Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 02:34 am GMT

PDB ID	:	6FJM
Title	:	tubulin-Disorazole Z complex
Authors	:	Menchon, G.; Prota, A.E.; Lucena Agell, D.; Bucher, P.; Jansen, R.; Irschik, H.; Mueller, R.; Paterson, I.; Diaz, J.F.; Altmann, K.-H.; Steinmetz, M.O.
Deposited on	:	2018-01-22
Resolution	:	2.10 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:

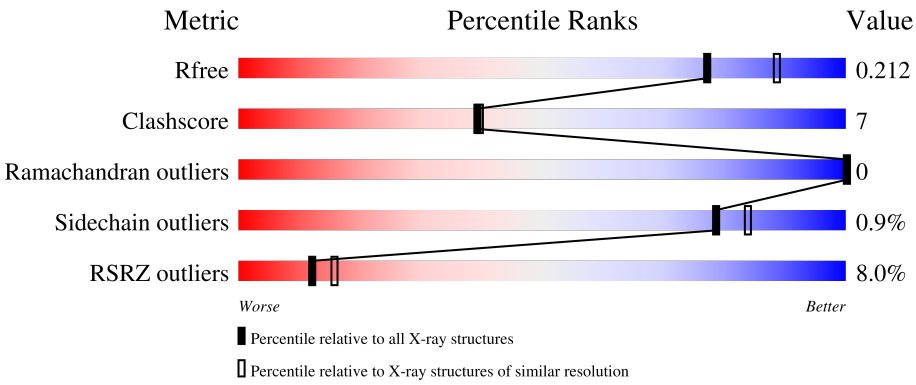
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	4% 82% 15% •
1	C	451	% 80% 18% •
2	B	445	3% 76% 20% •
2	D	445	5% 82% 14% •
3	E	143	10% 74% 12% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	27% 72% 17% • 9%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18583 atoms, of which 46 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	438	3428	2170	582	654	22	0	1	0
1	C	440	3463	2195	586	659	23	0	6	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	425	3359	2111	574	647	27	0	3	0
2	D	425	3341	2097	569	648	27	0	2	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1017	627	183	202	5	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

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

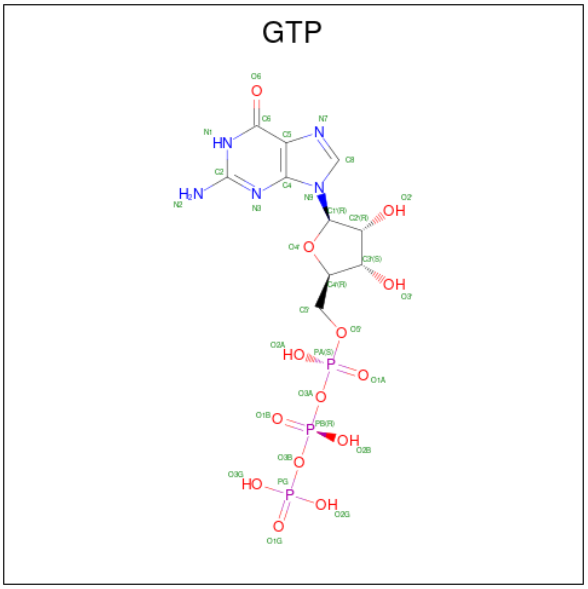
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	349	2849	1825	488	522	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0

- 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
			Total	Mg		
6	B	1	1	1	0	0
			Total	Mg		
6	C	1	1	1	0	0
			Total	Mg		
6	D	1	1	1	0	0

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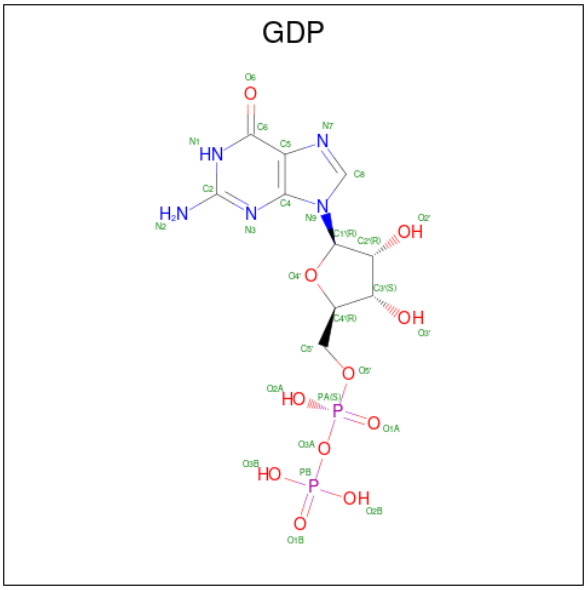
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

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

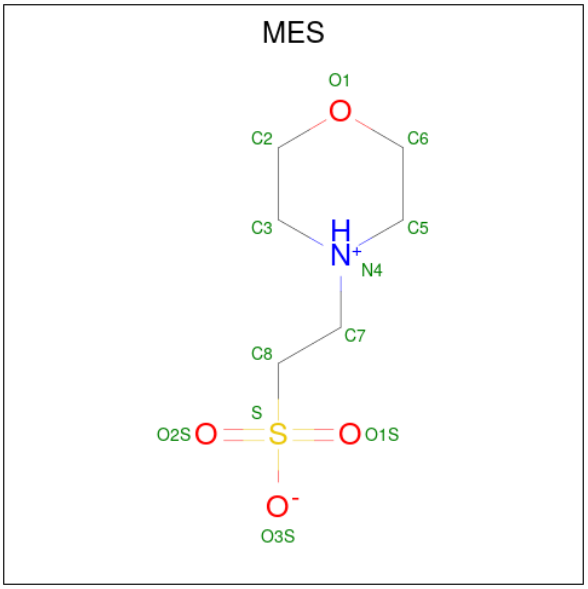
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	B	2	2	2	0	0
			Total	Ca		
7	C	1	1	1	0	0
			Total	Ca		
7	D	2	2	2	0	0
			Total	Ca		
7	E	1	1	1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



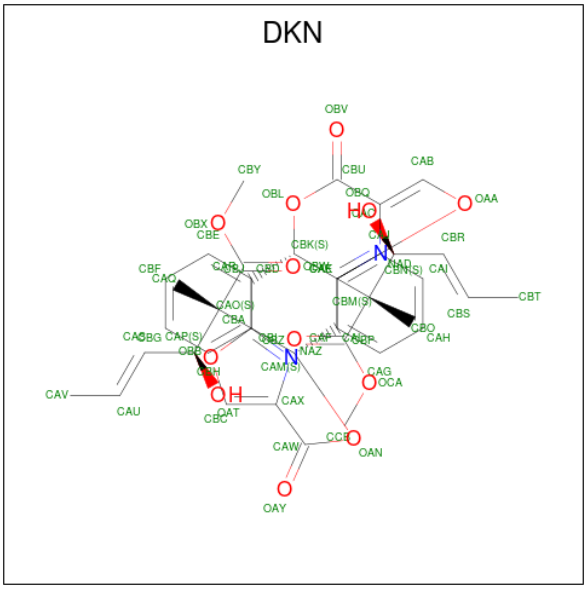
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
8	D	1	28	10	5	11	2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



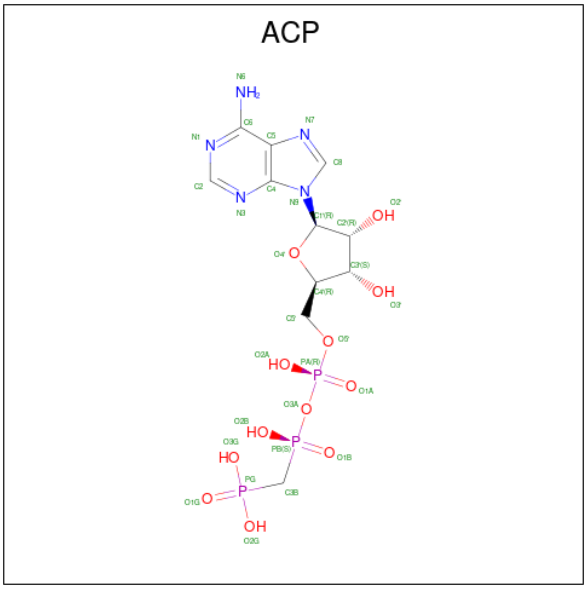
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is Disorazole Z (three-letter code: DKN) (formula: $C_{40}H_{46}N_2O_{12}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
10	D	1	100	40	46	2	12	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	F	1	31	11	5	12	3	0	0

- Molecule 12 is water.

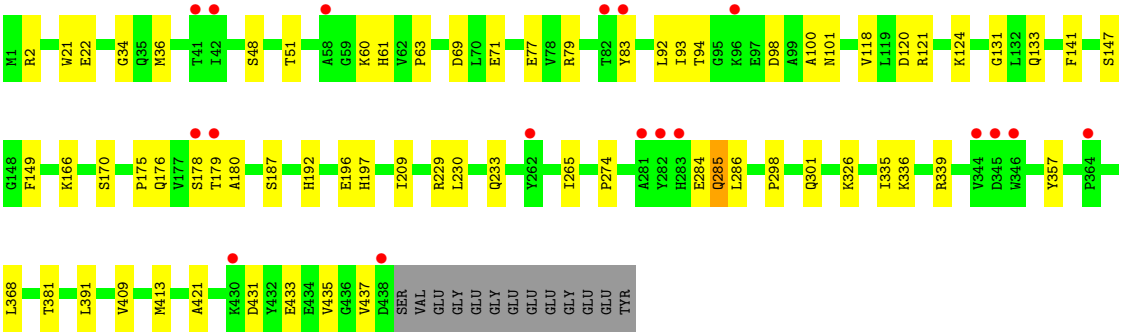
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	147	147	147	0	0
12	B	163	163	163	0	0
12	C	288	288	288	0	0
12	D	135	135	135	0	0
12	E	41	41	41	0	0
12	F	77	77	77	0	0

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.

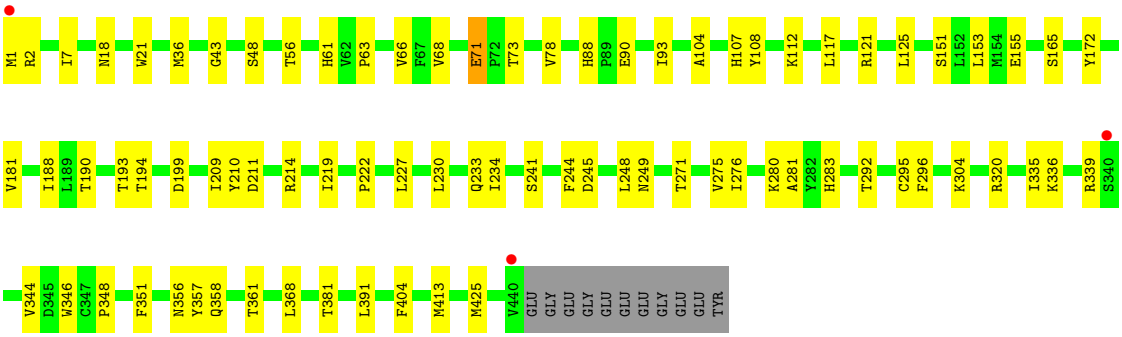
- Molecule 1: Tubulin alpha-1B chain

Chain A:



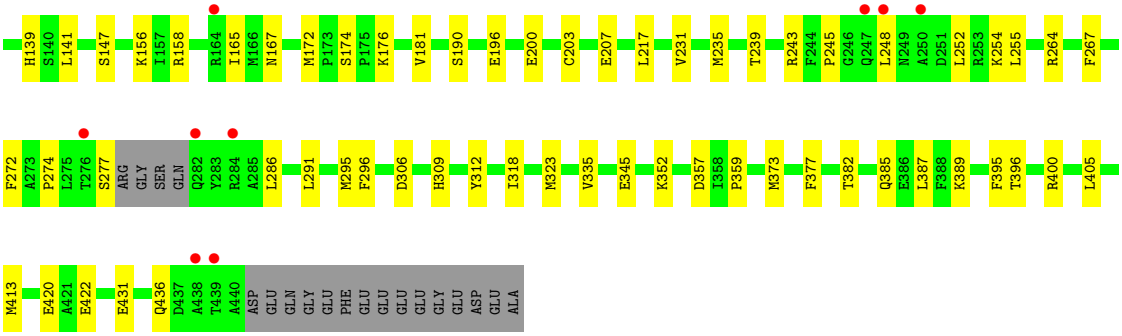
- Molecule 1: Tubulin alpha-1B chain

Chain C:



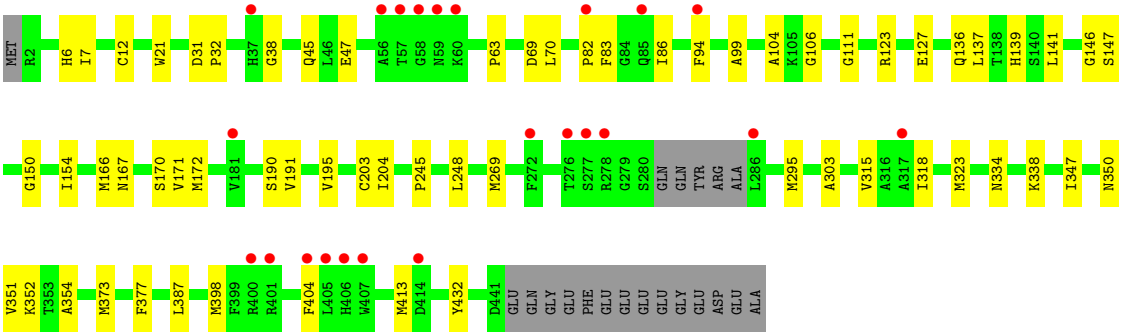
- Molecule 2: Tubulin beta-2B chain

Chain B:



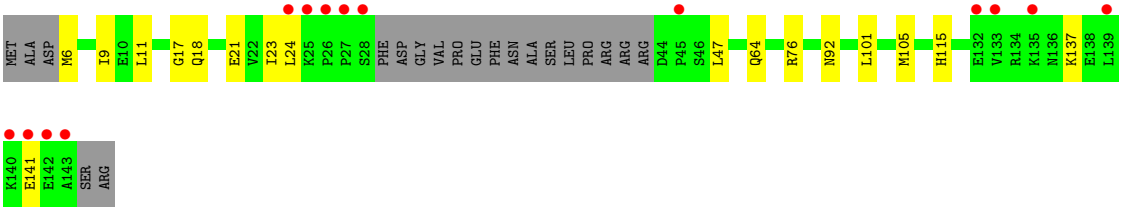
- Molecule 2: Tubulin beta-2B chain

Chain D:



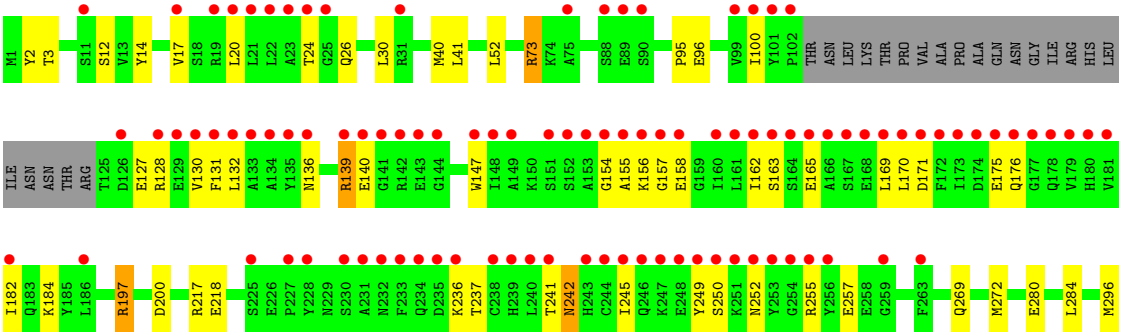
- Molecule 3: Stathmin-4

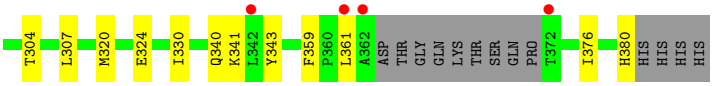
Chain E:



- Molecule 4: Tubulin tyrosine ligase

Chain F:




T304
L307
M320
E324
I330
Q340
K341
L342
Y343
F359
P360
L361
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
PRO
T372
I376
H380
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.39Å 157.63Å 179.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.97 – 2.10 55.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.97-2.10) 100.0 (55.97-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, R_{free}	0.179 , 0.213 0.179 , 0.212	Depositor DCC
R_{free} test set	8642 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18583	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: MES, DKN, GDP, GTP, CA, MG, ACP

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	0.27	0/3509	0.45	0/4764
1	C	0.30	0/3560	0.47	0/4835
2	B	0.29	0/3442	0.44	0/4662
2	D	0.27	0/3420	0.44	0/4632
3	E	0.26	0/1028	0.38	0/1364
4	F	0.26	0/2914	0.42	0/3936
All	All	0.28	0/17873	0.44	0/24193

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3428	0	3342	45	0
1	C	3463	0	3387	54	0
2	B	3359	0	3244	64	0
2	D	3341	0	3220	40	0
3	E	1017	0	1034	13	0
4	F	2849	0	2816	47	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	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	12	0	12	0	0
10	D	54	46	0	0	0
11	F	31	0	14	0	0
12	A	147	0	0	5	0
12	B	163	0	0	7	0
12	C	288	0	0	3	0
12	D	135	0	0	2	0
12	E	41	0	0	2	0
12	F	77	0	0	3	0
All	All	18537	46	17117	256	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 7.

All (256) 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:176:LYS:HD3	2:B:207:GLU:HG3	1.47	0.96
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.43	0.83
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.62	0.81
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.65	0.79
4:F:96:GLU:H	4:F:184:LYS:HE2	1.51	0.75
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.70	0.74
4:F:171:ASP:O	4:F:175:GLU:HG3	1.88	0.73
2:B:264:ARG:HD3	2:B:431:GLU:OE2	1.88	0.73
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.70	0.73
4:F:157:GLY:HA3	4:F:245:ILE:HD11	1.71	0.72
1:C:1:MET:HG2	1:C:2:ARG:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.72	0.70
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.07	0.70
2:D:432:TYR:OH	12:D:601:HOH:O	2.08	0.70
1:A:179:THR:HA	2:B:248:LEU:HD12	1.75	0.67
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.75	0.66
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.77	0.66
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.78	0.65
1:C:320:ARG:HA	1:C:356:ASN:O	1.96	0.65
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.80	0.64
1:C:283:HIS:HB2	12:C:617:HOH:O	1.97	0.64
4:F:237:THR:CG2	4:F:250:SER:HB3	2.27	0.63
1:C:165:SER:HA	1:C:199:ASP:OD2	1.98	0.63
1:A:285:GLN:HA	1:A:285:GLN:NE2	2.12	0.63
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.29	0.63
2:B:2:ARG:HB2	12:B:690:HOH:O	1.98	0.63
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.80	0.62
2:B:83:PHE:O	2:B:86:ILE:HG22	1.99	0.62
2:D:191:VAL:O	2:D:195:VAL:HG23	2.00	0.62
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.34	0.62
2:B:345:GLU:OE1	2:B:345:GLU:N	2.25	0.60
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.27	0.60
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.32	0.60
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.84	0.59
4:F:184:LYS:HE3	12:F:559:HOH:O	2.01	0.59
2:B:396:THR:O	2:B:400:ARG:HG2	2.03	0.59
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.36	0.58
12:B:730:HOH:O	1:C:2:ARG:HD2	2.03	0.58
4:F:252:ASN:OD1	4:F:255:ARG:HD2	2.03	0.58
2:D:323:MET:HB3	2:D:373:MET:HE2	1.85	0.58
2:D:171:VAL:HA	2:D:204:ILE:O	2.04	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.57
4:F:139:ARG:NH2	4:F:165:GLU:OE2	2.37	0.57
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.85	0.57
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.39	0.57
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.86	0.56
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.05	0.56
1:C:88[B]:HIS:HE1	1:C:90:GLU:HG3	1.71	0.56
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.41	0.56
1:C:271:THR:HG21	1:C:295:CYS:O	2.06	0.56
1:C:88[B]:HIS:CE1	1:C:90:GLU:HG3	2.41	0.56
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.87	0.55
2:B:35:SER:OG	2:B:60:LYS:HE2	2.05	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.42	0.55
2:D:136:GLN:HA	2:D:167:ASN:O	2.05	0.55
2:B:323:MET:HB3	2:B:373:MET:CE	2.37	0.55
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.89	0.55
2:D:323:MET:HB3	2:D:373:MET:CE	2.37	0.54
4:F:158:GLU:HB2	12:F:542:HOH:O	2.07	0.54
4:F:162:ILE:H	4:F:236:LYS:NZ	2.06	0.54
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.08	0.54
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.88	0.54
3:E:137:LYS:O	3:E:141:GLU:HG2	2.08	0.54
2:D:295:MET:CE	2:D:377:PHE:HB2	2.37	0.53
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.23	0.53
1:C:108:TYR:O	1:C:112:LYS:HG2	2.08	0.53
2:D:318:ILE:N	2:D:318:ILE:HD12	2.24	0.53
1:A:175:PRO:HA	1:A:178:SER:HB3	1.91	0.53
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.91	0.53
4:F:95:PRO:HA	4:F:184:LYS:HE2	1.91	0.53
2:B:136:GLN:HA	2:B:167:ASN:O	2.09	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.52
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.91	0.52
1:C:230:LEU:O	1:C:234:ILE:HD12	2.09	0.52
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.45	0.52
1:C:71:GLU:OE1	1:C:73:THR:HG23	2.09	0.52
2:B:123:ARG:O	2:B:127:GLU:HG3	2.10	0.52
12:C:676:HOH:O	3:E:115:HIS:HE1	1.92	0.52
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.93	0.51
4:F:237:THR:HG21	4:F:250:SER:HB3	1.93	0.51
4:F:341:LYS:HG2	4:F:341:LYS:O	2.10	0.51
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.46	0.51
4:F:280:GLU:HB2	12:F:510:HOH:O	2.12	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.12	0.50
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.26	0.50
1:C:190:THR:O	1:C:194:THR:HG23	2.11	0.50
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.43	0.50
1:A:265:ILE:O	1:A:265:ILE:HG22	2.12	0.49
1:C:107:HIS:HE1	1:C:155:GLU:OE1	1.95	0.49
1:A:120:ASP:HB2	12:A:626:HOH:O	2.12	0.49
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.47	0.49
1:A:196:GLU:HG2	12:A:668:HOH:O	2.11	0.49
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.95	0.49
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	1.94	0.49
2:B:88:ARG:HD2	12:B:742:HOH:O	2.13	0.49
4:F:127:GLU:HB3	4:F:130:VAL:CG2	2.42	0.49
1:C:104:ALA:HB2	1:C:413:MET:SD	2.53	0.49
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.49
2:D:172:MET:HE2	2:D:203:CYS:HA	1.95	0.49
4:F:242:ASN:OD1	4:F:242:ASN:N	2.45	0.49
4:F:269:GLN:HA	4:F:272:MET:CE	2.43	0.49
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.77	0.49
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.12	0.48
1:A:77:GLU:HG3	12:A:698:HOH:O	2.13	0.48
4:F:376:ILE:HD12	4:F:376:ILE:N	2.29	0.48
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.44	0.48
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.13	0.48
2:B:2:ARG:NH1	12:B:609:HOH:O	2.47	0.47
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.96	0.47
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.48	0.47
1:C:361:THR:HG23	12:C:616:HOH:O	2.14	0.47
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.21	0.47
1:A:298:PRO:HA	1:A:301:GLN:CD	2.35	0.47
2:B:133:GLN:OE1	2:B:252:LEU:N	2.39	0.47
2:B:147:SER:HG	2:B:190:SER:HG	1.57	0.47
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.96	0.47
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.96	0.47
1:A:79:ARG:HG2	1:A:92:LEU:CD1	2.44	0.47
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.15	0.47
1:C:296:PHE:HZ	1:C:351:PHE:HE2	1.61	0.47
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.96	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.50	0.47
4:F:245:ILE:O	4:F:249:TYR:HB2	2.15	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.47
2:D:7:ILE:O	2:D:137:LEU:HA	2.14	0.47
1:A:69:ASP:O	1:A:94:THR:HA	2.15	0.46
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.50	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.97	0.46
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.50	0.46
2:D:147:SER:HB2	2:D:190:SER:OG	2.16	0.46
2:B:156:LYS:HD3	3:E:76:ARG:CZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:THR:O	2:B:385:GLN:HG2	2.15	0.46
3:E:47:LEU:HD12	3:E:47:LEU:O	2.14	0.46
3:E:101:LEU:O	3:E:105:MET:HG2	2.16	0.46
2:B:323:MET:HB3	2:B:373:MET:HE2	1.98	0.46
1:A:229:ARG:NH1	12:A:607:HOH:O	2.49	0.46
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.98	0.46
3:E:6:MET:HA	3:E:23:ILE:O	2.16	0.46
3:E:141:GLU:HA	3:E:141:GLU:OE1	2.16	0.46
1:C:336:LYS:HZ1	1:C:351:PHE:HE1	1.63	0.46
1:C:43:GLY:HA2	1:C:56:THR:O	2.16	0.46
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.17	0.45
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.51	0.45
1:A:409:VAL:HA	1:A:413:MET:O	2.17	0.45
1:C:112:LYS:HE2	12:E:334:HOH:O	2.15	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.52	0.45
1:A:141:PHE:O	1:A:147:SER:HB3	2.17	0.45
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.44	0.45
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.47	0.45
2:B:323:MET:HB3	2:B:373:MET:HE1	1.99	0.45
4:F:155:ALA:O	4:F:156:LYS:HB2	2.16	0.45
4:F:163:SER:HB3	4:F:169:LEU:CD2	2.47	0.45
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.43	0.45
1:C:181[B]:VAL:HG21	1:C:404:PHE:CZ	2.53	0.44
2:D:295:MET:HE2	2:D:295:MET:HB2	1.82	0.44
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.99	0.44
2:B:309:HIS:O	2:B:436:GLN:NE2	2.51	0.44
4:F:320:MET:HG2	4:F:330:ILE:HG13	1.99	0.44
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.44
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.98	0.44
4:F:73:ARG:HA	4:F:73:ARG:HD3	1.59	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.44
3:E:64:GLN:HG2	12:E:337:HOH:O	2.17	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
1:A:120:ASP:O	1:A:124:LYS:HG3	2.18	0.43
1:A:176:GLN:HB2	12:A:679:HOH:O	2.18	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
2:B:47:GLU:OE1	2:B:245:PRO:HG3	2.17	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.43
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.99	0.43
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.99	0.43
4:F:40:MET:HE3	4:F:52:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.48	0.43
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.44	0.43
4:F:162:ILE:H	4:F:236:LYS:HZ1	1.67	0.43
4:F:237:THR:HG23	4:F:250:SER:HB3	2.00	0.43
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.83	0.43
2:D:123:ARG:O	2:D:127:GLU:HG3	2.18	0.43
1:A:431:ASP:O	1:A:435:VAL:HG23	2.17	0.43
2:B:26:ASP:HB3	12:B:616:HOH:O	2.17	0.43
1:C:48:SER:OG	1:C:245:ASP:HB2	2.18	0.43
2:D:146:GLY:O	2:D:150:GLY:HA3	2.19	0.43
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.88	0.43
4:F:3:THR:HB	4:F:30:LEU:HD11	2.00	0.43
4:F:96:GLU:N	4:F:184:LYS:HE2	2.28	0.43
2:B:217:LEU:HD13	2:B:277:SER:HB3	1.99	0.42
2:B:387:LEU:C	2:B:387:LEU:HD23	2.38	0.42
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.19	0.42
2:B:296:PHE:CE1	2:B:335:VAL:HG11	2.55	0.42
3:E:11:LEU:HD11	3:E:18:GLN:OE1	2.19	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.20	0.42
1:A:433:GLU:OE1	1:A:437:VAL:HG21	2.20	0.42
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.49	0.42
4:F:269:GLN:HA	4:F:272:MET:HE2	2.02	0.42
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	2.00	0.42
2:B:235:MET:HB3	2:B:235:MET:HE2	1.93	0.42
2:D:398:MET:CE	2:D:404:PHE:HD2	2.31	0.42
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.00	0.42
2:B:158:ARG:NH1	2:B:196:GLU:O	2.53	0.42
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.55	0.42
4:F:147:TRP:HB2	4:F:169:LEU:HD11	2.02	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.55	0.42
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.54	0.42
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.02	0.41
4:F:14:TYR:HA	4:F:17:VAL:HB	2.02	0.41
1:A:2:ARG:HB3	1:A:131:GLY:O	2.21	0.41
2:B:420:GLU:OE1	12:B:601:HOH:O	2.21	0.41
3:E:9:ILE:HG12	3:E:21:GLU:HB3	2.02	0.41
4:F:154:GLY:HA3	4:F:158:GLU:O	2.20	0.41
2:B:357:ASP:O	2:B:359:PRO:HD3	2.21	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.55	0.41
1:C:151[B]:SER:HA	1:C:194:THR:HG22	2.03	0.41
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.41
4:F:26:GLN:HE22	4:F:361:LEU:HA	1.86	0.41
2:B:239:THR:O	2:B:243:ARG:HG3	2.21	0.41
1:C:276:ILE:HD11	1:C:281:ALA:N	2.35	0.41
2:B:272:PHE:HE1	12:B:704:HOH:O	2.02	0.41
1:C:151[A]:SER:HA	1:C:194:THR:HG22	2.03	0.41
2:D:141:LEU:HD21	2:D:170:SER:HB3	2.02	0.41
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.41
4:F:136:ASN:O	4:F:140:GLU:HG2	2.20	0.41
1:C:276:ILE:HD11	1:C:280:LYS:C	2.41	0.41
2:D:83:PHE:O	2:D:86:ILE:HG22	2.21	0.41
1:C:241:SER:HA	1:C:249:ASN:OD1	2.21	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.41
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.21	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.41
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.61	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.03	0.41
1:A:2:ARG:HB2	1:A:133:GLN:CG	2.52	0.40
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.02	0.40
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.88	0.40
2:B:264:ARG:NH1	2:B:431:GLU:OE2	2.31	0.40
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.39	0.40
2:B:318:ILE:N	2:B:318:ILE:HD12	2.36	0.40
1:C:1:MET:CG	1:C:2:ARG:H	2.30	0.40
4:F:296:MET:SD	4:F:380:HIS:HB2	2.61	0.40
2:D:104:ALA:HB2	2:D:413:MET:SD	2.62	0.40
4:F:280:GLU:HA	4:F:284:LEU:HB2	2.03	0.40
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.56	0.40
2:D:167:ASN:ND2	12:D:610:HOH:O	2.53	0.40
1:A:48:SER:O	1:A:51[A]:THR:HG23	2.21	0.40
1:A:179:THR:HA	2:B:248:LEU:CD1	2.46	0.40
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.57	0.40
2:B:141:LEU:HD12	2:B:172:MET:SD	2.61	0.40
2:B:248:LEU:HD21	2:B:352:LYS:HB3	2.02	0.40
2:D:248:LEU:HD11	2:D:352:LYS:HB3	2.02	0.40
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.04	0.40
1:C:214:ARG:HG2	1:C:219:ILE:O	2.22	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	2.22	0.40
4:F:304:THR:HG22	4:F:307:LEU:HD12	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	437/451 (97%)	428 (98%)	9 (2%)	0	100	100
1	C	444/451 (98%)	434 (98%)	10 (2%)	0	100	100
2	B	424/445 (95%)	420 (99%)	4 (1%)	0	100	100
2	D	423/445 (95%)	418 (99%)	5 (1%)	0	100	100
3	E	120/143 (84%)	119 (99%)	1 (1%)	0	100	100
4	F	343/384 (89%)	332 (97%)	11 (3%)	0	100	100
All	All	2191/2319 (94%)	2151 (98%)	40 (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	370/379 (98%)	366 (99%)	4 (1%)	73	79
1	C	377/379 (100%)	375 (100%)	2 (0%)	88	92
2	B	370/383 (97%)	368 (100%)	2 (0%)	88	92
2	D	369/383 (96%)	368 (100%)	1 (0%)	92	95
3	E	111/127 (87%)	110 (99%)	1 (1%)	78	84
4	F	311/342 (91%)	304 (98%)	7 (2%)	50	55
All	All	1908/1993 (96%)	1891 (99%)	17 (1%)	78	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	284	GLU
1	A	285	GLN
1	A	381	THR
2	B	90	ASP
2	B	139	HIS
1	C	71	GLU
1	C	381	THR
2	D	139	HIS
3	E	92	ASN
4	F	12	SER
4	F	73	ARG
4	F	139	ARG
4	F	176	GLN
4	F	197	ARG
4	F	242	ASN
4	F	324	GLU

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

Mol	Chain	Res	Type
2	B	101	ASN
2	D	15	GLN
3	E	51	GLN
4	F	26	GLN
4	F	260	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	DKN	D	503	-	48,56,56	1.05	2 (4%)	46,76,76	3.14	18 (39%)
5	GTP	C	501	6	26,34,34	1.12	1 (3%)	32,54,54	1.31	5 (15%)
8	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.18	3 (10%)
9	MES	B	503	-	12,12,12	2.22	1 (8%)	14,16,16	2.08	3 (21%)
11	ACP	F	401	6	27,33,33	1.64	5 (18%)	32,52,52	1.31	3 (9%)
8	GDP	B	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.04	3 (10%)
5	GTP	A	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.34	5 (15%)

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	DKN	D	503	-	-	15/76/82/82	0/2/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	ACP	F	401	6	-	3/15/38/38	0/3/3/3
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.41	1.67	1.77
5	A	501	GTP	C5-C6	-4.06	1.39	1.47
5	C	501	GTP	C5-C6	-3.92	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O2B	-3.65	1.47	1.56
11	F	401	ACP	PB-O1B	3.37	1.59	1.51
11	F	401	ACP	C2'-C1'	-3.37	1.48	1.53
10	D	503	DKN	CAC-CBU	-2.65	1.45	1.50
11	F	401	ACP	PG-O3G	2.55	1.60	1.54
10	D	503	DKN	CAX-CAW	-2.53	1.45	1.50
8	D	501	GDP	C6-N1	-2.47	1.34	1.37
11	F	401	ACP	PG-O2G	2.46	1.60	1.54
8	B	501	GDP	C6-N1	-2.28	1.34	1.37
5	A	501	GTP	C2-N3	2.02	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	503	DKN	CAM-OAN-CAW	7.75	131.34	117.55
10	D	503	DKN	OAN-CAM-CAL	7.66	119.06	104.85
10	D	503	DKN	OCA-CBP-OBZ	-7.52	110.76	123.93
10	D	503	DKN	CBK-OBL-CBU	7.28	130.50	117.55
10	D	503	DKN	OBX-CAR-OBW	-6.74	112.13	123.93
9	B	503	MES	C5-N4-C3	6.43	123.31	108.83
10	D	503	DKN	OBL-CBK-CBJ	5.30	114.68	104.85
10	D	503	DKN	OCA-CBP-CBM	5.18	128.94	111.60
10	D	503	DKN	OBX-CAR-CAO	4.94	128.13	111.60
10	D	503	DKN	CCB-OCA-CBP	3.83	122.39	115.94
11	F	401	ACP	PB-O3A-PA	-3.67	120.92	132.56
11	F	401	ACP	N3-C2-N1	-3.61	123.03	128.68
8	D	501	GDP	PA-O3A-PB	-3.44	121.02	132.83
5	A	501	GTP	C5-C6-N1	3.03	119.31	113.95
10	D	503	DKN	CBO-CBM-CBP	3.01	116.95	108.60
5	A	501	GTP	C8-N7-C5	2.99	108.68	102.99
5	C	501	GTP	C8-N7-C5	2.97	108.65	102.99
5	C	501	GTP	C5-C6-N1	2.90	119.07	113.95
10	D	503	DKN	OBW-CAR-CAO	-2.85	119.73	125.75
5	A	501	GTP	PA-O3A-PB	-2.79	123.25	132.83
5	C	501	GTP	PA-O3A-PB	-2.70	123.56	132.83
10	D	503	DKN	OBZ-CBP-CBM	-2.58	120.30	125.75
10	D	503	DKN	CBY-OBX-CAR	2.58	120.29	115.94
11	F	401	ACP	C3'-C2'-C1'	2.57	104.85	100.98
10	D	503	DKN	CAQ-CAO-CAR	2.57	115.75	108.60
10	D	503	DKN	CAQ-CAO-CAM	-2.56	105.19	110.09
10	D	503	DKN	CBJ-CBK-CBM	2.55	121.87	115.09
5	C	501	GTP	C2-N1-C6	-2.48	120.52	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	GDP	C5-C6-N1	2.48	118.33	113.95
5	A	501	GTP	C2-N1-C6	-2.44	120.60	125.10
8	D	501	GDP	C8-N7-C5	2.32	107.41	102.99
10	D	503	DKN	CAL-CAK-CAJ	2.29	128.37	125.41
8	B	501	GDP	C8-N7-C5	2.28	107.33	102.99
8	D	501	GDP	C5-C6-N1	2.26	117.95	113.95
5	C	501	GTP	PB-O3B-PG	-2.23	125.18	132.83
9	B	503	MES	O2S-S-C8	2.15	109.50	106.92
8	B	501	GDP	PA-O3A-PB	-2.14	125.49	132.83
5	A	501	GTP	PB-O3B-PG	-2.09	125.64	132.83
10	D	503	DKN	OBL-CBK-CBM	2.04	112.39	107.50
9	B	503	MES	O1S-S-C8	2.01	109.33	106.92

There are no chirality outliers.

All (42) 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
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
10	D	503	DKN	CAM-CAO-CAR-OBW
10	D	503	DKN	CAM-CAO-CAR-OBX
10	D	503	DKN	CAO-CAR-OBX-CBY
10	D	503	DKN	CBK-CBM-CBN-CBR
10	D	503	DKN	CBK-CBM-CBN-OBQ
10	D	503	DKN	CBO-CBM-CBN-CBR
10	D	503	DKN	CBO-CBM-CBN-OBQ
10	D	503	DKN	CBP-CBM-CBN-OBQ
10	D	503	DKN	CBM-CBP-OCA-CCB
10	D	503	DKN	OBZ-CBP-OCA-CCB
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O3A
10	D	503	DKN	OBW-CAR-OBX-CBY
10	D	503	DKN	OAT-CAP-CAS-CAU
10	D	503	DKN	CAL-CAM-CAO-CAP
10	D	503	DKN	CAJ-CAK-CAL-CAM

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	C5'-O5'-PA-O2A
10	D	503	DKN	CBH-CBI-CBJ-CBK
5	C	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
9	B	503	MES	C8-C7-N4-C5

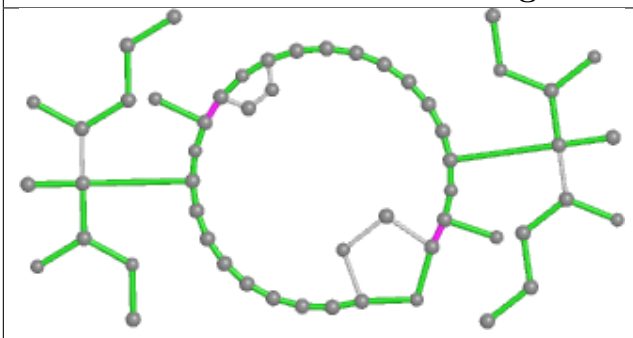
There are no ring outliers.

2 monomers are involved in 2 short contacts:

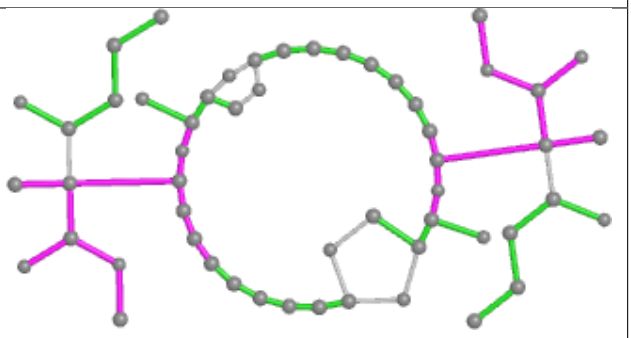
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
5	A	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

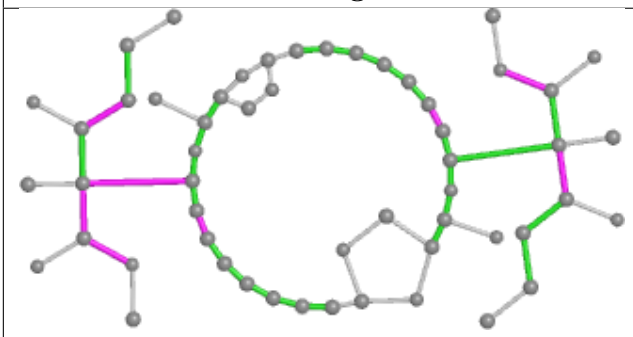
Ligand DKN D 503



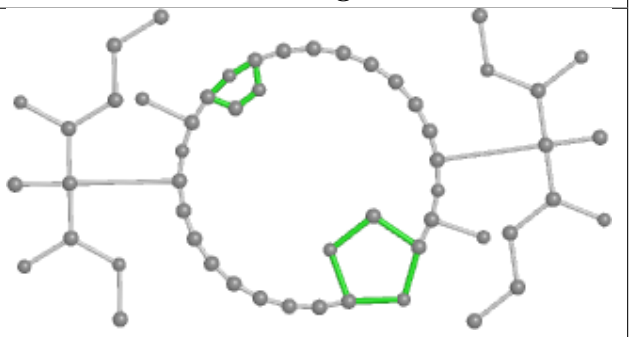
Bond lengths



Bond angles

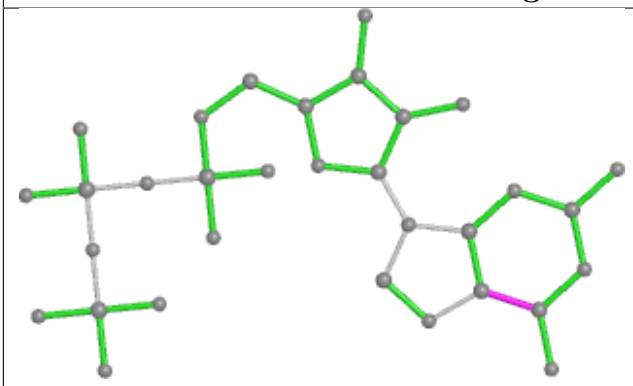


Torsions

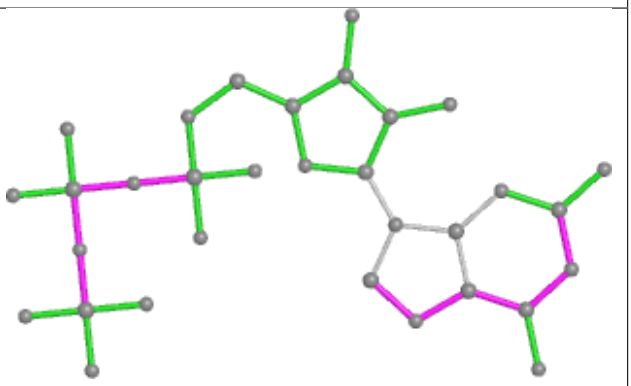


Rings

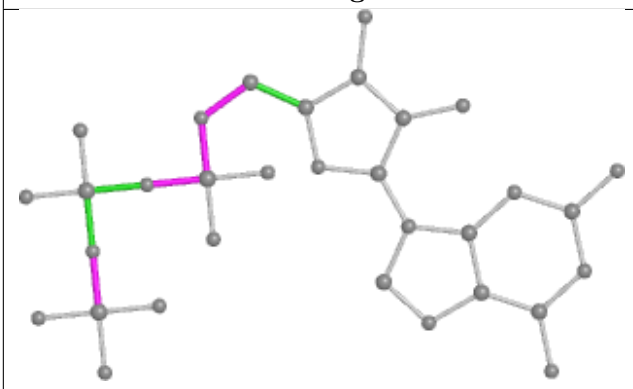
Ligand GTP C 501



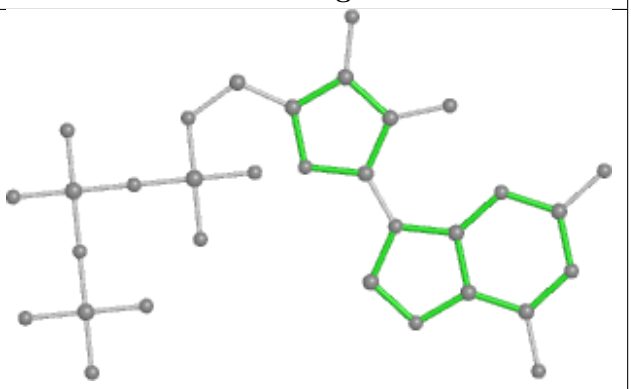
Bond lengths



Bond angles

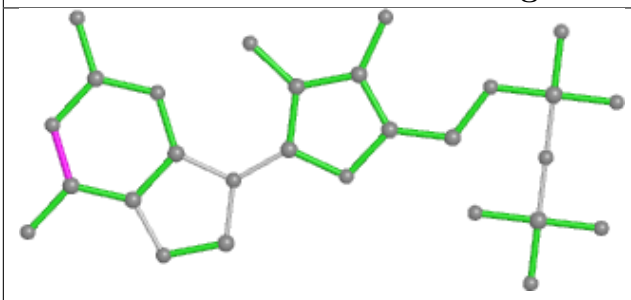


Torsions

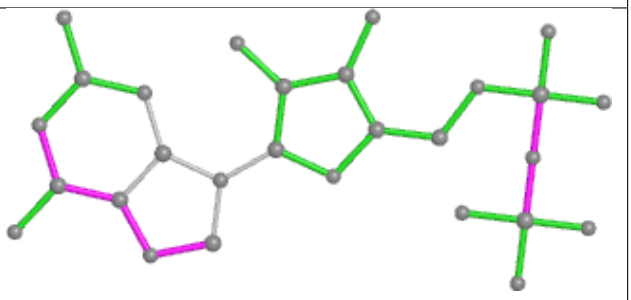


Rings

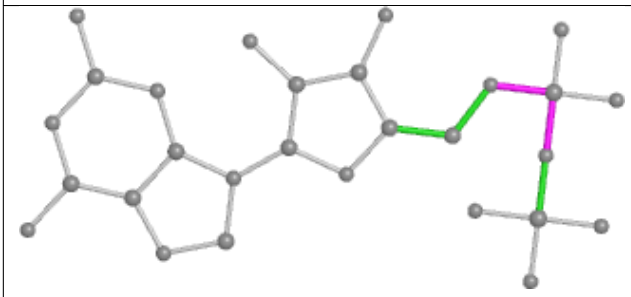
Ligand GDP D 501



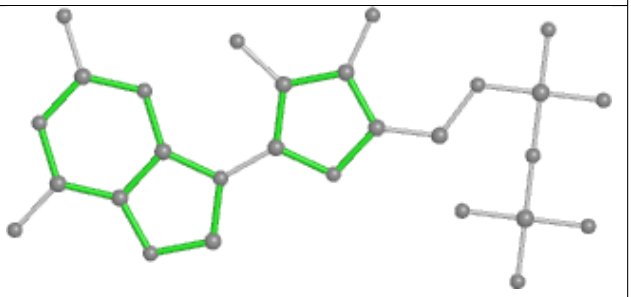
Bond lengths



Bond angles

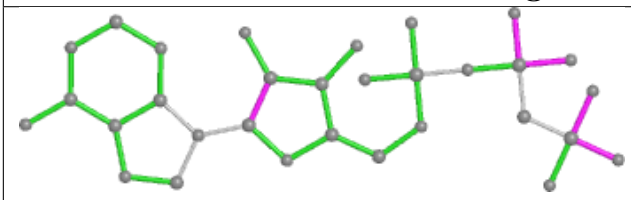


Torsions

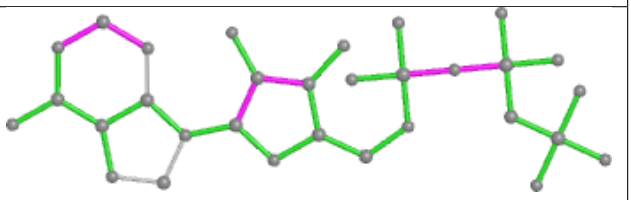


Rings

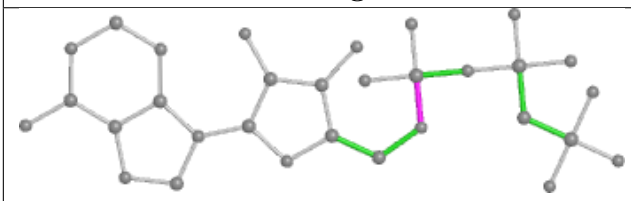
Ligand ACP F 401



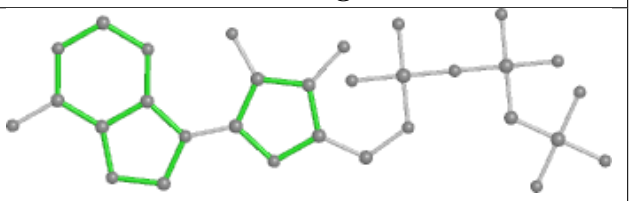
Bond lengths



Bond angles

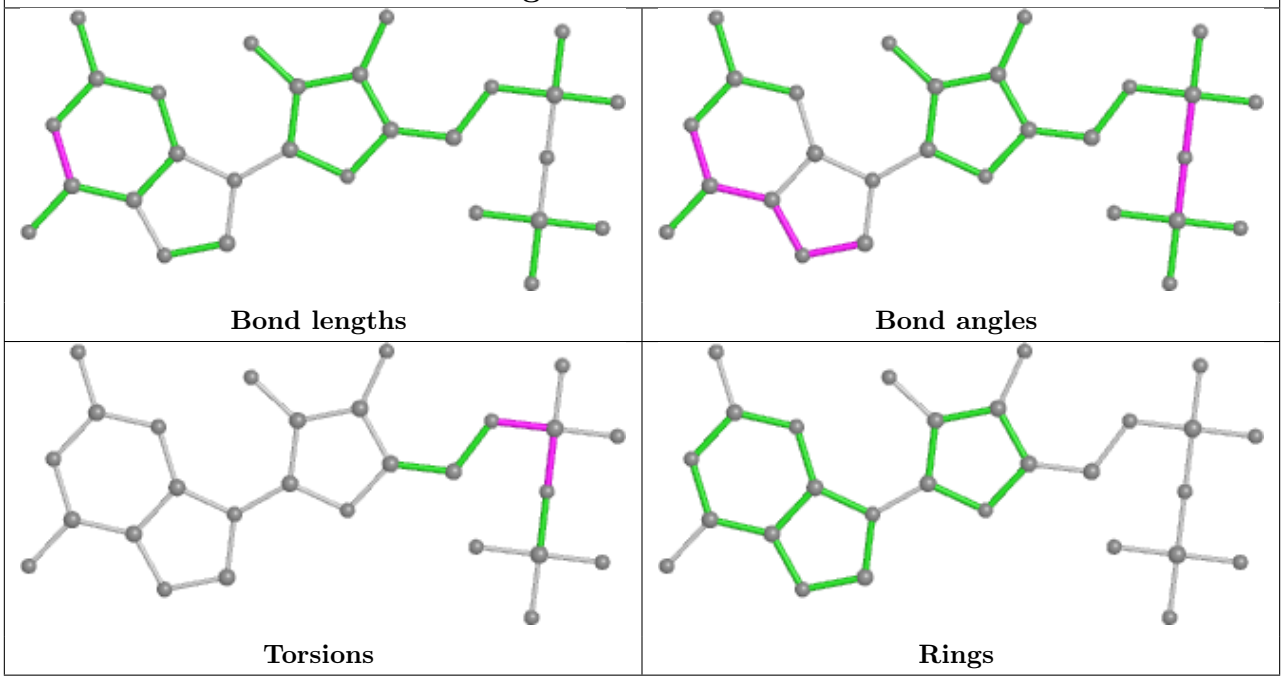


Torsions

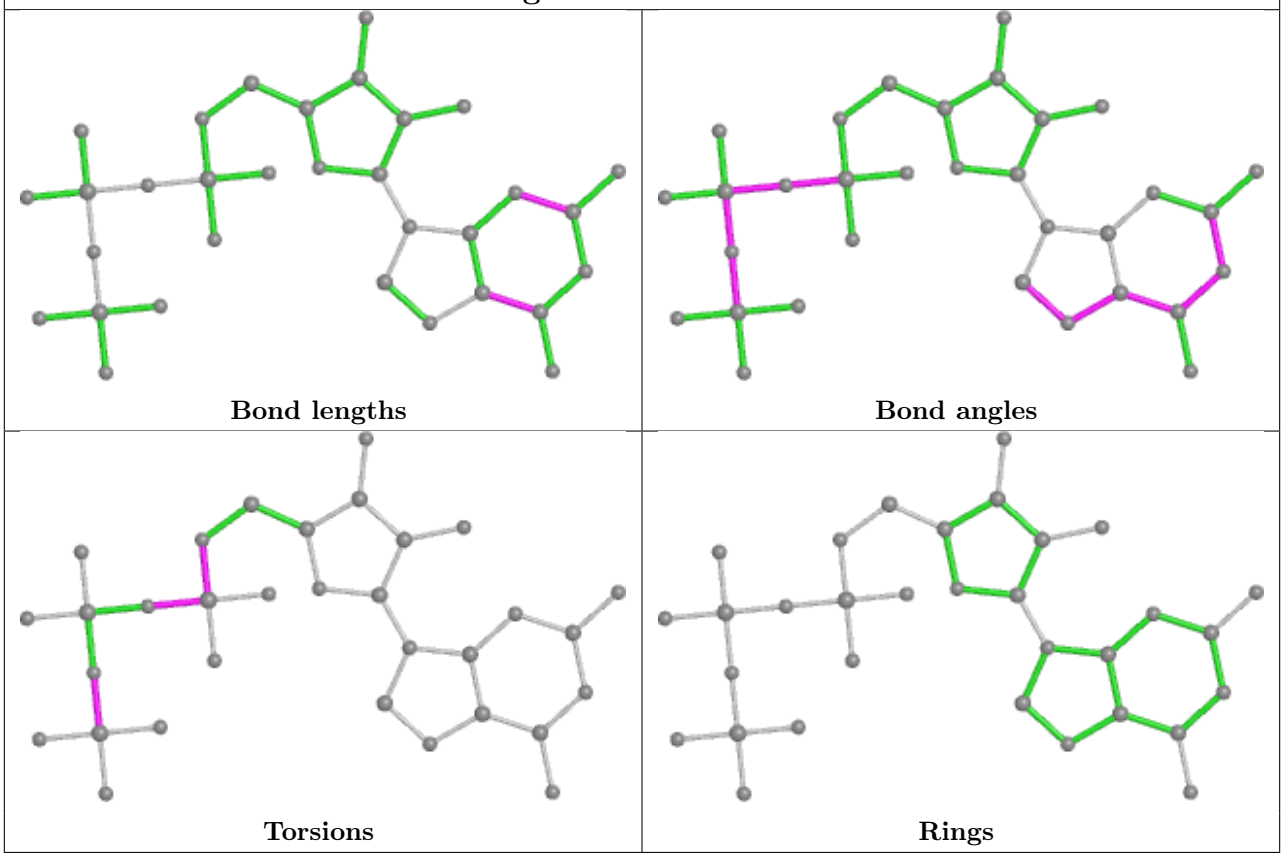


Rings

Ligand GDP B 501



Ligand GTP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	438/451 (97%)	0.35	18 (4%)	37	43	38, 56, 96, 165	0
1	C	440/451 (97%)	0.22	3 (0%)	87	89	31, 45, 75, 113	0
2	B	425/445 (95%)	0.31	15 (3%)	44	50	33, 55, 95, 133	0
2	D	425/445 (95%)	0.42	23 (5%)	25	31	38, 61, 94, 128	0
3	E	123/143 (86%)	0.64	14 (11%)	5	6	40, 70, 113, 142	0
4	F	349/384 (90%)	1.47	103 (29%)	0	0	46, 82, 156, 179	0
All	All	2200/2319 (94%)	0.52	176 (8%)	12	16	31, 58, 114, 179	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	8.8
4	F	173	ILE	8.7
4	F	89	GLU	8.2
4	F	157	GLY	7.9
4	F	249	TYR	7.7
4	F	130	VAL	7.2
4	F	233	PHE	7.0
4	F	99	VAL	6.7
4	F	20	LEU	6.5
4	F	135	TYR	6.5
4	F	161	LEU	6.2
2	D	57	THR	6.2
4	F	232	ASN	6.1
4	F	252	ASN	6.1
4	F	100	ILE	6.1
4	F	182	ILE	6.1
4	F	250	SER	6.1
4	F	132	LEU	6.0
4	F	253	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
4	F	179	VAL	5.9
4	F	166	ALA	5.8
4	F	231	ALA	5.8
3	E	26	PRO	5.7
4	F	170	LEU	5.6
4	F	172	PHE	5.5
3	E	143	ALA	5.4
1	A	282	TYR	5.4
4	F	131	PHE	5.4
4	F	234	GLN	5.1
4	F	244	CYS	5.1
4	F	101	TYR	5.1
4	F	245	ILE	5.1
1	C	340	SER	5.0
4	F	134	ALA	4.9
1	A	179	THR	4.9
1	A	346	TRP	4.8
4	F	22	LEU	4.8
2	B	58	GLY	4.7
4	F	251	LYS	4.5
4	F	176	GLN	4.5
4	F	129	GLU	4.5
4	F	248	GLU	4.4
4	F	24	THR	4.4
4	F	143	GLU	4.4
4	F	90	SER	4.4
4	F	165	GLU	4.3
4	F	177	GLY	4.3
4	F	23	ALA	4.3
4	F	227	PRO	4.3
4	F	178	GLN	4.3
4	F	168	GLU	4.2
4	F	174	ASP	4.2
4	F	236	LYS	4.1
2	B	438	ALA	4.1
2	D	56	ALA	4.1
3	E	25	LYS	4.1
4	F	162	ILE	4.1
4	F	17	VAL	4.0
4	F	136	ASN	4.0
4	F	167	SER	4.0
4	F	151	SER	4.0

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Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	4.0
1	A	438	ASP	4.0
2	D	286	LEU	3.9
1	A	262	TYR	3.9
2	B	439	THR	3.9
2	D	277	SER	3.9
4	F	160	ILE	3.9
3	E	24	LEU	3.9
4	F	259	GLY	3.8
4	F	154	GLY	3.8
4	F	240	LEU	3.8
3	E	141	GLU	3.8
4	F	361	LEU	3.8
2	B	59	ASN	3.7
4	F	152	SER	3.7
1	A	281	ALA	3.7
4	F	362	ALA	3.7
4	F	372	THR	3.7
1	A	345	ASP	3.6
4	F	235	ASP	3.6
4	F	142	ARG	3.6
4	F	163	SER	3.6
4	F	153	ALA	3.6
4	F	171	ASP	3.5
4	F	158	GLU	3.5
1	A	42	ILE	3.5
3	E	139	LEU	3.5
4	F	133	ALA	3.5
1	C	440	VAL	3.4
2	B	57	THR	3.4
4	F	164	SER	3.4
2	D	37	HIS	3.4
4	F	25	GLY	3.4
3	E	28	SER	3.4
2	D	59	ASN	3.3
2	D	276	THR	3.3
4	F	128	ARG	3.3
2	D	58	GLY	3.2
3	E	142	GLU	3.2
4	F	247	LYS	3.2
1	A	82	THR	3.2
4	F	238	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	230	SER	3.2
4	F	21	LEU	3.0
2	B	247	GLN	2.9
2	D	82	PRO	2.9
2	B	248	LEU	2.9
4	F	181	VAL	2.9
2	B	82	PRO	2.9
4	F	156	LYS	2.9
4	F	139	ARG	2.8
4	F	147	TRP	2.8
4	F	255	ARG	2.8
2	D	407	TRP	2.7
4	F	225	SER	2.7
2	D	60	LYS	2.7
4	F	102	PRO	2.7
4	F	239	HIS	2.7
2	D	400	ARG	2.7
4	F	144	GLY	2.6
1	C	1	MET	2.6
2	D	94	PHE	2.6
4	F	31	ARG	2.6
3	E	140	LYS	2.6
1	A	430	LYS	2.6
1	A	41	THR	2.5
2	B	37	HIS	2.5
4	F	342	LEU	2.5
1	A	83	TYR	2.5
2	D	85	GLN	2.4
4	F	149	ALA	2.4
1	A	178	SER	2.4
4	F	155	ALA	2.4
4	F	88	SER	2.4
3	E	132	GLU	2.4
4	F	140	GLU	2.4
2	B	284	ARG	2.4
2	D	414	ASP	2.4
4	F	243	HIS	2.4
4	F	256	TYR	2.4
4	F	175	GLU	2.3
2	D	317	ALA	2.3
2	B	250	ALA	2.3
1	A	344	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	401	ARG	2.3
2	D	406	HIS	2.3
2	D	272	PHE	2.3
2	D	404	PHE	2.3
2	D	278	ARG	2.3
1	A	58	ALA	2.3
4	F	126	ASP	2.2
2	B	282	GLN	2.2
4	F	19	ARG	2.2
3	E	45	PRO	2.2
4	F	263	PHE	2.2
4	F	254	GLY	2.2
4	F	141	GLY	2.2
2	D	405	LEU	2.2
1	A	96	LYS	2.2
4	F	228	TYR	2.2
1	A	283	HIS	2.2
2	B	38	GLY	2.2
4	F	11	SER	2.2
4	F	148	ILE	2.1
2	B	276	THR	2.1
3	E	133	VAL	2.1
1	A	364	PRO	2.1
2	B	164[A]	ARG	2.1
4	F	186	LEU	2.1
4	F	246	GLN	2.1
4	F	75	ALA	2.1
3	E	135	LYS	2.0
4	F	180	HIS	2.0
2	D	181	VAL	2.0
4	F	241	THR	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)

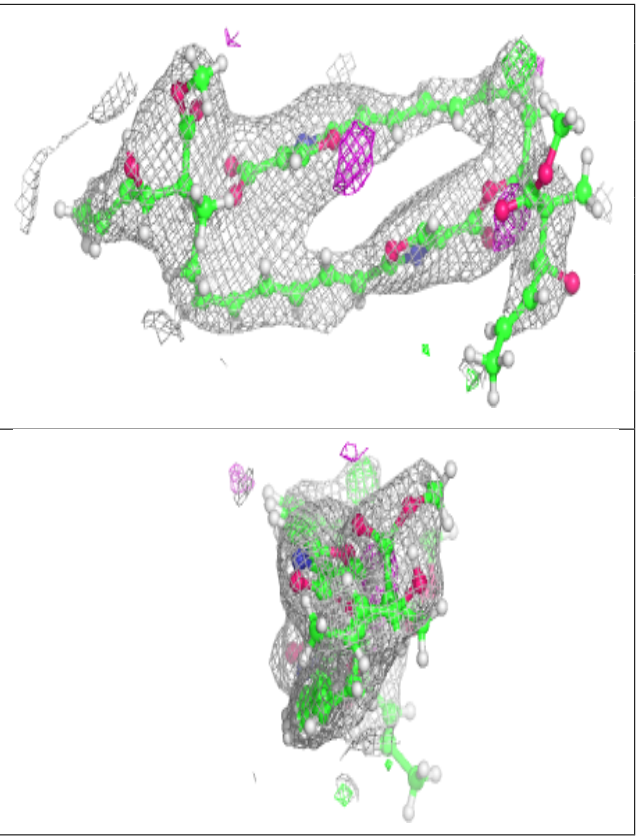
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	504	1/1	0.60	0.31	136,136,136,136	0
7	CA	D	505	1/1	0.73	0.18	118,118,118,118	0
7	CA	E	201	1/1	0.86	0.07	105,105,105,105	0
10	DKN	D	503	54/54	0.88	0.33	64,109,166,172	0
7	CA	D	504	1/1	0.90	0.31	99,99,99,99	0
6	MG	F	402	1/1	0.90	0.20	108,108,108,108	0
11	ACP	F	401	31/31	0.90	0.16	70,82,132,139	0
6	MG	A	502	1/1	0.92	0.15	38,38,38,38	0
9	MES	B	503	12/12	0.95	0.14	51,59,72,73	0
7	CA	A	503	1/1	0.96	0.08	81,81,81,81	0
8	GDP	D	501	28/28	0.97	0.11	49,56,64,71	0
7	CA	B	505	1/1	0.97	0.14	111,111,111,111	0
6	MG	D	502	1/1	0.98	0.04	51,51,51,51	0
5	GTP	A	501	32/32	0.98	0.16	32,39,44,52	0
8	GDP	B	501	28/28	0.99	0.13	33,38,42,45	0
7	CA	C	503	1/1	0.99	0.05	58,58,58,58	0
6	MG	C	502	1/1	0.99	0.14	33,33,33,33	0
5	GTP	C	501	32/32	0.99	0.14	29,33,40,42	0
6	MG	B	502	1/1	0.99	0.18	33,33,33,33	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.

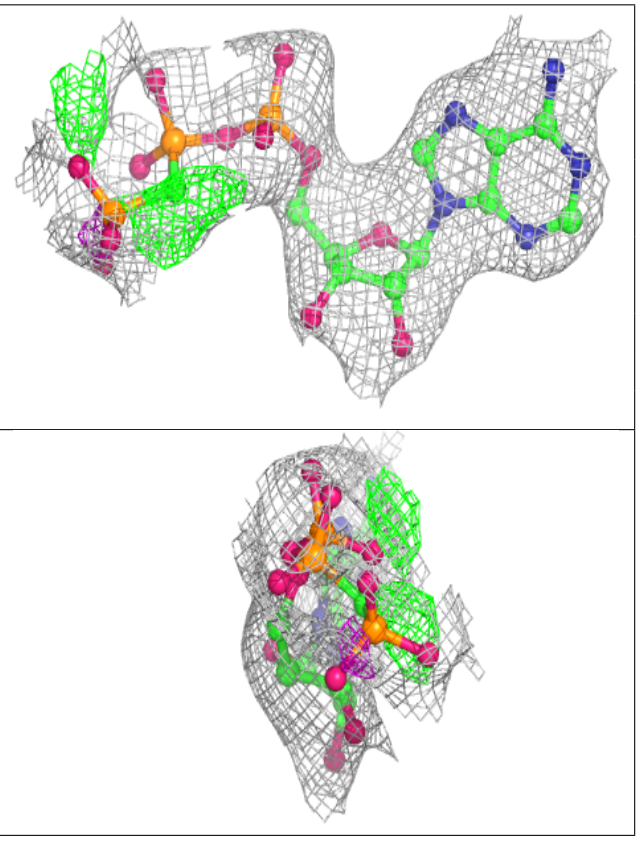
Electron density around DKN D 503:

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



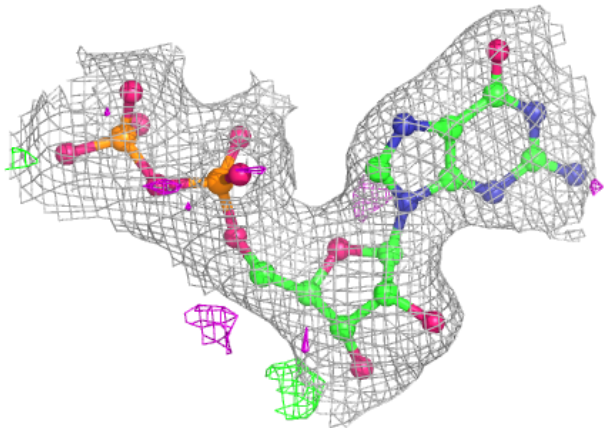
Electron density around ACP F 401:

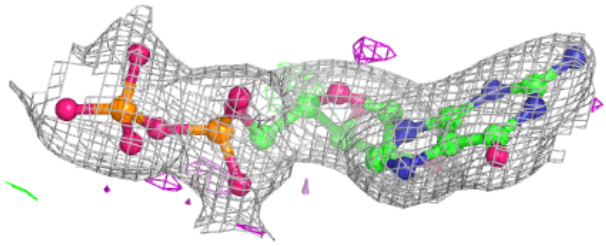
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP D 501:

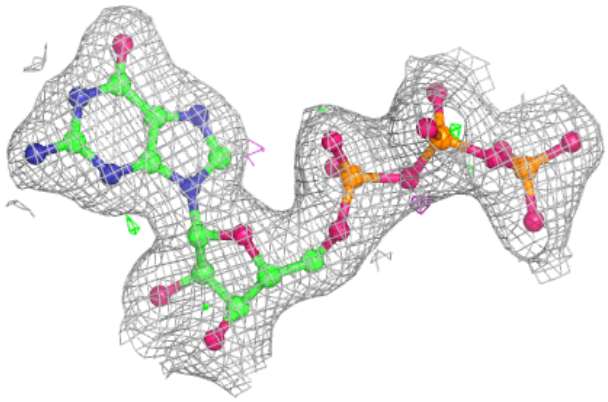
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

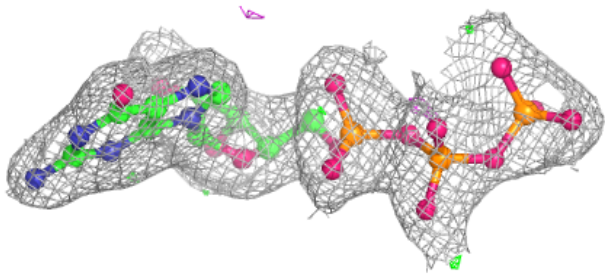


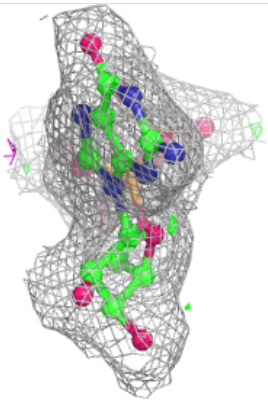


Electron density around GTP A 501:

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

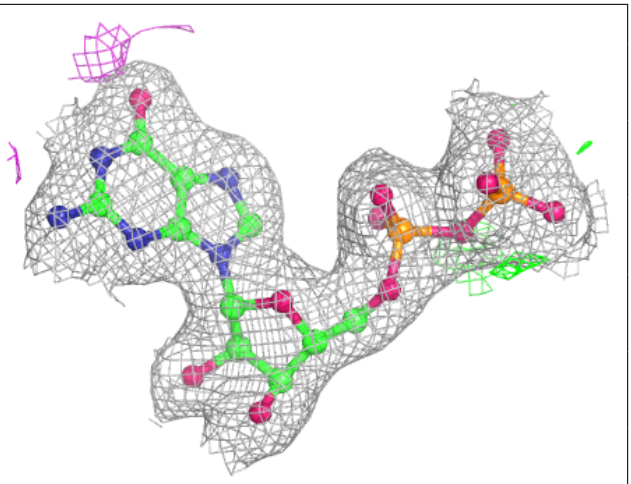


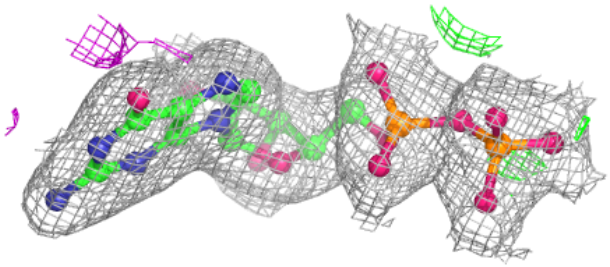


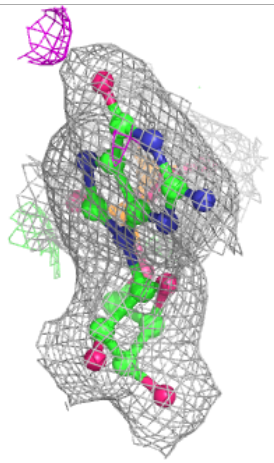


Electron density around GDP B 501:

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

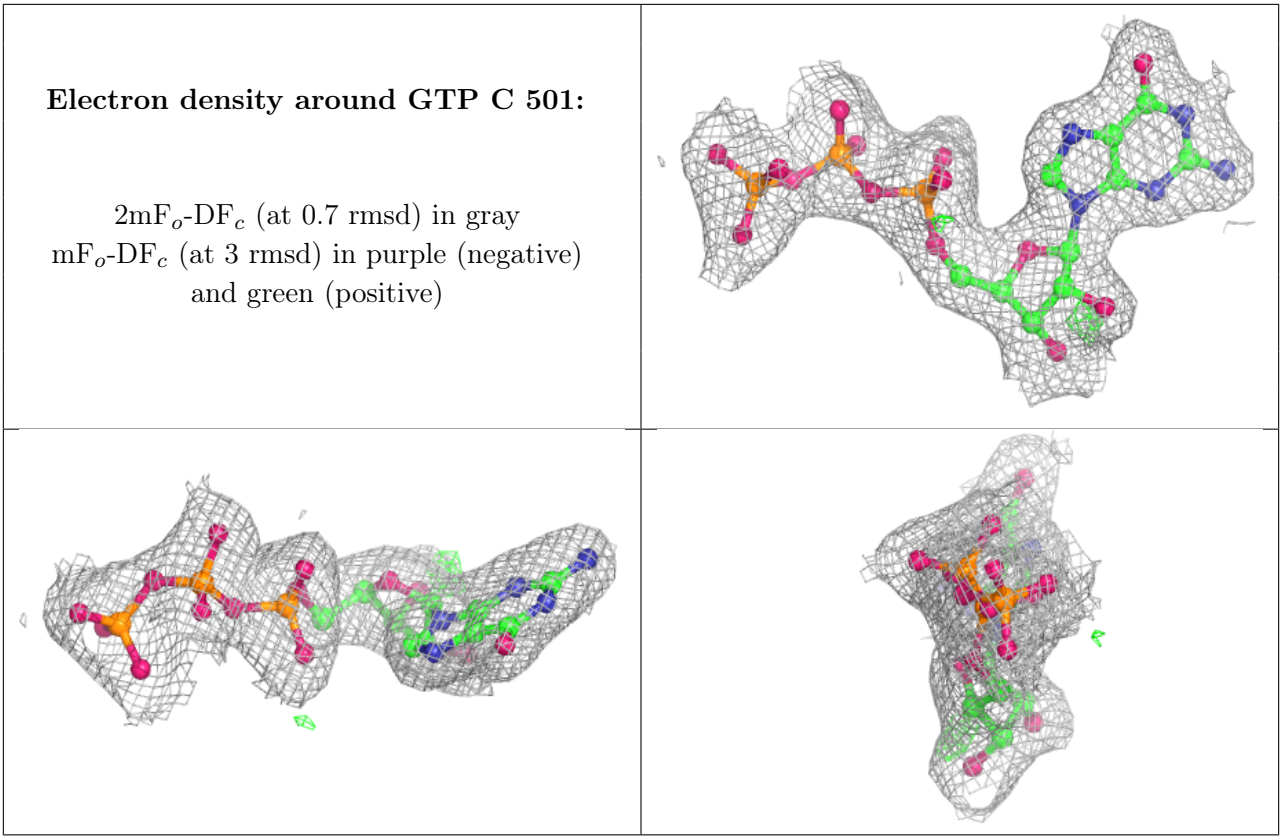






Electron density around GTP C 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.