Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2022 – 12:23 pm GMT

PDB ID	:	5LXT
Title	:	Tubulin-Discodermolide complex
Authors	:	Prota, A.E.; Steinmetz, M.O.
Deposited on	:	2016-09-22
Resolution	:	1.90 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 following versions of software and data (see references (i)) were used in the production of this report:

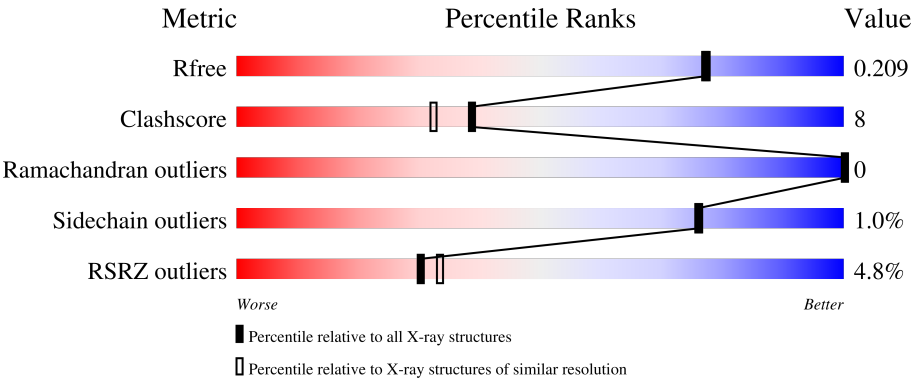
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	83% 14%
1	C	451	84% 14%
2	B	445	80% 16%
2	D	445	3% 80% 16%
3	E	143	2% 69% 17% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	19% 75% 17% 8%

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
9	MES	B	504	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 19693 atoms, of which 108 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	14	0
			3513	2230	589	669	25			
1	C	440	Total	C	N	O	S	0	14	0
			3499	2219	587	668	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	10	0
			3398	2137	579	654	28			
2	D	426	Total	C	N	O	S	0	6	0
			3366	2116	570	651	29			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	6	0
			1044	646	187	205	6			

There are 2 discrepancies between the modelled and reference sequences:

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

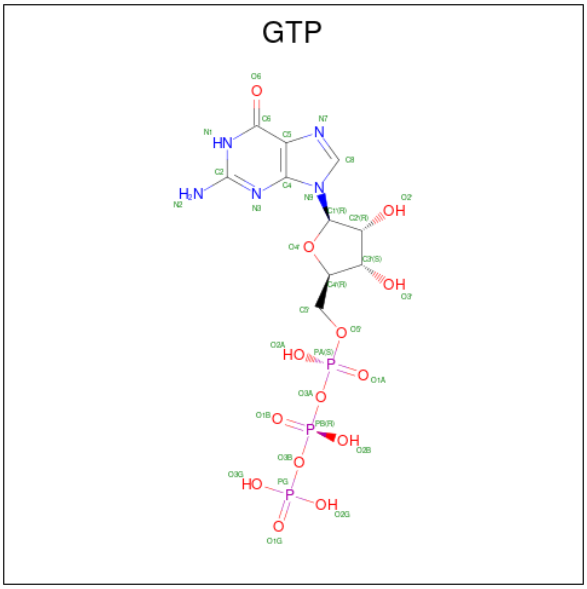
- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	354	Total	C	N	O	S	0	8	0
			2942	1890	508	529	15			

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	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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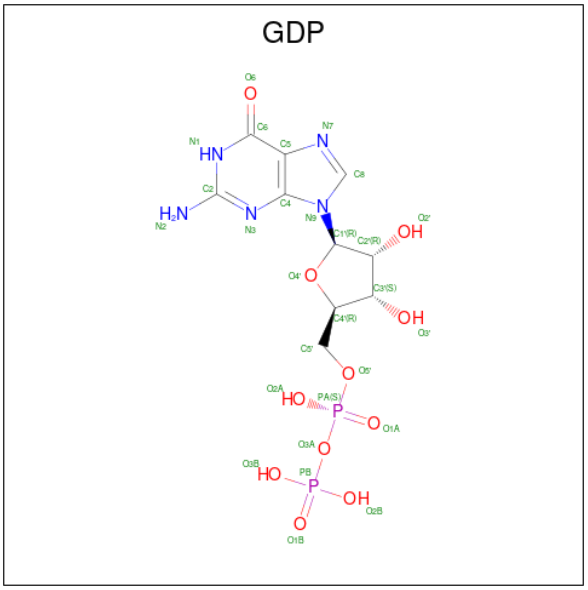
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

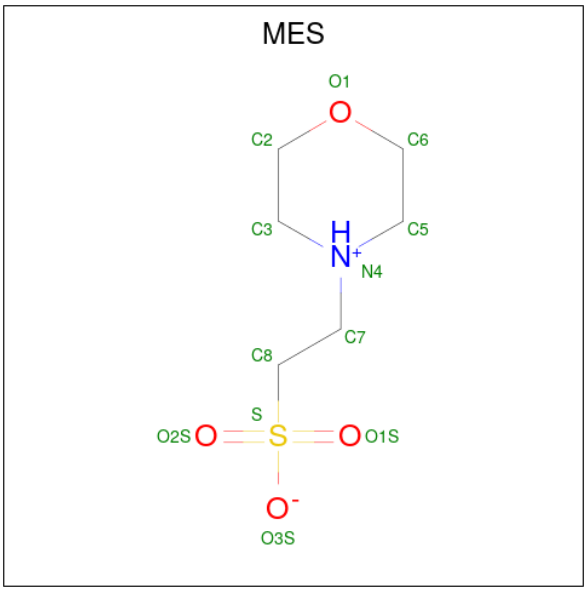
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



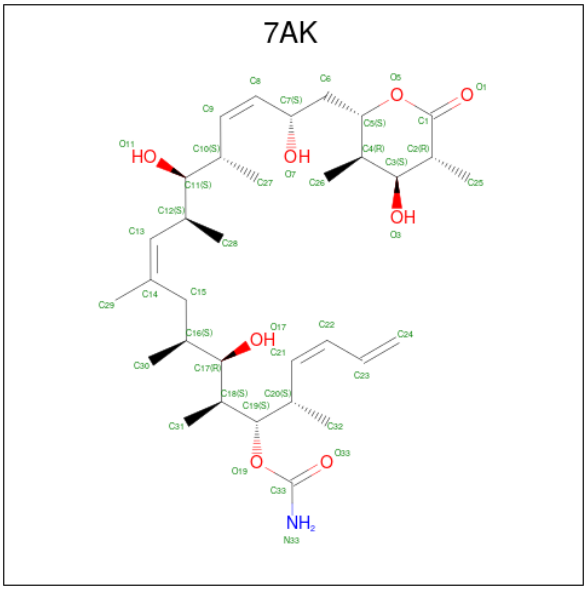
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

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



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

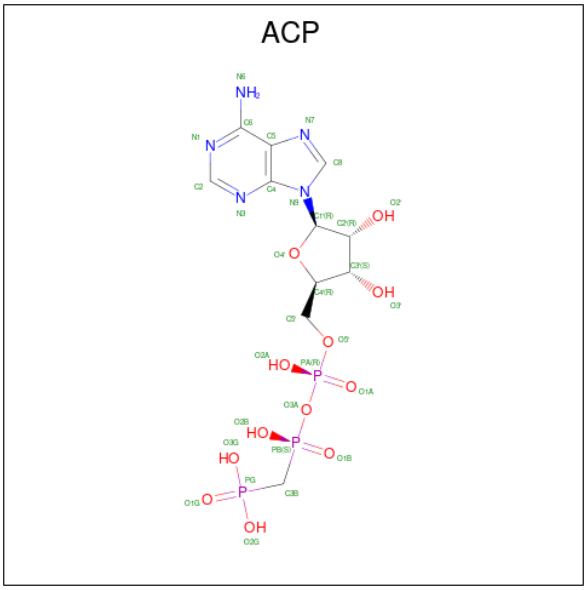
- Molecule 10 is (+)-Discodermolide (three-letter code: 7AK) (formula: $C_{33}H_{55}NO_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			96	33	54	1	8		
10	D	1	Total	C	H	N	O	0	0
			96	33	54	1	8		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-

letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

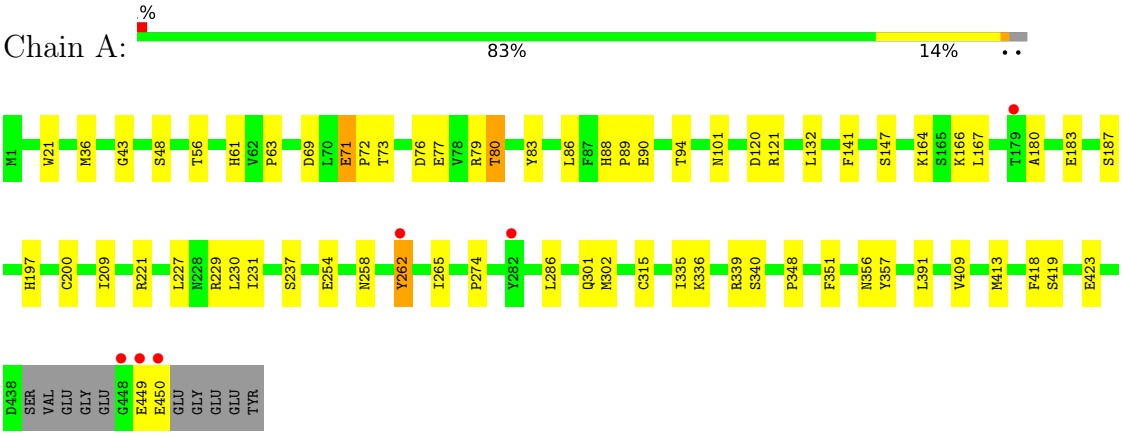
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	313	Total	O	0	0
			313	313		
12	B	307	Total	O	0	0
			307	307		
12	C	477	Total	O	0	0
			477	477		
12	D	226	Total	O	0	0
			226	226		
12	E	108	Total	O	0	0
			108	108		
12	F	136	Total	O	0	0
			136	136		

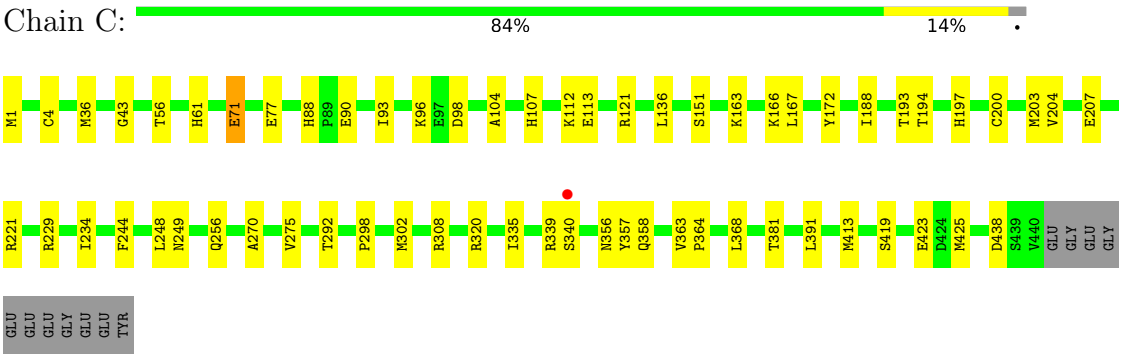
3 Residue-property plots (i)

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.

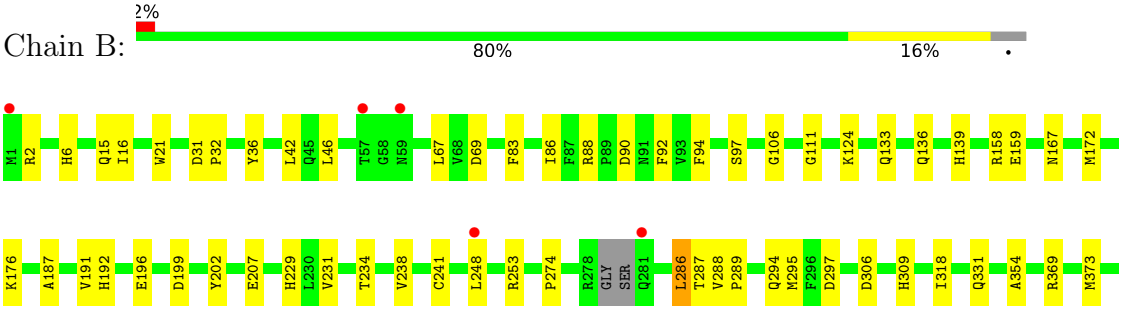
• Molecule 1: Tubulin alpha-1B chain

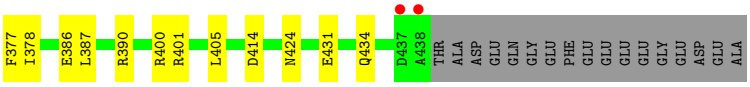


• Molecule 1: Tubulin alpha-1B chain

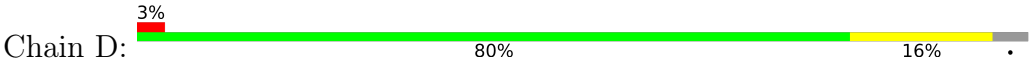


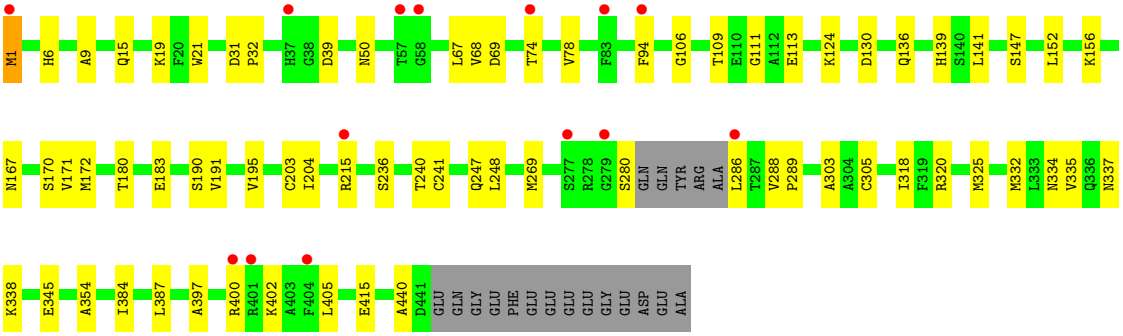
• Molecule 2: Tubulin beta-2B chain



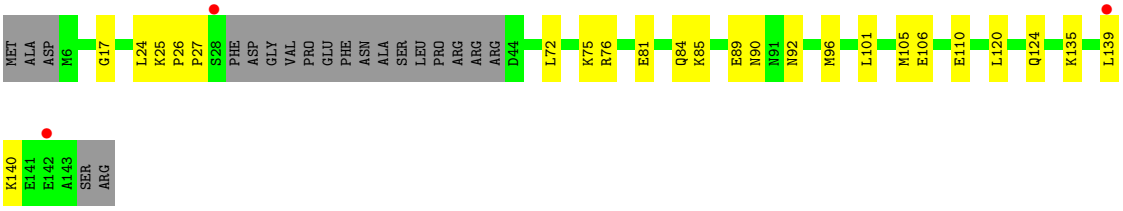


• Molecule 2: Tubulin beta-2B chain

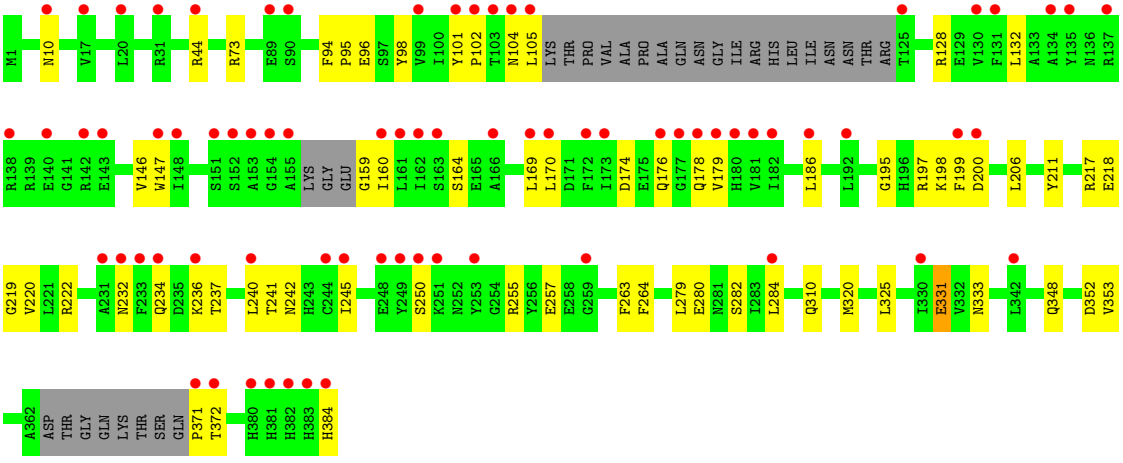




• Molecule 3: Stathmin-4



• Molecule 4: TUBULIN-TYROSINE LIGASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.50Å 157.79Å 180.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.25 – 1.90 78.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.25-1.90) 100.0 (78.89-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.173 , 0.208 0.174 , 0.209	Depositor DCC
R_{free} test set	11713 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	19693	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 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7AK, ACP, CA, GDP, GTP, MES, MG

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	0.30	0/3626	0.47	0/4921
1	C	0.36	0/3622	0.51	0/4921
2	B	0.32	0/3502	0.45	0/4741
2	D	0.29	0/3457	0.45	0/4682
3	E	0.30	0/1071	0.40	0/1422
4	F	0.25	0/3032	0.42	0/4096
All	All	0.31	0/18310	0.46	0/24783

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

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	3513	0	3453	48	0
1	C	3499	0	3442	51	0
2	B	3398	0	3306	56	0
2	D	3366	0	3264	54	1
3	E	1044	0	1071	19	0
4	F	2942	0	2932	48	1
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	1	0
9	B	12	0	13	6	0
10	B	42	54	0	1	0
10	D	42	54	0	0	0
11	F	31	0	14	4	0
12	A	313	0	0	8	0
12	B	307	0	0	11	0
12	C	477	0	0	10	0
12	D	226	0	0	9	0
12	E	108	0	0	3	0
12	F	136	0	0	2	0
All	All	19585	108	17543	268	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (268) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:401:ACP:H3B2	11:F:401:ACP:H5'2	1.39	1.02
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.38	1.01
1:A:450:GLU:HG3	4:F:333:ASN:HB3	1.51	0.90
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.52	0.90
1:C:256:GLN:NE2	12:C:601:HOH:O	2.09	0.86
2:D:147[B]:SER:HG	2:D:190:SER:HG	1.25	0.83
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.61	0.83
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.44	0.81
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.65	0.79
2:B:294:GLN:NE2	12:B:601:HOH:O	2.16	0.77
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.50	0.77
2:B:241[A]:CYS:SG	12:B:857:HOH:O	2.42	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:241[B]:CYS:SG	12:D:780:HOH:O	2.44	0.76
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.67	0.75
2:B:158:ARG:CZ	9:B:504:MES:H21	2.16	0.75
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.69	0.75
2:B:199:ASP:OD2	9:B:504:MES:H52	1.88	0.73
2:D:241[B]:CYS:SG	12:D:632:HOH:O	2.33	0.71
1:C:356[B]:ASN:ND2	1:C:358[B]:GLN:OE1	2.24	0.71
1:C:221:ARG:CG	2:D:325:MET:HG2	2.18	0.70
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.72	0.70
1:C:270:ALA:HB3	1:C:302:MET:CE	2.23	0.69
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.32	0.69
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.25	0.68
2:D:247:GLN:OE1	12:D:601:HOH:O	2.11	0.68
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.24	0.67
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.11	0.67
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.08	0.66
1:C:204:VAL:HG22	1:C:302:MET:SD	2.36	0.66
2:B:97:SER:HB2	12:B:700:HOH:O	1.96	0.65
1:C:438:ASP:OD1	12:C:602:HOH:O	2.14	0.65
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.37	0.64
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.27	0.64
2:D:215:ARG:NH1	12:D:605:HOH:O	2.30	0.64
2:B:424:ASN:HB3	12:B:613:HOH:O	1.97	0.64
2:D:106:GLY:O	2:D:111:GLY:HA3	1.99	0.63
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.79	0.63
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.99	0.63
1:C:358[B]:GLN:NE2	12:C:613:HOH:O	2.31	0.62
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.30	0.62
4:F:331:GLU:OE2	11:F:401:ACP:O1B	2.18	0.62
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.13	0.62
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.81	0.62
2:D:269[B]:MET:CE	2:D:305:CYS:HB2	2.29	0.62
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.14	0.61
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.31	0.60
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.84	0.60
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.36	0.60
1:A:132:LEU:O	1:A:164:LYS:NZ	2.34	0.59
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.85	0.58
1:C:1:MET:O	12:C:603:HOH:O	2.17	0.58
2:B:414:ASP:HB2	12:B:676:HOH:O	2.03	0.58
1:C:229:ARG:NE	1:C:363[B]:VAL:HG21	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:ARG:NH1	12:F:503:HOH:O	2.36	0.58
2:B:199:ASP:OD1	9:B:504:MES:H32	2.03	0.58
2:D:1:MET:N	2:D:130:ASP:OD2	2.36	0.58
2:D:1:MET:HA	2:D:1:MET:CE	2.34	0.58
2:B:431:GLU:O	2:B:434:GLN:HG2	2.04	0.58
2:B:369:ARG:O	10:B:505:7AK:O3	2.22	0.57
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.69	0.57
2:B:124:LYS:HD3	2:B:124:LYS:C	2.25	0.57
1:C:339:ARG:O	12:C:604:HOH:O	2.18	0.57
2:B:199:ASP:OD1	9:B:504:MES:H72	2.04	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.34	0.57
4:F:371:PRO:HA	4:F:372:THR:O	2.05	0.57
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.37	0.57
3:E:72:LEU:O	3:E:76:ARG:HG2	2.04	0.56
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.36	0.56
3:E:92:ASN:O	3:E:96:MET:HG2	2.06	0.56
12:B:602:HOH:O	3:E:76:ARG:HG3	2.06	0.56
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.71	0.55
4:F:371:PRO:HA	4:F:372:THR:HB	1.89	0.55
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.36	0.55
2:B:253[A]:ARG:NH2	9:B:504:MES:O2S	2.34	0.55
2:D:1:MET:SD	2:D:50:ASN:HB2	2.47	0.54
3:E:120:LEU:O	3:E:124:GLN:HG3	2.08	0.54
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.40	0.54
1:C:308:ARG:HG2	1:C:340:SER:HB2	1.90	0.54
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.08	0.54
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.90	0.54
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.53
2:B:274:PRO:HB3	2:B:286:LEU:HD11	1.90	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.53
1:C:207:GLU:OE2	12:C:605:HOH:O	2.19	0.53
4:F:159:GLY:C	4:F:160:ILE:HD12	2.29	0.53
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.91	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
1:C:43:GLY:HA2	1:C:56:THR:O	2.09	0.52
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.42	0.52
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.39	0.52
8:D:501:GDP:O3B	12:D:603:HOH:O	2.19	0.52
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.91	0.52
1:A:180:ALA:O	1:A:183:GLU:HG3	2.10	0.52
2:D:180:THR:O	2:D:183:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.91	0.52
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.45	0.52
1:C:229:ARG:CD	1:C:363[B]:VAL:HG21	2.40	0.51
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.92	0.51
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.25	0.51
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.26	0.51
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.34	0.51
1:C:229:ARG:HD3	1:C:363[B]:VAL:HG21	1.91	0.51
1:A:69:ASP:O	1:A:94:THR:HA	2.10	0.51
1:A:48:SER:HB2	12:A:705:HOH:O	2.11	0.51
3:E:101:LEU:O	3:E:105[A]:MET:HG2	2.10	0.51
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.26	0.51
2:B:297:ASP:HA	12:B:695:HOH:O	2.10	0.51
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	1.93	0.50
1:C:112:LYS:NZ	12:C:626:HOH:O	2.44	0.50
2:D:191:VAL:O	2:D:195:VAL:HG23	2.11	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.43	0.50
2:D:136:GLN:HA	2:D:167:ASN:O	2.10	0.50
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.94	0.50
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.92	0.50
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.94	0.49
4:F:371:PRO:HA	4:F:372:THR:C	2.31	0.49
2:D:109:THR:O	2:D:113:GLU:HG2	2.12	0.49
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.47	0.49
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.49
1:A:419:SER:O	1:A:423:GLU:HG3	2.13	0.48
1:C:203:MET:O	1:C:302:MET:HE3	2.12	0.48
3:E:81:GLU:HA	3:E:84[B]:GLN:HG2	1.93	0.48
1:A:77:GLU:HB2	12:A:670:HOH:O	2.13	0.48
1:A:237[B]:SER:HB2	12:A:656:HOH:O	2.14	0.48
1:C:163:LYS:HG3	3:E:90[A]:ASN:OD1	2.12	0.48
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.20	0.48
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.96	0.48
2:B:295:MET:CG	2:B:377:PHE:HB2	2.39	0.48
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.36	0.48
1:A:450:GLU:HB2	4:F:333:ASN:OD1	2.14	0.48
2:D:124:LYS:C	2:D:124:LYS:HD3	2.33	0.48
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.48
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.48	0.48
1:A:262:TYR:HD2	1:A:265:ILE:HG13	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269[B]:MET:HE1	2:D:305:CYS:HB2	1.96	0.48
2:B:192:HIS:ND1	12:B:613:HOH:O	2.35	0.47
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.95	0.47
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.96	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.95	0.47
4:F:10:ASN:HB2	4:F:44:ARG:NH2	2.25	0.47
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.95	0.47
2:B:318:ILE:N	2:B:318:ILE:HD12	2.29	0.47
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.30	0.47
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.14	0.47
11:F:401:ACP:O5'	11:F:401:ACP:H8	2.14	0.47
2:B:274:PRO:HB3	2:B:286:LEU:CD1	2.44	0.47
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.96	0.47
2:B:234:THR:O	2:B:238[A]:VAL:HG13	2.15	0.47
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.97	0.47
2:B:176:LYS:HG3	2:B:207:GLU:OE1	2.15	0.47
2:D:318:ILE:N	2:D:318:ILE:HD12	2.29	0.47
3:E:81:GLU:OE2	12:E:201:HOH:O	2.21	0.47
1:C:363[A]:VAL:HG13	1:C:364:PRO:HD2	1.97	0.47
1:C:77:GLU:OE2	12:C:606:HOH:O	2.20	0.46
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.97	0.46
1:A:90:GLU:O	1:A:121:ARG:HD2	2.14	0.46
1:A:315[A]:CYS:HG	1:A:351:PHE:HE2	1.63	0.46
3:E:84[A]:GLN:HG3	12:E:210:HOH:O	2.15	0.46
2:B:158:ARG:NE	9:B:504:MES:H21	2.30	0.46
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.97	0.46
12:B:705:HOH:O	3:E:75:LYS:HD2	2.15	0.46
2:D:236:SER:O	2:D:240[B]:THR:HG23	2.16	0.46
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.98	0.46
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.46	0.46
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	1.97	0.45
2:B:42:LEU:H	2:B:42:LEU:HD12	1.81	0.45
4:F:237:THR:HG21	4:F:250:SER:HB2	1.98	0.45
1:A:340:SER:O	12:A:601:HOH:O	2.21	0.45
1:A:43:GLY:HA2	1:A:56:THR:O	2.17	0.45
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.99	0.45
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.97	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.52	0.45
1:A:356:ASN:ND2	12:A:617:HOH:O	2.48	0.45
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.98	0.45
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:237:THR:CG2	4:F:250:SER:HB2	2.47	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.45
2:B:386:GLU:O	2:B:390:ARG:HG3	2.16	0.45
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.33	0.45
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.98	0.45
1:C:229:ARG:HD3	1:C:363[B]:VAL:CG2	2.46	0.45
2:D:19:LYS:HE2	12:D:784:HOH:O	2.16	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.17	0.45
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.44
2:B:373:MET:HE1	12:B:853:HOH:O	2.18	0.44
1:C:104:ALA:HB2	1:C:413:MET:SD	2.58	0.44
2:D:152:LEU:O	2:D:156:LYS:HG2	2.17	0.44
1:C:244:PHE:CD1	1:C:358[B]:GLN:HG2	2.53	0.44
1:C:221:ARG:HG3	2:D:325:MET:CG	2.28	0.44
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.43
4:F:198:LYS:HE3	4:F:320:MET:CE	2.48	0.43
1:C:308:ARG:HD2	12:C:821:HOH:O	2.18	0.43
3:E:140:LYS:HB3	3:E:140:LYS:HE2	1.82	0.43
2:B:159:GLU:OE2	12:B:602:HOH:O	2.21	0.43
2:D:1:MET:HA	2:D:1:MET:HE2	2.00	0.43
1:A:348:PRO:HG3	3:E:27:PRO:HD3	2.00	0.43
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	2.01	0.43
1:A:83:TYR:O	1:A:86:LEU:HB2	2.18	0.43
2:B:202:TYR:CZ	2:B:238[B]:VAL:HG11	2.53	0.43
1:C:234:ILE:HG21	1:C:302:MET:SD	2.59	0.43
4:F:240:LEU:HD12	4:F:240:LEU:N	2.34	0.43
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.51	0.43
2:B:306:ASP:O	2:B:309:HIS:HB2	2.18	0.43
4:F:280:GLU:HB2	12:F:560:HOH:O	2.17	0.43
2:D:167:ASN:ND2	12:D:622:HOH:O	2.51	0.42
2:D:345:GLU:HG3	2:D:440:ALA:HB2	2.00	0.42
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.42
4:F:101:TYR:CE2	4:F:179:VAL:HG22	2.54	0.42
3:E:106:GLU:O	3:E:110:GLU:HG3	2.19	0.42
1:A:77:GLU:O	1:A:80:THR:HG22	2.19	0.42
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.01	0.42
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.84	0.42
2:D:74:THR:O	2:D:78:VAL:HG23	2.19	0.42
4:F:232:ASN:OD1	4:F:234:GLN:HB3	2.20	0.42
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.02	0.42
1:A:339:ARG:HD3	12:A:730:HOH:O	2.19	0.42
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.54	0.42
2:D:141:LEU:HD21	2:D:170:SER:HB3	2.01	0.42
1:A:409:VAL:HA	1:A:413:MET:O	2.20	0.42
1:A:71:GLU:HG2	1:A:72:PRO:N	2.33	0.42
1:A:413:MET:CE	1:A:418:PHE:CE2	3.03	0.42
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.55	0.42
2:B:287:THR:HB	2:B:289:PRO:HD2	2.02	0.42
1:C:419:SER:O	1:C:423:GLU:HG3	2.20	0.42
2:D:203:CYS:SG	2:D:384[B]:ILE:HD11	2.60	0.42
4:F:199:PHE:HA	4:F:241:THR:HG21	2.01	0.42
2:B:187:ALA:O	2:B:191:VAL:HG23	2.20	0.42
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.35	0.42
1:C:356[B]:ASN:ND2	12:C:636:HOH:O	2.50	0.42
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.01	0.42
1:A:301:GLN:C	1:A:302[B]:MET:HE3	2.40	0.42
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.02	0.42
2:D:9:ALA:HA	2:D:68:VAL:O	2.19	0.42
2:B:196:GLU:HG3	12:E:263:HOH:O	2.20	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.89	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.54	0.41
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.93	0.41
2:B:238[B]:VAL:HG22	2:B:378:ILE:HD11	2.01	0.41
2:D:1:MET:HE1	12:D:759:HOH:O	2.19	0.41
2:D:74:THR:HB	12:D:671:HOH:O	2.19	0.41
2:D:248:LEU:HD23	2:D:354:ALA:HB2	2.02	0.41
2:B:42:LEU:HD12	2:B:42:LEU:N	2.36	0.41
2:D:15:GLN:O	2:D:19:LYS:HG2	2.20	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.02	0.41
1:A:449:GLU:OE2	12:A:602:HOH:O	2.22	0.41
3:E:135:LYS:HZ2	3:E:139:LEU:HD11	1.86	0.41
4:F:371:PRO:N	4:F:372:THR:HB	2.35	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.41
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.50	0.41
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.55	0.41
1:A:229:ARG:NH1	12:A:611:HOH:O	2.40	0.41
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.50	0.41
2:B:67:LEU:HD12	2:B:67:LEU:N	2.36	0.41
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.56	0.41
2:D:332:MET:O	2:D:335:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:206:LEU:HD23	4:F:353[A]:VAL:HG21	2.03	0.41
2:D:67:LEU:N	2:D:67:LEU:HD12	2.36	0.40
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.20	0.40
1:A:141:PHE:O	1:A:147:SER:HB3	2.22	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	2.22	0.40
2:D:286:LEU:O	2:D:286:LEU:HG	2.22	0.40
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.03	0.40
2:D:405:LEU:HD13	2:D:415:GLU:HG2	2.04	0.40
4:F:242:ASN:HD22	4:F:245:ILE:CD1	2.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:ASN:OD1	4:F:384:HIS:NE2[3_545]	2.18	0.02

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	451/451 (100%)	445 (99%)	6 (1%)	0	100	100
1	C	453/451 (100%)	441 (97%)	12 (3%)	0	100	100
2	B	432/445 (97%)	425 (98%)	7 (2%)	0	100	100
2	D	428/445 (96%)	422 (99%)	6 (1%)	0	100	100
3	E	125/143 (87%)	122 (98%)	3 (2%)	0	100	100
4	F	354/384 (92%)	343 (97%)	11 (3%)	0	100	100
All	All	2243/2319 (97%)	2198 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	385/379 (102%)	380 (99%)	5 (1%)	69	68
1	C	386/379 (102%)	384 (100%)	2 (0%)	88	89
2	B	379/383 (99%)	376 (99%)	3 (1%)	81	82
2	D	374/383 (98%)	370 (99%)	4 (1%)	73	73
3	E	116/127 (91%)	116 (100%)	0	100	100
4	F	325/342 (95%)	319 (98%)	6 (2%)	59	55
All	All	1965/1993 (99%)	1945 (99%)	20 (1%)	76	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	80	THR
1	A	120	ASP
1	A	221	ARG
1	A	262	TYR
2	B	139	HIS
2	B	229	HIS
2	B	286	LEU
1	C	71	GLU
1	C	381	THR
2	D	1	MET
2	D	39	ASP
2	D	139	HIS
2	D	280	SER
4	F	186	LEU
4	F	211	TYR
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	310	GLN
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	1.11	2 (7%)	33,54,54	1.90	6 (18%)
5	GTP	C	501	6	26,34,34	1.11	3 (11%)	33,54,54	1.92	7 (21%)
10	7AK	D	503	-	42,42,42	1.42	3 (7%)	50,58,58	1.67	9 (18%)
10	7AK	B	505	-	42,42,42	1.45	3 (7%)	50,58,58	1.50	7 (14%)
8	GDP	D	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.95	7 (22%)
11	ACP	F	401	6	27,33,33	1.98	7 (25%)	32,52,52	1.29	4 (12%)
9	MES	B	504	-	12,12,12	2.13	1 (8%)	14,16,16	1.13	1 (7%)
8	GDP	B	501	6	24,30,30	1.11	2 (8%)	31,47,47	1.92	7 (22%)

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	-	5/18/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
10	7AK	D	503	-	-	4/49/69/69	0/1/1/1
10	7AK	B	505	-	-	2/49/69/69	0/1/1/1
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
11	ACP	F	401	6	-	7/15/38/38	0/3/3/3
9	MES	B	504	-	-	2/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	7AK	O5-C1	7.41	1.45	1.34
9	B	504	MES	C8-S	-7.14	1.67	1.77
10	D	503	7AK	O5-C1	6.93	1.45	1.34
11	F	401	ACP	PG-O1G	5.40	1.61	1.50
10	D	503	7AK	O19-C33	4.33	1.45	1.35
10	B	505	7AK	O19-C33	4.16	1.45	1.35
11	F	401	ACP	PB-O1B	4.10	1.61	1.51
5	A	501	GTP	C5-C6	3.95	1.48	1.41
5	C	501	GTP	C5-C6	3.88	1.48	1.41
8	D	501	GDP	C5-C6	3.66	1.47	1.41
11	F	401	ACP	PB-O2B	-3.46	1.48	1.56
8	B	501	GDP	C5-C6	3.26	1.47	1.41
11	F	401	ACP	PB-O3A	3.23	1.62	1.58
11	F	401	ACP	PG-O2G	-2.83	1.48	1.54
11	F	401	ACP	PG-O3G	2.70	1.61	1.54
10	D	503	7AK	O5-C5	-2.63	1.42	1.46
8	B	501	GDP	O4'-C1'	2.55	1.44	1.41
11	F	401	ACP	C5-C4	2.48	1.47	1.40
10	B	505	7AK	O5-C5	-2.26	1.43	1.46
8	D	501	GDP	C5-C4	2.26	1.46	1.40
5	C	501	GTP	C5-C4	2.07	1.46	1.40
5	A	501	GTP	C5-C4	2.06	1.46	1.40
5	C	501	GTP	O4'-C1'	2.03	1.43	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	503	7AK	O19-C33-N33	5.54	119.19	110.58
10	B	505	7AK	O19-C33-N33	5.01	118.37	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	GDP	C4-C5-C6	-4.76	116.25	120.80
5	C	501	GTP	C2-N3-C4	4.66	120.68	115.36
5	A	501	GTP	C4-C5-C6	-4.56	116.44	120.80
8	D	501	GDP	C2-N3-C4	4.53	120.53	115.36
10	D	503	7AK	C29-C14-C13	-4.51	114.86	123.78
5	C	501	GTP	C2-N1-C6	4.49	123.06	115.93
8	D	501	GDP	C4-C5-C6	-4.41	116.59	120.80
5	A	501	GTP	C2-N1-C6	4.31	122.78	115.93
8	B	501	GDP	C2-N1-C6	4.27	122.71	115.93
5	C	501	GTP	C4-C5-C6	-4.24	116.75	120.80
8	B	501	GDP	C2-N3-C4	4.20	120.16	115.36
8	D	501	GDP	C2-N1-C6	4.17	122.56	115.93
10	B	505	7AK	C29-C14-C13	-4.13	115.61	123.78
5	A	501	GTP	C5-C6-N1	-4.09	117.84	123.43
5	A	501	GTP	C2-N3-C4	4.06	120.00	115.36
5	C	501	GTP	C5-C6-N1	-4.02	117.93	123.43
8	D	501	GDP	C5-C6-N1	-3.97	118.00	123.43
5	C	501	GTP	N3-C2-N1	-3.87	122.06	127.22
8	B	501	GDP	N3-C2-N1	-3.79	122.17	127.22
8	B	501	GDP	C5-C6-N1	-3.70	118.37	123.43
10	D	503	7AK	O33-C33-N33	-3.68	119.44	125.51
8	D	501	GDP	N3-C2-N1	-3.56	122.47	127.22
5	A	501	GTP	N3-C2-N1	-3.34	122.76	127.22
11	F	401	ACP	N3-C2-N1	-3.03	123.94	128.68
10	B	505	7AK	O33-C33-N33	-3.00	120.56	125.51
11	F	401	ACP	PB-O3A-PA	-2.99	123.07	132.56
9	B	504	MES	O3S-S-C8	2.97	110.58	105.77
11	F	401	ACP	C3'-C2'-C1'	2.95	105.41	100.98
10	B	505	7AK	C25-C2-C3	-2.61	108.11	112.93
10	B	505	7AK	O19-C33-O33	-2.59	121.07	123.69
10	D	503	7AK	C19-O19-C33	2.54	120.75	117.12
8	D	501	GDP	C4-C5-N7	-2.54	106.75	109.40
10	D	503	7AK	C25-C2-C3	-2.53	108.27	112.93
8	D	501	GDP	PA-O3A-PB	-2.52	124.19	132.83
11	F	401	ACP	C4-C5-N7	-2.47	106.83	109.40
10	D	503	7AK	C28-C12-C13	-2.46	105.96	110.05
10	B	505	7AK	C19-O19-C33	2.43	120.58	117.12
10	D	503	7AK	C15-C14-C13	2.34	126.93	121.39
10	D	503	7AK	O19-C33-O33	-2.30	121.37	123.69
10	D	503	7AK	C26-C4-C3	-2.26	109.11	112.15
8	B	501	GDP	C1'-N9-C4	-2.21	122.77	126.64
5	A	501	GTP	C4-C5-N7	-2.18	107.13	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	501	GTP	C4-C5-N7	-2.15	107.15	109.40
8	B	501	GDP	PA-O3A-PB	-2.10	125.60	132.83
10	B	505	7AK	C17-C18-C19	2.09	114.69	110.61
5	C	501	GTP	PA-O3A-PB	-2.04	125.83	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
10	D	503	7AK	C31-C18-C19-C20
10	D	503	7AK	C11-C10-C9-C8
10	B	505	7AK	C31-C18-C19-C20
10	B	505	7AK	C17-C18-C19-C20
10	D	503	7AK	C17-C18-C19-C20
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O1A
9	B	504	MES	N4-C7-C8-S
10	D	503	7AK	C15-C16-C17-C18

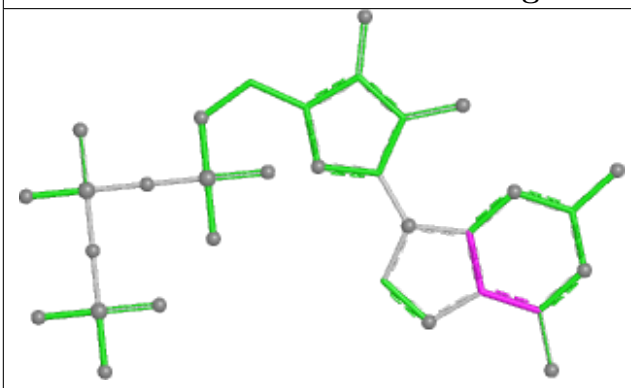
There are no ring outliers.

5 monomers are involved in 13 short contacts:

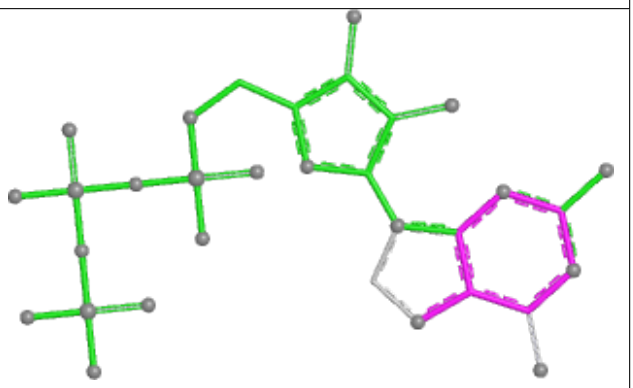
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	7AK	1	0
8	D	501	GDP	1	0
11	F	401	ACP	4	0
9	B	504	MES	6	0
8	B	501	GDP	1	0

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.

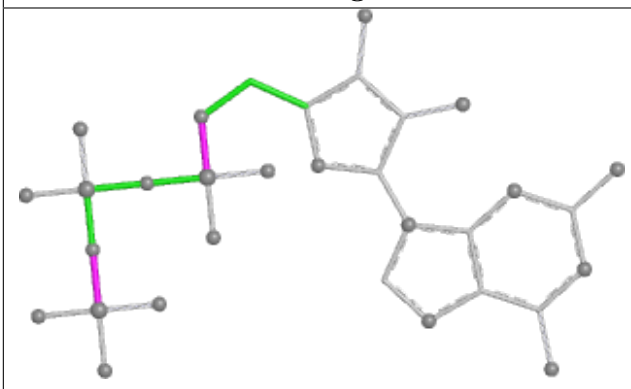
Ligand GTP A 501



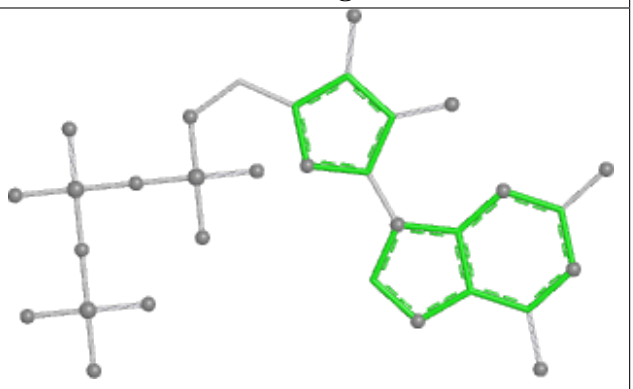
Bond lengths



Bond angles

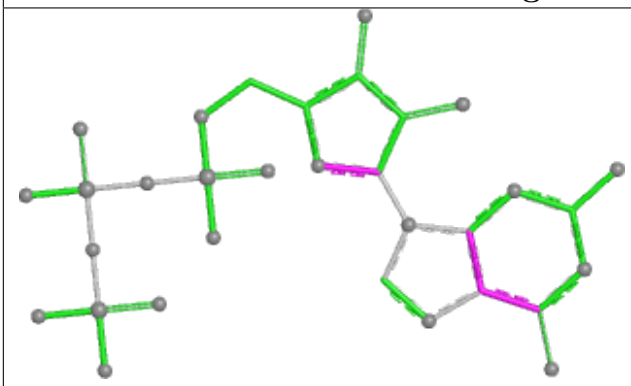


Torsions



Rings

Ligand GTP C 501



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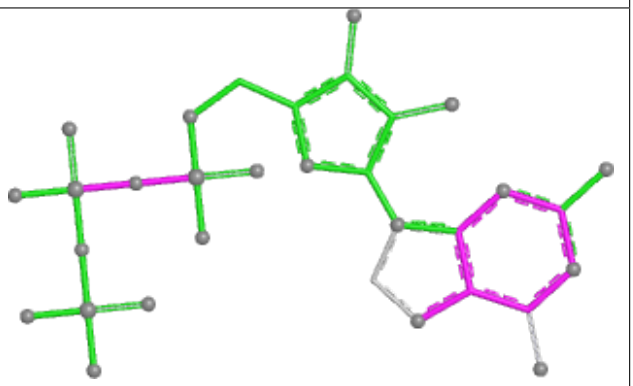

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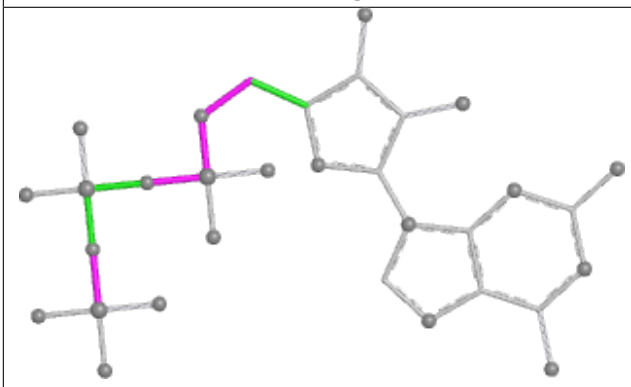

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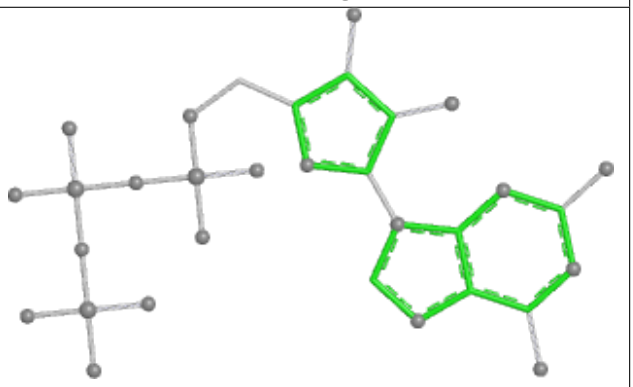
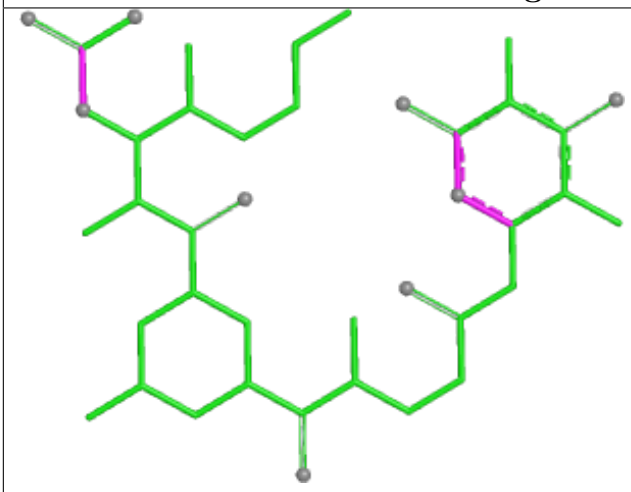
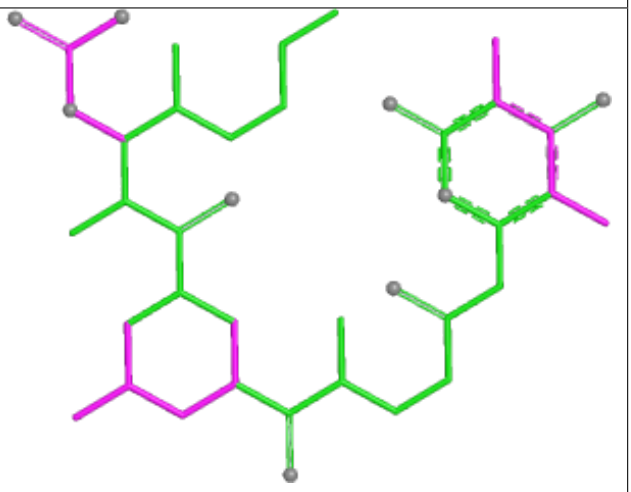


Rings

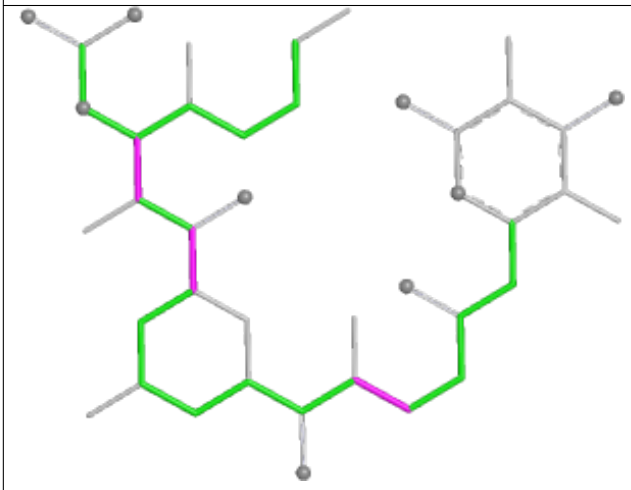
Ligand 7AK D 503



Bond lengths



Bond angles



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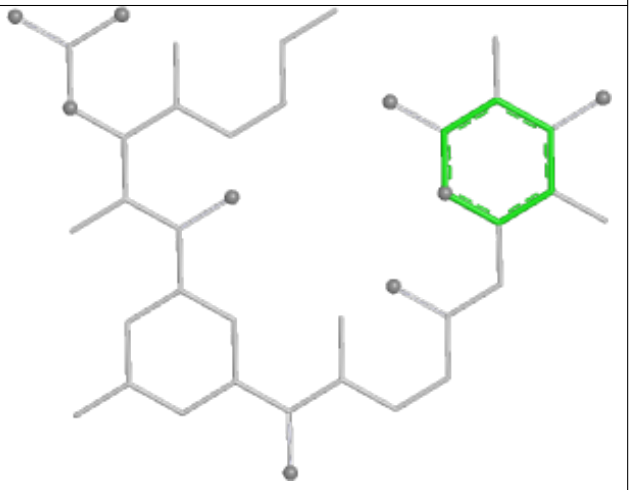
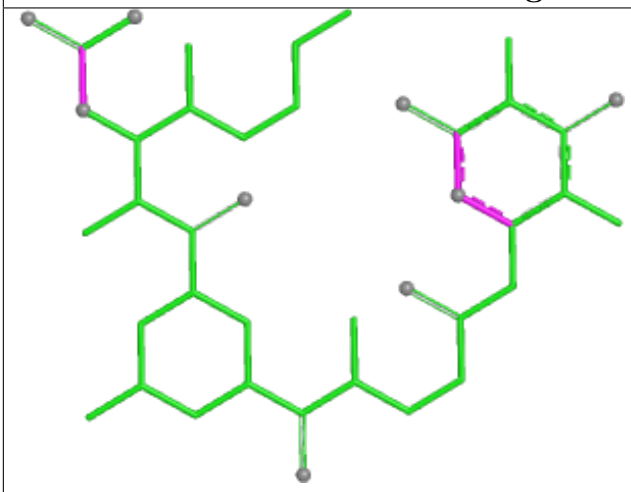


Rings

Ligand 7AK B 505



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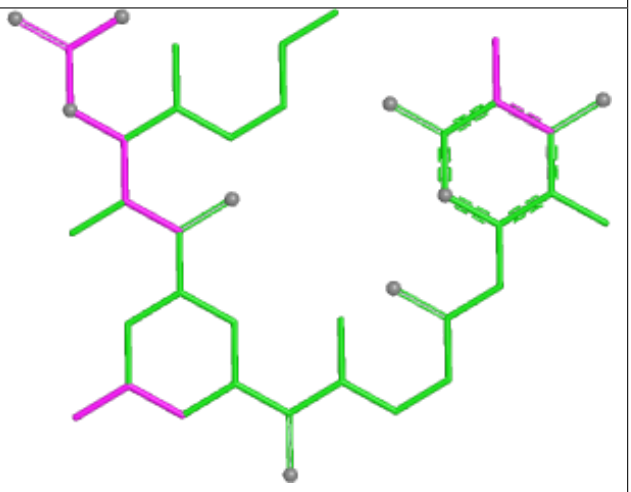
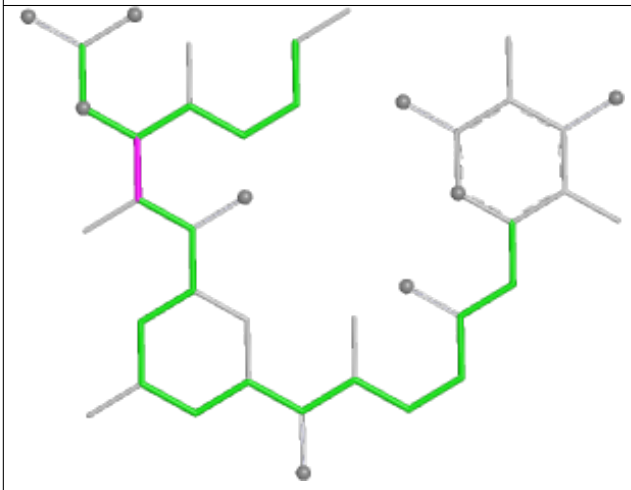
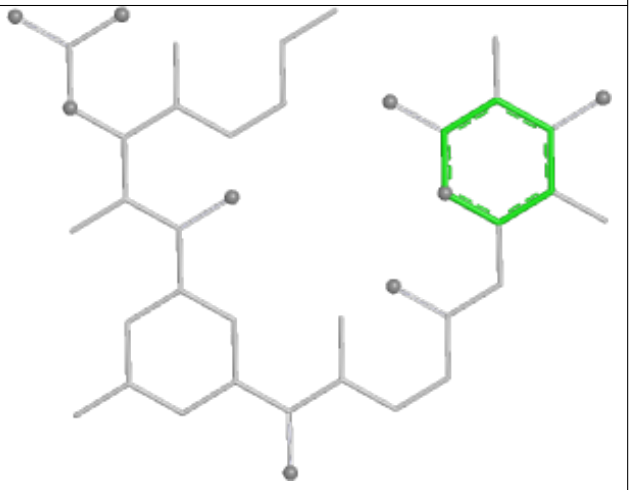


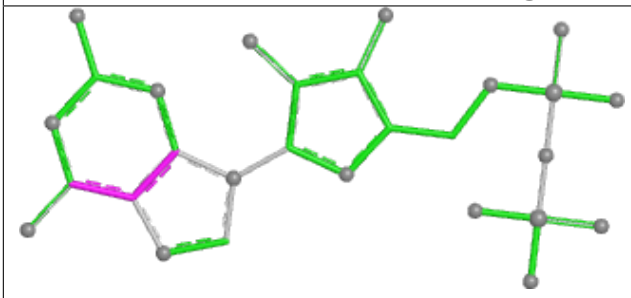
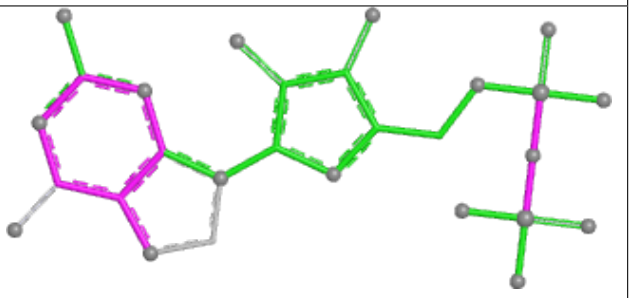
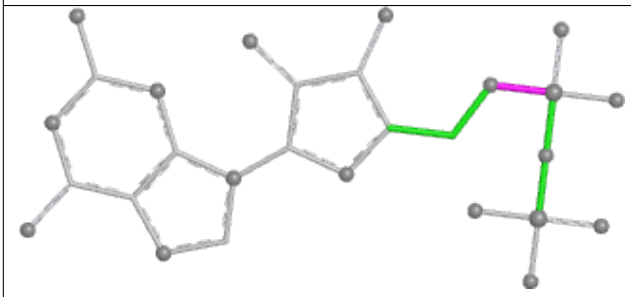
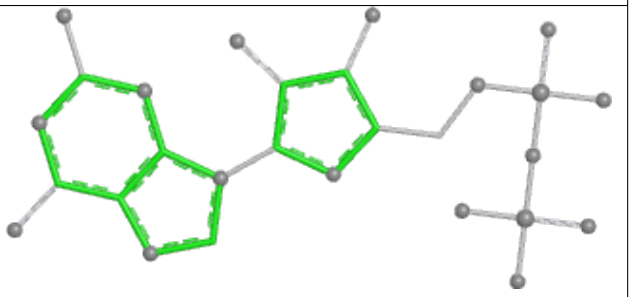
Bond angles

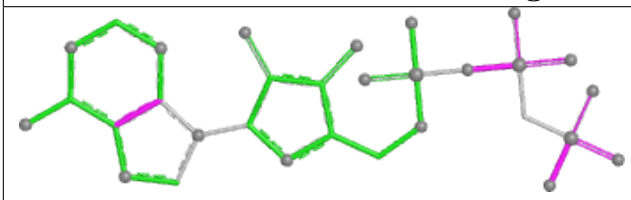
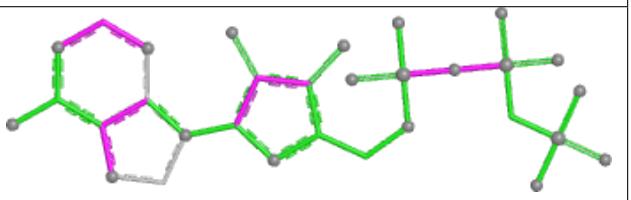
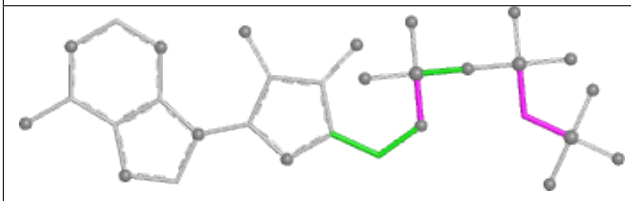
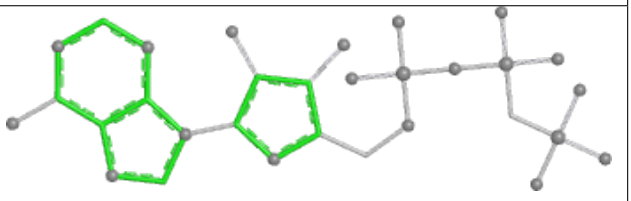


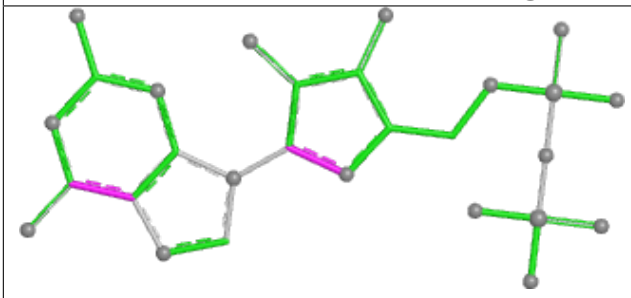
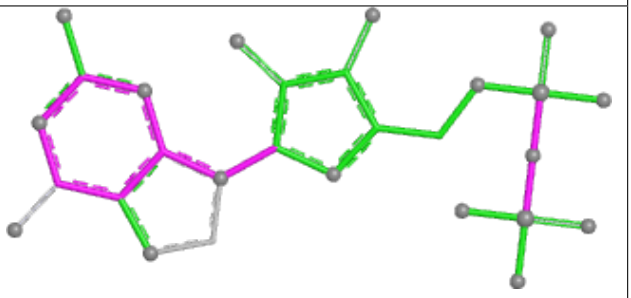
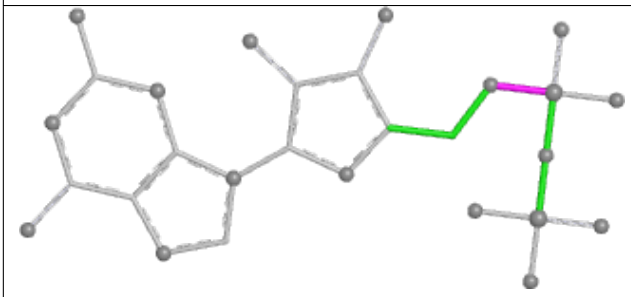
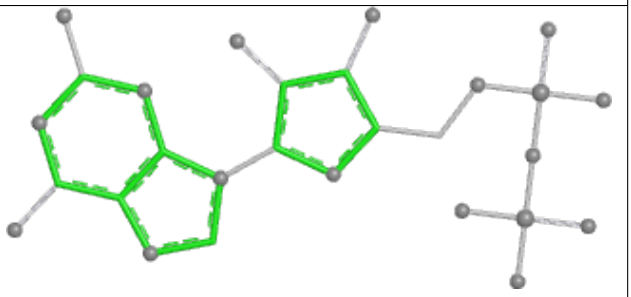
Torsions



Rings

Ligand GDP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACP F 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B 501	
 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	441/451 (97%)	-0.04	6 (1%) 75 77	25, 41, 69, 134	0
1	C	440/451 (97%)	0.15	1 (0%) 95 95	20, 32, 54, 89	0
2	B	426/445 (95%)	0.20	7 (1%) 72 74	22, 41, 74, 116	2 (0%)
2	D	426/445 (95%)	0.08	14 (3%) 46 49	27, 46, 77, 103	6 (1%)
3	E	123/143 (86%)	0.36	3 (2%) 59 62	31, 53, 91, 115	0
4	F	354/384 (92%)	1.06	74 (20%) 1 1	31, 64, 123, 158	0
All	All	2210/2319 (95%)	0.27	105 (4%) 30 33	20, 43, 89, 158	8 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	179	VAL	9.9
4	F	173	ILE	8.9
4	F	105	LEU	8.1
4	F	372	THR	6.4
4	F	178	GLN	6.2
4	F	152	SER	6.0
4	F	371	PRO	5.8
4	F	251	LYS	5.5
4	F	153	ALA	5.4
4	F	177	GLY	5.1
4	F	244	CYS	5.0
1	A	449	GLU	4.8
4	F	154	GLY	4.7
4	F	130	VAL	4.7
4	F	176	GLN	4.7
4	F	249	TYR	4.4
4	F	186	LEU	4.4
4	F	155	ALA	4.4
4	F	138	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	4.3
1	C	340	SER	4.3
2	B	438	ALA	4.3
4	F	231	ALA	4.2
4	F	134	ALA	4.2
4	F	147	TRP	4.1
2	B	1	MET	4.0
4	F	104	ASN	4.0
4	F	137	ARG	4.0
4	F	182	ILE	4.0
4	F	181	VAL	3.9
4	F	245	ILE	3.8
1	A	262	TYR	3.8
4	F	233	PHE	3.8
4	F	169	LEU	3.8
2	B	248	LEU	3.7
4	F	170	LEU	3.6
4	F	382	HIS	3.6
4	F	248	GLU	3.5
4	F	103	THR	3.4
4	F	131	PHE	3.4
4	F	44	ARG	3.4
4	F	160	ILE	3.3
2	D	404	PHE	3.2
1	A	179	THR	3.2
2	D	279	GLY	3.2
2	D	286	LEU	3.2
4	F	384	HIS	3.2
4	F	101	TYR	3.2
2	D	57	THR	3.2
4	F	250	SER	3.1
4	F	143	GLU	3.1
4	F	234	GLN	3.1
1	A	448	GLY	3.0
4	F	381	HIS	3.0
4	F	232	ASN	2.9
2	D	400	ARG	2.9
2	B	57	THR	2.9
2	D	94	PHE	2.9
4	F	383	HIS	2.9
4	F	253	TYR	2.9
1	A	450	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	240	LEU	2.9
4	F	380	HIS	2.7
4	F	166	ALA	2.7
4	F	162	ILE	2.7
4	F	17	VAL	2.7
2	D	74	THR	2.6
1	A	282	TYR	2.6
4	F	89	GLU	2.6
4	F	140	GLU	2.6
2	D	401	ARG	2.6
4	F	102	PRO	2.6
4	F	125	THR	2.6
4	F	31	ARG	2.5
4	F	148	ILE	2.5
4	F	342	LEU	2.5
4	F	10	ASN	2.5
2	D	1	MET	2.5
2	D	83	PHE	2.5
3	E	139	LEU	2.5
4	F	199	PHE	2.5
4	F	172	PHE	2.4
4	F	200	ASP	2.4
2	B	281	GLN	2.4
4	F	135	TYR	2.3
3	E	142	GLU	2.3
2	D	277	SER	2.3
4	F	163	SER	2.3
2	D	215	ARG	2.3
2	D	37	HIS	2.3
2	B	437	ASP	2.2
4	F	259	GLY	2.2
4	F	192	LEU	2.2
4	F	236	LYS	2.2
4	F	142	ARG	2.2
2	B	59	ASN	2.1
4	F	20	LEU	2.1
4	F	284[A]	LEU	2.1
3	E	28	SER	2.1
4	F	99	VAL	2.0
4	F	90	SER	2.0
4	F	151	SER	2.0
2	D	58	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	330	ILE	2.0
4	F	180	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)

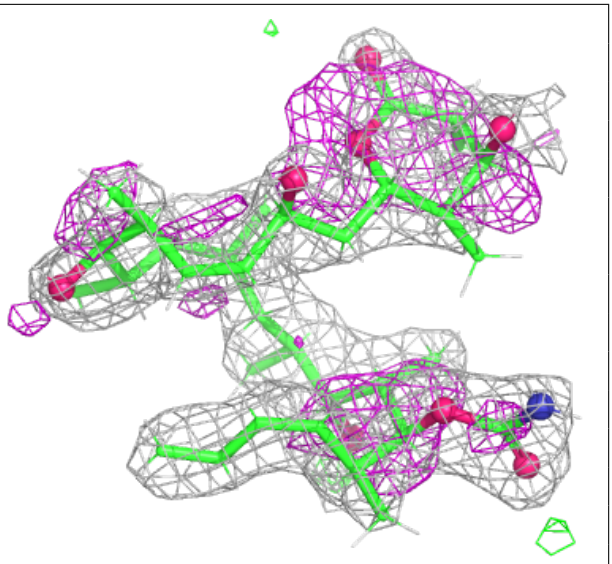
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

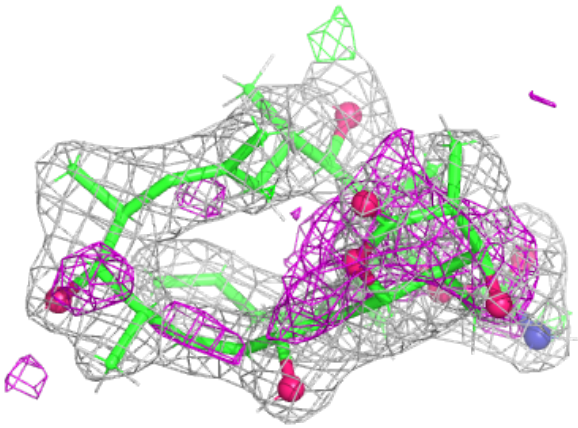
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	7AK	B	505	42/42	0.84	0.27	45,65,83,90	0
6	MG	F	402	1/1	0.90	0.05	65,65,65,65	0
6	MG	D	502	1/1	0.91	0.09	59,59,59,59	0
7	CA	B	503	1/1	0.94	0.07	75,75,75,75	0
10	7AK	D	503	42/42	0.94	0.21	44,57,69,74	0
11	ACP	F	401	31/31	0.95	0.12	53,58,105,124	0
9	MES	B	504	12/12	0.96	0.11	32,51,57,63	0
8	GDP	D	501	28/28	0.96	0.11	33,40,47,48	0
7	CA	A	503	1/1	0.97	0.09	51,51,51,51	0
6	MG	A	502	1/1	0.98	0.10	28,28,28,28	0
8	GDP	B	501	28/28	0.99	0.13	21,26,30,32	0
5	GTP	A	501	32/32	0.99	0.10	23,28,32,33	0
6	MG	C	502	1/1	0.99	0.14	24,24,24,24	0
7	CA	A	504	1/1	0.99	0.09	80,80,80,80	0
5	GTP	C	501	32/32	0.99	0.12	19,23,25,26	0
7	CA	C	503	1/1	0.99	0.10	41,41,41,41	0
6	MG	B	502	1/1	1.00	0.16	20,20,20,20	0

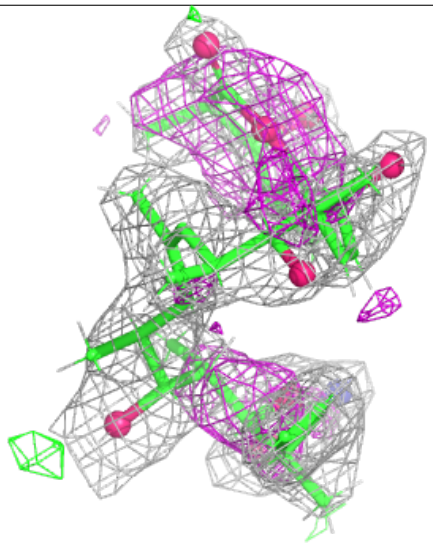
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7AK B 505:

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

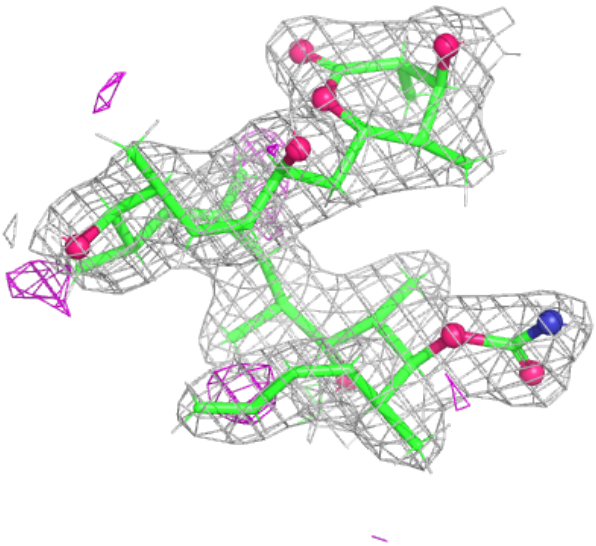


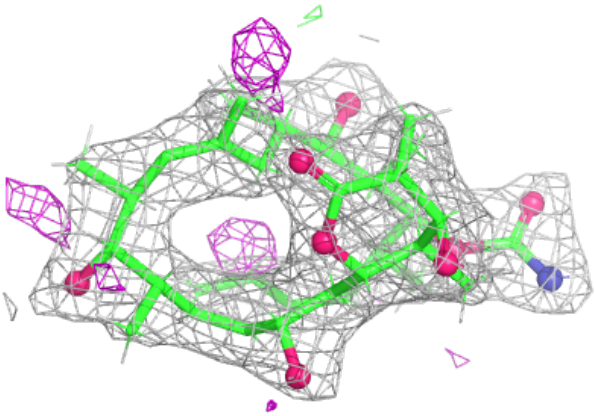


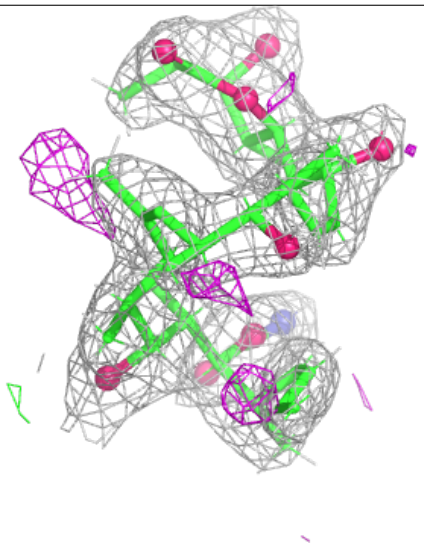


Electron density around 7AK D 503:

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

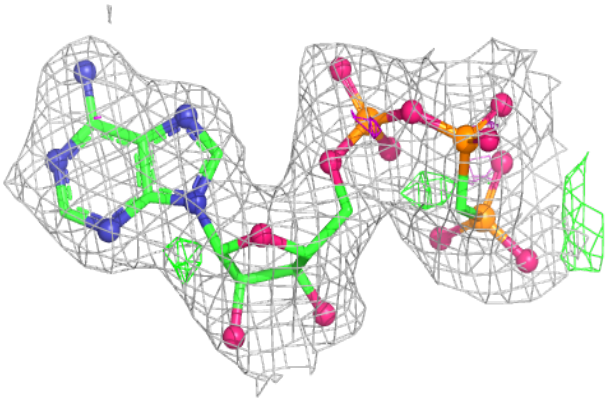


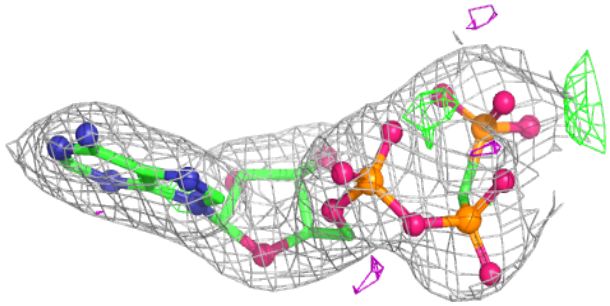


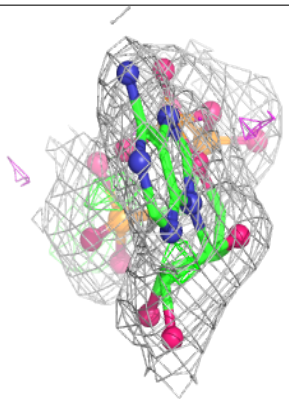


Electron density around ACP F 401:

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

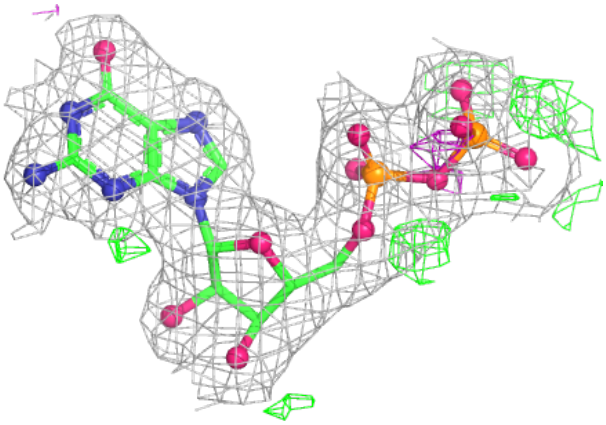


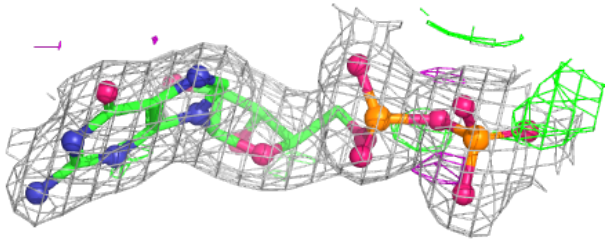


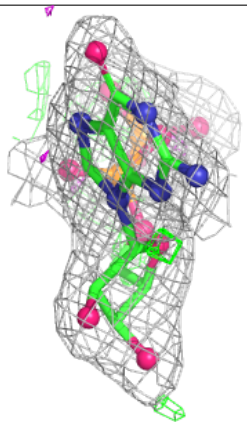


Electron density around GDP D 501:

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

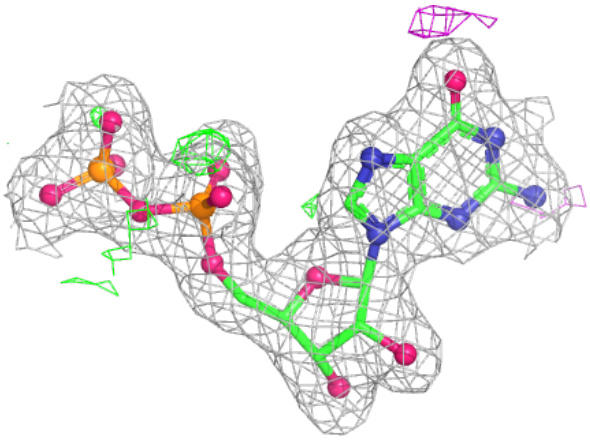


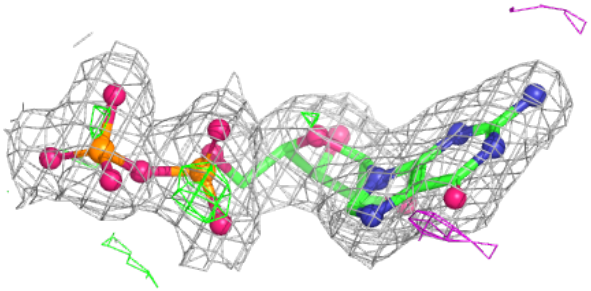


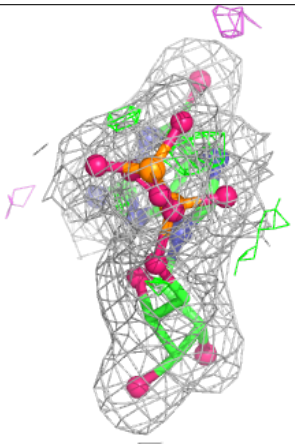


Electron density around GDP B 501:

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

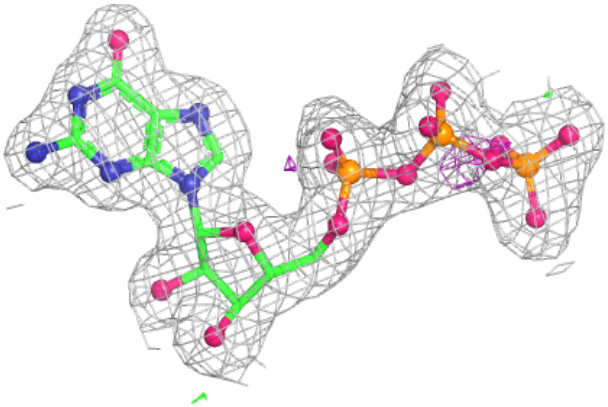


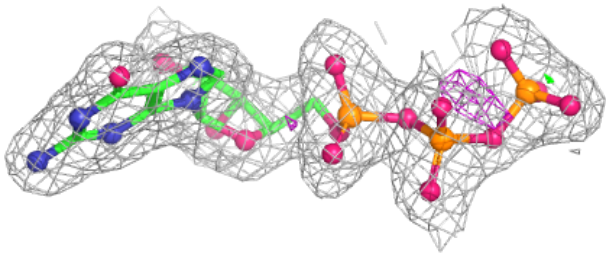


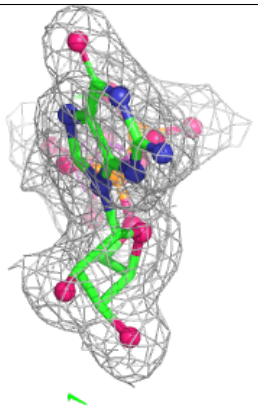


Electron density around GTP A 501:

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

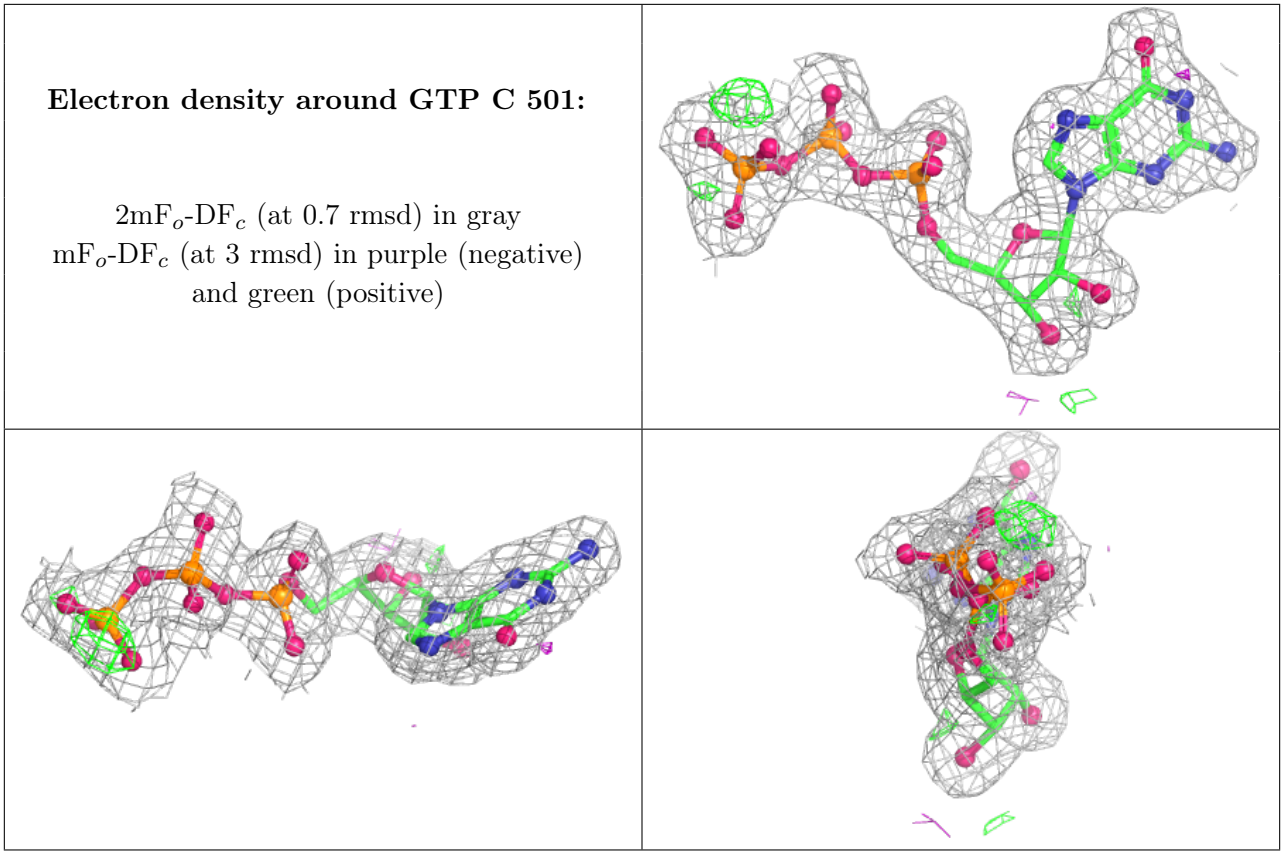






Electron density around GTP C 501:

$2mF_o$-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

There are no such residues in this entry.