Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 02:30 am GMT

PDB ID	:	2JAS
Title	:	Structure of deoxyadenosine kinase from M.mycoides with bound dATP
Authors	:	Welin, M.; Wang, L.; Eriksson, S.; Eklund, H.
Deposited on	:	2006-11-30
Resolution	:	2.70 Å(reported)

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

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

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

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

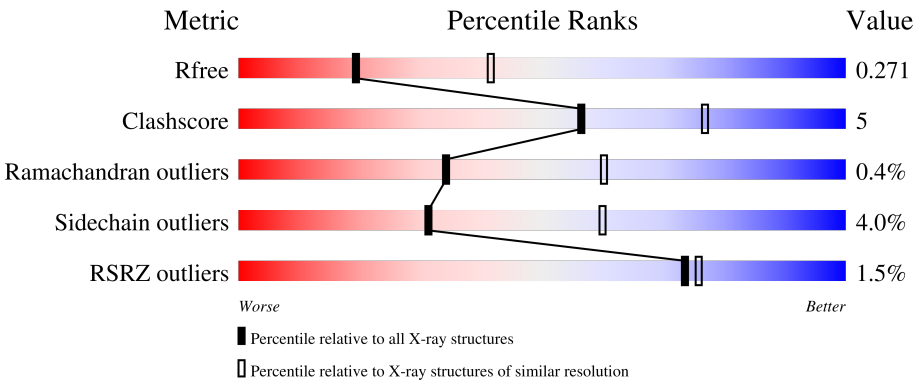
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	206	79% 16% 6%
1	B	206	2% 80% 13% • 6%
1	C	206	83% 9% • 5%
1	D	206	2% 83% 9% • 7%
1	E	206	2% 84% 9% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	206	78% 13% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9917 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.

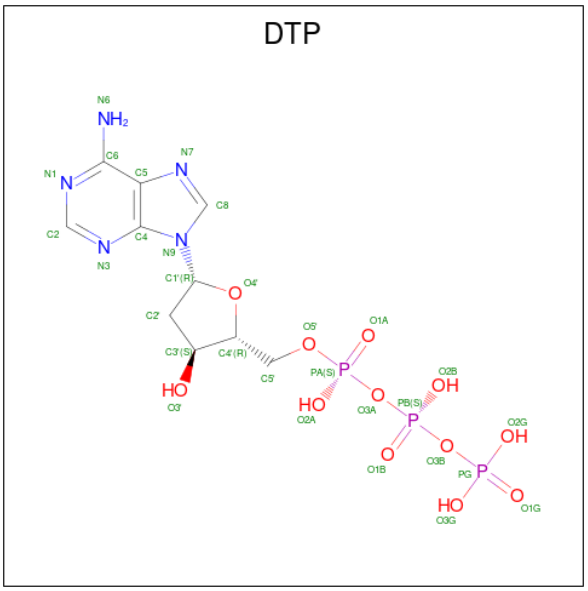
- Molecule 1 is a protein called DEOXYGUANOSINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1623	1054	256	308	5	0	0	0
1	B	193	1614	1048	254	307	5	0	0	0
1	C	195	1632	1060	258	309	5	0	0	0
1	D	192	1608	1045	253	305	5	0	0	0
1	E	194	1622	1054	255	308	5	0	0	0
1	F	193	1616	1048	256	307	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q93IG4
B	0	HIS	-	expression tag	UNP Q93IG4
C	0	HIS	-	expression tag	UNP Q93IG4
D	0	HIS	-	expression tag	UNP Q93IG4
E	0	HIS	-	expression tag	UNP Q93IG4
F	0	HIS	-	expression tag	UNP Q93IG4

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	2	Total O 2 2	0	0
4	C	5	Total O 5 5	0	0
4	D	1	Total O 1 1	0	0
4	E	3	Total O 3 3	0	0
4	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

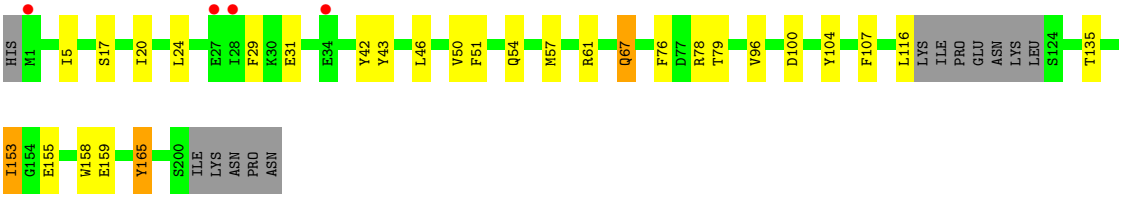
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DEOXYGUANOSINE KINASE

Chain A:

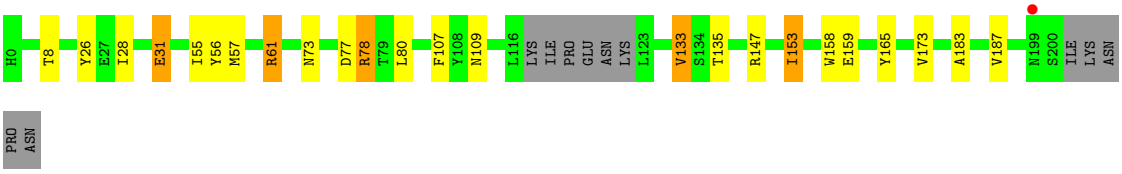
• Molecule 1: DEOXYGUANOSINE KINASE

Chain B:



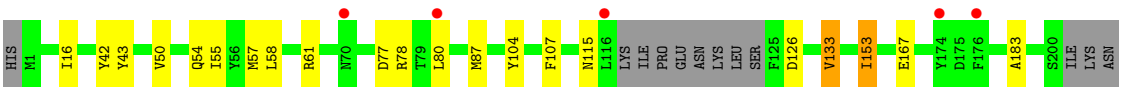
• Molecule 1: DEOXYGUANOSINE KINASE

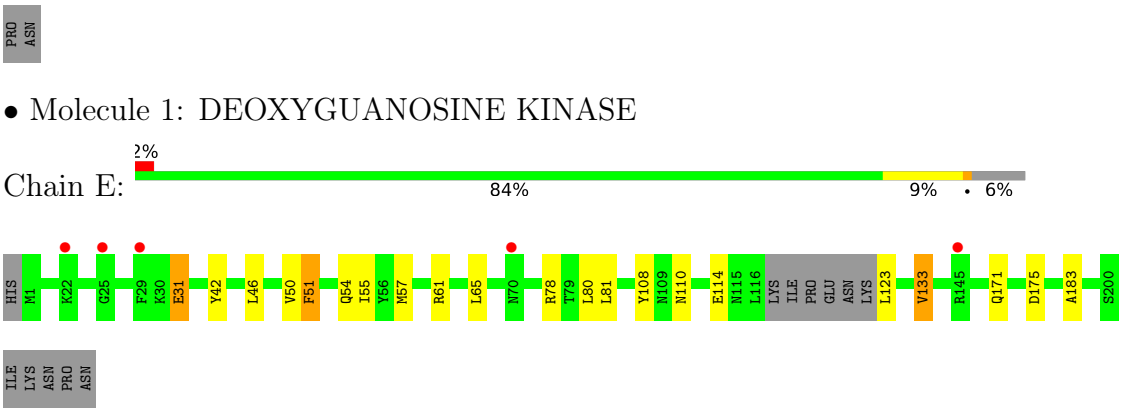
Chain C:



• Molecule 1: DEOXYGUANOSINE KINASE

Chain D:




PRO
ASN
• Molecule 1: DEOXYGUANOSINE KINASE
Chain E:
2%
84%
9%
6%
HIS M1 K22 G25 F29 K30 E31 Y42 L46 V50 F51 Q54 I55 Y56 M57 R61 L65 N70 R78 T79 L80 L81 Y108 N109 N110 E114 N115 L116 LYS ILE PRO GLU ASN LYS L123 V133 R145 Q171 D175 A183 S200
ILE
LYS
ASN
PRO
ASN
• Molecule 1: DEOXYGUANOSINE KINASE
Chain F:
78%
13%
6%
HO I20 E31 Y42 Y43 T49 V50 Q54 I55 Y56 M57 L58 R61 S62 L65 K69 E72 R78 T79 L80 M87 Y104 I105 D106 F107 V111 N115 LEU LYS ILE PRO GLU ASN LYS LEU S124 R132 V133 S134 T135 I153 W158 E159
Y165 E166 A183 I194 S200 ILE LYS ASN PRO ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.84Å 100.85Å 109.49Å 90.00° 124.58° 90.00°	Depositor
Resolution (Å)	47.00 – 2.70 47.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.00-2.70) 99.7 (47.11-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233 , 0.274 0.233 , 0.271	Depositor DCC
R_{free} test set	2373 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9917	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DTP

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	0.43	0/1653	0.51	0/2225
1	B	0.41	0/1644	0.52	0/2214
1	C	0.43	0/1663	0.57	0/2240
1	D	0.40	0/1638	0.54	0/2206
1	E	0.42	0/1652	0.53	0/2225
1	F	0.40	0/1647	0.54	0/2218
All	All	0.42	0/9897	0.53	0/13328

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1623	0	1633	20	0
1	B	1614	0	1620	19	0
1	C	1632	0	1638	12	0
1	D	1608	0	1615	13	0
1	E	1622	0	1631	13	0
1	F	1616	0	1616	26	0
2	A	30	0	12	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	12	3	0
2	C	30	0	12	1	0
2	D	30	0	12	2	0
2	E	30	0	12	1	0
2	F	30	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	5	0	0	1	0
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
All	All	9917	0	9825	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (99) 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)
1:F:31:GLU:HG2	1:F:61:ARG:HH12	1.11	1.09
1:E:55:ILE:HD11	1:F:55:ILE:HD11	1.42	0.99
1:A:133:VAL:HG13	1:A:183:ALA:HB3	1.64	0.77
1:C:55:ILE:HD11	1:D:55:ILE:HD11	1.69	0.74
1:A:96:VAL:HG13	1:A:100:ASP:HB2	1.70	0.74
1:F:31:GLU:HG2	1:F:61:ARG:NH1	1.96	0.73
1:E:133:VAL:HG13	1:E:183:ALA:HB3	1.71	0.72
1:A:56:TYR:HD2	1:A:57:MET:HE3	1.53	0.72
1:B:46:LEU:O	1:B:50:VAL:HG23	1.92	0.70
1:F:153:ILE:H	1:F:153:ILE:HD13	1.56	0.69
1:E:51:PHE:HE2	1:F:55:ILE:HD13	1.60	0.66
1:D:78:ARG:NH2	2:D:1201:DTP:O1A	2.29	0.65
1:E:46:LEU:O	1:E:50:VAL:HG23	1.98	0.64
1:F:43:TYR:CD2	1:F:153:ILE:HD12	2.35	0.62
1:F:78:ARG:NH2	2:F:1201:DTP:H5'1	2.15	0.61
1:C:153:ILE:H	1:C:153:ILE:HD13	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:GLU:CG	1:F:61:ARG:HH12	2.00	0.61
1:C:153:ILE:HD11	1:C:158:TRP:CZ2	2.37	0.60
1:D:153:ILE:H	1:D:153:ILE:HD13	1.66	0.59
1:C:133:VAL:HG13	1:C:183:ALA:HB3	1.84	0.59
1:F:69:LYS:HZ3	1:F:124:SER:N	2.01	0.58
1:B:42:TYR:CZ	2:B:1202:DTP:H2	2.39	0.57
1:B:153:ILE:H	1:B:153:ILE:HD13	1.70	0.57
1:A:46:LEU:O	1:A:50:VAL:HG23	2.04	0.57
1:A:57:MET:O	1:A:61:ARG:HG2	2.04	0.57
1:B:20:ILE:HG23	1:B:24:LEU:HD13	1.88	0.56
1:A:77:ASP:O	1:A:78:ARG:HB3	2.04	0.55
1:B:96:VAL:HG13	1:B:100:ASP:HB2	1.88	0.55
1:E:81:LEU:HA	1:E:108:TYR:OH	2.06	0.55
1:A:54:GLN:HE22	1:A:83:ASP:HB3	1.71	0.54
1:A:107:PHE:CZ	1:B:107:PHE:HZ	2.24	0.54
1:F:87:MET:HG2	1:F:104:TYR:CD2	2.43	0.54
1:E:31:GLU:HG2	1:E:61:ARG:HH12	1.72	0.54
1:F:133:VAL:HG13	1:F:183:ALA:HB3	1.89	0.53
1:B:135:THR:HG21	1:B:159:GLU:HG3	1.90	0.53
1:F:153:ILE:H	1:F:153:ILE:CD1	2.20	0.53
1:B:78:ARG:HG3	1:B:79:THR:N	2.24	0.53
1:F:78:ARG:HG3	1:F:79:THR:N	2.24	0.53
1:D:57:MET:O	1:D:61:ARG:HG2	2.08	0.53
1:B:51:PHE:HZ	1:B:100:ASP:HB3	1.75	0.52
1:D:87:MET:HG2	1:D:104:TYR:CD2	2.44	0.52
1:B:43:TYR:CD2	1:B:153:ILE:HD12	2.44	0.52
1:F:43:TYR:HD2	1:F:153:ILE:HD12	1.73	0.52
1:D:133:VAL:HG13	1:D:183:ALA:HB3	1.92	0.52
1:E:65:LEU:HD11	1:E:123:LEU:HD23	1.92	0.51
1:A:132:ARG:NH2	1:A:166:GLU:OE2	2.42	0.51
1:B:57:MET:O	1:B:61:ARG:HG2	2.10	0.51
1:A:153:ILE:HD11	1:A:158:TRP:CZ2	2.45	0.50
1:B:153:ILE:H	1:B:153:ILE:CD1	2.24	0.50
1:A:133:VAL:CG1	1:A:183:ALA:HB3	2.38	0.50
1:D:153:ILE:H	1:D:153:ILE:CD1	2.25	0.49
1:E:31:GLU:HG2	1:E:61:ARG:NH1	2.27	0.49
1:E:50:VAL:O	1:E:54:GLN:HG2	2.13	0.49
2:B:1202:DTP:H8	2:B:1202:DTP:H5'2	1.95	0.48
1:A:109:ASN:HD22	1:A:113:LEU:HD12	1.78	0.48
1:E:57:MET:O	1:E:61:ARG:HG2	2.13	0.48
1:D:42:TYR:CZ	2:D:1201:DTP:H2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HG3	1:C:80:LEU:HA	1.96	0.47
1:B:54:GLN:NE2	1:B:104:TYR:OH	2.47	0.47
1:D:54:GLN:O	1:D:58:LEU:HG	2.15	0.47
1:D:77:ASP:O	1:D:78:ARG:HB3	2.13	0.47
1:A:56:TYR:CD2	1:A:57:MET:HE3	2.41	0.47
1:C:26:TYR:CD2	1:C:73:ASN:HB3	2.49	0.47
1:B:153:ILE:HD11	1:B:158:TRP:CZ2	2.49	0.47
1:A:31:GLU:HA	1:A:64:GLN:HE22	1.80	0.47
1:D:43:TYR:CD2	1:D:153:ILE:HD12	2.50	0.47
1:C:8:THR:HG22	4:C:2001:HOH:O	2.14	0.46
1:C:56:TYR:HD2	1:C:57:MET:HE3	1.79	0.46
1:A:42:TYR:CZ	2:A:1201:DTP:H2	2.50	0.46
1:F:135:THR:HG21	1:F:159:GLU:HG3	1.97	0.46
1:A:78:ARG:HG3	1:A:79:THR:N	2.31	0.46
1:C:135:THR:HG21	1:C:159:GLU:HG3	1.97	0.46
1:F:20:ILE:HD11	1:F:194:ILE:HG21	1.98	0.46
1:F:153:ILE:HD11	1:F:158:TRP:CZ2	2.50	0.46
1:E:42:TYR:CZ	2:E:1201:DTP:H2	2.51	0.46
1:F:132:ARG:NH1	1:F:166:GLU:OE2	2.49	0.45
1:C:77:ASP:O	1:C:78:ARG:HB3	2.16	0.44
1:A:76:PHE:HE2	1:A:80:LEU:HD21	1.83	0.44
1:B:43:TYR:OH	2:B:1202:DTP:H2'1	2.18	0.44
1:F:42:TYR:CZ	2:F:1201:DTP:H2	2.53	0.43
1:F:58:LEU:O	1:F:62:SER:HB2	2.18	0.43
1:A:77:ASP:OD2	2:A:1201:DTP:O2B	2.35	0.43
1:C:31:GLU:H	1:C:31:GLU:HG3	1.64	0.43
1:C:107:PHE:CZ	1:D:107:PHE:HZ	2.35	0.43
2:C:1202:DTP:O2A	2:C:1202:DTP:O1B	2.35	0.43
1:D:153:ILE:HD13	1:D:153:ILE:N	2.32	0.43
1:A:65:LEU:O	1:A:69:LYS:HG3	2.19	0.42
1:A:65:LEU:HG	1:A:69:LYS:HE3	2.01	0.42
1:F:54:GLN:O	1:F:58:LEU:HG	2.19	0.42
1:F:107:PHE:O	1:F:111:VAL:HB	2.19	0.42
1:F:65:LEU:HB2	1:F:80:LEU:HD13	2.00	0.42
1:F:57:MET:O	1:F:61:ARG:HG3	2.20	0.41
1:B:5:ILE:HD13	1:B:17:SER:HB3	2.01	0.41
1:B:78:ARG:NH1	1:B:165:TYR:OH	2.54	0.41
1:F:57:MET:HA	1:F:57:MET:HE2	2.02	0.41
1:B:54:GLN:HG2	1:B:104:TYR:HE1	1.86	0.41
1:E:110:ASN:O	1:E:114:GLU:HG3	2.20	0.41
1:B:29:PHE:HE2	1:B:67:GLN:HG3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:PHE:CE2	1:F:55:ILE:HD13	2.48	0.41

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	190/206 (92%)	180 (95%)	9 (5%)	1 (0%)	29	54
1	B	189/206 (92%)	176 (93%)	13 (7%)	0	100	100
1	C	191/206 (93%)	174 (91%)	16 (8%)	1 (0%)	29	54
1	D	188/206 (91%)	173 (92%)	14 (7%)	1 (0%)	29	54
1	E	190/206 (92%)	182 (96%)	7 (4%)	1 (0%)	29	54
1	F	189/206 (92%)	183 (97%)	6 (3%)	0	100	100
All	All	1137/1236 (92%)	1068 (94%)	65 (6%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	D	115	ASN
1	E	78	ARG
1	C	78	ARG

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	181/193 (94%)	178 (98%)	3 (2%)	60	84
1	B	180/193 (93%)	173 (96%)	7 (4%)	32	61
1	C	182/193 (94%)	172 (94%)	10 (6%)	21	46
1	D	179/193 (93%)	172 (96%)	7 (4%)	32	61
1	E	181/193 (94%)	175 (97%)	6 (3%)	38	67
1	F	180/193 (93%)	170 (94%)	10 (6%)	21	45
All	All	1083/1158 (94%)	1040 (96%)	43 (4%)	31	60

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	165	TYR
1	A	200	SER
1	B	31	GLU
1	B	67	GLN
1	B	76	PHE
1	B	116	LEU
1	B	153	ILE
1	B	155	GLU
1	B	165	TYR
1	C	28	ILE
1	C	31	GLU
1	C	61	ARG
1	C	109	ASN
1	C	133	VAL
1	C	147	ARG
1	C	153	ILE
1	C	165	TYR
1	C	173	VAL
1	C	187	VAL
1	D	16	ILE
1	D	50	VAL
1	D	80	LEU
1	D	126	ASP
1	D	133	VAL
1	D	153	ILE
1	D	167	GLU
1	E	31	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	51	PHE
1	E	80	LEU
1	E	133	VAL
1	E	171	GLN
1	E	175	ASP
1	F	31	GLU
1	F	49	THR
1	F	50	VAL
1	F	54	GLN
1	F	87	MET
1	F	106	ASP
1	F	124	SER
1	F	133	VAL
1	F	153	ILE
1	F	165	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	109	ASN
1	B	54	GLN
1	B	199	ASN
1	C	54	GLN
1	C	94	ASN
1	D	98	GLN
1	D	102	ASN
1	D	199	ASN
1	F	109	ASN

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	DTP	F	1201	3	26,32,32	0.89	1 (3%)	30,50,50	1.45	4 (13%)
2	DTP	A	1201	3	26,32,32	0.89	1 (3%)	30,50,50	1.54	6 (20%)
2	DTP	D	1201	3	26,32,32	0.91	1 (3%)	30,50,50	1.45	4 (13%)
2	DTP	E	1201	3	26,32,32	0.91	2 (7%)	30,50,50	1.39	5 (16%)
2	DTP	B	1202	3	26,32,32	0.93	1 (3%)	30,50,50	1.49	6 (20%)
2	DTP	C	1202	3	26,32,32	0.90	1 (3%)	30,50,50	1.52	6 (20%)

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
2	DTP	F	1201	3	-	9/18/34/34	0/3/3/3
2	DTP	A	1201	3	-	10/18/34/34	0/3/3/3
2	DTP	D	1201	3	-	6/18/34/34	0/3/3/3
2	DTP	E	1201	3	-	2/18/34/34	0/3/3/3
2	DTP	B	1202	3	-	9/18/34/34	0/3/3/3
2	DTP	C	1202	3	-	1/18/34/34	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1202	DTP	C5-C4	2.69	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	DTP	C5-C4	2.55	1.47	1.40
2	E	1201	DTP	C5-C4	2.54	1.47	1.40
2	F	1201	DTP	C5-C4	2.52	1.47	1.40
2	B	1202	DTP	C5-C4	2.48	1.47	1.40
2	A	1201	DTP	C5-C4	2.33	1.47	1.40
2	E	1201	DTP	C2-N3	2.03	1.35	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1202	DTP	N3-C2-N1	-4.10	122.27	128.68
2	F	1201	DTP	N3-C2-N1	-3.77	122.78	128.68
2	E	1201	DTP	N3-C2-N1	-3.77	122.79	128.68
2	A	1201	DTP	N3-C2-N1	-3.75	122.81	128.68
2	D	1201	DTP	PA-O3A-PB	-3.48	120.87	132.83
2	B	1202	DTP	N3-C2-N1	-3.48	123.23	128.68
2	D	1201	DTP	N3-C2-N1	-3.41	123.35	128.68
2	C	1202	DTP	PA-O3A-PB	-3.31	121.48	132.83
2	B	1202	DTP	C4-C5-N7	-3.19	106.07	109.40
2	F	1201	DTP	PA-O3A-PB	-3.15	122.02	132.83
2	A	1201	DTP	PA-O3A-PB	-2.99	122.58	132.83
2	C	1202	DTP	PB-O3B-PG	-2.80	123.20	132.83
2	E	1201	DTP	PA-O3A-PB	-2.75	123.38	132.83
2	B	1202	DTP	PA-O3A-PB	-2.69	123.58	132.83
2	D	1201	DTP	C4-C5-N7	-2.55	106.74	109.40
2	A	1201	DTP	C4-C5-N7	-2.50	106.80	109.40
2	F	1201	DTP	C4-C5-N7	-2.49	106.80	109.40
2	A	1201	DTP	PB-O3B-PG	-2.45	124.42	132.83
2	E	1201	DTP	C4-C5-N7	-2.37	106.93	109.40
2	C	1202	DTP	C4-C5-N7	-2.37	106.93	109.40
2	C	1202	DTP	C2-N1-C6	2.34	122.75	118.75
2	A	1201	DTP	O3B-PG-O1G	-2.24	98.78	111.19
2	F	1201	DTP	C2-N1-C6	2.19	122.50	118.75
2	B	1202	DTP	PB-O3B-PG	-2.12	125.54	132.83
2	D	1201	DTP	C2-N1-C6	2.12	122.38	118.75
2	C	1202	DTP	O3G-PG-O2G	2.12	115.75	107.64
2	E	1201	DTP	PB-O3B-PG	-2.08	125.70	132.83
2	E	1201	DTP	C2-N1-C6	2.04	122.24	118.75
2	B	1202	DTP	O3G-PG-O2G	2.03	115.40	107.64
2	A	1201	DTP	C2-N1-C6	2.01	122.19	118.75
2	B	1202	DTP	O2B-PB-O1B	2.00	122.15	112.24

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	DTP	PB-O3B-PG-O2G
2	A	1201	DTP	C5'-O5'-PA-O2A
2	A	1201	DTP	C5'-O5'-PA-O3A
2	A	1201	DTP	C3'-C4'-C5'-O5'
2	B	1202	DTP	PB-O3B-PG-O2G
2	B	1202	DTP	C5'-O5'-PA-O3A
2	B	1202	DTP	O4'-C4'-C5'-O5'
2	D	1201	DTP	C5'-O5'-PA-O1A
2	D	1201	DTP	C5'-O5'-PA-O2A
2	F	1201	DTP	PB-O3B-PG-O2G
2	F	1201	DTP	C5'-O5'-PA-O2A
2	F	1201	DTP	C5'-O5'-PA-O3A
2	A	1201	DTP	O4'-C4'-C5'-O5'
2	B	1202	DTP	C3'-C4'-C5'-O5'
2	F	1201	DTP	C3'-C4'-C5'-O5'
2	F	1201	DTP	O4'-C4'-C5'-O5'
2	B	1202	DTP	PA-O3A-PB-O1B
2	B	1202	DTP	C4'-C5'-O5'-PA
2	F	1201	DTP	C4'-C5'-O5'-PA
2	B	1202	DTP	C5'-O5'-PA-O2A
2	D	1201	DTP	C4'-C5'-O5'-PA
2	C	1202	DTP	PB-O3A-PA-O2A
2	E	1201	DTP	PB-O3A-PA-O2A
2	A	1201	DTP	C4'-C5'-O5'-PA
2	A	1201	DTP	PB-O3A-PA-O1A
2	F	1201	DTP	PA-O3A-PB-O1B
2	F	1201	DTP	PB-O3B-PG-O1G
2	A	1201	DTP	PB-O3B-PG-O3G
2	B	1202	DTP	PB-O3B-PG-O3G
2	D	1201	DTP	PB-O3B-PG-O3G
2	F	1201	DTP	PB-O3B-PG-O3G
2	D	1201	DTP	C5'-O5'-PA-O3A
2	A	1201	DTP	PB-O3A-PA-O2A
2	B	1202	DTP	PA-O3A-PB-O2B
2	E	1201	DTP	PG-O3B-PB-O2B
2	D	1201	DTP	O4'-C4'-C5'-O5'
2	A	1201	DTP	PB-O3B-PG-O1G

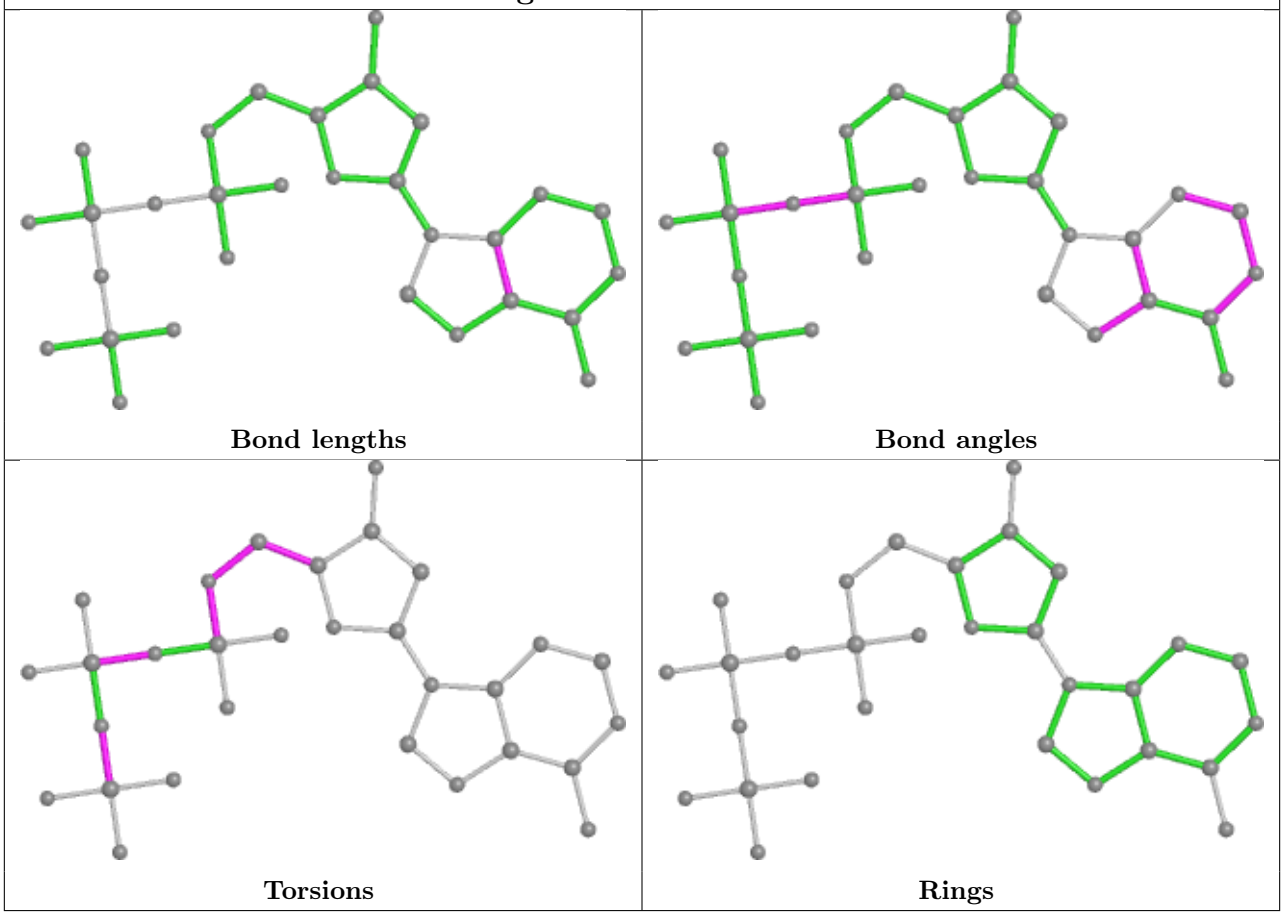
There are no ring outliers.

6 monomers are involved in 11 short contacts:

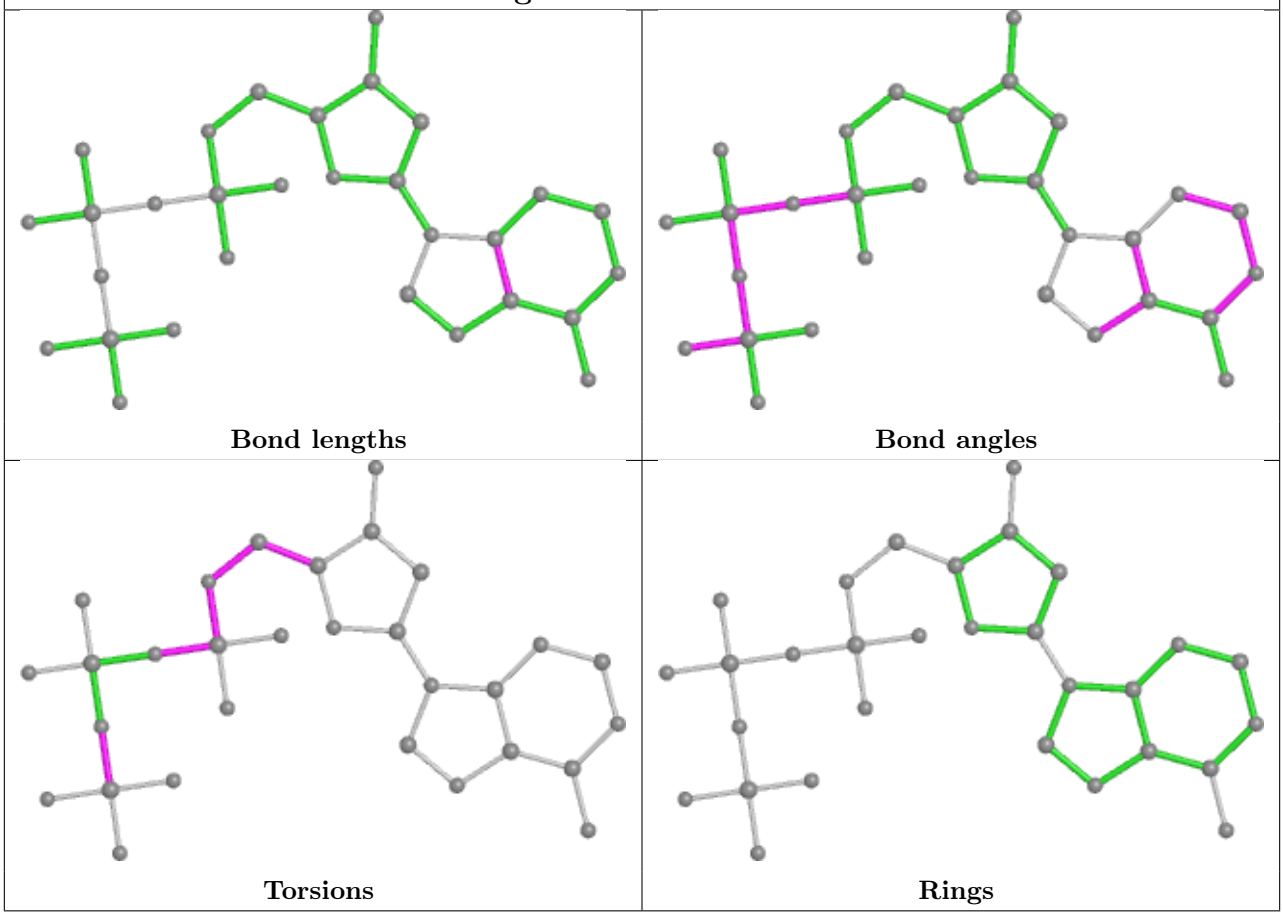
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1201	DTP	2	0
2	A	1201	DTP	2	0
2	D	1201	DTP	2	0
2	E	1201	DTP	1	0
2	B	1202	DTP	3	0
2	C	1202	DTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

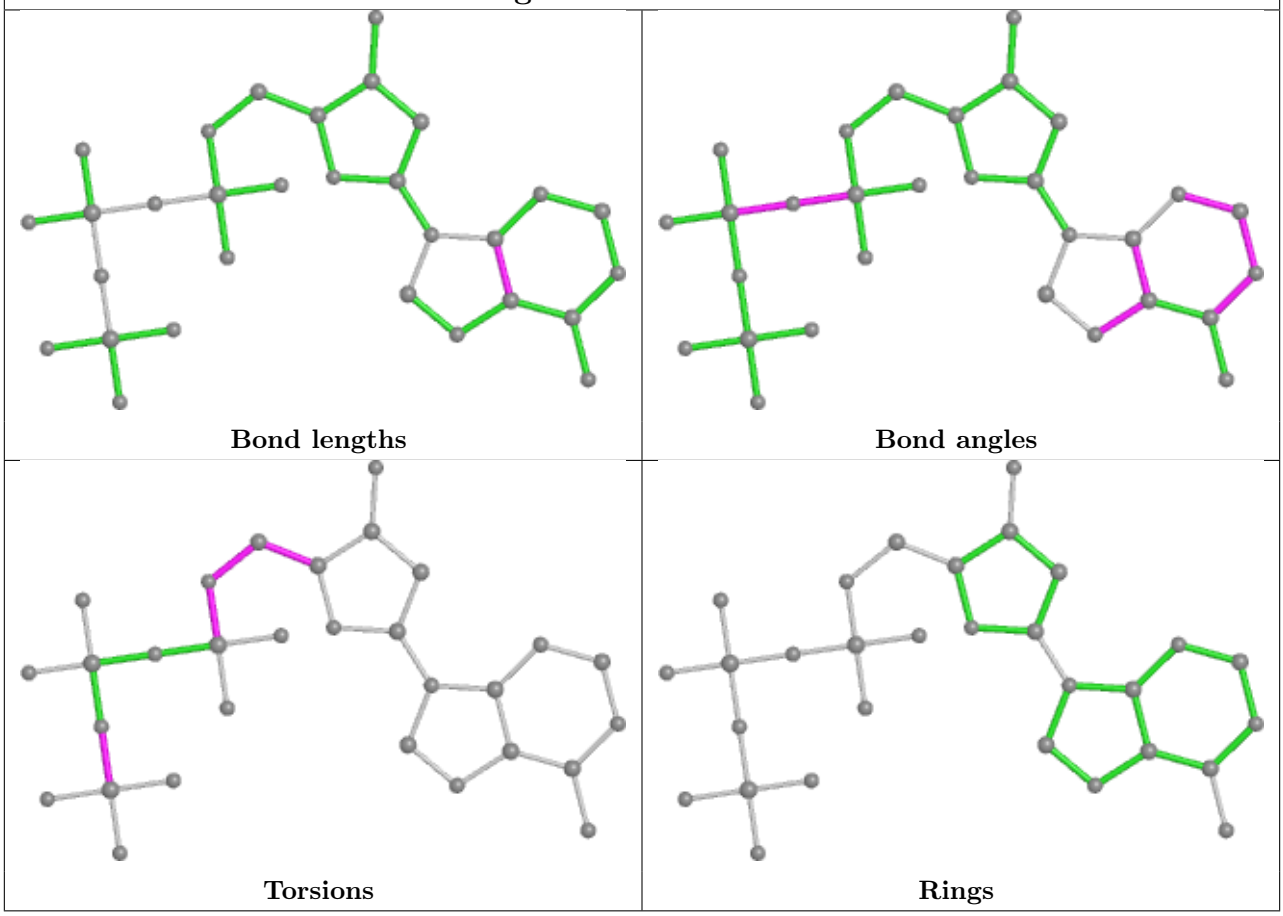
Ligand DTP F 1201



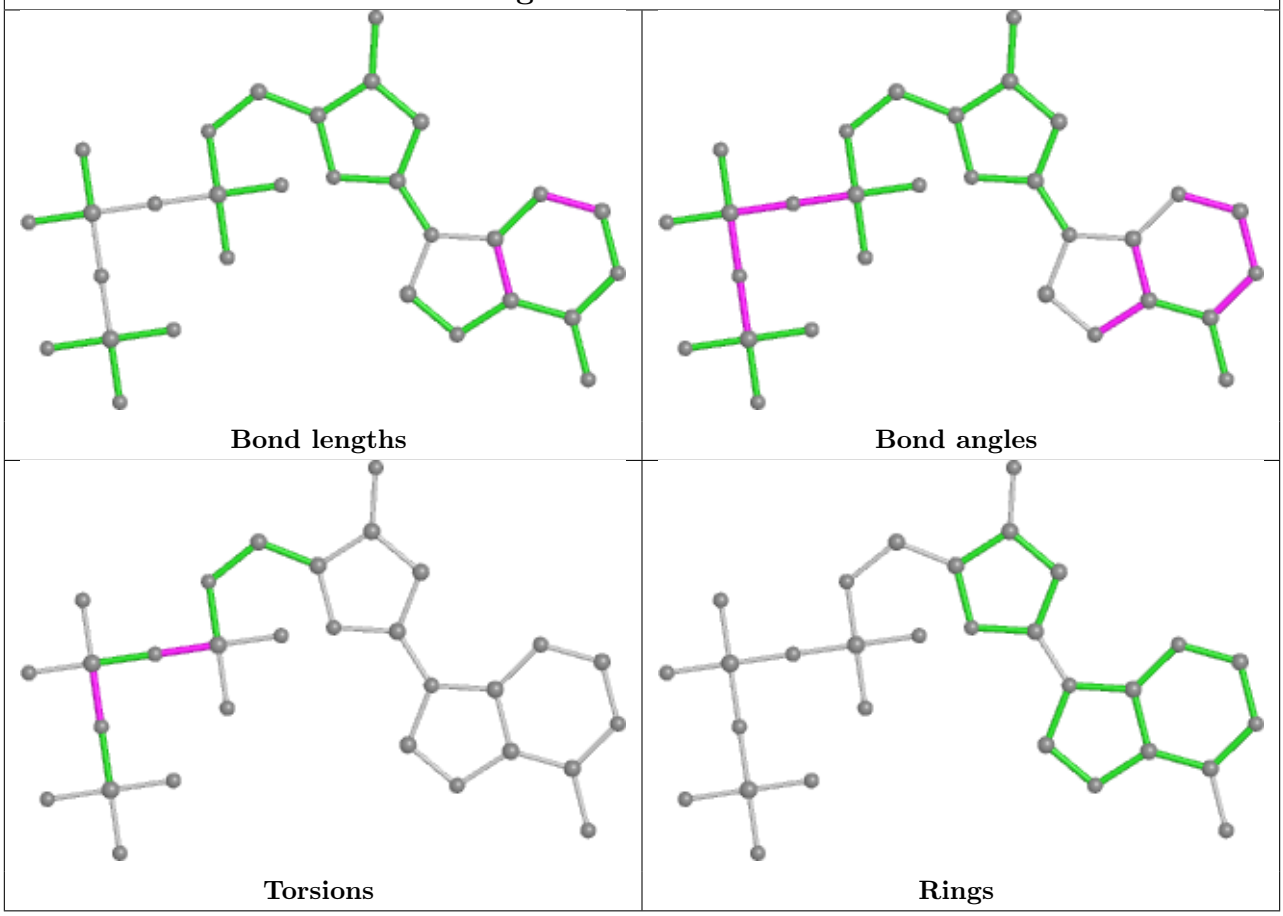
Ligand DTP A 1201



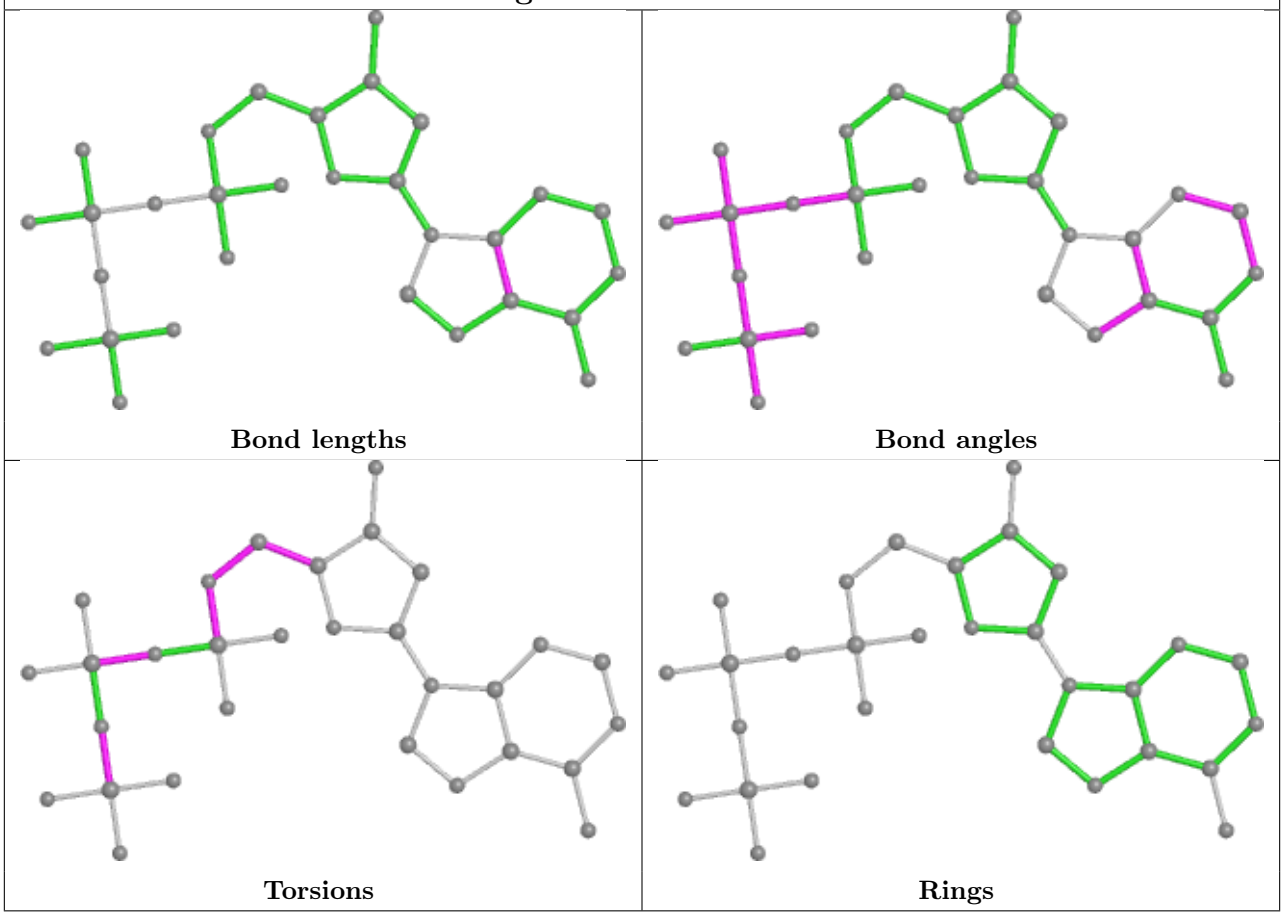
Ligand DTP D 1201



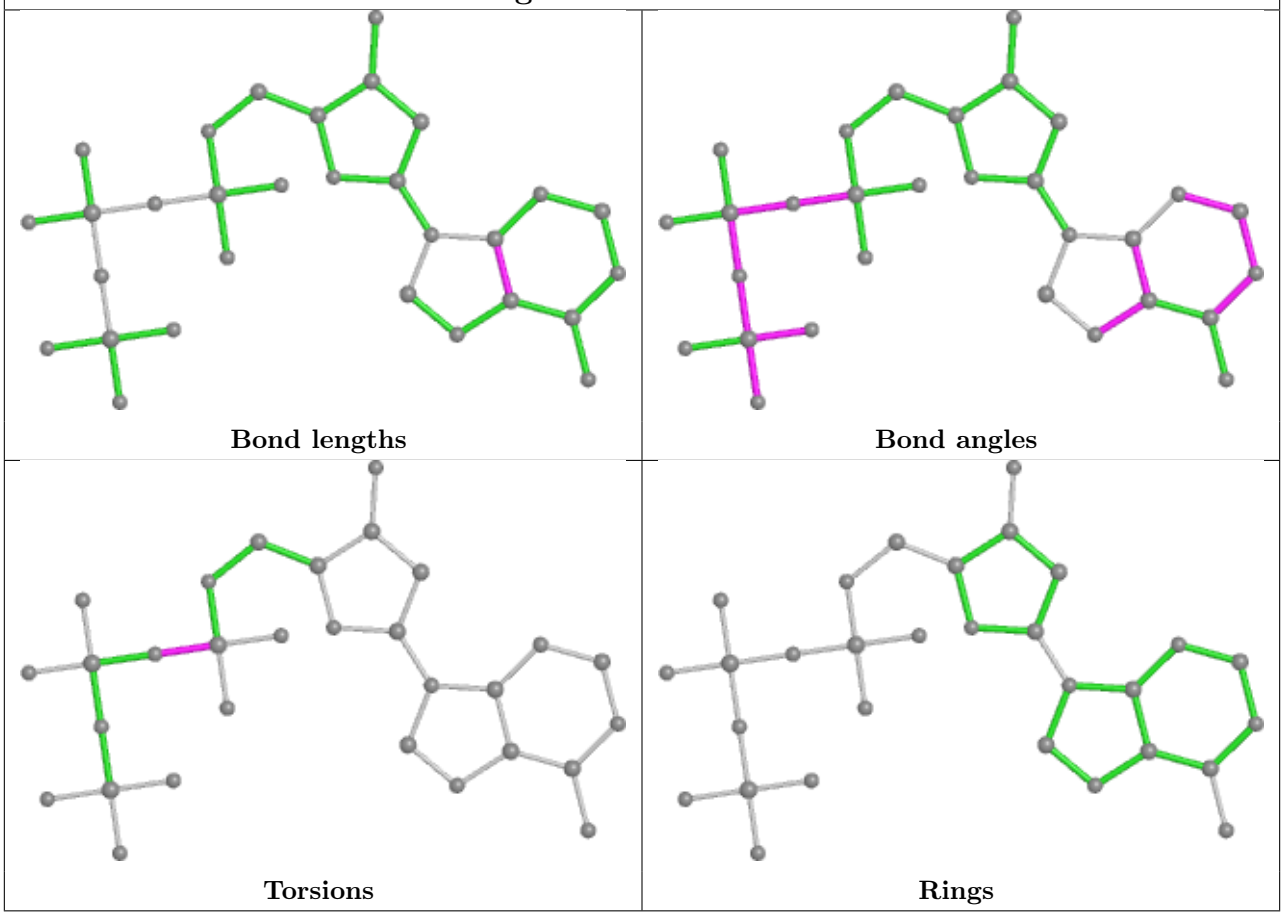
Ligand DTP E 1201



Ligand DTP B 1202



Ligand DTP C 1202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	194/206 (94%)	-0.24	1 (0%)	91	92	34, 39, 46, 55	0
1	B	193/206 (93%)	-0.09	4 (2%)	63	65	34, 39, 47, 54	0
1	C	195/206 (94%)	-0.27	1 (0%)	91	92	34, 39, 49, 51	0
1	D	192/206 (93%)	0.00	5 (2%)	56	57	34, 39, 46, 54	0
1	E	194/206 (94%)	0.02	5 (2%)	56	57	32, 41, 49, 54	0
1	F	193/206 (93%)	-0.16	1 (0%)	91	92	34, 39, 48, 52	0
All	All	1161/1236 (93%)	-0.12	17 (1%)	73	76	32, 39, 48, 55	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	ASN	4.3
1	D	80	LEU	3.6
1	D	174	TYR	3.4
1	D	116	LEU	2.7
1	E	22	LYS	2.6
1	D	176	PHE	2.5
1	F	72	GLU	2.4
1	E	25	GLY	2.4
1	E	145	ARG	2.4
1	A	66	LYS	2.4
1	B	27	GLU	2.3
1	B	1	MET	2.2
1	C	199	ASN	2.2
1	B	34	GLU	2.2
1	D	70	ASN	2.1
1	B	28	ILE	2.0
1	E	29	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)

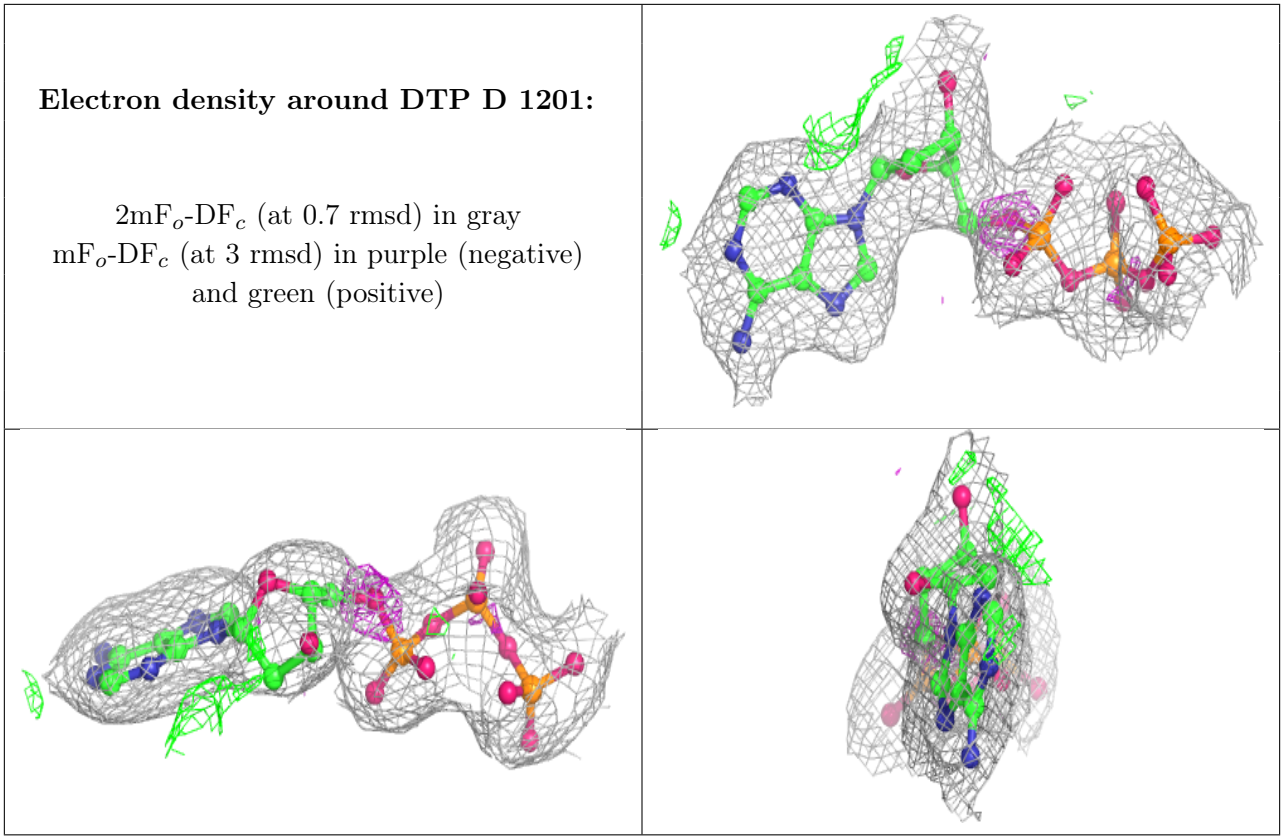
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	1202	1/1	0.73	0.16	67,67,67,67	0
3	MG	C	1201	1/1	0.86	0.29	46,46,46,46	0
3	MG	B	1201	1/1	0.86	0.28	47,47,47,47	0
3	MG	A	1202	1/1	0.89	0.19	44,44,44,44	0
3	MG	E	1202	1/1	0.90	0.22	60,60,60,60	0
3	MG	F	1202	1/1	0.94	0.16	46,46,46,46	0
2	DTP	D	1201	30/30	0.95	0.11	36,42,46,47	0
2	DTP	B	1202	30/30	0.96	0.10	33,35,38,39	0
2	DTP	A	1201	30/30	0.97	0.10	34,44,45,46	0
2	DTP	E	1201	30/30	0.97	0.11	37,41,48,48	0
2	DTP	F	1201	30/30	0.97	0.10	40,43,46,47	0
2	DTP	C	1202	30/30	0.98	0.09	26,28,32,33	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.

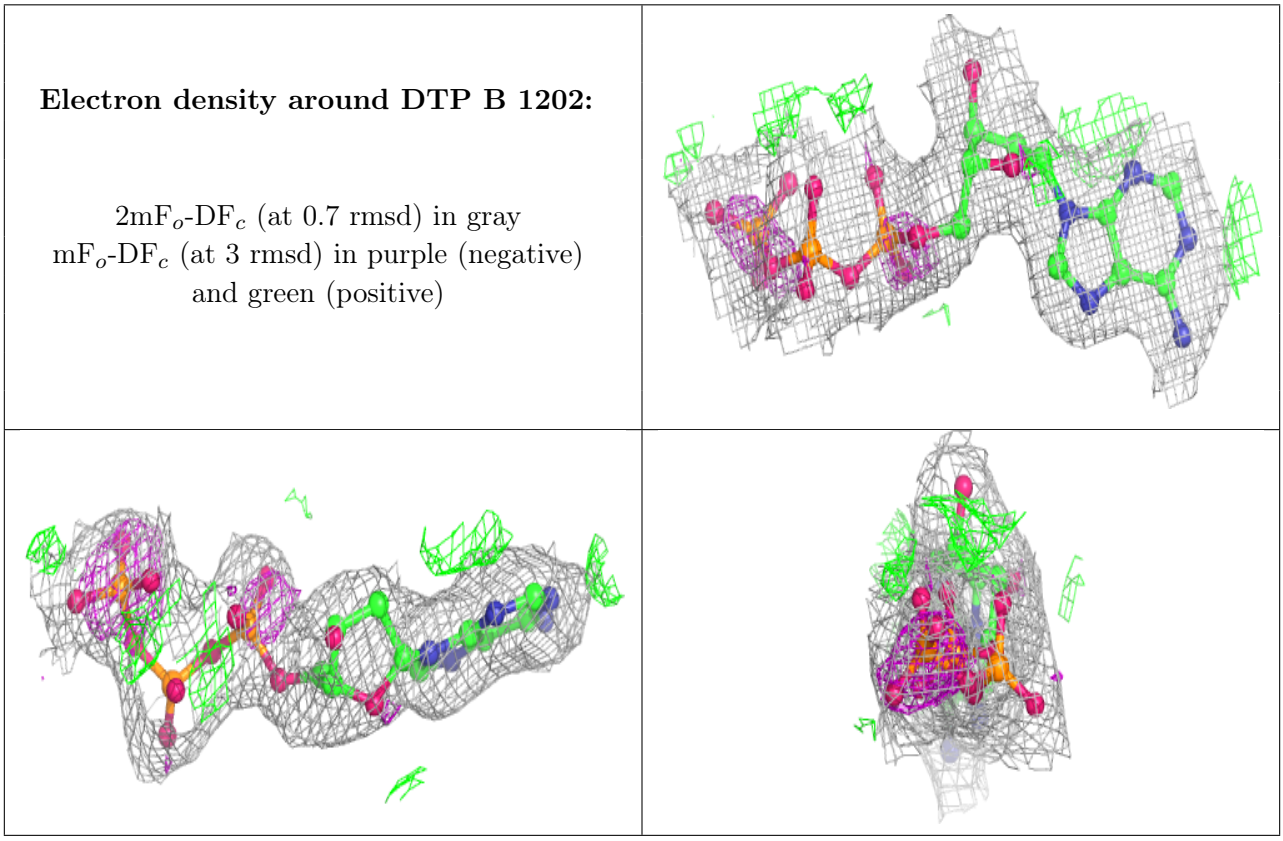
Electron density around DTP D 1201:

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



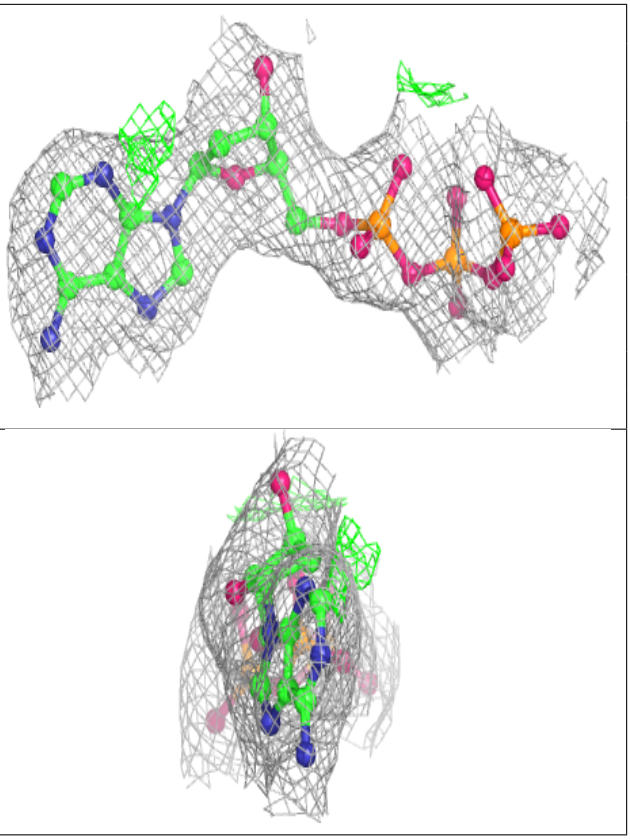
Electron density around DTP B 1202:

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



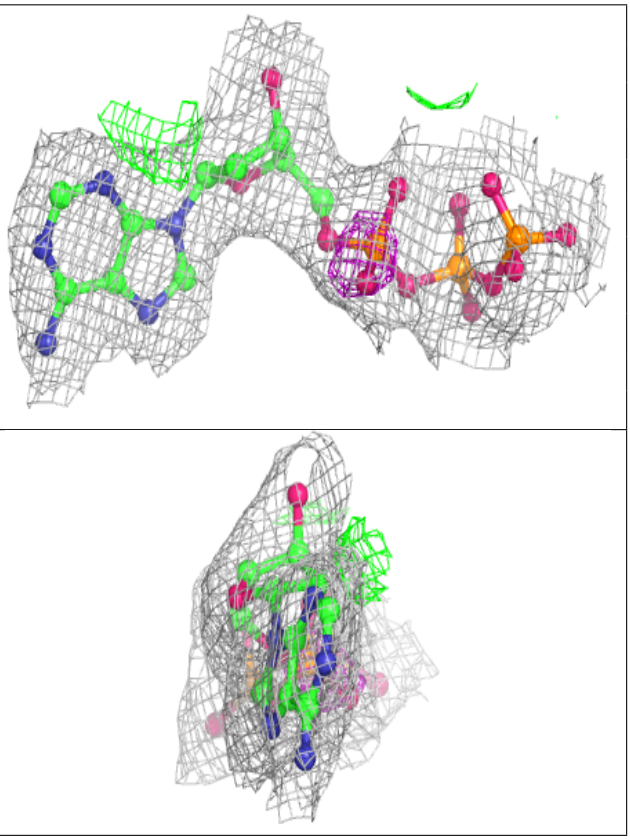
Electron density around DTP A 1201:

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



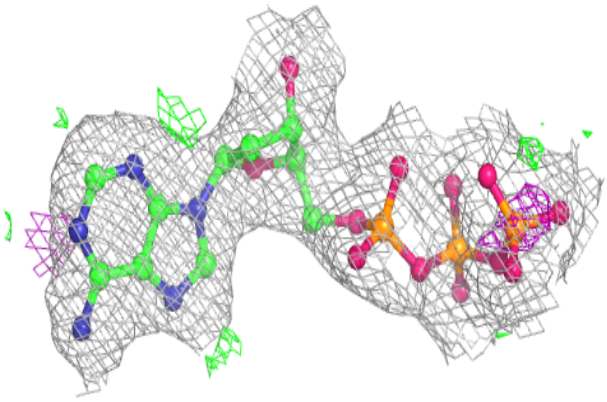
Electron density around DTP E 1201:

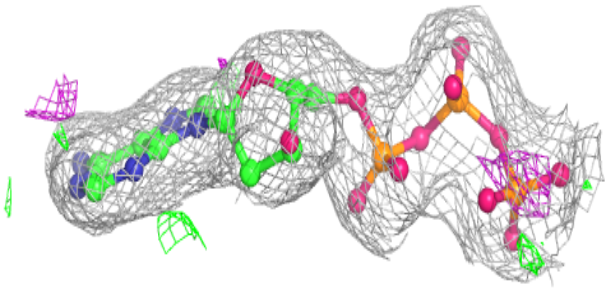
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

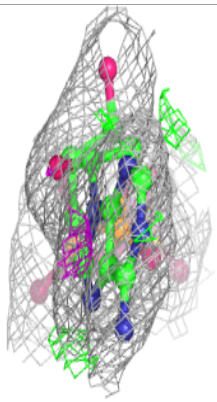


Electron density around DTP F 1201:

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

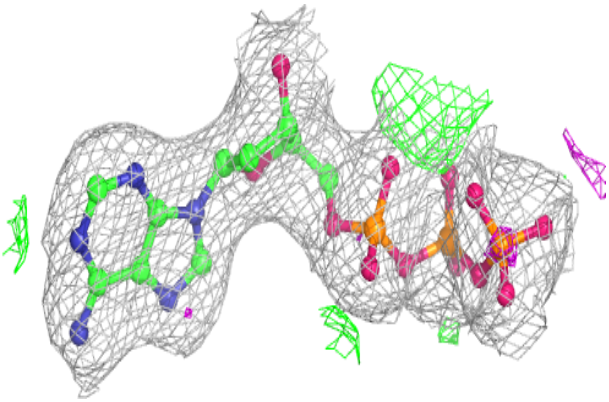


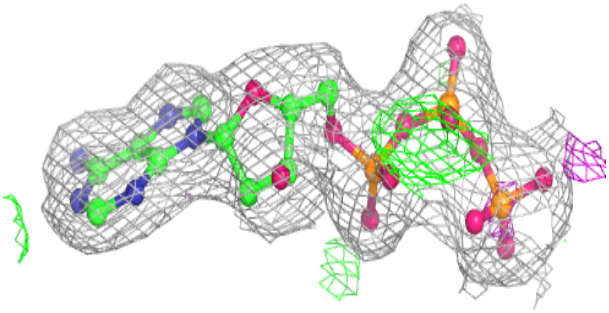


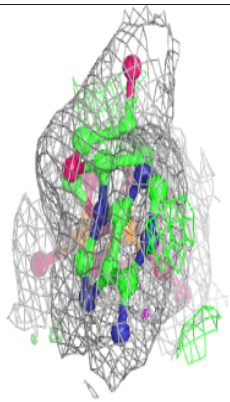


Electron density around DTP C 1202:

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







6.5 Other polymers (i)

There are no such residues in this entry.