Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 02:22 PM JST

PDB ID	:	7CNN
Title	:	vinorelbine in complex with tubulin
Authors	:	Wang, Y.X.; Wu, C.Y.
Deposited on	:	2020-08-02
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:

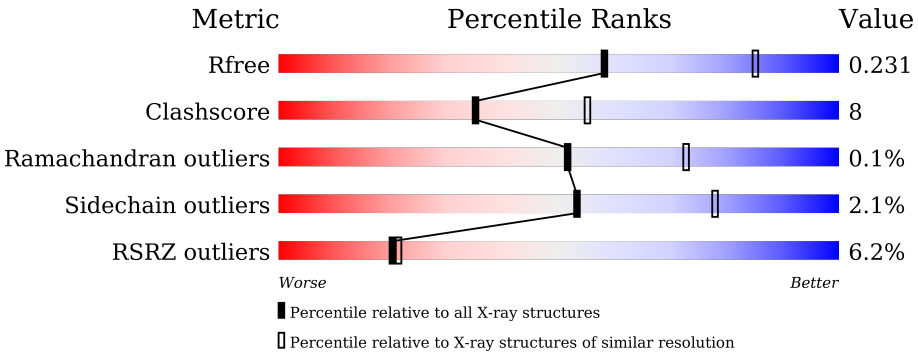
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	2% 84% 13% ·
1	C	451	83% 14% ·
2	B	445	2% 79% 17% ·
2	D	445	6% 74% 20% 6%
3	E	143	5% 69% 15% · 15%
4	F	384	22% 68% 22% •• 9%

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
10	MES	B	504	-	X	-	-
7	CA	B	503	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18183 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	6	0
			3453	2186	587	656	24			
1	C	440	Total	C	N	O	S	0	8	0
			3463	2192	584	662	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	4	0
			3398	2133	582	656	27			
2	D	420	Total	C	N	O	S	0	4	0
			3311	2082	561	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	4	0
			1031	637	186	202	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

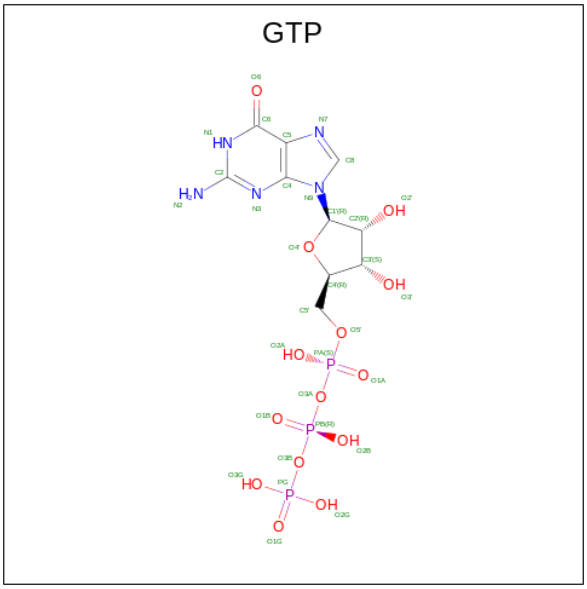
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	350	Total	C	N	O	S	0	4	0
			2894	1860	496	523	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		
5	D	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	C	1	Total	Mg	0	0
			1	1		

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

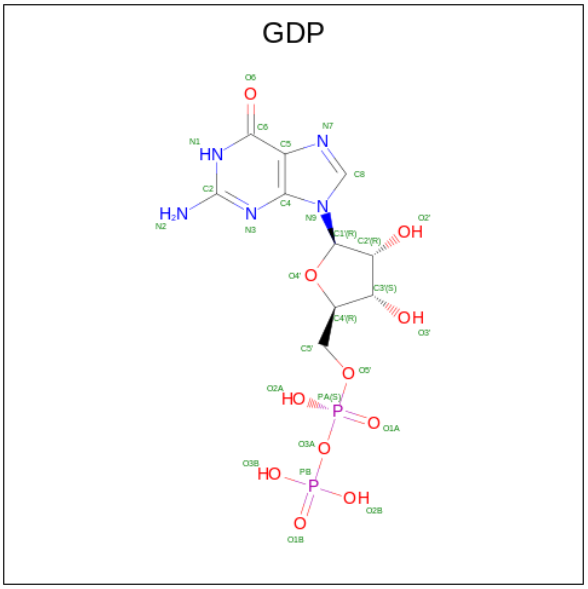
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	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).

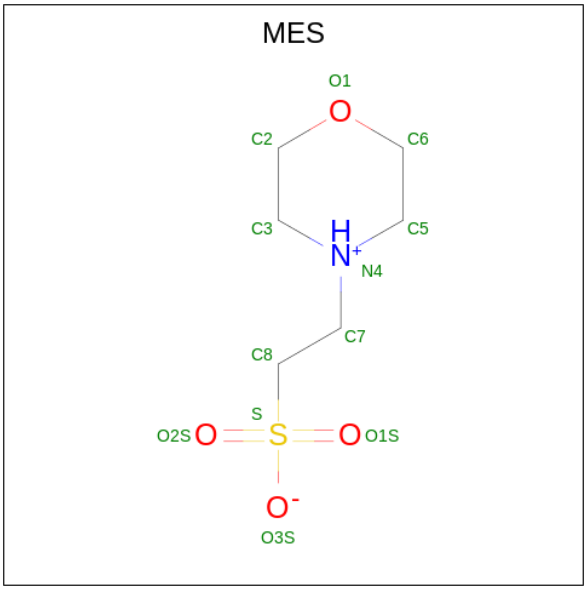
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



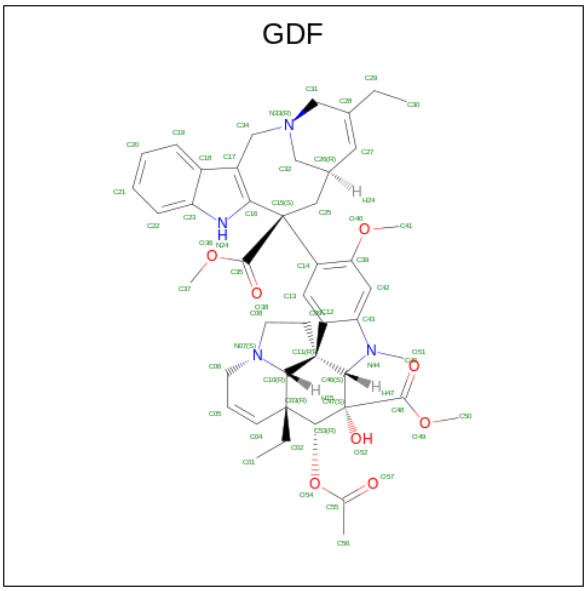
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is Vinorelbine (three-letter code: GDF) (formula: $C_{45}H_{54}N_4O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N O 57 45 4 8	0	0

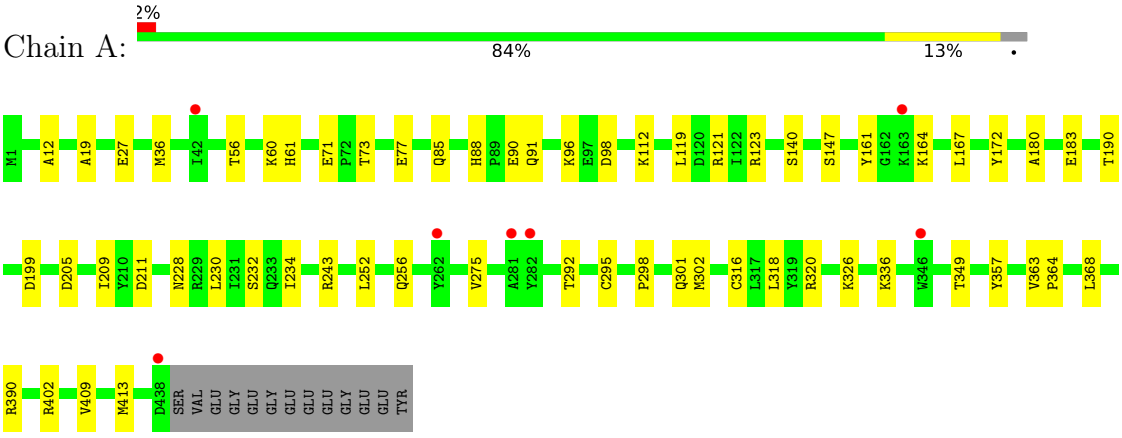
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	91	Total O 91 91	0	0
12	B	87	Total O 87 87	0	0
12	C	154	Total O 154 154	0	0
12	D	34	Total O 34 34	0	0
12	E	18	Total O 18 18	0	0
12	F	34	Total O 34 34	0	0

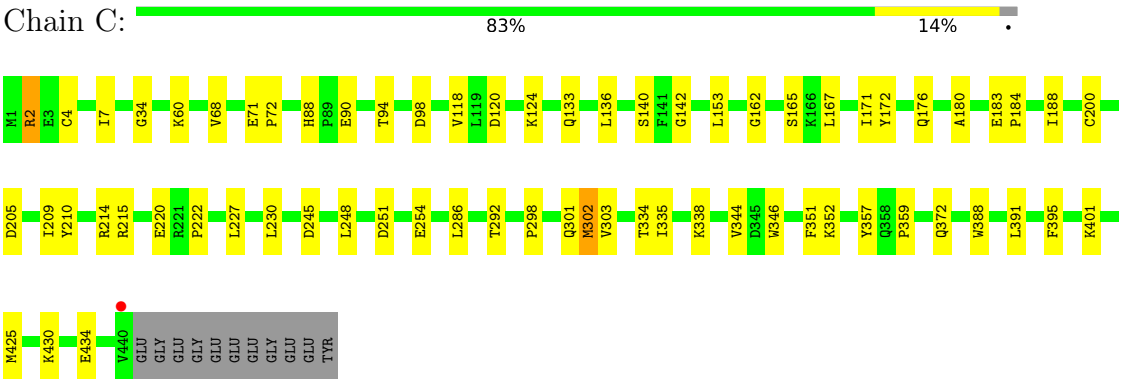
3 Residue-property plots (i)

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.

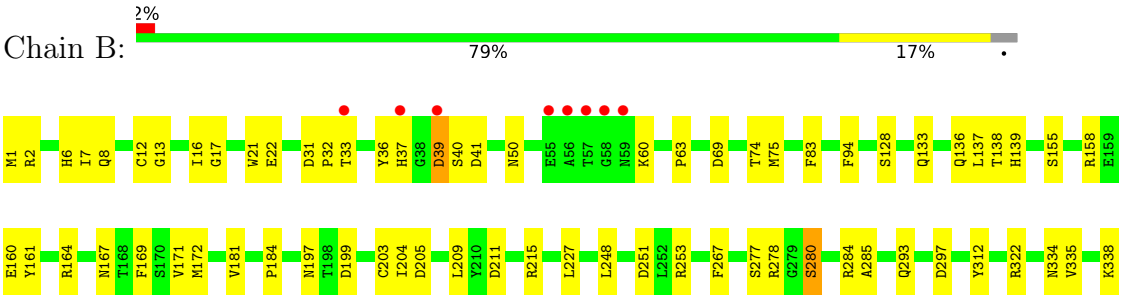
• Molecule 1: Tubulin alpha-1B chain

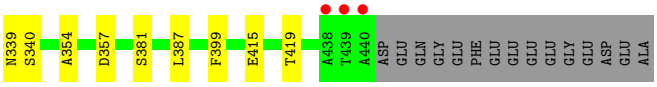


• Molecule 1: Tubulin alpha-1B chain



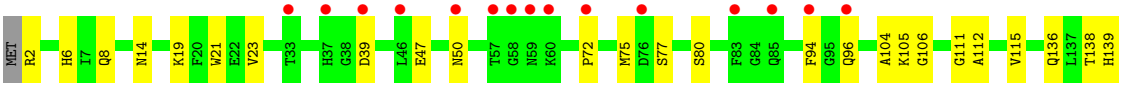
• Molecule 2: Tubulin beta chain

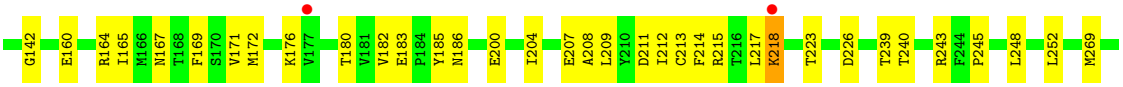


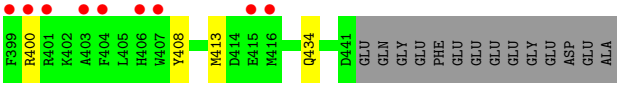


• Molecule 2: Tubulin beta chain

Chain D:

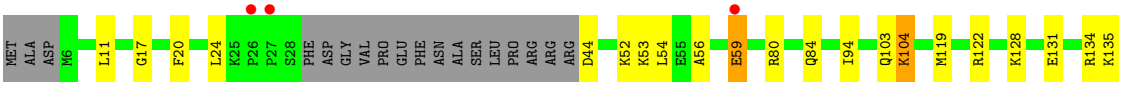


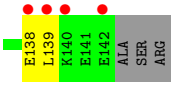




• Molecule 3: Stathmin-4

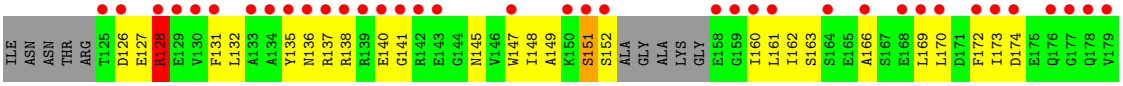
Chain E:

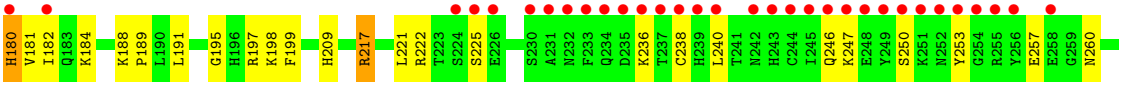


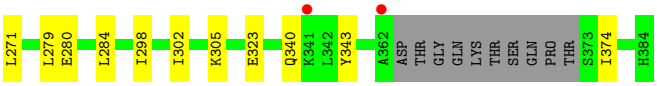


• Molecule 4: Tubulin tyrosine ligase

Chain F:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.88Å 156.13Å 183.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 2.50 49.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.96-2.50) 98.4 (49.96-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.199 , 0.229 0.200 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.4	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	0.94	EDS
Total number of atoms	18183	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: GDF, MG, GDP, CL, CA, MES, 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	0.45	0/3549	0.61	1/4817 (0.0%)
1	C	0.61	0/3562	0.66	0/4836
2	B	0.60	0/3485	0.65	1/4720 (0.0%)
2	D	0.52	0/3393	0.63	0/4597
3	E	0.57	0/1052	0.62	1/1396 (0.1%)
4	F	0.52	0/2974	0.67	2/4018 (0.0%)
All	All	0.54	0/18015	0.64	5/24384 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	128	ARG	NE-CZ-NH1	-12.23	114.19	120.30
3	E	44	ASP	CB-CG-OD2	5.61	123.34	118.30
2	B	297	ASP	CB-CG-OD1	5.59	123.33	118.30
4	F	32	LYS	CB-CA-C	-5.53	99.34	110.40
1	A	402	ARG	CG-CD-NE	-5.47	100.31	111.80

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	3453	0	3378	38	0
1	C	3463	0	3382	46	0
2	B	3398	0	3284	57	0
2	D	3311	0	3194	60	0
3	E	1031	0	1052	19	0
4	F	2894	0	2867	71	0
5	A	32	0	12	0	0
5	C	32	0	12	1	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	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	B	28	0	12	1	0
10	B	24	0	24	6	0
11	B	57	0	0	5	0
12	A	91	0	0	2	0
12	B	87	0	0	1	0
12	C	154	0	0	2	0
12	D	34	0	0	4	0
12	E	18	0	0	2	0
12	F	34	0	0	2	0
All	All	18183	0	17229	287	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 8.

All (287) 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:B:507:GDF:C03	11:B:507:GDF:C10	1.80	1.57
2:B:399:PHE:CE2	2:B:419:THR:HG22	2.10	0.86
2:B:399:PHE:HE2	2:B:419:THR:HG22	1.37	0.85
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.52	0.73
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.71	0.72
4:F:99:VAL:N	4:F:127:GLU:OE1	2.20	0.70
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:507:GDF:C10	11:B:507:GDF:C02	2.73	0.65
2:B:277:SER:HB2	2:B:280:SER:HB3	1.80	0.64
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.79	0.64
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.17	0.63
2:B:253:ARG:NH2	10:B:504:MES:O2S	2.26	0.63
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.81	0.63
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.34	0.62
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.80	0.62
4:F:135:TYR:O	4:F:145:ASN:ND2	2.32	0.62
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.81	0.62
4:F:31:ARG:HE	4:F:31:ARG:HA	1.65	0.62
4:F:138:ARG:HG3	4:F:138:ARG:HH11	1.65	0.61
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.41	0.61
4:F:138:ARG:HG3	4:F:138:ARG:NH1	2.15	0.61
4:F:148:ILE:HG13	4:F:162:ILE:HG13	1.81	0.61
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.17	0.60
1:C:188:ILE:HD13	1:C:395:PHE:HB2	1.83	0.60
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.84	0.60
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.84	0.60
4:F:128:ARG:O	4:F:131:PHE:HB3	2.02	0.60
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.35	0.59
11:B:507:GDF:C10	11:B:507:GDF:C53	2.77	0.59
1:A:60:LYS:HZ1	1:A:85:GLN:HG2	1.68	0.59
1:C:188:ILE:CD1	1:C:395:PHE:HB2	2.32	0.59
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.36	0.59
2:B:415:GLU:HG3	12:B:604:HOH:O	2.03	0.59
4:F:163:SER:HB3	4:F:169:LEU:HD22	1.84	0.58
2:B:1:MET:HG2	2:B:133:GLN:HB3	1.85	0.58
3:E:104:LYS:NZ	12:E:302:HOH:O	2.33	0.58
2:D:142:GLY:O	2:D:186:ASN:ND2	2.25	0.58
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.40	0.57
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.40	0.57
4:F:166:ALA:O	4:F:170:LEU:HB2	2.05	0.57
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.87	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.88	0.56
2:B:340[B]:SER:HG	4:F:34:ASN:HD21	1.48	0.56
1:C:430:LYS:CE	1:C:434:GLU:OE1	2.54	0.56
2:D:294:GLN:HA	2:D:297:ASP:HB2	1.87	0.56
4:F:103:THR:CG2	4:F:128:ARG:HH22	2.19	0.56
4:F:31:ARG:HA	4:F:31:ARG:NE	2.20	0.56
2:D:136:GLN:HA	2:D:167:ASN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:GLU:O	2:D:294:GLN:HG2	2.06	0.56
2:D:104:ALA:HB2	2:D:413:MET:CE	2.35	0.56
4:F:86:GLU:OE1	4:F:86:GLU:N	2.37	0.56
4:F:31:ARG:HD3	4:F:32:LYS:H	1.70	0.55
4:F:209:HIS:ND1	12:F:402:HOH:O	2.32	0.55
2:B:36:TYR:O	2:B:37:HIS:ND1	2.40	0.55
1:C:176:GLN:OE1	1:C:176:GLN:N	2.37	0.55
4:F:103:THR:HG23	4:F:128:ARG:HH22	1.72	0.55
2:D:106:GLY:O	2:D:111:GLY:HA3	2.05	0.55
2:D:164:ARG:HD2	12:D:713:HOH:O	2.07	0.55
2:B:199:ASP:OD1	10:B:504:MES:H32	2.06	0.55
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.42	0.55
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.89	0.55
2:D:171:VAL:HA	2:D:204:ILE:O	2.07	0.54
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.39	0.54
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.89	0.54
1:A:19:ALA:HB1	1:A:232:SER:OG	2.08	0.54
2:B:284:ARG:NH1	2:B:285:ALA:O	2.40	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.54
4:F:127:GLU:O	4:F:131:PHE:N	2.38	0.54
2:D:2:ARG:HH11	2:D:2:ARG:HB3	1.73	0.53
1:A:112:LYS:HE2	3:E:54:LEU:HB3	1.91	0.53
4:F:82:LYS:HE3	4:F:127:GLU:OE2	2.08	0.53
2:B:75:MET:HE1	2:B:94:PHE:HB3	1.90	0.53
2:B:50[B]:ASN:H	2:B:50[B]:ASN:ND2	2.07	0.53
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.89	0.53
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.90	0.53
4:F:160:ILE:HG22	4:F:161:LEU:H	1.74	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.53
2:B:69:ASP:OD2	2:B:74:THR:OG1	2.21	0.52
2:B:211:ASP:HB3	2:B:215:ARG:HH12	1.74	0.52
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.91	0.52
4:F:136:ASN:O	4:F:140:GLU:N	2.41	0.52
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.36	0.52
11:B:507:GDF:C03	11:B:507:GDF:C11	2.70	0.52
3:E:52:LYS:NZ	3:E:53:LYS:HE3	2.23	0.52
2:B:322:ARG:NH2	2:B:357:ASP:OD1	2.42	0.52
1:A:209:ILE:HD11	1:A:302:MET:SD	2.50	0.52
2:D:214:PHE:O	2:D:218:LYS:HA	2.10	0.52
2:B:340[B]:SER:OG	4:F:34:ASN:ND2	2.29	0.51
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:VAL:HG13	10:B:505:MES:H21	1.92	0.51
3:E:135:LYS:O	3:E:139:LEU:HD13	2.10	0.51
4:F:247:LYS:HB3	4:F:253:TYR:CE1	2.46	0.51
3:E:52:LYS:HZ3	3:E:53:LYS:HE3	1.76	0.51
4:F:70:LYS:HD2	4:F:76:SER:HB3	1.93	0.51
4:F:140:GLU:HG2	4:F:141:GLY:N	2.26	0.51
2:B:136:GLN:HA	2:B:167:ASN:O	2.11	0.51
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.26	0.50
4:F:101:TYR:HD2	4:F:126:ASP:HB2	1.76	0.50
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.93	0.50
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.92	0.50
1:C:188:ILE:HD13	1:C:395:PHE:CB	2.42	0.50
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.46	0.50
4:F:87:LEU:O	4:F:88:SER:OG	2.29	0.50
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.47	0.50
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.93	0.50
1:C:286:LEU:H	1:C:286:LEU:HD12	1.77	0.49
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.49
2:D:295:MET:CE	2:D:375:ALA:HB1	2.42	0.49
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.78	0.49
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.77	0.49
4:F:3:THR:HB	4:F:30:LEU:HD11	1.95	0.49
2:D:434:GLN:O	12:D:701:HOH:O	2.20	0.49
2:D:331:GLN:O	2:D:335:VAL:HG23	2.12	0.49
3:E:84:GLN:NE2	12:E:305:HOH:O	2.46	0.49
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.95	0.48
1:C:372:GLN:NE2	12:C:603:HOH:O	2.25	0.48
2:D:104:ALA:HB2	2:D:413:MET:HE3	1.95	0.48
1:C:209:ILE:HD11	1:C:302:MET:HG3	1.95	0.48
1:C:334:THR:HG23	1:C:338:LYS:HD2	1.96	0.48
4:F:199:PHE:CD2	4:F:221:LEU:HG	2.49	0.48
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.34	0.48
2:B:334:ASN:HD21	2:B:338:LYS:HE2	1.78	0.48
1:C:430:LYS:HD3	1:C:434:GLU:OE1	2.13	0.48
2:D:72:PRO:HG3	2:D:96:GLN:HA	1.96	0.48
4:F:138:ARG:HH12	4:F:184:LYS:HD3	1.79	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.48
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.79	0.47
2:D:208:ALA:O	2:D:212:ILE:HG13	2.14	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.47
4:F:103:THR:HG23	4:F:128:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.54	0.47
1:A:230:LEU:O	1:A:234:ILE:HD12	2.15	0.47
1:A:292:THR:O	1:A:295:CYS:HB2	2.15	0.47
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.49	0.47
2:D:272:PHE:O	2:D:300:ASN:HB3	2.15	0.47
4:F:88:SER:OG	4:F:90:SER:O	2.33	0.47
1:A:326:LYS:HD3	1:A:326:LYS:C	2.35	0.47
2:D:180:THR:HB	2:D:183:GLU:OE1	2.15	0.47
4:F:151:SER:OG	4:F:152:SER:N	2.48	0.47
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.97	0.47
4:F:160:ILE:HG22	4:F:161:LEU:N	2.29	0.47
1:C:430:LYS:O	1:C:434:GLU:HG3	2.15	0.47
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.50	0.46
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.50	0.46
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.78	0.46
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.46
1:C:430:LYS:NZ	1:C:434:GLU:OE1	2.47	0.46
2:B:172:MET:CE	2:B:387:LEU:HD21	2.45	0.46
2:D:211:ASP:HB3	2:D:215:ARG:HD2	1.98	0.46
4:F:247:LYS:HE3	4:F:247:LYS:HB2	1.68	0.46
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.16	0.46
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.98	0.46
2:B:75:MET:CE	2:B:94:PHE:HB3	2.45	0.46
1:C:68:VAL:HG21	1:C:118:VAL:HG21	1.98	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.45
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.17	0.45
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.98	0.45
2:B:160:GLU:HG2	2:B:161:TYR:CE1	2.49	0.45
1:A:228:ASN:O	1:A:232:SER:OG	2.31	0.45
2:D:223:THR:HG23	2:D:226:ASP:H	1.81	0.45
2:B:199:ASP:CG	10:B:504:MES:H32	2.36	0.45
2:D:2:ARG:HB3	2:D:2:ARG:NH1	2.31	0.45
2:D:104:ALA:HB2	2:D:413:MET:HE2	1.98	0.45
2:D:239:THR:O	2:D:243:ARG:HG3	2.17	0.45
4:F:188:LYS:HE2	4:F:323:GLU:OE2	2.17	0.45
4:F:169:LEU:H	4:F:169:LEU:HD23	1.80	0.45
4:F:126:ASP:OD1	4:F:127:GLU:N	2.49	0.45
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.45
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.99	0.45
4:F:149:ALA:HA	4:F:181:VAL:O	2.17	0.45
4:F:169:LEU:O	4:F:172:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.57	0.45
2:B:158:ARG:NH1	2:B:197:ASN:OD1	2.49	0.45
1:C:430:LYS:HD3	1:C:434:GLU:CD	2.37	0.45
3:E:56:ALA:O	3:E:59:GLU:HG3	2.16	0.45
3:E:134:ARG:O	3:E:138:GLU:HG3	2.16	0.45
1:A:211:ASP:HB3	12:A:602:HOH:O	2.15	0.45
2:B:33:THR:HB	2:B:60:LYS:HZ1	1.80	0.45
2:D:298:SER:HB2	2:D:307:PRO:HD2	1.97	0.45
2:B:33:THR:O	2:B:60:LYS:HE3	2.17	0.45
2:B:322:ARG:HD2	2:B:322:ARG:HA	1.78	0.44
1:C:2:ARG:HB3	1:C:133:GLN:HB2	1.99	0.44
2:D:215:ARG:O	2:D:218:LYS:HE2	2.17	0.44
2:D:369:ARG:HA	2:D:369:ARG:HD2	1.61	0.44
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.53	0.44
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.98	0.44
4:F:169:LEU:HA	4:F:172:PHE:HB3	1.99	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.52	0.44
2:D:320:ARG:O	2:D:373:MET:HA	2.18	0.44
2:D:105:LYS:NZ	12:D:709:HOH:O	2.50	0.44
2:D:167:ASN:ND2	2:D:200:GLU:HG3	2.33	0.44
4:F:12:SER:OG	12:F:401:HOH:O	2.21	0.44
2:B:181:VAL:O	2:B:184:PRO:HD2	2.18	0.44
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.00	0.44
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.53	0.43
4:F:102:PRO:HA	4:F:174:ASP:OD1	2.18	0.43
3:E:52:LYS:HZ3	3:E:53:LYS:HZ1	1.65	0.43
4:F:198:LYS:HG2	4:F:199:PHE:H	1.82	0.43
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.99	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.99	0.43
2:D:332:MET:O	2:D:336:GLN:HG3	2.18	0.43
1:A:336:LYS:HE3	1:A:349:THR:HG21	2.00	0.43
2:B:1:MET:HE1	2:B:251:ASP:OD1	2.19	0.43
2:B:16:ILE:HG13	2:B:17:GLY:N	2.32	0.43
2:B:36:TYR:OH	2:B:40:SER:O	2.35	0.43
2:B:205:ASP:O	2:B:209:LEU:HG	2.18	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.00	0.43
3:E:119:MET:HA	3:E:122:ARG:NH2	2.33	0.43
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.19	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
1:C:184:PRO:O	1:C:188:ILE:HD12	2.19	0.43
4:F:173:ILE:HD11	4:F:182:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:11:LEU:HD12	3:E:20:PHE:HB3	2.01	0.43
1:C:220:GLU:HG2	2:D:326:LYS:HD3	2.00	0.43
1:C:359:PRO:HB2	12:C:641:HOH:O	2.19	0.43
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.42
2:B:172:MET:HB2	2:B:205:ASP:HA	2.02	0.42
1:C:180:ALA:O	1:C:183:GLU:HG3	2.18	0.42
4:F:247:LYS:HB3	4:F:253:TYR:CZ	2.54	0.42
2:B:339:ASN:HB3	10:B:505:MES:H61	2.00	0.42
2:D:75:MET:HG3	2:D:94:PHE:CG	2.54	0.42
2:D:180:THR:O	2:D:183:GLU:HG3	2.18	0.42
2:B:8:GLN:HB2	2:B:13:GLY:O	2.20	0.42
1:C:205:ASP:CB	1:C:303:VAL:HA	2.50	0.42
4:F:149:ALA:HB2	4:F:169:LEU:HD12	2.02	0.42
3:E:52:LYS:HZ3	3:E:53:LYS:NZ	2.17	0.42
2:B:278:ARG:HE	2:B:278:ARG:HB2	1.59	0.42
1:C:298:PRO:HA	1:C:301:GLN:OE1	2.19	0.42
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.50	0.42
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.02	0.42
1:A:56:THR:OG1	1:A:60:LYS:HB3	2.20	0.42
1:A:90:GLU:HA	1:A:121:ARG:NH1	2.35	0.42
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.50	0.42
1:A:161:TYR:HB3	1:A:164:LYS:HG3	2.02	0.42
1:A:336:LYS:HD3	3:E:24:LEU:HD12	2.02	0.42
2:D:77:SER:O	2:D:80:SER:HB3	2.19	0.42
2:D:112:ALA:O	2:D:115:VAL:HG12	2.20	0.42
4:F:73:ARG:HG3	4:F:73:ARG:HH11	1.85	0.42
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.35	0.41
2:B:248:LEU:HD23	2:B:354:ALA:HB2	2.01	0.41
2:D:75:MET:HG3	2:D:94:PHE:CB	2.49	0.41
4:F:99:VAL:O	4:F:100:ILE:HD13	2.20	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.41
1:A:390[A]:ARG:HD2	4:F:54:HIS:CD2	2.55	0.41
1:C:388:TRP:CE3	1:C:425:MET:HE1	2.55	0.41
2:D:182:VAL:O	2:D:185:TYR:HB2	2.20	0.41
1:A:88:HIS:N	1:A:91:GLN:OE1	2.27	0.41
1:A:123:ARG:HA	1:A:123:ARG:HD3	1.85	0.41
2:D:176:LYS:NZ	2:D:207:GLU:OE2	2.27	0.41
4:F:246:GLN:O	4:F:250:SER:HB2	2.21	0.41
4:F:279:LEU:HG	4:F:284:LEU:HG	2.01	0.41
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:507:GDF:C10	11:B:507:GDF:C04	2.64	0.41
1:A:180:ALA:O	1:A:183:GLU:HG3	2.21	0.41
2:B:209:LEU:HB3	2:B:227:LEU:HG	2.03	0.41
1:A:320:ARG:HG3	12:A:618:HOH:O	2.20	0.41
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.41
1:C:72:PRO:HA	1:C:94:THR:HG21	2.03	0.41
1:C:351:PHE:CD1	1:C:351:PHE:N	2.88	0.41
3:E:135:LYS:HD2	3:E:135:LYS:HA	1.81	0.41
4:F:236:LYS:O	4:F:240:LEU:HB2	2.20	0.41
1:A:209:ILE:HG23	1:A:209:ILE:HD12	1.68	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.41
2:D:138:THR:HG22	2:D:169:PHE:HB2	2.03	0.41
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.02	0.41
2:D:400:ARG:HA	2:D:400:ARG:HD3	1.69	0.41
2:D:408:TYR:HB3	2:D:413:MET:HE3	2.02	0.41
3:E:80:ARG:HH11	3:E:80:ARG:HD2	1.73	0.41
4:F:217:ARG:HG2	4:F:374:ILE:O	2.21	0.41
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.96	0.41
2:B:158:ARG:CZ	10:B:504:MES:H21	2.51	0.41
2:D:204:ILE:CG2	2:D:209:LEU:HD11	2.50	0.41
4:F:21:LEU:O	4:F:24:THR:OG1	2.32	0.41
4:F:101:TYR:HD2	4:F:126:ASP:CB	2.34	0.40
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.03	0.40
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.04	0.40
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.57	0.40
4:F:184:LYS:HD2	4:F:184:LYS:HA	1.85	0.40
2:D:160:GLU:OE2	12:D:702:HOH:O	2.22	0.40
1:A:298:PRO:HA	1:A:301:GLN:CD	2.41	0.40
2:B:164[B]:ARG:HA	2:B:164[B]:ARG:HD2	1.91	0.40
2:D:274:PRO:HB3	2:D:286:LEU:HD22	2.04	0.40
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.40
3:E:52:LYS:HZ3	3:E:53:LYS:CE	2.33	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	442/451 (98%)	430 (97%)	12 (3%)	0	100	100
1	C	445/451 (99%)	437 (98%)	8 (2%)	0	100	100
2	B	432/445 (97%)	417 (96%)	15 (4%)	0	100	100
2	D	419/445 (94%)	404 (96%)	14 (3%)	1 (0%)	47	68
3	E	122/143 (85%)	118 (97%)	4 (3%)	0	100	100
4	F	346/384 (90%)	323 (93%)	22 (6%)	1 (0%)	41	61
All	All	2206/2319 (95%)	2129 (96%)	75 (3%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	32	LYS
2	D	340	SER

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	375/379 (99%)	373 (100%)	2 (0%)	88	96
1	C	378/379 (100%)	370 (98%)	8 (2%)	53	78
2	B	374/383 (98%)	366 (98%)	8 (2%)	53	78
2	D	366/383 (96%)	360 (98%)	6 (2%)	62	84
3	E	114/127 (90%)	110 (96%)	4 (4%)	36	62
4	F	319/342 (93%)	305 (96%)	14 (4%)	28	52
All	All	1926/1993 (97%)	1884 (98%)	42 (2%)	53	77

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	96	LYS
2	B	39[A]	ASP
2	B	39[B]	ASP
2	B	41	ASP
2	B	128	SER
2	B	139	HIS
2	B	155	SER
2	B	280	SER
2	B	293	GLN
1	C	2	ARG
1	C	71	GLU
1	C	165[A]	SER
1	C	165[B]	SER
1	C	215	ARG
1	C	245	ASP
1	C	251	ASP
1	C	302	MET
2	D	39	ASP
2	D	50	ASN
2	D	139	HIS
2	D	218	LYS
2	D	369	ARG
2	D	372	LYS
3	E	59	GLU
3	E	103	GLN
3	E	104	LYS
3	E	128	LYS
4	F	11	SER
4	F	70	LYS
4	F	105	LEU
4	F	128	ARG
4	F	137	ARG
4	F	151	SER
4	F	180	HIS
4	F	217	ARG
4	F	222	ARG
4	F	225	SER
4	F	238	CYS
4	F	271[A]	LEU
4	F	271[B]	LEU
4	F	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	358	GLN
2	D	8	GLN
2	D	15	GLN
2	D	167	ASN
2	D	426	ASN
3	E	103	GLN
4	F	333	ASN
4	F	340	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 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	1.24	2 (7%)	32,54,54	1.28	3 (9%)
11	GDF	B	507	-	57,65,65	4.54	27 (47%)	70,104,104	3.52	33 (47%)
5	GTP	C	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.35	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MES	B	504	-	12,12,12	2.25	4 (33%)	14,16,16	3.09	10 (71%)
5	GTP	D	602	6	26,34,34	1.16	2 (7%)	32,54,54	1.62	8 (25%)
9	GDP	B	501	6	24,30,30	0.96	0	30,47,47	1.19	3 (10%)
10	MES	B	505	-	12,12,12	2.42	1 (8%)	14,16,16	2.60	6 (42%)

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
11	GDF	B	507	-	-	5/30/127/127	0/7/9/9
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	D	602	6	-	5/18/38/38	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
10	MES	B	505	-	-	3/6/14/14	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	GDF	C43-C12	12.45	1.54	1.39
11	B	507	GDF	C43-N44	11.44	1.60	1.39
11	B	507	GDF	C03-C10	11.38	1.80	1.53
11	B	507	GDF	C47-C46	-9.40	1.21	1.56
11	B	507	GDF	C03-C04	-9.25	1.33	1.51
11	B	507	GDF	O52-C47	8.77	1.58	1.42
11	B	507	GDF	C04-C05	8.42	1.48	1.32
10	B	505	MES	C8-S	-7.59	1.66	1.77
11	B	507	GDF	C31-C28	7.18	1.64	1.50
11	B	507	GDF	C39-C14	6.73	1.51	1.39
11	B	507	GDF	C09-C11	-5.47	1.43	1.55
11	B	507	GDF	O36-C35	5.46	1.43	1.33
11	B	507	GDF	C31-N33	5.39	1.51	1.46
11	B	507	GDF	C11-C12	-5.21	1.43	1.51
11	B	507	GDF	C13-C14	5.20	1.47	1.39
10	B	504	MES	C8-S	-5.09	1.70	1.77
11	B	507	GDF	C17-C16	4.55	1.46	1.39
11	B	507	GDF	O54-C53	-4.54	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	GDF	C15-C35	4.42	1.57	1.53
11	B	507	GDF	O49-C48	4.17	1.41	1.33
11	B	507	GDF	O40-C39	4.13	1.43	1.37
5	C	501	GTP	C5-C6	-3.96	1.39	1.47
5	D	602	GTP	C5-C6	-3.91	1.39	1.47
5	A	501	GTP	C5-C6	-3.85	1.39	1.47
11	B	507	GDF	C42-C39	3.84	1.45	1.38
10	B	504	MES	O1S-S	3.80	1.56	1.45
10	B	504	MES	O2S-S	3.54	1.55	1.45
11	B	507	GDF	O54-C55	3.35	1.42	1.35
11	B	507	GDF	C46-N44	3.32	1.54	1.47
11	B	507	GDF	C32-N33	-3.29	1.41	1.46
11	B	507	GDF	C11-C10	-2.80	1.45	1.55
11	B	507	GDF	C21-C22	2.36	1.42	1.36
10	B	504	MES	O3S-S	2.30	1.55	1.47
5	D	602	GTP	C2-N3	2.26	1.38	1.33
5	A	501	GTP	O4'-C4'	-2.25	1.40	1.45
11	B	507	GDF	C34-N33	2.13	1.50	1.47
5	C	501	GTP	C5-C4	-2.10	1.37	1.43
11	B	507	GDF	C56-C55	2.07	1.56	1.49

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	507	GDF	C47-C46-N44	12.19	129.59	112.81
11	B	507	GDF	C43-N44-C46	-11.94	93.01	109.03
11	B	507	GDF	C11-C10-C03	-8.14	112.16	118.20
11	B	507	GDF	C45-N44-C46	7.93	138.55	119.21
11	B	507	GDF	O40-C39-C14	6.89	123.63	116.58
10	B	504	MES	C5-N4-C3	6.89	124.33	108.83
11	B	507	GDF	C53-O54-C55	-6.44	107.72	117.65
10	B	504	MES	O2S-S-C8	6.00	114.14	106.92
11	B	507	GDF	C26-C32-N33	5.85	118.25	110.08
11	B	507	GDF	C10-C03-C04	5.65	114.06	108.28
10	B	505	MES	O1S-S-C8	5.58	113.63	106.92
11	B	507	GDF	O36-C35-C15	4.84	118.60	111.32
11	B	507	GDF	O49-C48-C47	4.83	120.34	112.22
10	B	505	MES	C5-N4-C3	4.57	119.12	108.83
11	B	507	GDF	O40-C39-C42	-4.38	116.58	124.12
11	B	507	GDF	O54-C55-C56	4.18	118.77	111.09
11	B	507	GDF	O54-C53-C47	4.12	112.95	106.30
11	B	507	GDF	C09-C11-C12	-3.98	105.09	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	602	GTP	C5-C6-N1	3.68	120.46	113.95
11	B	507	GDF	O52-C47-C46	3.51	120.07	108.08
11	B	507	GDF	C06-N07-C08	3.50	126.60	115.90
5	D	602	GTP	PB-O3B-PG	-3.34	121.36	132.83
11	B	507	GDF	C53-C47-C46	-3.32	102.39	109.23
10	B	504	MES	O1-C6-C5	-3.24	104.66	111.80
5	A	501	GTP	C8-N7-C5	3.15	109.00	102.99
5	A	501	GTP	C2-N1-C6	-3.14	119.32	125.10
11	B	507	GDF	C13-C14-C39	3.11	121.23	116.78
11	B	507	GDF	C06-N07-C10	3.11	120.63	112.50
5	D	602	GTP	C8-N7-C5	3.11	108.92	102.99
5	A	501	GTP	C5-C6-N1	3.11	119.44	113.95
5	C	501	GTP	C8-N7-C5	3.04	108.79	102.99
9	B	501	GDP	C5-C6-N1	3.03	119.30	113.95
5	D	602	GTP	C2-N1-C6	-3.00	119.57	125.10
10	B	505	MES	C7-N4-C3	3.00	118.90	111.23
10	B	505	MES	O3S-S-C8	2.98	110.59	105.77
5	C	501	GTP	C5-C6-N1	2.91	119.09	113.95
11	B	507	GDF	C03-C10-N07	2.87	117.76	111.72
11	B	507	GDF	C12-C11-C46	-2.85	97.78	102.21
10	B	504	MES	C7-N4-C5	2.77	118.33	111.23
9	B	501	GDP	O6-C6-C5	-2.75	119.00	124.37
11	B	507	GDF	C42-C39-C14	-2.62	119.79	122.20
11	B	507	GDF	C47-C46-C11	2.61	119.57	114.18
5	C	501	GTP	C2-N1-C6	-2.60	120.31	125.10
9	B	501	GDP	C8-N7-C5	2.59	107.93	102.99
11	B	507	GDF	O49-C48-O51	-2.55	119.46	123.93
11	B	507	GDF	C03-C04-C05	-2.53	118.38	124.02
11	B	507	GDF	C12-C43-N44	-2.51	108.12	110.98
11	B	507	GDF	O51-C48-C47	-2.48	120.08	123.94
10	B	505	MES	C2-C3-N4	-2.48	106.34	110.10
11	B	507	GDF	C46-C11-C10	2.48	118.26	114.07
10	B	504	MES	C6-O1-C2	2.42	117.96	109.89
11	B	507	GDF	C09-C11-C10	2.41	107.07	101.82
10	B	504	MES	O1S-S-C8	2.37	109.77	106.92
10	B	504	MES	C7-N4-C3	2.37	117.29	111.23
5	C	501	GTP	PA-O3A-PB	-2.32	124.85	132.83
11	B	507	GDF	C06-C05-C04	2.31	126.80	123.02
11	B	507	GDF	C45-N44-C43	2.25	128.03	120.84
10	B	505	MES	O1-C2-C3	2.22	116.68	111.80
5	C	501	GTP	PB-O3B-PG	-2.21	125.23	132.83
5	D	602	GTP	O2G-PG-O3B	2.21	112.05	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	602	GTP	PA-O3A-PB	-2.21	125.24	132.83
5	C	501	GTP	O6-C6-C5	-2.21	120.06	124.37
5	D	602	GTP	O3G-PG-O3B	2.21	112.03	104.64
11	B	507	GDF	C41-O40-C39	-2.16	114.26	117.53
5	D	602	GTP	O6-C6-C5	-2.08	120.31	124.37
10	B	504	MES	C2-C3-N4	2.07	113.25	110.10
10	B	504	MES	C6-C5-N4	-2.07	106.96	110.10
11	B	507	GDF	O36-C35-O38	-2.05	120.34	123.93
10	B	504	MES	O2S-S-O1S	-2.02	106.96	113.95

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	602	GTP	C5'-O5'-PA-O1A
5	D	602	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O3S
10	B	505	MES	C8-C7-N4-C3
11	B	507	GDF	O51-C48-O49-C50
11	B	507	GDF	C47-C48-O49-C50
5	D	602	GTP	PB-O3B-PG-O1G
10	B	505	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O1G
5	D	602	GTP	PB-O3B-PG-O2G
5	D	602	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
11	B	507	GDF	C42-C39-O40-C41
10	B	504	MES	C7-C8-S-O2S
11	B	507	GDF	C14-C39-O40-C41
5	C	501	GTP	PB-O3B-PG-O1G
9	B	501	GDP	PB-O3A-PA-O2A
10	B	505	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	PB-O3A-PA-O1A
11	B	507	GDF	C31-C28-C29-C30

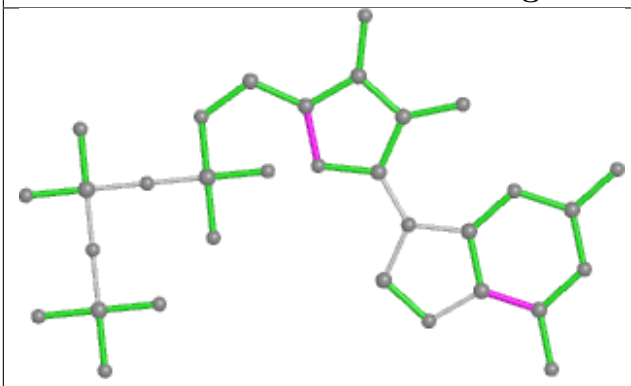
There are no ring outliers.

5 monomers are involved in 13 short contacts:

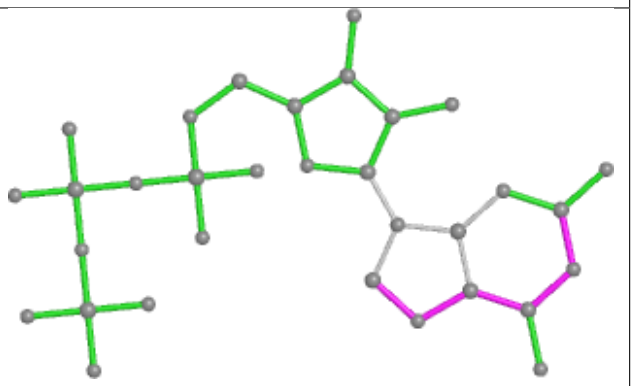
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	507	GDF	5	0
5	C	501	GTP	1	0
10	B	504	MES	4	0
9	B	501	GDP	1	0
10	B	505	MES	2	0

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.

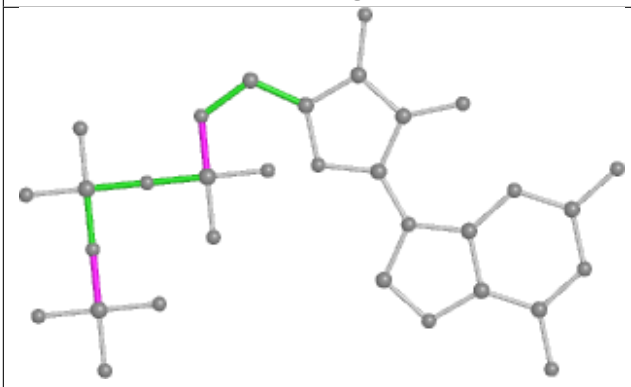
Ligand GTP A 501



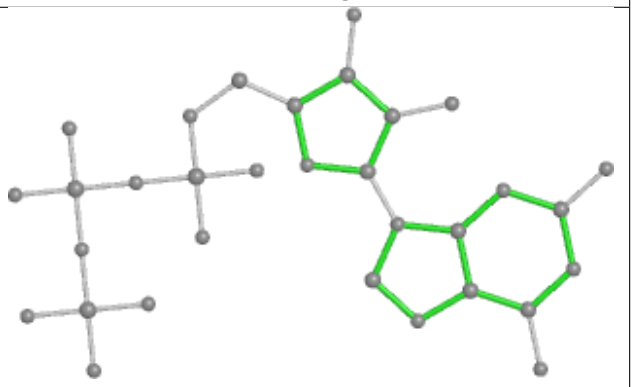
Bond lengths



Bond angles

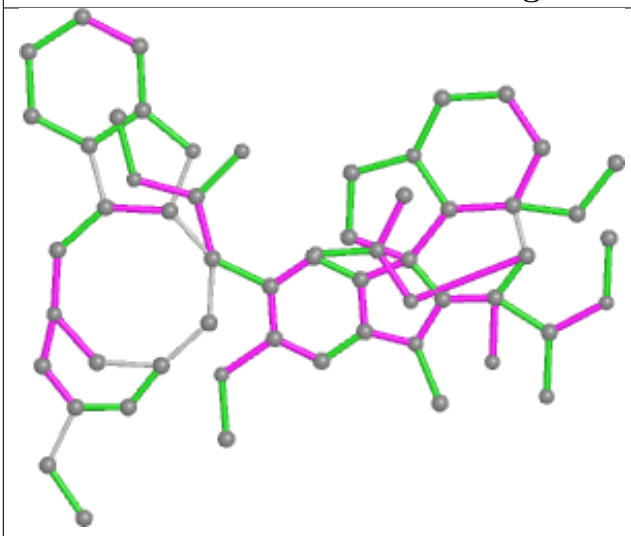


Torsions

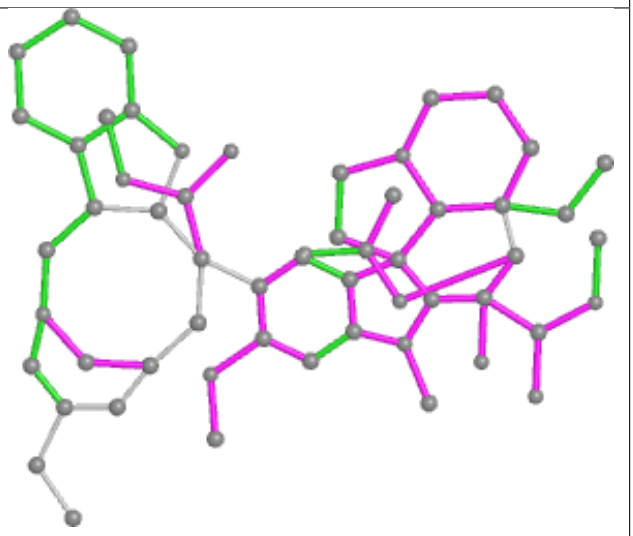


Rings

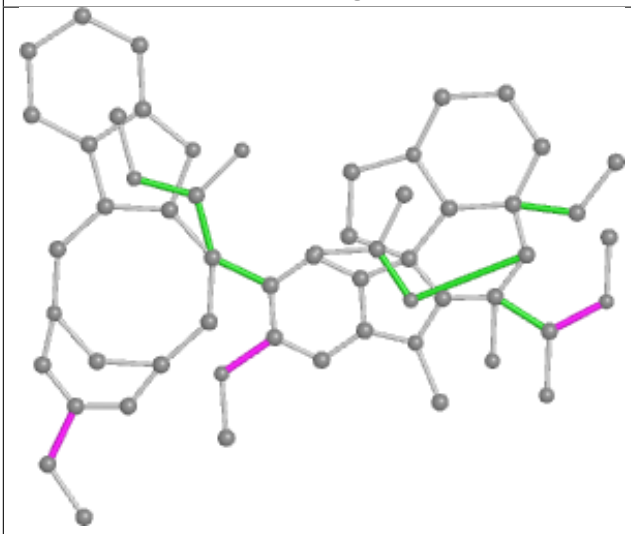
Ligand GDF B 507



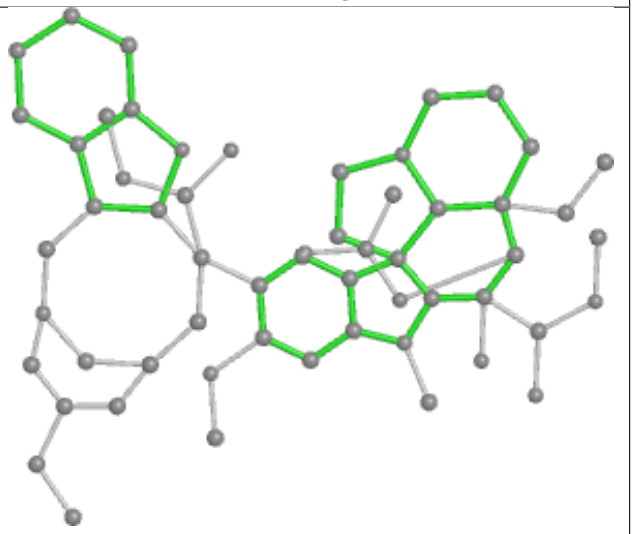
Bond lengths



Bond angles

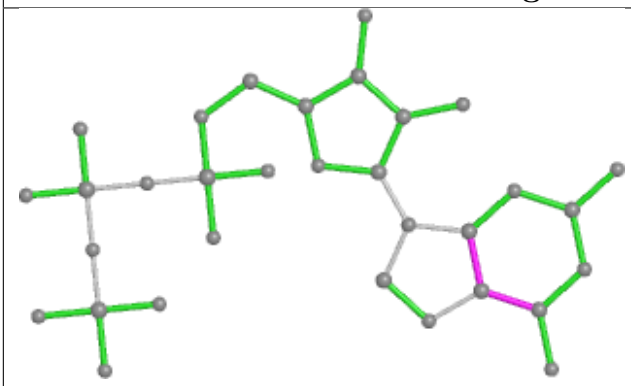


Torsions

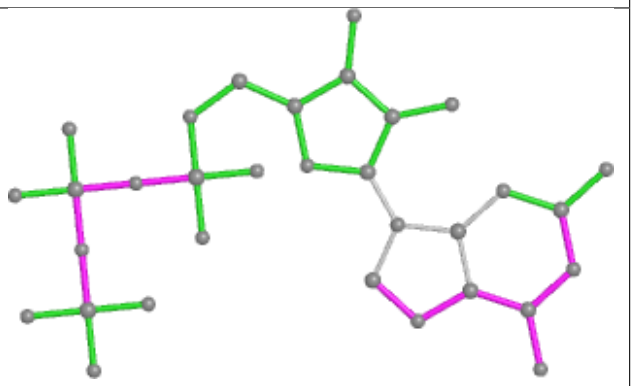


Rings

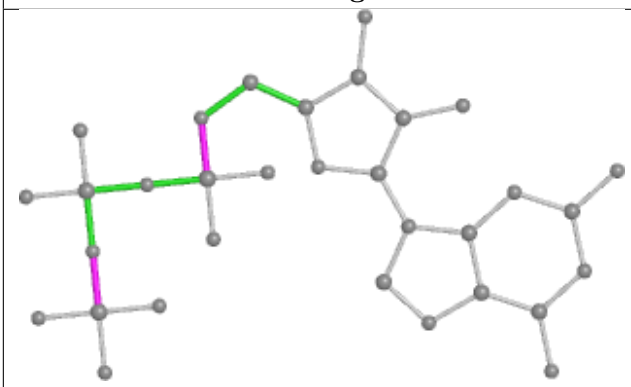
Ligand GTP C 501



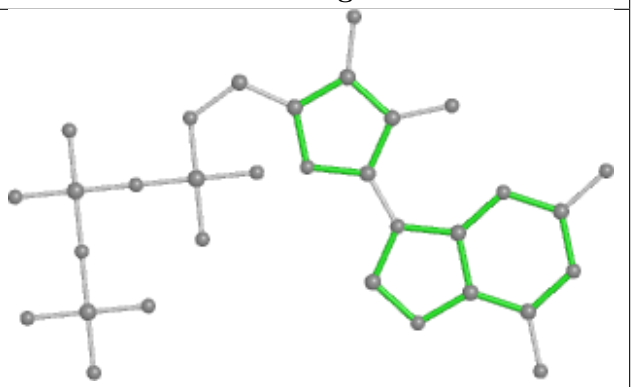
Bond lengths



Bond angles

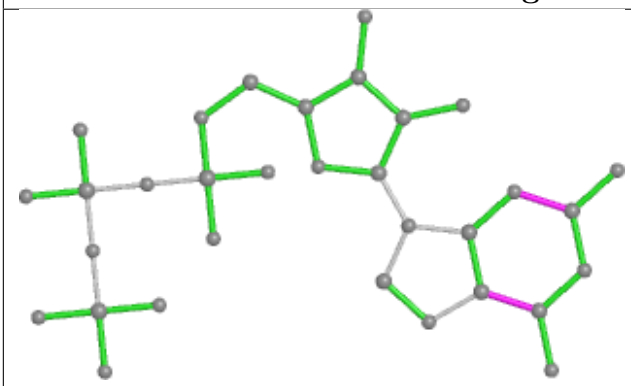


Torsions

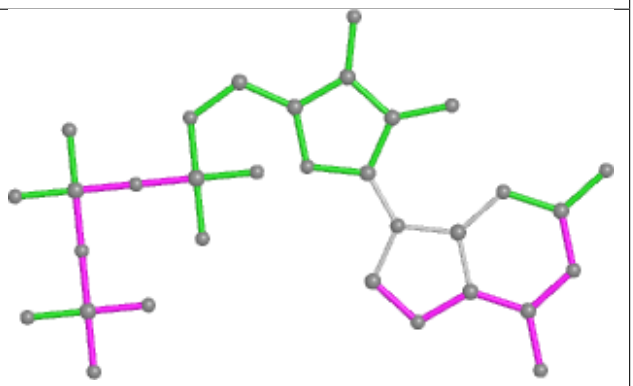


Rings

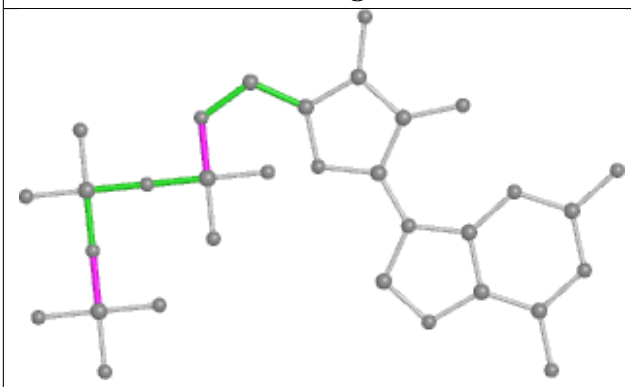
Ligand GTP D 602



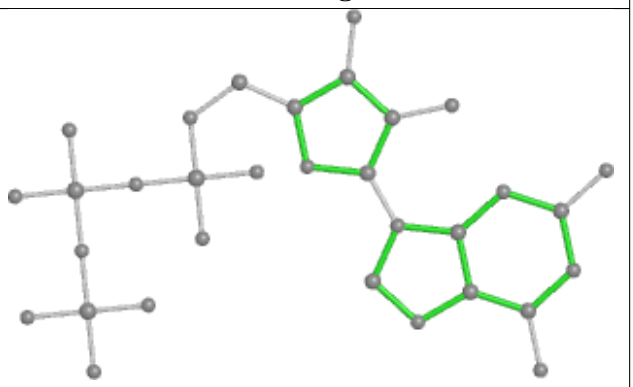
Bond lengths



Bond angles

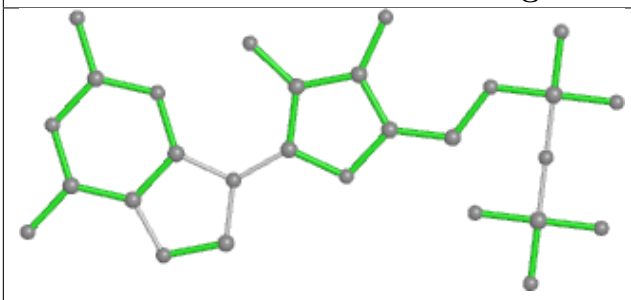


Torsions

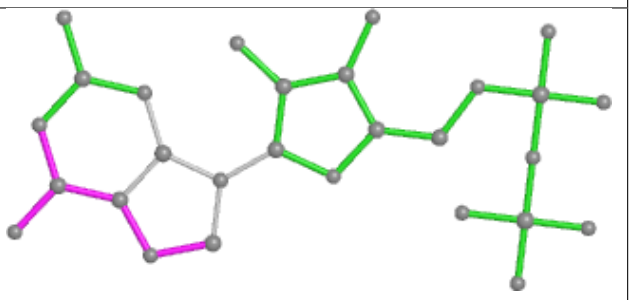


Rings

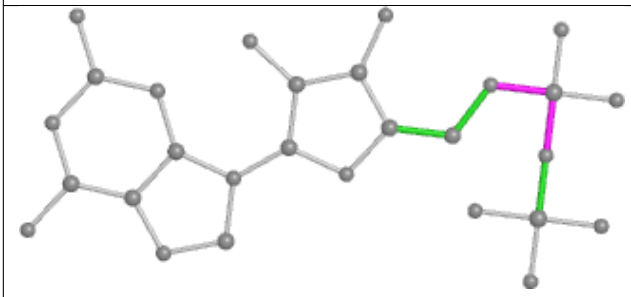
Ligand GDP B 501



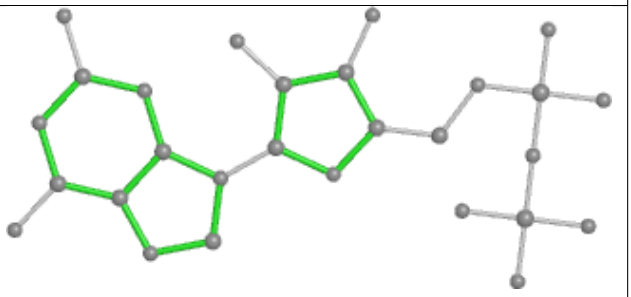
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	438/451 (97%)	0.04	7 (1%) 72 74	28, 41, 63, 80	0
1	C	440/451 (97%)	-0.20	1 (0%) 95 95	23, 35, 47, 56	1 (0%)
2	B	430/445 (96%)	-0.10	11 (2%) 56 59	22, 36, 62, 78	1 (0%)
2	D	420/445 (94%)	0.33	26 (6%) 20 21	32, 56, 78, 88	3 (0%)
3	E	122/143 (85%)	0.43	7 (5%) 23 25	36, 56, 78, 91	0
4	F	350/384 (91%)	1.02	84 (24%) 0 0	36, 68, 117, 136	0
All	All	2200/2319 (94%)	0.20	136 (6%) 20 21	22, 45, 83, 136	5 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	6.5
4	F	249	TYR	6.5
4	F	177	GLY	6.4
4	F	244	CYS	6.3
4	F	233	PHE	5.8
2	B	57	THR	5.8
2	D	57	THR	5.7
4	F	166	ALA	5.7
4	F	173	ILE	5.6
4	F	140	GLU	5.5
4	F	253	TYR	5.5
4	F	130	VAL	5.3
4	F	170	LEU	5.2
4	F	137	ARG	5.0
4	F	152	SER	4.8
4	F	141	GLY	4.8
4	F	255	ARG	4.6
4	F	251	LYS	4.6
4	F	362	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
4	F	256	TYR	4.4
4	F	104	ASN	4.3
2	D	58	GLY	4.3
1	C	440	VAL	4.1
4	F	245	ILE	4.0
1	A	282	TYR	4.0
4	F	133	ALA	4.0
4	F	235	ASP	4.0
4	F	142	ARG	4.0
4	F	243	HIS	4.0
4	F	176	GLN	3.9
4	F	134	ALA	3.8
4	F	103	THR	3.8
2	D	404	PHE	3.8
4	F	231	ALA	3.7
4	F	99	VAL	3.7
2	D	33	THR	3.7
2	D	218	LYS	3.6
4	F	125	THR	3.6
4	F	252	ASN	3.6
4	F	169	LEU	3.4
4	F	101	TYR	3.4
4	F	139	ARG	3.4
3	E	140	LYS	3.4
4	F	250	SER	3.4
4	F	151	SER	3.3
4	F	179	VAL	3.2
4	F	238	CYS	3.2
4	F	178	GLN	3.2
2	D	94	PHE	3.2
4	F	254	GLY	3.2
4	F	236	LYS	3.2
1	A	42	ILE	3.1
2	D	400	ARG	3.1
4	F	89	GLU	3.1
2	D	96	GLN	3.1
4	F	100	ILE	3.1
4	F	138	ARG	3.1
1	A	262	TYR	3.1
4	F	24	THR	3.1
4	F	182	ILE	3.0
4	F	246	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	56	ALA	3.0
4	F	128	ARG	3.0
2	D	401	ARG	2.9
3	E	142	GLU	2.9
1	A	438	ASP	2.9
4	F	239	HIS	2.9
4	F	136	ASN	2.9
4	F	143	GLU	2.9
1	A	346	TRP	2.9
4	F	248	GLU	2.9
3	E	27	PRO	2.9
4	F	247	LYS	2.9
3	E	138	GLU	2.8
4	F	131	PHE	2.8
2	D	37	HIS	2.8
4	F	150	LYS	2.8
4	F	10	ASN	2.8
4	F	129	GLU	2.8
4	F	172	PHE	2.8
4	F	174	ASP	2.8
1	A	281	ALA	2.7
2	D	83	PHE	2.7
4	F	161	LEU	2.7
2	D	415	GLU	2.7
2	D	59	ASN	2.7
4	F	234	GLN	2.7
4	F	17	VAL	2.7
4	F	226	GLU	2.6
2	B	59	ASN	2.6
2	D	50	ASN	2.6
3	E	26	PRO	2.6
2	B	439	THR	2.5
4	F	160	ILE	2.5
2	B	440	ALA	2.5
2	D	85	GLN	2.5
4	F	126	ASP	2.5
4	F	258	GLU	2.5
2	D	46	LEU	2.5
4	F	232	ASN	2.5
4	F	164	SER	2.4
2	D	407	TRP	2.4
4	F	147	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	438	ALA	2.4
4	F	225	SER	2.4
2	D	416	MET	2.4
2	D	60	LYS	2.4
2	D	76	ASP	2.4
4	F	135	TYR	2.3
4	F	90	SER	2.3
2	D	177	VAL	2.3
2	D	399	PHE	2.3
2	B	55	GLU	2.3
2	B	58	GLY	2.3
2	D	403	ALA	2.3
2	B	33	THR	2.3
2	D	406	HIS	2.3
1	A	163	LYS	2.2
4	F	168	GLU	2.2
4	F	240	LEU	2.2
2	D	39	ASP	2.2
4	F	242	ASN	2.2
4	F	158	GLU	2.1
4	F	237	THR	2.1
4	F	180	HIS	2.1
4	F	32	LYS	2.1
4	F	20	LEU	2.1
4	F	159	GLY	2.1
3	E	139	LEU	2.1
4	F	230	SER	2.0
3	E	59	GLU	2.0
4	F	224	SER	2.0
4	F	341	LYS	2.0
2	B	37	HIS	2.0
2	B	39[A]	ASP	2.0
2	D	72	PRO	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)

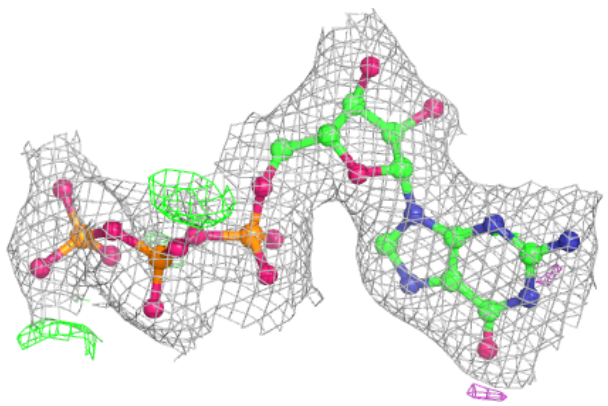
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

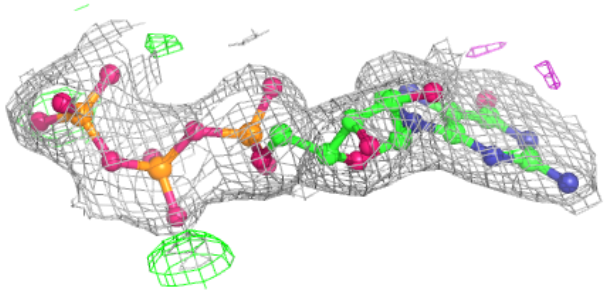
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	B	503	1/1	0.25	1.04	187,187,187,187	0
7	CA	E	201	1/1	0.74	0.17	91,91,91,91	0
6	MG	B	502	1/1	0.83	0.21	58,58,58,58	0
6	MG	B	506	1/1	0.87	0.57	89,89,89,89	0
6	MG	C	502	1/1	0.88	0.22	37,37,37,37	0
8	CL	A	504	1/1	0.88	0.11	51,51,51,51	0
6	MG	D	601	1/1	0.91	0.08	63,63,63,63	0
7	CA	C	503	1/1	0.94	0.12	50,50,50,50	0
7	CA	A	503	1/1	0.94	0.04	55,55,55,55	0
6	MG	A	502	1/1	0.94	0.48	44,44,44,44	0
5	GTP	D	602	32/32	0.95	0.13	51,63,81,84	0
11	GDF	B	507	57/57	0.95	0.16	35,41,50,56	0
10	MES	B	504	12/12	0.96	0.17	41,46,68,74	0
10	MES	B	505	12/12	0.97	0.17	32,41,63,67	0
5	GTP	C	501	32/32	0.98	0.17	28,34,38,40	0
5	GTP	A	501	32/32	0.98	0.23	28,39,58,59	0
9	GDP	B	501	28/28	0.98	0.15	18,22,29,30	0

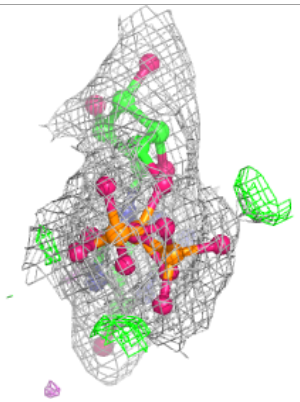
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

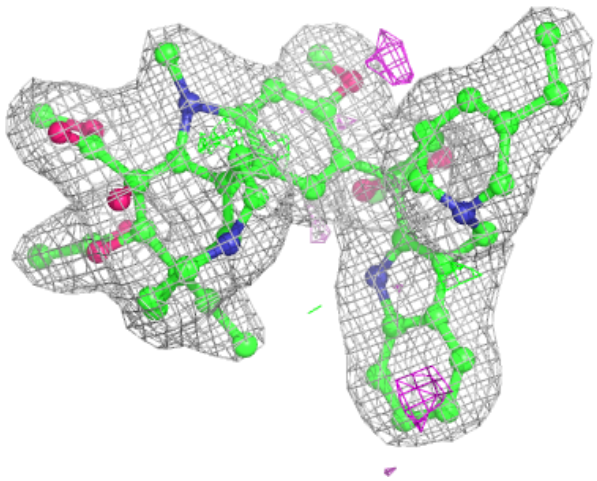


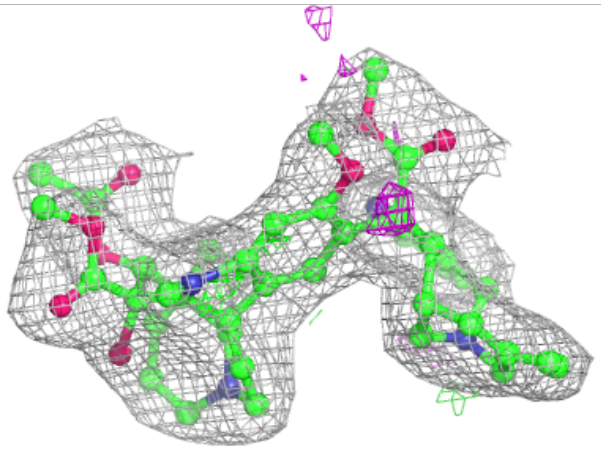


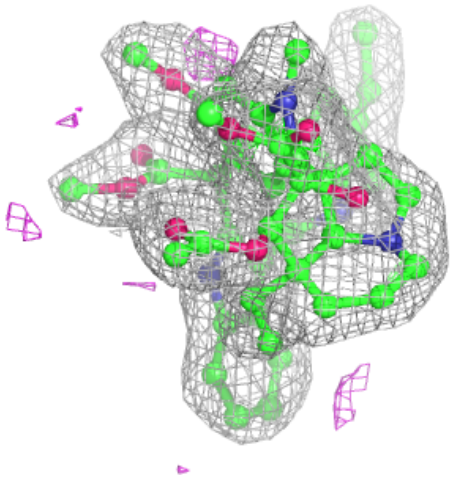


Electron density around GDF B 507:

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

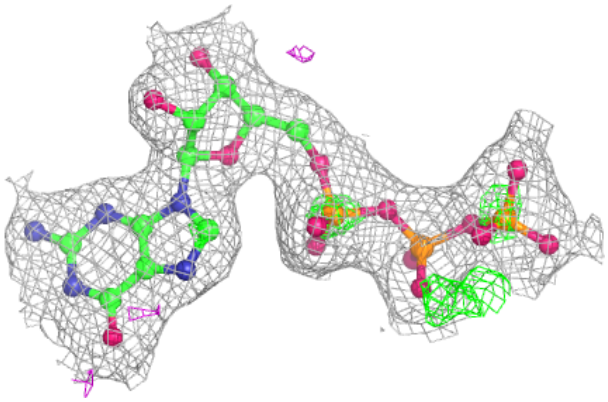


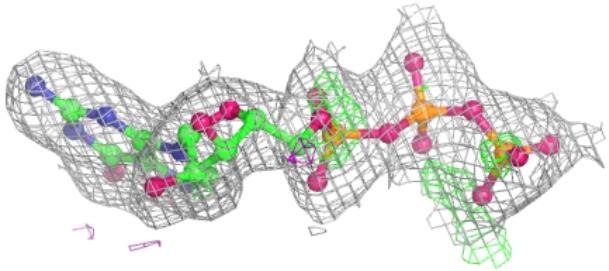


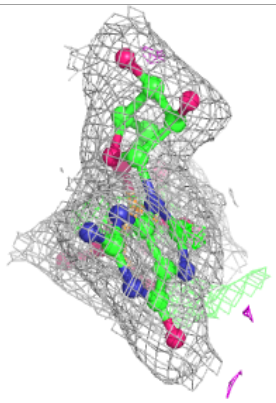


Electron density around GTP C 501:

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

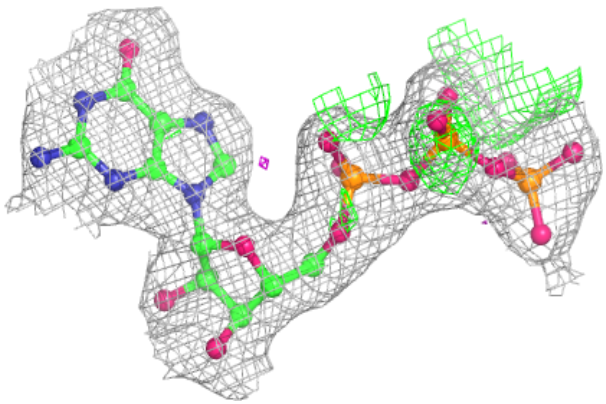


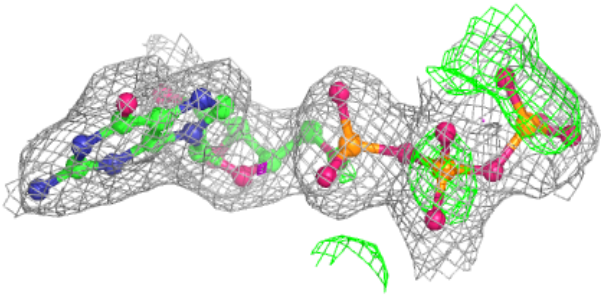


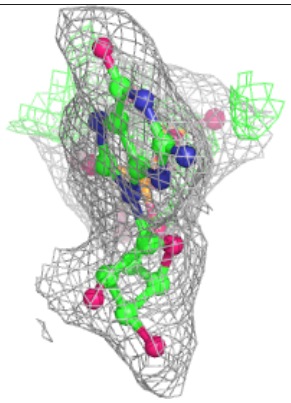


Electron density around GTP A 501:

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

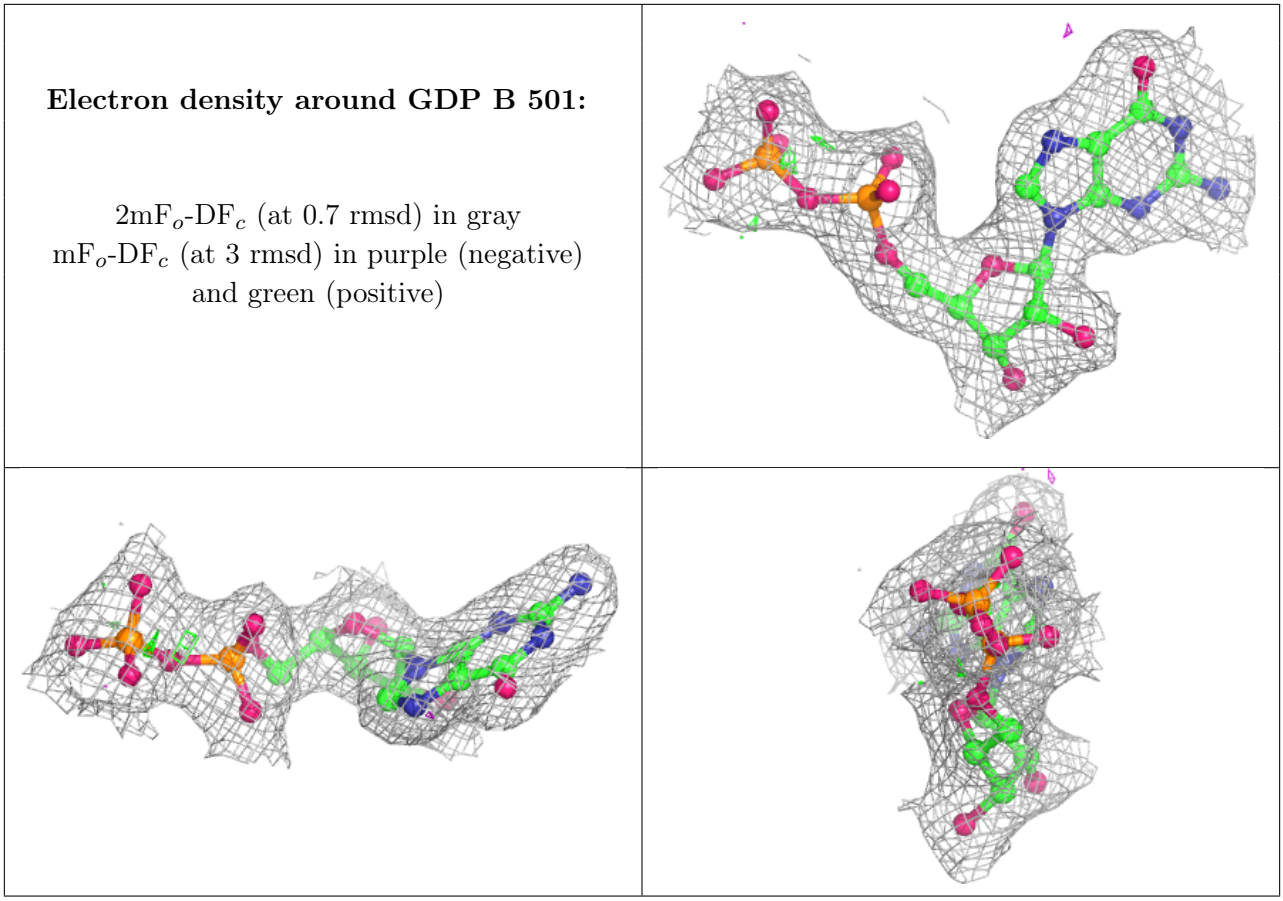






Electron density around GDP B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.