Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 04:38 AM EDT

PDB ID	:	7L05
Title	:	Complex of novel maytansinoid M24 bound to T2R-TTL (two tubulin alpha/beta heterodimers, RB3 stathmin-like domain, and tubulin tyrosine ligase)
Authors	:	Franklin, M.C.
Deposited on	:	2020-12-11
Resolution	:	2.21 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 ⓘ 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 ⓘ) were used in the production of this report:

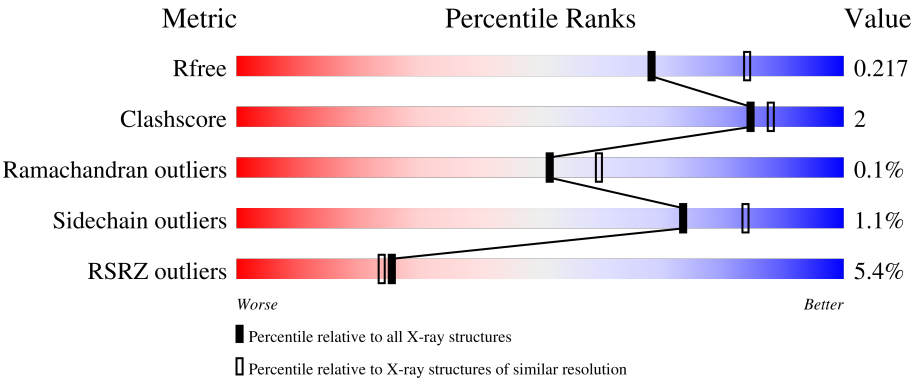
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	2% 93% . .
1	C	451	% 89% 9% .
2	B	445	2% 87% 7% 5%
2	D	445	5% 87% 7% 6%

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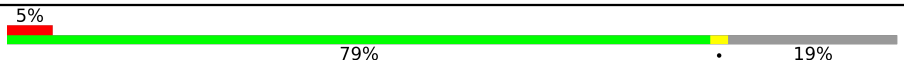
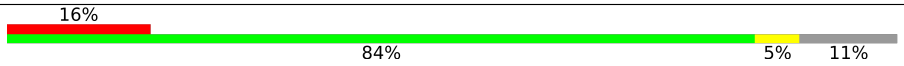
Mol	Chain	Length	Quality of chain
3	E	149	
4	F	384	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18587 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	1	0
			3434	2173	583	656	22			
1	C	440	Total	C	N	O	S	0	8	0
			3471	2197	586	664	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	5	0
			3325	2095	563	641	26			
2	D	420	Total	C	N	O	S	0	5	0
			3309	2082	558	643	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	3	0
			1017	629	184	198	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	cloning artifact	UNP P63043
E	146	HIS	-	expression tag	UNP P63043
E	147	HIS	-	expression tag	UNP P63043
E	148	HIS	-	expression tag	UNP P63043
E	149	HIS	-	expression tag	UNP P63043
E	150	HIS	-	expression tag	UNP P63043
E	151	HIS	-	expression tag	UNP P63043

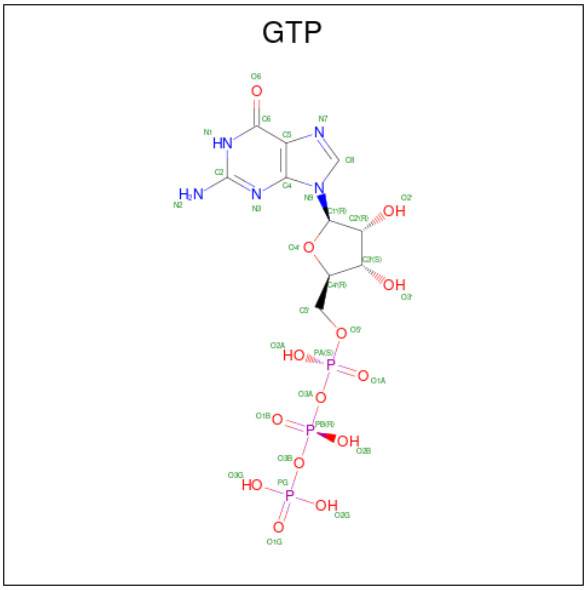
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	342	Total	C	N	O	S	0	4	0
			2838	1828	486	510	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

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

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

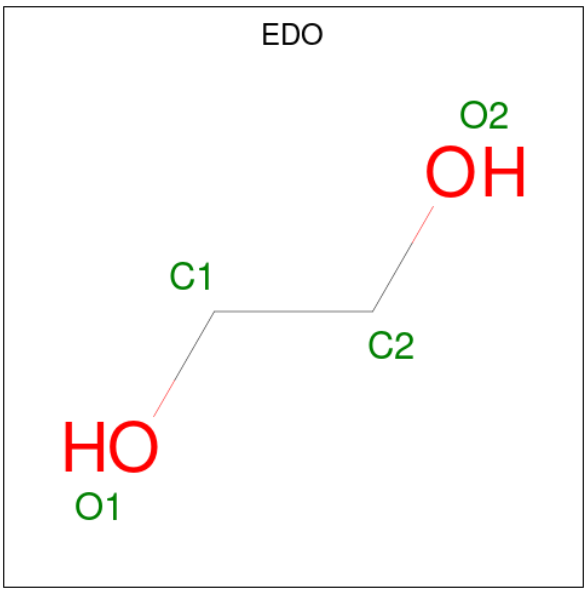
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

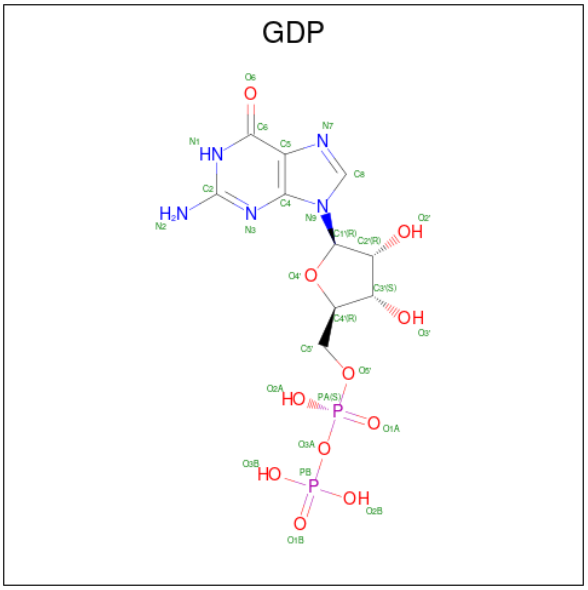
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



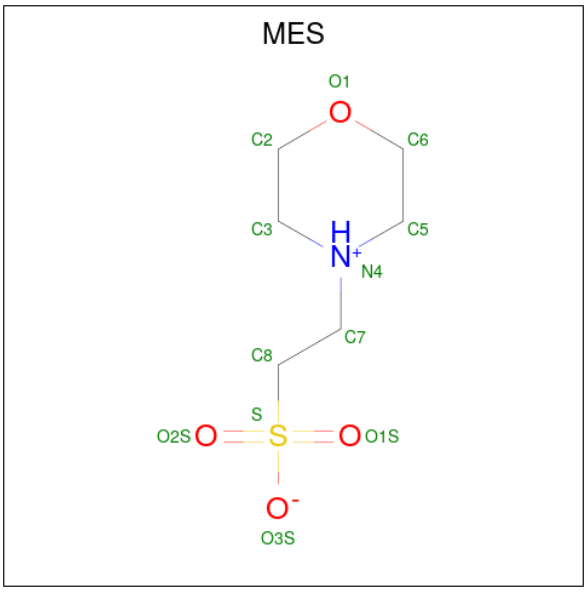
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

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



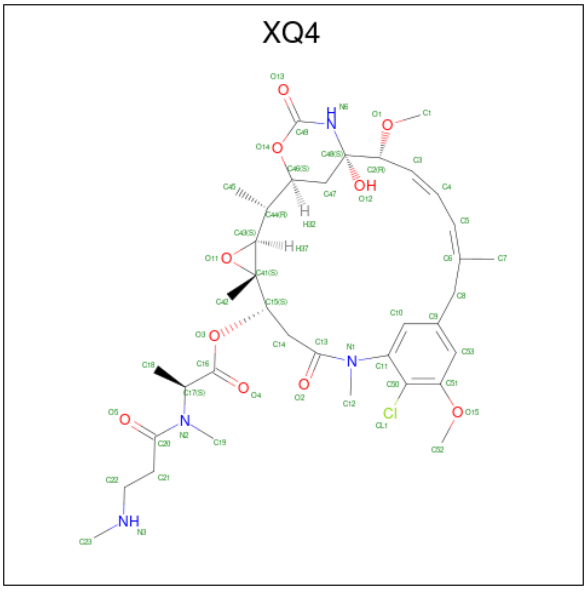
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O P 28 10 5 11 2	0	0
10	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



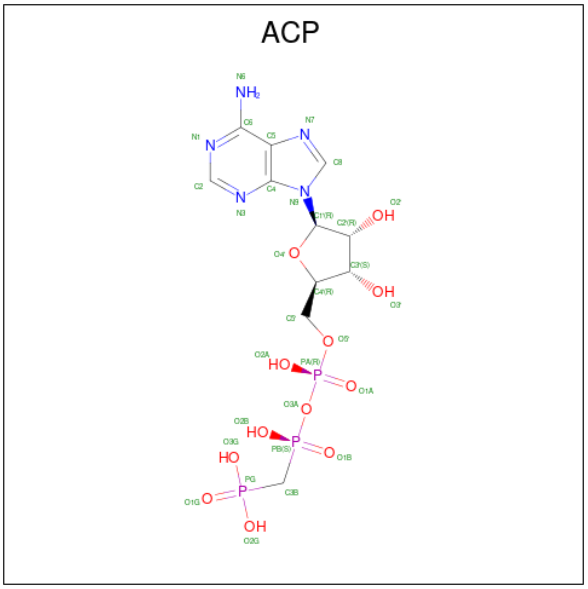
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 12 is (1S,2R,3S,5S,6S,16E,18E,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16,18-pentaen-6-yl (2S)-2-{methyl[3-(methylamino)propanoyl]amino}propanoate (non-preferred name) (three-letter code: XQ4) (formula: $C_{36}H_{51}ClN_4O_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	Cl	N	O	0	0
			51	36	1	4	10		

- 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
13	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 14 is water.

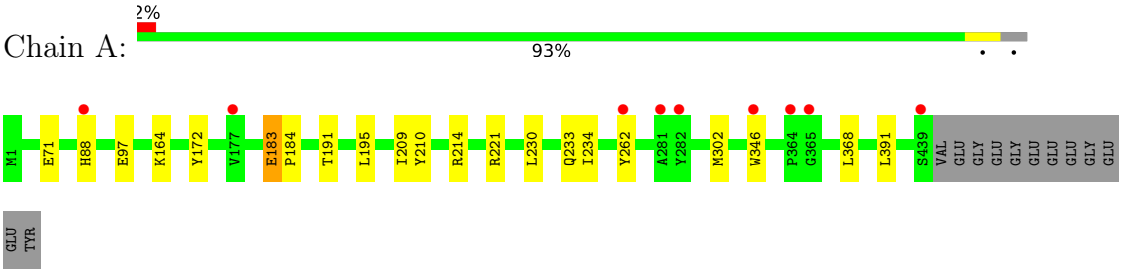
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	200	Total	O	0	0
			200	200		
14	B	176	Total	O	0	0
			176	176		
14	C	354	Total	O	0	0
			354	354		
14	D	100	Total	O	0	0
			100	100		
14	E	52	Total	O	0	0
			52	52		
14	F	75	Total	O	0	0
			75	75		

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.

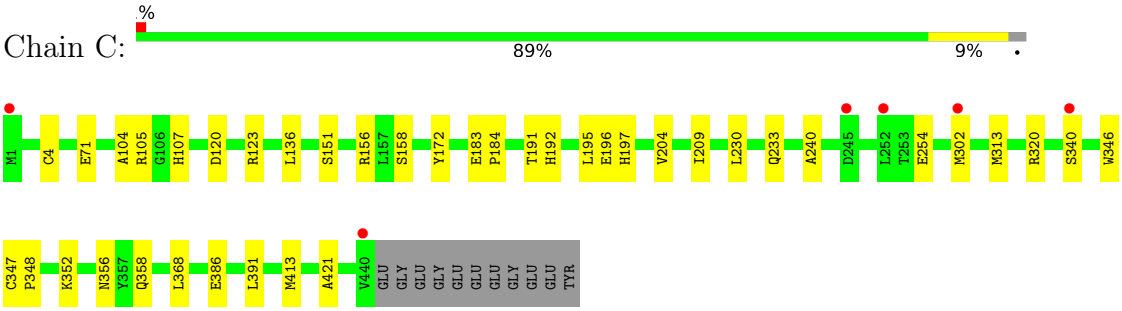
• Molecule 1: Tubulin alpha-1B chain

Chain A:



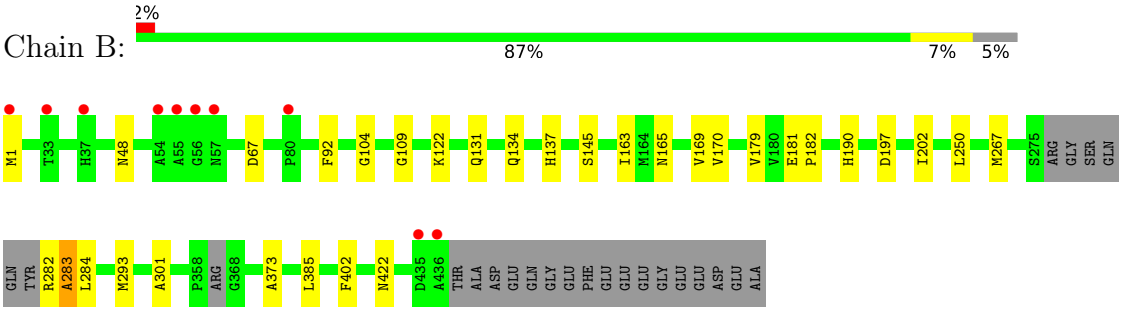
• Molecule 1: Tubulin alpha-1B chain

Chain C:



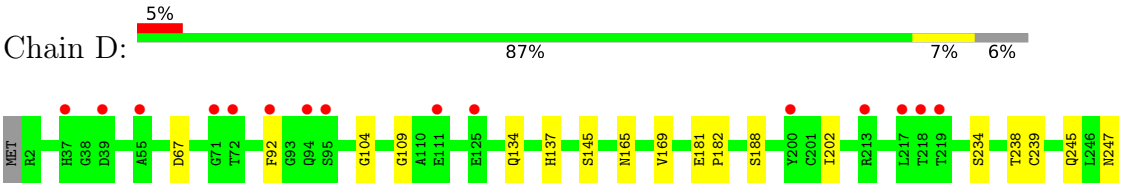
• Molecule 2: Tubulin beta chain

Chain B:



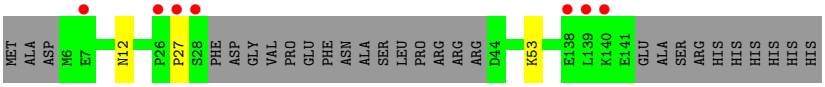
• Molecule 2: Tubulin beta chain

Chain D:



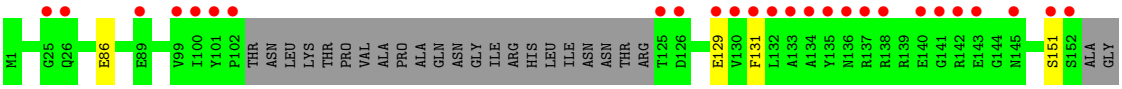
• Molecule 3: Stathmin-4

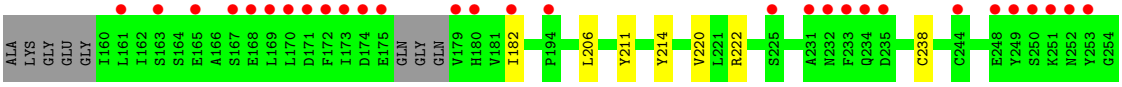
Chain E:

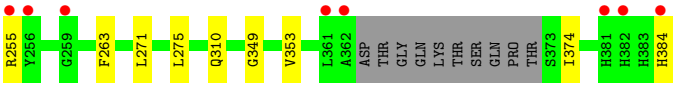


• Molecule 4: Tubulin Tyrosine Ligase

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	105.09Å 158.04Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.62 – 2.21 45.58 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.62-2.21) 97.8 (45.58-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.217 0.190 , 0.217	Depositor DCC
R_{free} test set	7466 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.7	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	0.95	EDS
Total number of atoms	18587	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACP, GDP, XQ4, EDO, GTP, CA, MG, MES

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	0.69	1/3515 (0.0%)	0.82	1/4772 (0.0%)
1	C	0.76	1/3573 (0.0%)	0.89	5/4853 (0.1%)
2	B	0.73	0/3412	0.81	1/4622 (0.0%)
2	D	0.68	0/3398	0.80	0/4605
3	E	0.76	0/1035	0.86	0/1373
4	F	0.68	0/2917	0.76	0/3941
All	All	0.71	2/17850 (0.0%)	0.82	7/24166 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	386	GLU	CD-OE2	5.26	1.31	1.25
1	A	183	GLU	CD-OE1	5.07	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	105	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	B	131	GLN	CB-CA-C	-5.67	99.05	110.40
1	A	88	HIS	CB-CA-C	5.49	121.38	110.40
1	C	123	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	156	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	120[A]	ASP	CB-CA-C	5.27	120.93	110.40
1	C	120[B]	ASP	CB-CA-C	5.27	120.93	110.40

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	3434	0	3346	10	0
1	C	3471	0	3392	22	0
2	B	3325	0	3222	23	0
2	D	3309	0	3190	19	1
3	E	1017	0	1040	1	0
4	F	2838	0	2818	6	1
5	A	32	0	12	0	0
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	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	A	4	0	6	0	0
9	B	8	0	12	0	0
10	B	28	0	12	0	0
10	D	28	0	12	0	0
11	B	12	0	13	3	0
12	D	51	0	0	0	0
13	F	31	0	14	0	0
14	A	200	0	0	0	0
14	B	176	0	0	1	0
14	C	354	0	0	2	0
14	D	100	0	0	4	0
14	E	52	0	0	1	0
14	F	75	0	0	0	0
All	All	18587	0	17101	79	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 2.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:HIS:CD2	2:B:422[A]:ASN:HD22	1.93	0.85
2:B:190:HIS:HD2	2:B:422[A]:ASN:HD22	1.23	0.81
1:A:209:ILE:HD11	1:A:302:MET:SD	2.26	0.74
2:B:170:VAL:HG11	2:B:385[A]:LEU:HD11	1.69	0.73
1:A:234:ILE:HD13	1:A:302:MET:SD	2.31	0.71
1:C:196:GLU:OE1	14:C:601:HOH:O	2.08	0.71
2:D:238[B]:THR:HG21	2:D:318:ARG:HD2	1.73	0.70
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.33	0.69
2:B:197:ASP:OD1	11:B:506:MES:H52	1.95	0.66
3:E:12:ASN:HB3	14:E:241:HOH:O	1.98	0.62
2:D:145[B]:SER:OG	2:D:188:SER:OG	2.12	0.59
1:C:204:VAL:HG22	1:C:302:MET:CE	2.34	0.57
1:C:356:ASN:OD1	1:C:358[B]:GLN:OE1	2.22	0.56
2:D:104:GLY:O	2:D:109:GLY:HA3	2.06	0.56
1:C:313:MET:O	1:C:347[A]:CYS:SG	2.63	0.56
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	2.95	0.55
2:D:239[B]:CYS:SG	14:D:689:HOH:O	2.59	0.55
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	3.00	0.54
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.43	0.54
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.44	0.53
2:D:134:GLN:HA	2:D:165:ASN:O	2.08	0.53
2:B:134:GLN:HA	2:B:165:ASN:O	2.09	0.53
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.91	0.53
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.44	0.53
2:B:197:ASP:OD2	11:B:506:MES:H32	2.08	0.52
2:D:245:GLN:OE1	14:D:601:HOH:O	2.18	0.52
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.90	0.52
2:B:104:GLY:O	2:B:109:GLY:HA3	2.10	0.52
1:C:158:SER:OG	1:C:197:HIS:HD2	1.95	0.50
2:D:332:ASN:HD21	2:D:336:LYS:HE3	1.76	0.50
2:D:234:SER:O	2:D:238[B]:THR:HG23	2.12	0.50
2:B:197:ASP:OD2	11:B:506:MES:H72	2.11	0.50
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.93	0.50
2:B:190:HIS:NE2	2:B:422[B]:ASN:OD1	2.45	0.49
2:B:165:ASN:ND2	14:B:606:HOH:O	2.46	0.49
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.95	0.49
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.43	0.48
2:B:190:HIS:HD2	2:B:422[A]:ASN:ND2	2.02	0.48
1:C:104:ALA:HB2	1:C:413:MET:SD	2.54	0.48
2:B:282:ARG:O	2:B:283:ALA:HB2	2.14	0.48
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.95	0.48
2:D:238[B]:THR:HG21	2:D:318:ARG:CD	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:343:GLU:HG3	2:D:438:ALA:HB2	1.96	0.47
1:C:240:ALA:HB1	1:C:356:ASN:HD22	1.79	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.97	0.47
2:D:169:VAL:HA	2:D:202:ILE:O	2.15	0.47
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	1.98	0.46
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.51	0.46
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.44
2:B:67:ASP:O	2:B:92:PHE:HA	2.17	0.44
2:D:306:ARG:NH2	14:D:608:HOH:O	2.50	0.44
2:B:169:VAL:HA	2:B:202:ILE:O	2.17	0.44
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.99	0.43
4:F:131:PHE:CZ	4:F:182:ILE:HG21	2.53	0.43
2:D:181:GLU:N	2:D:182:PRO:CD	2.81	0.43
2:D:293:MET:CE	2:D:373:ALA:HB1	2.49	0.43
1:C:158:SER:OG	1:C:197:HIS:CD2	2.72	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
1:A:191:THR:O	1:A:195:LEU:HB2	2.19	0.42
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.49	0.42
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.50	0.42
2:B:293:MET:HE3	2:B:373:ALA:HB1	2.01	0.42
2:D:67:ASP:O	2:D:92:PHE:HA	2.19	0.42
2:D:165:ASN:ND2	14:D:611:HOH:O	2.53	0.42
2:B:293:MET:CE	2:B:373:ALA:HB1	2.50	0.42
2:D:239[B]:CYS:SG	2:D:247:ASN:O	2.74	0.41
4:F:214:TYR:CE2	4:F:353[B]:VAL:CG1	3.04	0.41
2:B:181:GLU:N	2:B:182:PRO:CD	2.84	0.41
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.41
1:C:191:THR:O	1:C:195:LEU:HB2	2.20	0.41
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.02	0.41
2:B:48:ASN:ND2	2:B:48:ASN:H	2.18	0.41
1:C:356:ASN:ND2	14:C:618:HOH:O	2.53	0.41
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.40
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.03	0.40
1:A:97:GLU:HB2	2:B:1:MET:HG2	2.04	0.40
2:B:179:VAL:HG21	2:B:402:PHE:CZ	2.57	0.40
4:F:275[A]:LEU:HD13	4:F:275[A]:LEU:HA	1.91	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)
2:D:335:ASN:OD1	4:F:384:HIS:NE2[3_545]	2.08	0.12

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	438/451 (97%)	431 (98%)	7 (2%)	0	100 100
1	C	446/451 (99%)	435 (98%)	11 (2%)	0	100 100
2	B	420/445 (94%)	411 (98%)	8 (2%)	1 (0%)	47 54
2	D	419/445 (94%)	413 (99%)	6 (1%)	0	100 100
3	E	120/149 (80%)	119 (99%)	0	1 (1%)	19 18
4	F	336/384 (88%)	327 (97%)	9 (3%)	0	100 100
All	All	2179/2325 (94%)	2136 (98%)	41 (2%)	2 (0%)	51 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	ALA
3	E	27	PRO

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	371/379 (98%)	368 (99%)	3 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	379/379 (100%)	377 (100%)	2 (0%)	88 94
2	B	367/381 (96%)	363 (99%)	4 (1%)	73 84
2	D	366/381 (96%)	365 (100%)	1 (0%)	92 96
3	E	112/133 (84%)	111 (99%)	1 (1%)	78 87
4	F	314/342 (92%)	304 (97%)	10 (3%)	39 49
All	All	1909/1995 (96%)	1888 (99%)	21 (1%)	73 84

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	164	LYS
1	A	221	ARG
2	B	122	LYS
2	B	137	HIS
2	B	145	SER
2	B	284	LEU
1	C	71	GLU
1	C	340	SER
2	D	137	HIS
3	E	53	LYS
4	F	86	GLU
4	F	129	GLU
4	F	151	SER
4	F	211	TYR
4	F	222	ARG
4	F	238	CYS
4	F	255	ARG
4	F	271[A]	LEU
4	F	271[B]	LEU
4	F	310	GLN

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

Mol	Chain	Res	Type
1	A	128	GLN
2	B	165	ASN
2	B	190	HIS
1	C	107	HIS

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Mol	Chain	Res	Type
1	C	197	HIS
1	C	356	ASN
4	F	260	ASN
4	F	333	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	GDP	B	501	6	24,30,30	1.17	3 (12%)	30,47,47	1.16	4 (13%)
12	XQ4	D	503	-	52,54,54	1.67	7 (13%)	59,80,80	1.90	14 (23%)
13	ACP	F	502	6	27,33,33	0.86	1 (3%)	32,52,52	0.93	1 (3%)
5	GTP	A	501	6	26,34,34	0.99	3 (11%)	32,54,54	0.91	0
10	GDP	D	501	6	24,30,30	0.92	0	30,47,47	1.12	3 (10%)
9	EDO	A	506	-	3,3,3	0.13	0	2,2,2	0.13	0
9	EDO	B	504	-	3,3,3	0.14	0	2,2,2	0.30	0
9	EDO	B	505	-	3,3,3	0.42	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MES	B	506	-	12,12,12	0.86	0	14,16,16	1.53	4 (28%)
5	GTP	C	501	6	26,34,34	0.96	2 (7%)	32,54,54	0.90	1 (3%)

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	GDP	B	501	6	-	5/12/32/32	0/3/3/3
12	XQ4	D	503	-	-	16/61/88/88	0/2/4/4
13	ACP	F	502	6	-	7/15/38/38	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
10	GDP	D	501	6	-	4/12/32/32	0/3/3/3
9	EDO	A	506	-	-	1/1/1/1	-
9	EDO	B	504	-	-	1/1/1/1	-
9	EDO	B	505	-	-	1/1/1/1	-
11	MES	B	506	-	-	1/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	XQ4	O14-C49	6.89	1.45	1.35
12	D	503	XQ4	C41-C43	5.44	1.54	1.47
12	D	503	XQ4	O3-C16	4.41	1.44	1.34
12	D	503	XQ4	O11-C41	-3.55	1.41	1.45
12	D	503	XQ4	C50-CL1	3.41	1.80	1.72
10	B	501	GDP	O4'-C1'	3.17	1.45	1.41
5	C	501	GTP	C5-C6	-2.78	1.41	1.47
5	A	501	GTP	C5-C6	-2.46	1.42	1.47
10	B	501	GDP	C6-N1	-2.45	1.34	1.37
10	B	501	GDP	C2'-C1'	-2.36	1.50	1.53
13	F	502	ACP	PB-O2B	-2.33	1.50	1.56
12	D	503	XQ4	O3-C15	-2.26	1.42	1.46
12	D	503	XQ4	O14-C46	-2.21	1.43	1.46
5	A	501	GTP	C8-N7	-2.18	1.31	1.35
5	C	501	GTP	C5-C4	-2.08	1.37	1.43
5	A	501	GTP	C5-C4	-2.00	1.38	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	503	XQ4	C41-O11-C43	7.07	65.04	60.79
12	D	503	XQ4	O11-C43-C41	-4.80	56.42	59.83
12	D	503	XQ4	O15-C51-C50	4.10	120.39	115.53
12	D	503	XQ4	O3-C16-C17	3.39	118.16	110.80
12	D	503	XQ4	C46-O14-C49	-3.38	112.42	121.06
11	B	506	MES	C5-N4-C3	2.99	115.57	108.83
12	D	503	XQ4	C10-C11-C50	-2.98	118.73	122.53
11	B	506	MES	C6-C5-N4	2.78	114.32	110.10
12	D	503	XQ4	O3-C16-O4	-2.77	118.77	123.94
12	D	503	XQ4	O2-C13-C14	-2.76	117.22	122.20
11	B	506	MES	C2-C3-N4	2.74	114.25	110.10
10	D	501	GDP	O3B-PB-O1B	2.70	121.24	110.68
12	D	503	XQ4	O11-C41-C15	2.66	119.97	115.00
5	C	501	GTP	O6-C6-C5	2.64	129.54	124.37
12	D	503	XQ4	O15-C51-C53	-2.62	119.60	124.12
12	D	503	XQ4	C14-C15-C41	-2.54	109.25	114.60
12	D	503	XQ4	O11-C41-C42	2.41	117.62	114.17
10	D	501	GDP	C5-C6-N1	2.41	118.20	113.95
12	D	503	XQ4	C5-C4-C3	-2.35	118.83	124.53
10	B	501	GDP	PA-O3A-PB	-2.25	125.09	132.83
10	B	501	GDP	O3'-C3'-C4'	-2.16	104.80	111.05
10	B	501	GDP	C5-C6-N1	2.11	117.68	113.95
11	B	506	MES	O2S-S-C8	-2.09	104.40	106.92
12	D	503	XQ4	C12-N1-C13	2.07	122.57	119.15
13	F	502	ACP	C5-C6-N6	2.04	123.45	120.35
10	D	501	GDP	C8-N7-C5	2.04	106.87	102.99
10	B	501	GDP	C8-N7-C5	2.01	106.82	102.99

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O1A
11	B	506	MES	C8-C7-N4-C5
12	D	503	XQ4	C50-C51-O15-C52

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Mol	Chain	Res	Type	Atoms
12	D	503	XQ4	O3-C16-C17-N2
12	D	503	XQ4	O4-C16-C17-N2
12	D	503	XQ4	O5-C20-N2-C17
12	D	503	XQ4	C21-C20-N2-C17
12	D	503	XQ4	O5-C20-N2-C19
12	D	503	XQ4	C21-C20-N2-C19
13	F	502	ACP	C5'-O5'-PA-O1A
13	F	502	ACP	C5'-O5'-PA-O2A
12	D	503	XQ4	C53-C51-O15-C52
12	D	503	XQ4	C16-C17-N2-C19
12	D	503	XQ4	C18-C17-N2-C19
5	C	501	GTP	PB-O3B-PG-O3G
13	F	502	ACP	C3'-C4'-C5'-O5'
12	D	503	XQ4	C3-C2-O1-C1
5	A	501	GTP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O2A
13	F	502	ACP	PB-C3B-PG-O3G
13	F	502	ACP	O4'-C4'-C5'-O5'
12	D	503	XQ4	C45-C44-C46-C47
9	A	506	EDO	O1-C1-C2-O2
9	B	505	EDO	O1-C1-C2-O2
9	B	504	EDO	O1-C1-C2-O2
12	D	503	XQ4	C48-C2-O1-C1
12	D	503	XQ4	O2-C13-C14-C15
13	F	502	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O3A
13	F	502	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
10	B	501	GDP	PB-O3A-PA-O1A
10	B	501	GDP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O1A
12	D	503	XQ4	N1-C13-C14-C15
12	D	503	XQ4	C21-C22-N3-C23

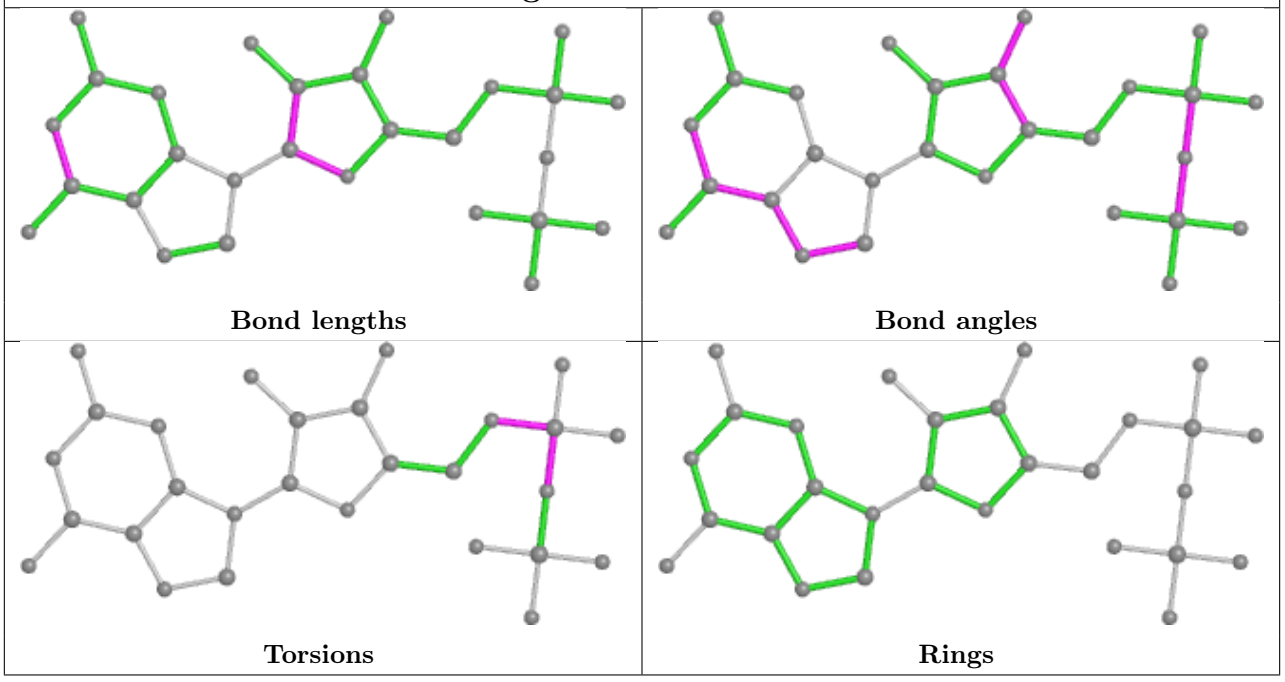
There are no ring outliers.

1 monomer is involved in 3 short contacts:

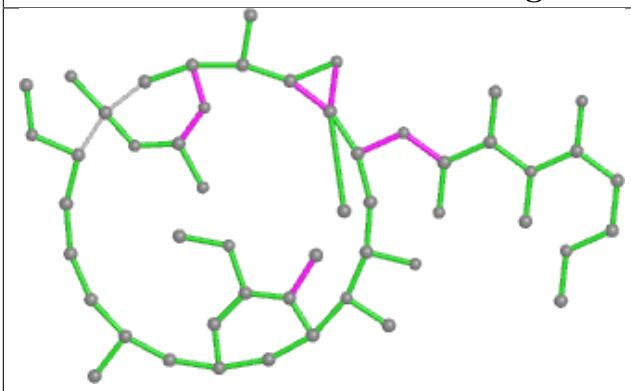
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	506	MES	3	0

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

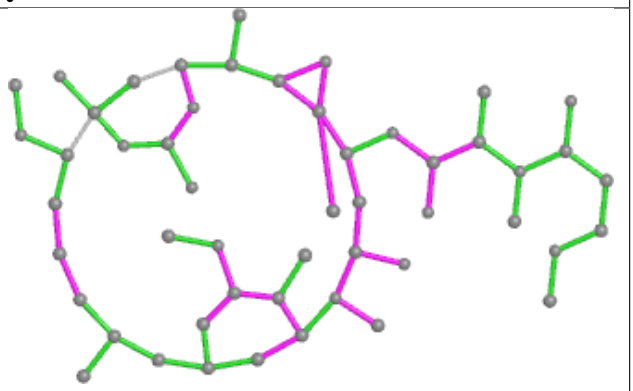
Ligand GDP B 501



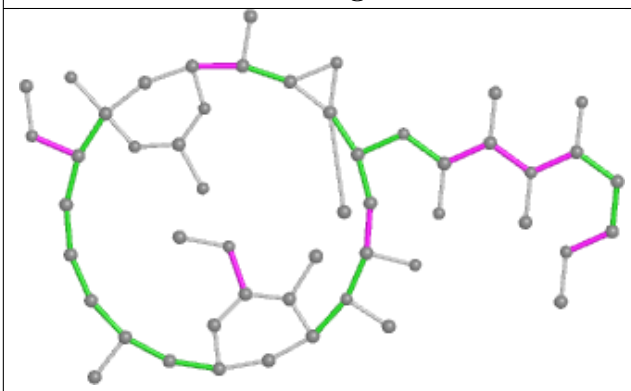
Ligand XQ4 D 503



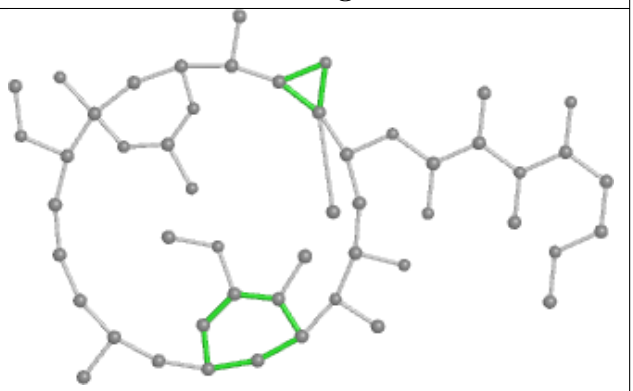
Bond lengths



Bond angles

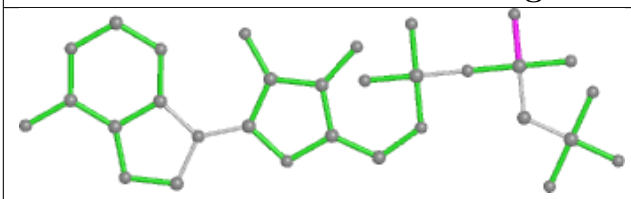


Torsions

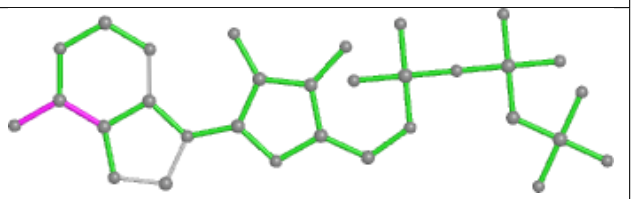


Rings

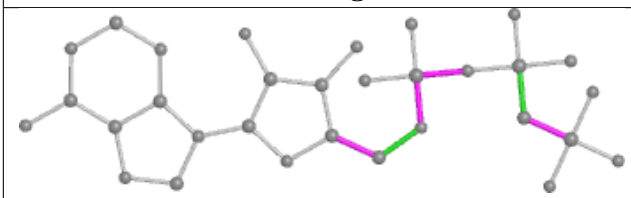
Ligand ACP F 502



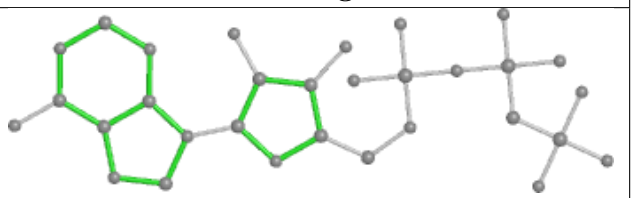
Bond lengths



Bond angles

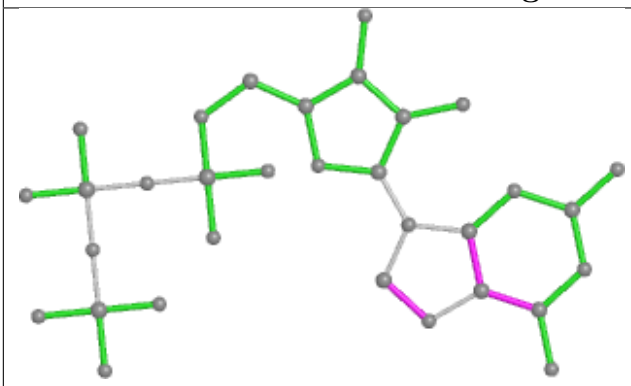


Torsions

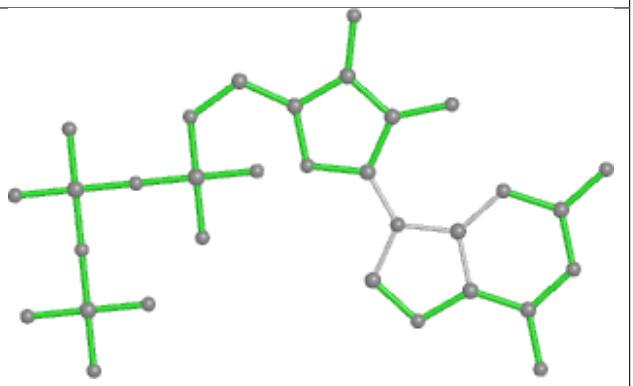


Rings

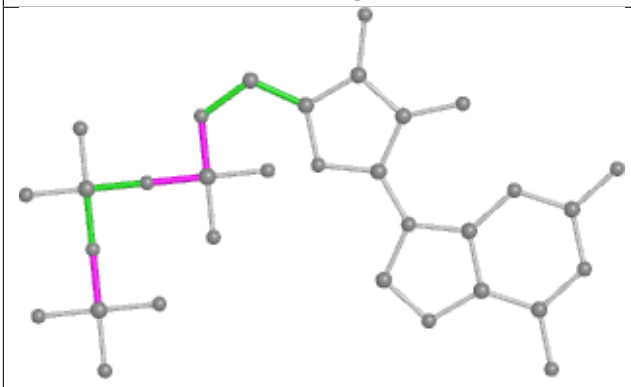
Ligand GTP A 501



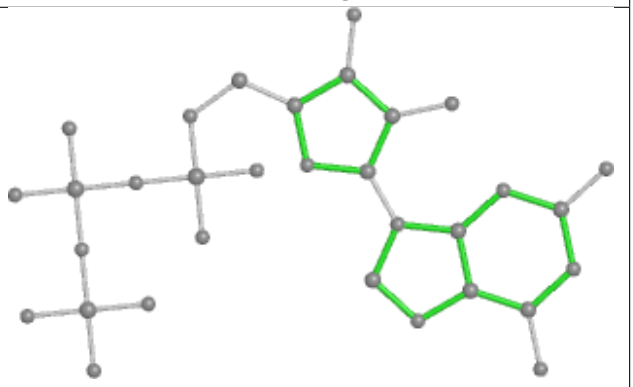
Bond lengths



Bond angles

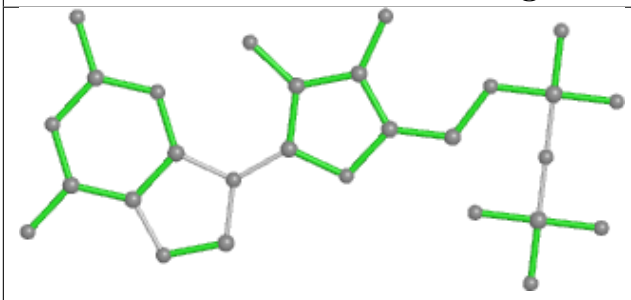


Torsions

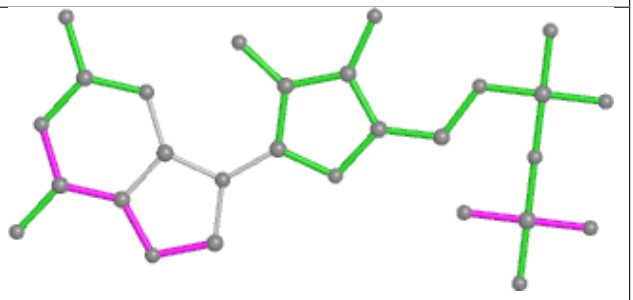


Rings

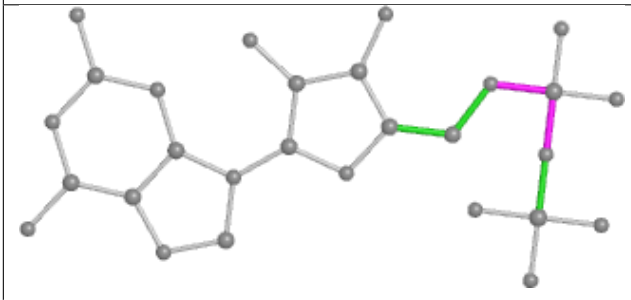
Ligand GDP D 501



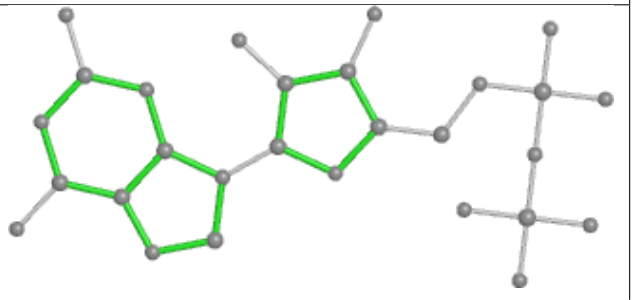
Bond lengths



Bond angles

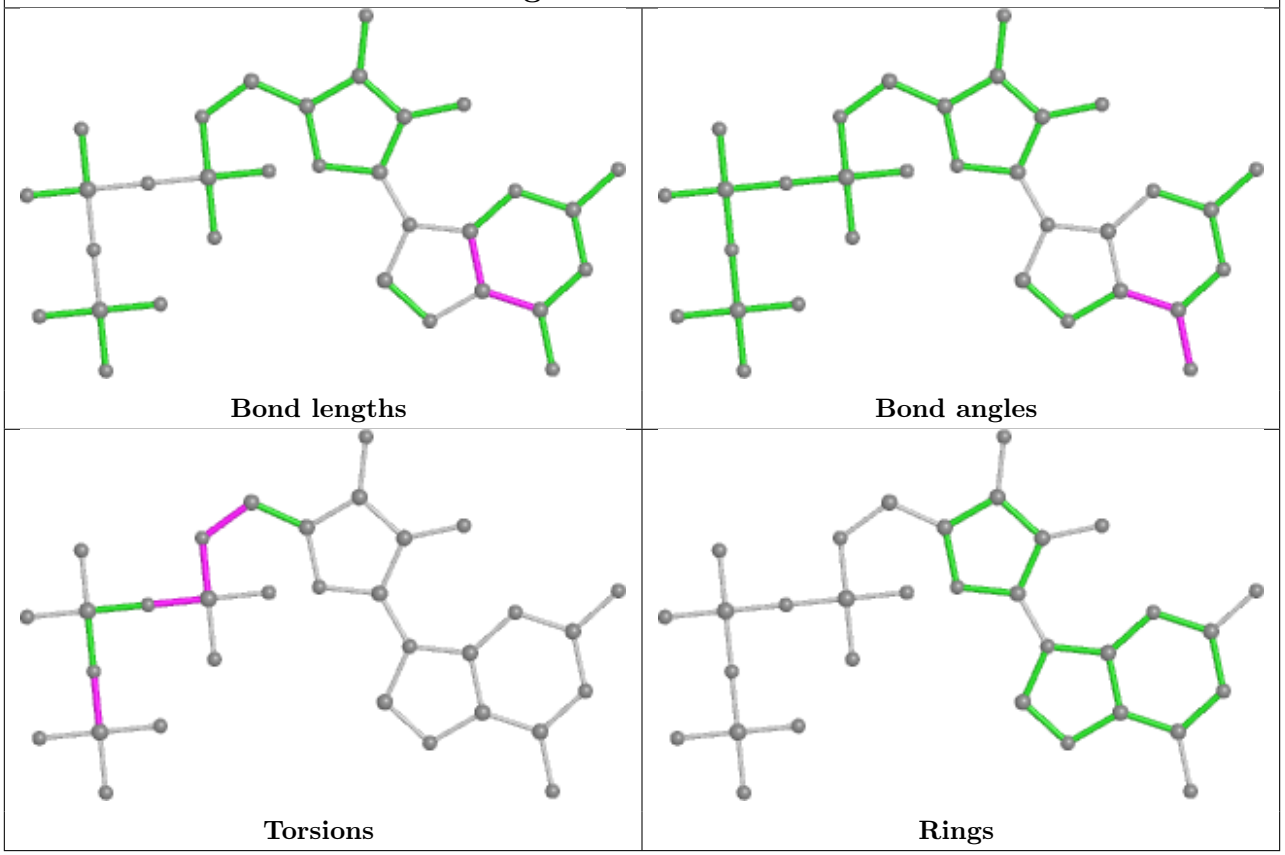


Torsions



Rings

Ligand GTP C 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	439/451 (97%)	-0.10	9 (2%) 63 61	20, 35, 66, 95	0
1	C	440/451 (97%)	-0.19	6 (1%) 75 73	16, 26, 46, 68	0
2	B	421/445 (94%)	-0.06	10 (2%) 59 57	17, 32, 59, 84	1 (0%)
2	D	420/445 (94%)	0.22	23 (5%) 25 23	22, 43, 74, 93	3 (0%)
3	E	121/149 (81%)	0.21	7 (5%) 23 21	25, 45, 86, 101	0
4	F	342/384 (89%)	0.61	63 (18%) 1 1	26, 55, 122, 135	0
All	All	2183/2325 (93%)	0.08	118 (5%) 25 24	16, 37, 81, 135	4 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	234	GLN	7.5
4	F	249	TYR	6.5
4	F	130	VAL	6.5
4	F	381	HIS	6.0
4	F	231	ALA	5.9
1	A	439	SER	5.9
4	F	134	ALA	5.8
2	B	1	MET	5.5
4	F	165	GLU	5.5
4	F	173	ILE	5.4
4	F	137	ARG	5.4
4	F	182	ILE	5.3
2	D	399	ARG	5.1
4	F	129	GLU	5.1
4	F	244	CYS	5.1
4	F	232	ASN	5.0
4	F	133	ALA	4.9
4	F	132	LEU	4.7
4	F	161	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
4	F	251	LYS	4.6
1	A	282	TYR	4.6
2	D	55	ALA	4.5
4	F	233	PHE	4.5
4	F	169	LEU	4.5
2	D	92	PHE	4.5
3	E	139	LEU	4.5
4	F	170	LEU	4.3
1	C	340	SER	4.2
2	D	95	SER	4.2
2	D	274	THR	4.1
4	F	102	PRO	4.1
4	F	248	GLU	4.1
4	F	125	THR	4.1
4	F	101	TYR	4.1
4	F	140	GLU	4.0
4	F	362	ALA	3.9
4	F	135	TYR	3.9
4	F	179	VAL	3.8
1	A	281	ALA	3.8
3	E	28	SER	3.8
4	F	143	GLU	3.8
4	F	174	ASP	3.8
1	C	440	VAL	3.8
1	A	262	TYR	3.5
2	D	219	THR	3.4
4	F	250	SER	3.4
2	B	435	ASP	3.3
4	F	382	HIS	3.3
1	A	365	GLY	3.2
3	E	27	PRO	3.2
4	F	256	TYR	3.2
2	B	55	ALA	3.2
4	F	171	ASP	3.1
2	B	56	GLY	3.1
4	F	136	ASN	3.1
3	E	140	LYS	3.0
4	F	384	HIS	3.0
3	E	7	GLU	3.0
4	F	131	PHE	3.0
4	F	142	ARG	2.9
4	F	235	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	172	PHE	2.9
2	B	57	ASN	2.9
4	F	361	LEU	2.9
2	B	37	HIS	2.9
4	F	126	ASP	2.9
2	B	80	PRO	2.8
2	D	398	ARG	2.8
2	D	72	THR	2.8
2	D	218	THR	2.8
2	D	71	GLY	2.7
2	D	111	GLU	2.7
3	E	138	GLU	2.7
2	B	436	ALA	2.7
4	F	151	SER	2.7
4	F	163	SER	2.7
4	F	175	GLU	2.7
4	F	141	GLY	2.7
1	A	346	TRP	2.6
4	F	25	GLY	2.6
4	F	168	GLU	2.6
4	F	138	ARG	2.6
4	F	167	SER	2.6
4	F	253	TYR	2.6
3	E	26	PRO	2.5
4	F	152	SER	2.4
4	F	89	GLU	2.4
2	D	37	HIS	2.4
2	B	33	THR	2.4
1	A	88	HIS	2.3
1	C	302	MET	2.3
1	A	177	VAL	2.3
4	F	26	GLN	2.3
4	F	99	VAL	2.3
4	F	100	ILE	2.3
2	B	54	ALA	2.3
2	D	217	LEU	2.3
2	D	414	MET	2.2
4	F	255	ARG	2.2
4	F	259	GLY	2.2
2	D	125	GLU	2.2
4	F	225	SER	2.2
1	C	245	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	213	ARG	2.2
1	C	1	MET	2.2
4	F	180	HIS	2.1
1	C	252	LEU	2.1
4	F	145	ASN	2.1
2	D	402	PHE	2.1
2	D	412	ASP	2.1
2	D	408	GLY	2.1
2	D	39	ASP	2.1
4	F	194	PRO	2.1
2	D	200	TYR	2.1
4	F	252	ASN	2.0
2	D	94	GLN	2.0
1	A	364	PRO	2.0
2	D	250	LEU	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, 95^{th} 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
9	EDO	A	506	4/4	0.74	0.21	57,59,59,60	0
13	ACP	F	502	31/31	0.85	0.15	49,69,87,94	0
7	CA	B	503	1/1	0.86	0.15	61,61,61,61	0
12	XQ4	D	503	51/51	0.87	0.23	52,66,102,112	0
6	MG	F	501	1/1	0.88	0.08	62,62,62,62	0
7	CA	A	505	1/1	0.89	0.07	69,69,69,69	0
8	CL	A	504	1/1	0.92	0.11	57,57,57,57	0
7	CA	A	503	1/1	0.93	0.09	44,44,44,44	0

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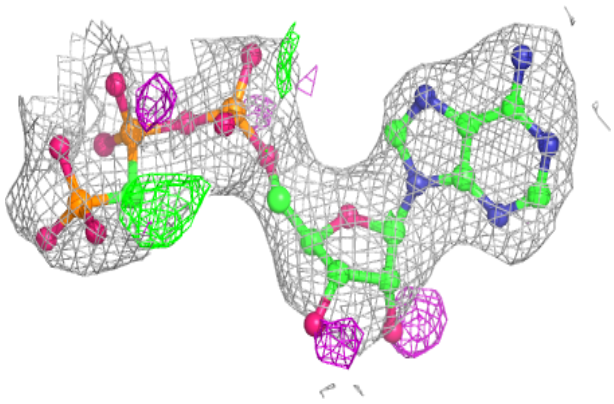
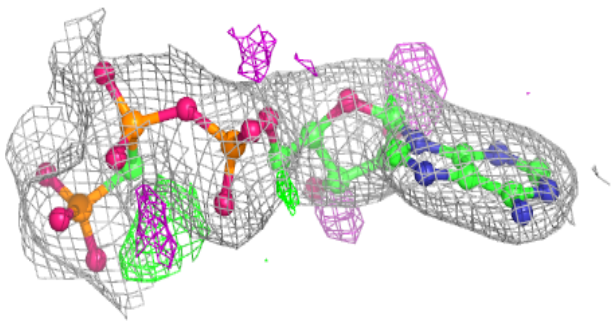
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	B	504	4/4	0.93	0.11	46,47,48,48	0
6	MG	D	502	1/1	0.94	0.11	47,47,47,47	0
9	EDO	B	505	4/4	0.94	0.12	39,40,40,40	0
11	MES	B	506	12/12	0.96	0.09	32,34,37,41	0
10	GDP	D	501	28/28	0.97	0.09	32,37,41,45	0
6	MG	C	502	1/1	0.97	0.15	17,17,17,17	0
6	MG	A	502	1/1	0.98	0.11	21,21,21,21	0
7	CA	C	503	1/1	0.98	0.03	28,28,28,28	0
6	MG	B	502	1/1	0.99	0.11	13,13,13,13	0
5	GTP	C	501	32/32	0.99	0.11	13,14,16,18	0
5	GTP	A	501	32/32	0.99	0.14	17,19,20,22	0
10	GDP	B	501	28/28	0.99	0.13	13,17,19,21	0

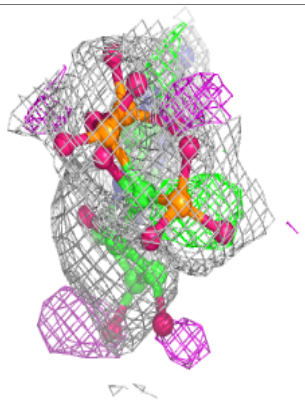
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 502:

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

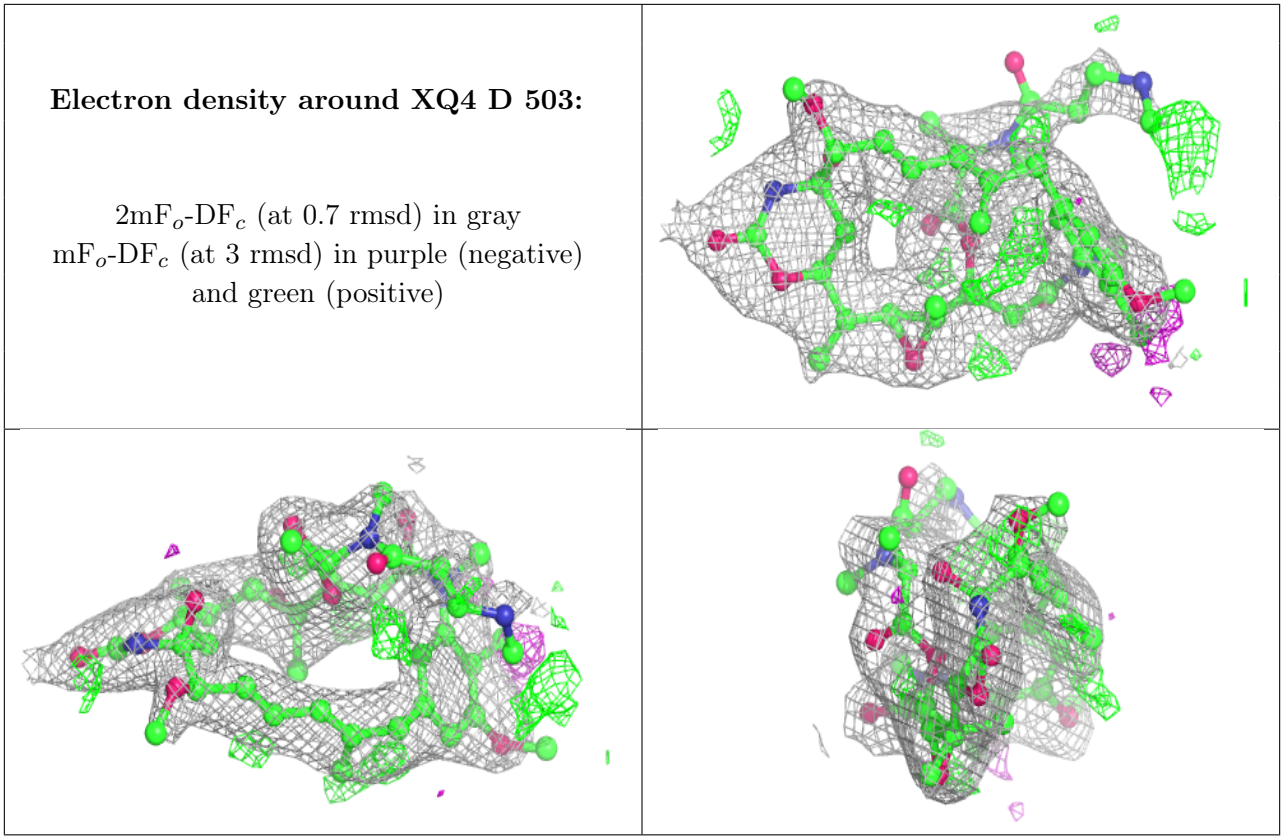






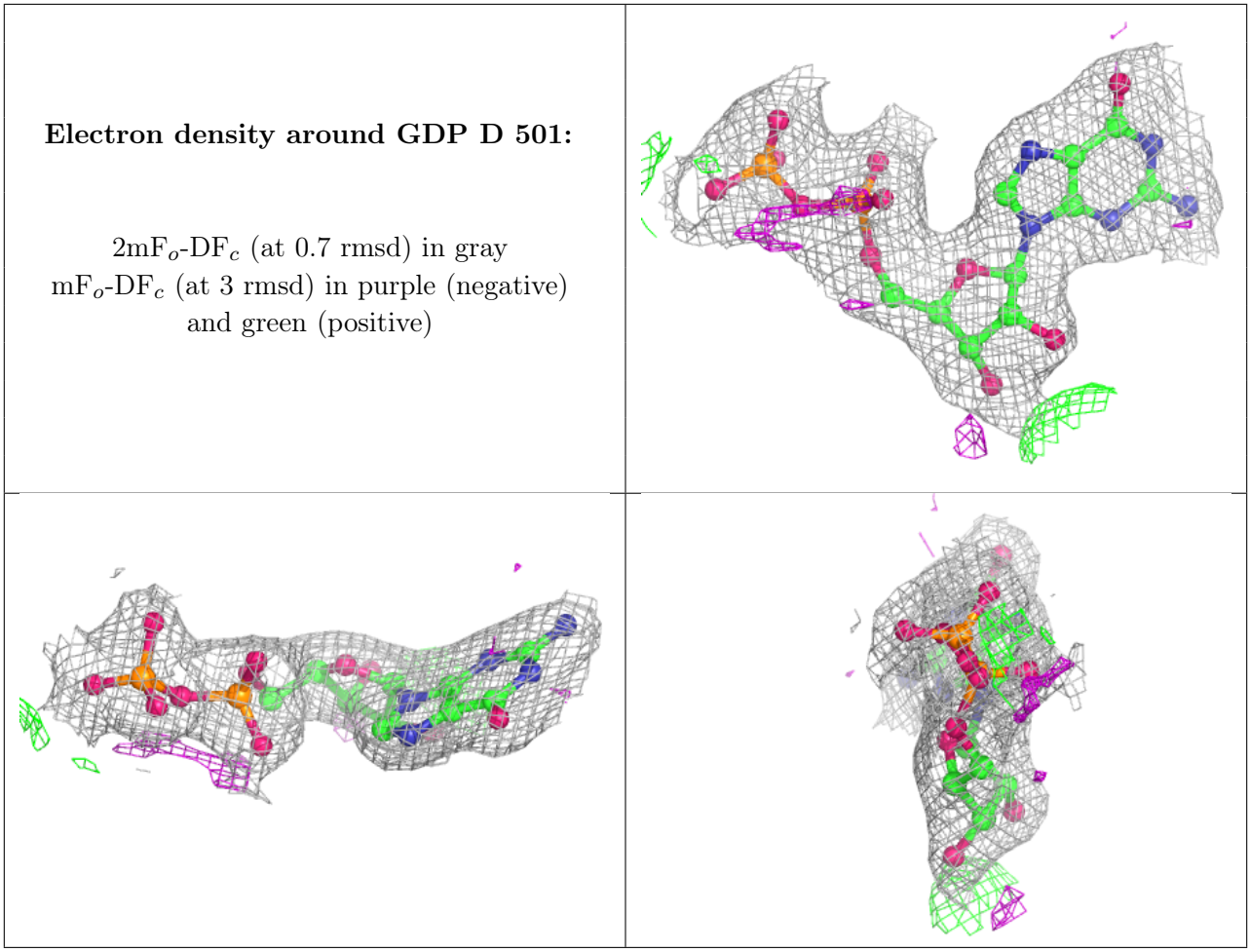
Electron density around XQ4 D 503:

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



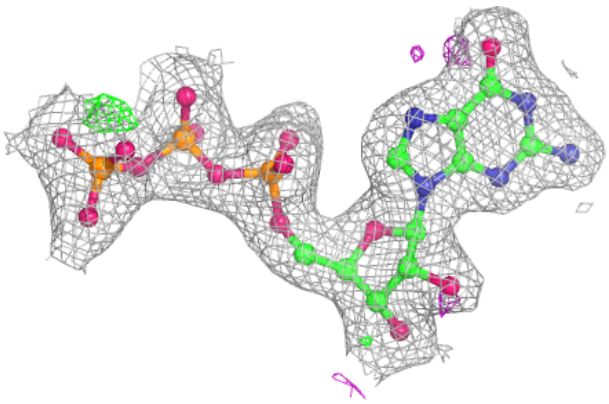
Electron density around GDP D 501:

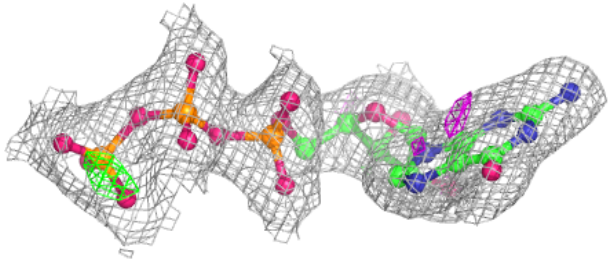
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

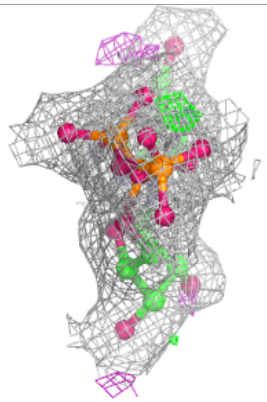


Electron density around GTP C 501:

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

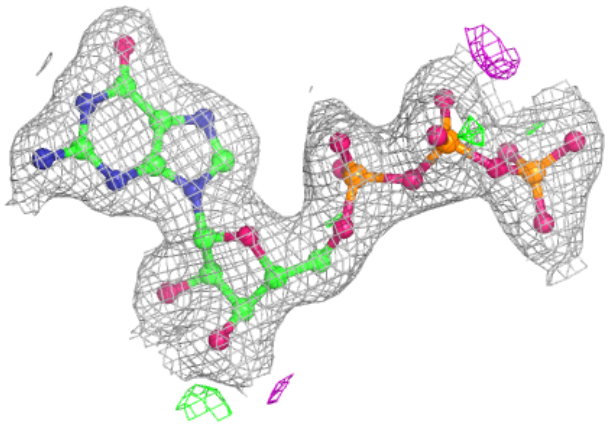


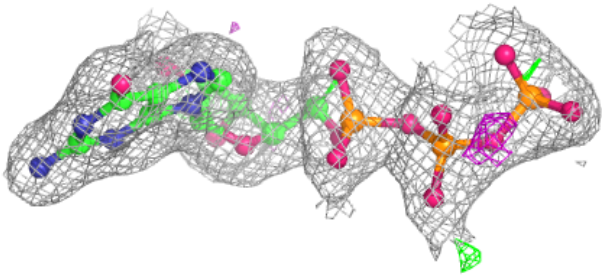


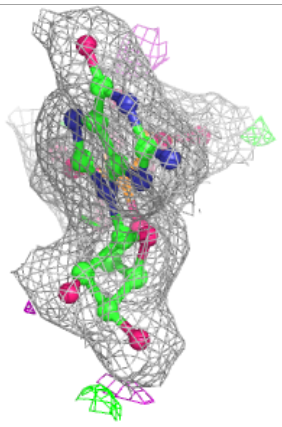


Electron density around GTP A 501:

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

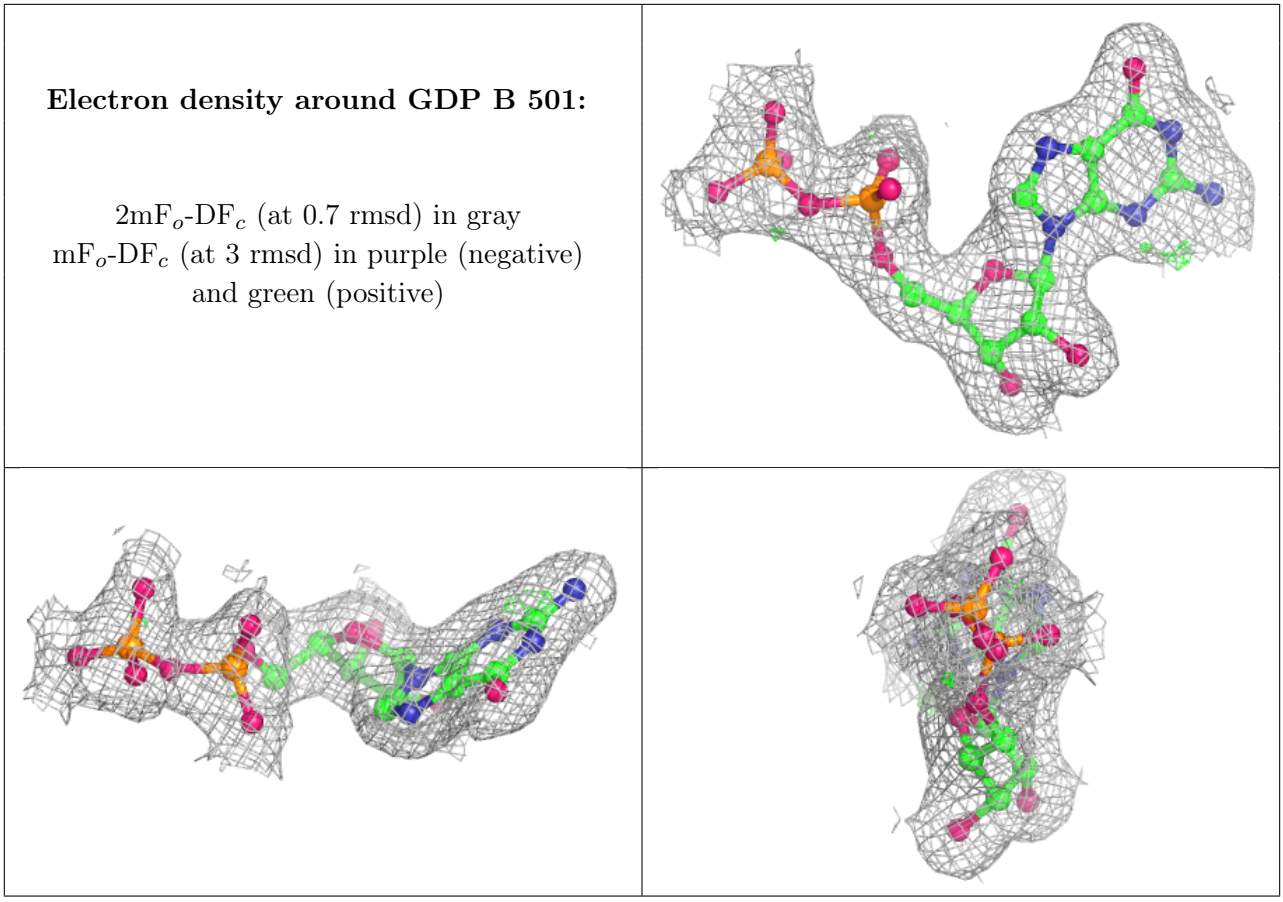






Electron density around GDP B 501:

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



6.5 Other polymers

There are no such residues in this entry.