Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 02:54 PM EDT

PDB ID	:	4LRL
Title	:	Structure of an Enterococcus Faecalis HD-domain protein complexed with dGTP and dTTP
Authors	:	Vorontsov, I.I.; Minasov, G.; Shuvalova, L.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2013-07-19
Resolution	:	2.35 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:

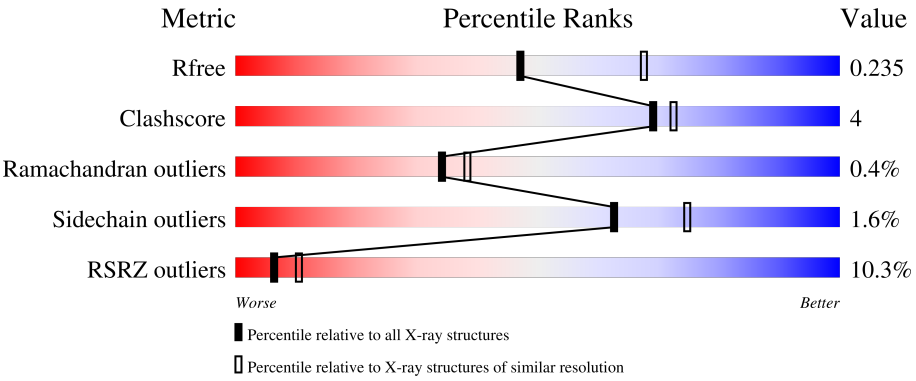
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	480	5% 86% 8% 6%
1	B	480	8% 81% 12% 7%
1	C	480	6% 85% 10% 5%
1	D	480	19% 80% 11% 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15805 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 HD domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	6	0
			3751	2404	636	698	13			
1	B	445	Total	C	N	O	S	0	5	0
			3688	2370	622	683	13			
1	C	455	Total	C	N	O	S	0	5	0
			3777	2422	641	702	12			
1	D	439	Total	C	N	O	S	0	3	0
			3631	2329	611	678	13			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q836G9
A	-22	HIS	-	expression tag	UNP Q836G9
A	-21	HIS	-	expression tag	UNP Q836G9
A	-20	HIS	-	expression tag	UNP Q836G9
A	-19	HIS	-	expression tag	UNP Q836G9
A	-18	HIS	-	expression tag	UNP Q836G9
A	-17	HIS	-	expression tag	UNP Q836G9
A	-16	SER	-	expression tag	UNP Q836G9
A	-15	SER	-	expression tag	UNP Q836G9
A	-14	GLY	-	expression tag	UNP Q836G9
A	-13	VAL	-	expression tag	UNP Q836G9
A	-12	ASP	-	expression tag	UNP Q836G9
A	-11	LEU	-	expression tag	UNP Q836G9
A	-10	GLY	-	expression tag	UNP Q836G9
A	-9	THR	-	expression tag	UNP Q836G9
A	-8	GLU	-	expression tag	UNP Q836G9
A	-7	ASN	-	expression tag	UNP Q836G9
A	-6	LEU	-	expression tag	UNP Q836G9
A	-5	TYR	-	expression tag	UNP Q836G9
A	-4	PHE	-	expression tag	UNP Q836G9
A	-3	GLN	-	expression tag	UNP Q836G9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q836G9
A	-1	ASN	-	expression tag	UNP Q836G9
A	0	ALA	-	expression tag	UNP Q836G9
B	-23	MET	-	expression tag	UNP Q836G9
B	-22	HIS	-	expression tag	UNP Q836G9
B	-21	HIS	-	expression tag	UNP Q836G9
B	-20	HIS	-	expression tag	UNP Q836G9
B	-19	HIS	-	expression tag	UNP Q836G9
B	-18	HIS	-	expression tag	UNP Q836G9
B	-17	HIS	-	expression tag	UNP Q836G9
B	-16	SER	-	expression tag	UNP Q836G9
B	-15	SER	-	expression tag	UNP Q836G9
B	-14	GLY	-	expression tag	UNP Q836G9
B	-13	VAL	-	expression tag	UNP Q836G9
B	-12	ASP	-	expression tag	UNP Q836G9
B	-11	LEU	-	expression tag	UNP Q836G9
B	-10	GLY	-	expression tag	UNP Q836G9
B	-9	THR	-	expression tag	UNP Q836G9
B	-8	GLU	-	expression tag	UNP Q836G9
B	-7	ASN	-	expression tag	UNP Q836G9
B	-6	LEU	-	expression tag	UNP Q836G9
B	-5	TYR	-	expression tag	UNP Q836G9
B	-4	PHE	-	expression tag	UNP Q836G9
B	-3	GLN	-	expression tag	UNP Q836G9
B	-2	SER	-	expression tag	UNP Q836G9
B	-1	ASN	-	expression tag	UNP Q836G9
B	0	ALA	-	expression tag	UNP Q836G9
C	-23	MET	-	expression tag	UNP Q836G9
C	-22	HIS	-	expression tag	UNP Q836G9
C	-21	HIS	-	expression tag	UNP Q836G9
C	-20	HIS	-	expression tag	UNP Q836G9
C	-19	HIS	-	expression tag	UNP Q836G9
C	-18	HIS	-	expression tag	UNP Q836G9
C	-17	HIS	-	expression tag	UNP Q836G9
C	-16	SER	-	expression tag	UNP Q836G9
C	-15	SER	-	expression tag	UNP Q836G9
C	-14	GLY	-	expression tag	UNP Q836G9
C	-13	VAL	-	expression tag	UNP Q836G9
C	-12	ASP	-	expression tag	UNP Q836G9
C	-11	LEU	-	expression tag	UNP Q836G9
C	-10	GLY	-	expression tag	UNP Q836G9
C	-9	THR	-	expression tag	UNP Q836G9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q836G9
C	-7	ASN	-	expression tag	UNP Q836G9
C	-6	LEU	-	expression tag	UNP Q836G9
C	-5	TYR	-	expression tag	UNP Q836G9
C	-4	PHE	-	expression tag	UNP Q836G9
C	-3	GLN	-	expression tag	UNP Q836G9
C	-2	SER	-	expression tag	UNP Q836G9
C	-1	ASN	-	expression tag	UNP Q836G9
C	0	ALA	-	expression tag	UNP Q836G9
D	-23	MET	-	expression tag	UNP Q836G9
D	-22	HIS	-	expression tag	UNP Q836G9
D	-21	HIS	-	expression tag	UNP Q836G9
D	-20	HIS	-	expression tag	UNP Q836G9
D	-19	HIS	-	expression tag	UNP Q836G9
D	-18	HIS	-	expression tag	UNP Q836G9
D	-17	HIS	-	expression tag	UNP Q836G9
D	-16	SER	-	expression tag	UNP Q836G9
D	-15	SER	-	expression tag	UNP Q836G9
D	-14	GLY	-	expression tag	UNP Q836G9
D	-13	VAL	-	expression tag	UNP Q836G9
D	-12	ASP	-	expression tag	UNP Q836G9
D	-11	LEU	-	expression tag	UNP Q836G9
D	-10	GLY	-	expression tag	UNP Q836G9
D	-9	THR	-	expression tag	UNP Q836G9
D	-8	GLU	-	expression tag	UNP Q836G9
D	-7	ASN	-	expression tag	UNP Q836G9
D	-6	LEU	-	expression tag	UNP Q836G9
D	-5	TYR	-	expression tag	UNP Q836G9
D	-4	PHE	-	expression tag	UNP Q836G9
D	-3	GLN	-	expression tag	UNP Q836G9
D	-2	SER	-	expression tag	UNP Q836G9
D	-1	ASN	-	expression tag	UNP Q836G9
D	0	ALA	-	expression tag	UNP Q836G9

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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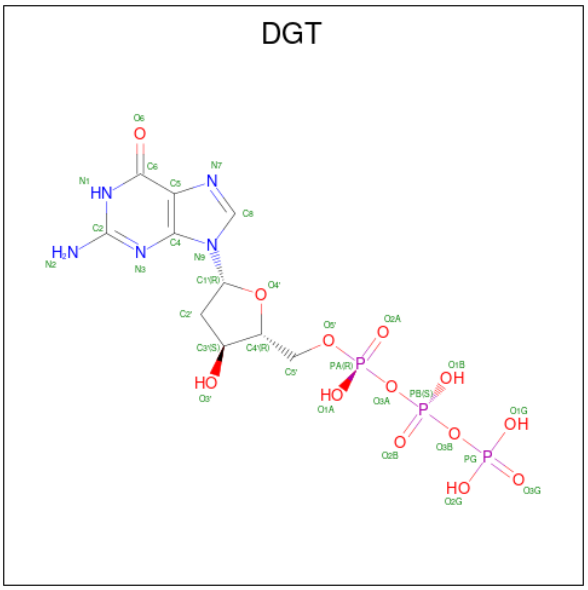
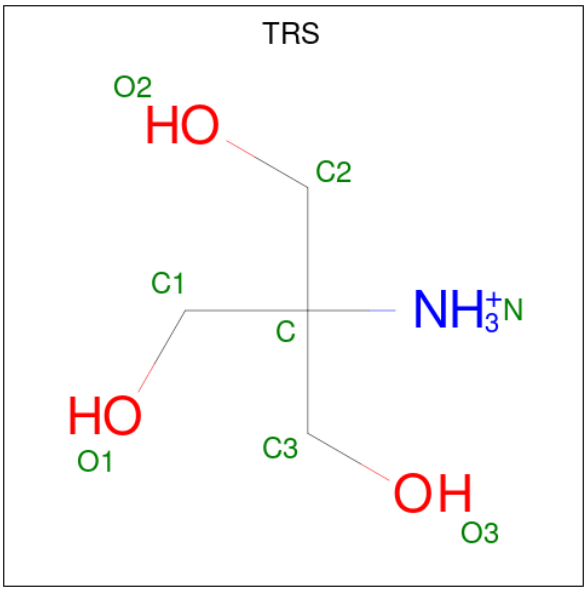
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ni 1 1	0	0

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



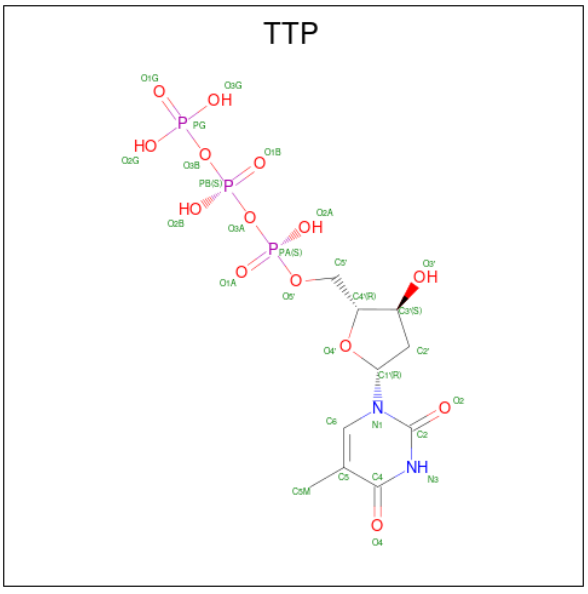
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 10 5 13 3	0	0
3	B	1	Total C N O P 31 10 5 13 3	0	0
3	C	1	Total C N O P 31 10 5 13 3	0	0
3	D	1	Total C N O P 31 10 5 13 3	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



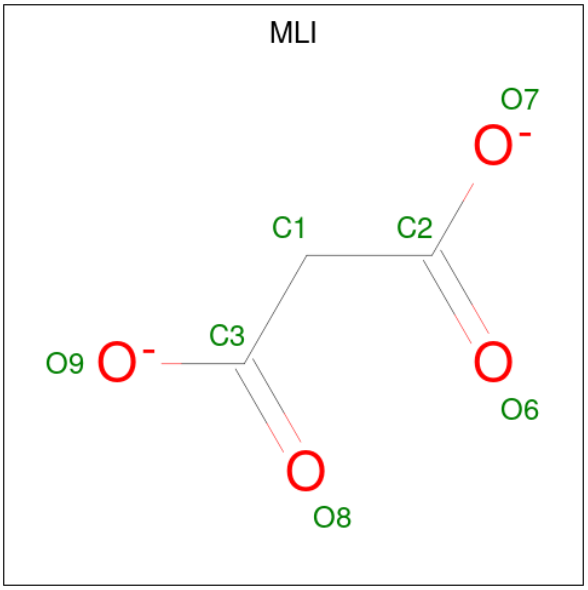
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
5	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	3	4		
6	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is water.

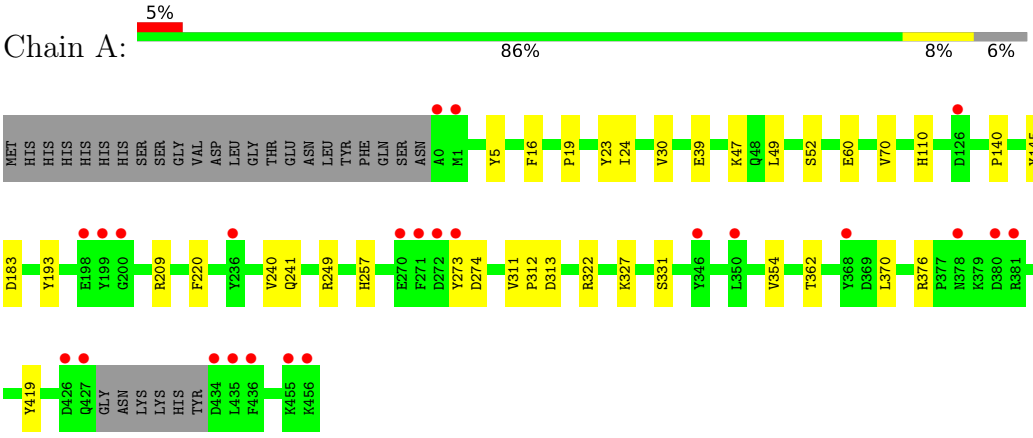
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	241	Total	O	0	0
			241	241		
7	B	193	Total	O	0	0
			193	193		
7	C	168	Total	O	0	0
			168	168		
7	D	132	Total	O	0	0
			132	132		

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.

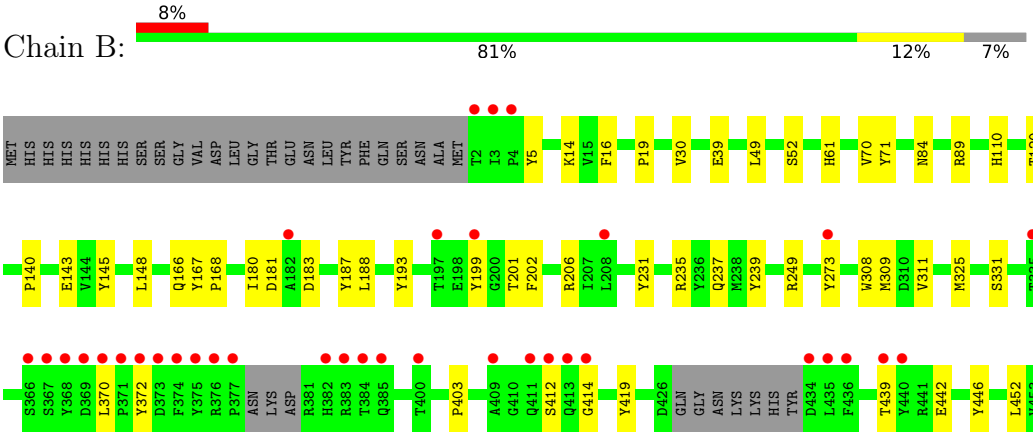
• Molecule 1: HD domain protein

Chain A:



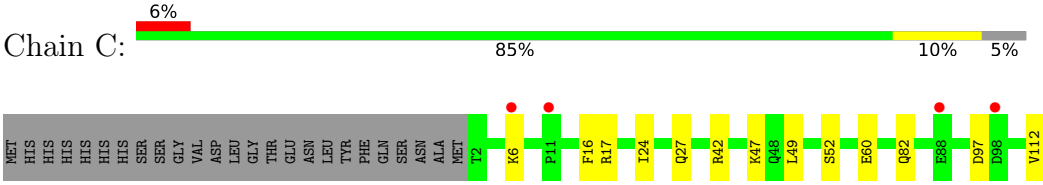
• Molecule 1: HD domain protein

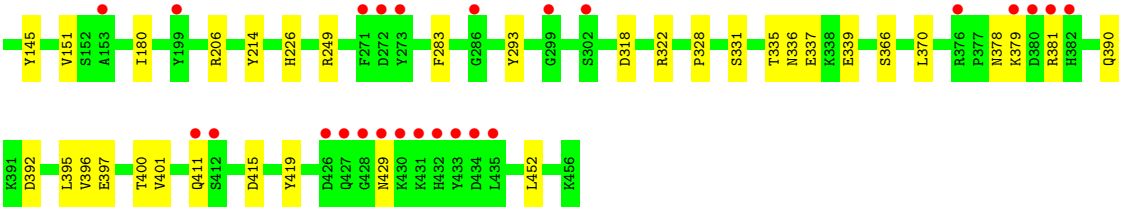
Chain B:



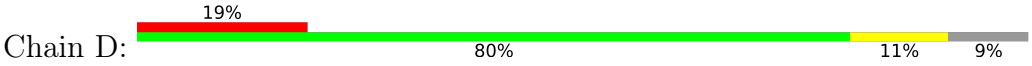
• Molecule 1: HD domain protein

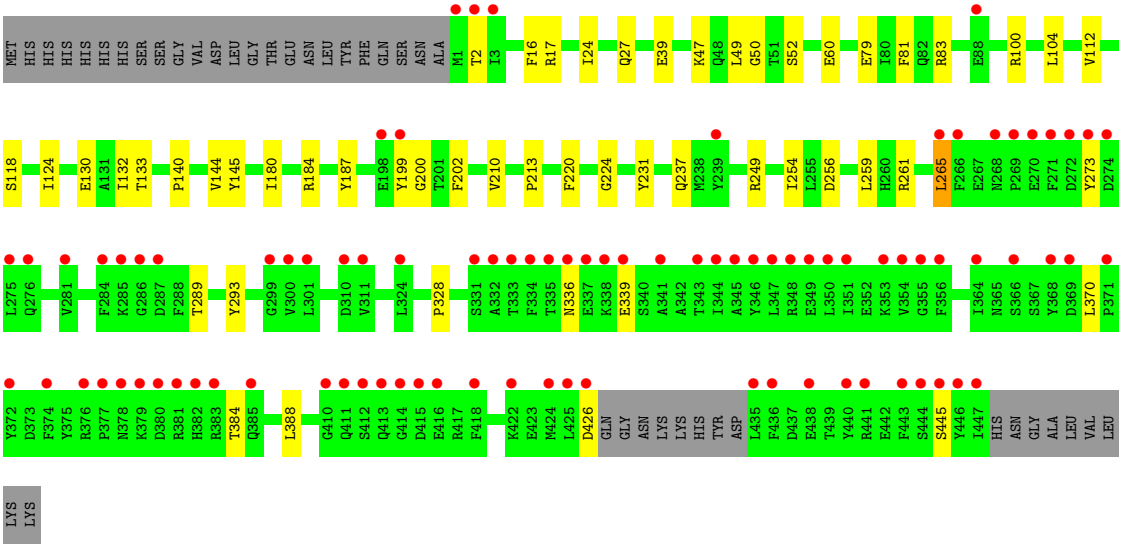
Chain C:





• Molecule 1: HD domain protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.54Å 144.62Å 155.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.35 29.86 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.86-2.35) 99.5 (29.86-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.184 , 0.235 0.184 , 0.235	Depositor DCC
R_{free} test set	4304 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15805	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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.*

[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: TTP, NI, TRS, MLI, DGT

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	0.48	0/3856	0.57	0/5221
1	B	0.45	0/3795	0.56	0/5138
1	C	0.42	0/3887	0.56	0/5263
1	D	0.42	0/3730	0.54	1/5053 (0.0%)
All	All	0.44	0/15268	0.55	1/20675 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	200	GLY	N-CA-C	-5.12	100.31	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	199	TYR	Peptide

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	3751	0	3665	23	0
1	B	3688	0	3608	41	0
1	C	3777	0	3695	24	0
1	D	3631	0	3545	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	8	0	12	0	0
4	B	16	0	24	0	0
5	B	29	0	13	0	0
5	D	29	0	13	2	0
6	B	7	0	2	0	0
6	C	7	0	2	0	0
7	A	241	0	0	3	0
7	B	193	0	0	2	0
7	C	168	0	0	0	0
7	D	132	0	0	2	0
All	All	15805	0	14627	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 4.

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)
1:B:188:LEU:HD11	1:B:235:ARG:HG3	1.52	0.92
1:B:273:TYR:CE2	1:B:311:VAL:HG22	2.08	0.88
1:C:366:SER:HB2	1:C:415:ASP:O	1.87	0.74
1:B:239:TYR:CE2	1:B:372:TYR:HB3	2.25	0.72
1:A:331:SER:HB3	1:A:419:TYR:CE2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ARG:HD3	1:B:370:LEU:HD11	1.73	0.68
1:C:249:ARG:HD3	1:C:370:LEU:HD11	1.74	0.68
1:D:16:PHE:HB2	1:D:24:ILE:HB	1.78	0.66
1:C:49:LEU:HB3	1:C:52:SER:HB2	1.76	0.66
1:B:120:THR:O	1:B:124:ILE:HD12	1.95	0.66
1:B:239:TYR:HE2	1:B:372:TYR:CB	2.08	0.65
1:B:446:TYR:CE2	1:B:455:LYS:HB2	2.32	0.65
1:A:311:VAL:HG12	1:A:313:ASP:H	1.61	0.64
1:D:336:ASN:HB2	1:D:339:GLU:HB2	1.79	0.63
1:B:403:PRO:HD2	1:C:411:GLN:HE21	1.64	0.63
1:B:331:SER:HB3	1:B:419:TYR:CE2	2.35	0.62
1:A:49:LEU:HB3	1:A:52:SER:HB2	1.80	0.62
1:D:180:ILE:HG12	1:D:231:TYR:CE2	2.35	0.61
1:B:14:LYS:NZ	3:B:502:DGT:O2A	2.35	0.60
1:A:209:ARG:NH2	7:A:744:HOH:O	2.35	0.59
1:A:140:PRO:HA	1:A:145:TYR:CD2	2.38	0.59
1:B:331:SER:HB3	1:B:419:TYR:CD2	2.38	0.58
1:B:237[B]:GLN:HA	1:B:237[B]:GLN:OE1	2.03	0.58
1:B:239:TYR:CE2	1:B:372:TYR:CB	2.84	0.57
1:C:16:PHE:HB2	1:C:24:ILE:HB	1.86	0.57
1:B:140:PRO:HA	1:B:145:TYR:CD2	2.39	0.57
1:A:47:LYS:HD2	7:A:696:HOH:O	2.05	0.56
1:D:39:GLU:HG2	1:D:144:VAL:HG23	1.88	0.55
1:C:390:GLN:HB2	1:C:392:ASP:OD1	2.07	0.55
5:D:503:TTP:O1A	5:D:503:TTP:O3G	2.25	0.55
1:C:378:ASN:HB3	1:C:381:ARG:HB2	1.90	0.54
1:B:239:TYR:HE2	1:B:372:TYR:HB3	1.66	0.54
1:D:254:ILE:HD11	1:D:328:PRO:HA	1.91	0.53
1:D:49:LEU:HB3	1:D:52:SER:HB2	1.90	0.53
1:B:201:THR:HG21	7:B:734:HOH:O	2.09	0.53
1:C:397:GLU:O	1:C:400:THR:HB	2.10	0.52
1:C:214:TYR:CE1	1:C:395:LEU:HD11	2.45	0.51
1:B:273:TYR:CZ	1:B:311:VAL:HG22	2.44	0.51
1:D:124:ILE:HD11	1:D:256:ASP:HA	1.93	0.51
1:B:239:TYR:HE2	1:B:372:TYR:HB2	1.75	0.50
1:C:331:SER:HB3	1:C:419:TYR:CD2	2.46	0.50
1:B:70:VAL:HG21	1:B:110:HIS:CE1	2.46	0.50
1:C:400:THR:HG22	1:C:401:VAL:HG13	1.94	0.50
1:B:308:TRP:HA	1:B:311:VAL:HG23	1.94	0.50
1:B:49:LEU:HB3	1:B:52:SER:HB2	1.94	0.49
1:B:235:ARG:O	1:B:239:TYR:HD1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LYS:HD3	1:C:60[A]:GLU:OE1	2.13	0.49
1:D:47:LYS:HD3	1:D:60[A]:GLU:OE1	2.13	0.49
1:D:140:PRO:HA	1:D:145:TYR:CD2	2.49	0.48
1:D:261:ARG:O	1:D:265:LEU:HG	2.14	0.47
1:C:112:VAL:HG12	1:C:133:THR:HG23	1.96	0.47
1:A:23:TYR:CE1	1:C:206:ARG:HD3	2.49	0.47
1:B:180:ILE:HG12	1:B:231:TYR:CE2	2.48	0.47
1:C:283:PHE:HZ	1:C:293:TYR:HA	1.80	0.47
1:D:79[A]:GLU:CD	1:D:100:ARG:HH22	2.18	0.47
1:B:5:TYR:CE2	1:B:30:VAL:HG22	2.50	0.47
1:D:254:ILE:CD1	1:D:328:PRO:HA	2.44	0.47
1:B:70:VAL:HG22	1:B:183:ASP:HA	1.97	0.47
1:C:6:LYS:HB2	1:C:151:VAL:HG13	1.97	0.47
7:A:818:HOH:O	1:B:325[B]:MET:SD	2.61	0.46
1:D:81:PHE:CE2	1:D:213:PRO:HD3	2.50	0.46
1:D:289:THR:HB	7:D:648:HOH:O	2.14	0.46
1:A:5:TYR:CE2	1:A:30:VAL:HG22	2.50	0.46
1:B:39:GLU:OE1	1:B:143:GLU:HB2	2.15	0.46
1:B:202:PHE:HA	7:B:724:HOH:O	2.15	0.46
1:A:331:SER:HB3	1:A:419:TYR:CD2	2.51	0.46
1:B:239:TYR:CZ	1:B:372:TYR:HB3	2.51	0.46
1:A:47:LYS:HE3	1:A:60:GLU:HA	1.97	0.46
1:B:199:TYR:CE1	1:C:226:HIS:HB3	2.51	0.45
1:D:100:ARG:O	1:D:104:LEU:HG	2.17	0.45
1:D:249:ARG:HD3	1:D:370:LEU:HD11	1.98	0.45
1:B:137:ILE:HG23	1:B:148:LEU:CD1	2.46	0.45
1:A:376:ARG:HH11	1:A:412:SER:HA	1.82	0.45
1:A:19:PRO:HB2	1:A:193:TYR:CE2	2.52	0.45
1:A:180:ILE:O	1:A:180:ILE:HG23	2.17	0.44
1:C:336:ASN:HB3	1:C:339:GLU:HG2	1.99	0.44
1:A:181:ASP:OD2	1:A:183:ASP:HB3	2.17	0.44
1:B:19:PRO:HB2	1:B:193:TYR:CE2	2.52	0.44
1:D:220:PHE:O	1:D:388:LEU:HA	2.17	0.44
1:B:309:MET:HE2	1:B:309:MET:HB3	1.74	0.44
1:B:84:ASN:O	1:B:89:ARG:NH1	2.51	0.44
1:A:16:PHE:HB2	1:A:24:ILE:HB	2.01	0.43
1:D:237[A]:GLN:HA	1:D:237[A]:GLN:OE1	2.18	0.43
1:C:331:SER:HB3	1:C:419:TYR:CE2	2.54	0.43
1:A:322:ARG:HG2	1:A:327:LYS:HB2	2.01	0.42
1:C:82:GLN:OE1	1:C:97:ASP:HB2	2.20	0.42
1:A:240:VAL:HG23	1:A:241:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HD3	1:A:370:LEU:HD11	2.01	0.42
1:A:257:HIS:HE1	1:A:362:THR:O	2.02	0.42
1:C:17:ARG:HD2	1:C:17:ARG:HA	1.92	0.42
1:D:17:ARG:HB2	5:D:503:TTP:H1'	2.01	0.42
1:C:140:PRO:HA	1:C:145:TYR:CD2	2.55	0.42
1:D:124:ILE:HD13	1:D:259:LEU:HB2	2.01	0.42
1:D:210:VAL:HG11	1:D:224:GLY:HA3	2.02	0.42
1:B:167:TYR:CD1	1:B:168:PRO:HD2	2.55	0.41
1:D:112:VAL:HG12	1:D:133:THR:HG23	2.02	0.41
1:B:181:ASP:OD2	1:B:183:ASP:HB3	2.20	0.41
1:A:60:GLU:OE1	1:B:61:HIS:HA	2.20	0.41
1:C:379:LYS:HE2	1:C:379:LYS:HB3	1.93	0.41
1:D:202:PHE:HA	7:D:667:HOH:O	2.20	0.41
1:B:353:LYS:HE2	1:B:439:THR:OG1	2.21	0.41
1:D:132:ILE:HG21	1:D:293:TYR:CE2	2.55	0.41
1:D:184:ARG:HA	1:D:187:TYR:CE2	2.55	0.41
1:B:239:TYR:OH	1:B:372:TYR:HB3	2.20	0.41
1:C:318:ASP:OD2	1:C:322:ARG:HD2	2.21	0.41
1:D:39:GLU:HG2	1:D:144:VAL:CG2	2.50	0.41
1:B:239:TYR:CE2	1:B:372:TYR:HB2	2.55	0.41
1:A:70:VAL:HG21	1:A:110:HIS:CE1	2.55	0.40
1:A:220:PHE:O	1:A:388:LEU:HA	2.21	0.40
1:A:273:TYR:CG	1:A:274:ASP:N	2.89	0.40
1:B:412:SER:C	1:B:414:GLY:H	2.25	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	453/480 (94%)	436 (96%)	14 (3%)	3 (1%)	22 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	444/480 (92%)	429 (97%)	15 (3%)	0	100	100
1	C	458/480 (95%)	440 (96%)	16 (4%)	2 (0%)	34	38
1	D	438/480 (91%)	417 (95%)	19 (4%)	2 (0%)	29	32
All	All	1793/1920 (93%)	1722 (96%)	64 (4%)	7 (0%)	34	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	SER
1	C	429	ASN
1	D	50	GLY
1	D	445	SER
1	C	180	ILE
1	A	180	ILE
1	A	312	PRO

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	410/430 (95%)	408 (100%)	2 (0%)	88	94
1	B	404/430 (94%)	397 (98%)	7 (2%)	60	72
1	C	413/430 (96%)	406 (98%)	7 (2%)	60	72
1	D	398/430 (93%)	389 (98%)	9 (2%)	50	61
All	All	1625/1720 (94%)	1600 (98%)	25 (2%)	62	76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	354	VAL
1	B	16	PHE
1	B	71	TYR

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Mol	Chain	Res	Type
1	B	166	GLN
1	B	187	TYR
1	B	206	ARG
1	B	442	GLU
1	B	452	LEU
1	C	27	GLN
1	C	42	ARG
1	C	328	PRO
1	C	335	THR
1	C	337	GLU
1	C	396	VAL
1	C	452	LEU
1	D	2	THR
1	D	27	GLN
1	D	83	ARG
1	D	118	SER
1	D	130	GLU
1	D	265	LEU
1	D	273	TYR
1	D	384	THR
1	D	426	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	411	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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	DGT	A	502	-	26,33,33	0.80	0	32,52,52	1.48	5 (15%)
6	MLI	C	503	-	6,6,6	1.13	0	7,7,7	0.79	0
5	TTP	B	503	-	26,30,30	1.35	4 (15%)	39,47,47	1.81	8 (20%)
3	DGT	C	502	-	26,33,33	0.82	1 (3%)	32,52,52	1.24	4 (12%)
3	DGT	B	502	-	26,33,33	0.88	1 (3%)	32,52,52	1.29	4 (12%)
3	DGT	D	502	-	26,33,33	0.99	1 (3%)	32,52,52	1.19	2 (6%)
4	TRS	B	505	-	7,7,7	0.47	0	9,9,9	0.39	0
6	MLI	B	504	-	6,6,6	1.09	0	7,7,7	0.93	0
5	TTP	D	503	-	26,30,30	1.26	3 (11%)	39,47,47	2.07	8 (20%)
4	TRS	B	506	-	7,7,7	0.47	0	9,9,9	0.29	0
4	TRS	A	503	-	7,7,7	0.49	0	9,9,9	0.33	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
3	DGT	A	502	-	-	4/18/34/34	0/3/3/3
6	MLI	C	503	-	-	2/4/4/4	-
5	TTP	B	503	-	-	2/22/34/34	0/2/2/2
3	DGT	C	502	-	-	5/18/34/34	0/3/3/3
3	DGT	B	502	-	-	5/18/34/34	0/3/3/3
3	DGT	D	502	-	-	4/18/34/34	0/3/3/3
4	TRS	B	505	-	-	6/9/9/9	-
6	MLI	B	504	-	-	2/4/4/4	-
5	TTP	D	503	-	-	4/22/34/34	0/2/2/2
4	TRS	B	506	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	A	503	-	-	3/9/9/9	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	TTP	C6-C5	3.70	1.40	1.34
5	D	503	TTP	C2-N1	3.25	1.43	1.38
3	D	502	DGT	C6-N1	-3.22	1.33	1.37
5	D	503	TTP	C6-C5	2.95	1.39	1.34
3	B	502	DGT	C6-N1	-2.67	1.33	1.37
5	B	503	TTP	C2-N1	2.60	1.42	1.38
5	B	503	TTP	C4-C5	-2.29	1.41	1.44
3	C	502	DGT	C6-N1	-2.20	1.34	1.37
5	B	503	TTP	C4-N3	-2.19	1.34	1.38
5	D	503	TTP	C4-C5	-2.18	1.41	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	503	TTP	C5-C4-N3	6.53	120.88	115.31
5	D	503	TTP	C4-N3-C2	-5.35	120.43	127.35
5	B	503	TTP	C5-C4-N3	5.26	119.80	115.31
5	B	503	TTP	C4-N3-C2	-4.43	121.62	127.35
3	A	502	DGT	PB-O3B-PG	-4.27	118.18	132.83
5	B	503	TTP	N3-C2-N1	3.93	120.10	114.89
5	D	503	TTP	O4-C4-C5	-3.83	120.46	124.90
5	D	503	TTP	C5-C6-N1	-3.74	119.49	123.34
5	D	503	TTP	N3-C2-N1	3.57	119.63	114.89
5	B	503	TTP	C5-C6-N1	-3.33	119.91	123.34
3	C	502	DGT	PB-O3B-PG	-3.30	121.52	132.83
5	D	503	TTP	C5M-C5-C6	-3.19	118.58	122.85
5	D	503	TTP	C5M-C5-C4	3.05	122.12	118.77
3	A	502	DGT	O6-C6-C5	-2.92	118.66	124.37
3	B	502	DGT	PA-O3A-PB	-2.82	123.16	132.83
3	B	502	DGT	PB-O3B-PG	-2.81	123.17	132.83
3	D	502	DGT	PB-O3B-PG	-2.79	123.24	132.83
5	B	503	TTP	C5M-C5-C6	-2.66	119.29	122.85
3	B	502	DGT	C5-C6-N1	2.65	118.63	113.95
5	B	503	TTP	O4'-C1'-N1	2.64	112.59	107.86
5	B	503	TTP	C5M-C5-C4	2.54	121.57	118.77
3	D	502	DGT	C5-C6-N1	2.52	118.41	113.95
3	A	502	DGT	C5-C6-N1	2.51	118.39	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	DGT	C8-N7-C5	2.40	107.56	102.99
3	C	502	DGT	PA-O3A-PB	-2.36	124.71	132.83
5	D	503	TTP	O4'-C1'-N1	2.34	112.05	107.86
3	C	502	DGT	O6-C6-C5	-2.26	119.95	124.37
5	B	503	TTP	O4-C4-C5	-2.25	122.29	124.90
3	A	502	DGT	O2G-PG-O1G	2.13	115.78	107.64
3	C	502	DGT	C5-C6-N1	2.11	117.67	113.95
3	A	502	DGT	C8-N7-C5	2.08	106.95	102.99

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	DGT	O4'-C4'-C5'-O5'
3	A	502	DGT	C3'-C4'-C5'-O5'
3	B	502	DGT	PB-O3B-PG-O2G
3	B	502	DGT	C5'-O5'-PA-O2A
3	C	502	DGT	O4'-C4'-C5'-O5'
3	C	502	DGT	C3'-C4'-C5'-O5'
3	D	502	DGT	PB-O3B-PG-O1G
3	D	502	DGT	PB-O3B-PG-O2G
4	B	505	TRS	C2-C-C3-O3
5	B	503	TTP	PB-O3B-PG-O3G
5	D	503	TTP	C5'-O5'-PA-O1A
6	B	504	MLI	C2-C1-C3-O9
4	B	505	TRS	C1-C-C2-O2
4	B	505	TRS	C1-C-C3-O3
4	B	506	TRS	C3-C-C1-O1
6	B	504	MLI	C2-C1-C3-O8
6	C	503	MLI	C3-C1-C2-O7
3	A	502	DGT	PB-O3A-PA-O2A
6	C	503	MLI	C3-C1-C2-O6
5	D	503	TTP	C5'-O5'-PA-O3A
3	B	502	DGT	PB-O3A-PA-O2A
3	C	502	DGT	PB-O3A-PA-O1A
4	A	503	TRS	N-C-C3-O3
4	B	505	TRS	N-C-C2-O2
4	B	505	TRS	N-C-C3-O3
4	B	506	TRS	N-C-C1-O1
5	D	503	TTP	PG-O3B-PB-O1B
5	D	503	TTP	C5'-O5'-PA-O2A
4	A	503	TRS	C2-C-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	505	TRS	C3-C-C2-O2
4	B	506	TRS	C2-C-C1-O1
3	D	502	DGT	O4'-C4'-C5'-O5'
3	B	502	DGT	PB-O3B-PG-O1G
5	B	503	TTP	PB-O3B-PG-O2G
3	B	502	DGT	C5'-O5'-PA-O3A
3	A	502	DGT	PB-O3A-PA-O1A
3	C	502	DGT	PG-O3B-PB-O2B
3	C	502	DGT	PB-O3A-PA-O2A
4	A	503	TRS	C1-C-C3-O3
3	D	502	DGT	C5'-O5'-PA-O2A

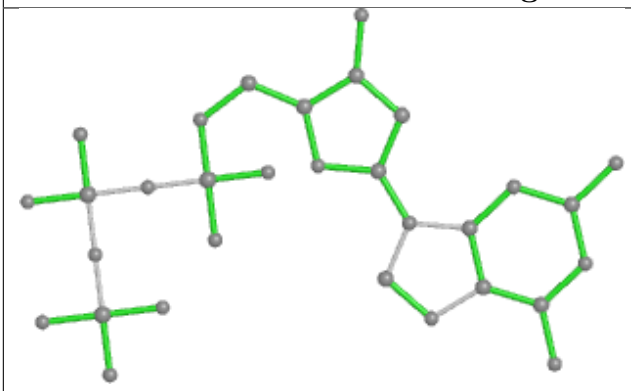
There are no ring outliers.

2 monomers are involved in 3 short contacts:

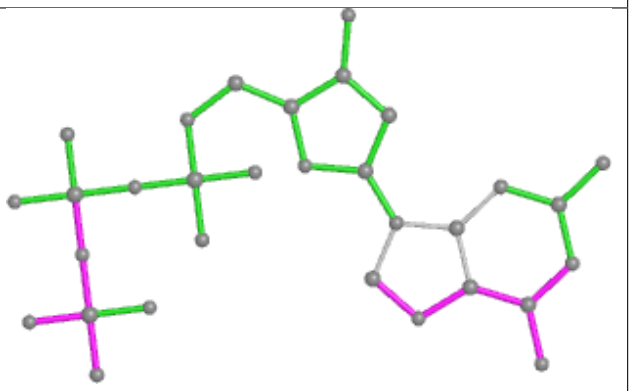
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	DGT	1	0
5	D	503	TTP	2	0

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.

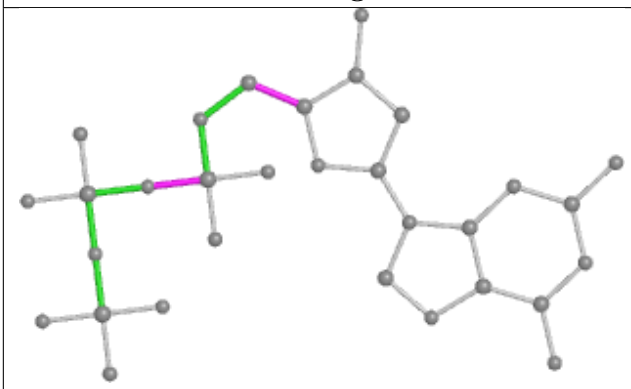
Ligand DGT A 502



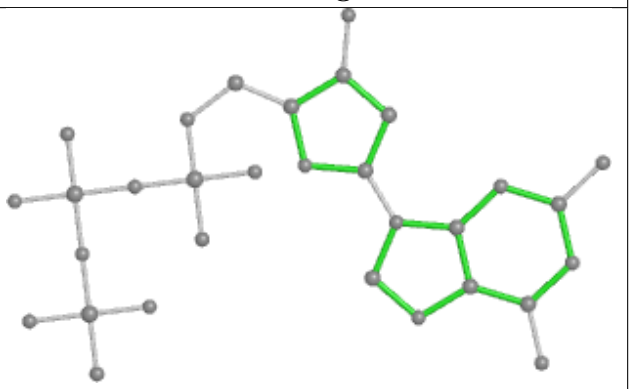
Bond lengths



Bond angles

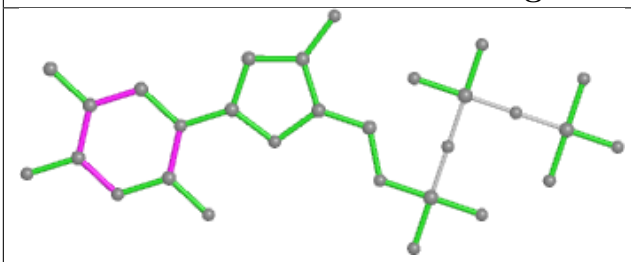


Torsions

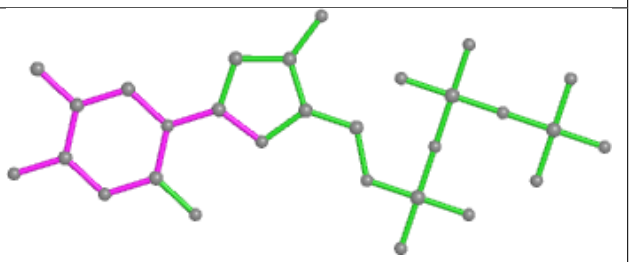


Rings

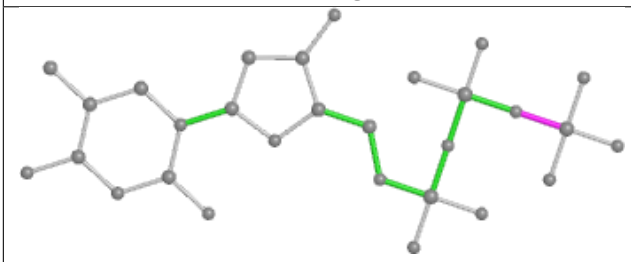
Ligand TTP B 503



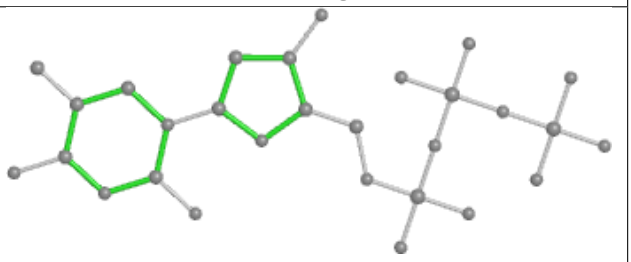
Bond lengths



Bond angles

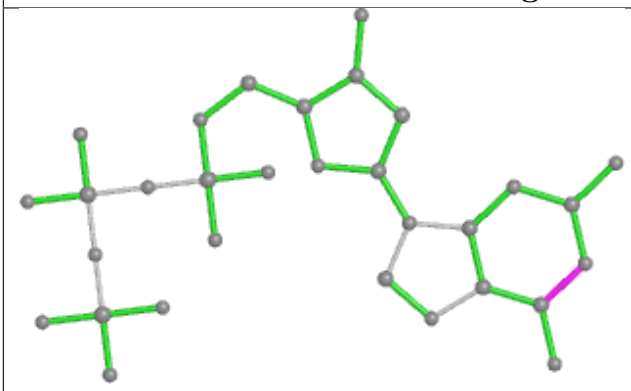


Torsions

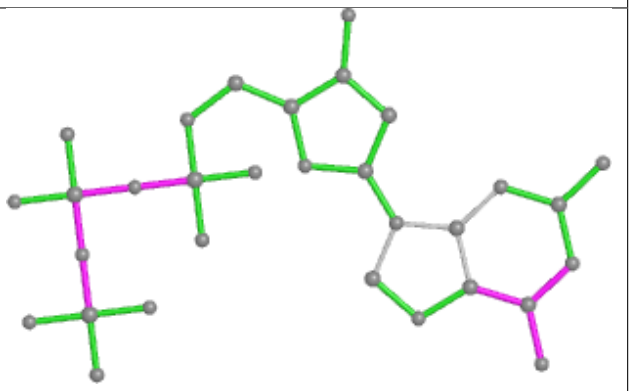


Rings

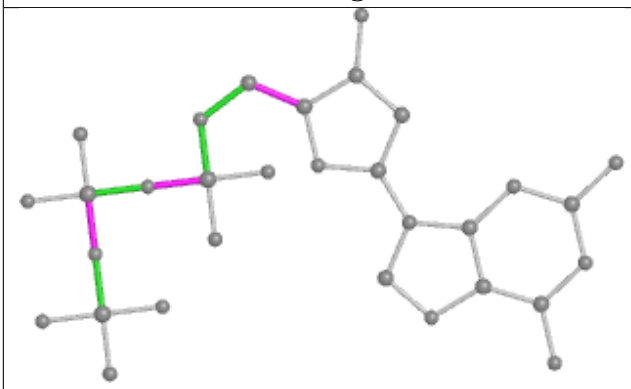
Ligand DGT C 502



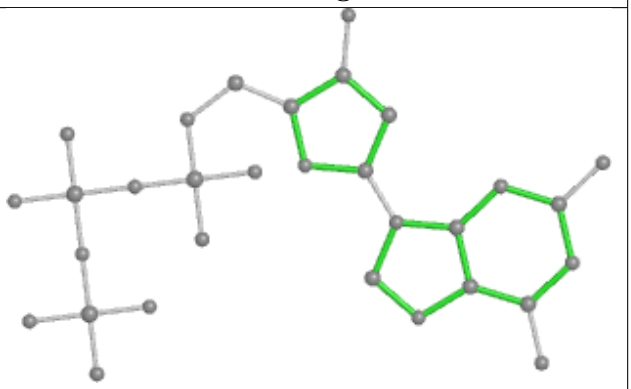
Bond lengths



Bond angles

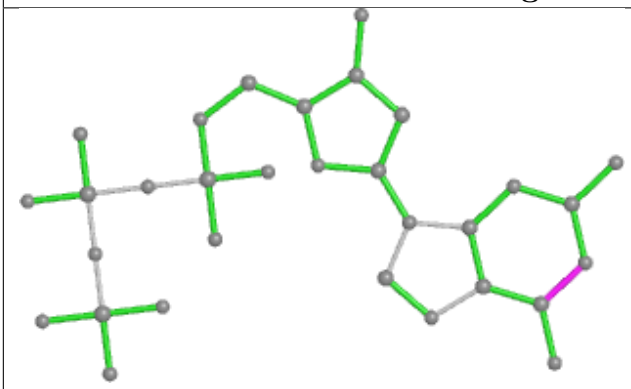


Torsions

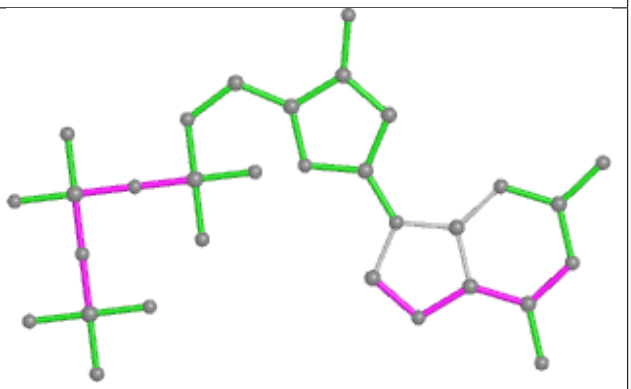


Rings

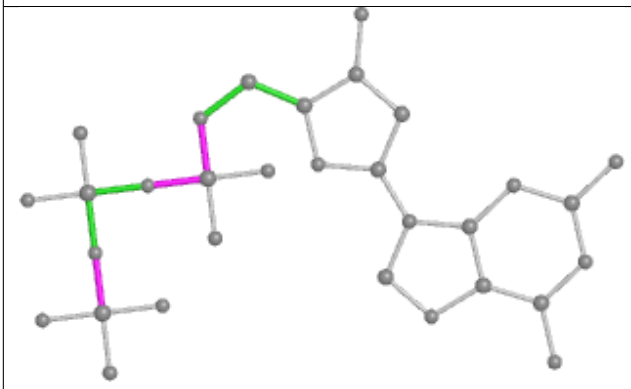
Ligand DGT B 502



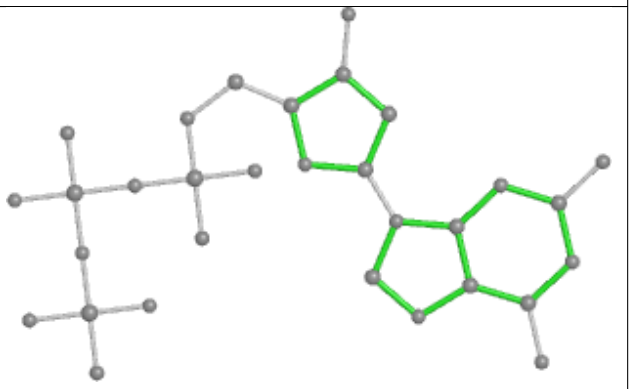
Bond lengths



Bond angles

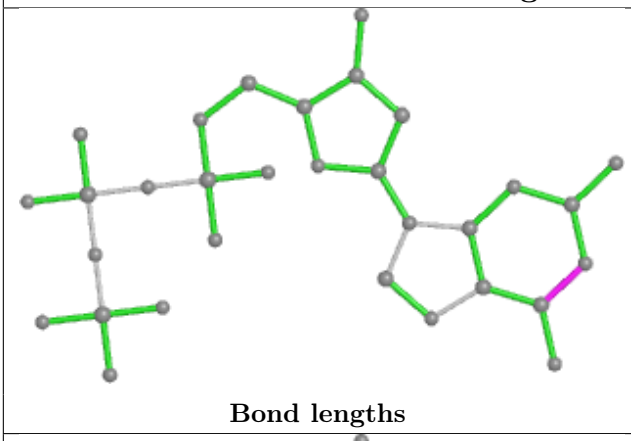


Torsions

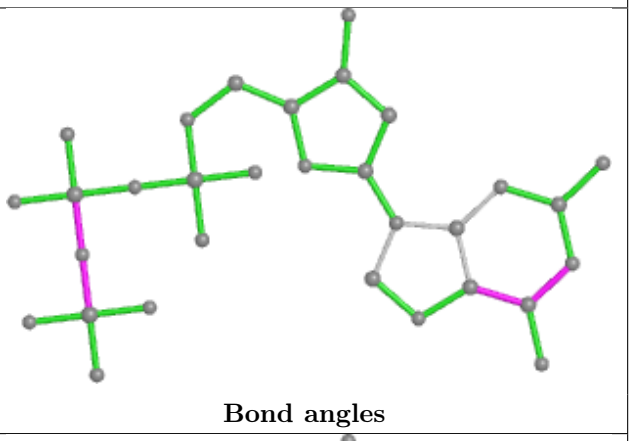


Rings

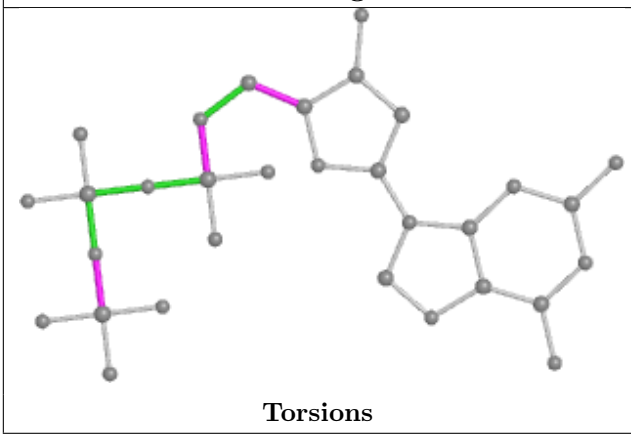
Ligand DGT D 502



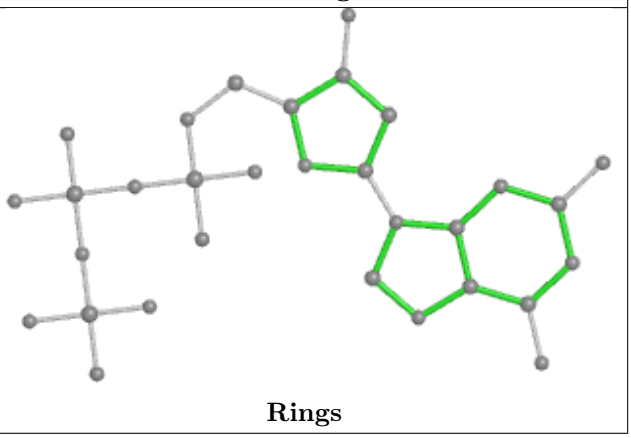
Bond lengths



Bond angles

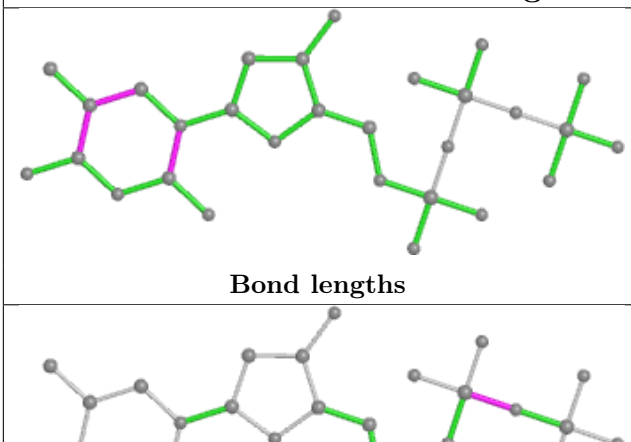


Torsions

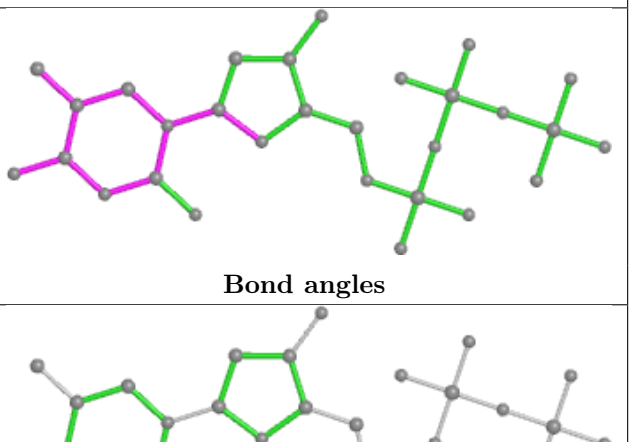


Rings

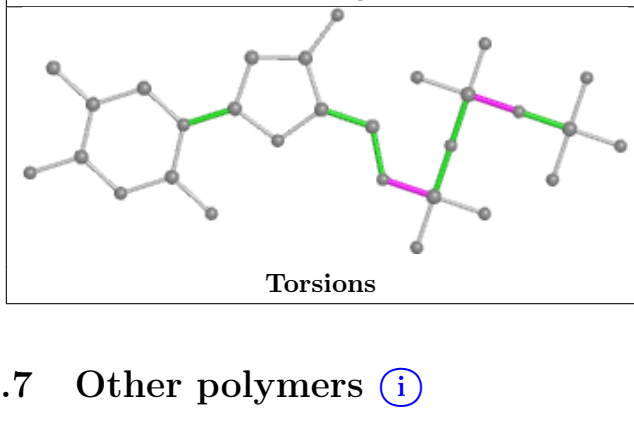
Ligand TTP D 503



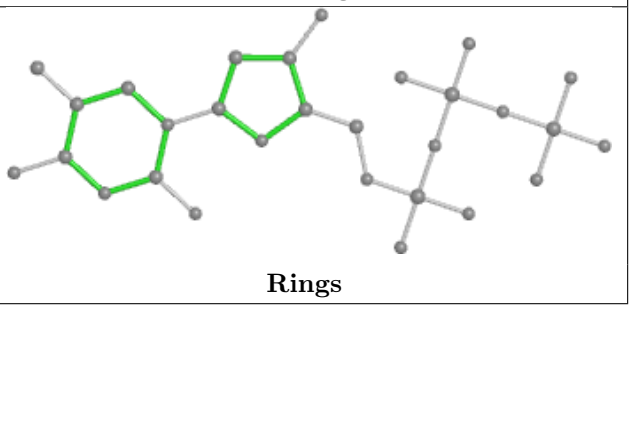
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	451/480 (93%)	0.12	26 (5%) 23 33	21, 38, 74, 117	0
1	B	445/480 (92%)	0.37	40 (8%) 9 14	25, 46, 94, 160	0
1	C	455/480 (94%)	0.21	29 (6%) 19 28	27, 45, 79, 150	0
1	D	439/480 (91%)	0.86	90 (20%) 1 1	28, 53, 148, 252	0
All	All	1790/1920 (93%)	0.39	185 (10%) 6 10	21, 45, 106, 252	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	432	HIS	9.9
1	D	368	TYR	9.4
1	D	1	MET	8.7
1	D	435	LEU	8.6
1	D	346	TYR	8.1
1	C	430	LYS	8.1
1	D	273	TYR	7.9
1	C	433	TYR	7.7
1	D	374	PHE	7.6
1	D	381	ARG	7.5
1	C	429	ASN	7.3
1	D	425	LEU	7.1
1	D	334	PHE	7.0
1	B	375	TYR	6.5
1	D	271	PHE	6.5
1	A	435	LEU	6.4
1	B	368	TYR	6.4
1	A	273	TYR	6.3
1	D	440	TYR	6.3
1	A	380	ASP	6.2
1	D	383	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	374[A]	PHE	5.9
1	D	335	THR	5.9
1	A	1	MET	5.7
1	D	436	PHE	5.7
1	C	434	ASP	5.6
1	D	424	MET	5.5
1	D	443	PHE	5.5
1	D	270	GLU	5.3
1	D	269	PRO	5.2
1	C	428	GLY	5.2
1	C	412	SER	5.2
1	B	456	LYS	5.2
1	C	427	GLN	5.2
1	B	377	PRO	5.1
1	D	355	GLY	5.0
1	B	436	PHE	5.0
1	D	380	ASP	5.0
1	B	435	LEU	4.9
1	D	274	ASP	4.9
1	D	379	LYS	4.8
1	D	354	VAL	4.8
1	B	372	TYR	4.6
1	B	434	ASP	4.6
1	D	378	ASN	4.6
1	A	368	TYR	4.5
1	D	199	TYR	4.5
1	D	2	THR	4.4
1	D	414	GLY	4.4
1	D	426	ASP	4.4
1	C	273	TYR	4.4
1	A	434	ASP	4.4
1	D	353	LYS	4.3
1	D	422	LYS	4.3
1	B	382	HIS	4.3
1	D	344	ILE	4.3
1	D	441	ARG	4.3
1	C	272	ASP	4.3
1	D	418	PHE	4.2
1	A	272	ASP	4.2
1	D	351	ILE	4.1
1	C	435	LEU	4.1
1	C	431	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	411	GLN	4.0
1	B	384	THR	4.0
1	D	371	PRO	3.9
1	A	427	GLN	3.8
1	A	426	ASP	3.8
1	B	2	THR	3.8
1	A	200	GLY	3.7
1	B	369	ASP	3.7
1	D	332	ALA	3.7
1	A	270	GLU	3.7
1	C	11	PRO	3.7
1	A	198	GLU	3.7
1	D	382	HIS	3.7
1	D	285	LYS	3.6
1	B	412	SER	3.6
1	D	350	LEU	3.6
1	B	455	LYS	3.6
1	D	356	PHE	3.5
1	D	343	THR	3.5
1	D	347	LEU	3.5
1	B	371	PRO	3.4
1	B	413	GLN	3.4
1	D	341	ALA	3.4
1	C	411	GLN	3.3
1	D	438	GLU	3.3
1	A	0	ALA	3.3
1	A	199	TYR	3.3
1	D	372	TYR	3.2
1	C	88	GLU	3.2
1	B	383	ARG	3.2
1	D	412	SER	3.2
1	D	198	GLU	3.2
1	D	310	ASP	3.2
1	D	338	LYS	3.2
1	D	300	VAL	3.1
1	D	377	PRO	3.1
1	D	281	VAL	3.1
1	D	369	ASP	3.1
1	D	268	ASN	3.0
1	D	339	GLU	3.0
1	A	378	ASN	3.0
1	C	286	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	426	ASP	3.0
1	B	376	ARG	2.9
1	B	409	ALA	2.9
1	A	412	SER	2.9
1	D	348	ARG	2.9
1	A	436	PHE	2.9
1	D	272	ASP	2.9
1	A	381	ARG	2.9
1	D	410	GLY	2.9
1	B	199	TYR	2.9
1	D	284	PHE	2.9
1	D	366	SER	2.9
1	B	414	GLY	2.9
1	D	311	VAL	2.8
1	D	349	GLU	2.8
1	D	413	GLN	2.8
1	D	447	ILE	2.8
1	B	370	LEU	2.8
1	A	346	TYR	2.8
1	B	400	THR	2.7
1	B	411	GLN	2.7
1	D	88	GLU	2.7
1	D	301	LEU	2.7
1	A	271	PHE	2.7
1	B	454	LEU	2.7
1	D	333	THR	2.6
1	C	376	ARG	2.6
1	D	286	GLY	2.6
1	B	273	TYR	2.6
1	D	287	ASP	2.6
1	D	275	LEU	2.6
1	D	324	LEU	2.5
1	C	271	PHE	2.5
1	A	236[A]	TYR	2.5
1	C	381	ARG	2.5
1	B	3	ILE	2.5
1	D	3	ILE	2.5
1	D	266	PHE	2.5
1	D	411	GLN	2.4
1	D	415	ASP	2.4
1	A	350	LEU	2.4
1	B	373	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	446	TYR	2.4
1	D	337	GLU	2.4
1	D	445	SER	2.4
1	D	331	SER	2.4
1	D	299	GLY	2.3
1	B	385	GLN	2.3
1	C	380	ASP	2.3
1	D	239	TYR	2.3
1	D	336	ASN	2.3
1	D	416	GLU	2.3
1	D	345	ALA	2.3
1	A	456	LYS	2.2
1	B	335	THR	2.2
1	D	265	LEU	2.2
1	A	455	LYS	2.2
1	C	6	LYS	2.2
1	B	182	ALA	2.2
1	B	439	THR	2.2
1	D	276	GLN	2.2
1	C	379	LYS	2.2
1	D	376	ARG	2.1
1	A	126	ASP	2.1
1	B	197	THR	2.1
1	C	153	ALA	2.1
1	B	366	SER	2.1
1	B	367	SER	2.1
1	B	208	LEU	2.1
1	D	364	ILE	2.1
1	D	444	SER	2.1
1	B	339	GLU	2.0
1	C	382	HIS	2.0
1	C	299	GLY	2.0
1	B	4	PRO	2.0
1	D	385	GLN	2.0
1	B	440	TYR	2.0
1	C	199	TYR	2.0
1	C	98	ASP	2.0
1	C	302	SER	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)

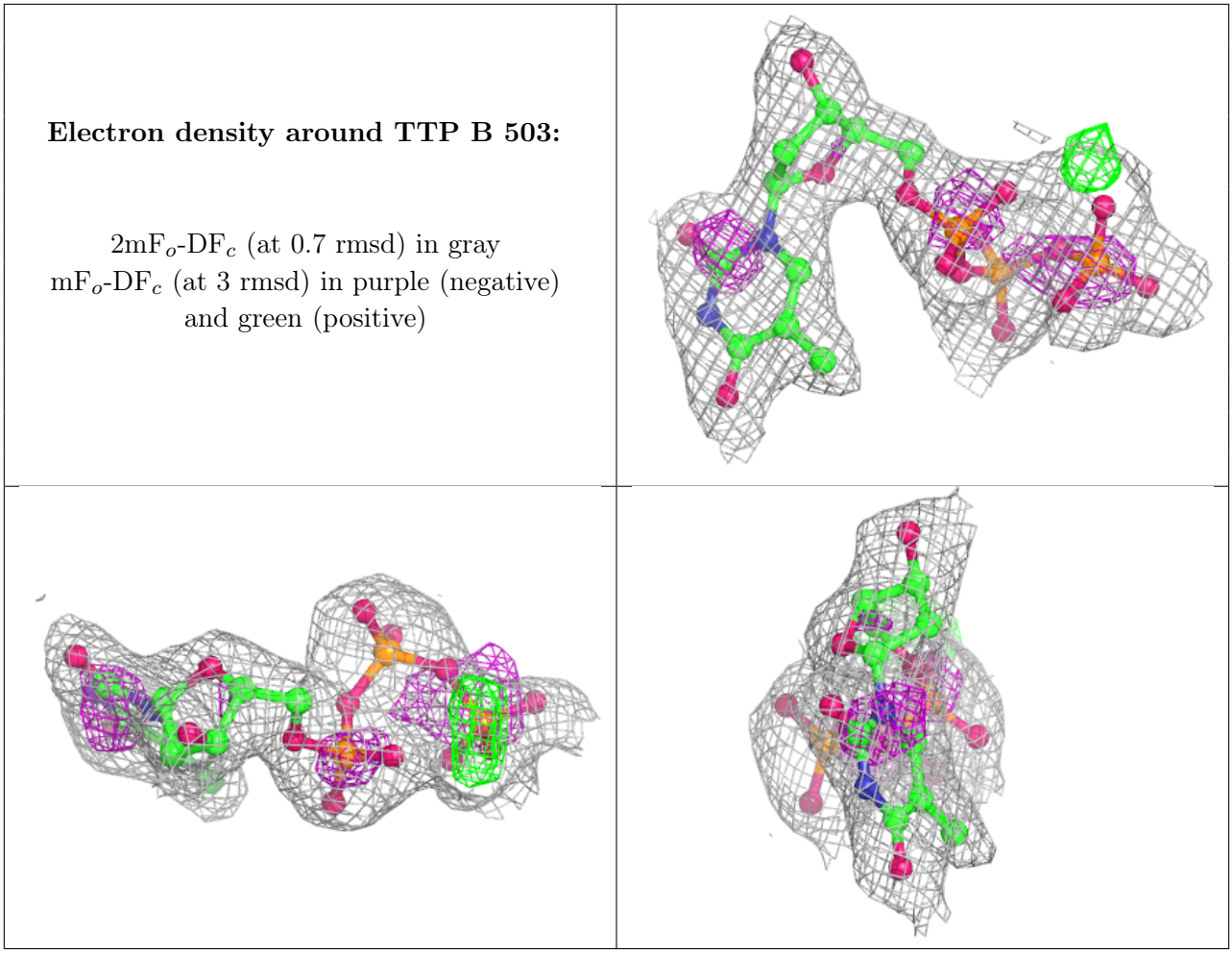
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	MLI	B	504	7/7	0.69	0.27	52,53,53,53	7
4	TRS	B	506	8/8	0.77	0.31	61,61,61,61	8
4	TRS	A	503	8/8	0.80	0.22	48,49,49,49	8
6	MLI	C	503	7/7	0.83	0.13	52,53,53,54	7
4	TRS	B	505	8/8	0.88	0.21	42,43,44,45	8
5	TTP	B	503	29/29	0.91	0.13	37,40,56,58	4
5	TTP	D	503	29/29	0.91	0.14	45,49,63,64	4
3	DGT	C	502	31/31	0.93	0.11	35,46,66,67	4
3	DGT	D	502	31/31	0.95	0.14	26,38,58,59	4
3	DGT	A	502	31/31	0.95	0.12	19,34,53,56	4
3	DGT	B	502	31/31	0.96	0.11	28,37,55,57	4
2	NI	D	501	1/1	0.98	0.06	48,48,48,48	0
2	NI	B	501	1/1	0.99	0.03	52,52,52,52	0
2	NI	A	501	1/1	1.00	0.06	35,35,35,35	0
2	NI	C	501	1/1	1.00	0.05	46,46,46,46	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.

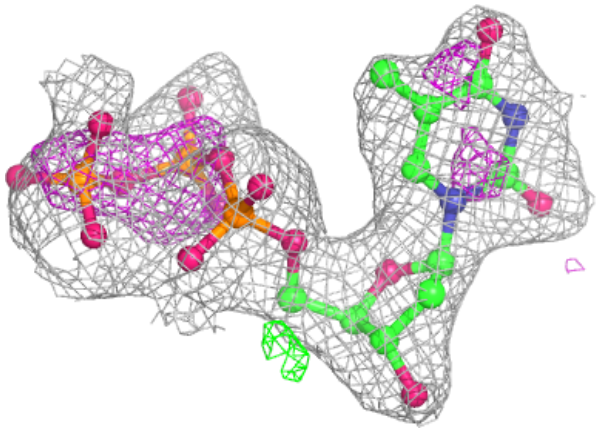
Electron density around TTP B 503:

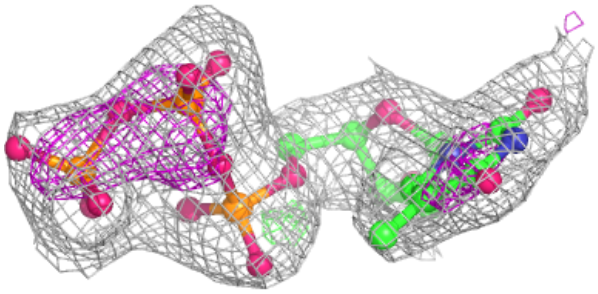
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

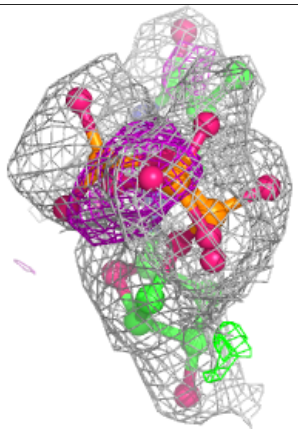


Electron density around TTP D 503:

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

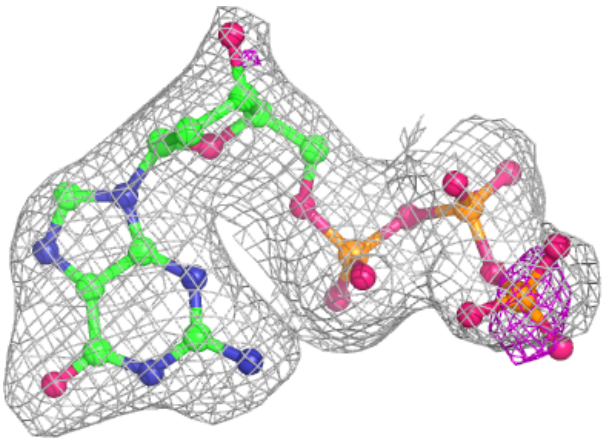


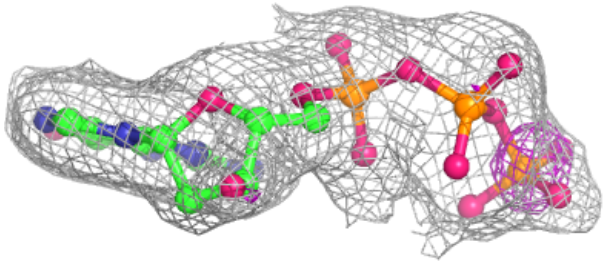


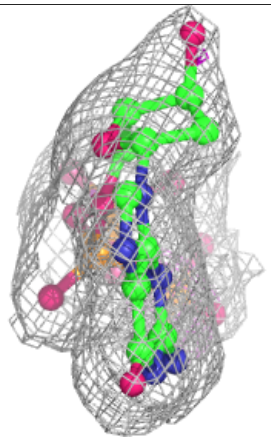


Electron density around DGT C 502:

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

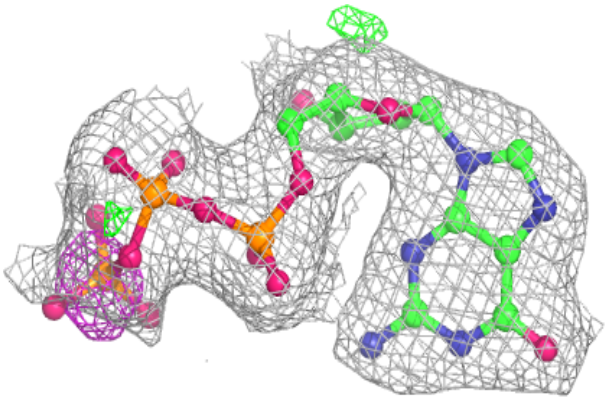


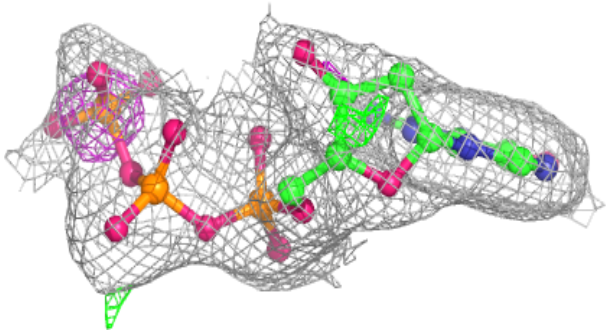


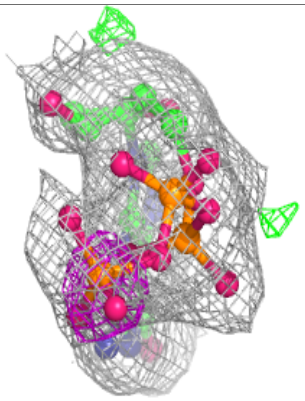


Electron density around DGT D 502:

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

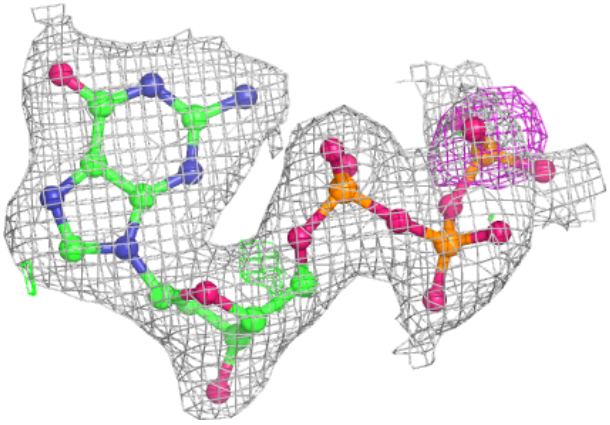


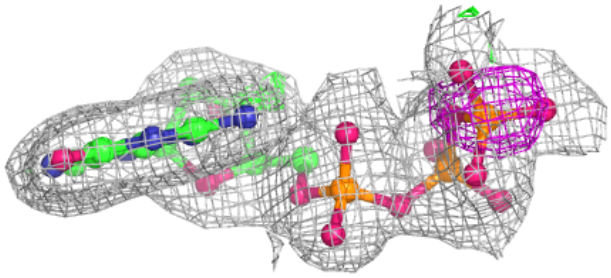


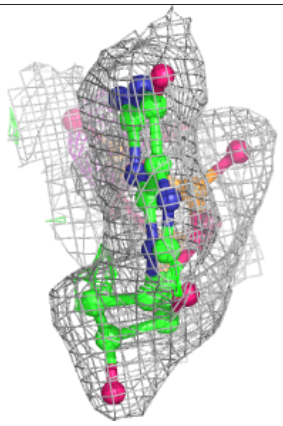


Electron density around DGT A 502:

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

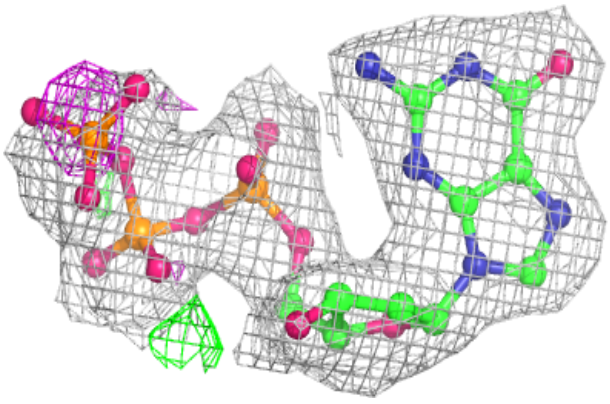


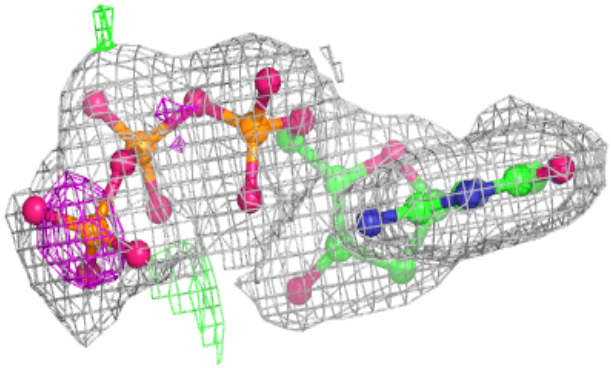


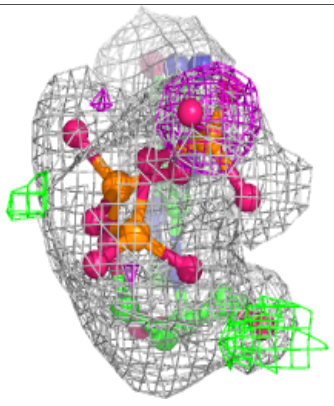


Electron density around DGT B 502:

$2mF_o$-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.