Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 09:18 AM EST

PDB ID	:	6BS2
Title	:	Tubulin-RB3_SLD-TTL in complex with heterocyclic pyrimidine compound 8b
Authors	:	Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on	:	2017-12-01
Resolution	:	2.65 Å(reported)

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

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

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

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

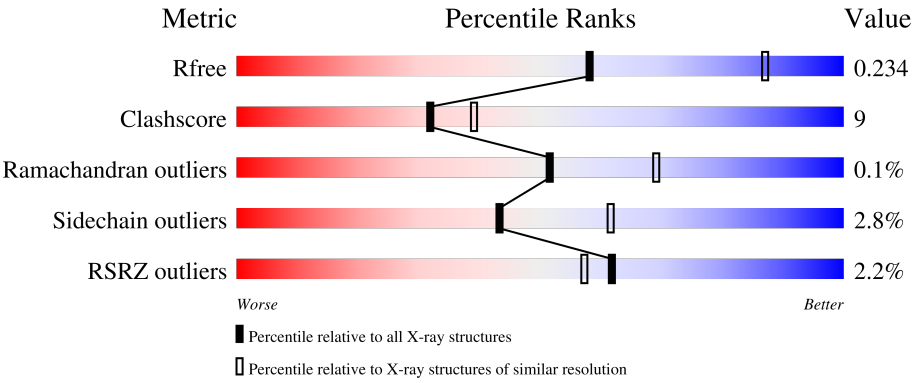
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.65 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.



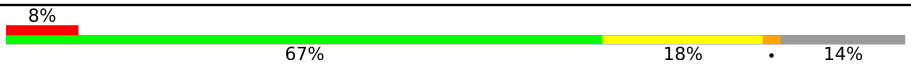
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	450	82% 14% •
1	C	450	80% 17% • •
2	B	445	2% 78% 17% • •
2	D	445	2% 74% 20% 5%
3	E	143	2% 69% 15% • 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17633 atoms, of which 14 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	437	Total	C	N	O	S	0	0	0
			3404	2155	579	648	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3355	2107	573	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3307	2079	562	639	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

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

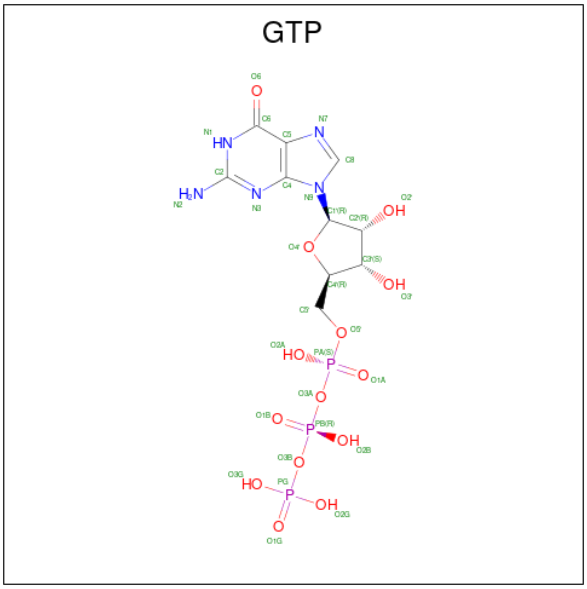
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2707	1741	464	488	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

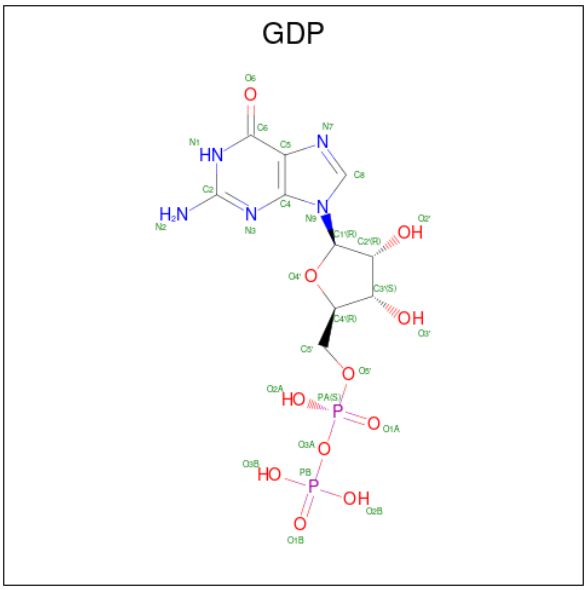
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

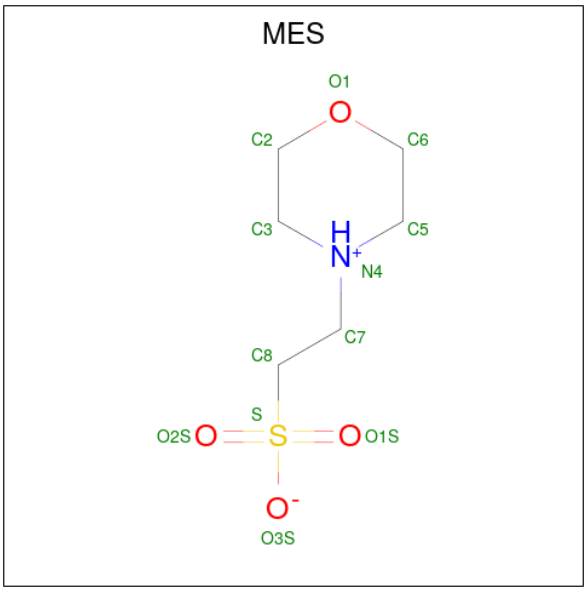
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

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



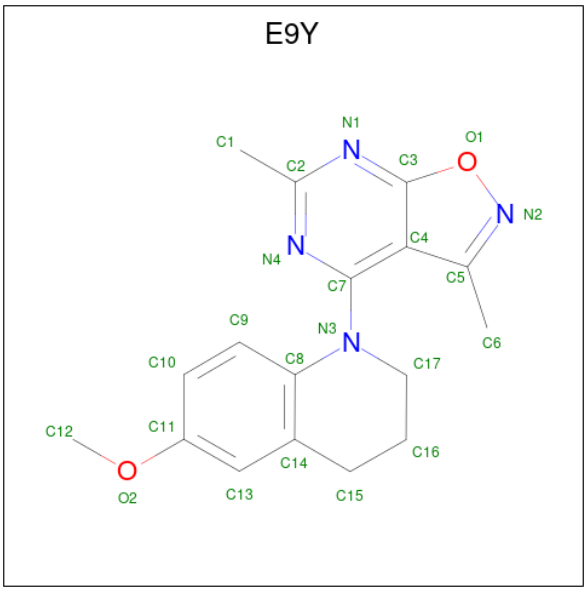
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

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



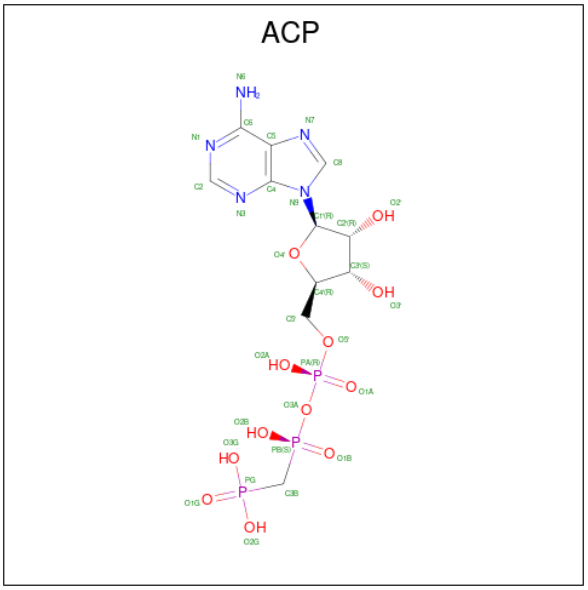
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 1-(3,6-dimethyl[1,2]oxazolo[5,4-d]pyrimidin-4-yl)-6-methoxy-1,2,3,4-tetrahydroquinoline (three-letter code: E9Y) (formula: $C_{17}H_{18}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O 23 17 4 2	0	0
10	D	1	Total C N O 23 17 4 2	0	0

- 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 H N O P 45 11 14 5 12 3	0	0

- Molecule 12 is water.

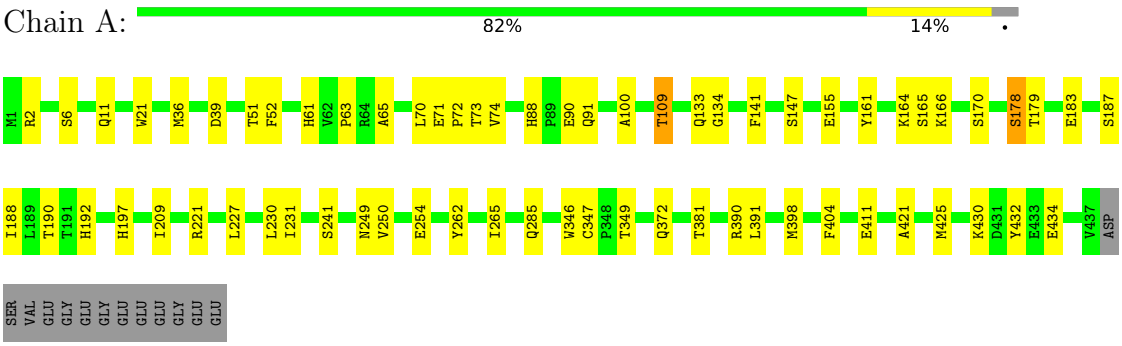
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	40	Total O 40 40	0	0
12	B	37	Total O 37 37	0	0
12	C	56	Total O 56 56	0	0
12	D	23	Total O 23 23	0	0
12	E	2	Total O 2 2	0	0
12	F	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

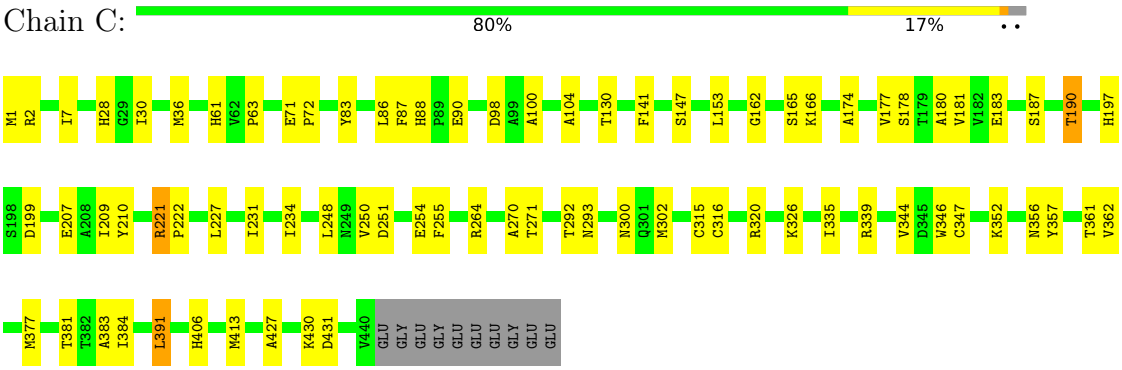
• Molecule 1: Tubulin alpha-1B chain

Chain A:



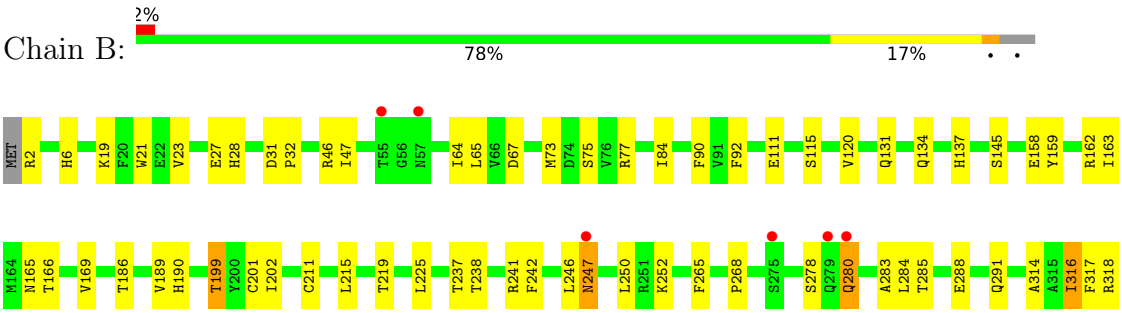
• Molecule 1: Tubulin alpha-1B chain

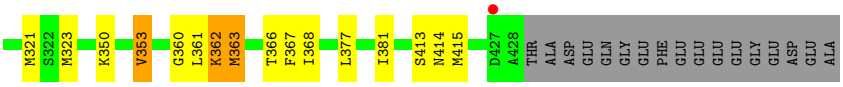
Chain C:



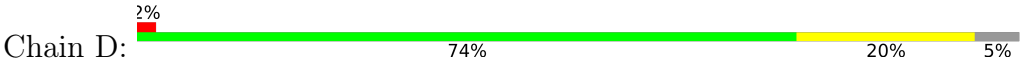
• Molecule 2: Tubulin beta-2B chain

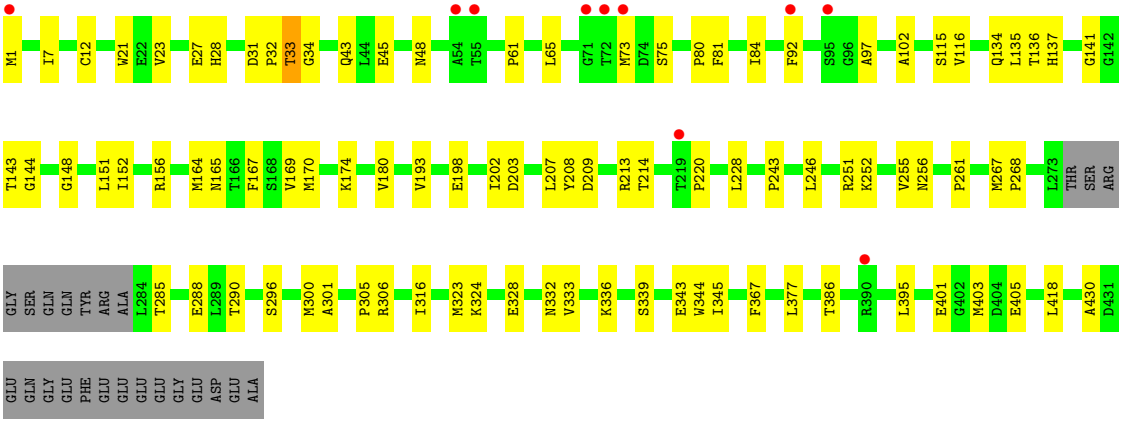
Chain B:



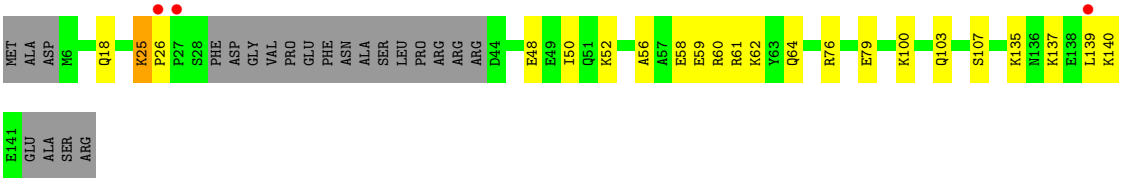


• Molecule 2: Tubulin beta-2B chain

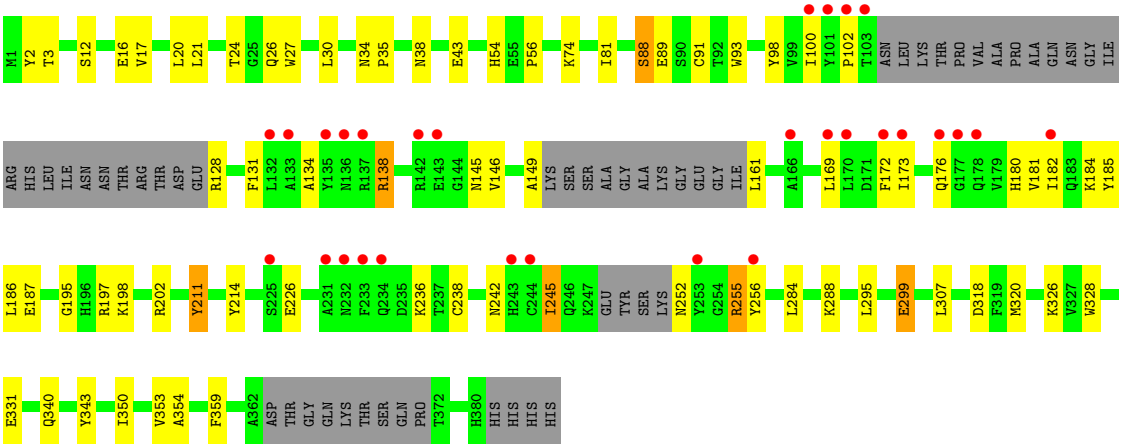




• Molecule 3: Stathmin-4



• 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	105.10Å 157.60Å 181.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.65 49.75 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.75-2.65) 97.3 (49.75-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.181 , 0.234 0.181 , 0.234	Depositor DCC
R_{free} test set	4223 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17633	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: E9Y, ACP, GDP, MG, CA, GTP, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.42	0/3482	0.61	0/4730
1	C	0.48	2/3515 (0.1%)	0.66	0/4772
2	B	0.45	1/3430 (0.0%)	0.62	0/4647
2	D	0.38	0/3380	0.59	0/4578
3	E	0.44	0/1008	0.53	0/1337
4	F	0.36	0/2769	0.55	0/3743
All	All	0.42	3/17584 (0.0%)	0.60	0/23807

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	111	GLU	CG-CD	5.28	1.59	1.51
1	C	347	CYS	CB-SG	-5.06	1.73	1.81
1	C	315	CYS	CB-SG	-5.01	1.73	1.81

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	3404	0	3305	54	0
1	C	3437	0	3349	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3355	0	3227	64	0
2	D	3307	0	3184	66	0
3	E	1000	0	1018	19	0
4	F	2707	0	2667	57	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	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	F	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	3	0
9	B	24	0	24	1	0
9	C	12	0	12	2	0
10	B	23	0	0	2	0
10	D	23	0	0	0	0
11	F	31	14	14	0	0
12	A	40	0	0	0	0
12	B	37	0	0	0	0
12	C	56	0	0	1	0
12	D	23	0	0	1	0
12	E	2	0	0	0	0
12	F	12	0	0	2	0
All	All	17619	14	16848	305	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 9.

All (305) 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)
2:B:283:ALA:HA	2:B:362:LYS:HE3	1.21	1.09
2:B:321:MET:HB3	2:B:363:MET:HE1	1.36	1.06
4:F:24:THR:HG23	4:F:26:GLN:H	1.33	0.93
1:C:221:ARG:HD2	2:D:323:MET:HG2	1.48	0.92
1:A:71:GLU:OE1	1:A:73:THR:HB	1.70	0.90
1:C:381:THR:HG22	1:C:383:ALA:H	1.36	0.89
2:B:283:ALA:CA	2:B:362:LYS:HE3	2.03	0.88
1:A:109:THR:HG21	1:A:411:GLU:OE2	1.78	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:O	2:B:247:ASN:ND2	2.15	0.79
2:B:362:LYS:HD2	2:B:363:MET:CG	2.13	0.78
1:C:221:ARG:CD	2:D:323:MET:HG2	2.13	0.78
4:F:21:LEU:O	4:F:24:THR:HG22	1.84	0.77
4:F:149:ALA:HB2	4:F:161:LEU:HB3	1.68	0.76
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.66	0.76
4:F:172:PHE:O	4:F:176:GLN:HG2	1.86	0.74
1:A:262:TYR:HE2	1:A:346:TRP:CZ2	2.06	0.73
1:A:88:HIS:N	1:A:91:GLN:OE1	2.19	0.73
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.71	0.73
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.70	0.73
1:A:285:GLN:HG3	1:A:372:GLN:NE2	2.05	0.71
1:A:349:THR:OG1	3:E:25:LYS:HE3	1.88	0.71
2:B:186:THR:HA	2:B:415:MET:CE	2.21	0.71
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.72	0.70
4:F:245:ILE:HG22	4:F:245:ILE:O	1.91	0.70
1:C:28:HIS:HB3	1:C:36:MET:HE1	1.74	0.70
2:B:134:GLN:HA	2:B:165:ASN:O	1.92	0.69
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.28	0.68
4:F:149:ALA:O	4:F:180:HIS:ND1	2.26	0.68
4:F:242:ASN:HB2	4:F:245:ILE:HB	1.76	0.67
1:C:427:ALA:HA	1:C:430:LYS:HE3	1.76	0.67
2:B:186:THR:HA	2:B:415:MET:HE1	1.75	0.67
4:F:149:ALA:CB	4:F:161:LEU:HB3	2.24	0.67
2:B:2:ARG:NH2	2:B:131:GLN:HB3	2.11	0.66
3:E:56:ALA:O	3:E:59:GLU:HG3	1.96	0.66
1:A:166:LYS:HE2	1:A:197:HIS:O	1.95	0.66
2:B:186:THR:HG23	2:B:415:MET:HE3	1.77	0.65
4:F:226:GLU:OE1	4:F:252:ASN:HB2	1.97	0.65
2:B:362:LYS:HD2	2:B:363:MET:HG3	1.77	0.65
1:C:209:ILE:HD11	1:C:302:MET:CE	2.27	0.64
2:D:143:THR:HB	8:D:501:GDP:O1B	1.97	0.64
2:B:283:ALA:HA	2:B:362:LYS:CE	2.14	0.63
4:F:98:TYR:O	4:F:181:VAL:HG23	1.98	0.63
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.80	0.63
2:D:80:PRO:O	2:D:81:PHE:HB2	1.98	0.62
1:C:264:ARG:HD3	9:C:503:MES:H81	1.81	0.62
2:B:323:MET:SD	2:B:353:VAL:HG21	2.39	0.62
2:D:134:GLN:HA	2:D:165:ASN:O	1.99	0.62
4:F:24:THR:HG21	4:F:27:TRP:HD1	1.64	0.61
1:A:109:THR:CG2	1:A:411:GLU:HB3	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:LYS:O	2:D:328:GLU:HG3	2.01	0.61
2:D:285:THR:OG1	2:D:288:GLU:HG3	1.99	0.61
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.82	0.61
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.65	0.61
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.81	0.61
2:D:97:ALA:HB2	2:D:143:THR:OG1	2.01	0.61
2:B:284:LEU:H	2:B:362:LYS:CE	2.14	0.60
2:D:170:MET:CE	2:D:377:LEU:HD21	2.30	0.60
3:E:25:LYS:HD2	3:E:26:PRO:O	2.01	0.60
2:B:362:LYS:HD2	2:B:363:MET:HG2	1.82	0.60
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.84	0.60
1:C:147:SER:O	1:C:190:THR:HG23	2.02	0.60
2:D:34:GLY:HA2	2:D:84:ILE:HD11	1.84	0.60
2:B:316:ILE:HG23	2:B:366:THR:HB	1.84	0.60
2:D:316:ILE:N	2:D:316:ILE:HD12	2.15	0.60
2:B:283:ALA:HB1	2:B:362:LYS:HD3	1.84	0.60
2:D:1:MET:HA	2:D:48:ASN:ND2	2.17	0.59
4:F:146:VAL:HG12	4:F:187:GLU:OE2	2.02	0.59
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.84	0.59
1:A:36:MET:HE3	1:A:61:HIS:CE1	2.38	0.59
1:A:349:THR:HB	3:E:25:LYS:HG3	1.84	0.59
2:B:280:GLN:HG3	2:B:280:GLN:O	2.02	0.59
2:B:283:ALA:CB	2:B:362:LYS:HD3	2.33	0.59
2:D:401:GLU:HA	3:E:137:LYS:CD	2.33	0.58
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.84	0.58
1:A:346:TRP:CZ3	1:A:347:CYS:SG	2.97	0.58
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.86	0.58
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.69	0.58
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.38	0.58
1:A:179:THR:HA	2:B:350:LYS:HD2	1.86	0.58
2:B:285:THR:OG1	2:B:288:GLU:HG3	2.04	0.57
2:B:362:LYS:CD	2:B:363:MET:HG3	2.34	0.57
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.39	0.57
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.39	0.57
2:D:73:MET:SD	2:D:92:PHE:HB3	2.44	0.57
3:E:56:ALA:HA	3:E:59:GLU:HG2	1.87	0.57
4:F:245:ILE:O	4:F:245:ILE:CG2	2.53	0.56
4:F:138:ARG:HB3	4:F:145:ASN:ND2	2.20	0.56
1:C:100:ALA:HA	2:D:252:LYS:HG2	1.88	0.56
1:A:39:ASP:OD1	1:A:61:HIS:HE1	1.87	0.56
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:LEU:H	2:B:362:LYS:HE2	1.71	0.56
2:D:156:ARG:HD3	12:D:612:HOH:O	2.04	0.56
1:A:36:MET:CE	1:A:61:HIS:CE1	2.89	0.56
2:D:395:LEU:HD21	2:D:405:GLU:HG2	1.88	0.55
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.04	0.55
1:C:1:MET:HB3	1:C:130:THR:OG1	2.07	0.55
2:B:169:VAL:HA	2:B:202:ILE:O	2.06	0.55
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.42	0.55
1:A:187:SER:CB	1:A:391:LEU:HD21	2.37	0.55
2:B:158:GLU:HG2	2:B:159:TYR:CE2	2.41	0.55
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.42	0.55
4:F:211:TYR:CE2	4:F:299:GLU:HG2	2.43	0.54
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.54
1:A:430:LYS:NZ	1:A:434:GLU:OE1	2.30	0.54
2:D:401:GLU:HA	3:E:137:LYS:HD3	1.88	0.54
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.38	0.54
2:B:46:ARG:NH1	2:B:242:PHE:O	2.40	0.54
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.89	0.53
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.89	0.53
4:F:184:LYS:NZ	12:F:501:HOH:O	2.40	0.53
4:F:169:LEU:O	4:F:173:ILE:HG13	2.08	0.53
2:D:213:ARG:O	2:D:214:THR:HB	2.09	0.53
2:B:189:VAL:HB	2:B:415:MET:HE2	1.92	0.52
2:D:228:LEU:HB3	2:D:300:MET:HE3	1.91	0.52
1:A:100:ALA:HA	2:B:252:LYS:HG2	1.91	0.52
1:A:262:TYR:CE2	1:A:346:TRP:CH2	2.97	0.52
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.40	0.52
1:C:221:ARG:NE	2:D:323:MET:HG2	2.25	0.52
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.91	0.51
1:C:63:PRO:HG2	1:C:87:PHE:CE2	2.45	0.51
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.92	0.51
1:A:227:LEU:O	1:A:231:ILE:HG13	2.11	0.51
2:D:377:LEU:C	2:D:377:LEU:HD23	2.31	0.50
3:E:140:LYS:HG3	3:E:140:LYS:O	2.11	0.50
4:F:16:GLU:O	4:F:20:LEU:HD23	2.11	0.50
2:B:64:ILE:CD1	2:B:120:VAL:HG22	2.40	0.50
2:B:186:THR:HA	2:B:415:MET:HE3	1.93	0.50
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	2.93	0.50
1:C:104:ALA:HB2	1:C:413:MET:SD	2.52	0.50
1:A:178:SER:HB2	1:A:183:GLU:OE1	2.12	0.50
2:B:189:VAL:HB	2:B:415:MET:CE	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:HG12	1:C:36:MET:CE	2.42	0.50
2:B:237:THR:O	2:B:241:ARG:HG3	2.11	0.50
2:D:81:PHE:O	2:D:84:ILE:HG22	2.11	0.50
2:B:166:THR:OG1	2:B:199:THR:HB	2.11	0.50
1:A:155:GLU:HB3	3:E:50:ILE:HD11	1.94	0.50
2:B:65:LEU:HD22	2:B:90:PHE:CE2	2.47	0.50
1:C:30:ILE:HG12	1:C:36:MET:HE2	1.94	0.50
1:C:270:ALA:O	1:C:302:MET:HG2	2.12	0.50
4:F:3:THR:O	4:F:38:ASN:HB2	2.12	0.50
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.93	0.49
4:F:17:VAL:O	4:F:21:LEU:HG	2.12	0.49
1:A:141:PHE:O	1:A:147:SER:HB3	2.12	0.49
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.47	0.49
10:B:505:E9Y:C9	10:B:505:E9Y:C6	2.90	0.49
1:C:165:SER:HA	1:C:199:ASP:OD1	2.12	0.49
2:D:332:ASN:HD21	2:D:336:LYS:HE3	1.76	0.49
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.28	0.49
2:D:33:THR:O	2:D:33:THR:CG2	2.61	0.49
4:F:89:GLU:C	4:F:91:CYS:H	2.16	0.49
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.48	0.48
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.48	0.48
2:B:238:THR:HG21	2:B:318:ARG:HD3	1.94	0.48
3:E:56:ALA:O	3:E:59:GLU:CG	2.60	0.48
1:C:361:THR:HG22	1:C:362:VAL:N	2.28	0.48
9:B:503:MES:H51	9:B:503:MES:H81	1.61	0.48
1:C:166:LYS:HE2	1:C:197:HIS:O	2.14	0.48
4:F:195:GLY:C	4:F:197:ARG:HG3	2.34	0.48
2:D:169:VAL:HA	2:D:202:ILE:O	2.13	0.48
3:E:59:GLU:HG3	3:E:60:ARG:N	2.28	0.48
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.48
3:E:100:LYS:O	3:E:103:GLN:HG3	2.13	0.48
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.14	0.48
2:D:174:LYS:HD2	2:D:208:TYR:CD2	2.49	0.48
3:E:59:GLU:HG3	3:E:60:ARG:H	1.78	0.48
2:B:219:THR:HG21	1:C:326:LYS:HA	1.96	0.47
2:B:268:PRO:HA	2:B:367:PHE:O	2.14	0.47
2:D:116:VAL:HG11	2:D:151:LEU:HD21	1.95	0.47
4:F:146:VAL:HG13	4:F:185:TYR:HB3	1.97	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
4:F:146:VAL:HG12	4:F:187:GLU:CD	2.35	0.47
4:F:255:ARG:HD2	4:F:256:TYR:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:MET:CE	1:A:404:PHE:CD2	2.97	0.47
2:D:116:VAL:CG1	2:D:151:LEU:HD21	2.45	0.47
4:F:146:VAL:CG1	4:F:187:GLU:HG2	2.45	0.47
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.50	0.47
2:D:203:ASP:O	2:D:207:LEU:HG	2.15	0.47
2:D:141:GLY:HA3	8:D:501:GDP:O3A	2.14	0.47
1:C:255:PHE:CE1	1:C:352:LYS:HG2	2.50	0.46
4:F:186:LEU:CD1	4:F:320:MET:HG2	2.45	0.46
2:D:208:TYR:CE1	2:D:220:PRO:HD2	2.50	0.46
1:C:83:TYR:HD1	1:C:86:LEU:HD22	1.81	0.46
1:C:234:ILE:HG12	1:C:302:MET:CE	2.45	0.46
1:A:36:MET:HB3	1:A:61:HIS:CD2	2.51	0.46
4:F:56:PRO:HD2	12:F:503:HOH:O	2.16	0.46
1:A:241:SER:HB2	1:A:249:ASN:O	2.16	0.45
2:B:377:LEU:HD23	2:B:381:ILE:HD12	1.98	0.45
1:C:391:LEU:HA	1:C:391:LEU:HD23	1.69	0.45
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.99	0.45
4:F:211:TYR:CE2	4:F:299:GLU:CG	3.00	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.45
1:C:30:ILE:CG1	1:C:36:MET:CE	2.94	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.45
2:B:283:ALA:CA	2:B:362:LYS:CE	2.85	0.45
2:B:360:GLY:O	2:B:361:LEU:HD23	2.16	0.45
2:D:144:GLY:O	2:D:148:GLY:HA3	2.16	0.45
1:A:36:MET:HB3	1:A:61:HIS:NE2	2.32	0.45
2:B:317:PHE:HB2	2:B:353:VAL:HG12	1.97	0.45
4:F:16:GLU:HG3	4:F:20:LEU:HD23	1.98	0.45
2:B:2:ARG:HG2	2:B:2:ARG:HH11	1.81	0.45
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.98	0.45
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.51	0.45
2:D:23:VAL:O	2:D:27:GLU:HG3	2.16	0.45
1:C:83:TYR:CD1	1:C:86:LEU:HD22	2.52	0.45
2:B:211:CYS:HA	2:B:215:LEU:HB2	1.99	0.45
2:D:251:ARG:O	2:D:255:VAL:HG23	2.17	0.45
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.56	0.45
2:D:268:PRO:HA	2:D:367:PHE:O	2.17	0.45
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.77	0.45
1:C:141:PHE:HB3	1:C:187:SER:OG	2.17	0.45
2:D:102:ALA:HB2	2:D:403:MET:SD	2.57	0.45
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.44	0.44
4:F:81:ILE:O	4:F:88:SER:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:B:19:LYS:HB3	2:B:19:LYS:HE3	1.80	0.44
4:F:131:PHE:CE1	4:F:182:ILE:HD11	2.53	0.44
1:A:51:THR:HG22	1:A:52:PHE:CD1	2.53	0.44
2:D:296:SER:HB2	2:D:305:PRO:HD2	2.00	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.44
2:D:28:HIS:HA	2:D:43:GLN:HB3	2.00	0.44
1:A:6:SER:O	1:A:65:ALA:HA	2.18	0.44
2:B:73:MET:CE	2:B:92:PHE:HD1	2.31	0.44
1:C:177:VAL:HG23	12:C:642:HOH:O	2.18	0.44
3:E:48:GLU:O	3:E:52:LYS:HB2	2.18	0.44
1:C:316:CYS:O	1:C:377:MET:HG3	2.18	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
2:D:34:GLY:CA	2:D:84:ILE:HD11	2.46	0.43
4:F:88:SER:OG	4:F:89:GLU:HB2	2.18	0.43
2:B:23:VAL:O	2:B:27:GLU:HG3	2.17	0.43
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.53	0.43
2:D:246:LEU:HD23	2:D:246:LEU:HA	1.78	0.43
3:E:135:LYS:HG2	3:E:139:LEU:HD13	2.00	0.43
2:B:362:LYS:H	2:B:362:LYS:HG3	1.62	0.43
1:C:227:LEU:O	1:C:231:ILE:HG13	2.19	0.43
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.11	0.43
2:B:314:ALA:HB3	2:B:368:ILE:HB	2.01	0.43
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.99	0.43
2:D:65:LEU:N	2:D:65:LEU:HD12	2.34	0.43
2:B:65:LEU:N	2:B:65:LEU:HD12	2.34	0.43
2:B:247:ASN:CG	2:B:247:ASN:O	2.57	0.43
3:E:60:ARG:O	3:E:64:GLN:HG3	2.19	0.43
1:A:2:ARG:CB	1:A:133:GLN:HG2	2.48	0.43
2:D:344:TRP:CE3	2:D:345:ILE:HG13	2.54	0.43
4:F:202:ARG:NE	4:F:318:ASP:OD1	2.42	0.43
2:D:152:ILE:HG23	2:D:164:MET:HG2	2.00	0.43
1:A:249:ASN:N	1:A:254:GLU:OE2	2.53	0.42
2:D:7:ILE:O	2:D:135:LEU:HA	2.18	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.42
2:B:2:ARG:CZ	2:B:131:GLN:HB3	2.49	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.48	0.42
1:C:30:ILE:CG1	1:C:36:MET:HE2	2.48	0.42
2:D:193:VAL:CG2	2:D:418:LEU:HD22	2.49	0.42
2:B:247:ASN:ND2	2:B:247:ASN:O	2.52	0.42
4:F:181:VAL:CG2	4:F:182:ILE:N	2.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:295:LEU:HD23	4:F:295:LEU:HA	1.88	0.42
1:C:221:ARG:HE	2:D:323:MET:CG	2.32	0.42
2:D:165:ASN:HA	2:D:198:GLU:O	2.20	0.42
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.53	0.42
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.42
10:B:505:E9Y:C6	10:B:505:E9Y:C8	2.98	0.42
2:D:12:CYS:SG	2:D:169:VAL:HG21	2.60	0.42
4:F:326:LYS:HD3	4:F:328:TRP:CZ2	2.55	0.42
1:C:147:SER:O	1:C:190:THR:CG2	2.68	0.42
2:B:28:HIS:HB3	2:B:47:ILE:HD12	2.01	0.42
2:D:84:ILE:HD12	2:D:84:ILE:HA	1.93	0.42
4:F:284:LEU:O	4:F:288:LYS:HG3	2.20	0.42
2:D:45:GLU:OE1	2:D:243:PRO:HG3	2.19	0.41
1:A:134:GLY:HA3	1:A:165:SER:O	2.19	0.41
2:B:284:LEU:N	2:B:362:LYS:HE2	2.34	0.41
2:B:377:LEU:CD2	2:B:381:ILE:HD12	2.50	0.41
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.80	0.41
1:C:250:VAL:HG11	1:C:352:LYS:HE3	2.02	0.41
4:F:3:THR:HB	4:F:30:LEU:HD11	2.02	0.41
2:B:67:ASP:O	2:B:92:PHE:HA	2.21	0.41
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.41
2:B:73:MET:HE2	2:B:92:PHE:CD1	2.56	0.41
2:D:170:MET:HE2	2:D:170:MET:HB3	1.86	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HG3	2.03	0.41
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.82	0.41
1:C:30:ILE:HD11	1:C:36:MET:HE3	2.02	0.41
2:D:174:LYS:HE3	2:D:209:ASP:OD1	2.21	0.41
3:E:76:ARG:HD3	3:E:79:GLU:OE1	2.20	0.41
1:A:71:GLU:OE1	1:A:73:THR:CB	2.55	0.41
1:A:285:GLN:HE21	1:A:372:GLN:HG3	1.86	0.41
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.51	0.41
2:D:343:GLU:CG	2:D:430:ALA:HB2	2.45	0.41
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.51	0.41
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.50	0.41
1:A:51:THR:HG22	1:A:52:PHE:HD1	1.86	0.41
1:C:271:THR:HG23	1:C:300:ASN:O	2.20	0.41
2:D:193:VAL:HG21	2:D:418:LEU:HD22	2.03	0.41
4:F:88:SER:HA	4:F:89:GLU:HA	1.79	0.41
4:F:236:LYS:HE3	4:F:236:LYS:HB2	1.90	0.41
2:B:323:MET:HE2	2:B:323:MET:HB3	1.79	0.40
1:C:431:ASP:HB3	9:C:503:MES:H51	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:THR:HG22	2:D:167:PHE:HB2	2.03	0.40
4:F:350:ILE:O	4:F:354:ALA:HB3	2.22	0.40
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.04	0.40
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.85	0.40
4:F:74:LYS:NZ	4:F:331:GLU:HG3	2.36	0.40
4:F:181:VAL:HG22	4:F:182:ILE:N	2.35	0.40
4:F:214:TYR:CE2	4:F:353:VAL:HG11	2.56	0.40
1:C:181:VAL:HG12	2:D:256:ASN:OD1	2.22	0.40
4:F:24:THR:HG23	4:F:26:GLN:N	2.17	0.40
4:F:134:ALA:O	4:F:138:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	426 (98%)	9 (2%)	0	100	100
1	C	438/450 (97%)	428 (98%)	9 (2%)	1 (0%)	47	64
2	B	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	404 (97%)	13 (3%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	322/384 (84%)	299 (93%)	21 (6%)	2 (1%)	25	37
All	All	2154/2317 (93%)	2085 (97%)	66 (3%)	3 (0%)	51	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLY
4	F	102	PRO
4	F	245	ILE

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	365/378 (97%)	360 (99%)	5 (1%)	67	81
1	C	371/378 (98%)	363 (98%)	8 (2%)	52	70
2	B	368/383 (96%)	350 (95%)	18 (5%)	25	38
2	D	363/383 (95%)	355 (98%)	8 (2%)	52	70
3	E	109/127 (86%)	105 (96%)	4 (4%)	34	50
4	F	294/342 (86%)	285 (97%)	9 (3%)	40	57
All	All	1870/1991 (94%)	1818 (97%)	52 (3%)	43	61

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	THR
1	A	178	SER
1	A	221	ARG
1	A	250	VAL
1	A	381	THR
2	B	75	SER
2	B	77	ARG
2	B	84	ILE
2	B	115	SER
2	B	137	HIS
2	B	145	SER
2	B	162	ARG
2	B	199	THR
2	B	225	LEU
2	B	247	ASN
2	B	278	SER
2	B	280	GLN
2	B	291	GLN
2	B	316	ILE
2	B	353	VAL
2	B	362	LYS
2	B	363	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	413	SER
1	C	2	ARG
1	C	178	SER
1	C	190	THR
1	C	221	ARG
1	C	251	ASP
1	C	293	ASN
1	C	384	ILE
1	C	391	LEU
2	D	33	THR
2	D	75	SER
2	D	115	SER
2	D	137	HIS
2	D	180	VAL
2	D	306	ARG
2	D	339	SER
2	D	386	THR
3	E	18	GLN
3	E	25	LYS
3	E	62	LYS
3	E	107	SER
4	F	12	SER
4	F	43	GLU
4	F	88	SER
4	F	138	ARG
4	F	211	TYR
4	F	238	CYS
4	F	255	ARG
4	F	299	GLU
4	F	307	LEU

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

Mol	Chain	Res	Type
1	A	61	HIS
1	A	285	GLN
1	A	372	GLN
2	B	165	ASN
1	C	356	ASN
3	E	18	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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	E9Y	B	505	-	22,26,26	0.86	2 (9%)	24,38,38	1.14	2 (8%)
5	GTP	C	501	7	26,34,34	1.12	2 (7%)	32,54,54	1.45	5 (15%)
9	MES	B	502	-	12,12,12	2.11	1 (8%)	14,16,16	2.17	4 (28%)
10	E9Y	D	502	-	22,26,26	0.84	1 (4%)	24,38,38	1.14	2 (8%)
8	GDP	B	501	7	24,30,30	0.96	1 (4%)	30,47,47	1.14	3 (10%)
5	GTP	A	501	7	26,34,34	1.19	1 (3%)	32,54,54	1.48	8 (25%)
9	MES	B	503	-	12,12,12	2.13	1 (8%)	14,16,16	1.86	3 (21%)
8	GDP	D	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.14	3 (10%)
9	MES	C	503	-	12,12,12	1.91	1 (8%)	14,16,16	2.01	3 (21%)
11	ACP	F	402	7	27,33,33	5.68	6 (22%)	32,52,52	1.83	5 (15%)

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
10	E9Y	B	505	-	-	3/6/16/16	0/4/4/4
5	GTP	C	501	7	-	6/18/38/38	0/3/3/3
9	MES	B	502	-	-	2/6/14/14	0/1/1/1
10	E9Y	D	502	-	-	4/6/16/16	0/4/4/4
8	GDP	B	501	7	-	3/12/32/32	0/3/3/3
5	GTP	A	501	7	-	6/18/38/38	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
8	GDP	D	501	-	-	5/12/32/32	0/3/3/3
9	MES	C	503	-	-	1/6/14/14	0/1/1/1
11	ACP	F	402	7	-	4/15/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	PB-O3A	27.27	1.88	1.58
11	F	402	ACP	PA-O5'	8.11	1.92	1.59
9	B	503	MES	C8-S	-7.01	1.67	1.77
9	B	502	MES	C8-S	-6.90	1.67	1.77
9	C	503	MES	C8-S	-6.18	1.68	1.77
5	A	501	GTP	C5-C6	-4.06	1.39	1.47
11	F	402	ACP	C5'-C4'	3.89	1.63	1.51
5	C	501	GTP	C5-C6	-3.75	1.39	1.47
11	F	402	ACP	O5'-C5'	-3.13	1.32	1.44
11	F	402	ACP	C2-N1	2.93	1.39	1.33
8	D	501	GDP	C6-N1	-2.71	1.33	1.37
8	B	501	GDP	C6-N1	-2.62	1.34	1.37
11	F	402	ACP	O3'-C3'	-2.51	1.37	1.43
10	B	505	E9Y	C3-N1	-2.22	1.30	1.35
10	D	502	E9Y	C3-N1	-2.15	1.30	1.35
5	C	501	GTP	C2-N3	2.13	1.38	1.33
10	B	505	E9Y	C7-N3	2.01	1.43	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	502	MES	C5-N4-C3	6.31	123.04	108.83
11	F	402	ACP	O5'-PA-O1A	-5.25	88.55	109.07
11	F	402	ACP	O1B-PB-C3B	4.78	121.72	109.07
9	C	503	MES	C5-N4-C3	4.61	119.21	108.83
9	B	503	MES	C5-N4-C3	4.41	118.77	108.83
10	D	502	E9Y	C4-C7-N4	-4.32	119.55	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	505	E9Y	C4-C7-N4	-4.32	119.55	124.05
11	F	402	ACP	O1G-PG-C3B	-3.96	102.70	111.24
9	C	503	MES	O3S-S-C8	3.82	111.94	105.77
5	A	501	GTP	O2G-PG-O3B	3.31	115.73	104.64
9	B	503	MES	O3S-S-C8	3.29	111.08	105.77
5	C	501	GTP	PB-O3B-PG	-3.24	121.71	132.83
5	C	501	GTP	C8-N7-C5	3.19	109.07	102.99
11	F	402	ACP	O2A-PA-O5'	-3.02	93.73	107.75
8	B	501	GDP	PA-O3A-PB	-2.94	122.75	132.83
5	A	501	GTP	PA-O3A-PB	-2.88	122.93	132.83
5	C	501	GTP	PA-O3A-PB	-2.88	122.93	132.83
5	A	501	GTP	C8-N7-C5	2.88	108.47	102.99
5	A	501	GTP	C5-C6-N1	2.85	118.98	113.95
9	B	502	MES	O1S-S-C8	2.84	110.34	106.92
8	D	501	GDP	C8-N7-C5	2.76	108.24	102.99
5	A	501	GTP	PB-O3B-PG	-2.66	123.70	132.83
5	C	501	GTP	C5-C6-N1	2.62	118.58	113.95
5	A	501	GTP	C2-N1-C6	-2.50	120.49	125.10
5	C	501	GTP	C2-N1-C6	-2.50	120.50	125.10
9	B	502	MES	O3S-S-C8	2.45	109.72	105.77
8	D	501	GDP	O3B-PB-O3A	2.44	112.81	104.64
9	C	503	MES	O2S-S-C8	2.39	109.80	106.92
9	B	503	MES	O1S-S-C8	2.39	109.79	106.92
10	B	505	E9Y	C2-N1-C3	2.37	117.45	115.52
8	B	501	GDP	C5-C6-N1	2.35	118.11	113.95
10	D	502	E9Y	C2-N1-C3	2.27	117.36	115.52
5	A	501	GTP	O6-C6-C5	-2.26	119.95	124.37
5	A	501	GTP	N2-C2-N1	2.20	121.39	116.71
11	F	402	ACP	O2B-PB-C3B	2.11	115.22	106.58
8	B	501	GDP	O6-C6-C5	-2.09	120.29	124.37
8	D	501	GDP	O4'-C1'-C2'	-2.08	103.88	106.93
9	B	502	MES	C2-C3-N4	2.01	113.16	110.10

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	C	503	MES	N4-C7-C8-S
10	B	505	E9Y	C4-C7-N3-C17
10	D	502	E9Y	C4-C7-N3-C17
10	D	502	E9Y	C4-C7-N3-C8
10	D	502	E9Y	N4-C7-N3-C8
11	F	402	ACP	PG-C3B-PB-O1B
11	F	402	ACP	C5'-O5'-PA-O2A
11	F	402	ACP	C5'-O5'-PA-O3A
10	D	502	E9Y	N4-C7-N3-C17
10	B	505	E9Y	N4-C7-N3-C17
9	B	502	MES	C8-C7-N4-C3
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
11	F	402	ACP	C5'-O5'-PA-O1A
9	B	502	MES	C8-C7-N4-C5
10	B	505	E9Y	N4-C7-N3-C8
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

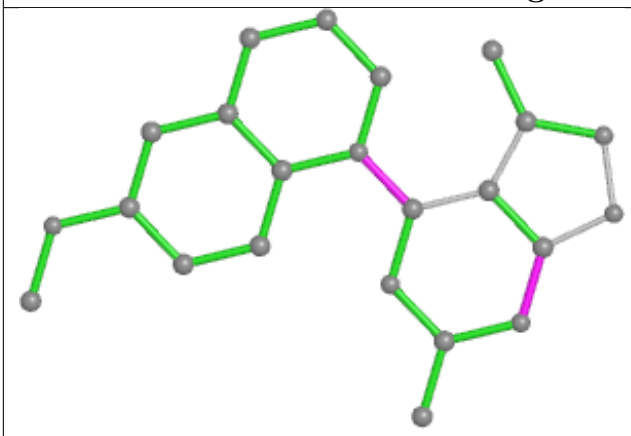
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	E9Y	2	0
9	B	503	MES	1	0
8	D	501	GDP	3	0
9	C	503	MES	2	0

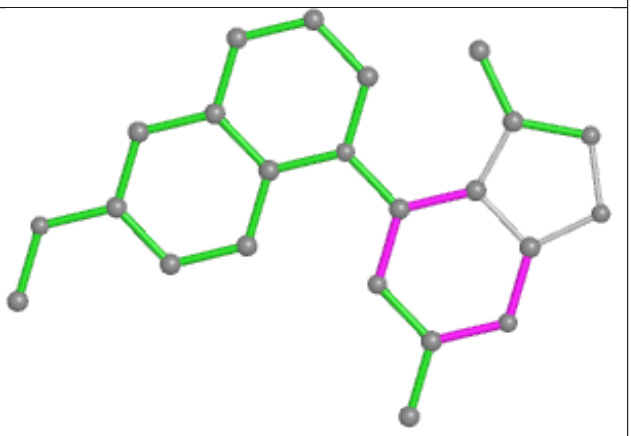
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

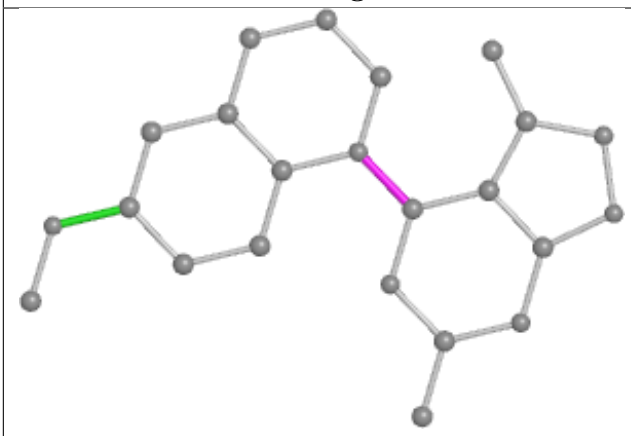
Ligand E9Y B 505



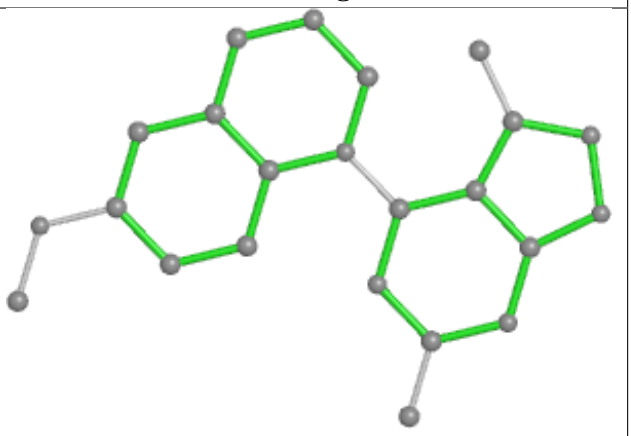
Bond lengths



Bond angles

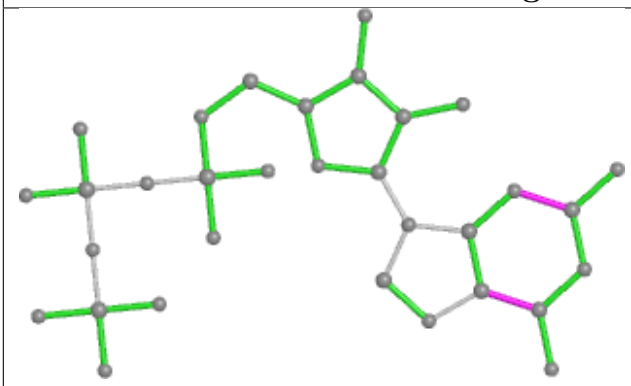


Torsions

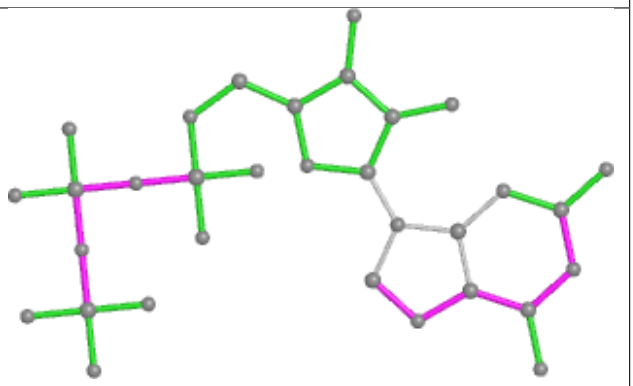


Rings

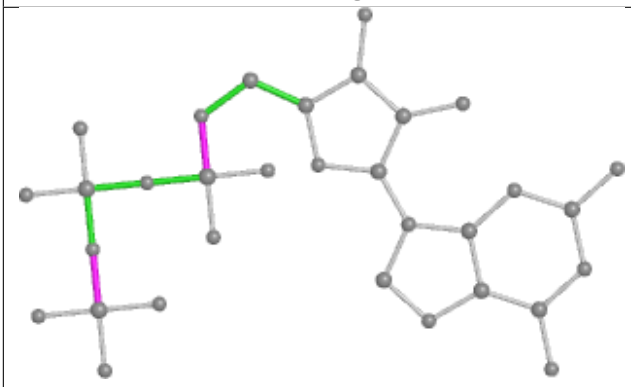
Ligand GTP C 501



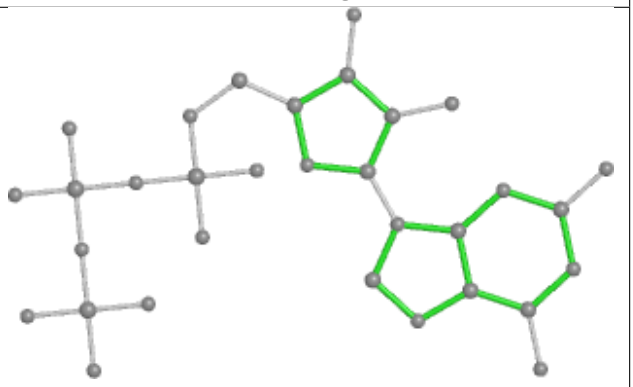
Bond lengths



Bond angles

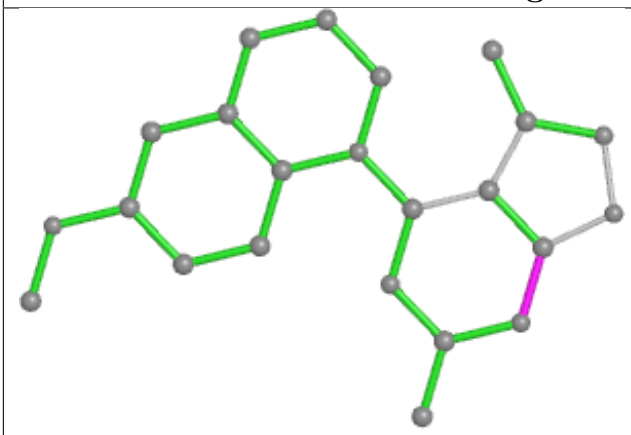


Torsions

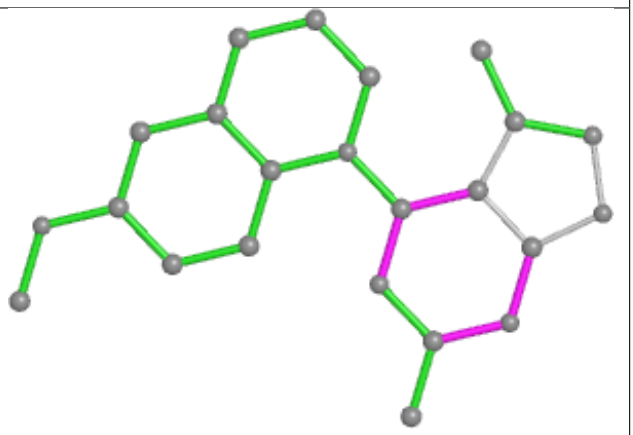


Rings

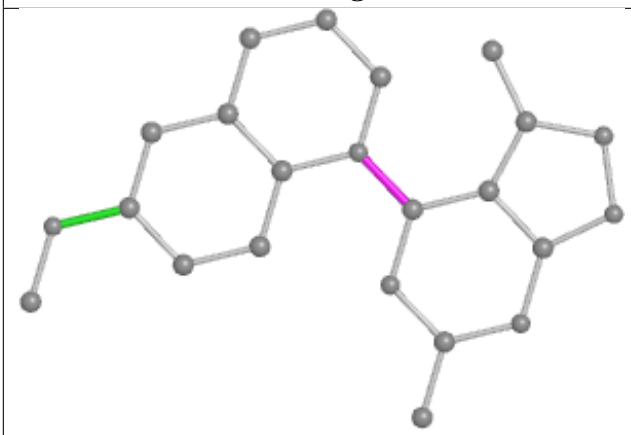
Ligand E9Y D 502



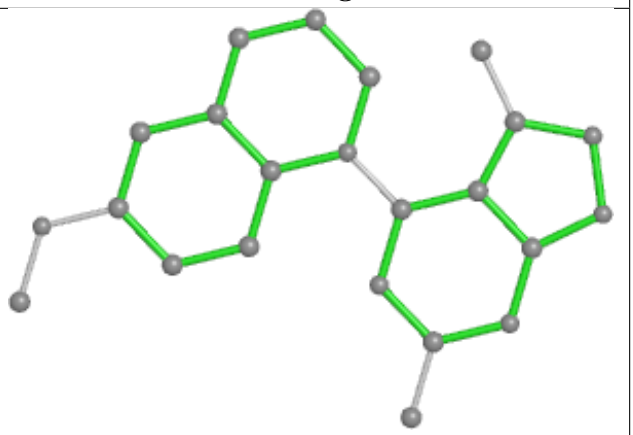
Bond lengths



Bond angles

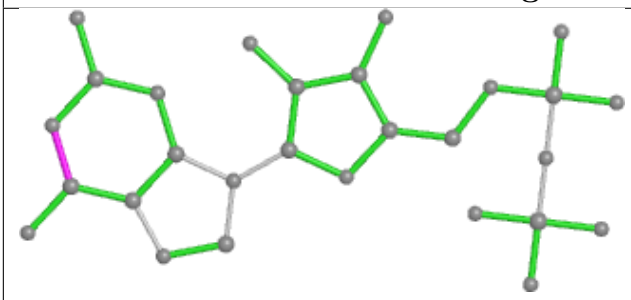


Torsions

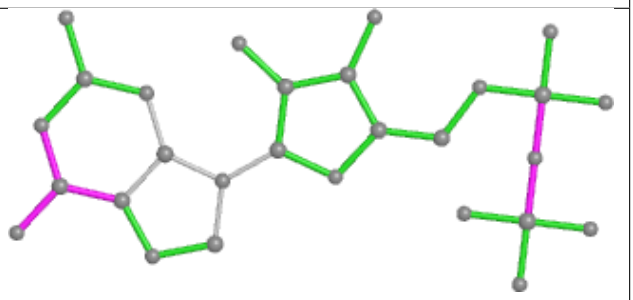


Rings

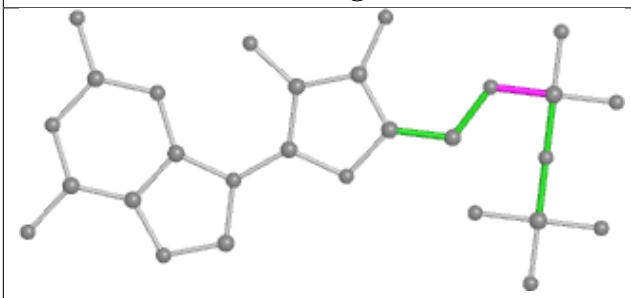
Ligand GDP B 501



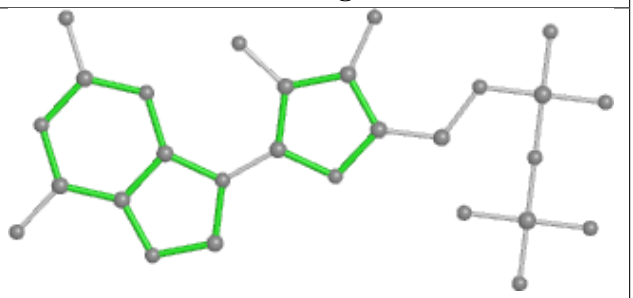
Bond lengths



Bond angles

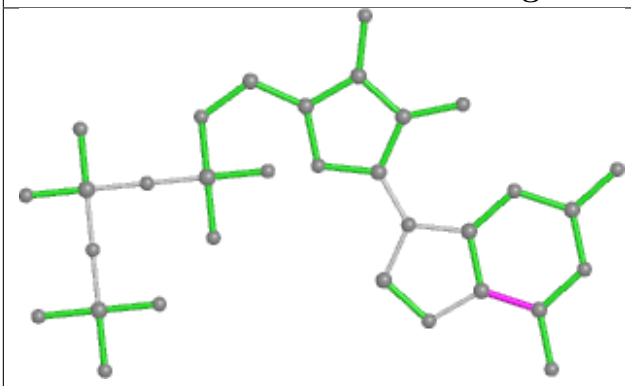


Torsions

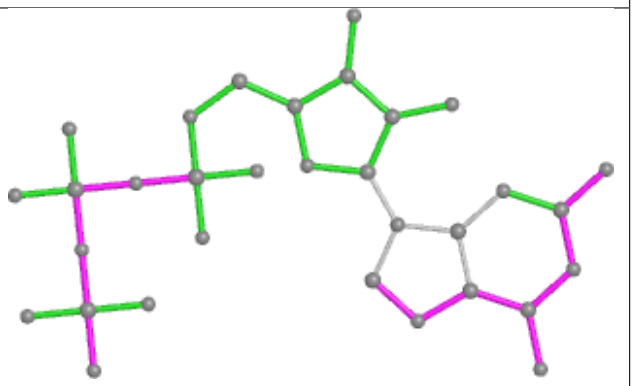


Rings

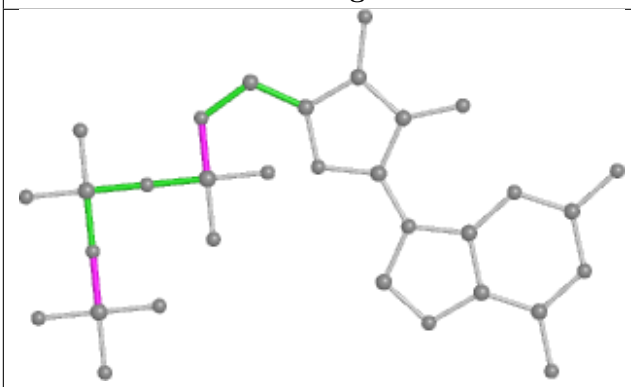
Ligand GTP A 501



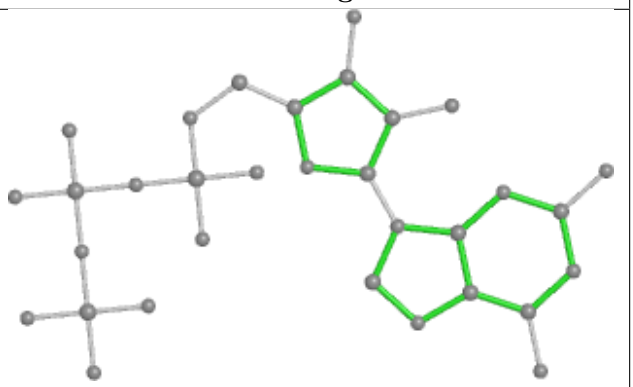
Bond lengths



Bond angles

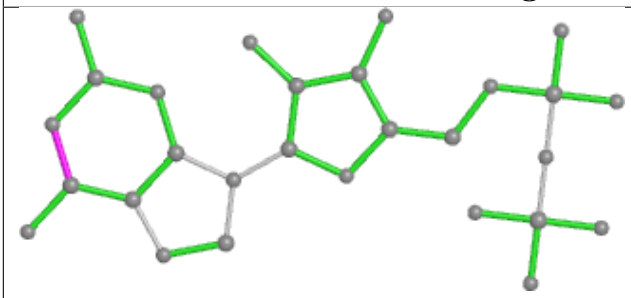


Torsions

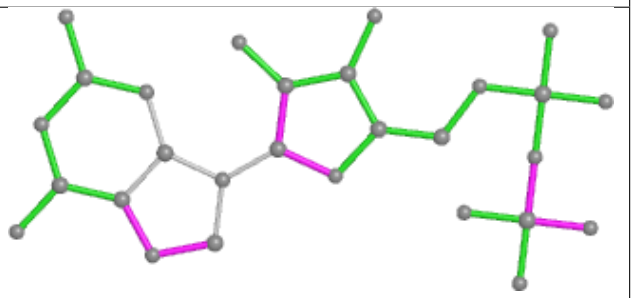


Rings

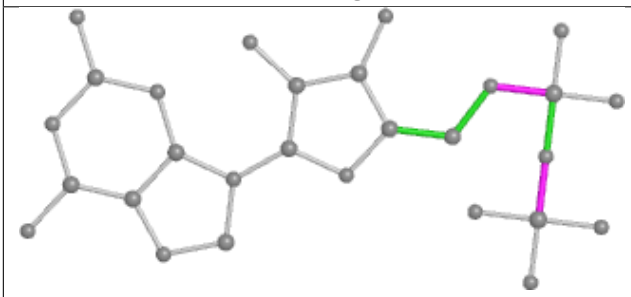
Ligand GDP D 501



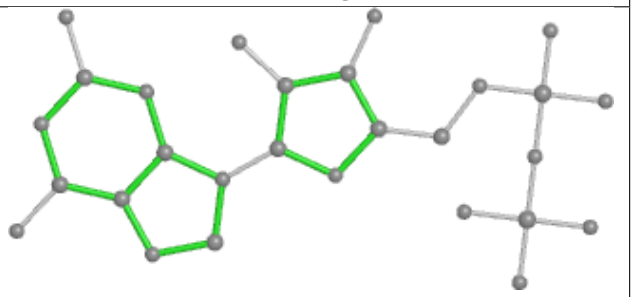
Bond lengths



Bond angles

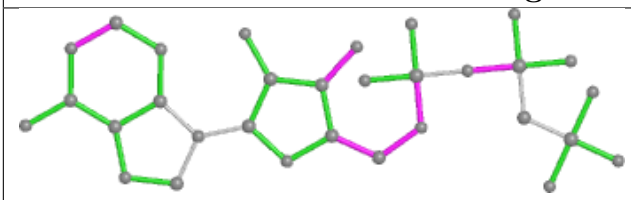


Torsions

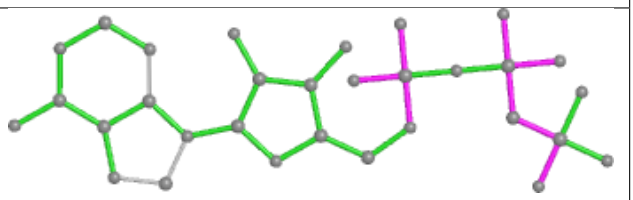


Rings

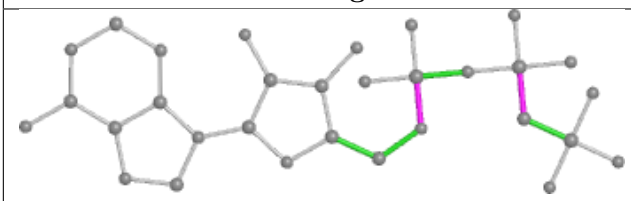
Ligand ACP F 402



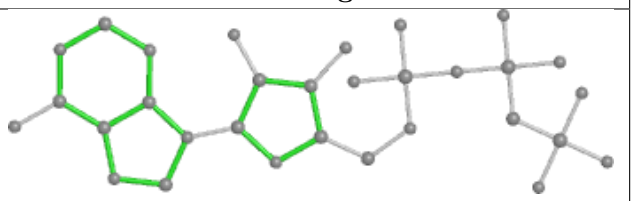
Bond lengths



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	437/450 (97%)	-0.49	0 100 100	22, 39, 69, 97	0
1	C	440/450 (97%)	-0.62	0 100 100	16, 28, 54, 86	0
2	B	427/445 (95%)	-0.40	7 (1%) 72 69	18, 36, 75, 124	0
2	D	421/445 (94%)	-0.18	10 (2%) 59 54	25, 53, 90, 135	0
3	E	121/143 (84%)	-0.13	3 (2%) 57 53	28, 51, 85, 109	0
4	F	332/384 (86%)	0.28	29 (8%) 10 8	30, 60, 124, 148	0
All	All	2178/2317 (94%)	-0.30	49 (2%) 62 57	16, 42, 89, 148	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	279	GLN	5.3
2	D	72	THR	5.2
4	F	169	LEU	4.0
4	F	101	TYR	3.9
4	F	100	ILE	3.9
4	F	102	PRO	3.8
4	F	234	GLN	3.7
4	F	233	PHE	3.7
4	F	178	GLN	3.6
2	B	57	ASN	3.5
2	D	92	PHE	3.4
4	F	143	GLU	3.4
4	F	177	GLY	3.3
2	B	55	THR	3.1
4	F	182	ILE	3.1
4	F	176	GLN	3.0
2	D	1	MET	2.9
4	F	135	TYR	2.9
4	F	253	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	133	ALA	2.8
3	E	139	LEU	2.8
4	F	132	LEU	2.8
4	F	244	CYS	2.7
4	F	137	ARG	2.7
4	F	136	ASN	2.7
2	D	219	THR	2.7
3	E	26	PRO	2.6
2	D	390	ARG	2.6
4	F	142	ARG	2.6
3	E	27	PRO	2.5
4	F	232	ASN	2.5
2	D	95	SER	2.4
2	D	73	MET	2.4
2	D	55	THR	2.4
4	F	231	ALA	2.4
4	F	173	ILE	2.4
4	F	103	THR	2.3
2	B	427	ASP	2.3
2	D	54	ALA	2.2
4	F	225	SER	2.2
2	B	247	ASN	2.1
4	F	256	TYR	2.1
4	F	243	HIS	2.1
2	B	275	SER	2.1
4	F	166	ALA	2.1
4	F	170	LEU	2.0
2	D	71	GLY	2.0
2	B	280	GLN	2.0
4	F	172	PHE	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)

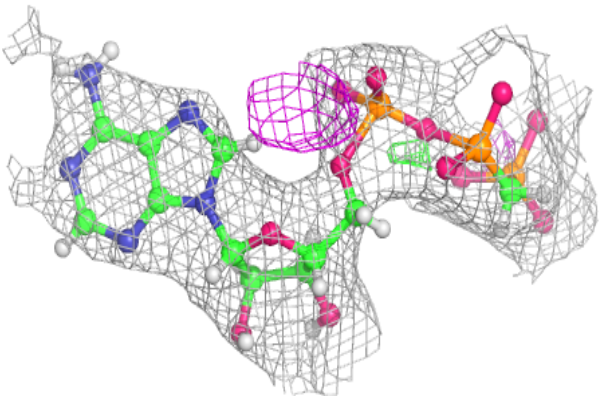
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

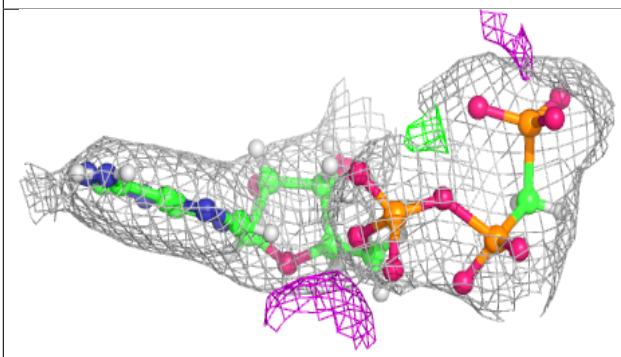
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MES	C	503	12/12	0.83	0.34	61,66,96,102	12
11	ACP	F	402	31/31	0.91	0.16	59,76,94,109	0
7	MG	F	401	1/1	0.92	0.11	59,59,59,59	0
6	CA	A	502	1/1	0.95	0.06	59,59,59,59	0
8	GDP	D	501	28/28	0.96	0.12	34,40,57,60	0
10	E9Y	D	502	23/23	0.96	0.17	30,38,63,69	0
9	MES	B	503	12/12	0.96	0.17	59,64,68,72	0
10	E9Y	B	505	23/23	0.97	0.16	27,37,52,62	0
7	MG	C	504	1/1	0.97	0.18	18,18,18,18	0
9	MES	B	502	12/12	0.97	0.12	28,34,56,56	0
7	MG	B	504	1/1	0.98	0.25	22,22,22,22	0
5	GTP	A	501	32/32	0.99	0.17	20,26,30,30	0
6	CA	C	502	1/1	0.99	0.07	37,37,37,37	0
8	GDP	B	501	28/28	0.99	0.16	18,22,28,31	0
7	MG	A	503	1/1	0.99	0.13	18,18,18,18	0
5	GTP	C	501	32/32	0.99	0.13	17,25,27,27	0

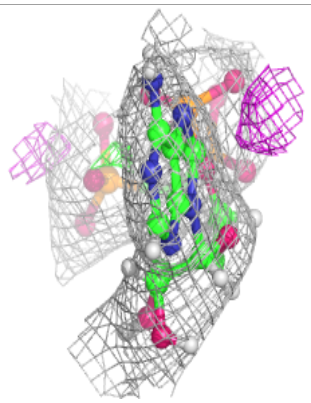
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

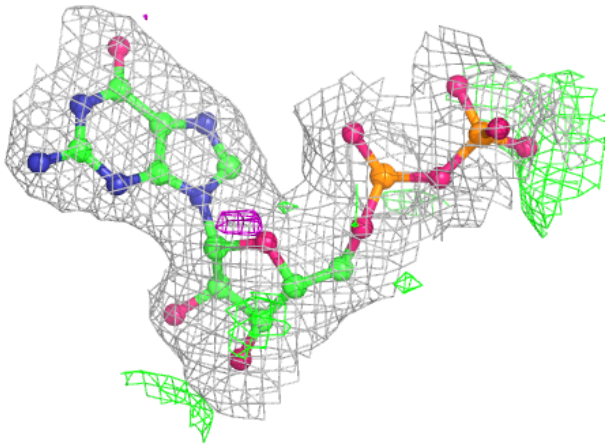


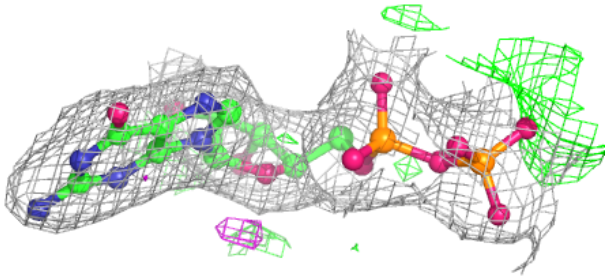


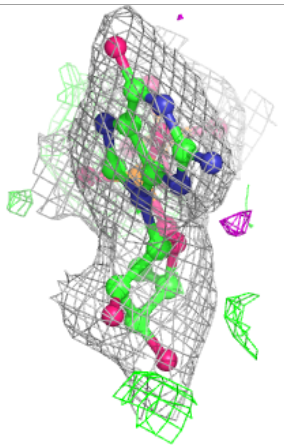


Electron density around GDP D 501:

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

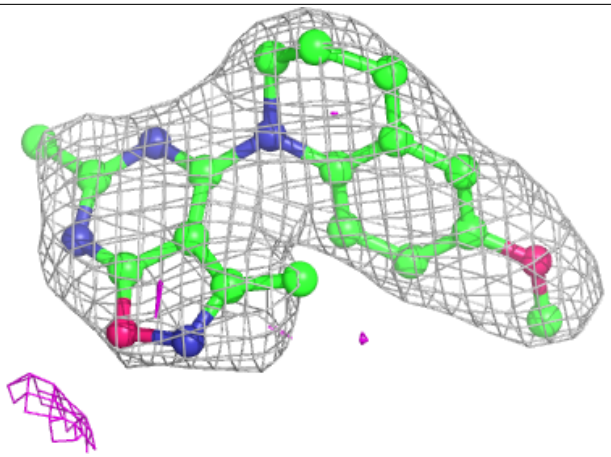


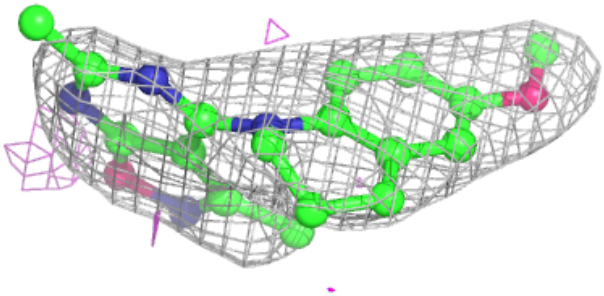


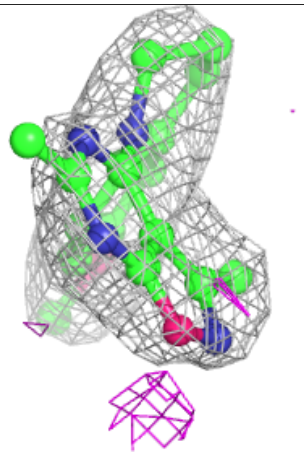


Electron density around E9Y D 502:

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

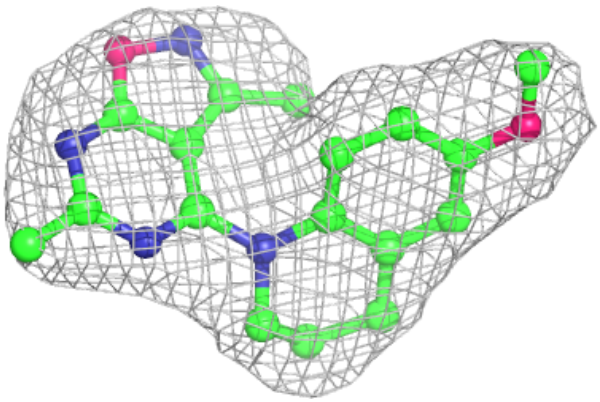


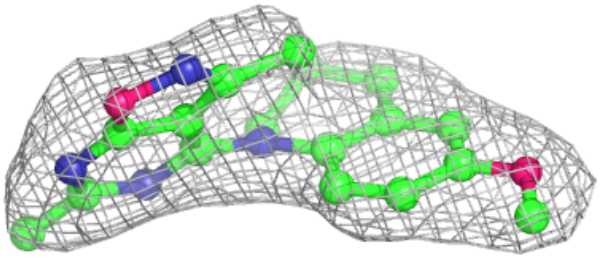


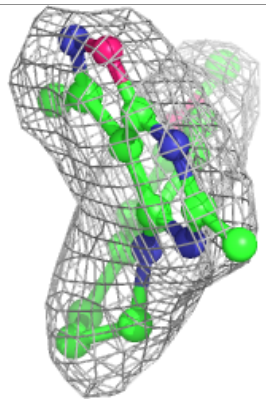


Electron density around E9Y B 505:

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

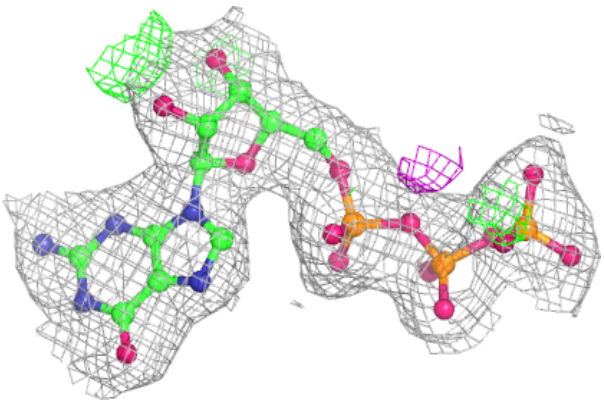


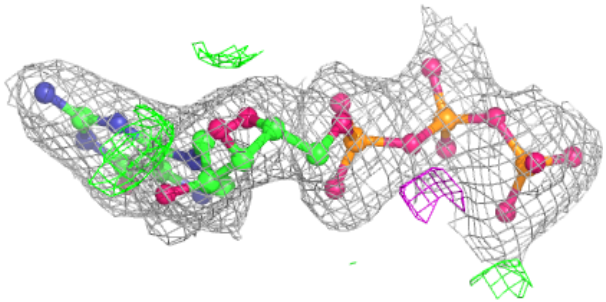


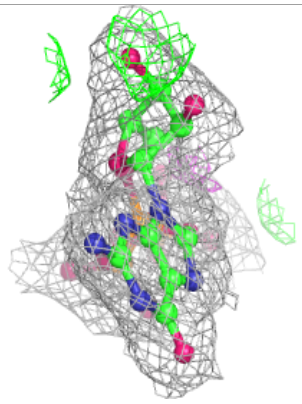


Electron density around GTP A 501:

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

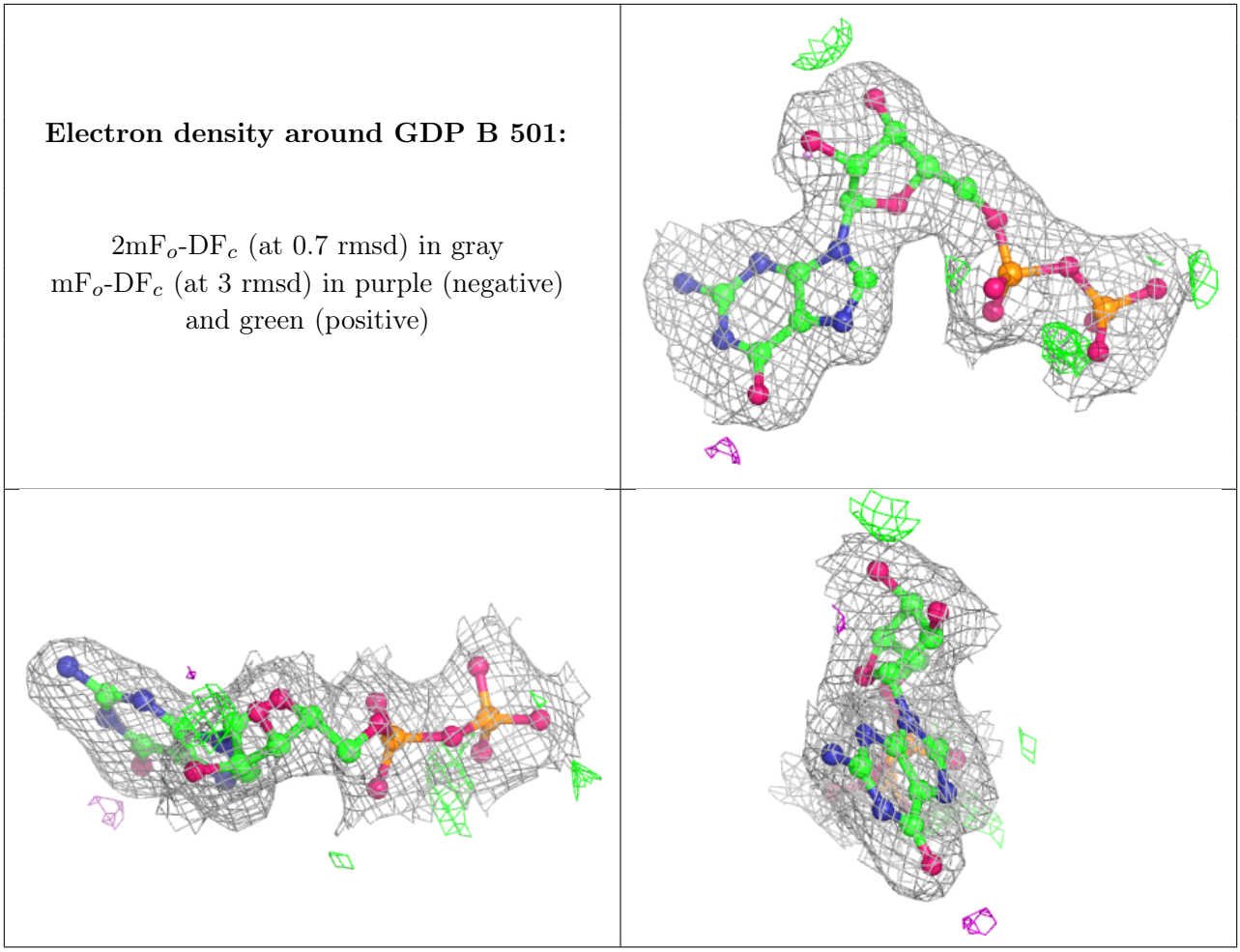






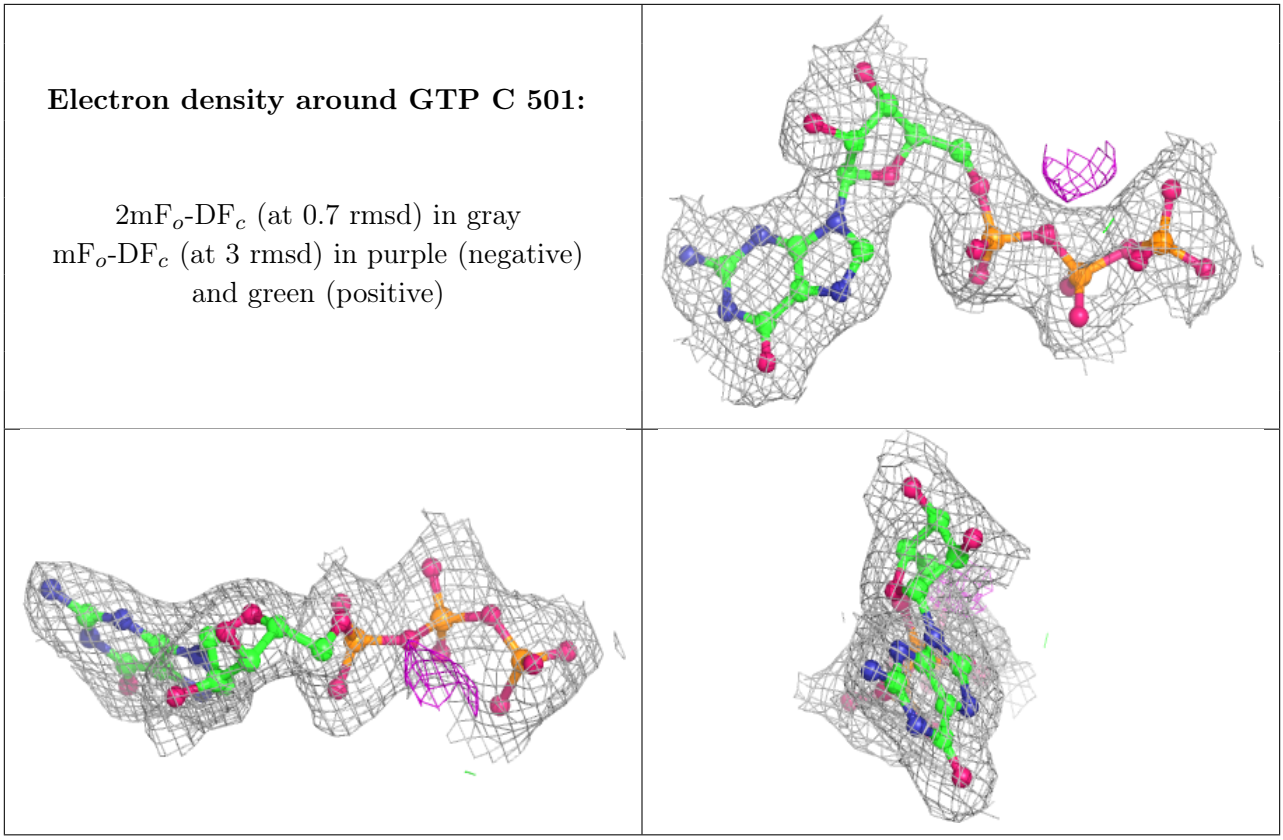
Electron density around GDP B 501:

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



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.