



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:51 AM UTC

PDB ID : 6Y4N / pdb_00006y4n
Title : Structure of Tubulin Tyrosine Ligase in Complex with Tb116
Authors : Gavriluk, J.; Nocek, B.; Rigol, S.; Nicolaou, K.C.; Stoll, V.
Deposited on : 2020-02-21
Resolution : 2.85 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

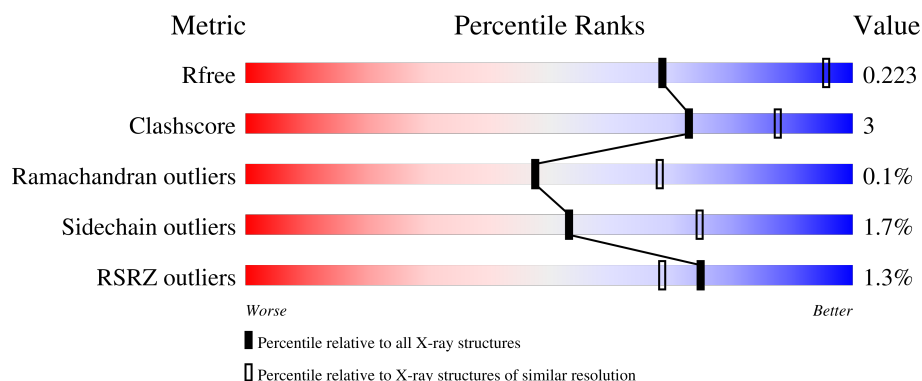
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	% 92% 5% .
1	C	451	% 87% 9% ..
2	B	445	87% 9% .
2	D	445	2% 89% 7% .
3	E	143	% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	2% 83% 7% 10%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 18400 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	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	5	0
			3484	2202	594	665	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	2	0
			3401	2134	582	658	27			
2	D	428	Total	C	N	O	S	0	1	0
			3367	2112	578	651	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	47	MET	-	expression tag	UNP P63043
E	48	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	1	0
			2851	1826	488	522	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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

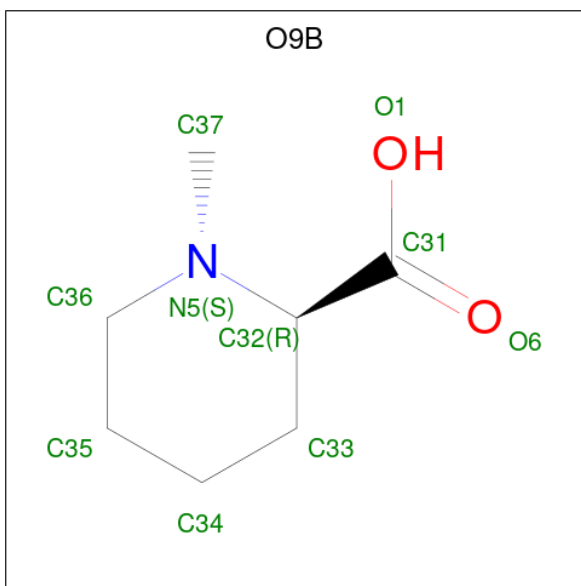
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





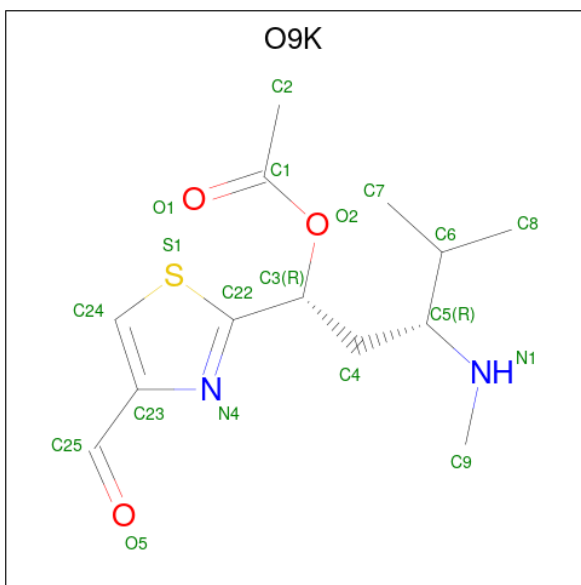
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (2 {R})-1-methylpiperidine-2-carboxylic acid (CCD ID: O9B) (formula: C₇H₁₃NO₂).



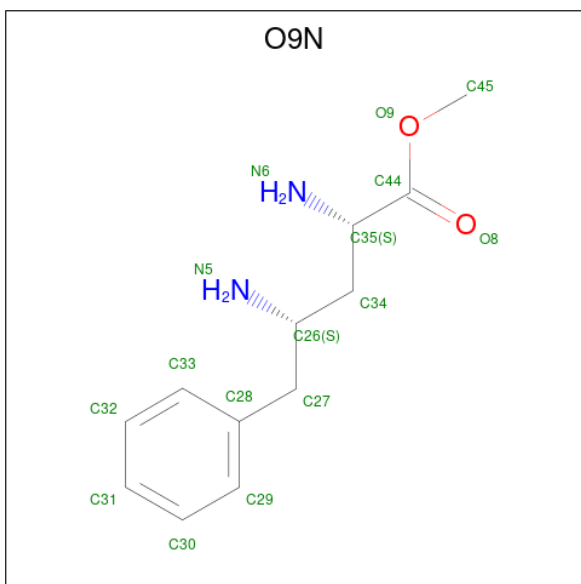
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			9	7	1	1		

- Molecule 11 is [(1 {R}),3 {R}]-1-(4-methanoyl-1,3-thiazol-2-yl)-4-methyl-3-(methylamino)pentyl ethanoate (CCD ID: O9K) (formula: C₁₃H₂₀N₂O₃S).



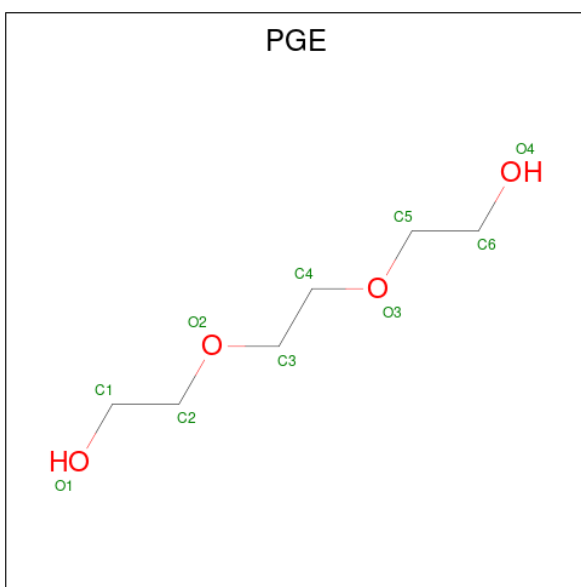
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			19	13	2	3	1		

- Molecule 12 is methyl (2 {S},4 {S})-2,4-bis(azanyl)-5-phenyl-pentanoate (CCD ID: O9N) (formula: $C_{12}H_{18}N_2O_2$).



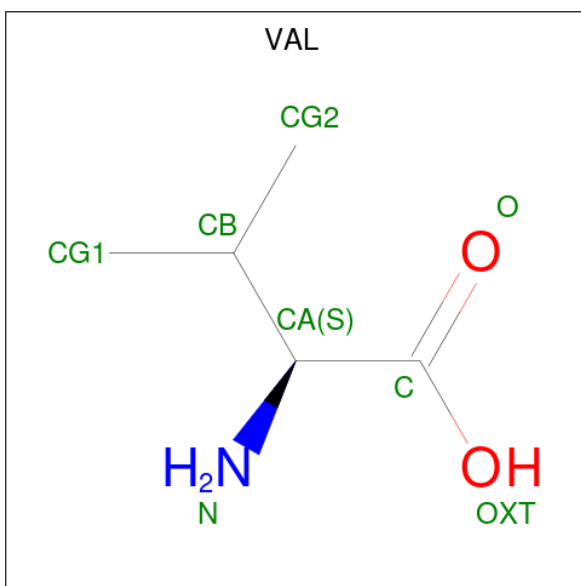
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 13 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



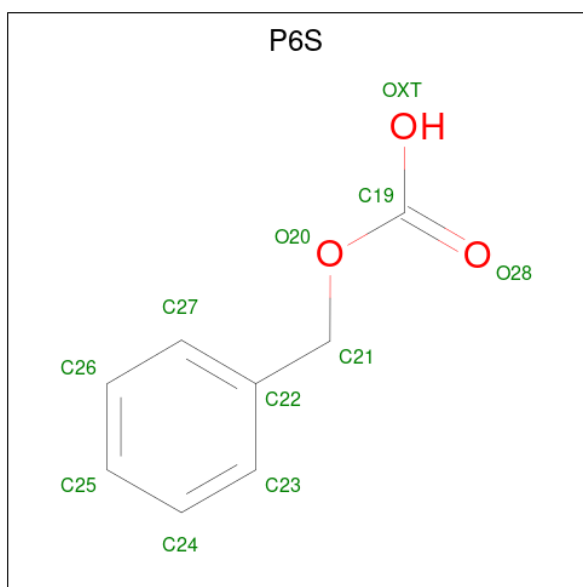
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 14 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



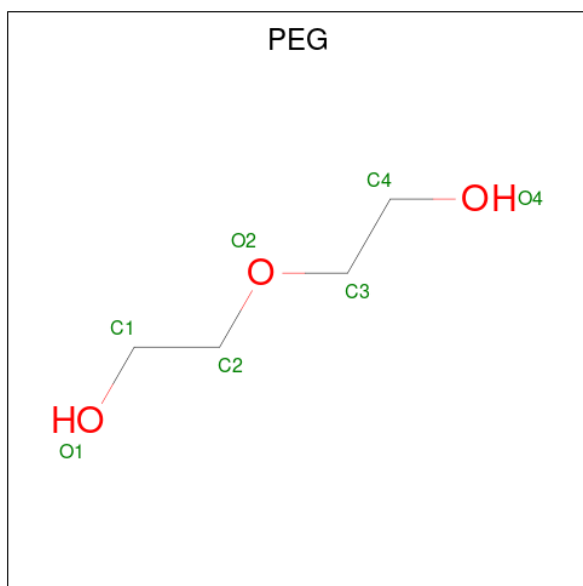
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 15 is benzyl hydrogen carbonate (CCD ID: P6S) (formula: $C_8H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			10	8	2		

- Molecule 16 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



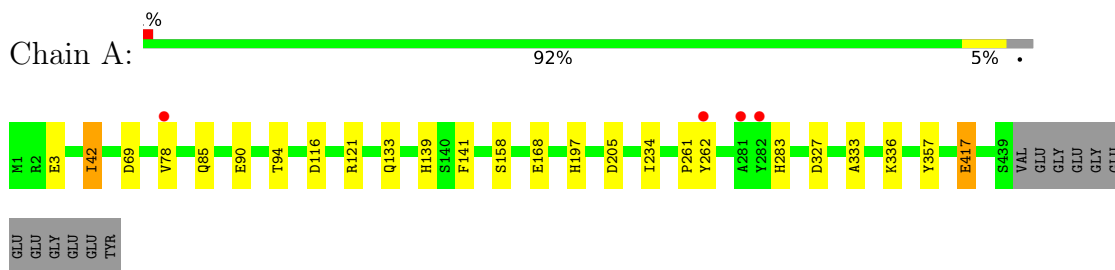
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 17 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

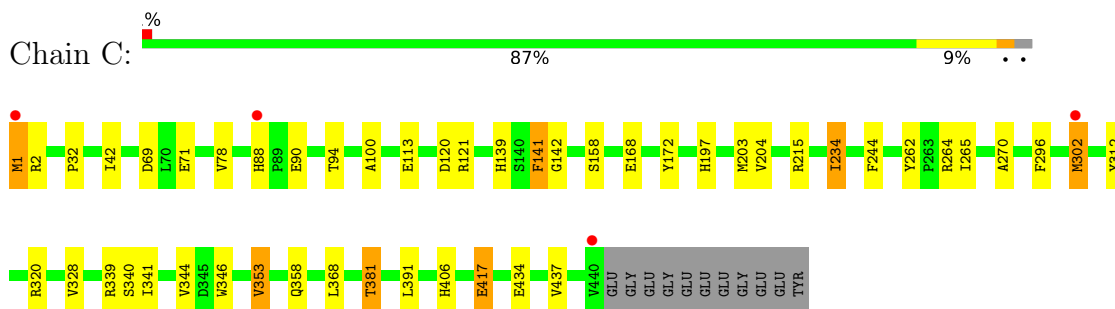
3 Residue-property plots [i](#)

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.

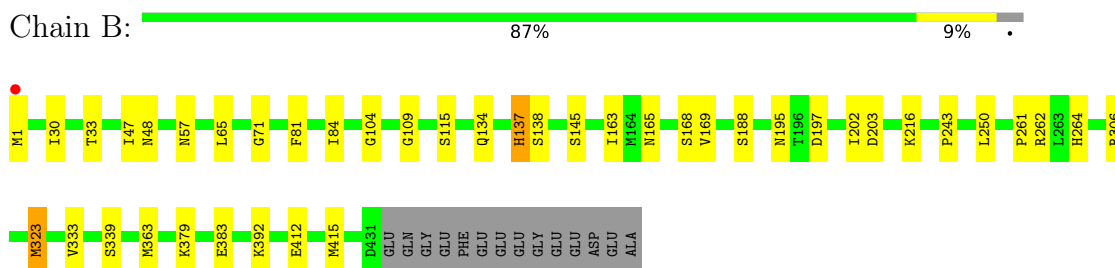
- Molecule 1: Tubulin alpha-1B chain



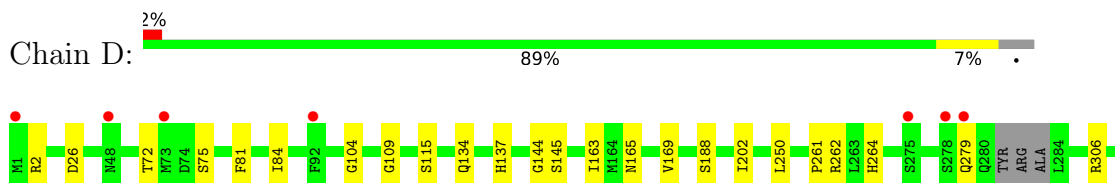
- Molecule 1: Tubulin alpha-1B chain

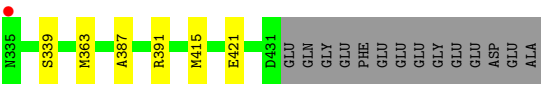


- Molecule 2: Tubulin beta chain

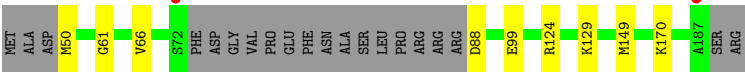
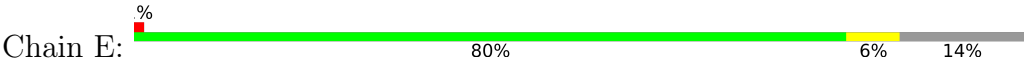


- Molecule 2: Tubulin beta chain

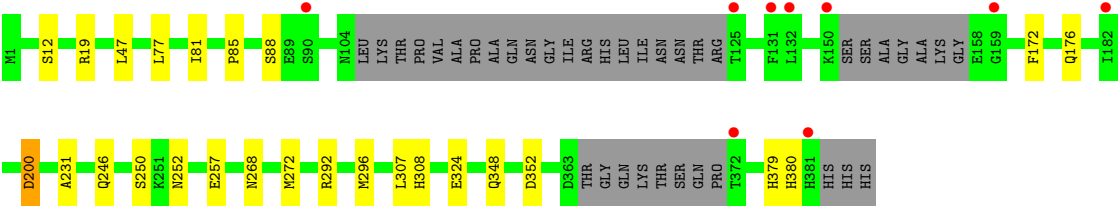
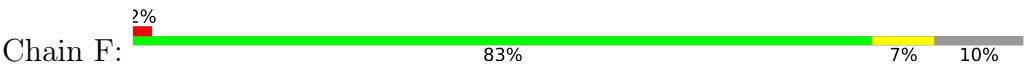




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.28Å 154.97Å 183.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.93 – 2.85 78.93 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.93-2.85) 100.0 (78.93-2.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.7 (6-FEB-2020)	Depositor
R, R_{free}	0.183 , 0.220 0.183 , 0.223	Depositor DCC
R_{free} test set	3527 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18400	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, P6S, O9B, MG, CA, ACP, MES, GTP, O9K, O9N, GDP, PEG

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	0.78	0/3508	1.03	4/4762 (0.1%)
1	C	0.78	0/3563	1.03	5/4837 (0.1%)
2	B	0.77	1/3476 (0.0%)	1.00	1/4709 (0.0%)
2	D	0.75	1/3440 (0.0%)	1.00	0/4659
3	E	0.77	0/1022	1.08	0/1356
4	F	0.77	1/2916 (0.0%)	0.99	1/3939 (0.0%)
All	All	0.77	3/17925 (0.0%)	1.02	11/24262 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	415	MET	SD-CE	-9.89	1.54	1.79
2	D	415	MET	SD-CE	-5.93	1.64	1.79
4	F	231	ALA	CA-C	5.07	1.58	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	PHE	CA-CB-CG	7.32	121.11	113.80
1	C	141	PHE	CA-CB-CG	7.16	120.96	113.80
1	C	353	VAL	CA-C-N	6.61	126.15	121.65
1	C	353	VAL	C-N-CA	6.61	126.15	121.65
1	C	78	VAL	N-CA-C	-5.68	105.31	110.82
1	C	142	GLY	N-CA-C	5.50	119.81	112.77
4	F	200	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	203	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	78	VAL	N-CA-C	-5.13	105.84	110.82
1	A	327	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	417	GLU	CB-CG-CD	5.07	121.22	112.60

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	3430	0	3339	15	0
1	C	3484	0	3386	33	0
2	B	3401	0	3275	25	0
2	D	3367	0	3246	16	0
3	E	1014	0	1029	9	0
4	F	2851	0	2808	14	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	12	0	13	2	0
10	B	9	0	0	0	0
11	B	19	0	0	0	0
12	B	16	0	0	0	0
13	C	10	0	14	4	0
14	C	7	0	8	0	0
15	C	10	0	0	0	0
16	D	7	0	10	0	0
17	F	31	0	14	0	0
18	A	116	0	0	8	0
18	B	143	0	0	11	0
18	C	174	0	0	11	0
18	D	67	0	0	6	0
18	E	31	0	0	7	0
18	F	70	0	0	4	0
All	All	18400	0	17190	111	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 3.

All (111) 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)
3:E:149:MET:HB3	18:E:223:HOH:O	1.42	1.14
1:C:215:ARG:HB2	18:C:1208:HOH:O	1.68	0.91
3:E:149:MET:CB	18:E:223:HOH:O	2.06	0.88
1:C:113:GLU:HG3	18:C:1197:HOH:O	1.72	0.88
1:A:261:PRO:HD2	18:A:1147:HOH:O	1.74	0.86
1:C:120:ASP:HB2	18:C:1230:HOH:O	1.76	0.86
2:D:262:ARG:NH1	18:D:1101:HOH:O	2.12	0.83
1:A:262:TYR:CE1	18:A:1214:HOH:O	2.33	0.81
1:A:262:TYR:CD1	18:A:1214:HOH:O	2.39	0.75
4:F:246:GLN:O	4:F:250:SER:HB3	1.87	0.74
2:D:306:ARG:NH1	18:D:1103:HOH:O	2.19	0.74
2:D:72:THR:HG23	18:D:1162:HOH:O	1.88	0.73
1:C:381:THR:CG2	18:C:1131:HOH:O	2.39	0.71
1:C:381:THR:HG23	18:C:1131:HOH:O	1.91	0.71
18:B:1161:HOH:O	3:E:129:LYS:HE2	1.92	0.70
2:D:2:ARG:NH1	18:D:1104:HOH:O	2.23	0.69
2:B:197:ASP:OD2	9:B:1003:MES:H52	1.93	0.69
1:A:85:GLN:HB2	18:A:1105:HOH:O	1.94	0.67
1:C:262:TYR:HB3	13:C:1004:PGE:H42	1.78	0.65
2:B:57:ASN:HA	18:B:1102:HOH:O	1.97	0.63
3:E:88:ASP:N	18:E:201:HOH:O	2.30	0.63
1:C:296:PHE:CE2	1:C:341:ILE:HD11	2.33	0.63
2:D:81:PHE:O	2:D:84:ILE:HG22	1.99	0.62
2:B:323:MET:HB2	18:B:1177:HOH:O	2.02	0.60
2:B:104:GLY:O	2:B:109:GLY:HA3	2.01	0.60
2:B:197:ASP:OD1	9:B:1003:MES:H32	2.01	0.60
2:D:421:GLU:HB2	18:D:1101:HOH:O	2.02	0.59
1:A:116:ASP:HB2	18:A:1138:HOH:O	2.03	0.58
3:E:124:ARG:NH2	18:E:202:HOH:O	2.36	0.57
4:F:19:ARG:HG3	18:F:1147:HOH:O	2.05	0.57
4:F:292:ARG:HD2	18:F:1151:HOH:O	2.06	0.56
1:A:262:TYR:HE1	18:A:1214:HOH:O	1.80	0.55
2:D:115:SER:OG	18:D:1102:HOH:O	2.18	0.55
2:B:306:ARG:HD3	18:B:1200:HOH:O	2.06	0.55
2:B:1:MET:HE3	2:B:48:ASN:HB2	1.87	0.54
1:C:88[B]:HIS:HD2	1:C:90[B]:GLU:H	1.56	0.54
4:F:379:HIS:HD2	18:F:1149:HOH:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:99:GLU:HB3	18:E:217:HOH:O	2.08	0.53
2:B:392:LYS:HG3	18:B:1140:HOH:O	2.09	0.53
4:F:296[B]:MET:SD	4:F:380:HIS:ND1	2.81	0.53
2:B:137:HIS:HE1	2:B:168:SER:OG	1.92	0.53
1:C:1:MET:HG3	1:C:2:ARG:N	2.25	0.52
4:F:77:LEU:O	4:F:81:ILE:HG12	2.10	0.52
2:D:134:GLN:HA	2:D:165:ASN:O	2.10	0.52
1:C:417:GLU:HG2	18:C:1107:HOH:O	2.11	0.51
2:B:134:GLN:HA	2:B:165:ASN:O	2.10	0.51
1:C:320:ARG:HG3	18:C:1176:HOH:O	2.11	0.50
2:B:81:PHE:O	2:B:84:ILE:HG22	2.12	0.50
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.94	0.50
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.49
1:C:270:ALA:HB3	1:C:302[B]:MET:HE2	1.95	0.48
2:B:216:LYS:HE2	18:B:1205:HOH:O	2.14	0.48
1:C:203:MET:O	1:C:302[B]:MET:HE3	2.13	0.48
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.94	0.48
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.49	0.48
1:C:234:ILE:HG13	1:C:302[A]:MET:HE2	1.96	0.48
4:F:172:PHE:O	4:F:176:GLN:HG2	2.14	0.48
2:B:261:PRO:O	2:B:264:HIS:HD2	1.97	0.47
2:D:145:SER:HG	2:D:188:SER:HG	1.62	0.47
2:D:261:PRO:O	2:D:264:HIS:HD2	1.96	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.47
1:C:139:HIS:HE1	1:C:168:GLU:OE1	1.98	0.47
4:F:292:ARG:NH2	18:F:1103:HOH:O	2.47	0.46
2:B:412[B]:GLU:OE2	2:B:412[B]:GLU:HA	2.16	0.46
1:C:434:GLU:O	1:C:437:VAL:HG22	2.16	0.46
2:B:145:SER:HG	2:B:188:SER:HG	1.63	0.46
1:A:139:HIS:HE1	1:A:168:GLU:OE1	1.98	0.46
2:D:387:ALA:O	2:D:391:ARG:NH1	2.49	0.45
2:B:138:SER:HB2	18:B:1144:HOH:O	2.15	0.45
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.97	0.45
1:C:90[B]:GLU:O	1:C:121:ARG:HD2	2.16	0.45
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.52	0.44
3:E:149:MET:HB2	18:E:223:HOH:O	1.95	0.44
1:A:333:ALA:O	1:A:336:LYS:HG2	2.18	0.44
1:C:69:ASP:O	1:C:94:THR:HA	2.18	0.44
1:C:406:HIS:HD2	18:C:1256:HOH:O	2.00	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CE2	3:E:61:GLY:HA2	2.53	0.43
2:B:262:ARG:HD2	18:B:1228:HOH:O	2.18	0.43
2:D:104:GLY:O	2:D:109:GLY:HA3	2.19	0.43
2:B:30:ILE:CD1	2:B:47:ILE:HD11	2.48	0.43
2:B:262:ARG:CD	18:B:1228:HOH:O	2.67	0.43
4:F:85:PRO:O	4:F:88:SER:OG	2.31	0.43
4:F:296[B]:MET:CE	4:F:380:HIS:ND1	2.82	0.43
2:B:379:LYS:O	2:B:383:GLU:HG3	2.18	0.43
1:C:158:SER:OG	1:C:197:HIS:HD2	2.01	0.43
1:C:204:VAL:HG22	1:C:302[B]:MET:SD	2.59	0.43
1:A:205:ASP:OD2	18:A:1101:HOH:O	2.22	0.42
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.52	0.42
1:C:264:ARG:CD	13:C:1004:PGE:H62	2.49	0.42
1:C:264:ARG:HD3	13:C:1004:PGE:H62	2.00	0.42
4:F:47:LEU:C	4:F:47:LEU:HD23	2.45	0.42
1:C:100:ALA:HB2	18:C:1155:HOH:O	2.19	0.42
1:C:141:PHE:HE1	18:C:1268:HOH:O	2.03	0.42
2:D:137:HIS:HD2	2:D:144:GLY:O	2.03	0.42
1:A:158:SER:OG	1:A:197:HIS:HD2	2.02	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.19	0.42
2:B:243:PRO:HA	18:B:1107:HOH:O	2.18	0.42
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.50	0.41
4:F:268:ASN:O	4:F:272:MET:HG3	2.20	0.41
1:A:42:ILE:HA	18:A:1107:HOH:O	2.20	0.41
1:C:32:PRO:O	18:C:1101:HOH:O	2.22	0.41
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.55	0.41
2:B:65:LEU:N	2:B:65:LEU:HD12	2.36	0.41
2:D:72:THR:HA	2:D:75:SER:OG	2.20	0.41
1:C:262:TYR:CB	13:C:1004:PGE:H42	2.45	0.41
2:B:195:ASN:ND2	18:B:1108:HOH:O	2.43	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.40
3:E:50:MET:N	18:E:204:HOH:O	2.53	0.40
1:A:3:GLU:O	1:A:133:GLN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	437/451 (97%)	422 (97%)	15 (3%)	0	100	100
1	C	443/451 (98%)	430 (97%)	13 (3%)	0	100	100
2	B	431/445 (97%)	418 (97%)	12 (3%)	1 (0%)	43	62
2	D	425/445 (96%)	412 (97%)	12 (3%)	1 (0%)	43	62
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	339/384 (88%)	325 (96%)	14 (4%)	0	100	100
All	All	2194/2319 (95%)	2126 (97%)	66 (3%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	279	GLN
2	B	71	GLY

5.3.2 Protein sidechains

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	370/379 (98%)	366 (99%)	4 (1%)	65	81
1	C	376/379 (99%)	364 (97%)	12 (3%)	34	59
2	B	372/381 (98%)	365 (98%)	7 (2%)	50	72
2	D	369/381 (97%)	366 (99%)	3 (1%)	73	86
3	E	110/127 (87%)	108 (98%)	2 (2%)	51	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	F	313/342 (92%)	308 (98%)	5 (2%)	55 76
All	All	1910/1989 (96%)	1877 (98%)	33 (2%)	53 75

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	234	ILE
1	A	283	HIS
1	A	417	GLU
2	B	33	THR
2	B	115	SER
2	B	137	HIS
2	B	323	MET
2	B	333	VAL
2	B	339	SER
2	B	363	MET
1	C	1	MET
1	C	42	ILE
1	C	71	GLU
1	C	234	ILE
1	C	265	ILE
1	C	302[A]	MET
1	C	302[B]	MET
1	C	339	ARG
1	C	340	SER
1	C	368	LEU
1	C	381	THR
1	C	417	GLU
2	D	26	ASP
2	D	339	SER
2	D	363	MET
3	E	66	VAL
3	E	170	LYS
4	F	12	SER
4	F	200	ASP
4	F	252	ASN
4	F	257	GLU
4	F	324	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	139	HIS
1	A	197	HIS
1	A	256	GLN
1	A	300	ASN
1	A	358	GLN
1	A	372	GLN
1	A	393	HIS
2	B	89	ASN
2	B	94	GLN
2	B	137	HIS
2	B	190	HIS
2	B	264	HIS
2	B	329	GLN
2	B	337	ASN
2	B	414	ASN
2	B	426	GLN
1	C	11	GLN
1	C	85	GLN
1	C	139	HIS
1	C	197	HIS
1	C	283	HIS
1	C	329	ASN
1	C	393	HIS
2	D	137	HIS
2	D	190	HIS
2	D	195	ASN
2	D	264	HIS
2	D	280	GLN
2	D	329	GLN
2	D	337	ASN
2	D	414	ASN
3	E	108	GLN
3	E	115	HIS
4	F	45	ASN
4	F	269	GLN
4	F	306	HIS
4	F	333	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	1001	6	33,34,34	0.43	0	50,54,54	0.50	0
8	GDP	B	1001	6	29,30,30	0.27	0	45,47,47	0.43	0
5	GTP	D	1001	6	33,34,34	0.41	0	50,54,54	0.54	1 (2%)
9	MES	B	1003	-	12,12,12	0.70	0	15,16,16	0.62	0
5	GTP	C	1001	6	33,34,34	0.43	0	50,54,54	0.51	0
11	O9K	B	1005	12,14	18,19,19	0.57	0	19,25,25	1.06	1 (5%)
17	ACP	F	1001	6	31,33,33	1.72	10 (32%)	47,52,52	1.79	10 (21%)
16	PEG	D	1003	-	6,6,6	0.18	0	5,5,5	0.07	0
15	P6S	C	1006	12	9,10,11	0.22	0	10,11,13	0.26	0
12	O9N	B	1006	15,11	15,16,16	0.24	0	16,20,20	0.36	0
14	VAL	C	1005	10,11	4,6,7	0.63	0	6,7,9	0.91	1 (16%)
13	PGE	C	1004	-	9,9,9	0.24	0	8,8,8	0.28	0
10	O9B	B	1004	14	7,9,10	0.49	0	7,11,13	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	1001	6	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	1001	6	-	4/16/32/32	0/3/3/3
5	GTP	D	1001	6	-	3/22/38/38	0/3/3/3
9	MES	B	1003	-	-	4/6/14/14	0/1/1/1
5	GTP	C	1001	6	-	8/22/38/38	0/3/3/3
11	O9K	B	1005	12,14	-	1/20/20/20	0/1/1/1
17	ACP	F	1001	6	-	4/19/38/38	0/3/3/3
16	PEG	D	1003	-	-	0/4/4/4	-
15	P6S	C	1006	12	-	1/4/4/5	0/1/1/1
12	O9N	B	1006	15,11	-	2/14/14/14	0/1/1/1
14	VAL	C	1005	10,11	-	1/5/6/8	-
13	PGE	C	1004	-	-	5/7/7/7	-
10	O9B	B	1004	14	-	0/1/13/15	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	1001	ACP	C5-C4	4.65	1.47	1.39
17	F	1001	ACP	PG-O2G	3.34	1.62	1.55
17	F	1001	ACP	PG-O3G	3.16	1.62	1.55
17	F	1001	ACP	C5-C6	2.58	1.48	1.41
17	F	1001	ACP	PB-O3A	2.57	1.61	1.58
17	F	1001	ACP	C5-N7	-2.53	1.34	1.39
17	F	1001	ACP	PA-O3A	2.40	1.62	1.59
17	F	1001	ACP	PB-O2B	2.25	1.61	1.56
17	F	1001	ACP	C8-N7	2.12	1.35	1.31
17	F	1001	ACP	C4-N9	-2.06	1.33	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	1001	ACP	C5-C4-N3	-5.74	118.82	126.72
17	F	1001	ACP	N3-C4-N9	4.77	135.27	127.17
17	F	1001	ACP	C2-N3-C4	3.83	121.17	111.83
17	F	1001	ACP	N3-C2-N1	-3.65	123.05	128.58
17	F	1001	ACP	C4-C5-N7	-3.04	107.11	110.58
17	F	1001	ACP	C4-N9-C8	2.66	108.53	105.74
11	B	1005	O9K	C9-N1-C5	2.44	117.30	114.39
5	D	1001	GTP	O5'-PA-O1A	2.38	118.36	108.94
17	F	1001	ACP	O2G-PG-O1G	-2.26	106.54	112.39
17	F	1001	ACP	C5-N7-C8	2.20	106.90	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	1001	ACP	PB-O3A-PA	-2.16	125.33	132.37
17	F	1001	ACP	C2-N1-C6	2.03	122.07	118.73
14	C	1005	VAL	O-C-CA	-2.01	119.60	124.77

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	GTP	C5'-O5'-PA-O3A
5	A	1001	GTP	C5'-O5'-PA-O1A
5	C	1001	GTP	C5'-O5'-PA-O3A
5	C	1001	GTP	C5'-O5'-PA-O1A
5	D	1001	GTP	C5'-O5'-PA-O3A
5	D	1001	GTP	C5'-O5'-PA-O1A
8	B	1001	GDP	C5'-O5'-PA-O3A
8	B	1001	GDP	C5'-O5'-PA-O1A
9	B	1003	MES	C8-C7-N4-C5
9	B	1003	MES	C7-C8-S-O2S
9	B	1003	MES	C7-C8-S-O3S
17	F	1001	ACP	PG-C3B-PB-O1B
17	F	1001	ACP	PG-C3B-PB-O2B
17	F	1001	ACP	PG-C3B-PB-O3A
17	F	1001	ACP	C5'-O5'-PA-O1A
13	C	1004	PGE	O3-C5-C6-O4
13	C	1004	PGE	O2-C3-C4-O3
9	B	1003	MES	C7-C8-S-O1S
12	B	1006	O9N	N6-C35-C44-O8
5	A	1001	GTP	C5'-O5'-PA-O2A
5	C	1001	GTP	C5'-O5'-PA-O2A
5	D	1001	GTP	C5'-O5'-PA-O2A
8	B	1001	GDP	C5'-O5'-PA-O2A
5	A	1001	GTP	PB-O3A-PA-O2A
5	C	1001	GTP	PB-O3A-PA-O2A
14	C	1005	VAL	O-C-CA-CB
13	C	1004	PGE	C6-C5-O3-C4
8	B	1001	GDP	PB-O3A-PA-O2A
13	C	1004	PGE	C4-C3-O2-C2
5	C	1001	GTP	PB-O3B-PG-O1G
11	B	1005	O9K	C4-C5-C6-C8
5	A	1001	GTP	PB-O3B-PG-O3G
5	C	1001	GTP	PB-O3B-PG-O2G
5	C	1001	GTP	PB-O3B-PG-O3G

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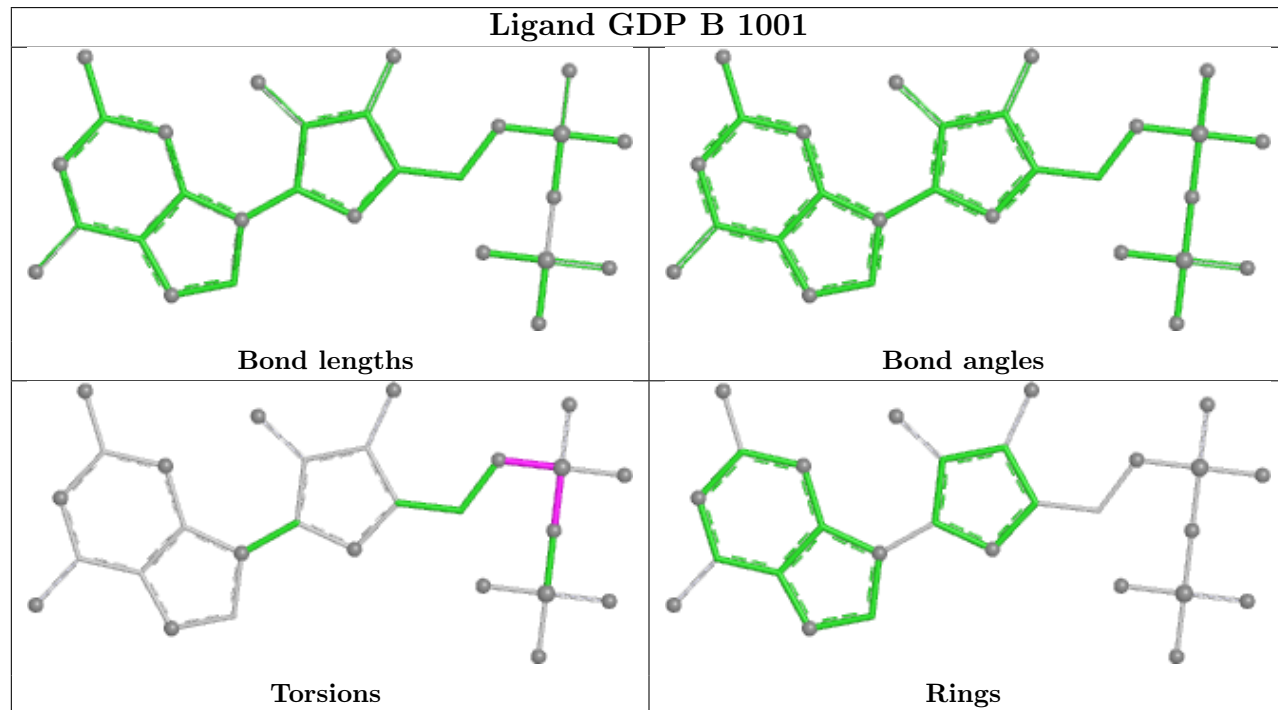
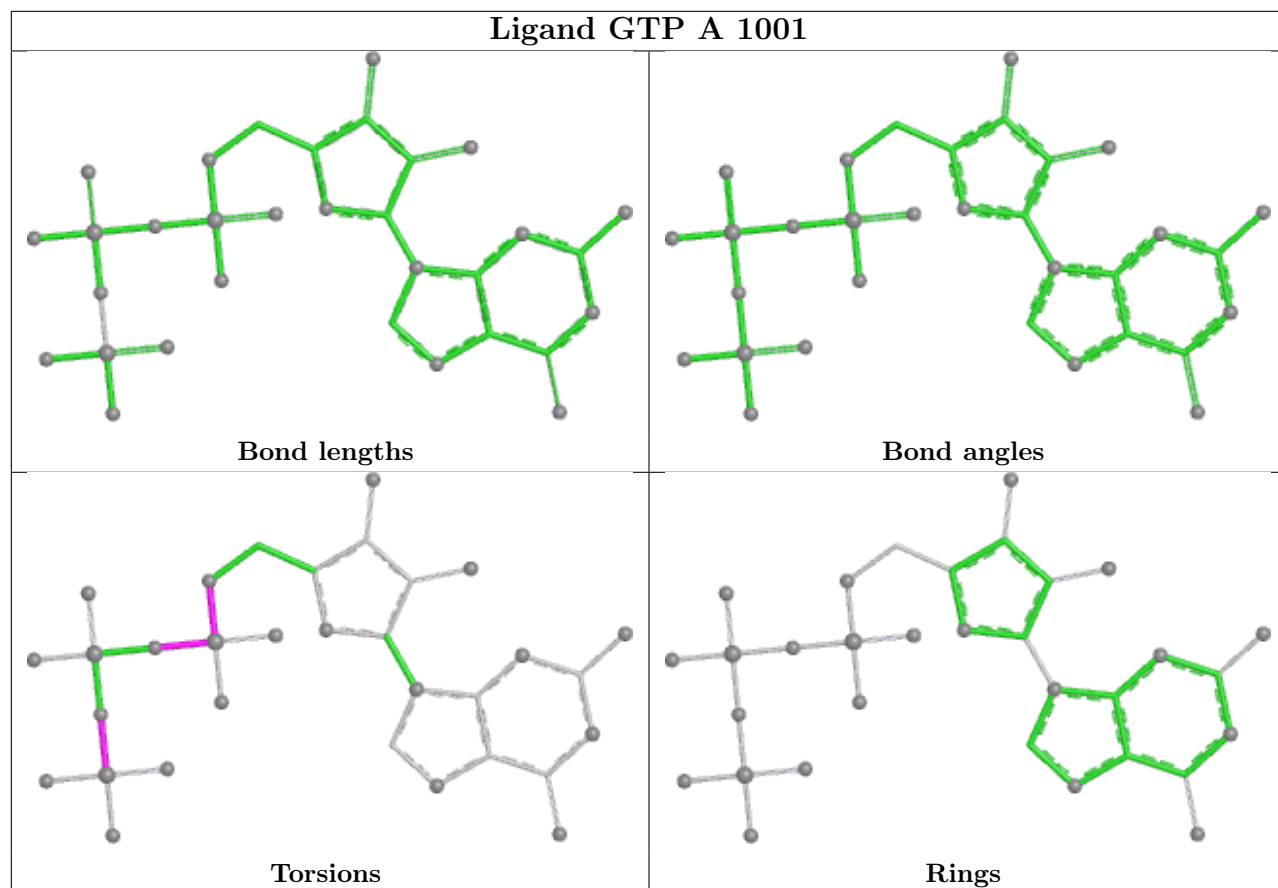
Mol	Chain	Res	Type	Atoms
5	A	1001	GTP	PB-O3A-PA-O1A
5	C	1001	GTP	PB-O3A-PA-O1A
13	C	1004	PGE	C1-C2-O2-C3
15	C	1006	P6S	C22-C21-O20-C19
5	A	1001	GTP	PB-O3B-PG-O1G
12	B	1006	O9N	N6-C35-C44-O9

There are no ring outliers.

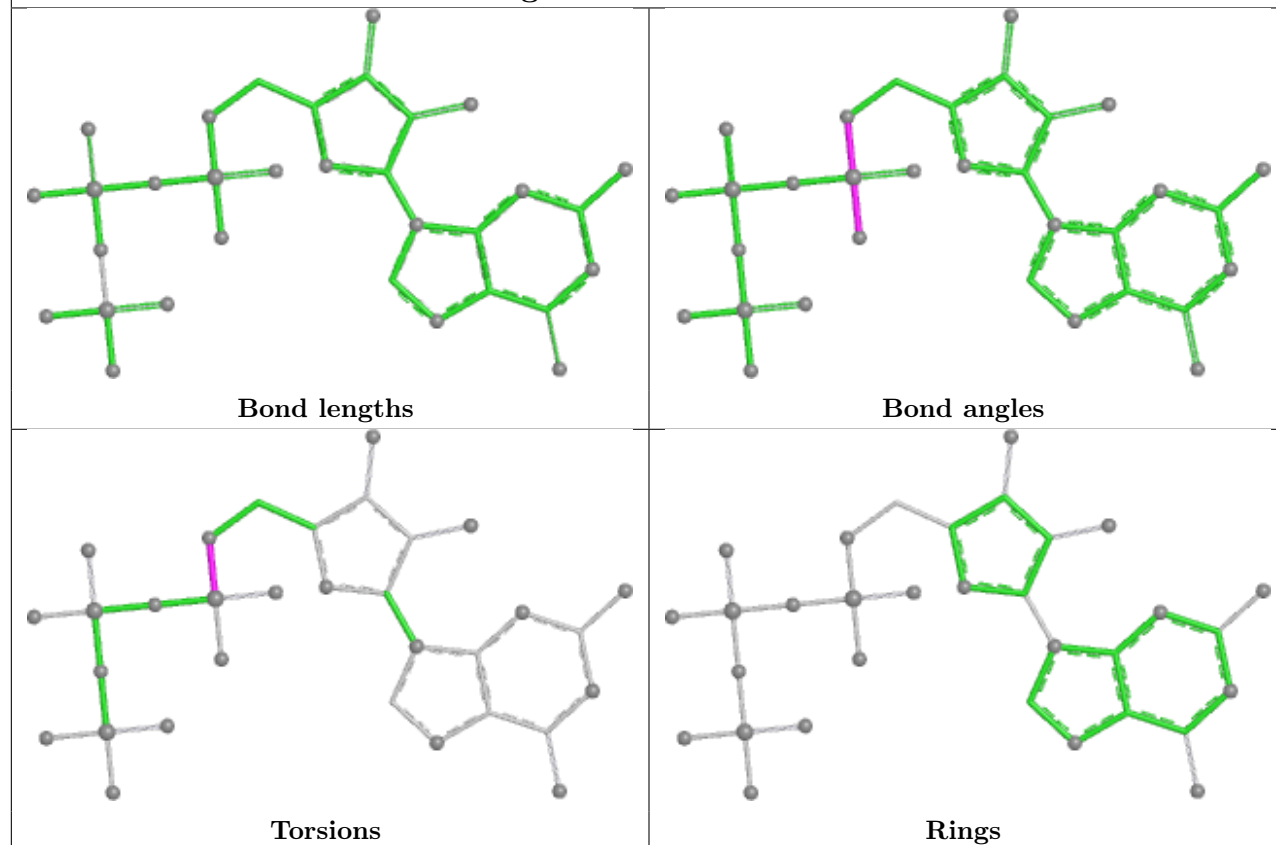
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1003	MES	2	0
13	C	1004	PGE	4	0

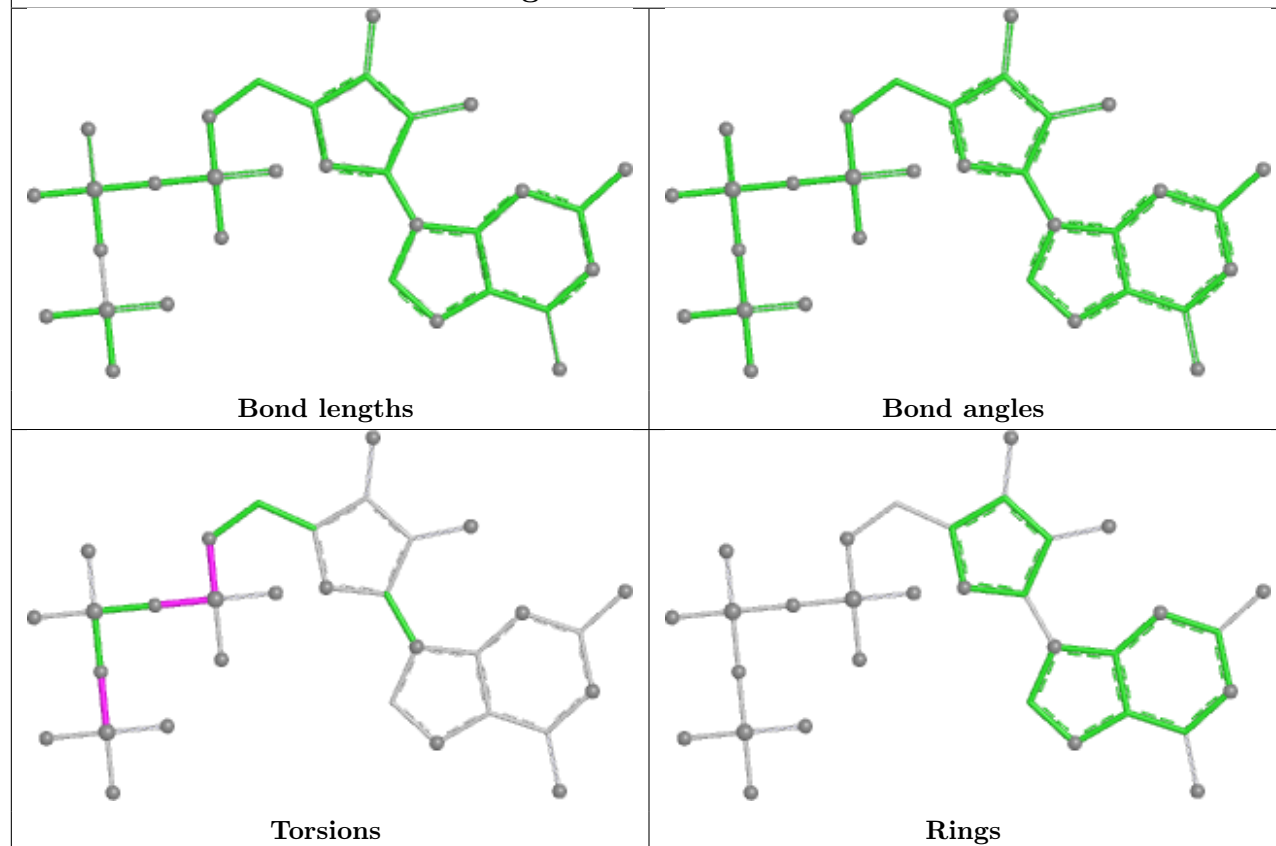
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

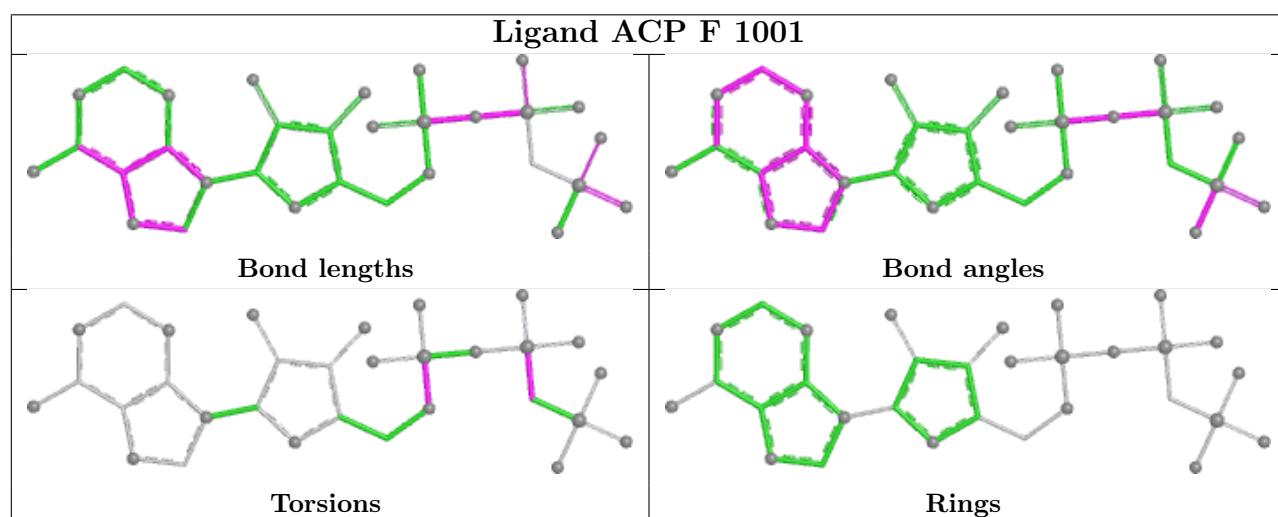
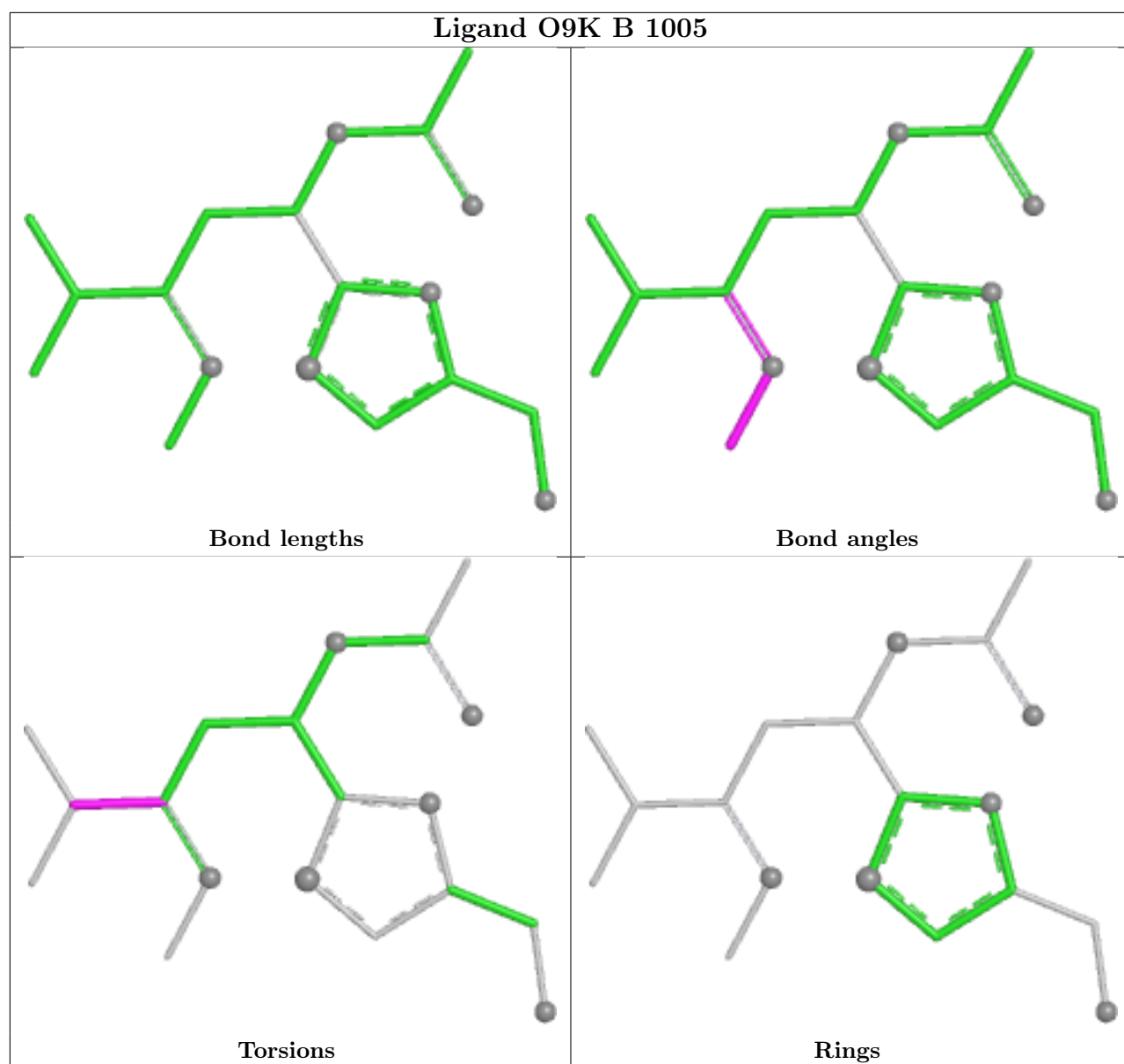


Ligand GTP D 1001



Ligand GTP C 1001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	-0.11	4 (0%) 81 76	37, 57, 83, 98	0
1	C	440/451 (97%)	-0.29	4 (0%) 81 76	24, 48, 65, 87	5 (1%)
2	B	431/445 (96%)	-0.33	1 (0%) 91 91	23, 49, 79, 99	2 (0%)
2	D	428/445 (96%)	0.07	8 (1%) 66 59	31, 69, 92, 123	1 (0%)
3	E	123/143 (86%)	-0.05	2 (1%) 70 64	46, 66, 92, 107	0
4	F	346/384 (90%)	0.14	9 (2%) 57 48	28, 76, 143, 179	1 (0%)
All	All	2207/2319 (95%)	-0.11	28 (1%) 75 68	23, 59, 98, 179	9 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	150	LYS	3.8
4	F	125	THR	3.8
2	B	1	MET	3.6
1	C	88[A]	HIS	3.0
4	F	381	HIS	2.9
1	C	1	MET	2.9
2	D	1	MET	2.6
1	C	302[A]	MET	2.5
4	F	131	PHE	2.5
2	D	73	MET	2.4
2	D	92	PHE	2.3
1	A	262	TYR	2.3
4	F	132	LEU	2.3
1	A	282	TYR	2.3
4	F	90	SER	2.2
2	D	335	ASN	2.2
2	D	279	GLN	2.2
1	A	78	VAL	2.1
1	C	440	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	278	SER	2.1
4	F	182	ILE	2.1
4	F	159	GLY	2.1
4	F	372	THR	2.1
1	A	281	ALA	2.1
3	E	187	ALA	2.1
2	D	275	SER	2.0
3	E	72	SER	2.0
2	D	48	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

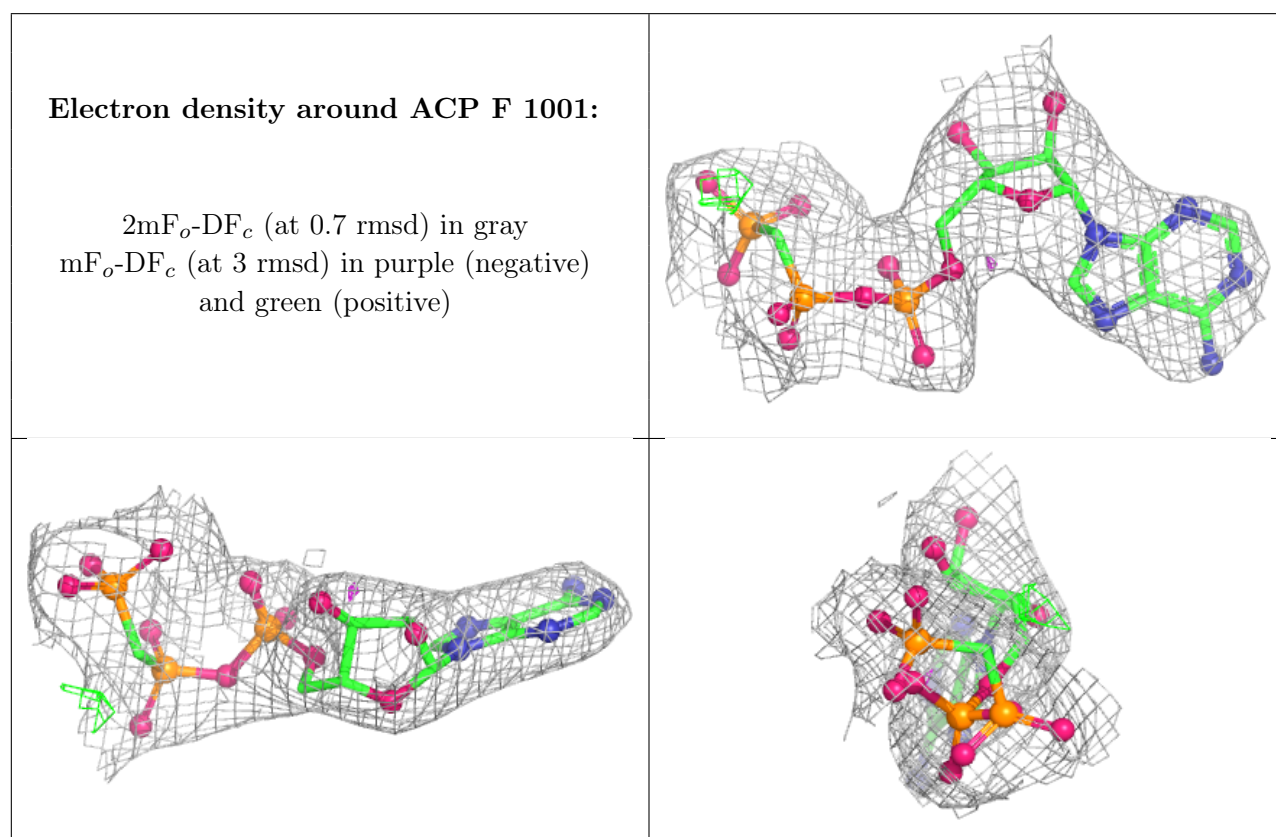
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	PGE	C	1004	10/10	0.81	0.22	70,70,71,71	0
16	PEG	D	1003	7/7	0.81	0.15	93,93,94,94	0
15	P6S	C	1006	10/11	0.83	0.16	71,74,74,74	0
6	MG	F	1002	1/1	0.90	0.10	68,68,68,68	0
12	O9N	B	1006	16/16	0.91	0.11	58,59,69,69	0
17	ACP	F	1001	31/31	0.92	0.08	91,94,105,105	0
9	MES	B	1003	12/12	0.95	0.09	65,65,68,68	0
11	O9K	B	1005	19/19	0.96	0.09	47,54,57,57	0
14	VAL	C	1005	7/8	0.97	0.08	44,45,46,47	0
7	CA	C	1003	1/1	0.97	0.05	64,64,64,64	0
5	GTP	D	1001	32/32	0.97	0.06	65,68,75,75	0
10	O9B	B	1004	9/10	0.97	0.08	42,43,46,46	0
8	GDP	B	1001	28/28	0.98	0.06	38,39,40,41	0
6	MG	B	1002	1/1	0.98	0.19	58,58,58,58	0

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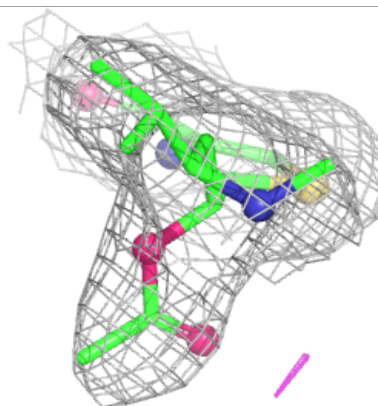
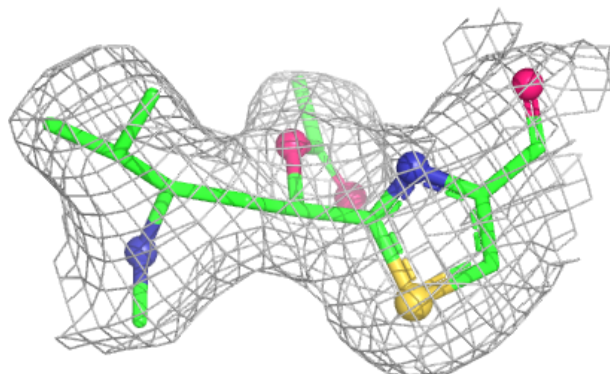
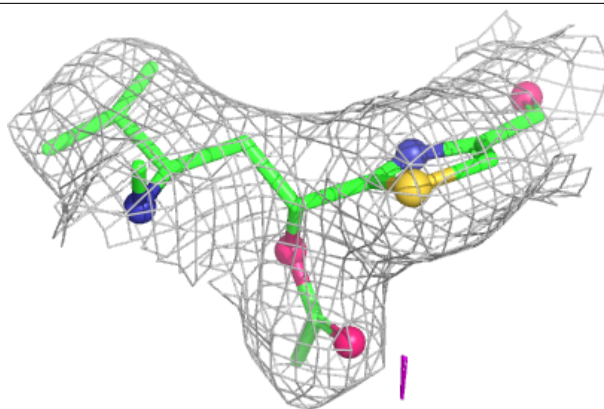
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	C	1001	32/32	0.98	0.06	41,43,45,46	0
7	CA	A	1003	1/1	0.98	0.07	80,80,80,80	0
5	GTP	A	1001	32/32	0.98	0.06	44,46,48,48	0
6	MG	A	1002	1/1	0.99	0.05	45,45,45,45	0
6	MG	D	1002	1/1	1.00	0.02	64,64,64,64	0
6	MG	C	1002	1/1	1.00	0.04	42,42,42,42	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.

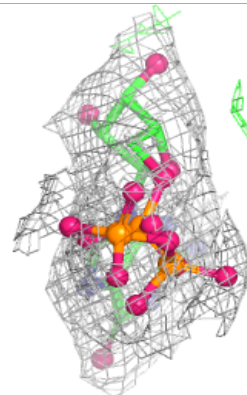
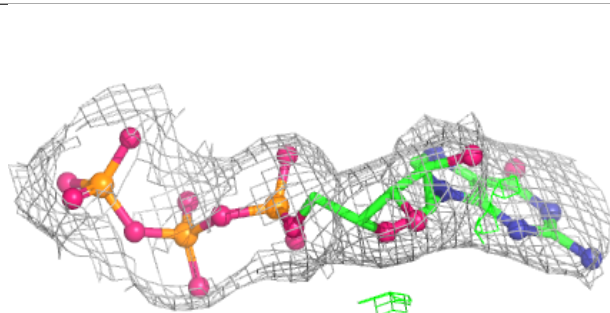
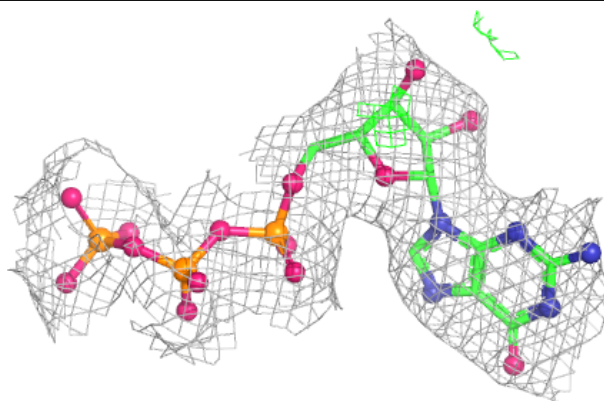


Electron density around O9K B 1005:

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

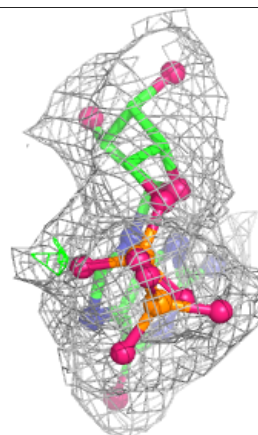
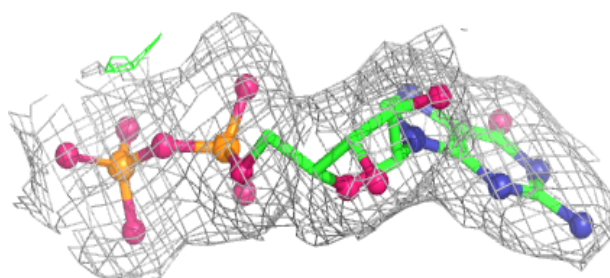
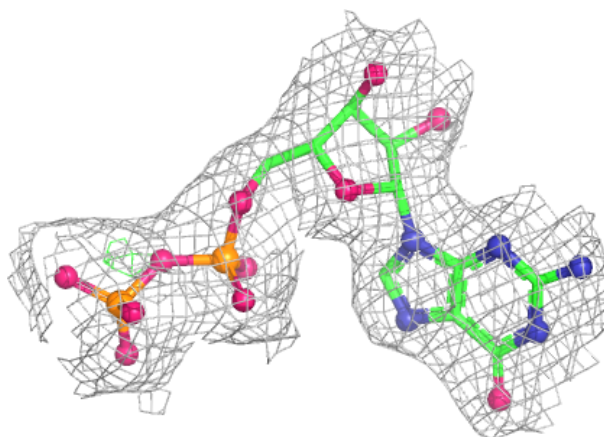
**Electron density around GTP D 1001:**

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

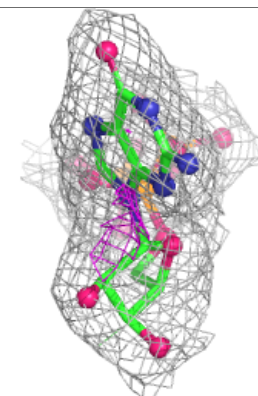
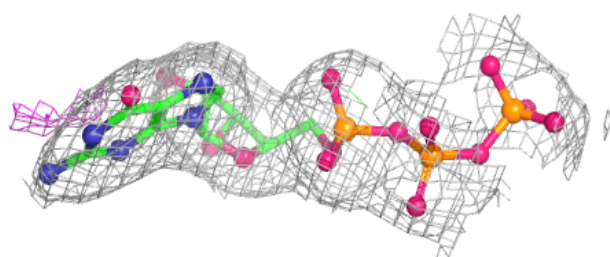
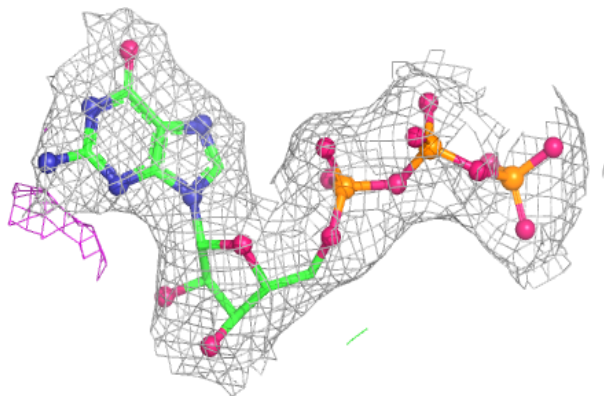


Electron density around GDP B 1001:

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

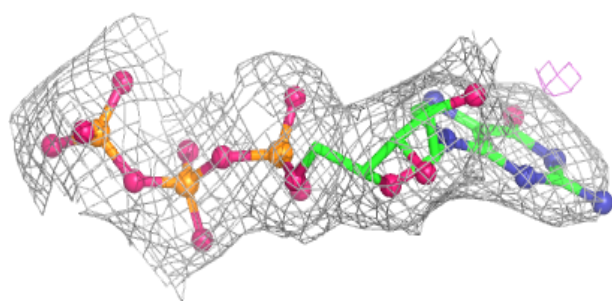
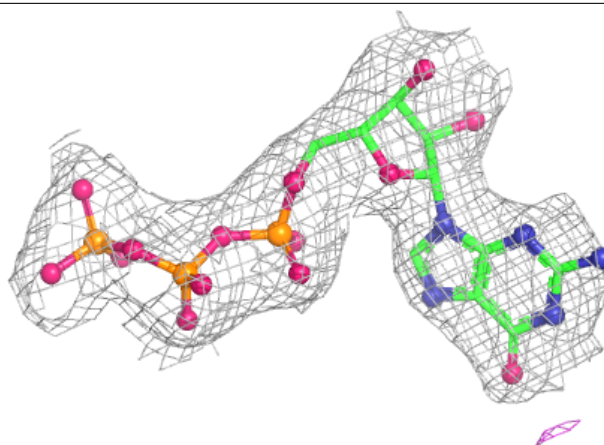
**Electron density around GTP C 1001:**

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



Electron density around GTP A 1001:

$2mF_o-DF_c$ (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.