



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:08 pm BST

PDB ID : 4TV9
Title : Tubulin-PM060184 complex
Authors : Prota, A.E.; Bargsten, K.; Diaz, J.F.; Marsh, M.; Cuevas, C.; Liniger, M.; Neuhaus, C.; Andreu, J.M.; Altmann, K.H.; Steinmetz, M.O.
Deposited on : 2014-06-26
Resolution : 2.00 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 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 : 2.11
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) : 2.11

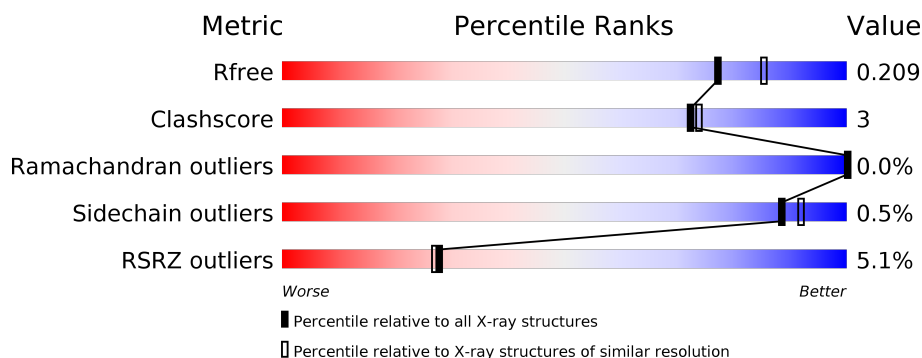
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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 $\leq 5\%$. 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	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> </div>
1	C	451	<div> <div style="width: 90%;"></div> <div style="width: 7%;"></div> <div style="width: 3%;"></div> </div>
2	B	445	<div> <div style="width: 86%;"></div> <div style="width: 9%;"></div> <div style="width: 5%;"></div> </div>
2	D	445	<div> <div style="width: 85%;"></div> <div style="width: 9%;"></div> <div style="width: 5%;"></div> </div>
3	E	143	<div> <div style="width: 80%;"></div> <div style="width: 6%;"></div> <div style="width: 15%;"></div> </div>
4	F	384	<div> <div style="width: 21%;"></div> <div style="width: 76%;"></div> <div style="width: 11%;"></div> <div style="width: 12%;"></div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18487 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	13	0
			3490	2217	587	661	25			
1	C	440	Total	C	N	O	S	0	15	0
			3506	2222	588	672	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	10	0
			3366	2123	566	649	28			
2	D	421	Total	C	N	O	S	0	6	0
			3333	2099	562	644	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	4	0
			1027	634	184	204	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	338	Total	C	N	O	S	0	7	0
			2796	1805	467	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	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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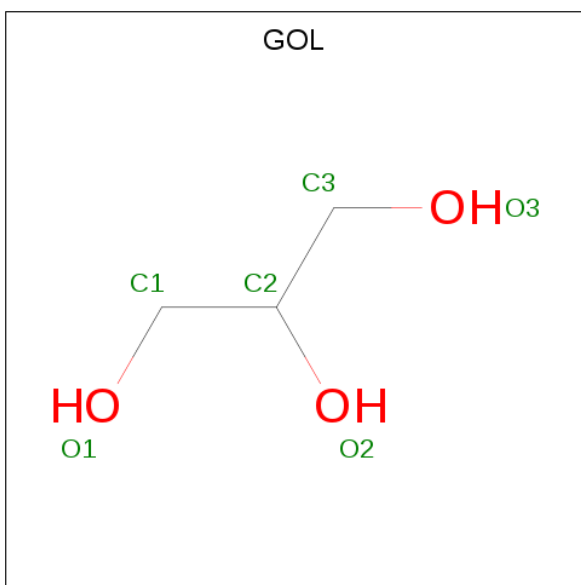
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

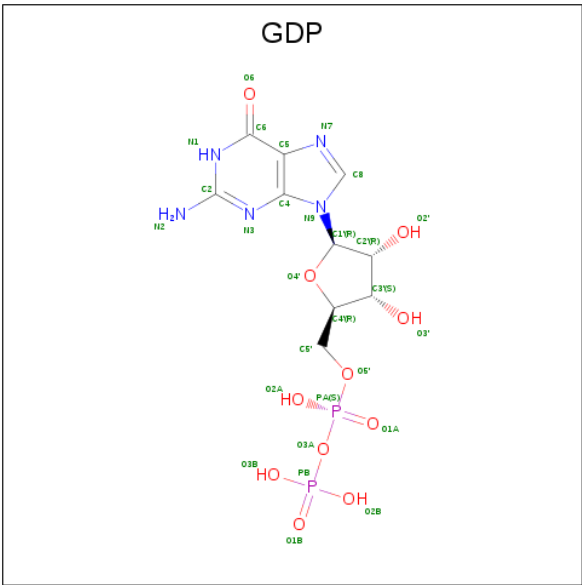
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



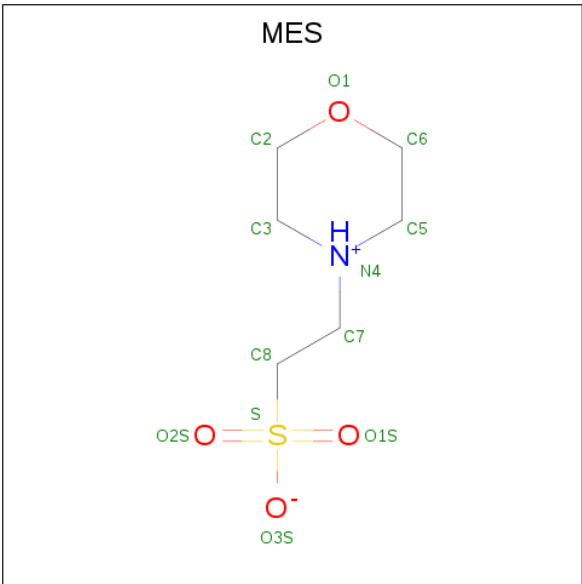
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



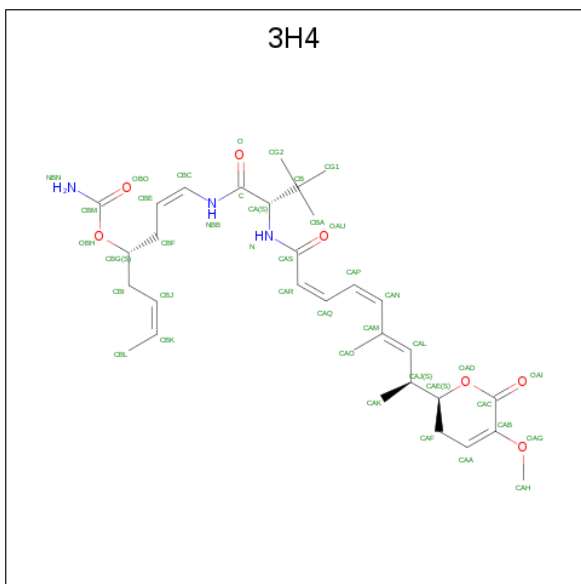
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



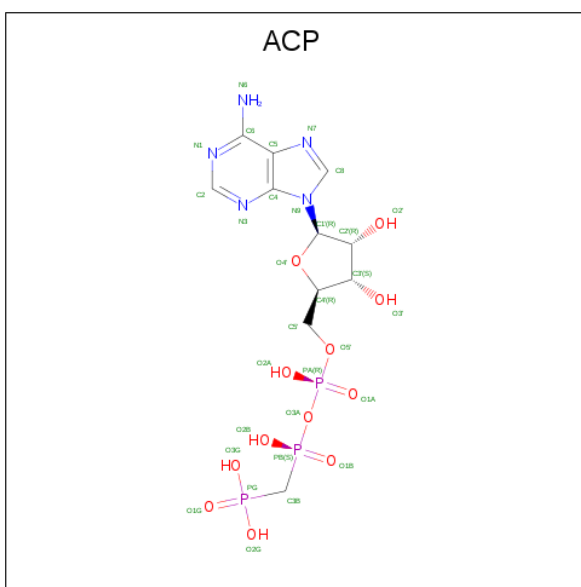
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (1Z,4S,6Z)-1-[(N-{(2Z,4Z,6E,8S)-8-[(2S)-5-methoxy-6-oxo-3,6-dihydro-2H-pyran-2-yl]-6-methylnona-2,4,6-trienoyl}-3-methyl-L-valyl)amino]octa-1,6-dien-4-yl carbamate (three-letter code: 3H4) (formula: C₃₁H₄₅N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			41	31	3	7		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

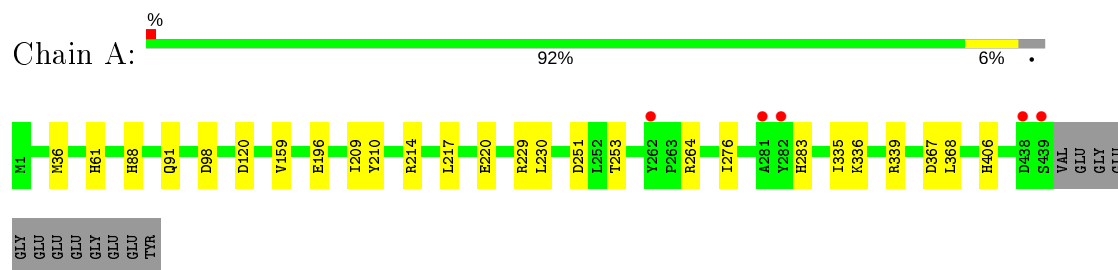
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	143	Total	O	0	0
			143	143		
13	B	134	Total	O	0	0
			134	134		
13	C	245	Total	O	0	0
			245	245		
13	D	119	Total	O	0	0
			119	119		
13	E	42	Total	O	0	0
			42	42		
13	F	63	Total	O	0	0
			63	63		

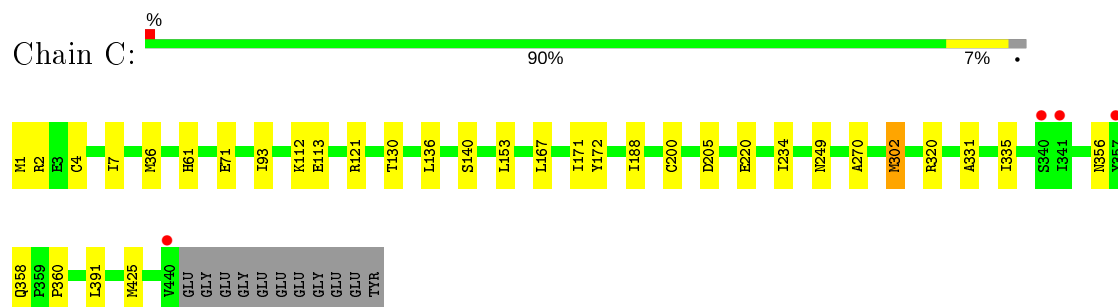
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

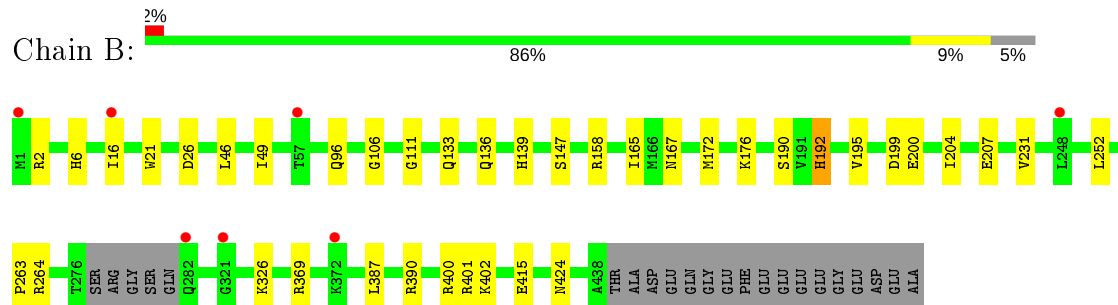
- Molecule 1: Tubulin alpha-1B chain



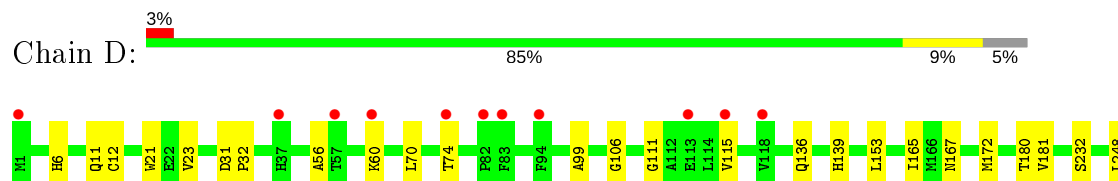
- Molecule 1: Tubulin alpha-1B chain

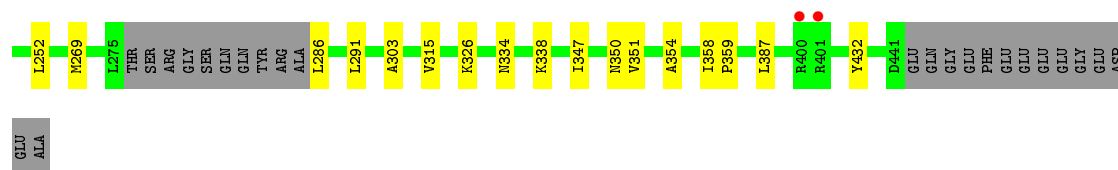


- Molecule 2: Tubulin beta-2B chain

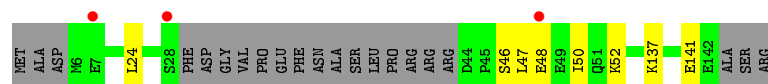
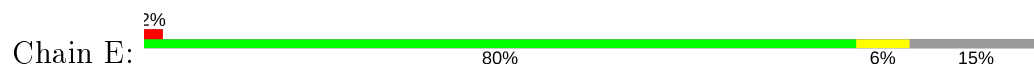


- Molecule 2: Tubulin beta-2B chain

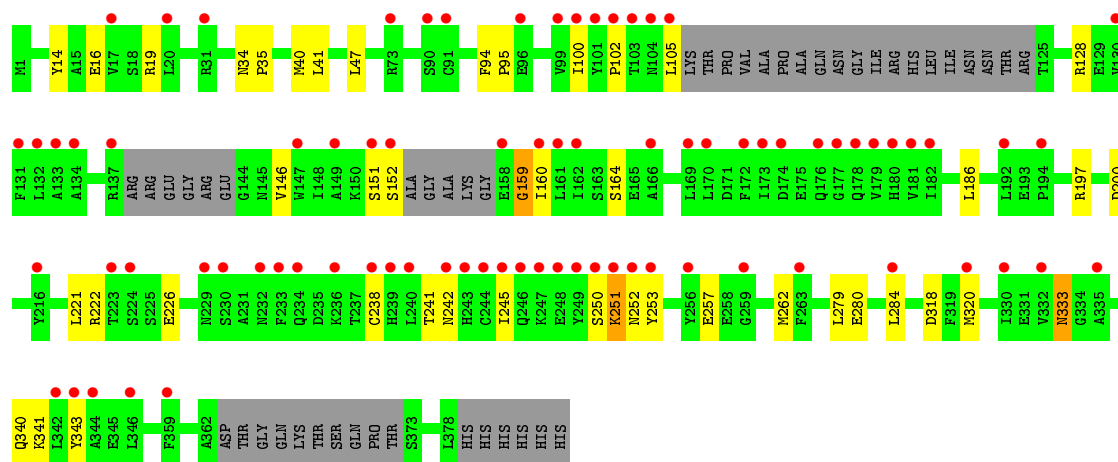
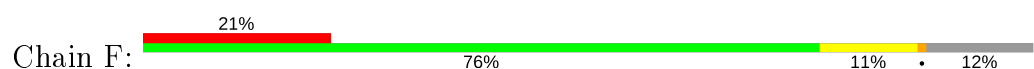




• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.20Å 157.29Å 180.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.04 – 2.00 78.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.04-2.00) 99.9 (78.64-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.180 , 0.208 0.182 , 0.209	Depositor DCC
R_{free} test set	9969 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18487	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, 3H4, CA, GTP, ACP, 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	0.22	0/3607	0.40	0/4897
1	C	0.24	0/3626	0.42	0/4926
2	B	0.23	0/3470	0.39	0/4699
2	D	0.22	0/3424	0.38	0/4640
3	E	0.21	0/1047	0.32	0/1390
4	F	0.21	0/2878	0.38	0/3890
All	All	0.23	0/18052	0.39	0/24442

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	3490	0	3444	16	0
1	C	3506	0	3439	20	0
2	B	3366	0	3273	26	0
2	D	3333	0	3233	26	0
3	E	1027	0	1050	5	0
4	F	2796	0	2799	27	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	C	1	0	0	0	0
8	A	6	0	8	1	0
8	B	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	13	5	0
11	D	41	0	45	10	0
12	F	31	0	14	2	0
13	A	143	0	0	2	0
13	B	134	0	0	1	0
13	C	245	0	0	0	0
13	D	119	0	0	1	0
13	E	42	0	0	0	0
13	F	63	0	0	3	0
All	All	18487	0	17374	120	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 3.

All (120) 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)
11:D:503:3H4:CAQ	11:D:503:3H4:H13	1.80	1.09
11:D:503:3H4:H18	11:D:503:3H4:CAO	1.91	1.00
11:D:503:3H4:H18	11:D:503:3H4:H13	0.95	0.92
2:D:181:VAL:HG12	11:D:503:3H4:CAQ	2.17	0.74
2:B:264:ARG:NH2	2:B:424:ASN:OD1	2.26	0.69
2:D:432:TYR:OH	13:D:719:HOH:O	2.13	0.64
2:D:181:VAL:HG12	11:D:503:3H4:CAR	2.27	0.64
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.81	0.63
11:D:503:3H4:H17	11:D:503:3H4:OAU	1.98	0.62
2:D:180:THR:O	11:D:503:3H4:H40	2.01	0.60
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.50	0.60
1:A:229[B]:ARG:NH1	1:A:367:ASP:OD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.19	0.59
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.68	0.59
1:A:264:ARG:NH1	13:A:698:HOH:O	2.28	0.58
4:F:200:ASP:OD1	4:F:222:ARG:NH2	2.37	0.58
2:B:402:LYS:NZ	2:B:415:GLU:OE2	2.35	0.58
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.85	0.58
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.85	0.58
4:F:333:ASN:ND2	13:F:562:HOH:O	2.37	0.57
2:D:181:VAL:CG1	11:D:503:3H4:CAR	2.83	0.56
4:F:251:LYS:HE2	4:F:253:TYR:HB3	1.88	0.56
4:F:16:GLU:OE2	4:F:19:ARG:NH1	2.39	0.55
2:B:158:ARG:CZ	10:B:503:MES:H21	2.36	0.55
2:B:96:GLN:O	1:C:2:ARG:NH1	2.40	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.91	0.53
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.43	0.52
1:C:356[B]:ASN:ND2	1:C:358[B]:GLN:OE1	2.42	0.52
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.91	0.52
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.91	0.52
1:A:220:GLU:HB3	2:B:326:LYS:HD3	1.92	0.51
2:B:199:ASP:OD2	10:B:503:MES:H52	2.11	0.51
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.92	0.51
1:C:234:ILE:HG21	1:C:302:MET:SD	2.51	0.51
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.44	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.28	0.51
2:B:199:ASP:OD1	10:B:503:MES:H32	2.11	0.51
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.92	0.50
2:D:286:LEU:HD21	2:D:291:LEU:HD13	1.93	0.50
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.92	0.50
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.93	0.50
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.52	0.50
8:A:504:GOL:O1	10:B:503:MES:O1S	2.22	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.49
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.47	0.49
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.45	0.49
2:D:334:ASN:OD1	2:D:338:LYS:NZ	2.32	0.49
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.96	0.48
4:F:159:GLY:H	4:F:160:ILE:HD12	1.78	0.48
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.96	0.48
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.96	0.48
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:VAL:HG21	2:D:232:SER:HB3	1.96	0.47
4:F:242:ASN:HB2	4:F:245:ILE:HG13	1.96	0.47
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.97	0.47
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.47	0.47
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.97	0.46
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.98	0.46
1:A:196:GLU:OE2	13:A:698:HOH:O	2.20	0.46
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.97	0.46
2:B:26:ASP:OD1	2:B:369:ARG:NH1	2.48	0.45
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.99	0.45
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.98	0.45
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.51	0.45
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.99	0.44
1:A:276:ILE:HD13	1:A:283:HIS:NE2	2.32	0.44
2:D:358:ILE:HA	2:D:359:PRO:HD3	1.78	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.00	0.44
1:A:159:VAL:HG11	3:E:47:LEU:HB2	2.00	0.44
4:F:226:GLU:HB2	4:F:238:CYS:HB3	2.00	0.44
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.36	0.44
2:D:136:GLN:HA	2:D:167:ASN:O	2.18	0.44
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.43
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.43
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.31	0.43
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.99	0.43
4:F:40:MET:HE2	4:F:47:LEU:HG	2.00	0.43
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.99	0.43
1:C:220:GLU:HB2	2:D:326:LYS:HD3	2.00	0.43
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.01	0.43
1:C:1:MET:HB3	1:C:130:THR:OG1	2.18	0.43
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.01	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
1:A:251:ASP:OD1	1:A:253:THR:OG1	2.30	0.42
3:E:48:GLU:HG2	3:E:52:LYS:HE2	2.01	0.42
2:D:11:GLN:HA	2:D:74:THR:HG21	2.00	0.42
2:D:56:ALA:HB3	2:D:60:LYS:HB3	2.01	0.42
4:F:151:SER:OG	4:F:152:SER:N	2.52	0.42
2:B:136:GLN:HA	2:B:167:ASN:O	2.20	0.42
3:E:137:LYS:O	3:E:141:GLU:HG2	2.19	0.42
2:B:192:HIS:O	2:B:195[B]:VAL:HG22	2.19	0.42
4:F:146:VAL:HG22	4:F:164:SER:HB3	2.00	0.42
2:D:181:VAL:CG1	11:D:503:3H4:CAQ	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.50	0.41
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.01	0.41
2:B:158:ARG:HG3	10:B:503:MES:H62	2.01	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.41
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.02	0.41
4:F:34:ASN:HA	4:F:35:PRO:HD3	1.83	0.41
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.01	0.41
11:D:503:3H4:CAP	11:D:503:3H4:OAU	2.68	0.41
4:F:14:TYR:OH	13:F:519:HOH:O	2.20	0.41
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.95	0.41
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.56	0.41
2:D:115:VAL:HG23	2:D:153:LEU:HD23	2.01	0.41
4:F:242:ASN:HD21	12:F:401:ACP:H5'2	1.85	0.41
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.56	0.41
1:A:406:HIS:CD2	2:B:263:PRO:HG3	2.56	0.41
2:B:390:ARG:NE	13:B:701:HOH:O	2.54	0.41
2:B:46:LEU:HA	2:B:49:ILE:HB	2.03	0.41
1:C:320:ARG:HG3	1:C:360:PRO:HG3	2.03	0.41
4:F:341:LYS:NZ	13:F:554:HOH:O	2.54	0.41
4:F:221:LEU:HB2	4:F:262:MET:HB3	2.02	0.40
3:E:46:SER:O	3:E:50:ILE:HG12	2.22	0.40
4:F:250:SER:O	4:F:251:LYS:HD2	2.22	0.40
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.21	0.40
1:C:331:ALA:O	1:C:335:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	450/451 (100%)	442 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	453/451 (100%)	446 (98%)	7 (2%)	0	100	100
2	B	429/445 (96%)	421 (98%)	8 (2%)	0	100	100
2	D	423/445 (95%)	415 (98%)	8 (2%)	0	100	100
3	E	122/143 (85%)	121 (99%)	1 (1%)	0	100	100
4	F	335/384 (87%)	320 (96%)	14 (4%)	1 (0%)	41	37
All	All	2212/2319 (95%)	2165 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	159	GLY

5.3.2 Protein sidechains ⓘ

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	383/379 (101%)	382 (100%)	1 (0%)	92	95
1	C	386/379 (102%)	384 (100%)	2 (0%)	88	92
2	B	375/383 (98%)	373 (100%)	2 (0%)	88	92
2	D	370/383 (97%)	369 (100%)	1 (0%)	92	95
3	E	114/127 (90%)	114 (100%)	0	100	100
4	F	312/342 (91%)	309 (99%)	3 (1%)	76	81
All	All	1940/1993 (97%)	1931 (100%)	9 (0%)	88	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASP
2	B	139	HIS
2	B	192	HIS
1	C	71	GLU
1	C	302	MET

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Mol	Chain	Res	Type
2	D	139	HIS
4	F	251	LYS
4	F	252	ASN
4	F	333	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	136	GLN
2	B	167	ASN
4	F	180	HIS
4	F	183	GLN
4	F	243	HIS
4	F	252	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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
12	ACP	F	401	6	27,33,33	1.65	6 (22%)	32,52,52	1.40	4 (12%)
8	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.36	0
10	MES	B	503	-	12,12,12	2.29	1 (8%)	14,16,16	1.27	1 (7%)
11	3H4	D	503	-	40,41,41	0.96	1 (2%)	48,54,54	1.32	9 (18%)
9	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.95	7 (22%)
8	GOL	B	504	-	5,5,5	0.38	0	5,5,5	0.26	0
5	GTP	A	501	6	26,34,34	1.15	2 (7%)	33,54,54	1.91	7 (21%)
9	GDP	B	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.86	6 (19%)
5	GTP	C	501	6	26,34,34	1.14	2 (7%)	33,54,54	1.86	7 (21%)

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
12	ACP	F	401	6	-	6/15/38/38	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	3H4	D	503	-	-	2/46/59/59	0/1/1/1
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3
8	GOL	B	504	-	-	2/4/4/4	-
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.70	1.66	1.77
9	D	501	GDP	C6-C5	4.14	1.48	1.41
5	A	501	GTP	C6-C5	4.09	1.48	1.41
12	F	401	ACP	PB-O1B	4.08	1.61	1.51
5	C	501	GTP	C6-C5	4.05	1.48	1.41
9	B	501	GDP	C6-C5	3.92	1.48	1.41
12	F	401	ACP	PB-O2B	-3.37	1.48	1.56
12	F	401	ACP	PB-O3A	2.84	1.61	1.58
12	F	401	ACP	PG-O3G	2.83	1.61	1.54
12	F	401	ACP	PG-O2G	2.82	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	C5-C4	2.53	1.47	1.40
11	D	503	3H4	OAD-CAE	-2.49	1.43	1.46
9	D	501	GDP	C5-C4	2.43	1.47	1.40
5	A	501	GTP	C5-C4	2.36	1.47	1.40
5	C	501	GTP	C5-C4	2.34	1.47	1.40
9	B	501	GDP	C5-C4	2.25	1.46	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	4.91	120.96	115.36
9	D	501	GDP	C2-N3-C4	4.82	120.87	115.36
5	A	501	GTP	C2-N3-C4	4.82	120.86	115.36
9	B	501	GDP	C2-N3-C4	4.42	120.40	115.36
5	A	501	GTP	C6-N1-C2	4.29	122.74	115.93
9	B	501	GDP	C6-C5-C4	-4.28	116.71	120.80
9	B	501	GDP	C6-N1-C2	4.15	122.53	115.93
5	A	501	GTP	C6-C5-C4	-4.13	116.86	120.80
5	C	501	GTP	C6-N1-C2	4.09	122.42	115.93
9	D	501	GDP	C6-N1-C2	4.08	122.42	115.93
9	D	501	GDP	C6-C5-C4	-4.08	116.91	120.80
5	C	501	GTP	C5-C6-N1	-4.02	117.94	123.43
5	A	501	GTP	C5-C6-N1	-4.01	117.94	123.43
9	D	501	GDP	C5-C6-N1	-3.92	118.07	123.43
9	B	501	GDP	C5-C6-N1	-3.91	118.08	123.43
5	C	501	GTP	C6-C5-C4	-3.84	117.13	120.80
12	F	401	ACP	PA-O3A-PB	-3.70	120.84	132.56
5	A	501	GTP	N3-C2-N1	-3.58	122.44	127.22
5	C	501	GTP	N3-C2-N1	-3.45	122.63	127.22
9	D	501	GDP	N3-C2-N1	-3.35	122.75	127.22
9	B	501	GDP	N3-C2-N1	-3.35	122.75	127.22
12	F	401	ACP	C3'-C2'-C1'	3.34	106.00	100.98
12	F	401	ACP	N3-C2-N1	-3.15	123.75	128.68
11	D	503	3H4	OAU-CAS-N	-3.12	118.22	122.35
11	D	503	3H4	OAG-CAB-CAA	-2.99	121.42	126.40
11	D	503	3H4	O-C-NBB	-2.85	120.31	123.68
11	D	503	3H4	CB-CA-C	-2.79	110.19	112.81
9	D	501	GDP	PA-O3A-PB	-2.75	123.40	132.83
12	F	401	ACP	C4-C5-N7	-2.68	106.61	109.40
9	D	501	GDP	C4-C5-N7	-2.61	106.68	109.40
10	B	503	MES	O3S-S-C8	2.53	109.85	105.77
5	C	501	GTP	C4-C5-N7	-2.49	106.81	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C4-C5-N7	-2.43	106.87	109.40
11	D	503	3H4	CAH-OAG-CAB	-2.35	112.62	116.96
11	D	503	3H4	OAD-CAE-CAJ	2.34	110.57	105.72
9	B	501	GDP	C4-C5-N7	-2.34	106.97	109.40
11	D	503	3H4	OBH-CBM-NBN	2.21	114.01	110.58
5	A	501	GTP	PA-O3A-PB	-2.17	125.36	132.83
11	D	503	3H4	CBG-CBF-CBE	-2.05	110.18	114.98
5	C	501	GTP	PA-O3A-PB	-2.04	125.82	132.83
11	D	503	3H4	OAG-CAB-CAC	2.02	115.74	111.75

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O2G
12	F	401	ACP	PB-C3B-PG-O3G
12	F	401	ACP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O3A
10	B	503	MES	C8-C7-N4-C5
11	D	503	3H4	CAR-CAS-N-CA
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
8	B	504	GOL	O1-C1-C2-C3
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	504	GOL	O1-C1-C2-O2
8	A	504	GOL	O1-C1-C2-O2
9	D	501	GDP	C5'-O5'-PA-O3A
8	A	504	GOL	O1-C1-C2-C3
12	F	401	ACP	C5'-O5'-PA-O1A
11	D	503	3H4	CAM-CAN-CAP-CAQ
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A

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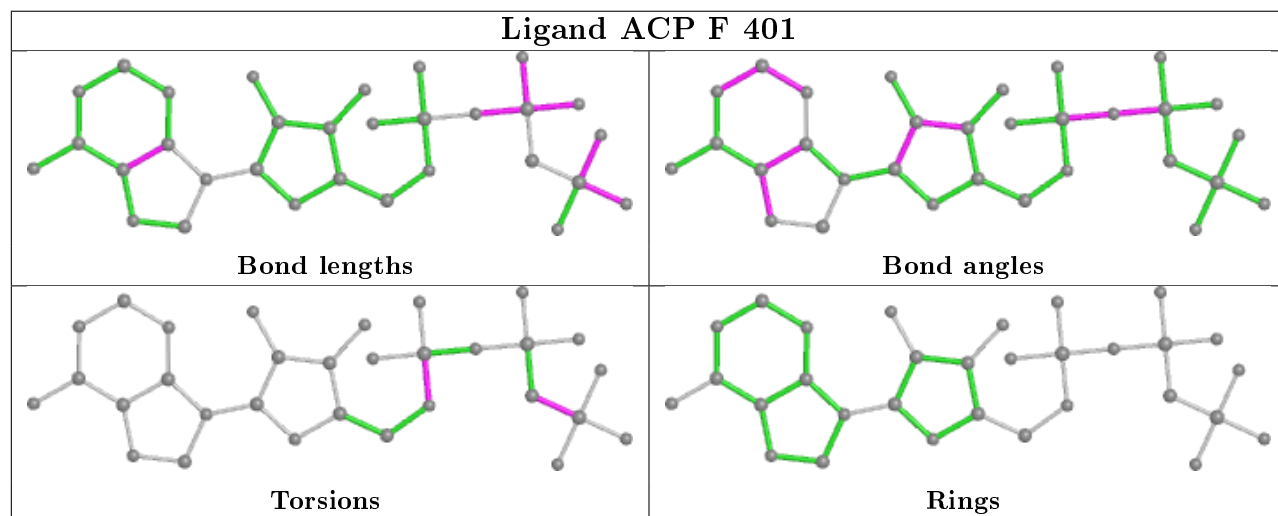
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O1G

There are no ring outliers.

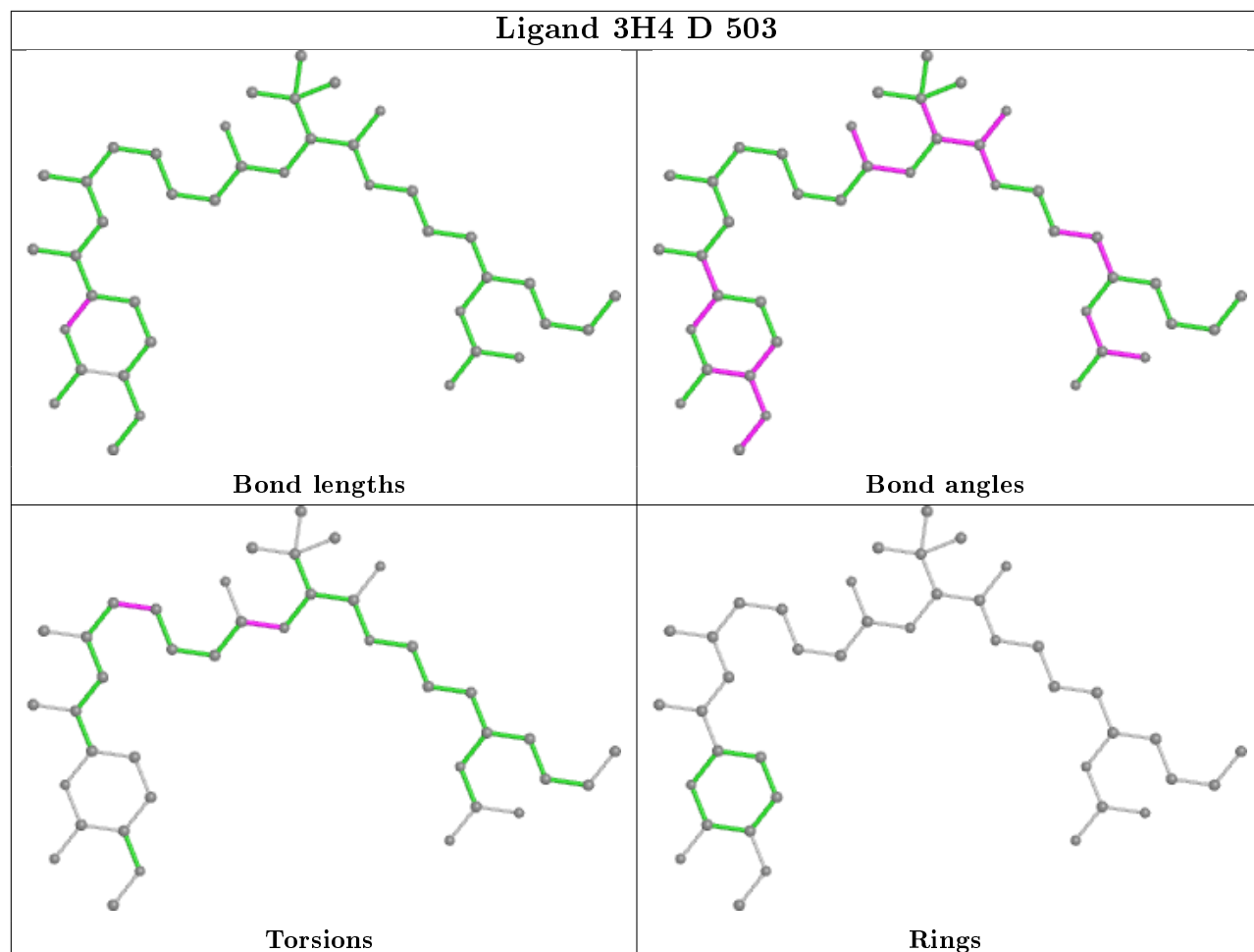
6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	2	0
8	A	504	GOL	1	0
10	B	503	MES	5	0
11	D	503	3H4	10	0
9	D	501	GDP	1	0
5	A	501	GTP	1	0

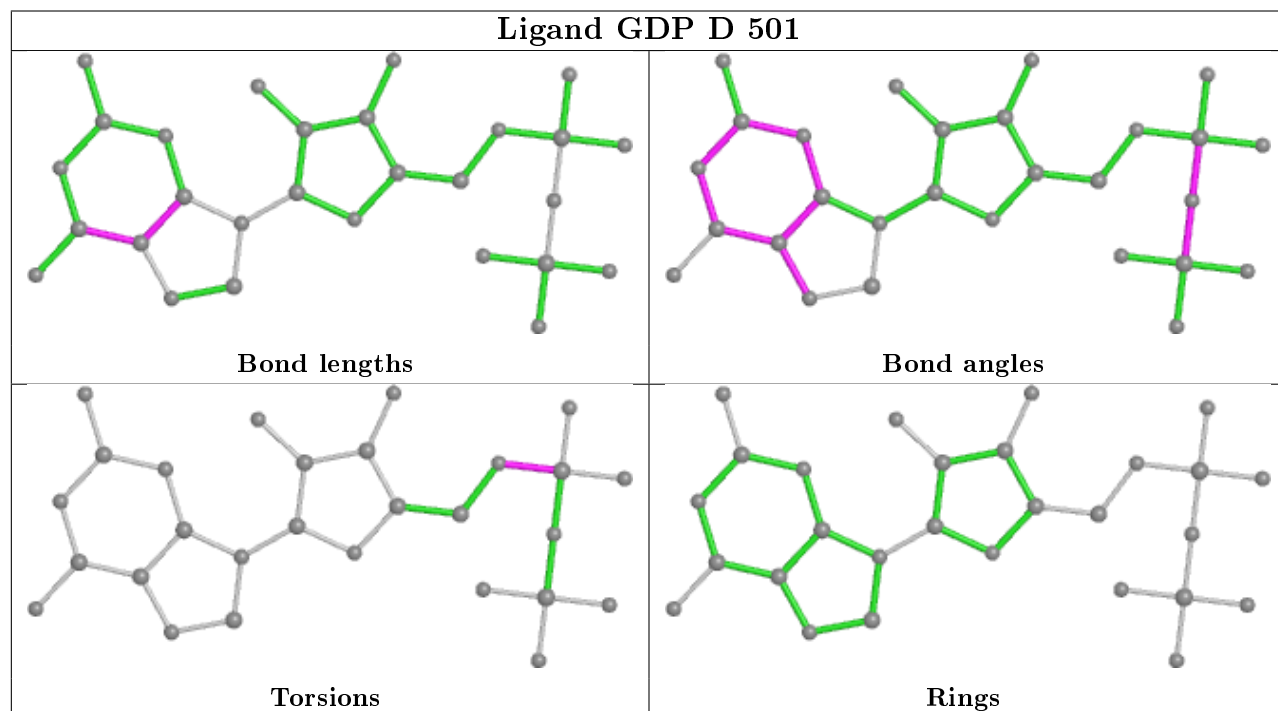
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

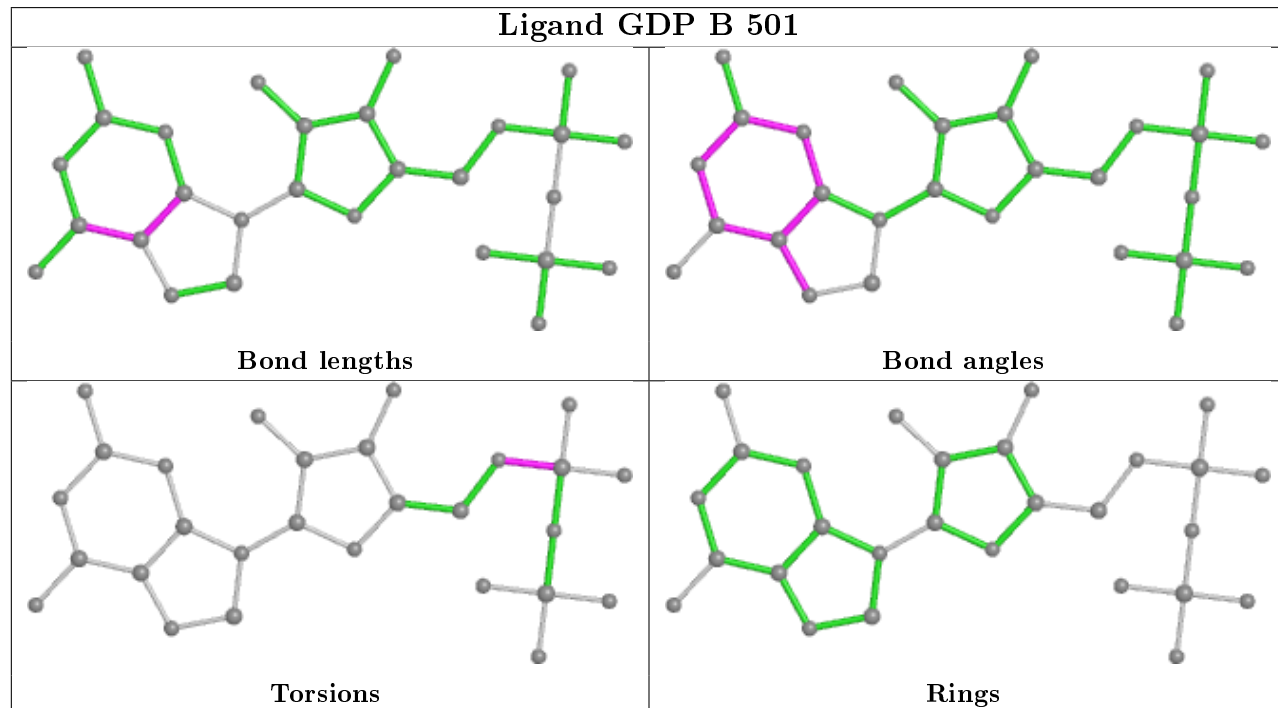
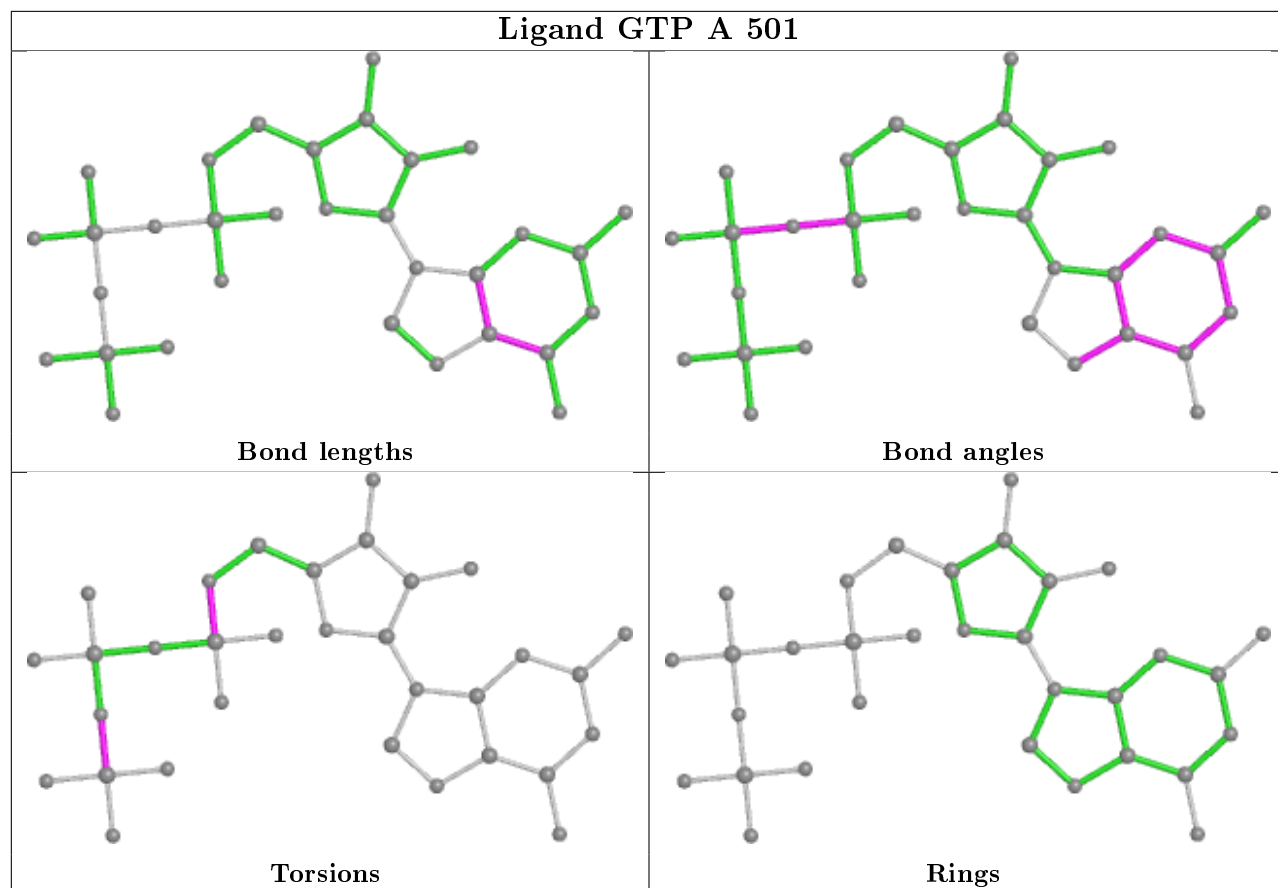


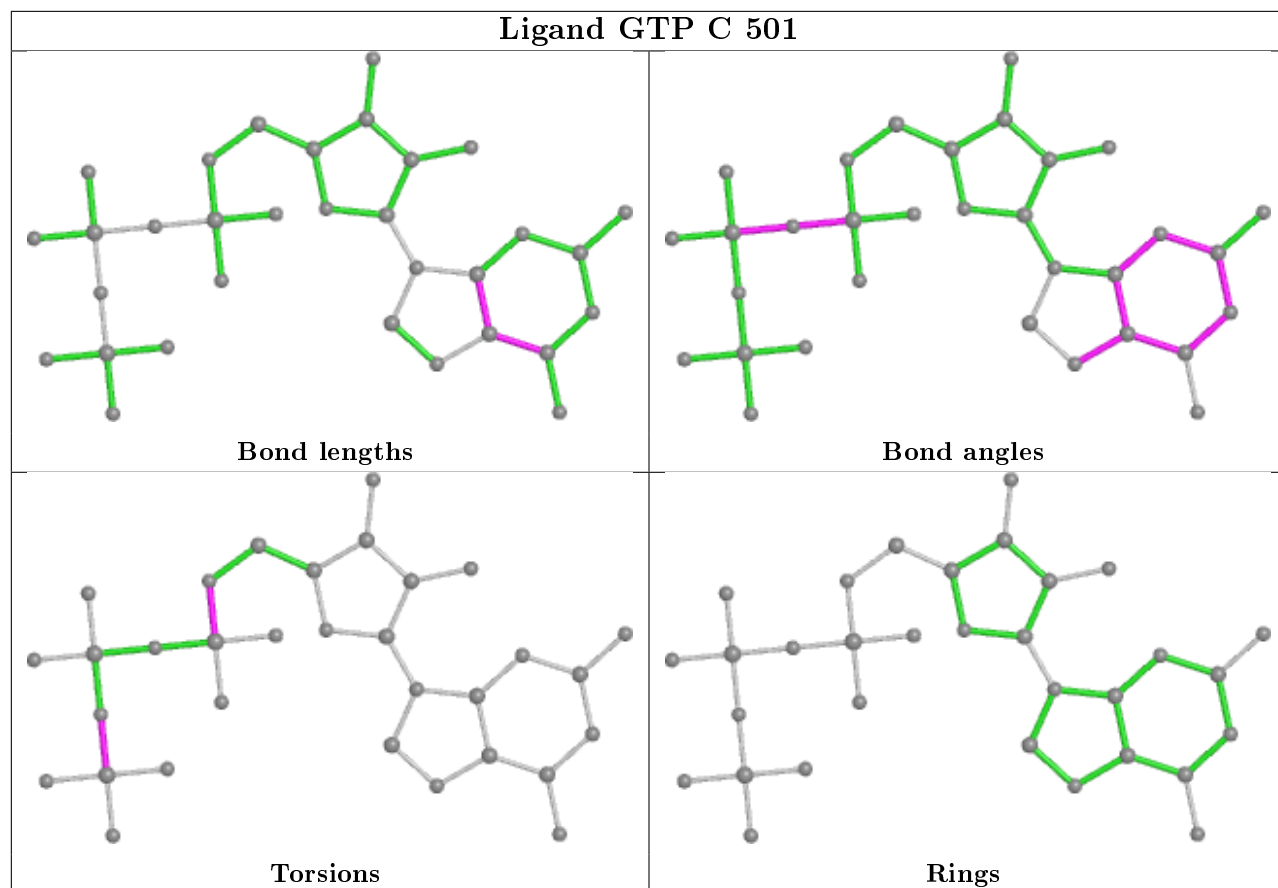
Ligand 3H4 D 503



Ligand GDP D 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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	0.19	5 (1%)	80 79	35, 56, 91, 137	0
1	C	440/451 (97%)	0.38	4 (0%)	84 83	30, 43, 68, 115	0
2	B	423/445 (95%)	0.37	7 (1%)	70 68	33, 53, 90, 139	2 (0%)
2	D	421/445 (94%)	0.28	13 (3%)	49 48	37, 60, 90, 114	5 (1%)
3	E	122/143 (85%)	0.57	3 (2%)	57 56	40, 69, 108, 124	0
4	F	338/384 (88%)	1.30	80 (23%)	0 0	45, 78, 145, 175	0
All	All	2183/2319 (94%)	0.47	112 (5%)	28 27	30, 56, 104, 175	7 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	8.3
1	A	439	SER	7.1
4	F	177	GLY	6.3
4	F	232	ASN	6.3
4	F	248	GLU	6.2
2	B	1	MET	6.1
4	F	161	LEU	5.8
4	F	233	PHE	5.7
4	F	244	CYS	5.7
4	F	245	ILE	5.7
4	F	253	TYR	5.6
4	F	173	ILE	5.4
4	F	176	GLN	5.2
4	F	130	VAL	5.1
4	F	182	ILE	5.1
4	F	251	LYS	5.0
4	F	320	MET	4.8
4	F	181	VAL	4.6
4	F	100	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	178	GLN	4.4
2	B	57	THR	4.4
4	F	179	VAL	4.4
4	F	169	LEU	4.3
4	F	236	LYS	4.3
4	F	99	VAL	4.3
4	F	103	THR	4.0
4	F	234	GLN	4.0
4	F	240	LEU	3.9
4	F	344	ALA	3.8
4	F	20	LEU	3.7
4	F	250	SER	3.7
2	B	248	LEU	3.6
4	F	105	LEU	3.5
4	F	239	HIS	3.4
4	F	242	ASN	3.4
2	D	1	MET	3.3
1	A	262	TYR	3.3
4	F	152	SER	3.3
4	F	160	ILE	3.3
4	F	342	LEU	3.3
2	D	83	PHE	3.2
4	F	149	ALA	3.2
4	F	151	SER	3.2
4	F	162	ILE	3.2
4	F	17	VAL	3.1
4	F	147	TRP	2.9
4	F	166	ALA	2.9
1	C	340	SER	2.9
4	F	102	PRO	2.9
4	F	238	CYS	2.9
4	F	335	ALA	2.9
4	F	192	LEU	2.9
4	F	343	TYR	2.8
4	F	284[A]	LEU	2.8
4	F	158	GLU	2.8
1	A	282	TYR	2.8
4	F	247	LYS	2.8
1	A	281	ALA	2.7
3	E	7	GLU	2.7
4	F	90	SER	2.6
4	F	224	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	2.6
1	A	438	ASP	2.6
4	F	134	ALA	2.6
2	D	94	PHE	2.6
3	E	48	GLU	2.6
4	F	133	ALA	2.6
2	D	82	PRO	2.6
3	E	28	SER	2.5
4	F	101	TYR	2.5
4	F	174	ASP	2.5
4	F	216	TYR	2.5
4	F	259	GLY	2.5
4	F	246	GLN	2.5
2	D	57	THR	2.4
4	F	346	LEU	2.4
4	F	104	ASN	2.4
4	F	330	ILE	2.4
4	F	137	ARG	2.4
4	F	194	PRO	2.4
4	F	252	ASN	2.4
4	F	263	PHE	2.4
2	D	401	ARG	2.3
1	C	357	TYR	2.3
4	F	91	CYS	2.3
4	F	132	LEU	2.3
4	F	96	GLU	2.3
2	D	118	VAL	2.3
4	F	31	ARG	2.3
1	C	341	ILE	2.3
2	D	60	LYS	2.2
2	D	115	VAL	2.2
4	F	172	PHE	2.2
4	F	73	ARG	2.2
4	F	223	THR	2.2
4	F	229	ASN	2.2
2	B	372	LYS	2.2
1	C	440	VAL	2.2
2	B	321	GLY	2.2
2	B	16[A]	ILE	2.1
2	D	37	HIS	2.1
2	D	400	ARG	2.1
4	F	359	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	180	HIS	2.1
4	F	243	HIS	2.1
2	B	282	GLN	2.0
2	D	113	GLU	2.0
4	F	256	TYR	2.0
4	F	332	VAL	2.0
4	F	230	SER	2.0
2	D	74	THR	2.0
4	F	170	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 carbohydrates 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
6	MG	F	402	1/1	0.61	0.10	74,74,74,74	0
8	GOL	A	504	6/6	0.83	0.13	67,85,89,92	0
8	GOL	B	504	6/6	0.84	0.23	80,81,82,84	0
10	MES	B	503	12/12	0.90	0.17	63,73,86,91	0
6	MG	D	502	1/1	0.91	0.07	52,52,52,52	0
11	3H4	D	503	41/41	0.91	0.17	55,73,81,83	0
12	ACP	F	401	31/31	0.92	0.17	69,82,127,162	0
6	MG	A	502	1/1	0.92	0.10	38,38,38,38	0
9	GDP	D	501	28/28	0.94	0.15	48,57,65,71	0
6	MG	C	502	1/1	0.94	0.10	34,34,34,34	0
7	CA	A	503	1/1	0.96	0.08	72,72,72,72	0
5	GTP	A	501	32/32	0.98	0.14	31,40,43,57	0
5	GTP	C	501	32/32	0.98	0.15	28,34,36,38	0
7	CA	C	503	1/1	0.99	0.11	56,56,56,56	0

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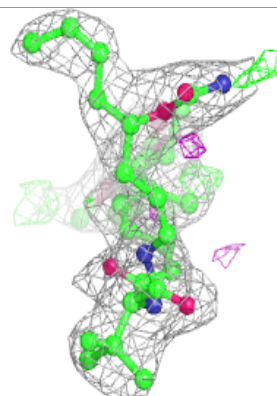
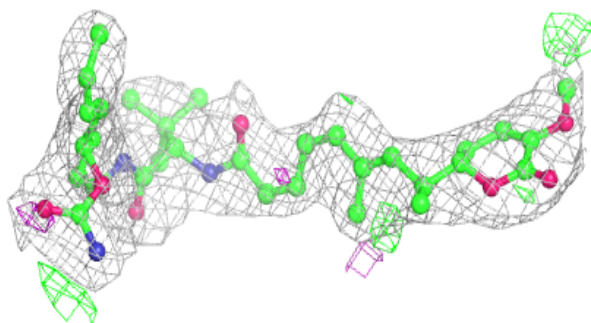
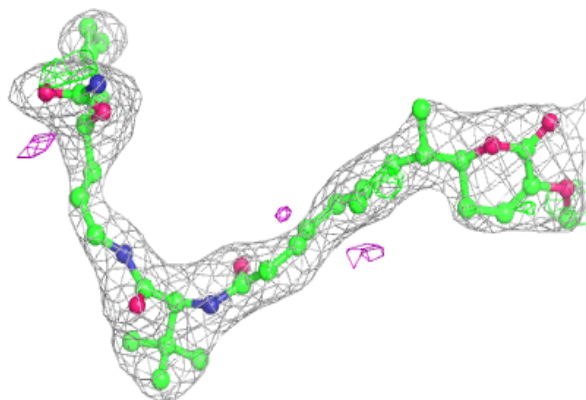
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	GDP	B	501	28/28	0.99	0.15	30,36,40,42	0
6	MG	B	502	1/1	0.99	0.18	30,30,30,30	0

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.

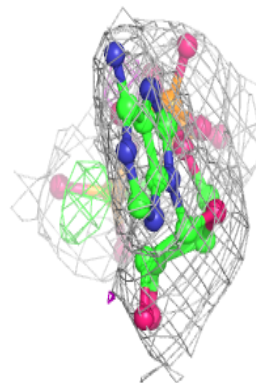
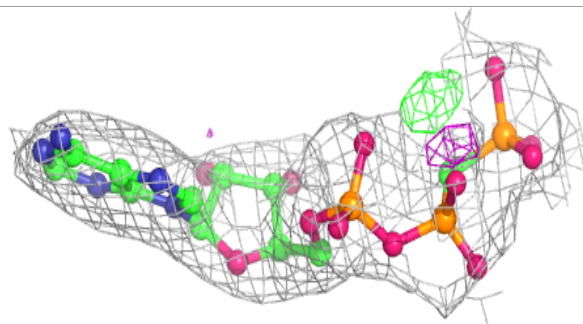
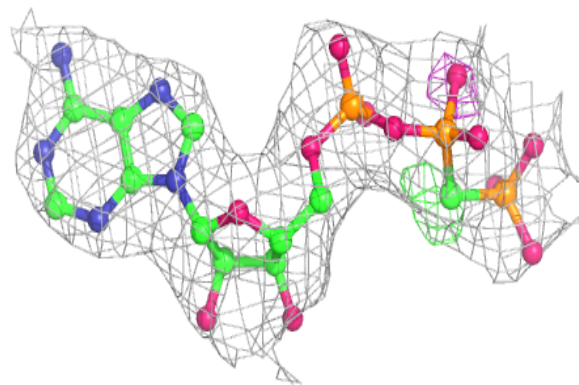
Electron density around 3H4 D 503:

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

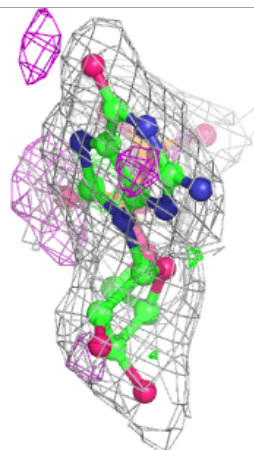
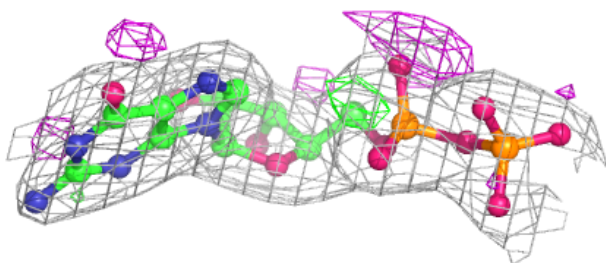
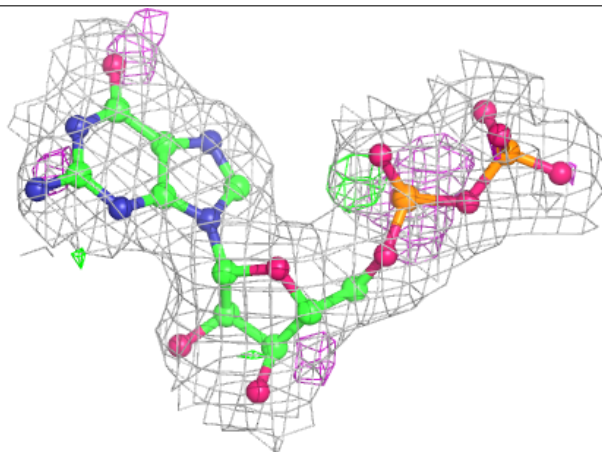


Electron density around ACP F 401:

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

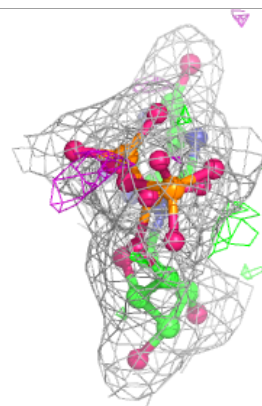
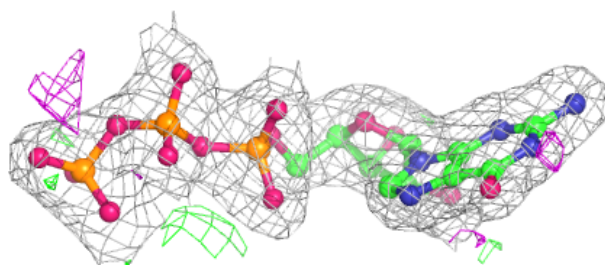
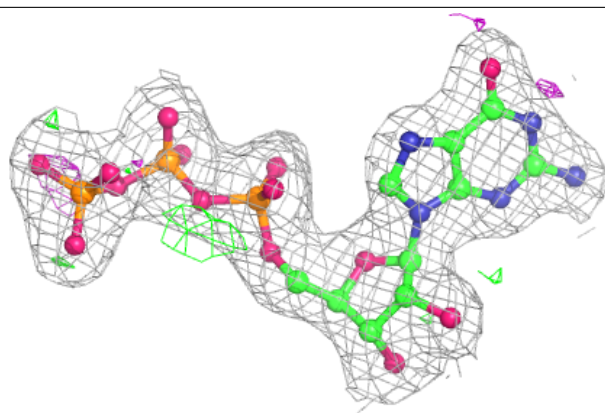
**Electron density around GDP D 501:**

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

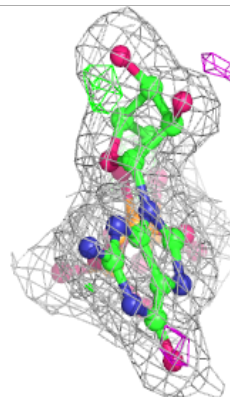
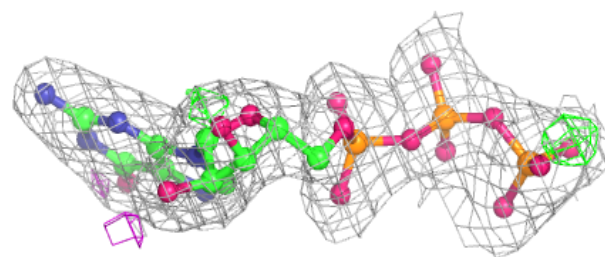
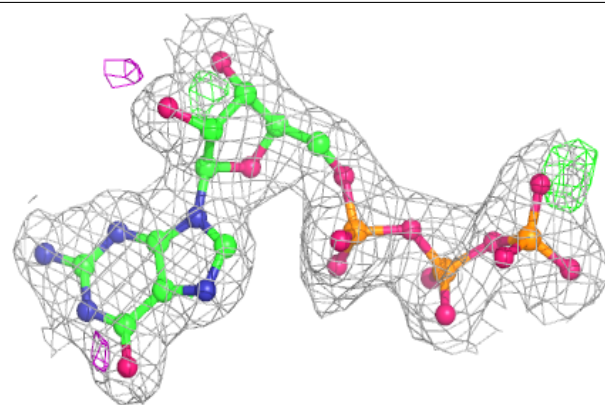


Electron density around GTP A 501:

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

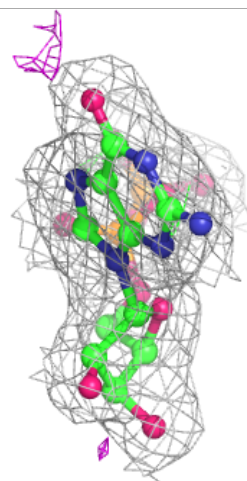
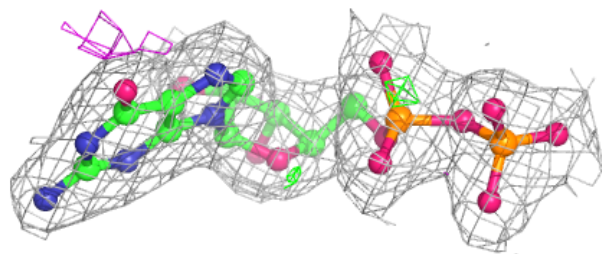
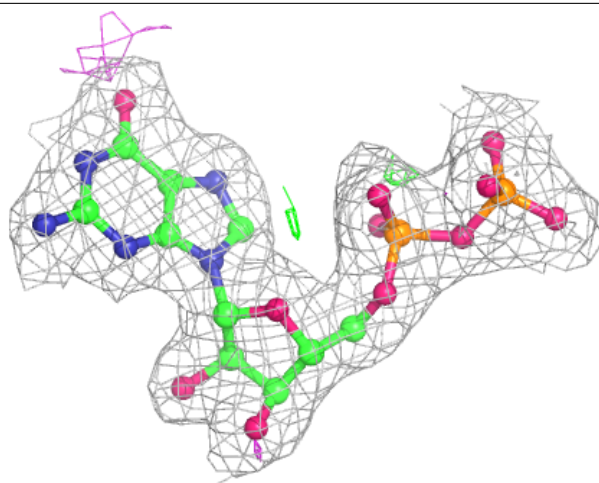
**Electron density around GTP C 501:**

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



Electron density around GDP B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.