Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 04:57 AM EDT

PDB ID	:	4I4T
Title	:	Crystal structure of tubulin-RB3-TTL-Zampanolide complex
Authors	:	Prota, A.E.; Steinmetz, M.O.
Deposited on	:	2012-11-28
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

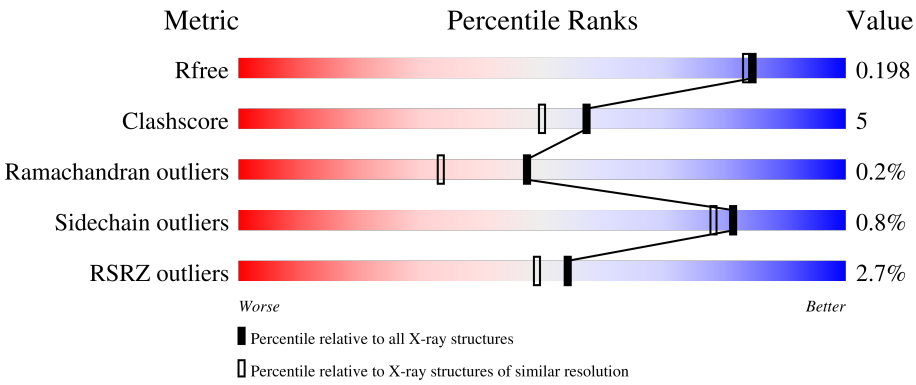
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	450	2%, 89%, 10%, •
1	C	450	87%, 10%, •
2	B	445	.%, 82%, 12%, 6%
2	D	445	2%, 88%, 9%, •
3	E	143	.%, 77%, 9%, 14%

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Mol	Chain	Length	Quality of chain
4	F	384	8% 84% 9% 7%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 37713 atoms, of which 17968 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	447	7106	2266	3537	599	679	25	0	17	0
1	C	440	7045	2249	3503	588	678	27	0	24	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	420	6753	2149	3350	569	656	29	0	22	0
2	D	431	6752	2151	3330	580	662	29	0	8	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	123	2131	649	1082	188	206	6	0	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

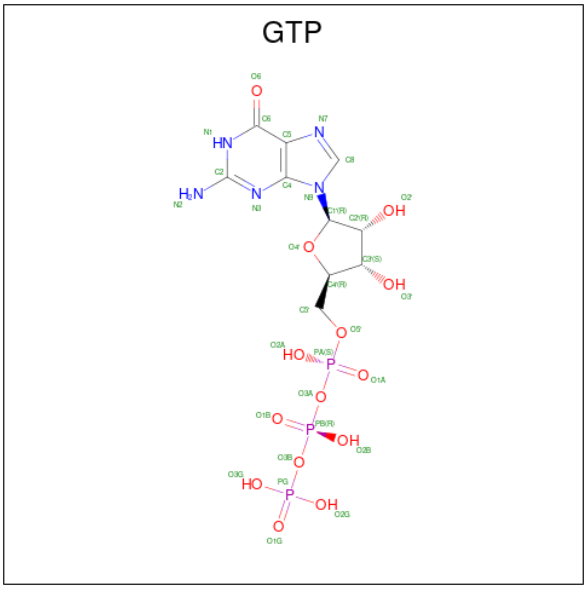
- Molecule 4 is a protein called Tubulin Tyrosine ligase, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	357	5964	1914	2991	508	536	15	0	11	0

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
			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	2	2	2	0	0

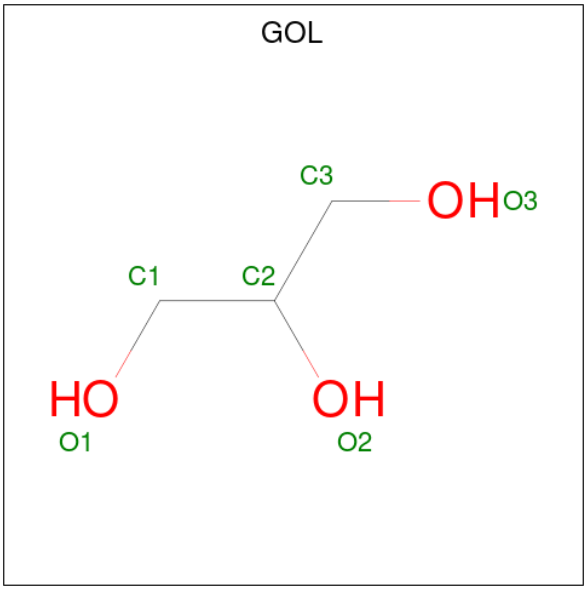
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

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



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

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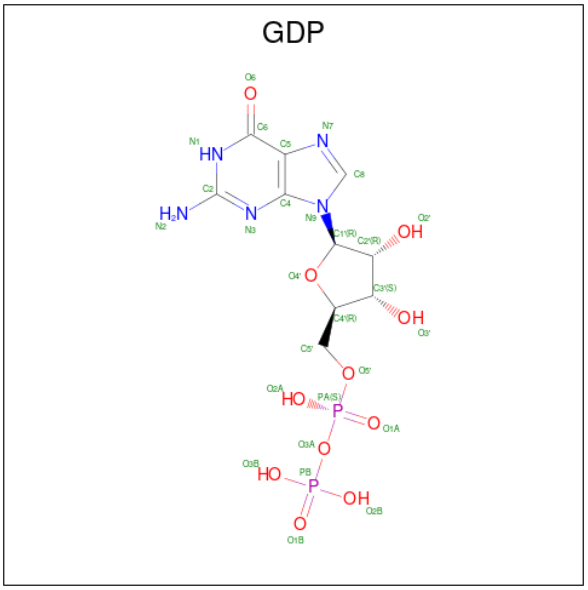
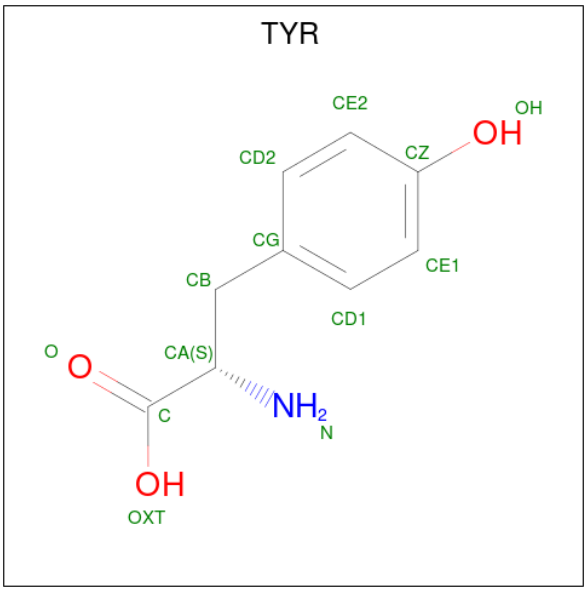
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	A	1	14	3	8	3	0	0
			Total	C	H	O		
9	B	1	14	3	8	3	0	0
			Total	C	H	O		
9	B	1	14	3	8	3	0	0
			Total	C	H	O		
9	F	1	14	3	8	3	0	0
			Total	C	H	O		
9	F	1	14	3	8	3	0	0

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



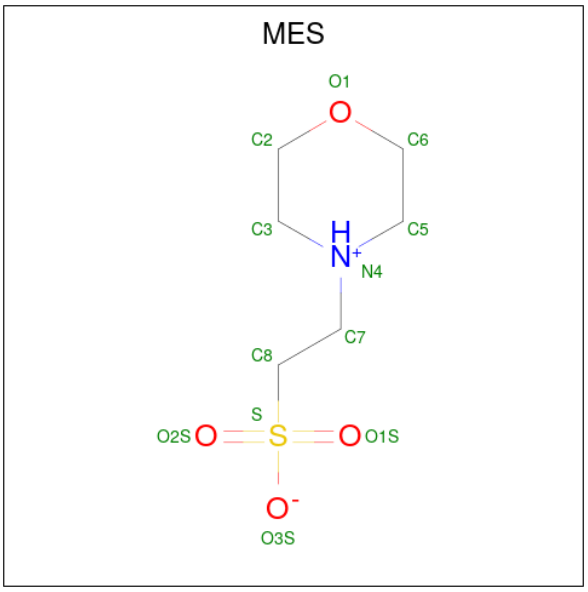
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
10	B	1	38	10	10	5	11	2	0	0
			Total	C	H	N	O	P		
10	D	1	38	10	10	5	11	2	0	0

- Molecule 11 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
11	B	1	24	9	11	1	3	0	0

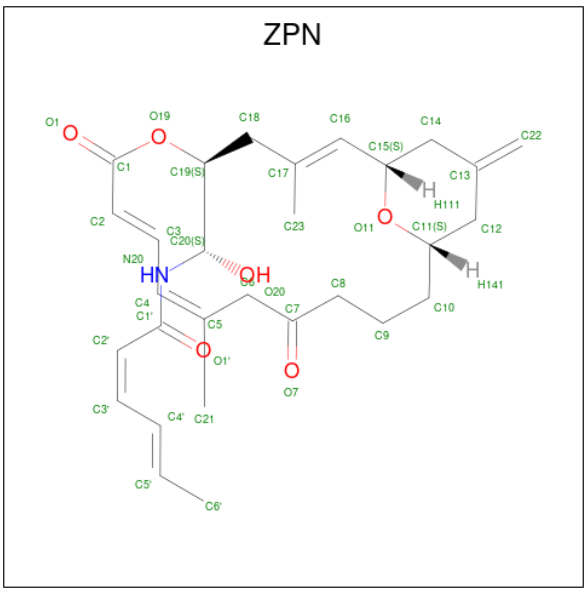
- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
12	B	1	25	6	13	1	4	1	0	0

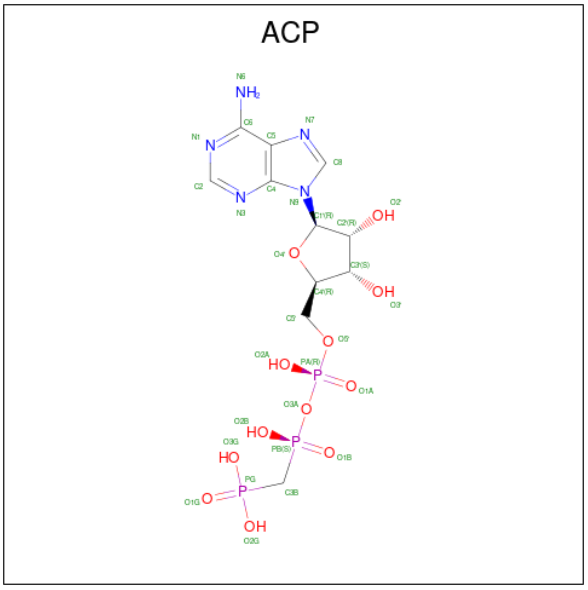
- Molecule 13 is (2Z,4E)-N-[(S)-[(1S,2E,5S,8E,10Z,17S)-3,11-dimethyl-19-methylidene-7,13-dioxo-6,21-dioxabicyclo[15.3.1]henicosa-2,8,10-trien-5-yl](hydroxy)methyl]hexa-2,4-dienamide

(three-letter code: ZPN) (formula: $C_{29}H_{39}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
13	D	1	74	29	38	1	6	0	0

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
14	F	1	48	11	17	5	12	3	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	316	316	316	0	0
			Total	O		
15	B	235	235	235	0	0
			Total	O		
15	C	417	417	417	0	0
			Total	O		
15	D	265	265	265	0	0
			Total	O		
15	E	81	81	81	0	0
			Total	O		
15	F	208	208	208	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: 2% 89% 10%

M1 E22 C25 M36 D46 H61 D76 R79 Y83 R84 Q85 L86 F87 H88 P89 E90 N102 R105 R121 H192 I209 R221 R229 L230 I231 V250 E254 N258 A281 Y282 H283 E284 Q285 P298 Q301 M302 Y312

C315 I335 K336 T337 K338 R339 Y357 Q372 T381 K394 E411 G412 M413 F418 A421 V440 E441 G444 GLU GLU GLU G448 E449 E450

• Molecule 1: Tubulin alpha-1B chain

Chain C: 87% 10%

M1 R2 E3 C4 E71 I93 D98 A104 R121 Q133 L136 S151 L167 Y172 V181 V182 E183 P184 H192 T193 T194 C200 I209 R221 Q233 I234 L248 N249 V250 D251 A270 V275 L286 T292 E297 M302

R320 I335 S340 W346 C347 N356 Y357 Q358 T361 D367 L368 L391 D392 F404 M413 A421 E429 V440 GLU GLY GLU GLY GLU GLU GLY GLU GLU

• Molecule 2: Tubulin beta-2B chain

Chain B: % 82% 12% 6%

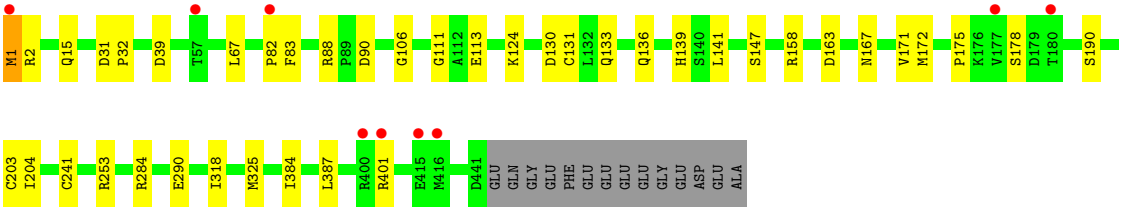
M1 R2 H6 I16 K19 F20 W21 D31 P32 A56 K60 D69 F94 S97 G106 G111 K124 D130 T138 H139 S140 L141 R158 M172 V177 V191 H192 V195 D199 E200 T201 Y202 D205 N206 E207 Y210 D211

T223 L227 S232 V238 C241 L248 R253 R264 T276 S277 ARG GLY SER GLN GLN TYR ARG ALA L286 T287 V288 P289 M295 I318 S340 L371 F377 L387 R400 R401 E422 S423 N424 E431 D437 A438 THR ALA ASP GLU GLN GLY

GLU PHE GLU GLU GLU GLU GLY GLU ASP GLU ALA

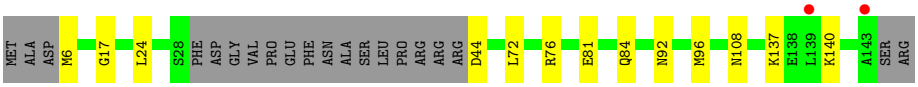
• Molecule 2: Tubulin beta-2B chain

Chain D: 2% 88% 9%



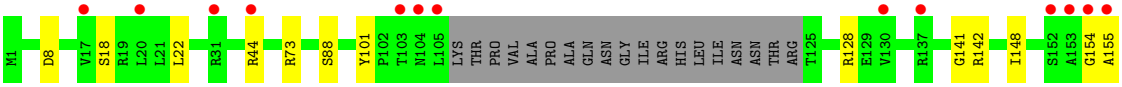
- Molecule 3: Stathmin-4

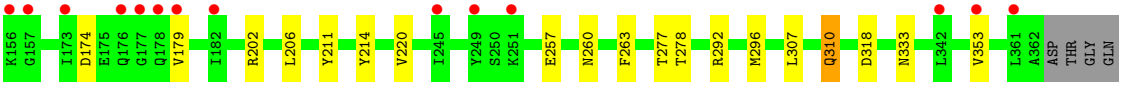
Chain E:

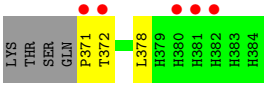


- Molecule 4: Tubulin Tyrosine ligase, TTL

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	104.77Å 158.64Å 179.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.32 – 1.80 79.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (79.32-1.80) 99.8 (79.32-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.171 , 0.204 0.165 , 0.198	Depositor DCC
R_{free} test set	13945 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	37713	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACP, CL, CA, MG, ZPN, GTP, GDP, 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	0.41	0/3698	0.57	0/5015
1	C	0.49	0/3695	0.60	0/5020
2	B	0.44	0/3549	0.56	0/4805
2	D	0.36	0/3521	0.52	0/4771
3	E	0.39	0/1079	0.47	0/1433
4	F	0.38	0/3076	0.52	0/4157
All	All	0.42	0/18618	0.55	0/25201

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	3569	3537	3524	44	0
1	C	3542	3503	3480	32	0
2	B	3403	3350	3330	40	0
2	D	3422	3330	3321	27	0
3	E	1049	1082	1077	10	0
4	F	2973	2991	2978	32	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	2	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	18	24	24	2	0
9	B	12	16	16	1	0
9	F	12	16	16	1	0
10	B	28	10	12	0	0
10	D	28	10	12	0	0
11	B	13	11	8	0	0
12	B	12	13	13	4	0
13	D	36	38	38	2	0
14	F	31	17	14	1	0
15	A	316	0	0	9	0
15	B	235	0	0	9	0
15	C	417	0	0	6	0
15	D	265	0	0	6	0
15	E	81	0	0	2	0
15	F	208	0	0	2	0
All	All	19745	17968	17887	178	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 5.

All (178) 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)
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.07	0.94
2:D:241[B]:CYS:SG	15:D:792:HOH:O	2.30	0.89
2:B:241[B]:CYS:SG	15:B:768:HOH:O	2.31	0.88
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.21	0.81
2:B:253[A]:ARG:NH1	12:B:507:MES:O2S	2.17	0.77
1:A:46:ASP:OD1	15:A:868:HOH:O	2.04	0.74
3:E:44:ASP:OD2	15:E:258:HOH:O	2.07	0.73
1:A:339:ARG:O	15:A:815:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253[A]:ARG:NH2	12:B:507:MES:O2S	2.23	0.71
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.24	0.70
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.31	0.69
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.32	0.69
1:A:22:GLU:OE1	15:A:816:HOH:O	2.11	0.68
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.34	0.68
1:A:105[B]:ARG:CD	1:A:411:GLU:OE1	2.42	0.68
2:B:424:ASN:HB3	15:B:826:HOH:O	1.95	0.67
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	2.88	0.66
1:A:229[B]:ARG:NH1	15:A:816:HOH:O	2.28	0.66
2:B:422:GLU:OE2	15:B:801:HOH:O	2.15	0.64
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.30	0.64
2:D:88:ARG:NH1	15:D:806:HOH:O	2.33	0.62
1:A:105[B]:ARG:HD3	1:A:411:GLU:OE1	2.00	0.61
2:B:202:TYR:CZ	2:B:238[B]:VAL:HG11	2.35	0.61
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.82	0.61
2:B:97:SER:HB2	15:B:823:HOH:O	1.99	0.60
4:F:310:GLN:NE2	15:F:946:HOH:O	2.33	0.60
1:C:181[B]:VAL:HG12	15:D:611:HOH:O	2.00	0.60
1:A:450:GLU:OE1	4:F:333:ASN:HB3	2.01	0.60
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.32	0.59
2:B:192:HIS:O	2:B:195[B]:VAL:HG22	2.02	0.58
1:C:286:LEU:HB2	15:C:905:HOH:O	2.02	0.58
1:A:450:GLU:OXT	4:F:202:ARG:NH2	2.36	0.58
1:A:90:GLU:O	1:A:121:ARG:HD2	2.04	0.57
4:F:101:TYR:CE1	4:F:179:VAL:HG22	2.39	0.57
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.34	0.57
2:B:264:ARG:NH2	2:B:431[A]:GLU:OE2	2.37	0.57
2:B:253[A]:ARG:CZ	12:B:507:MES:O2S	2.54	0.56
3:E:108[B]:ASN:ND2	15:E:271:HOH:O	2.39	0.55
1:C:356[B]:ASN:ND2	15:C:651:HOH:O	2.41	0.54
1:A:411:GLU:OE2	9:A:506:GOL:C3	2.55	0.54
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.89	0.54
1:A:105[B]:ARG:HG2	1:A:411:GLU:HG3	1.90	0.54
2:B:192:HIS:ND1	15:B:826:HOH:O	2.34	0.54
1:C:209:ILE:HD11	1:C:302[A]:MET:SD	2.48	0.53
2:D:318:ILE:N	2:D:318:ILE:HD12	2.24	0.53
2:B:19:LYS:HB3	2:B:232:SER:OG	2.08	0.53
2:B:158:ARG:CZ	12:B:507:MES:H21	2.39	0.53
1:C:361:THR:HG23	15:C:1012:HOH:O	2.08	0.53
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356[B]:ASN:ND2	1:C:358[B]:GLN:OE1	2.43	0.52
13:D:503:ZPN:H81	13:D:503:ZPN:C4	2.40	0.51
4:F:206:LEU:HD23	4:F:353[A]:VAL:HG21	1.91	0.51
2:D:141:LEU:HD12	2:D:172:MET:SD	2.51	0.51
4:F:206:LEU:CD2	4:F:353[A]:VAL:CG2	2.89	0.51
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.41	0.51
1:C:270:ALA:CB	1:C:302[B]:MET:SD	2.99	0.51
2:D:284:ARG:HD3	2:D:290:GLU:OE2	2.11	0.51
1:C:181[B]:VAL:HG11	1:C:404:PHE:CZ	2.47	0.50
4:F:292:ARG:NH1	4:F:296[B]:MET:SD	2.85	0.50
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.94	0.50
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.50
4:F:277[A]:THR:HG22	4:F:278:THR:H	1.77	0.50
1:A:450:GLU:CG	4:F:333:ASN:HB3	2.42	0.49
4:F:296[A]:MET:SD	9:F:704:GOL:H2	2.52	0.49
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.92	0.49
2:B:205:ASP:OD1	2:B:207:GLU:N	2.45	0.49
2:B:192:HIS:CD2	15:B:825:HOH:O	2.64	0.49
4:F:371:PRO:CA	4:F:372:THR:HB	2.42	0.48
2:B:211:ASP:OD2	15:B:803:HOH:O	2.20	0.48
4:F:18:SER:O	4:F:22:LEU:HD22	2.13	0.48
9:B:505:GOL:H2	15:B:802:HOH:O	2.14	0.48
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.49	0.48
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.45	0.47
1:A:102:ASN:HB3	1:A:105[B]:ARG:HG3	1.97	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.47
1:C:133:GLN:NE2	15:C:964:HOH:O	2.44	0.47
1:C:251[B]:ASP:OD2	15:C:692:HOH:O	2.20	0.47
2:D:203:CYS:SG	2:D:384[B]:ILE:HD11	2.55	0.47
3:E:137:LYS:HA	3:E:140:LYS:HD2	1.97	0.47
1:A:413:MET:CE	1:A:418:PHE:CE1	2.98	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.47
2:B:295[B]:MET:CG	2:B:377:PHE:HB2	2.44	0.47
2:D:171:VAL:HA	2:D:204:ILE:O	2.15	0.47
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.50	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.46
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.46
1:A:105[B]:ARG:HD2	1:A:411:GLU:OE1	2.16	0.46
2:D:2:ARG:NH1	2:D:130:ASP:OD2	2.48	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.46
2:D:241[B]:CYS:SG	15:D:682:HOH:O	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.98	0.46
2:D:175:PRO:HA	2:D:178:SER:HB2	1.97	0.46
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.45	0.46
2:B:124:LYS:HD3	2:B:124:LYS:C	2.35	0.46
3:E:72:LEU:O	3:E:76:ARG:HG2	2.16	0.45
4:F:8:ASP:OD2	4:F:44:ARG:NH1	2.49	0.45
1:A:285:GLN:HG3	1:A:372[B]:GLN:NE2	2.31	0.45
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.46	0.45
4:F:371:PRO:HA	4:F:372:THR:HB	1.98	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.16	0.45
4:F:318:ASP:OD2	14:F:703:ACP:O3G	2.35	0.45
2:B:205:ASP:OD1	2:B:207:GLU:CB	2.65	0.45
4:F:310:GLN:CD	15:F:946:HOH:O	2.55	0.45
4:F:371:PRO:HA	4:F:372:THR:C	2.37	0.45
2:B:387:LEU:HD23	2:B:387:LEU:C	2.38	0.45
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.99	0.45
1:A:411:GLU:OE2	9:A:506:GOL:H31	2.16	0.45
1:C:183:GLU:N	1:C:184:PRO:CD	2.80	0.44
1:A:88:HIS:HE1	15:A:737:HOH:O	2.00	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.52	0.44
1:A:450:GLU:HG3	4:F:333:ASN:HB3	1.99	0.44
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	1.98	0.44
1:C:221:ARG:HG3	2:D:325:MET:HG3	1.99	0.44
2:D:113:GLU:HG3	15:D:822:HOH:O	2.17	0.44
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.53	0.44
2:D:15:GLN:HG2	15:D:808:HOH:O	2.18	0.44
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.33	0.44
2:B:177:VAL:HG21	2:B:210:TYR:HB2	2.00	0.43
2:B:318:ILE:HD12	2:B:318:ILE:N	2.33	0.43
2:B:2:ARG:NH1	2:B:130:ASP:OD2	2.51	0.43
2:B:199:ASP:C	2:B:200:GLU:HG3	2.38	0.43
2:B:202:TYR:CZ	2:B:238[B]:VAL:CG1	3.01	0.43
3:E:92:ASN:O	3:E:96:MET:HG2	2.18	0.43
4:F:257:GLU:HG2	4:F:260:ASN:HA	2.01	0.43
3:E:81:GLU:HA	3:E:84[B]:GLN:HG2	2.00	0.43
2:D:1:MET:N	2:D:131:CYS:SG	2.67	0.43
2:B:141:LEU:HD12	2:B:172:MET:SD	2.58	0.43
2:D:1:MET:HB2	2:D:133:GLN:HG2	2.00	0.43
1:A:394:LYS:NZ	15:A:896:HOH:O	2.37	0.42
4:F:18:SER:O	4:F:22:LEU:CD2	2.68	0.42
13:D:503:ZPN:H31	13:D:503:ZPN:H61	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:HB2	1:A:89:PRO:HD2	2.00	0.42
2:D:124:LYS:C	2:D:124:LYS:HD3	2.39	0.42
1:A:83:TYR:O	1:A:86:LEU:HB2	2.20	0.42
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.01	0.42
1:C:367:ASP:OD1	15:C:861:HOH:O	2.22	0.42
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.60	0.42
1:A:357:TYR:CE1	3:E:17:GLY:HA2	2.55	0.42
1:A:441:GLU:HB2	4:F:73:ARG:HG3	2.02	0.42
2:B:276:THR:CG2	2:B:277:SER:N	2.83	0.42
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.29	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.49	0.42
1:A:298:PRO:HA	1:A:301:GLN:CD	2.40	0.42
4:F:371:PRO:N	4:F:372:THR:HB	2.35	0.42
1:A:283:HIS:HE1	15:A:617:HOH:O	2.03	0.41
1:A:441:GLU:HB2	4:F:73:ARG:CG	2.50	0.41
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.02	0.41
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.34	0.41
2:D:136:GLN:HA	2:D:167:ASN:O	2.20	0.41
4:F:214:TYR:CE2	4:F:353[B]:VAL:HG11	2.55	0.41
2:B:191:VAL:O	2:B:195[A]:VAL:HG23	2.20	0.41
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.38	0.41
3:E:6:MET:SD	3:E:24:LEU:CD2	3.08	0.41
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.02	0.41
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.02	0.41
2:D:147[A]:SER:HB2	2:D:190:SER:HG	1.85	0.41
1:A:336:LYS:NZ	15:A:804:HOH:O	2.53	0.41
2:B:195[B]:VAL:HG21	15:B:826:HOH:O	2.21	0.41
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.41
2:D:163:ASP:O	2:D:253:ARG:NH2	2.54	0.41
4:F:371:PRO:HA	4:F:372:THR:O	2.21	0.41
1:A:105[B]:ARG:NH2	15:A:873:HOH:O	2.52	0.41
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	2.02	0.41
1:A:312:TYR:CD2	1:A:315[B]:CYS:SG	3.14	0.40
2:B:205:ASP:OD1	2:B:207:GLU:HB3	2.21	0.40
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.04	0.40
4:F:141:GLY:O	4:F:142:ARG:HB2	2.22	0.40
4:F:148:ILE:O	4:F:148:ILE:HG23	2.22	0.40
2:B:16[A]:ILE:HD11	2:B:138[A]:THR:HB	2.03	0.40
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.04	0.40
2:D:82:PRO:O	2:D:83:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HG2	1:A:85:GLN:N	2.37	0.40
1:A:209[A]:ILE:CD1	1:A:302[A]:MET:SD	3.07	0.40
2:B:223:THR:O	2:B:227:LEU:HD13	2.21	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	460/450 (102%)	448 (97%)	12 (3%)	0	100	100
1	C	462/450 (103%)	448 (97%)	13 (3%)	1 (0%)	47	33
2	B	438/445 (98%)	432 (99%)	6 (1%)	0	100	100
2	D	437/445 (98%)	429 (98%)	8 (2%)	0	100	100
3	E	126/143 (88%)	126 (100%)	0	0	100	100
4	F	362/384 (94%)	352 (97%)	7 (2%)	3 (1%)	19	7
All	All	2285/2317 (99%)	2235 (98%)	46 (2%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ARG
4	F	155	ALA
4	F	88	SER
4	F	154	GLY

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	392/378 (104%)	390 (100%)	2 (0%)	88	87
1	C	395/378 (104%)	393 (100%)	2 (0%)	88	87
2	B	386/383 (101%)	383 (99%)	3 (1%)	81	78
2	D	380/383 (99%)	375 (99%)	5 (1%)	69	62
3	E	117/127 (92%)	117 (100%)	0	100	100
4	F	330/342 (96%)	327 (99%)	3 (1%)	78	75
All	All	2000/1991 (100%)	1985 (99%)	15 (1%)	81	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
1	A	381	THR
2	B	139	HIS
2	B	371[A]	LEU
2	B	371[B]	LEU
1	C	71	GLU
1	C	297	GLU
2	D	1	MET
2	D	39	ASP
2	D	139	HIS
2	D	158	ARG
2	D	401	ARG
4	F	211	TYR
4	F	307	LEU
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
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 26 ligands modelled in this entry, 11 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.14	3 (9%)
9	GOL	F	705	-	5,5,5	0.39	0	5,5,5	0.19	0
12	MES	B	507	-	12,12,12	2.36	1 (8%)	14,16,16	1.19	1 (7%)
9	GOL	A	506	-	5,5,5	0.13	0	5,5,5	0.48	0
9	GOL	B	504	-	5,5,5	0.47	0	5,5,5	0.71	0
10	GDP	B	501	6	24,30,30	1.21	2 (8%)	30,47,47	1.25	3 (10%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.16	2 (6%)
11	TYR	B	506	-	12,13,13	0.69	1 (8%)	16,17,17	0.91	2 (12%)
9	GOL	B	505	-	5,5,5	0.31	0	5,5,5	0.54	0
9	GOL	A	508	-	5,5,5	0.36	0	5,5,5	0.49	0
13	ZPN	D	503	2	36,37,37	0.81	1 (2%)	35,48,48	1.61	5 (14%)
10	GDP	D	501	6	24,30,30	1.17	1 (4%)	30,47,47	1.06	2 (6%)
14	ACP	F	703	6	27,33,33	1.12	2 (7%)	32,52,52	1.65	7 (21%)
9	GOL	F	704	-	5,5,5	0.36	0	5,5,5	0.28	0
9	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
9	GOL	F	705	-	-	2/4/4/4	-
12	MES	B	507	-	-	5/6/14/14	0/1/1/1
9	GOL	A	506	-	-	2/4/4/4	-
9	GOL	B	504	-	-	4/4/4/4	-
10	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
11	TYR	B	506	-	-	4/8/8/8	0/1/1/1
9	GOL	B	505	-	-	2/4/4/4	-
9	GOL	A	508	-	-	2/4/4/4	-
13	ZPN	D	503	2	-	6/41/53/53	0/1/2/2
10	GDP	D	501	6	-	3/12/32/32	0/3/3/3
14	ACP	F	703	6	-	2/15/38/38	0/3/3/3
9	GOL	F	704	-	-	1/4/4/4	-
9	GOL	A	507	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	507	MES	C8-S	-8.00	1.66	1.77
5	C	501	GTP	C5-C6	-3.89	1.39	1.47
10	B	501	GDP	O4'-C1'	3.88	1.46	1.41
5	A	501	GTP	C6-N1	-3.11	1.33	1.37
13	D	503	ZPN	C20-N20	3.05	1.47	1.43
10	D	501	GDP	C6-N1	-3.05	1.33	1.37
10	B	501	GDP	C6-N1	-2.79	1.33	1.37
5	A	501	GTP	PG-O3G	-2.55	1.45	1.54
14	F	703	ACP	PG-O1G	-2.26	1.45	1.50
14	F	703	ACP	PG-O2G	2.18	1.59	1.54
11	B	506	TYR	OXT-C	-2.02	1.23	1.30
5	C	501	GTP	C2-N3	2.01	1.38	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	503	ZPN	O19-C19-C18	5.96	122.19	107.05
14	F	703	ACP	PB-O3A-PA	-4.07	119.65	132.56
14	F	703	ACP	N3-C2-N1	-3.90	122.58	128.68
13	D	503	ZPN	O1'-C1'-N20	-3.10	118.26	122.35
5	C	501	GTP	C8-N7-C5	3.06	108.81	102.99
13	D	503	ZPN	C19-O19-C1	2.85	121.69	117.45
10	B	501	GDP	O6-C6-C5	-2.76	118.97	124.37
14	F	703	ACP	C3'-C2'-C1'	2.71	105.06	100.98
14	F	703	ACP	PA-O5'-C5'	-2.59	106.50	121.68
13	D	503	ZPN	C3'-C4'-C5'	-2.55	119.87	124.69
10	B	501	GDP	C5-C6-N1	2.53	118.41	113.95
10	D	501	GDP	C8-N7-C5	2.48	107.72	102.99
11	B	506	TYR	OXT-C-O	-2.45	118.54	124.09
5	C	501	GTP	C5-C6-N1	2.42	118.23	113.95
10	B	501	GDP	O2B-PB-O3A	2.41	112.70	104.64
11	B	506	TYR	OXT-C-CA	2.35	121.40	113.38
10	D	501	GDP	C5-C6-N1	2.33	118.06	113.95
5	A	501	GTP	C8-N7-C5	2.27	107.32	102.99
5	A	501	GTP	C5-C6-N1	2.22	117.87	113.95
14	F	703	ACP	O4'-C4'-C3'	2.15	109.38	105.11
14	F	703	ACP	O2A-PA-O1A	2.14	122.83	112.24
14	F	703	ACP	O3G-PG-O1G	-2.12	106.79	112.39
12	B	507	MES	O1S-S-C8	2.12	109.46	106.92
13	D	503	ZPN	O19-C1-O1	-2.10	119.93	123.35
5	A	501	GTP	O6-C6-C5	-2.03	120.41	124.37

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	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
9	A	506	GOL	O1-C1-C2-O2
9	A	506	GOL	O1-C1-C2-C3
9	A	508	GOL	O1-C1-C2-C3
9	B	504	GOL	O1-C1-C2-O2
9	B	504	GOL	O1-C1-C2-C3
9	B	504	GOL	C1-C2-C3-O3
9	B	505	GOL	O1-C1-C2-C3
10	B	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O2A
12	B	507	MES	C8-C7-N4-C5
12	B	507	MES	C7-C8-S-O1S
12	B	507	MES	C7-C8-S-O2S
11	B	506	TYR	OXT-C-CA-N
9	A	507	GOL	O1-C1-C2-O2
9	A	507	GOL	O1-C1-C2-C3
9	F	705	GOL	O1-C1-C2-C3
9	B	504	GOL	O2-C2-C3-O3
9	F	705	GOL	O1-C1-C2-O2
13	D	503	ZPN	O1-C1-O19-C19
11	B	506	TYR	CA-CB-CG-CD1
12	B	507	MES	C7-C8-S-O3S
11	B	506	TYR	CA-CB-CG-CD2
9	B	505	GOL	O1-C1-C2-O2
13	D	503	ZPN	C17-C18-C19-O19
9	A	508	GOL	O1-C1-C2-O2
11	B	506	TYR	O-C-CA-N
5	A	501	GTP	PB-O3B-PG-O3G
13	D	503	ZPN	O7-C7-C8-C9
13	D	503	ZPN	C11-C10-C9-C8
14	F	703	ACP	O4'-C4'-C5'-O5'
13	D	503	ZPN	C17-C18-C19-C20
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	F	704	GOL	O1-C1-C2-O2
10	B	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	501	GDP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
10	B	501	GDP	PB-O3A-PA-O2A
14	F	703	ACP	C5'-O5'-PA-O2A
13	D	503	ZPN	C18-C19-C20-N20
12	B	507	MES	C8-C7-N4-C3

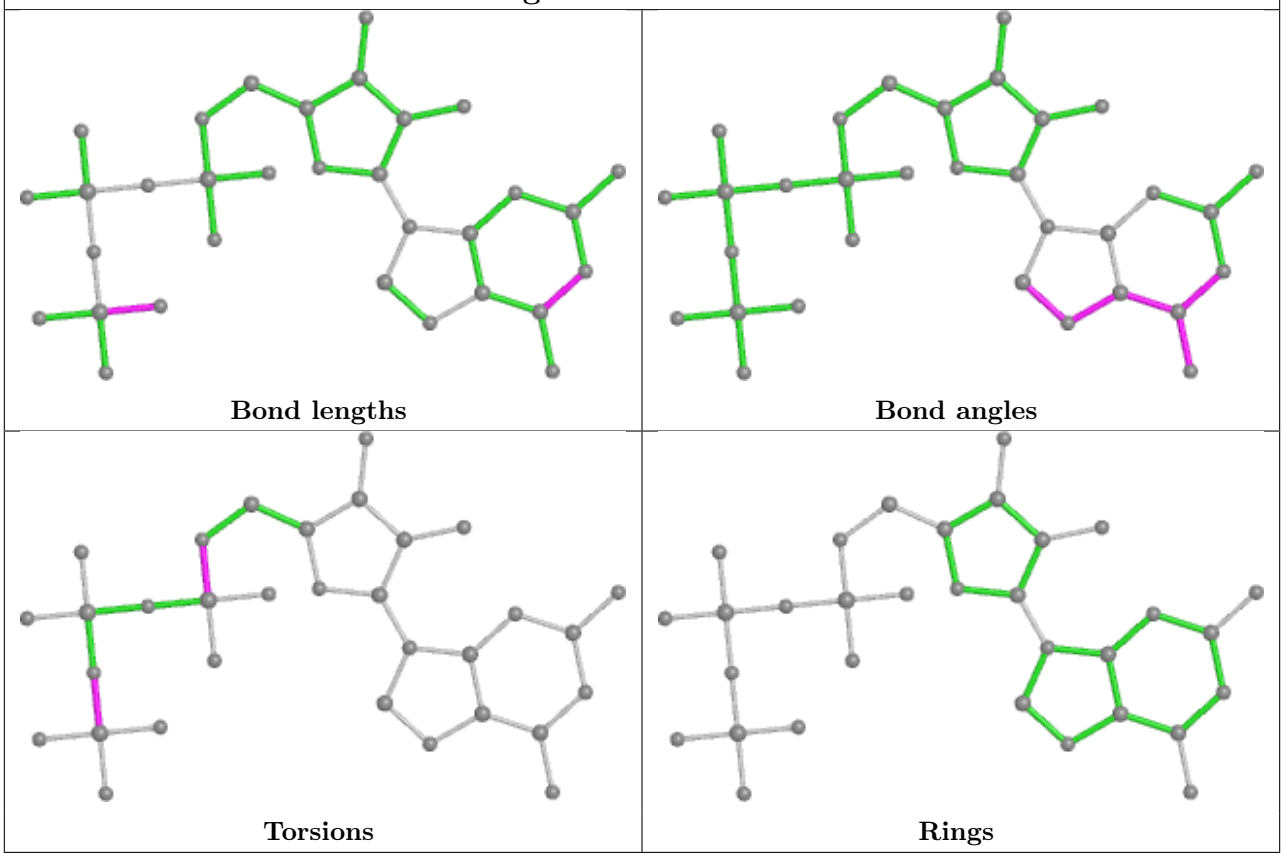
There are no ring outliers.

6 monomers are involved in 11 short contacts:

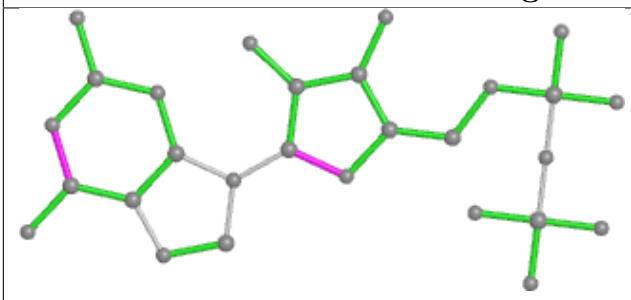
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	507	MES	4	0
9	A	506	GOL	2	0
9	B	505	GOL	1	0
13	D	503	ZPN	2	0
14	F	703	ACP	1	0
9	F	704	GOL	1	0

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

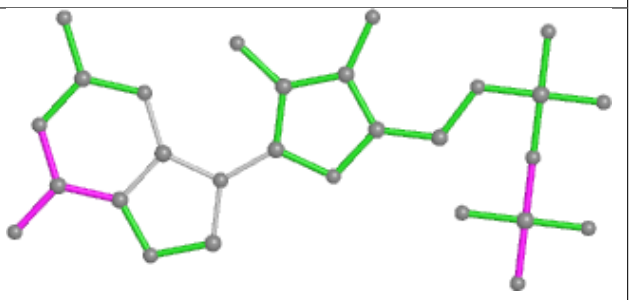
Ligand GTP A 501



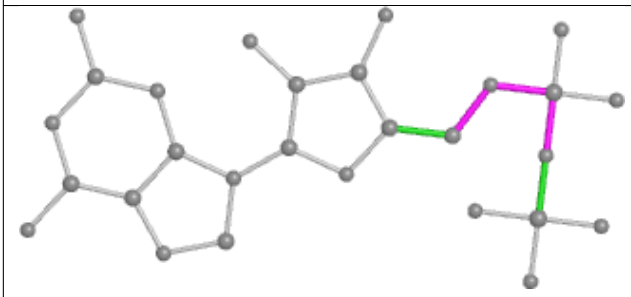
Ligand GDP B 501



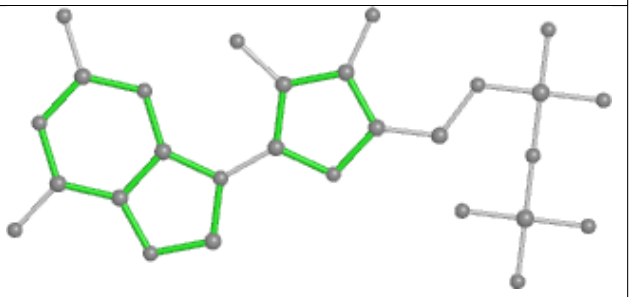
Bond lengths



Bond angles

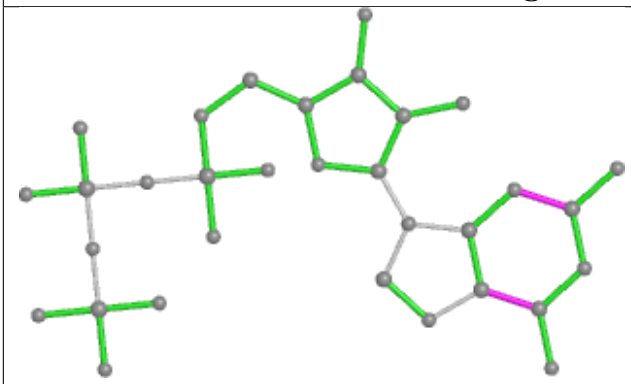


Torsions

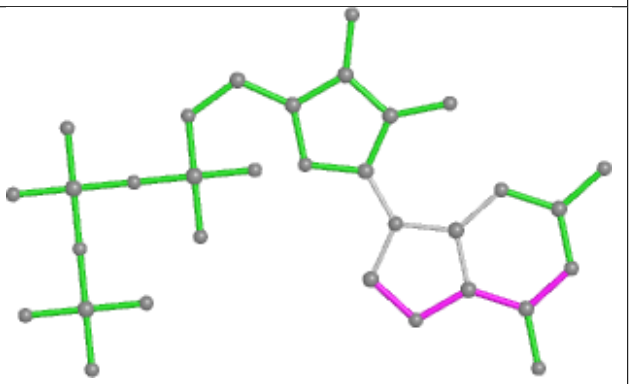


Rings

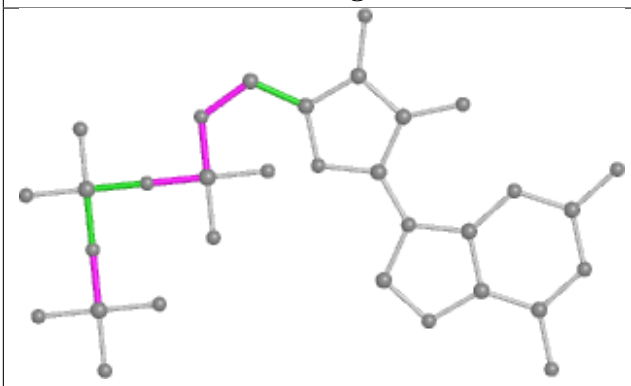
Ligand GTP C 501



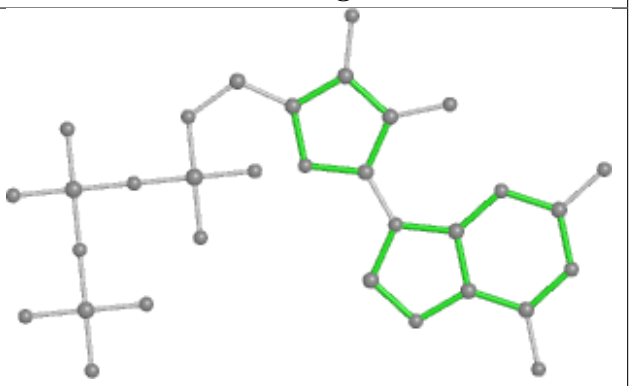
Bond lengths



Bond angles

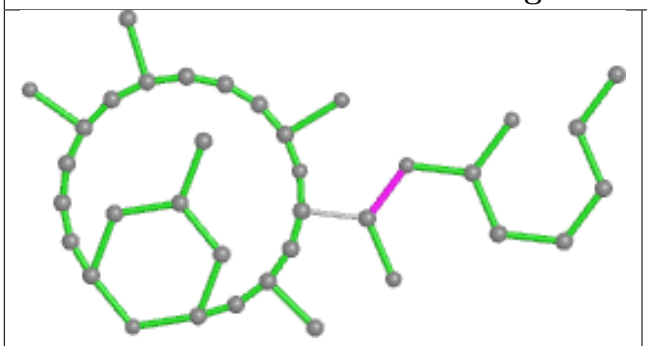


Torsions

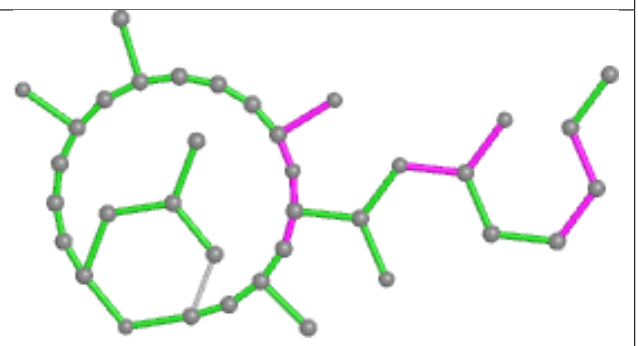


Rings

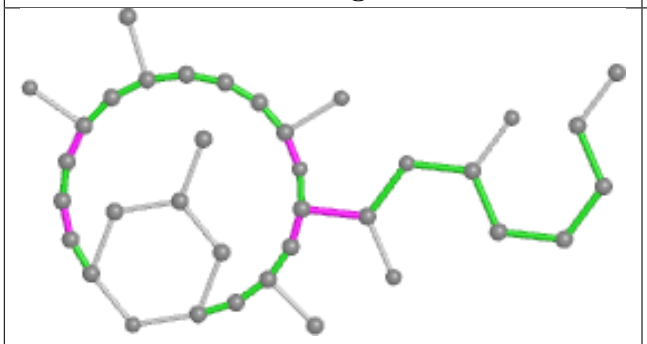
Ligand ZPN D 503



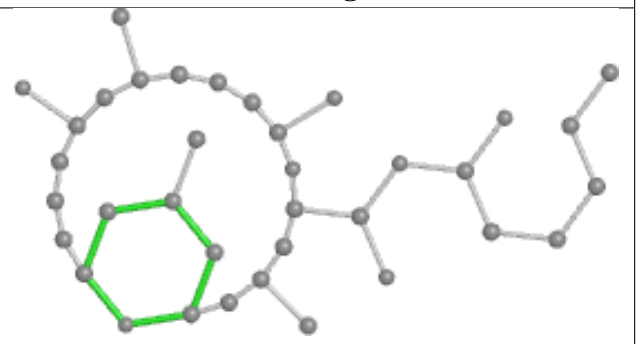
Bond lengths



Bond angles

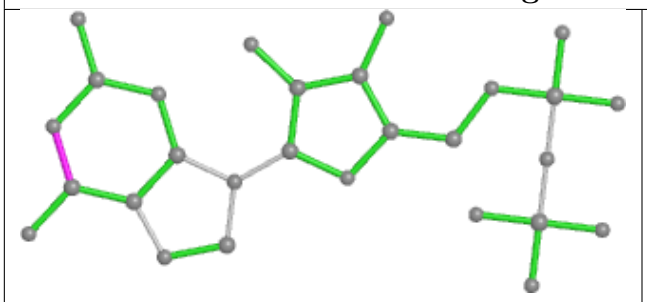


Torsions

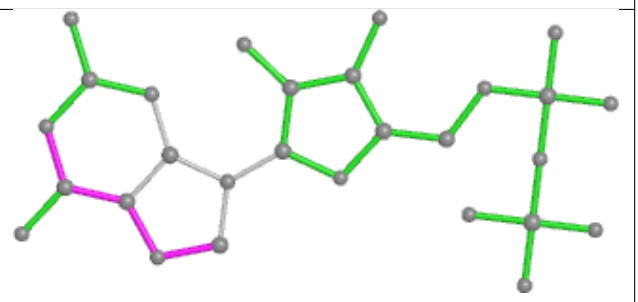


Rings

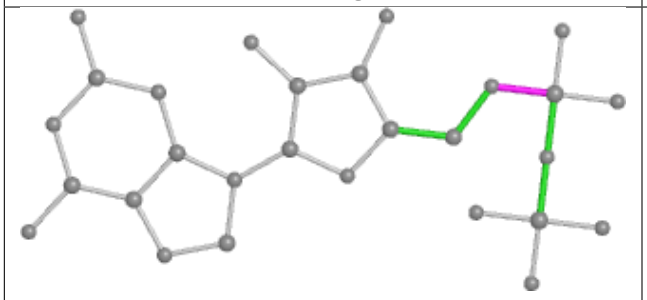
Ligand GDP D 501



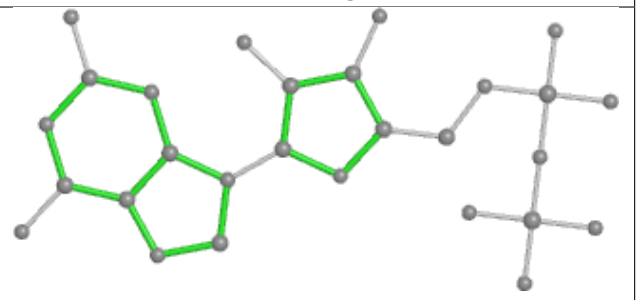
Bond lengths



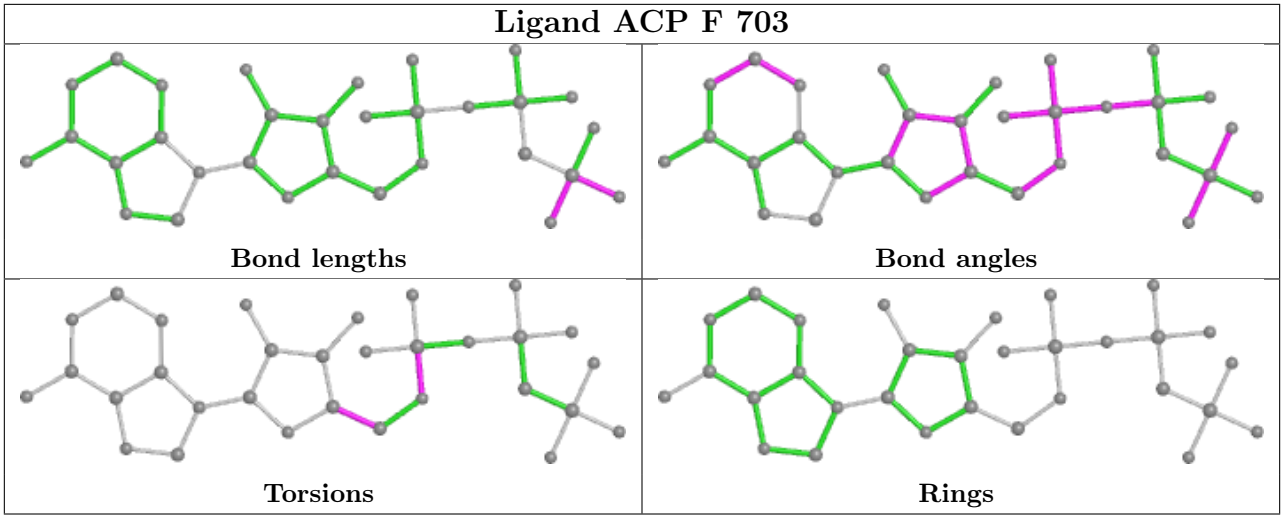
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	447/450 (99%)	-0.05	9 (2%)	65	61	24, 38, 69, 134	0
1	C	440/450 (97%)	0.16	2 (0%)	91	89	20, 30, 53, 84	0
2	B	420/445 (94%)	0.11	6 (1%)	75	72	23, 40, 72, 106	2 (0%)
2	D	431/445 (96%)	-0.06	9 (2%)	63	59	24, 40, 71, 105	6 (1%)
3	E	123/143 (86%)	0.19	2 (1%)	72	68	27, 52, 89, 112	0
4	F	357/384 (92%)	0.44	32 (8%)	9	7	28, 51, 100, 117	0
All	All	2218/2317 (95%)	0.11	60 (2%)	54	49	20, 40, 77, 134	8 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	6.1
1	A	448	GLY	6.0
4	F	155	ALA	5.4
4	F	372	THR	5.2
2	B	276	THR	5.0
4	F	177	GLY	4.8
1	A	440	VAL	4.4
4	F	153	ALA	4.3
4	F	371	PRO	4.3
2	B	438	ALA	4.3
2	D	57	THR	3.9
4	F	249	TYR	3.9
2	D	82	PRO	3.8
2	D	1	MET	3.8
4	F	31	ARG	3.8
2	B	437	ASP	3.6
3	E	143	ALA	3.6
4	F	105	LEU	3.3
4	F	157	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	154	GLY	3.2
4	F	251	LYS	3.1
4	F	156	LYS	3.1
4	F	381	HIS	3.0
4	F	245	ILE	2.9
2	D	400	ARG	2.9
4	F	380	HIS	2.9
3	E	139	LEU	2.9
1	C	1	MET	2.8
4	F	130	VAL	2.7
1	A	444	GLY	2.7
1	C	340	SER	2.7
2	D	401	ARG	2.6
4	F	361	LEU	2.6
4	F	44	ARG	2.5
2	D	415	GLU	2.5
2	D	177	VAL	2.5
1	A	282	TYR	2.5
4	F	179	VAL	2.4
1	A	450	GLU	2.4
4	F	20	LEU	2.3
4	F	382	HIS	2.3
1	A	281	ALA	2.3
1	A	338	LYS	2.3
4	F	152	SER	2.3
2	D	416	MET	2.3
4	F	182	ILE	2.2
4	F	103	THR	2.2
4	F	176	GLN	2.2
1	A	449	GLU	2.2
4	F	17	VAL	2.2
4	F	137	ARG	2.1
4	F	178	GLN	2.1
2	B	288	VAL	2.1
4	F	353[A]	VAL	2.1
2	B	248	LEU	2.1
2	B	340[A]	SER	2.0
4	F	104	ASN	2.0
4	F	342	LEU	2.0
1	A	441	GLU	2.0
2	D	180	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)

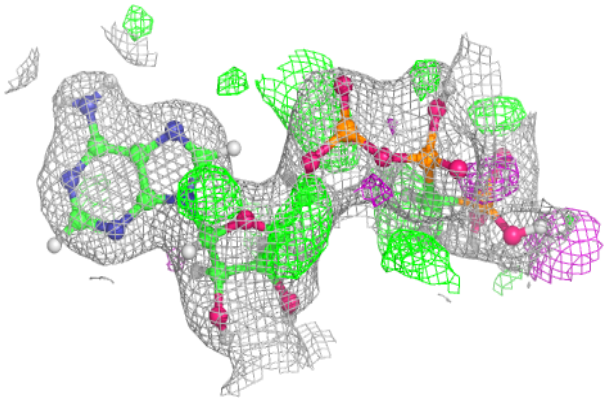
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

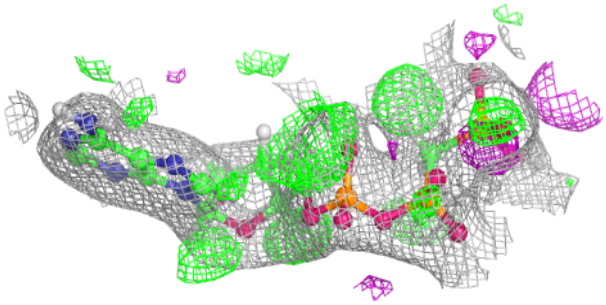
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GOL	F	705	6/6	0.71	0.22	55,84,101,116	0
11	TYR	B	506	13/13	0.81	0.23	72,94,112,113	0
6	MG	F	701	1/1	0.84	0.21	68,68,68,68	0
7	CA	B	503	1/1	0.85	0.15	76,76,76,76	0
9	GOL	B	505	6/6	0.85	0.24	55,85,113,120	0
9	GOL	F	704	6/6	0.86	0.23	50,87,105,109	0
6	MG	D	502	1/1	0.88	0.18	62,62,62,62	0
14	ACP	F	703	31/31	0.90	0.12	42,56,93,104	0
9	GOL	A	508	6/6	0.91	0.13	37,58,70,70	0
9	GOL	A	506	6/6	0.92	0.10	29,65,85,87	0
9	GOL	B	504	6/6	0.93	0.15	45,63,96,111	0
7	CA	A	505	1/1	0.93	0.13	80,80,80,80	0
8	CL	A	504	1/1	0.93	0.15	56,56,56,56	0
12	MES	B	507	12/12	0.94	0.12	35,51,67,72	0
6	MG	F	702	1/1	0.94	0.08	38,38,38,38	0
13	ZPN	D	503	36/36	0.95	0.10	29,39,73,81	0
9	GOL	A	507	6/6	0.96	0.15	53,107,124,134	0
7	CA	A	503	1/1	0.97	0.14	44,44,44,44	0
10	GDP	D	501	28/28	0.97	0.09	33,37,46,49	0
10	GDP	B	501	28/28	0.98	0.14	22,27,36,37	0
5	GTP	A	501	32/32	0.98	0.12	21,26,33,34	0
6	MG	C	502	1/1	0.99	0.17	23,23,23,23	0
7	CA	C	503	1/1	0.99	0.13	39,39,39,39	0
5	GTP	C	501	32/32	0.99	0.13	16,22,27,30	0
6	MG	A	502	1/1	0.99	0.18	27,27,27,27	0
6	MG	B	502	1/1	1.00	0.25	21,21,21,21	0

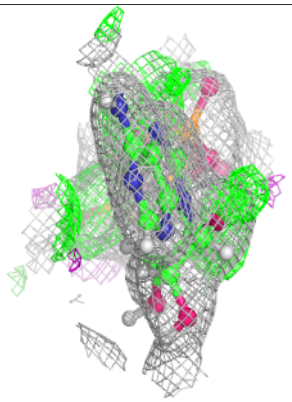
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 703:

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

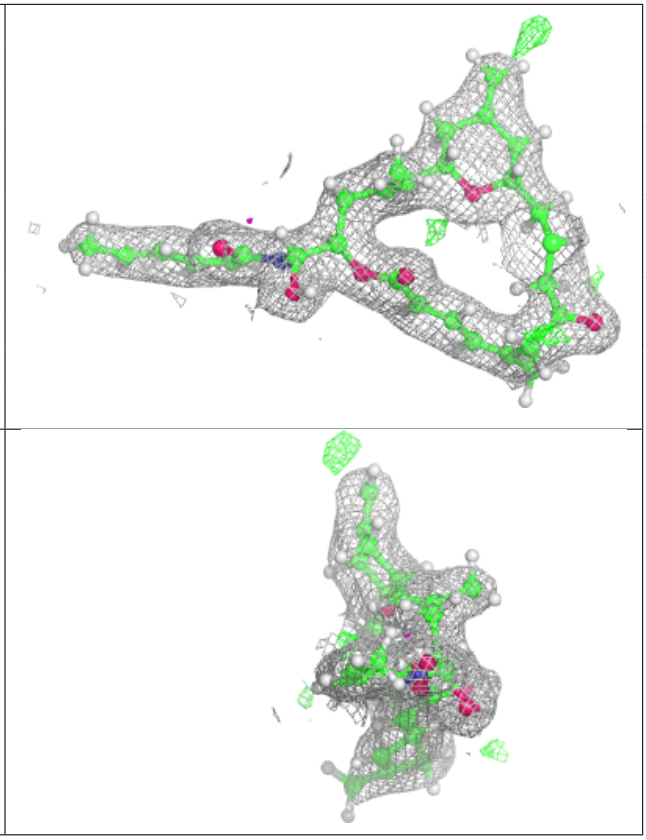






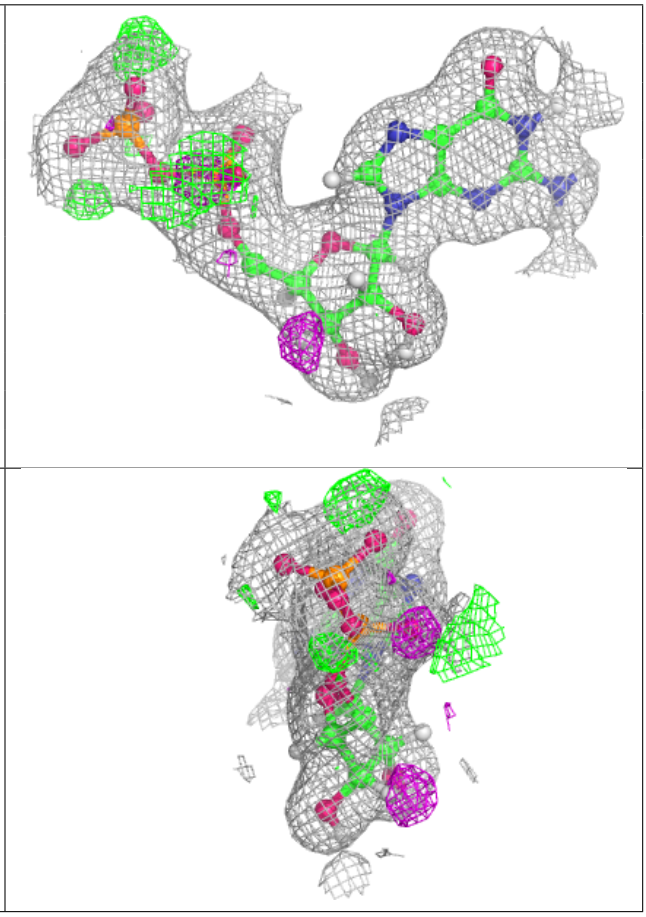
Electron density around ZPN D 503:

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



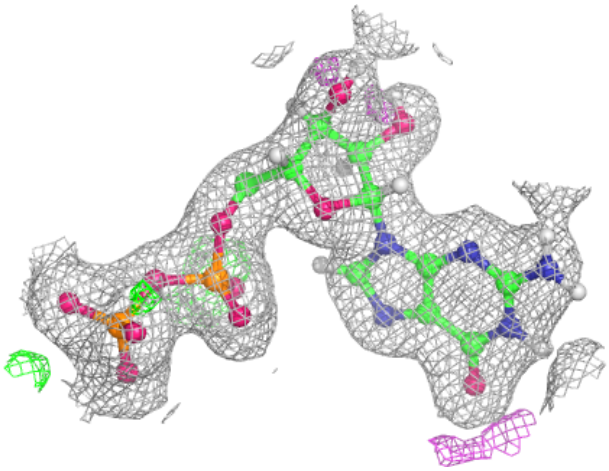
Electron density around GDP D 501:

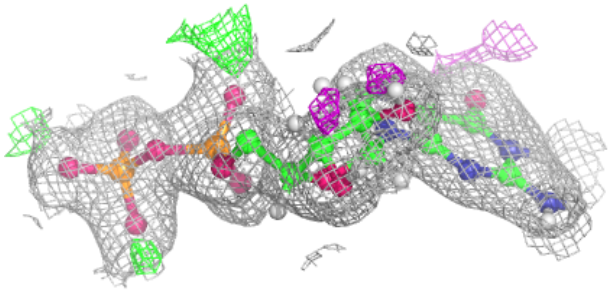
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

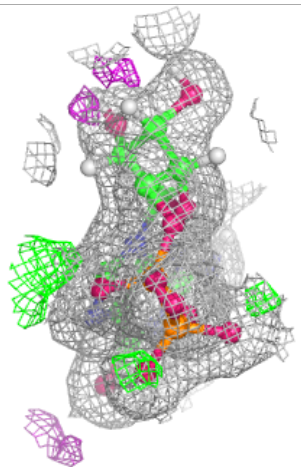


Electron density around GDP B 501:

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

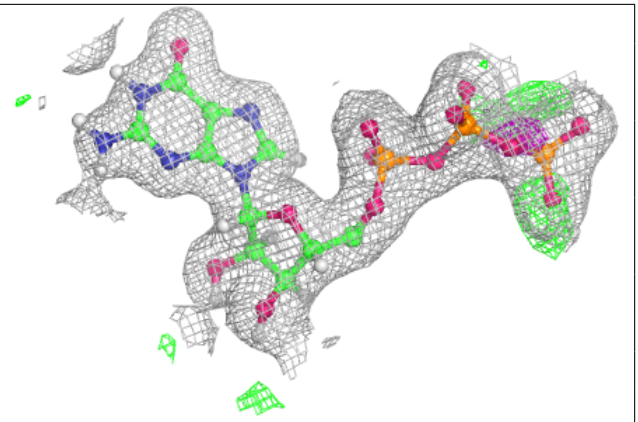


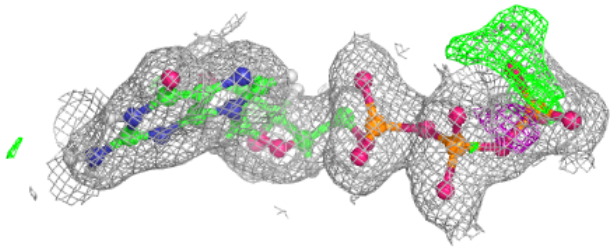


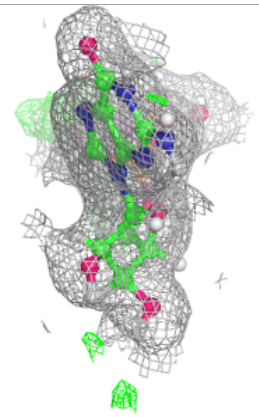


Electron density around GTP A 501:

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

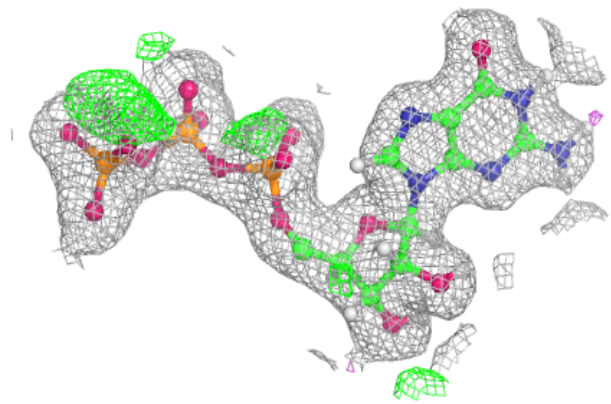


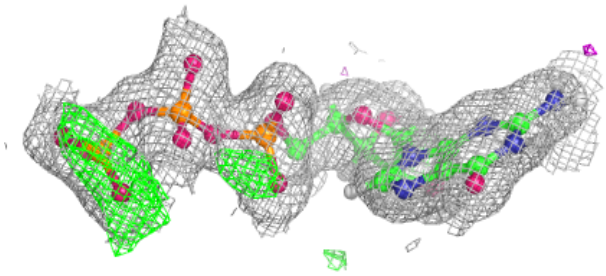


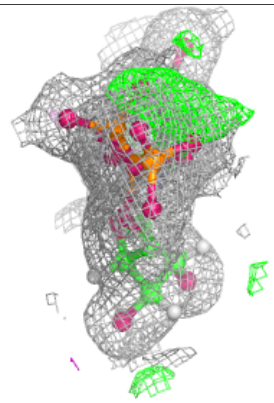


Electron density around GTP C 501:

$2mF_o$-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.