Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 01:55 PM EDT

PDB ID	:	4O2A
Title	:	Tubulin-BAL27862 complex
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Deposited on	:	2013-12-17
Resolution	:	2.50 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:

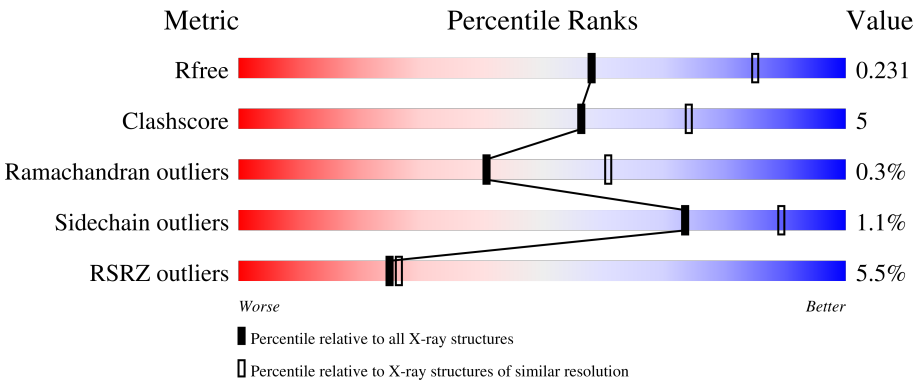
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	.% 87% 10% •
1	C	451	88% 9% • •
2	B	445	.% 82% 12% 6%
2	D	445	3% 79% 14% • 5%
3	E	143	3% 83% • 13%

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Mol	Chain	Length	Quality of chain
4	F	384	24% 72% 14% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	2RR	D	604	-	-	X	X
14	ADP	F	401	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 18043 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
			Total	C	N	O	S			
1	A	439	3487	2214	587	662	24	0	12	0
1	C	440	3504	2224	587	667	26	0	15	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	418	3371	2127	566	650	28	0	16	0
2	D	421	3324	2091	562	643	28	0	4	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	124	1045	646	188	205	6	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

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

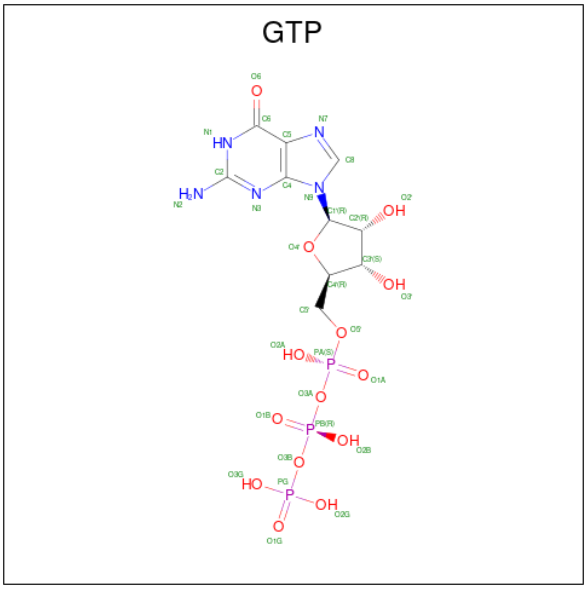
- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	331	2740	1766	465	495	14	0	4	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
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		
6	B	2	Total	Mg	0	0
			2	2		
6	D	2	Total	Mg	0	0
			2	2		

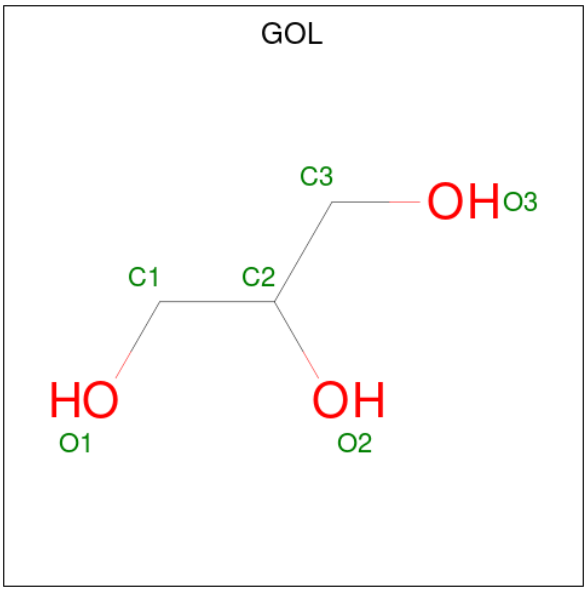
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

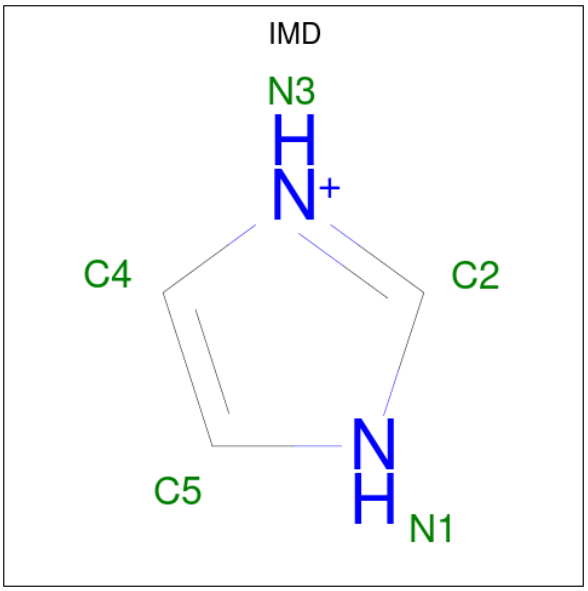
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

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



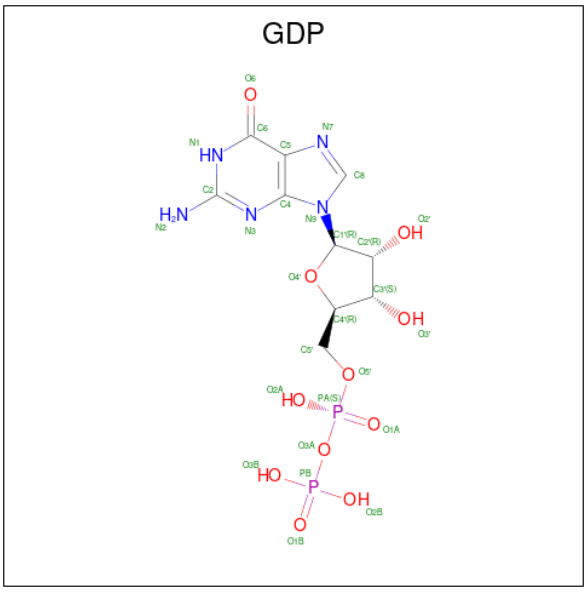
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0

- Molecule 10 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



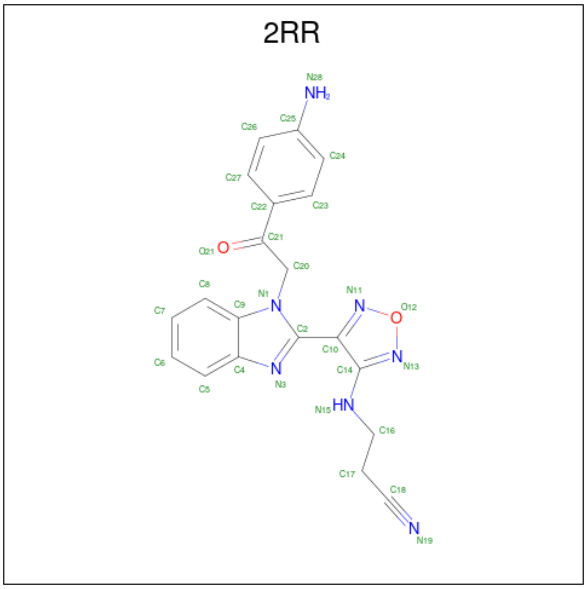
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
10	A	1	5	3	2	0	0

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



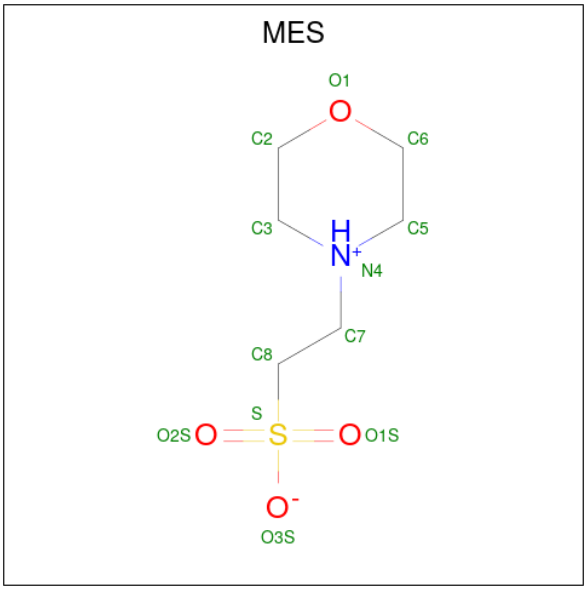
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
11	D	1	28	10	5	11	2	0	0

- Molecule 12 is 3-[(4-{1-[2-(4-aminophenyl)-2-oxoethyl]-1H-benzimidazol-2-yl}-1,2,5-oxadiazol-3-yl)amino]propanenitrile (three-letter code: 2RR) (formula: $C_{20}H_{17}N_7O_2$).



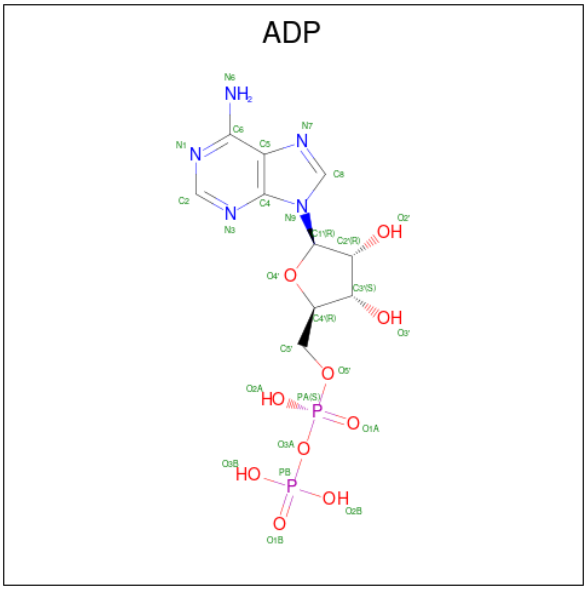
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	B	1	29	20	7	2	0	0
			Total	C	N	O		
12	D	1	29	20	7	2	0	0

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



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

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	F	1	27	10	5	10	2	0	0

- Molecule 15 is water.

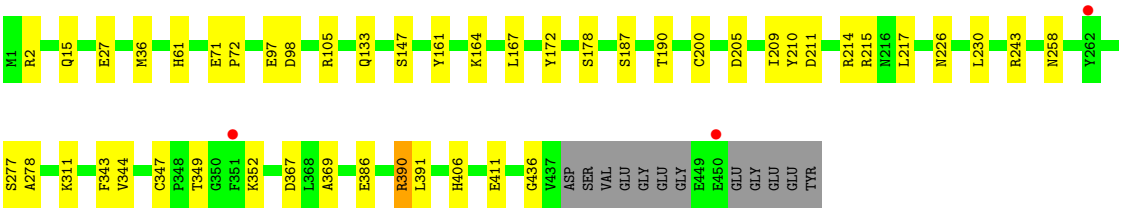
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	63	63	63	0	0
15	B	70	70	70	0	0
15	C	144	144	144	0	0
15	D	26	26	26	0	0
15	E	13	13	13	0	0
15	F	18	18	18	0	0

3 Residue-property plots (i)

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

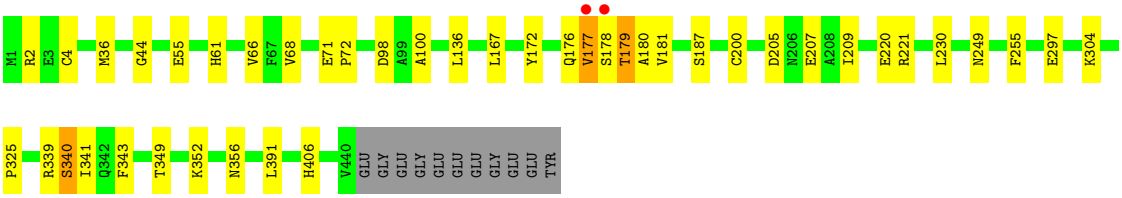
• Molecule 1: Tubulin alpha-1B chain

Chain A:



• Molecule 1: Tubulin alpha-1B chain

Chain C:

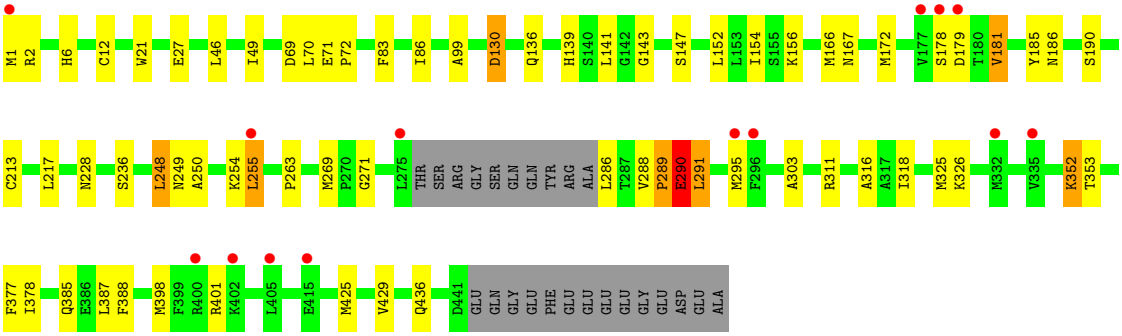


• Molecule 2: Tubulin beta-2B chain

Chain B:

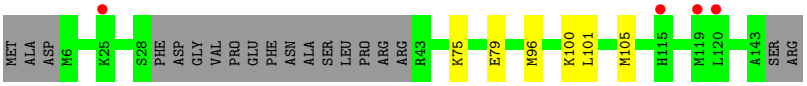
• Molecule 2: Tubulin beta-2B chain

Chain D:



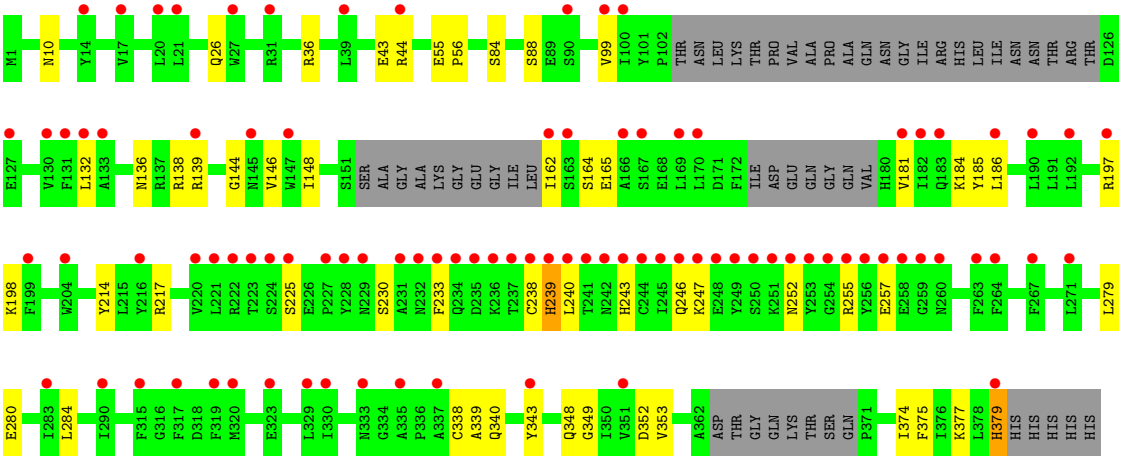
- Molecule 3: Stathmin-4

Chain E:



- Molecule 4: TUBULIN-TYROSINE LIGASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.53Å 158.12Å 179.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.36 – 2.50 78.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.36-2.50) 99.7 (78.45-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.194 , 0.232 0.195 , 0.231	Depositor DCC
R_{free} test set	5155 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.2	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	18043	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: GDP, MES, IMD, CL, GOL, 2RR, MG, CA, ADP, GTP

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	0.21	0/3600	0.38	0/4886
1	C	0.23	0/3628	0.40	0/4926
2	B	0.22	0/3489	0.38	0/4724
2	D	0.22	0/3409	0.42	2/4619 (0.0%)
3	E	0.20	0/1069	0.31	0/1419
4	F	0.22	0/2815	0.37	0/3801
All	All	0.22	0/18010	0.39	2/24375 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	289	PRO	C-N-CA	5.32	135.00	121.70
2	D	289	PRO	CA-C-N	5.01	128.22	117.20

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	3487	0	3433	25	0
1	C	3504	0	3447	32	0
2	B	3371	0	3289	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3324	0	3215	49	0
3	E	1045	0	1066	3	0
4	F	2740	0	2729	37	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	6	0	8	0	0
10	A	5	0	5	0	0
11	B	28	0	12	2	0
11	D	28	0	12	2	0
12	B	29	0	17	2	0
12	D	29	0	17	17	0
13	B	12	0	12	2	0
14	F	27	0	12	3	0
15	A	63	0	0	0	0
15	B	70	0	0	1	0
15	C	144	0	0	1	0
15	D	26	0	0	1	0
15	E	13	0	0	0	0
15	F	18	0	0	2	0
All	All	18043	0	17298	176	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 (176) 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)
4:F:238:CYS:SG	4:F:239:HIS:CE1	2.03	1.50
4:F:238:CYS:SG	4:F:239:HIS:ND1	2.11	1.22
1:C:180:ALA:N	12:D:604:2RR:H16	1.87	0.89
4:F:238:CYS:SG	4:F:239:HIS:HE1	1.67	0.85
4:F:225:SER:H	4:F:246:GLN:HE22	1.30	0.78
12:D:604:2RR:H14	12:D:604:2RR:N3	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ALA:CA	12:D:604:2RR:H16	2.16	0.76
1:C:179:THR:C	12:D:604:2RR:H16	2.06	0.75
2:B:287:THR:HG22	2:B:289:PRO:HD2	1.71	0.72
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.37	0.72
1:C:341:ILE:HD12	1:C:341:ILE:N	2.05	0.71
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.72	0.70
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.25	0.69
2:B:1:MET:SD	2:B:253[B]:ARG:NH1	2.66	0.69
4:F:184:LYS:O	14:F:401:ADP:N6	2.30	0.65
4:F:36:ARG:NH2	15:F:513:HOH:O	2.31	0.64
2:B:1:MET:HB3	2:B:133:GLN:HG2	1.79	0.64
1:C:220:GLU:HG2	2:D:326:LYS:HD3	1.79	0.64
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.79	0.63
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.82	0.62
1:C:207:GLU:HG2	1:C:304:LYS:HE3	1.82	0.62
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.32	0.61
2:D:178:SER:HB3	2:D:179:ASP:HA	1.83	0.61
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.20	0.60
1:C:180:ALA:HB2	12:D:604:2RR:H17	1.84	0.58
2:D:289:PRO:HB2	2:D:290:GLU:HB2	1.84	0.58
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.84	0.58
2:D:352:LYS:HE3	2:D:353:THR:H	1.69	0.58
2:D:255:LEU:HG	12:D:604:2RR:C26	2.34	0.58
11:B:501:GDP:O1A	15:B:639:HOH:O	2.16	0.58
2:B:311:ARG:NH2	2:B:343:PHE:O	2.37	0.57
1:A:98:ASP:O	1:A:105[B]:ARG:NH2	2.37	0.57
1:A:211[B]:ASP:OD2	1:A:215:ARG:NH2	2.38	0.57
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.38	0.56
2:D:248:LEU:HD12	2:D:250:ALA:HB2	1.87	0.56
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.88	0.56
1:C:177:VAL:HG13	1:C:178:SER:H	1.71	0.56
4:F:26:GLN:NE2	15:F:514:HOH:O	2.39	0.55
1:C:221:ARG:NH1	2:D:325:MET:SD	2.80	0.55
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.89	0.55
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.55
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.54
4:F:132:LEU:O	4:F:136:ASN:ND2	2.39	0.54
4:F:139:ARG:NH1	4:F:165:GLU:OE1	2.40	0.54
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.89	0.54
2:D:311:ARG:NH1	2:D:436:GLN:O	2.39	0.54
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:10:ASN:HB2	4:F:44:ARG:HH12	1.72	0.54
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.90	0.53
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.39	0.53
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.89	0.53
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.42	0.52
2:D:185:TYR:OH	2:D:398:MET:O	2.26	0.52
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.90	0.52
2:D:228:ASN:OD1	11:D:602:GDP:N1	2.29	0.52
4:F:184:LYS:NZ	4:F:185:TYR:O	2.42	0.52
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.52
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.92	0.52
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.91	0.52
2:B:2:ARG:NH1	2:B:130:ASP:OD2	2.42	0.52
2:D:289:PRO:CB	2:D:290:GLU:HB2	2.40	0.51
2:D:46:LEU:HA	2:D:49:ILE:HB	1.92	0.51
1:A:217:LEU:HA	1:A:277:SER:HB3	1.93	0.51
2:B:253[A]:ARG:NH1	13:B:505:MES:O3S	2.38	0.51
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.92	0.51
4:F:99:VAL:HA	4:F:181:VAL:HG12	1.93	0.51
2:B:188:THR:HA	2:B:425:MET:HE1	1.93	0.50
1:C:339:ARG:HB2	1:C:341:ILE:HD11	1.93	0.50
4:F:243:HIS:O	4:F:247:LYS:N	2.40	0.50
2:B:161:TYR:HB3	2:B:164:ARG:HG2	1.94	0.50
1:C:255:PHE:CD1	1:C:352:LYS:HD3	2.47	0.50
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.94	0.50
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.93	0.50
1:C:180:ALA:HA	12:D:604:2RR:H16	1.94	0.49
2:D:318:ILE:HD11	12:D:604:2RR:C24	2.42	0.49
2:D:178:SER:CB	2:D:179:ASP:HA	2.42	0.49
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.94	0.49
2:D:1:MET:SD	15:D:717:HOH:O	2.60	0.49
4:F:239:HIS:ND1	4:F:239:HIS:N	2.60	0.49
2:D:143:GLY:O	2:D:186:ASN:ND2	2.46	0.48
4:F:243:HIS:HA	4:F:246:GLN:HB3	1.96	0.48
2:B:334:ASN:O	2:B:338:LYS:HG2	2.13	0.48
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.96	0.48
2:D:388:PHE:HD1	2:D:425:MET:HE3	1.78	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.48
2:D:12:CYS:HB2	11:D:602:GDP:C8	2.48	0.47
4:F:186:LEU:N	14:F:401:ADP:N1	2.47	0.47
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:GLU:HG2	1:C:339:ARG:HH22	1.80	0.47
1:C:341:ILE:N	1:C:341:ILE:CD1	2.73	0.47
1:A:386:GLU:O	1:A:390:ARG:HG2	2.14	0.47
2:D:271:GLY:HA3	2:D:377:PHE:HB3	1.97	0.47
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.49	0.46
4:F:138:ARG:NH1	4:F:144:GLY:O	2.47	0.46
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.98	0.46
4:F:252:ASN:HD21	4:F:255:ARG:HH21	1.62	0.46
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.51	0.46
2:D:255:LEU:CG	12:D:604:2RR:C26	2.94	0.46
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.80	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.46
1:A:97:GLU:HG2	1:A:105[B]:ARG:HH22	1.81	0.46
2:D:255:LEU:HG	12:D:604:2RR:C27	2.46	0.46
1:A:147:SER:HB2	1:A:190:THR:HB	1.98	0.46
12:D:604:2RR:C21	12:D:604:2RR:N11	2.80	0.45
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.17	0.45
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.98	0.45
2:B:199:ASP:OD2	13:B:505:MES:H52	2.17	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.52	0.45
2:D:152:LEU:O	2:D:156:LYS:HG2	2.17	0.45
2:D:255:LEU:HD21	12:D:604:2RR:C26	2.46	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.99	0.45
4:F:198:LYS:HD3	4:F:239:HIS:HA	1.97	0.45
2:B:303:ALA:O	2:B:305:CYS:N	2.50	0.45
1:A:2:ARG:O	1:A:133:GLN:NE2	2.47	0.45
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.45
4:F:230:SER:O	4:F:233:PHE:CZ	2.70	0.45
2:B:188:THR:HG23	2:B:425:MET:HE3	1.98	0.44
2:B:360:PRO:HG2	2:B:371[A]:LEU:HB2	1.99	0.44
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.99	0.44
2:D:295:MET:CG	2:D:377:PHE:HB2	2.48	0.44
1:C:44:GLY:HA2	1:C:55:GLU:HB2	1.99	0.44
2:D:288:VAL:HA	2:D:291:LEU:HB2	1.99	0.44
12:B:504:2RR:C20	12:B:504:2RR:N11	2.81	0.44
2:D:255:LEU:HD21	12:D:604:2RR:H3	1.98	0.44
2:B:238:VAL:HG23	2:B:239:THR:HG23	2.00	0.44
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.49	0.44
1:C:180:ALA:HB2	12:D:604:2RR:C17	2.48	0.44
2:D:69:ASP:OD1	2:D:70:LEU:N	2.50	0.44
2:B:12:CYS:HB2	11:B:501:GDP:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:VAL:HG11	2:B:153:LEU:HD11	2.00	0.43
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.53	0.43
2:B:70:LEU:HD12	2:B:99:ALA:HB2	2.01	0.43
2:D:2:ARG:NH1	2:D:130:ASP:HB3	2.33	0.43
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.00	0.43
2:B:318:ILE:HG13	2:B:354:ALA:HB3	2.00	0.43
1:C:343:PHE:CD1	1:C:349:THR:HG23	2.53	0.43
2:B:360:PRO:HG2	2:B:371[B]:LEU:HB2	2.01	0.43
2:D:385:GLN:HB2	2:D:429:VAL:HG13	2.00	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.92	0.43
3:E:101:LEU:O	3:E:105[A]:MET:HG2	2.19	0.43
1:C:181[A]:VAL:HG22	12:D:604:2RR:C6	2.49	0.43
2:D:141:LEU:HD22	2:D:190:SER:HB3	2.01	0.43
2:D:316:ALA:HB3	2:D:378:ILE:HB	2.01	0.42
4:F:377:LYS:HE2	4:F:379:HIS:CE1	2.54	0.42
2:B:221:THR:HG21	1:C:325:PRO:HB2	2.00	0.42
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.59	0.42
4:F:84:SER:O	4:F:88:SER:N	2.45	0.42
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.19	0.42
1:A:105[B]:ARG:HG2	1:A:411:GLU:HG3	2.00	0.42
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.02	0.42
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	2.02	0.42
2:D:71:GLU:HA	2:D:72:PRO:HD3	1.89	0.42
2:D:27:GLU:OE1	2:D:236:SER:OG	2.34	0.42
2:D:288:VAL:O	2:D:291:LEU:N	2.49	0.42
2:B:320:ARG:HD3	2:B:360:PRO:HD3	2.02	0.42
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.01	0.42
4:F:240:LEU:HD23	14:F:401:ADP:H4'	2.01	0.42
2:D:255:LEU:CD2	12:D:604:2RR:H3	2.50	0.42
2:D:289:PRO:CA	2:D:290:GLU:HB2	2.49	0.42
2:D:352:LYS:HB2	12:D:604:2RR:C4	2.49	0.42
3:E:96:MET:HB3	3:E:100:LYS:HE3	2.01	0.42
4:F:55:GLU:HA	4:F:56:PRO:HD3	1.91	0.42
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.02	0.41
12:B:504:2RR:N11	12:B:504:2RR:H1	2.34	0.41
1:C:340:SER:HB3	15:C:699:HOH:O	2.19	0.41
2:D:136:GLN:HA	2:D:167:ASN:O	2.20	0.41
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.45	0.41
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.56	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.02	0.41
4:F:43:GLU:OE2	4:F:43:GLU:N	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:217:ARG:HE	4:F:374:ILE:HA	1.85	0.41
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.21	0.40
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.43	0.40
2:D:83:PHE:O	2:D:86:ILE:HG22	2.21	0.40
2:D:288:VAL:C	2:D:291:LEU:H	2.25	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	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	47	68
1	C	453/451 (100%)	443 (98%)	9 (2%)	1 (0%)	47	68
2	B	430/445 (97%)	417 (97%)	11 (3%)	2 (0%)	29	48
2	D	421/445 (95%)	402 (96%)	17 (4%)	2 (0%)	29	48
3	E	125/143 (87%)	124 (99%)	1 (1%)	0	100	100
4	F	325/384 (85%)	313 (96%)	12 (4%)	0	100	100
All	All	2201/2319 (95%)	2130 (97%)	65 (3%)	6 (0%)	41	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	290	GLU
2	D	181	VAL
1	C	177	VAL
1	A	178	SER
2	B	304	ALA
2	B	82	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	382/379 (101%)	381 (100%)	1 (0%)	92	97
1	C	386/379 (102%)	382 (99%)	4 (1%)	76	90
2	B	378/383 (99%)	374 (99%)	4 (1%)	73	89
2	D	368/383 (96%)	357 (97%)	11 (3%)	41	68
3	E	115/127 (91%)	115 (100%)	0	100	100
4	F	303/342 (89%)	301 (99%)	2 (1%)	84	94
All	All	1932/1993 (97%)	1910 (99%)	22 (1%)	73	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	ARG
2	B	139	HIS
2	B	167[A]	ASN
2	B	167[B]	ASN
2	B	323	MET
1	C	2	ARG
1	C	176	GLN
1	C	179	THR
1	C	340	SER
2	D	130	ASP
2	D	139	HIS
2	D	181	VAL
2	D	248	LEU
2	D	249	ASN
2	D	255	LEU
2	D	286	LEU
2	D	290	GLU
2	D	291	LEU
2	D	352	LYS
2	D	401	ARG
4	F	239	HIS
4	F	379	HIS

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
2	B	8	GLN

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	$\#\|Z\| > 2$
12	2RR	D	604	-	25,32,32	1.23	2 (8%)	29,44,44	1.66	6 (20%)
11	GDP	D	602	6	24,30,30	0.95	1 (4%)	30,47,47	1.22	4 (13%)
9	GOL	A	505	-	5,5,5	0.38	0	5,5,5	0.25	0
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.48	5 (15%)
11	GDP	B	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.16	3 (10%)
10	IMD	A	506	-	3,5,5	0.42	0	4,5,5	0.59	0
5	GTP	A	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.49	6 (18%)
13	MES	B	505	-	12,12,12	2.29	1 (8%)	14,16,16	2.44	7 (50%)
14	ADP	F	401	-	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	2RR	B	504	-	25,32,32	1.21	2 (8%)	29,44,44	1.65	5 (17%)

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	2RR	D	604	-	-	2/11/17/17	0/4/4/4
11	GDP	D	602	6	-	5/12/32/32	0/3/3/3
9	GOL	A	505	-	-	2/4/4/4	-
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
11	GDP	B	501	-	-	4/12/32/32	0/3/3/3
10	IMD	A	506	-	-	-	0/1/1/1
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
13	MES	B	505	-	-	2/6/14/14	0/1/1/1
14	ADP	F	401	-	-	2/12/32/32	0/3/3/3
12	2RR	B	504	-	-	0/11/17/17	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	505	MES	C8-S	-7.69	1.66	1.77
12	D	604	2RR	C14-N15	4.19	1.41	1.34
12	B	504	2RR	C14-N15	4.09	1.41	1.34
5	A	501	GTP	C5-C6	-4.01	1.39	1.47
5	C	501	GTP	C5-C6	-3.95	1.39	1.47
12	D	604	2RR	C22-C21	-2.51	1.45	1.49
12	B	504	2RR	C22-C21	-2.48	1.45	1.49
14	F	401	ADP	C5-C4	2.45	1.47	1.40
11	B	501	GDP	C6-N1	-2.34	1.34	1.37
11	D	602	GDP	C6-N1	-2.29	1.34	1.37
5	C	501	GTP	C2-N3	2.16	1.38	1.33
5	A	501	GTP	C2-N3	2.14	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	505	MES	C5-N4-C3	5.30	120.77	108.83
12	D	604	2RR	C16-N15-C14	-4.88	114.68	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	504	2RR	C16-N15-C14	-4.78	114.85	122.95
12	B	504	2RR	C10-C2-N1	-3.50	121.12	126.06
13	B	505	MES	C7-N4-C5	3.48	120.13	111.23
12	D	604	2RR	C21-C20-N1	3.46	115.75	110.95
14	F	401	ADP	N3-C2-N1	-3.31	123.51	128.68
5	A	501	GTP	PA-O3A-PB	-3.30	121.51	132.83
5	C	501	GTP	PB-O3B-PG	-3.27	121.60	132.83
14	F	401	ADP	PA-O3A-PB	-3.23	121.75	132.83
5	A	501	GTP	C5-C6-N1	3.14	119.50	113.95
14	F	401	ADP	C3'-C2'-C1'	3.14	105.70	100.98
5	C	501	GTP	PA-O3A-PB	-3.13	122.09	132.83
5	C	501	GTP	C5-C6-N1	3.11	119.45	113.95
5	A	501	GTP	PB-O3B-PG	-3.11	122.14	132.83
12	D	604	2RR	C10-C2-N1	-3.09	121.70	126.06
13	B	505	MES	C7-N4-C3	3.08	119.10	111.23
5	C	501	GTP	C8-N7-C5	3.03	108.77	102.99
5	A	501	GTP	C8-N7-C5	3.01	108.73	102.99
11	D	602	GDP	PA-O3A-PB	-2.98	122.60	132.83
13	B	505	MES	C6-C5-N4	-2.97	105.60	110.10
11	B	501	GDP	PA-O3A-PB	-2.86	123.00	132.83
5	C	501	GTP	C2-N1-C6	-2.80	119.95	125.10
5	A	501	GTP	C2-N1-C6	-2.78	119.97	125.10
11	D	602	GDP	C3'-C2'-C1'	2.58	104.86	100.98
14	F	401	ADP	C4-C5-N7	-2.55	106.74	109.40
12	B	504	2RR	C8-C9-C4	2.48	125.35	121.30
13	B	505	MES	O3S-S-C8	2.44	109.72	105.77
11	D	602	GDP	C8-N7-C5	2.36	107.48	102.99
11	B	501	GDP	C5-C6-N1	2.35	118.10	113.95
11	B	501	GDP	C8-N7-C5	2.34	107.44	102.99
12	B	504	2RR	C7-C8-C9	-2.27	115.09	119.44
13	B	505	MES	O2S-S-C8	2.24	109.61	106.92
12	D	604	2RR	C8-C9-C4	2.21	124.91	121.30
13	B	505	MES	C2-C3-N4	-2.15	106.85	110.10
11	D	602	GDP	C5-C6-N1	2.10	117.67	113.95
12	B	504	2RR	C24-C25-C26	2.09	121.39	118.15
12	D	604	2RR	C7-C8-C9	-2.08	115.45	119.44
12	D	604	2RR	C24-C25-C26	2.08	121.38	118.15
5	A	501	GTP	O6-C6-C5	-2.03	120.41	124.37

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
9	A	505	GOL	O1-C1-C2-C3
11	B	501	GDP	C5'-O5'-PA-O1A
11	B	501	GDP	C5'-O5'-PA-O2A
11	D	602	GDP	C5'-O5'-PA-O1A
11	D	602	GDP	C5'-O5'-PA-O2A
12	D	604	2RR	N15-C16-C17-C18
13	B	505	MES	C8-C7-N4-C5
14	F	401	ADP	O4'-C4'-C5'-O5'
14	F	401	ADP	C3'-C4'-C5'-O5'
9	A	505	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
11	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
12	D	604	2RR	C21-C20-N1-C2
13	B	505	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	B	501	GDP	C5'-O5'-PA-O3A
11	D	602	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
11	D	602	GDP	PB-O3A-PA-O1A
11	D	602	GDP	PB-O3A-PA-O2A

There are no ring outliers.

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	604	2RR	17	0
11	D	602	GDP	2	0
11	B	501	GDP	2	0
5	A	501	GTP	1	0
13	B	505	MES	2	0
14	F	401	ADP	3	0

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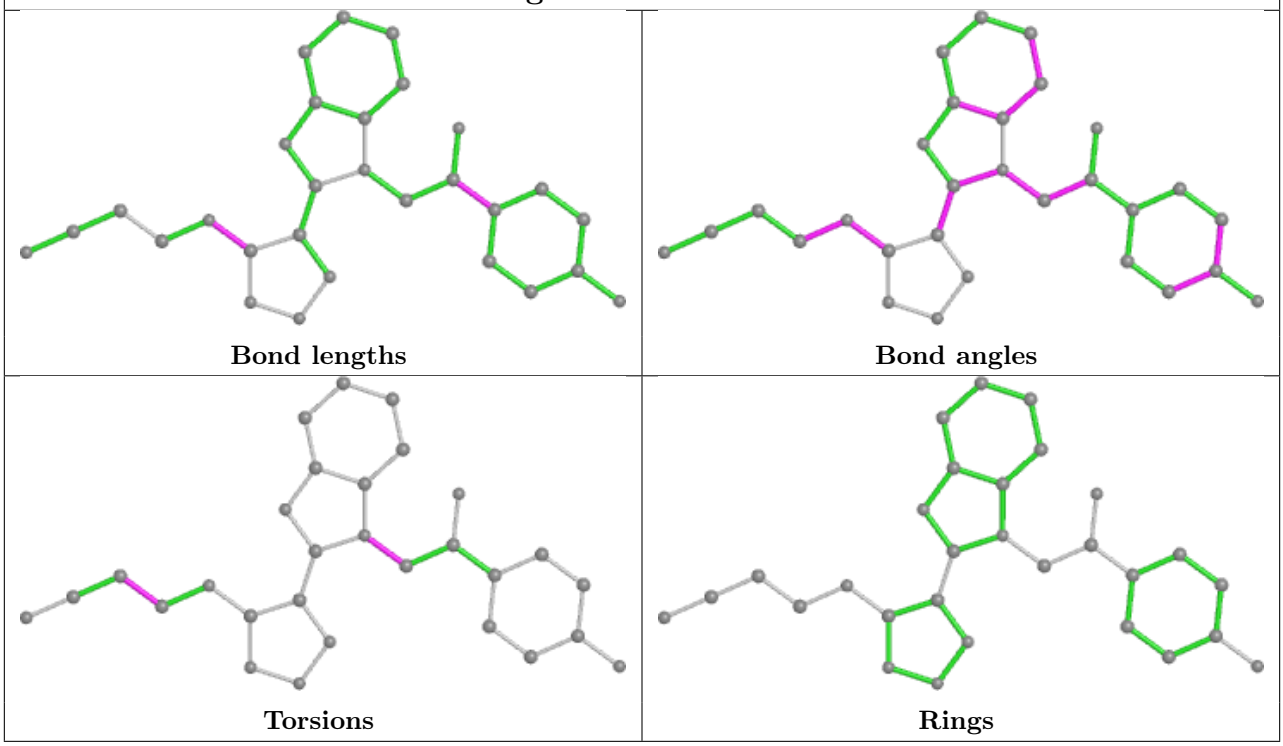
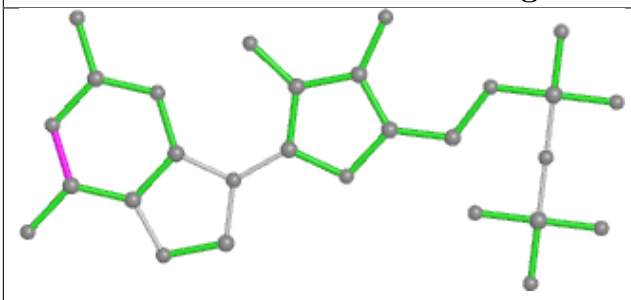
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	504	2RR	2	0

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.

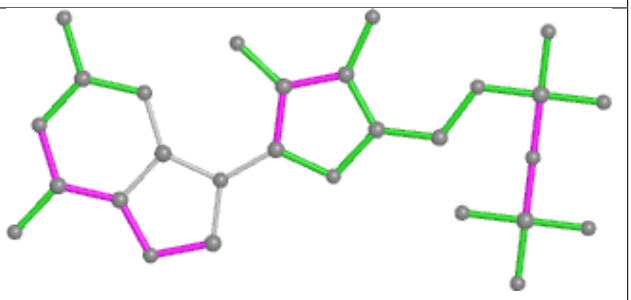
Ligand 2RR D 604



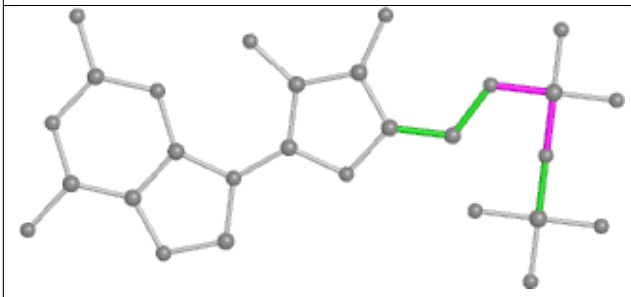
Ligand GDP D 602



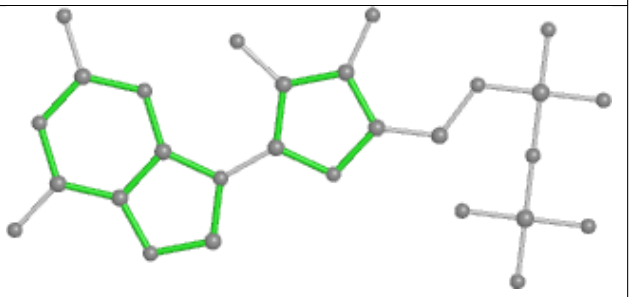
Bond lengths



Bond angles

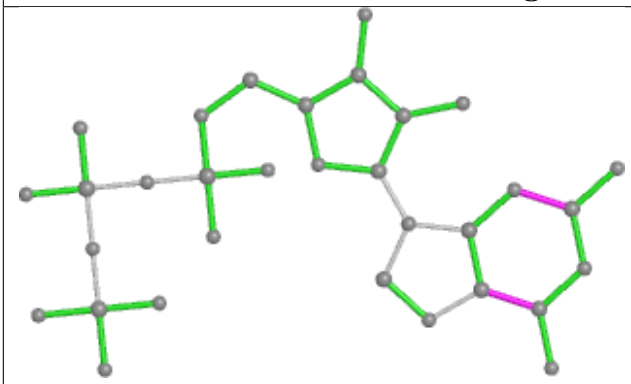


Torsions

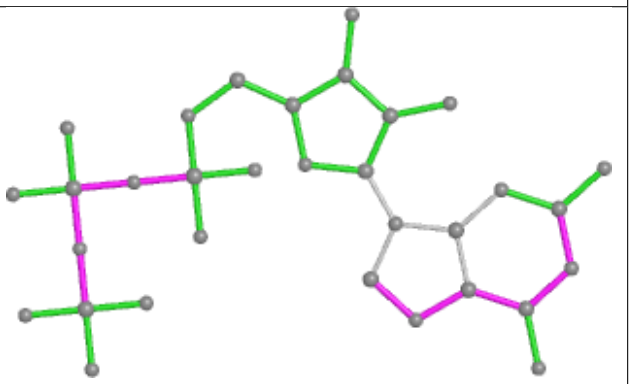


Rings

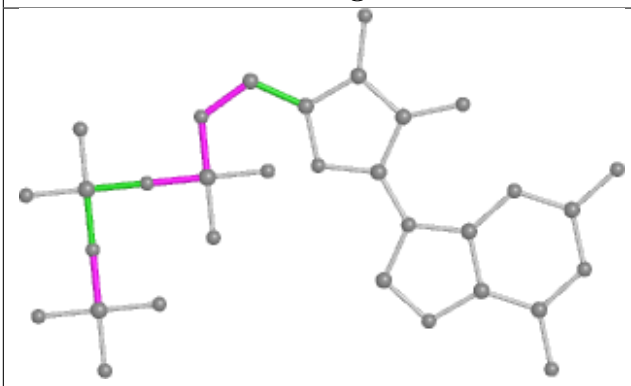
Ligand GTP C 501



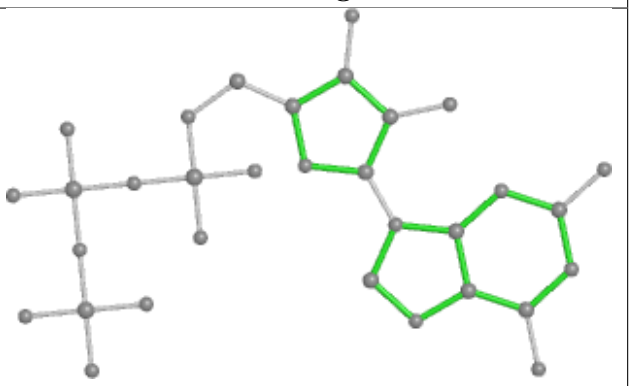
Bond lengths



Bond angles

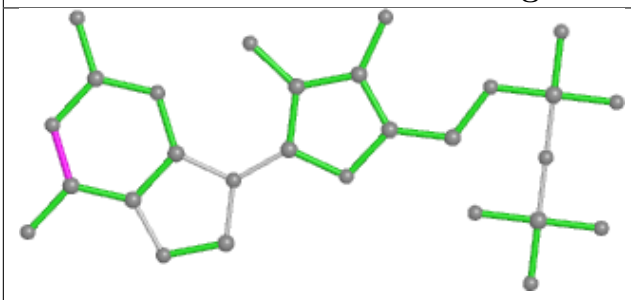


Torsions

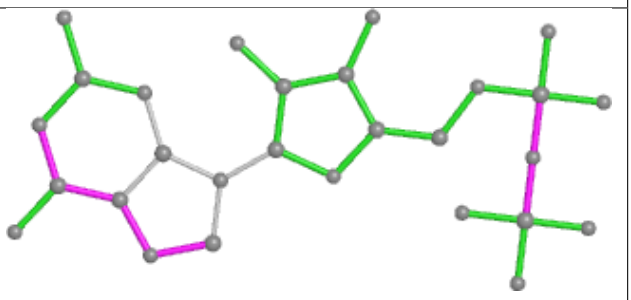


Rings

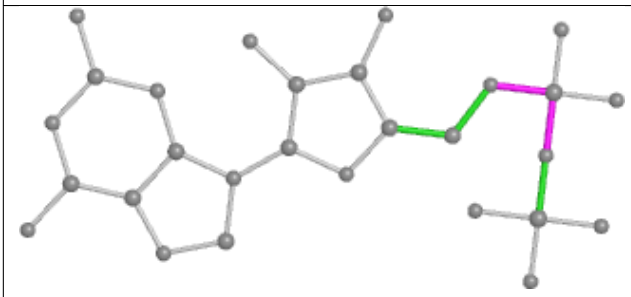
Ligand GDP B 501



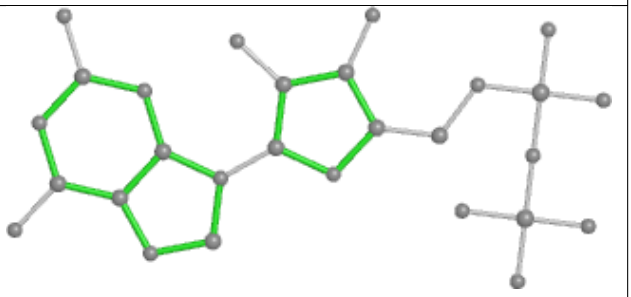
Bond lengths



Bond angles

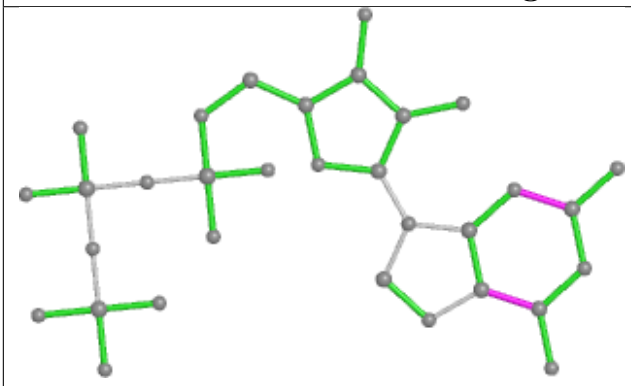


Torsions

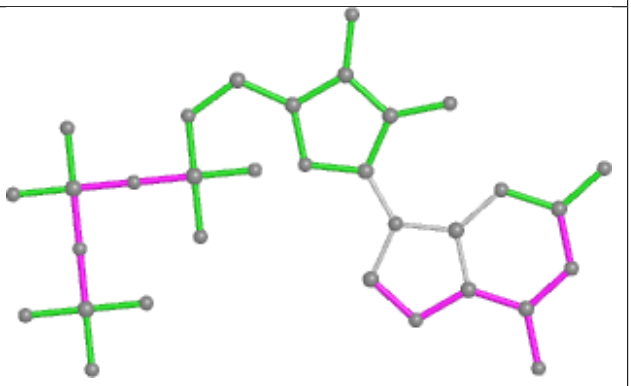


Rings

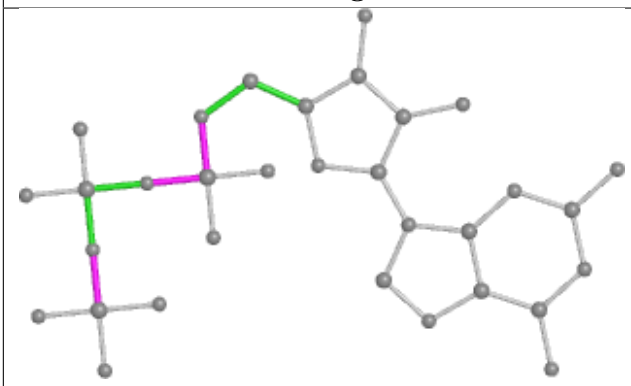
Ligand GTP A 501



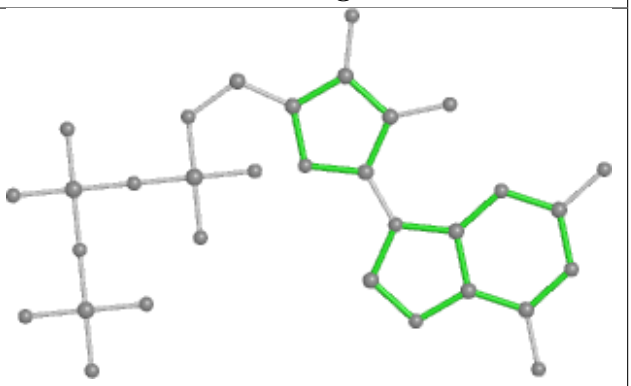
Bond lengths



Bond angles

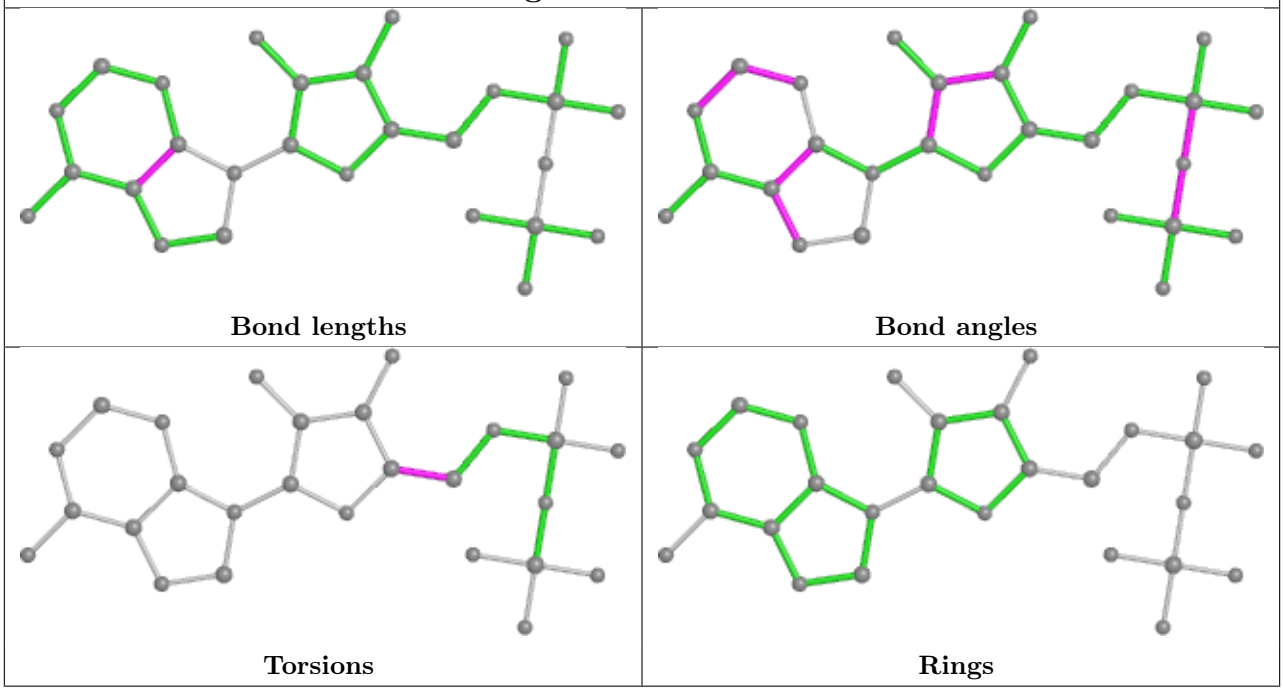


Torsions

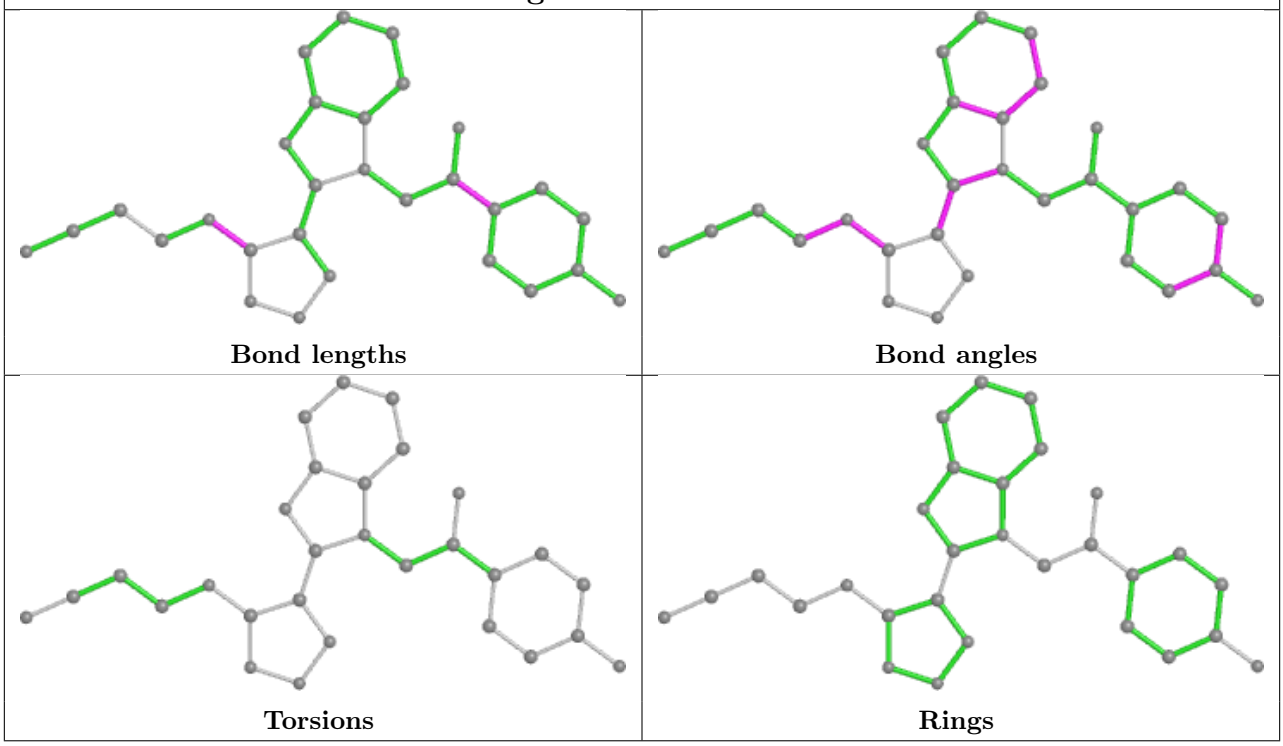


Rings

Ligand ADP F 401



Ligand 2RR B 504



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	439/451 (97%)	0.14	3 (0%)	87	89	25, 44, 77, 114	0
1	C	440/451 (97%)	0.11	2 (0%)	91	91	15, 31, 65, 98	0
2	B	418/445 (93%)	0.23	4 (0%)	82	84	19, 41, 78, 112	2 (0%)
2	D	421/445 (94%)	0.26	14 (3%)	46	50	24, 58, 93, 116	6 (1%)
3	E	124/143 (86%)	0.40	4 (3%)	47	51	32, 58, 102, 130	0
4	F	331/384 (86%)	1.35	93 (28%)	0	0	32, 65, 143, 162	0
All	All	2173/2319 (93%)	0.37	120 (5%)	25	26	15, 47, 99, 162	8 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	8.9
4	F	249	TYR	8.1
4	F	240	LEU	7.8
4	F	251	LYS	7.8
4	F	253	TYR	7.5
4	F	233	PHE	7.3
4	F	252	ASN	7.1
4	F	250	SER	6.5
4	F	241	THR	6.4
4	F	243	HIS	6.0
1	C	177	VAL	5.3
4	F	234	GLN	5.2
4	F	229	ASN	5.0
4	F	242	ASN	4.9
2	B	438	ALA	4.9
4	F	232	ASN	4.9
4	F	166	ALA	4.9
4	F	170	LEU	4.8
4	F	245	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	4.8
4	F	256	TYR	4.6
2	D	402	LYS	4.4
2	D	335	VAL	4.3
4	F	231	ALA	4.2
2	B	437	ASP	4.1
4	F	169	LEU	4.1
4	F	182	ILE	3.9
4	F	379	HIS	3.8
4	F	248	GLU	3.7
4	F	330	ILE	3.7
4	F	238	CYS	3.7
2	D	400	ARG	3.7
4	F	239	HIS	3.7
4	F	99	VAL	3.6
4	F	257	GLU	3.6
4	F	133	ALA	3.5
4	F	131	PHE	3.4
4	F	228	TYR	3.4
4	F	224	SER	3.4
4	F	259	GLY	3.3
1	A	450	GLU	3.3
4	F	181	VAL	3.3
4	F	162	ILE	3.1
2	D	179	ASP	3.1
4	F	225	SER	3.1
2	D	1	MET	3.1
3	E	25	LYS	3.0
4	F	263	PHE	3.0
4	F	127	GLU	3.0
2	D	332	MET	3.0
4	F	254	GLY	3.0
4	F	147	TRP	3.0
2	D	295	MET	3.0
4	F	319	PHE	2.9
4	F	246	GLN	2.9
4	F	199	PHE	2.9
3	E	119	MET	2.9
4	F	315	PHE	2.9
4	F	320	MET	2.8
2	D	275	LEU	2.8
4	F	351	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	255	ARG	2.8
4	F	247	LYS	2.7
4	F	236	LYS	2.7
2	D	296	PHE	2.7
4	F	329	LEU	2.7
4	F	20	LEU	2.7
4	F	192	LEU	2.6
2	D	415	GLU	2.6
4	F	258	GLU	2.6
4	F	17	VAL	2.6
4	F	333	ASN	2.6
1	C	178	SER	2.6
4	F	235	ASP	2.6
4	F	221	LEU	2.5
4	F	260	ASN	2.5
1	A	262	TYR	2.5
4	F	130	VAL	2.5
4	F	283	ILE	2.5
4	F	197	ARG	2.5
4	F	190	LEU	2.5
4	F	167	SER	2.5
4	F	222	ARG	2.5
2	D	405	LEU	2.5
4	F	14	TYR	2.5
4	F	271[A]	LEU	2.5
4	F	323	GLU	2.5
4	F	343	TYR	2.5
4	F	220	VAL	2.4
4	F	100	ILE	2.4
4	F	237	THR	2.4
3	E	120	LEU	2.4
4	F	163	SER	2.4
4	F	264	PHE	2.4
4	F	21	LEU	2.4
2	D	255	LEU	2.3
4	F	290	ILE	2.3
2	B	59	ASN	2.3
4	F	44	ARG	2.3
4	F	183	GLN	2.3
2	D	177	VAL	2.2
4	F	335	ALA	2.2
4	F	39	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	204	TRP	2.2
4	F	227	PRO	2.2
4	F	145	ASN	2.2
2	D	178	SER	2.2
4	F	27	TRP	2.2
4	F	31	ARG	2.1
4	F	90	SER	2.1
4	F	223	THR	2.1
2	B	358	ILE	2.1
4	F	186	LEU	2.1
4	F	216	TYR	2.1
1	A	351	PHE	2.1
4	F	317	PHE	2.1
4	F	337	ALA	2.0
4	F	267	PHE	2.0
4	F	139	ARG	2.0
3	E	115[A]	HIS	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
14	ADP	F	401	27/27	0.69	0.62	165,168,234,394	0
12	2RR	D	604	29/29	0.75	0.64	60,72,78,80	0
8	CL	A	504	1/1	0.78	0.14	78,78,78,78	0
9	GOL	A	505	6/6	0.81	0.20	90,97,99,99	0
10	IMD	A	506	5/5	0.84	0.23	92,92,94,95	0
6	MG	D	601	1/1	0.88	0.15	23,23,23,23	0

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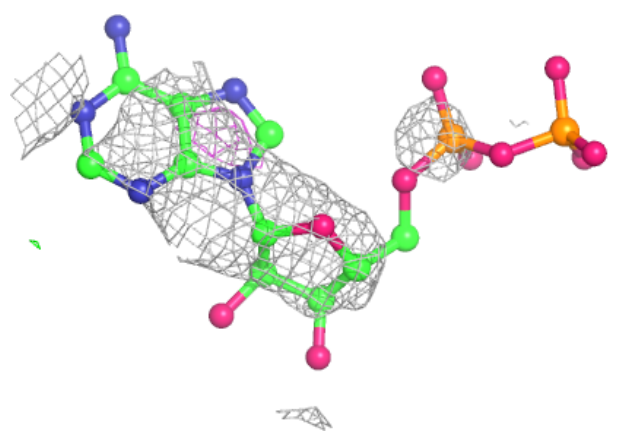
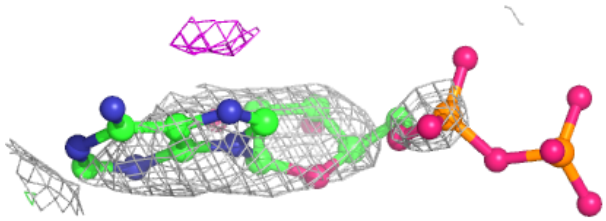
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	B	503	1/1	0.89	0.32	81,81,81,81	0
6	MG	A	502	1/1	0.90	0.16	25,25,25,25	0
6	MG	B	502	1/1	0.93	0.33	47,47,47,47	0
12	2RR	B	504	29/29	0.95	0.16	34,47,54,55	0
7	CA	A	503	1/1	0.95	0.13	62,62,62,62	0
11	GDP	D	602	28/28	0.95	0.17	35,44,62,69	0
13	MES	B	505	12/12	0.96	0.16	41,50,67,67	0
6	MG	D	603	1/1	0.97	0.07	44,44,44,44	0
7	CA	E	700	1/1	0.97	0.19	84,84,84,84	0
11	GDP	B	501	28/28	0.97	0.18	18,27,36,43	0
5	GTP	A	501	32/32	0.97	0.17	13,31,36,67	0
6	MG	B	506	1/1	0.98	0.12	42,42,42,42	0
7	CA	C	502	1/1	0.98	0.16	58,58,58,58	0
5	GTP	C	501	32/32	0.98	0.15	11,22,35,62	0

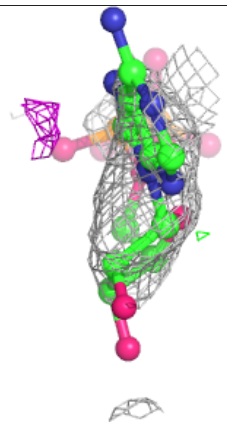
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

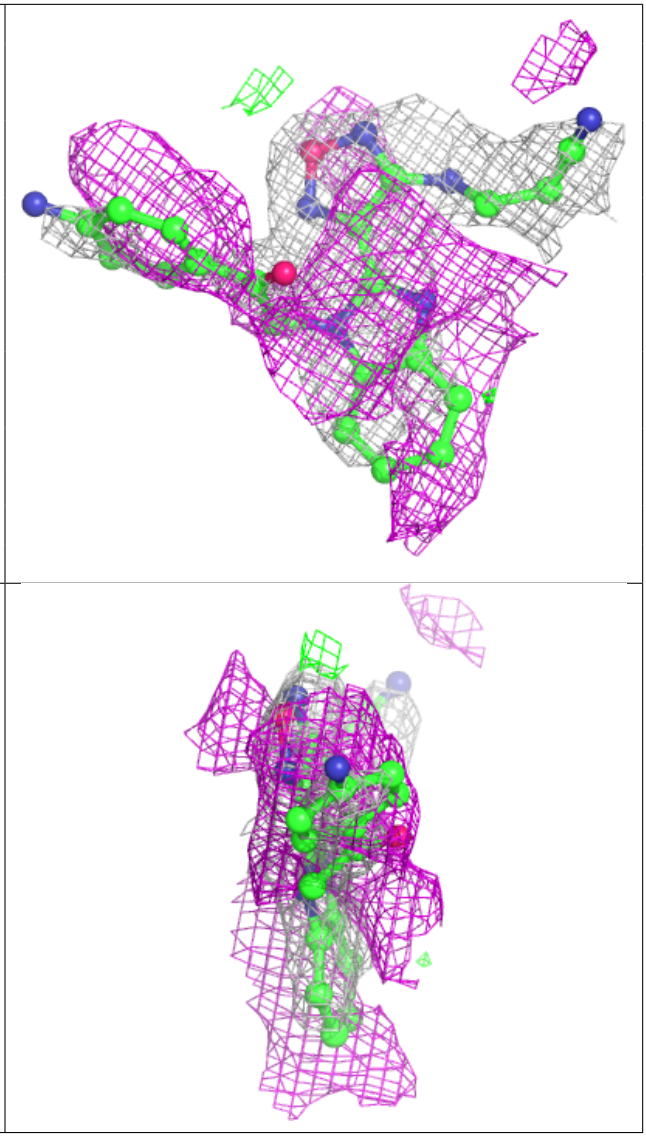






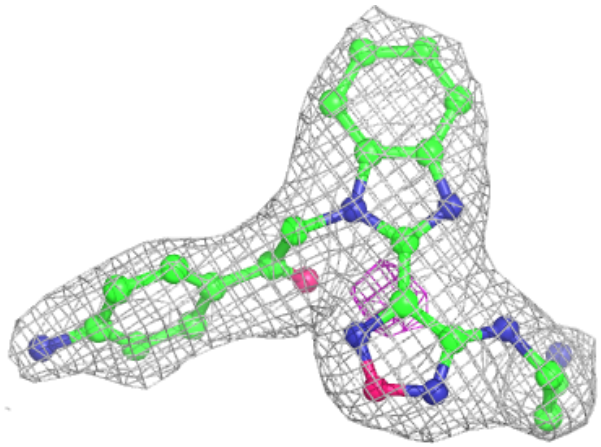
Electron density around 2RR D 604:

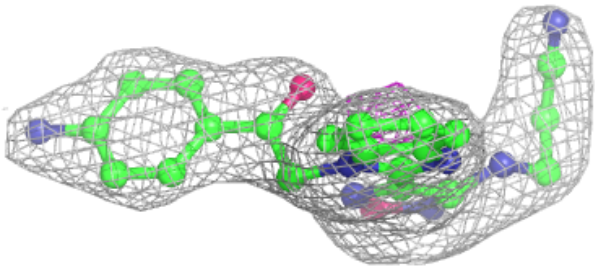
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

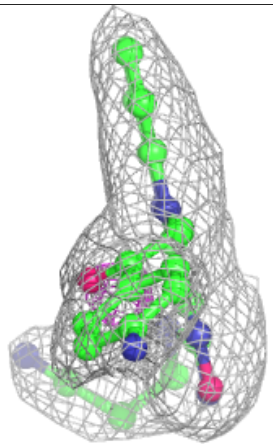


Electron density around 2RR B 504:

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

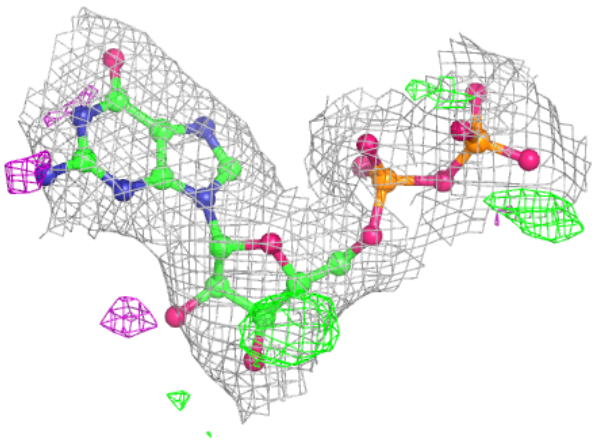


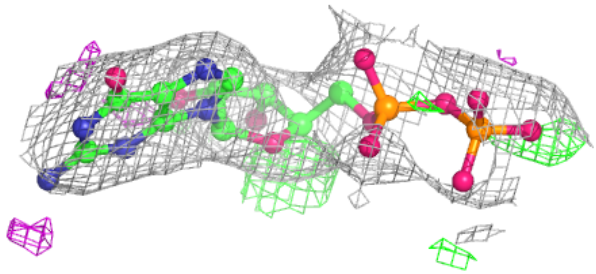


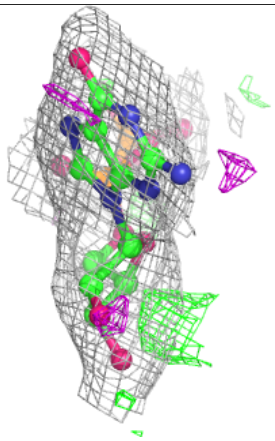


Electron density around GDP D 602:

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

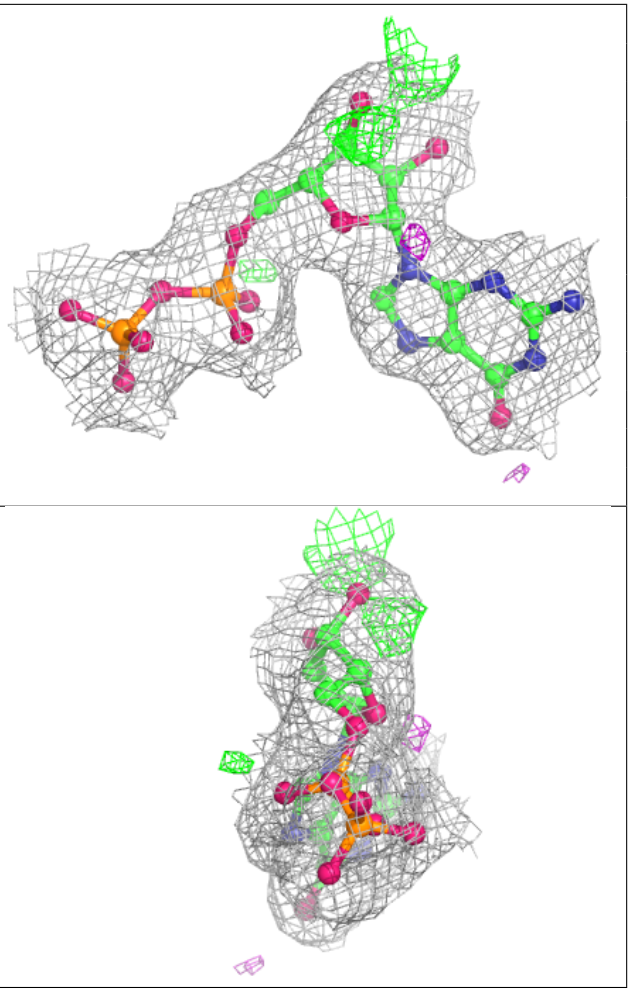






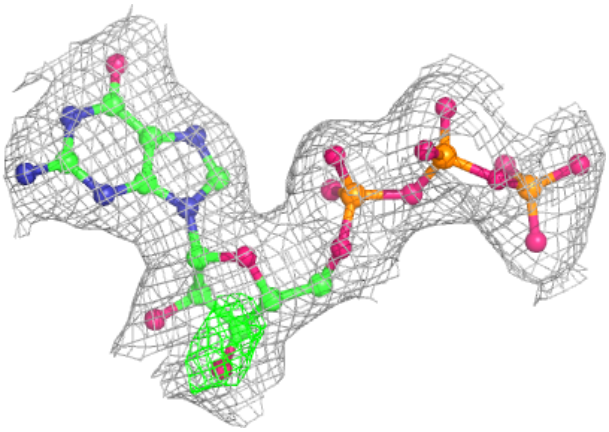
Electron density around GDP B 501:

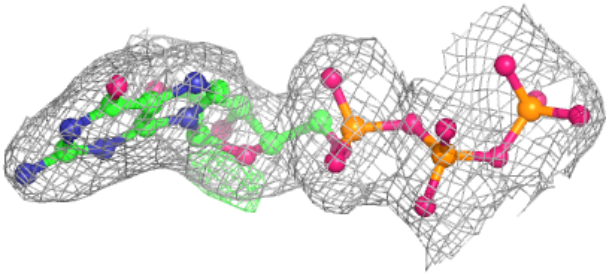
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

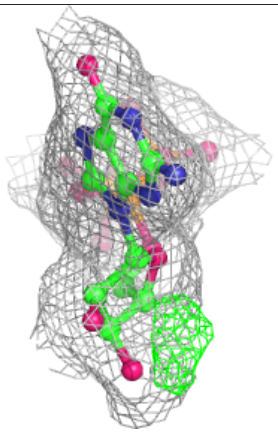


Electron density around GTP A 501:

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

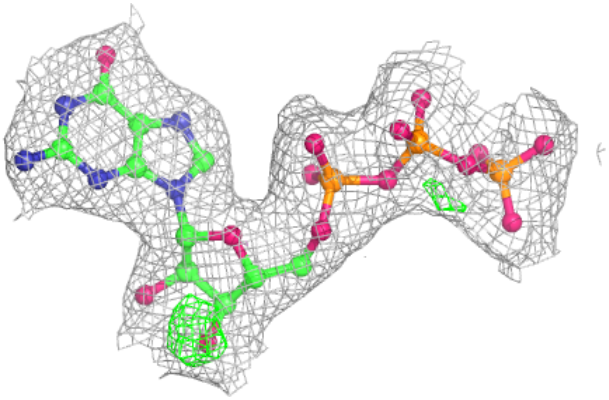


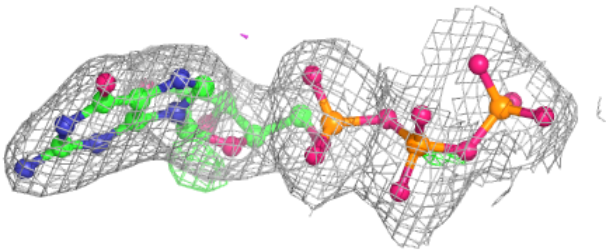


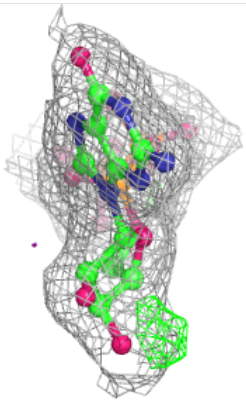


Electron density around GTP C 501:

$2mF_o$-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.