17	VAL	2.0
2	D	87	PRO	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)

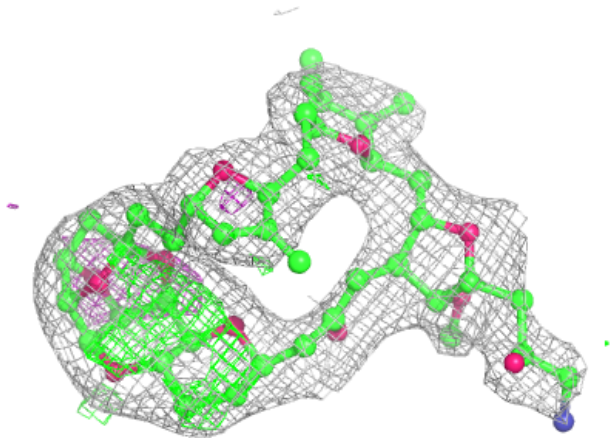
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

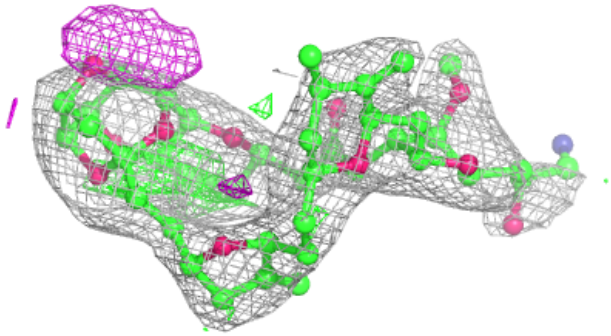
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	B	505	1/1	0.68	0.17	94,94,94,94	0
7	CA	A	503	1/1	0.80	0.08	82,82,82,82	0
7	CA	B	504	1/1	0.84	0.15	101,101,101,101	0
12	6K9	D	503	52/52	0.84	0.26	63,84,94,96	0
7	CA	A	506	1/1	0.85	0.05	96,96,96,96	0
6	MG	D	501	1/1	0.86	0.14	63,63,63,63	0
8	GOL	A	504	6/6	0.88	0.26	65,78,85,90	0
13	ACP	F	402	31/31	0.88	0.16	80,88,105,112	0
11	G2X	C	605	31/31	0.89	0.22	43,58,74,77	0
8	GOL	A	505	6/6	0.91	0.20	77,92,101,110	0
11	G2X	C	601	31/31	0.93	0.21	51,58,76,80	0
6	MG	B	502	1/1	0.93	0.14	65,65,65,65	0
5	GTP	D	502	32/32	0.95	0.14	55,64,81,87	0
6	MG	F	401	1/1	0.95	0.09	79,79,79,79	0
6	MG	C	603	1/1	0.96	0.17	40,40,40,40	0
7	CA	C	604	1/1	0.96	0.34	75,75,75,75	0
5	GTP	A	501	32/32	0.97	0.21	43,51,67,82	0
5	GTP	C	602	32/32	0.97	0.19	31,49,64,78	0
9	GDP	B	501	28/28	0.97	0.18	31,55,77,92	0
10	MES	B	503	12/12	0.97	0.16	48,59,71,73	0
6	MG	A	502	1/1	0.98	0.20	47,47,47,47	0
7	CA	C	606	1/1	0.99	0.11	47,47,47,47	0

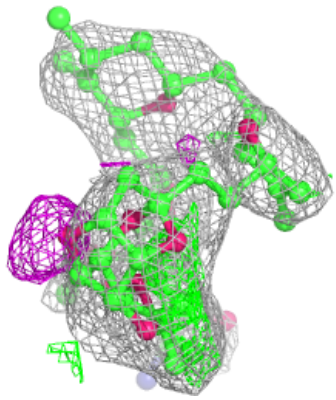
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6K9 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)

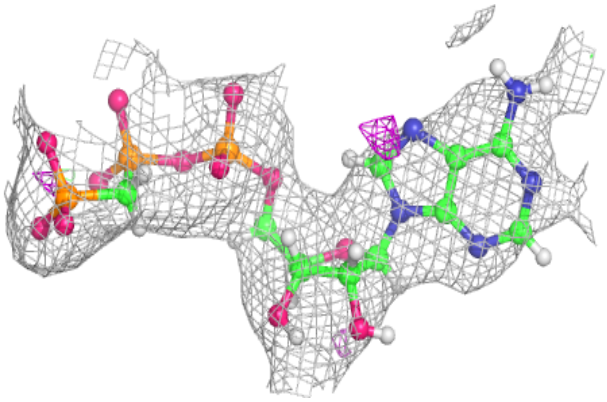


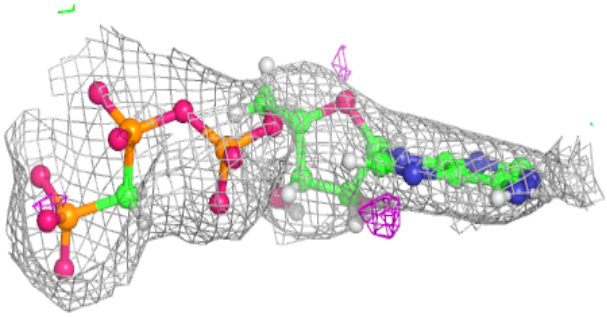


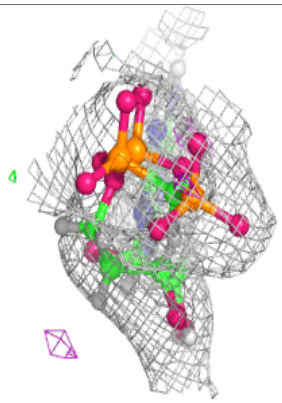


Electron density around ACP F 402:

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

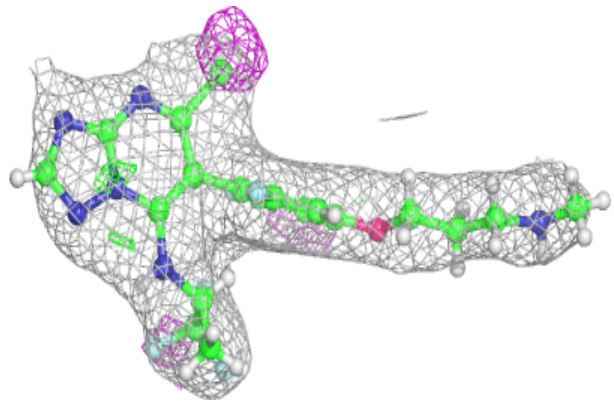


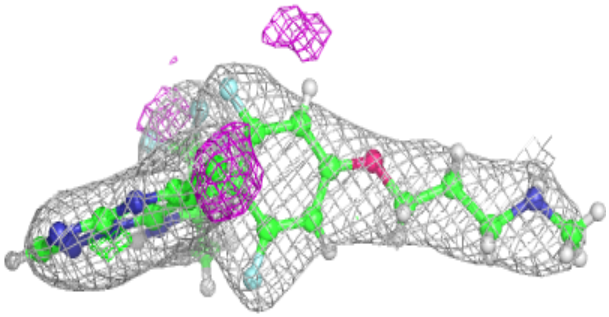


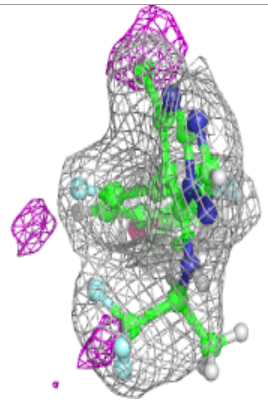


Electron density around G2X C 605:

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

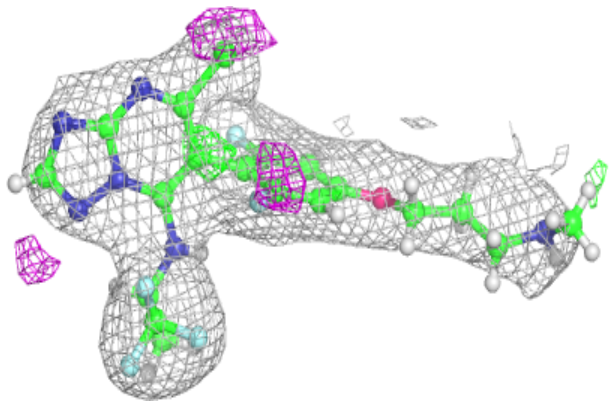


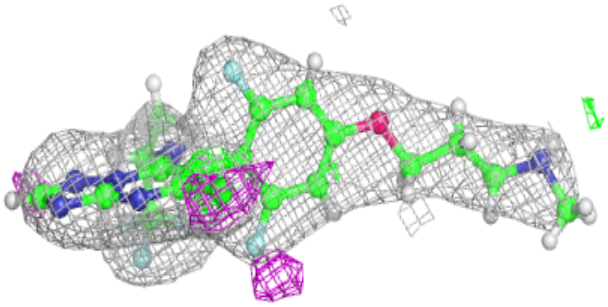


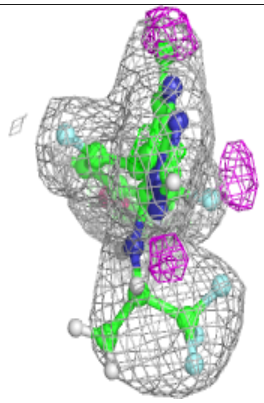


Electron density around G2X C 601:

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

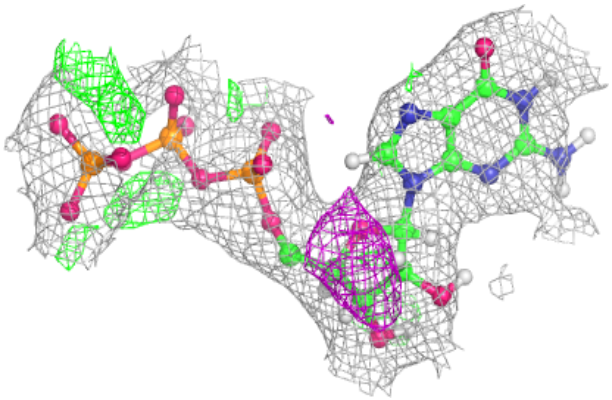


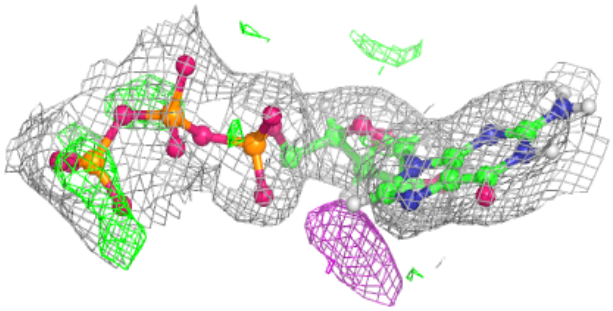


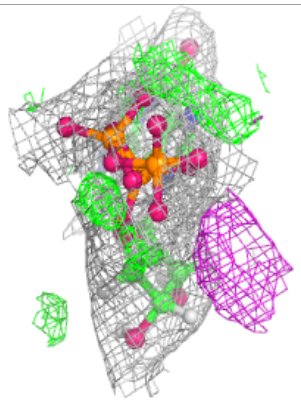


Electron density around GTP D 502:

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

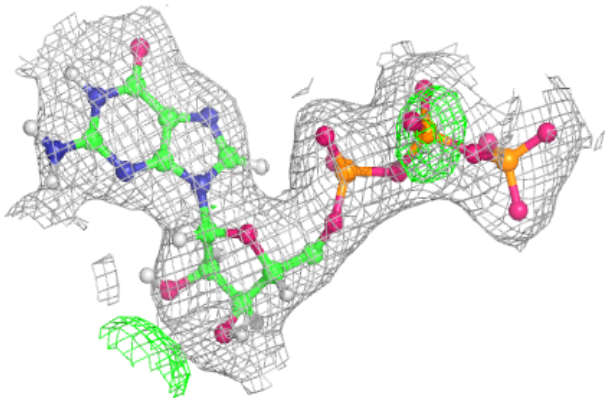


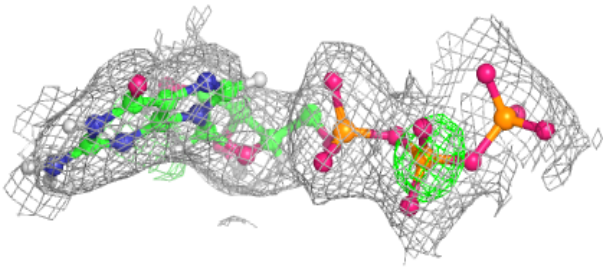


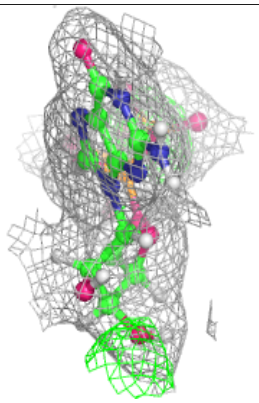


Electron density around GTP A 501:

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

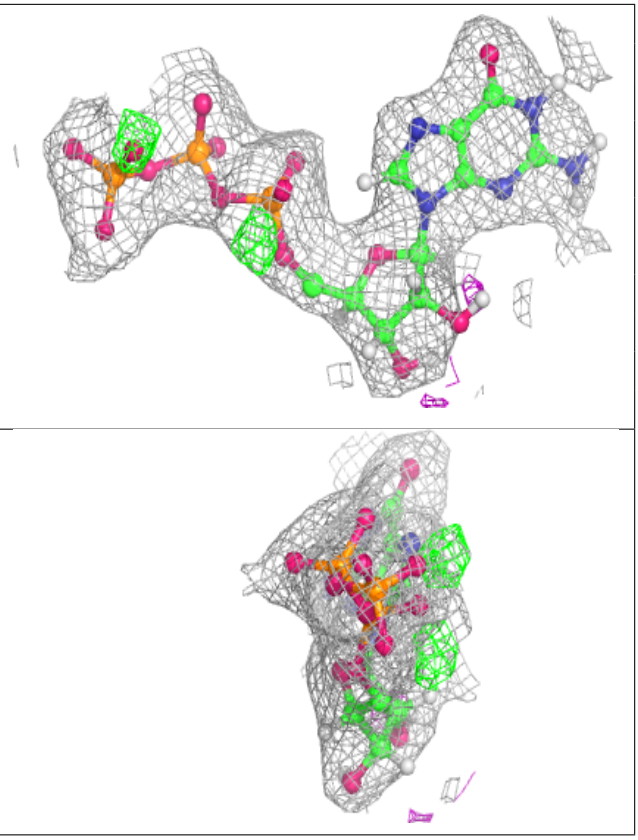






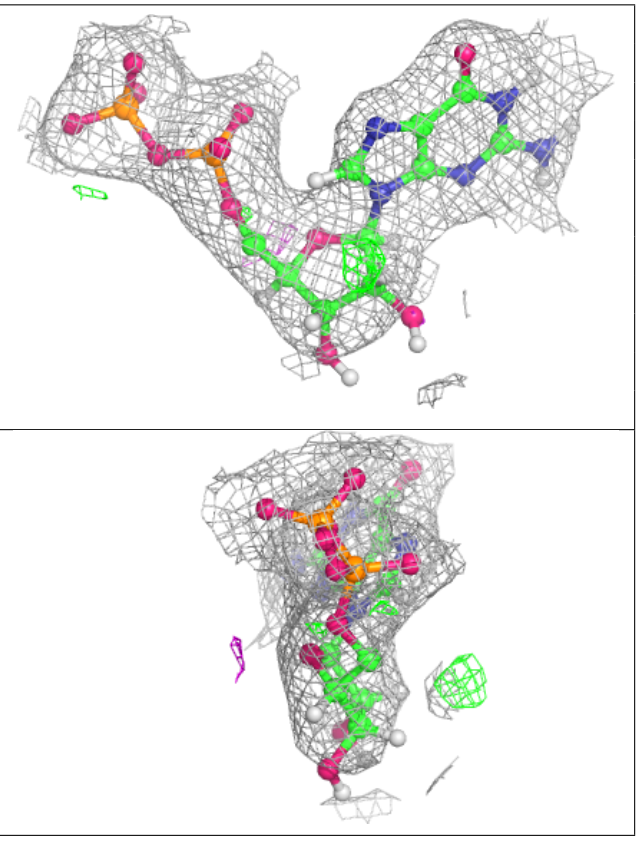
Electron density around GTP C 602:

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



Electron density around GDP B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.