



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:25 PM UTC

PDB ID : 3IRH / pdb_00003irh
Title : Structure of an Enterococcus Faecalis HD-domain protein complexed with dGTP and dATP
Authors : Vorontsov, I.I.; Minasov, G.; Shuvalova, L.; Brunzelle, J.S.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-08-24
Resolution : 2.40 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

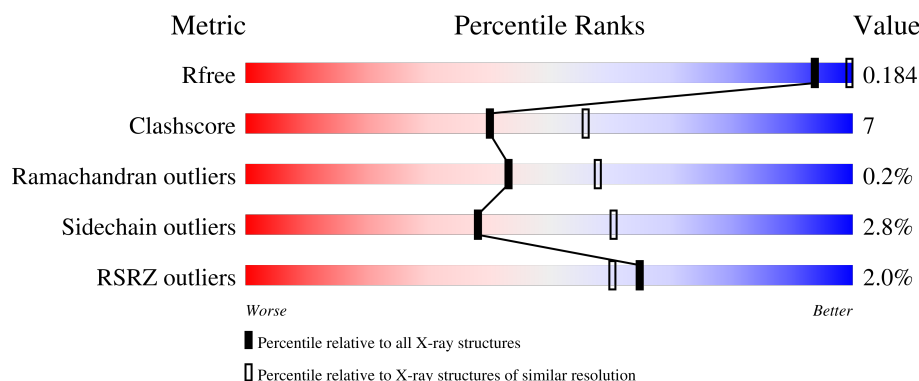
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	480	0.184 78% 15% • 6%
1	B	480	3% 75% 16% • 7%
1	C	480	0.184 80% 14% 5%
1	D	480	3% 74% 15% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15380 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	450	Total	C	N	O	S	0	3	0
			3735	2392	637	694	12			
1	B	445	Total	C	N	O	S	0	5	0
			3694	2362	631	688	13			
1	C	454	Total	C	N	O	S	0	2	0
			3757	2406	640	698	13			
1	D	434	Total	C	N	O	S	0	5	0
			3597	2302	611	672	12			

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 CALCIUM ION (CCD ID: CA) (formula: Ca).

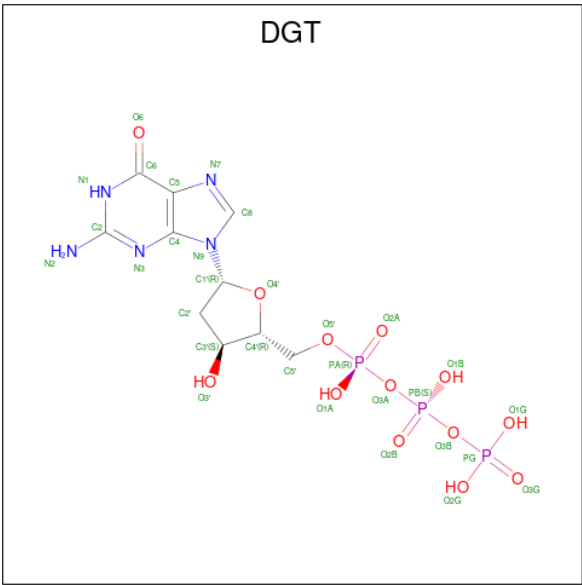
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

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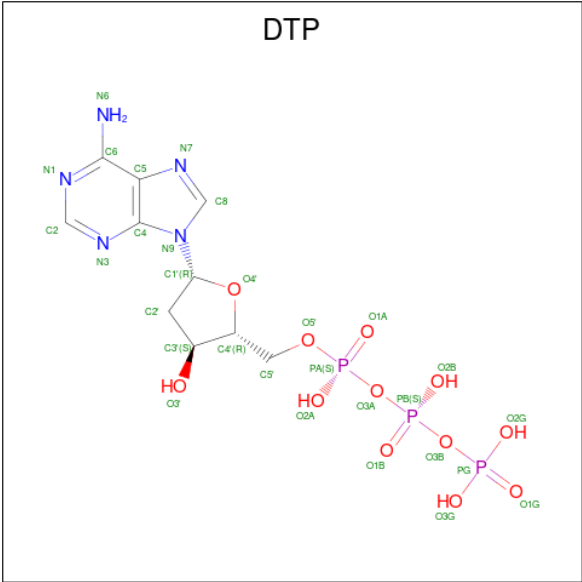
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: 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	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

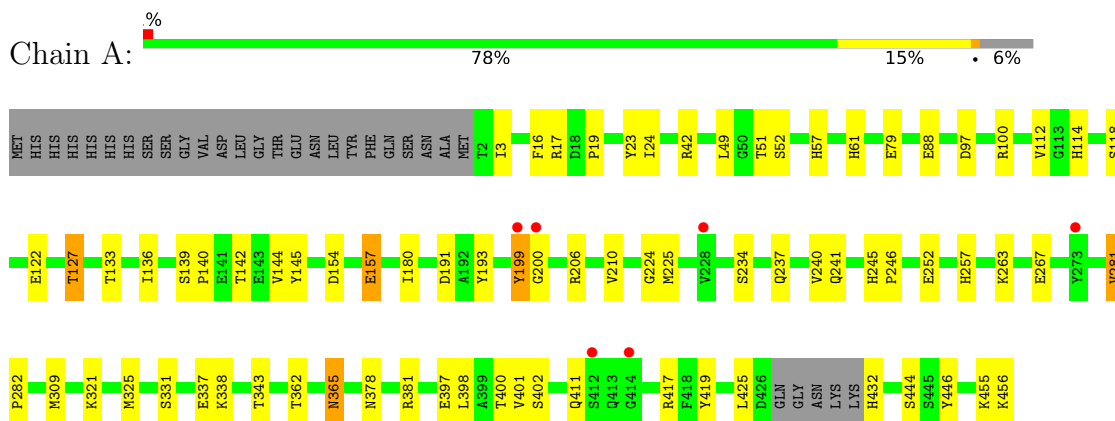
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		
5	B	111	Total	O	0	0
			111	111		
5	C	100	Total	O	0	0
			100	100		
5	D	104	Total	O	0	0
			104	104		

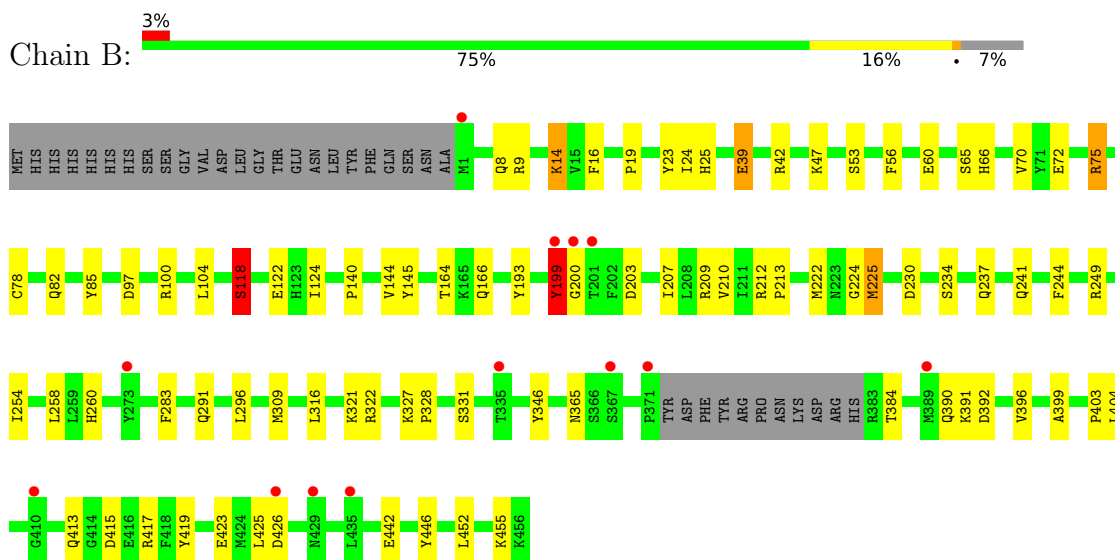
3 Residue-property plots [i](#)

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.

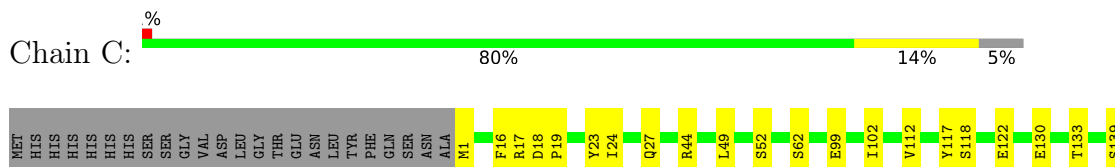
• Molecule 1: HD domain protein

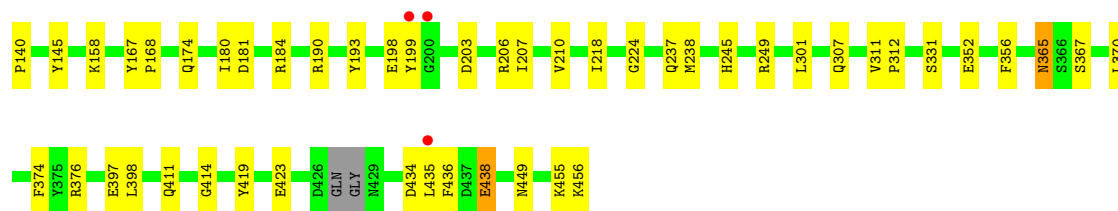


• Molecule 1: HD domain protein

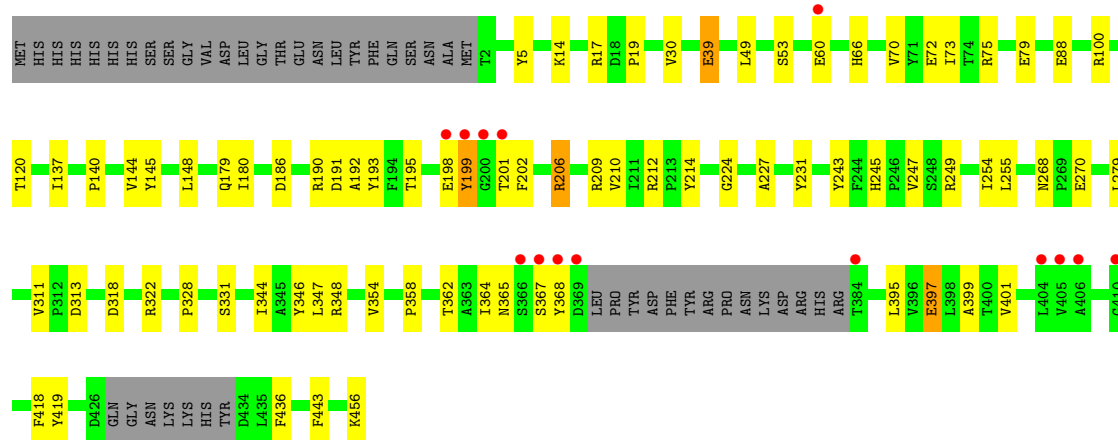
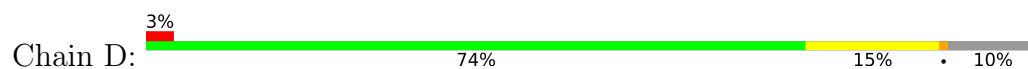


• Molecule 1: HD domain protein





● Molecule 1: HD domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.25Å 188.66Å 67.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.40) 99.1 (30.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.244 0.187 , 0.184	Depositor DCC
R_{free} test set	3759 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.6	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	0.94	EDS
Total number of atoms	15380	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 12.99% 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: CA, DTP, 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	0.58	1/3828 (0.0%)	0.87	3/5183 (0.1%)
1	B	0.60	0/3782	0.87	2/5118 (0.0%)
1	C	0.57	0/3850	0.86	5/5211 (0.1%)
1	D	0.60	0/3684	0.89	5/4985 (0.1%)
All	All	0.59	1/15144 (0.0%)	0.87	15/20497 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	VAL	CA-CB	6.81	1.58	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	TYR	N-CA-C	-7.29	104.01	113.12
1	C	139	SER	CA-C-N	6.87	126.84	119.28
1	C	139	SER	C-N-CA	6.87	126.84	119.28
1	D	199	TYR	N-CA-C	-6.17	104.62	111.71
1	A	402	SER	CA-C-N	5.67	125.34	119.05
1	A	402	SER	C-N-CA	5.67	125.34	119.05
1	B	118	SER	N-CA-C	5.45	117.65	111.11
1	D	202	PHE	N-CA-C	-5.32	102.17	110.42
1	C	398	LEU	N-CA-C	5.30	116.74	111.07
1	D	212	ARG	N-CA-C	5.18	114.26	108.25
1	A	398	LEU	N-CA-C	5.09	117.22	111.11
1	D	346	TYR	CA-C-N	5.08	127.34	120.38
1	D	346	TYR	C-N-CA	5.08	127.34	120.38
1	C	245	HIS	CA-C-N	5.01	124.80	119.28
1	C	245	HIS	C-N-CA	5.01	124.80	119.28

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	3735	0	3640	48	0
1	B	3694	0	3617	55	0
1	C	3757	0	3670	46	0
1	D	3597	0	3518	66	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	1	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	2	0
4	B	30	0	12	0	0
4	D	30	0	12	3	0
5	A	94	0	0	1	0
5	B	111	0	0	0	0
5	C	100	0	0	1	0
5	D	104	0	0	2	0
All	All	15380	0	14517	196	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 7.

All (196) 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:D:198:GLU:HG2	1:D:201:THR:HG23	1.21	1.20
1:B:222:MET:HE1	1:B:396:VAL:HG11	1.44	0.99
1:B:237:GLN:HG3	5:C:461:HOH:O	1.71	0.90
1:B:249:ARG:HD2	1:B:365:ASN:HD21	1.37	0.89
1:D:198:GLU:HG2	1:D:201:THR:CG2	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:VAL:HG11	1:D:224:GLY:HA3	1.61	0.81
1:D:249:ARG:HD2	1:D:365:ASN:HD21	1.45	0.81
1:B:423:GLU:HA	1:B:426:ASP:HB2	1.62	0.81
1:A:365:ASN:HB2	1:A:419:TYR:HE1	1.45	0.79
1:A:309:MET:HE1	1:A:325:MET:HE2	1.63	0.79
1:D:198:GLU:CG	1:D:201:THR:HG23	2.11	0.76
1:B:140:PRO:HA	1:B:145:TYR:CD2	2.22	0.75
1:C:112:VAL:HG12	1:C:133:THR:HG23	1.68	0.74
1:A:309:MET:CE	1:A:321:LYS:HA	2.19	0.73
1:D:192:ALA:HB1	1:D:198:GLU:HA	1.70	0.73
1:C:203:ASP:OD2	1:C:206:ARG:HG3	1.89	0.72
1:B:210:VAL:HG11	1:B:224:GLY:HA3	1.70	0.72
1:C:181:ASP:OD2	1:C:184:ARG:HG3	1.89	0.71
1:B:249:ARG:HH11	1:B:365:ASN:ND2	1.88	0.71
1:C:62:SER:N	1:D:60:GLU:OE1	2.24	0.71
1:C:374:PHE:HB2	1:C:376:ARG:HH21	1.56	0.70
1:D:249:ARG:HD2	1:D:365:ASN:ND2	2.07	0.69
1:B:75:ARG:HB3	1:B:104:LEU:HD21	1.75	0.69
1:D:192:ALA:HB1	1:D:198:GLU:HG3	1.76	0.67
1:D:186:ASP:OD2	1:D:190:ARG:NH1	2.28	0.67
1:D:348:ARG:HE	1:D:362:THR:HG21	1.60	0.66
1:A:309:MET:HE2	1:A:321:LYS:HA	1.75	0.66
1:C:18:ASP:OD1	1:C:190:ARG:NH2	2.28	0.66
1:A:446:TYR:CE2	1:A:455:LYS:HB2	2.32	0.65
1:A:17:ARG:HE	1:C:206:ARG:NH1	1.95	0.64
1:B:423:GLU:HA	1:B:426:ASP:CB	2.27	0.64
1:D:79[A]:GLU:HG2	1:D:100[A]:ARG:NH2	2.13	0.64
1:A:210:VAL:HG11	1:A:224:GLY:HA3	1.80	0.63
1:C:17:ARG:HH22	1:D:199:TYR:HE1	1.46	0.63
1:A:199:TYR:HB3	1:A:237:GLN:HB3	1.80	0.63
1:B:39:GLU:HG2	1:B:144:VAL:HG23	1.80	0.63
1:B:203:ASP:OD2	1:D:17:ARG:NH2	2.27	0.63
1:A:240:VAL:HG23	1:A:241:GLN:HG3	1.80	0.62
1:C:140:PRO:HA	1:C:145:TYR:CD2	2.34	0.62
1:C:365:ASN:C	1:C:365:ASN:HD22	2.08	0.62
1:A:23:TYR:HE1	1:C:206:ARG:HG2	1.64	0.61
1:B:392:ASP:H	1:C:449:ASN:HD21	1.48	0.61
1:A:365:ASN:HB2	1:A:419:TYR:CE1	2.32	0.60
1:B:403:PRO:HD2	1:C:411:GLN:HE22	1.67	0.60
1:A:42[B]:ARG:NH2	1:A:112:VAL:O	2.32	0.58
1:C:249:ARG:HD3	1:C:370:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:GLU:HG3	1:D:399:ALA:H	1.69	0.57
1:D:322:ARG:NH2	5:D:479:HOH:O	2.29	0.57
1:C:16:PHE:HB2	1:C:24:ILE:HB	1.88	0.56
4:D:459:DTP:H5'1	4:D:459:DTP:H8	1.88	0.56
1:A:140:PRO:HA	1:A:145:TYR:CD2	2.40	0.56
1:C:455:LYS:O	1:C:456:LYS:C	2.48	0.56
1:A:16:PHE:HB2	1:A:24:ILE:HB	1.88	0.56
1:A:309:MET:HE3	1:A:321:LYS:HA	1.87	0.56
1:D:368:TYR:CE1	4:D:459:DTP:H2'2	2.41	0.55
1:B:249:ARG:HH11	1:B:365:ASN:HD21	1.53	0.55
1:A:122:GLU:HG2	1:A:127:THR:HG22	1.88	0.55
1:D:72:GLU:OE1	1:D:75:ARG:NH1	2.39	0.55
1:B:230:ASP:OD1	1:C:237:GLN:CD	2.50	0.55
1:A:263:LYS:O	1:A:267:GLU:HG2	2.07	0.54
1:D:331:SER:HB3	1:D:419:TYR:CE2	2.42	0.54
1:D:19:PRO:HB2	1:D:193:TYR:CE2	2.43	0.54
1:D:140:PRO:HA	1:D:145:TYR:CD2	2.43	0.54
1:B:19:PRO:HB2	1:B:193:TYR:CE2	2.44	0.53
1:B:47:LYS:HD3	1:B:60:GLU:OE1	2.07	0.53
1:D:5:TYR:CE2	1:D:30:VAL:HG22	2.43	0.53
1:A:23:TYR:CE1	1:C:206:ARG:HG2	2.44	0.53
1:A:343:THR:OG1	1:A:456:LYS:OXT	2.23	0.53
1:C:210:VAL:HG11	1:C:224:GLY:HA3	1.91	0.53
1:D:268:ASN:OD1	1:D:270:GLU:HG2	2.08	0.53
1:D:311:VAL:HG12	1:D:313:ASP:H	1.74	0.53
1:D:254:ILE:CD1	1:D:328:PRO:HA	2.40	0.52
1:D:186:ASP:OD1	1:D:190:ARG:NH1	2.42	0.52
1:D:79[A]:GLU:HG2	1:D:100[A]:ARG:HH22	1.74	0.51
1:D:186:ASP:CG	1:D:190:ARG:NH1	2.69	0.51
1:A:142:THR:HG22	1:A:145:TYR:H	1.74	0.51
1:B:322:ARG:HG2	1:B:327:LYS:HB2	1.93	0.51
1:C:331:SER:HB3	1:C:419:TYR:CE2	2.46	0.50
1:B:39:GLU:HG2	1:B:144:VAL:CG2	2.42	0.50
1:D:362:THR:CG2	1:D:418:PHE:CE1	2.95	0.50
1:C:44:ARG:NH1	1:D:53:SER:O	2.44	0.50
1:C:49:LEU:HB3	1:C:52:SER:HB2	1.94	0.49
1:D:247:VAL:HG21	3:D:458:DGT:H5'	1.93	0.49
1:C:307:GLN:HE22	1:D:279:LEU:HD21	1.77	0.49
1:A:51:THR:OG1	1:A:252[B]:GLU:HG3	2.11	0.49
1:B:212[A]:ARG:HG2	1:B:213:PRO:HD2	1.92	0.49
1:C:367:SER:OG	1:C:414:GLY:HA2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:TYR:CD2	4:D:459:DTP:H1'	2.48	0.49
1:A:331:SER:OG	1:A:417:ARG:NH1	2.45	0.49
1:D:348:ARG:HH21	1:D:362:THR:HG22	1.78	0.49
1:C:102:ILE:HD11	1:C:158:LYS:HB3	1.94	0.49
1:D:245:HIS:HD2	1:D:247:VAL:H	1.61	0.48
1:D:254:ILE:HD11	1:D:328:PRO:HA	1.95	0.48
1:A:397:GLU:O	1:A:400:THR:HB	2.13	0.48
1:D:120:THR:HG21	1:D:255:LEU:HG	1.95	0.48
1:D:75:ARG:NH2	1:D:79[A]:GLU:OE2	2.46	0.48
1:A:200:GLY:HA2	1:A:234:SER:HB3	1.96	0.48
1:B:392:ASP:N	1:C:449:ASN:HD21	2.12	0.48
1:B:249:ARG:NH2	1:B:415:ASP:OD2	2.45	0.47
1:B:283:PHE:CE2	1:B:296:LEU:HD11	2.49	0.47
1:D:348:ARG:HE	1:D:362:THR:CG2	2.25	0.47
1:D:362:THR:HA	1:D:419:TYR:O	2.14	0.47
1:A:61:HIS:HE1	1:A:191:ASP:OD1	1.97	0.47
1:C:434:ASP:C	1:C:436:PHE:H	2.20	0.47
1:D:362:THR:HG23	1:D:418:PHE:CE1	2.49	0.47
1:A:97:ASP:OD2	1:A:100:ARG:NH1	2.47	0.47
1:C:19:PRO:HB2	1:C:193:TYR:CE2	2.50	0.47
1:D:192:ALA:CB	1:D:198:GLU:HG3	2.43	0.47
1:B:124:ILE:HD12	1:B:260:HIS:HB2	1.97	0.47
1:C:331:SER:HB3	1:C:419:TYR:CD2	2.50	0.47
1:A:112:VAL:HG12	1:A:133:THR:HG23	1.95	0.47
1:B:222:MET:HE1	1:B:396:VAL:CG1	2.32	0.47
1:A:365:ASN:CB	1:A:419:TYR:HE1	2.22	0.47
1:B:25:HIS:HD2	1:B:72:GLU:OE2	1.99	0.46
1:B:75:ARG:HB3	1:B:104:LEU:CD2	2.44	0.46
1:D:39:GLU:HG2	1:D:144:VAL:HG23	1.96	0.46
3:A:458:DGT:O2B	1:B:14:LYS:NZ	2.48	0.46
1:D:249:ARG:HH11	1:D:365:ASN:ND2	2.14	0.46
1:A:154:ASP:O	1:A:157:GLU:HG3	2.15	0.46
1:A:365:ASN:HD22	1:A:365:ASN:HA	1.56	0.46
1:A:79:GLU:OE2	1:A:100:ARG:NH2	2.48	0.46
1:C:435:LEU:HA	1:C:438:GLU:HB2	1.98	0.46
1:D:331:SER:HB3	1:D:419:TYR:CD2	2.50	0.46
1:B:331:SER:HB3	1:B:419:TYR:CE2	2.51	0.45
1:C:99:GLU:O	1:C:102:ILE:HG22	2.16	0.45
1:A:142:THR:CG2	1:A:144:VAL:HB	2.46	0.45
1:B:85:TYR:OH	1:B:212[B]:ARG:CZ	2.65	0.45
1:B:346:TYR:OH	1:B:442:GLU:OE2	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:TYR:CE1	1:D:395:LEU:HD11	2.52	0.45
1:A:19:PRO:HB2	1:A:193:TYR:CE2	2.52	0.45
1:D:72:GLU:CD	1:D:75:ARG:NH1	2.75	0.44
1:A:61:HIS:CD2	1:A:61:HIS:H	2.33	0.44
1:B:200:GLY:HA2	1:B:234:SER:HB3	1.98	0.44
1:C:434:ASP:C	1:C:436:PHE:N	2.75	0.44
1:A:118:SER:O	1:A:122:GLU:HG3	2.17	0.44
1:B:254:ILE:CD1	1:B:328:PRO:HA	2.48	0.44
1:D:79[B]:GLU:CD	1:D:100[B]:ARG:HH12	2.25	0.44
1:B:78:CYS:HB3	1:B:100:ARG:HD2	2.00	0.44
1:B:66:HIS:O	1:B:70:VAL:HG23	2.18	0.44
1:D:331:SER:HA	1:D:418:PHE:O	2.18	0.44
1:B:82:GLN:OE1	1:B:97:ASP:HB2	2.17	0.43
1:D:358:PRO:O	1:D:362:THR:HB	2.18	0.43
1:B:16:PHE:HB2	1:B:24:ILE:HB	2.00	0.43
1:D:137:ILE:HG23	1:D:148:LEU:CD1	2.48	0.43
1:B:53:SER:HA	1:B:56:PHE:O	2.19	0.43
1:C:118:SER:O	1:C:122:GLU:HG3	2.18	0.43
1:D:180:ILE:HG12	1:D:231:TYR:CE2	2.53	0.43
1:A:206:ARG:HG3	1:C:23:TYR:HE1	1.83	0.43
1:A:57:HIS:HD2	1:B:65:SER:HB3	1.84	0.43
1:B:391:LYS:HB2	1:C:449:ASN:HD22	1.83	0.43
1:C:44:ARG:NH2	3:D:458:DGT:N7	2.67	0.43
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.77	0.43
1:D:347:LEU:HD22	1:D:443:PHE:CD1	2.54	0.43
1:B:225:MET:HE3	1:B:225:MET:HB2	1.64	0.43
1:B:118:SER:O	1:B:122:GLU:HG3	2.19	0.43
1:B:384:THR:HG21	1:B:399:ALA:HB2	2.01	0.43
1:C:352:GLU:HA	1:C:356:PHE:O	2.19	0.42
1:D:100[B]:ARG:NH2	5:D:461:HOH:O	2.23	0.42
1:D:245:HIS:CD2	1:D:247:VAL:H	2.35	0.42
1:D:344:ILE:HD13	1:D:364:ILE:HD11	2.01	0.42
1:D:145:TYR:CD2	1:D:145:TYR:C	2.97	0.42
1:A:17:ARG:NE	1:C:206:ARG:NH1	2.65	0.42
1:C:311:VAL:HA	1:C:312:PRO:HD3	1.92	0.42
1:D:354:VAL:O	1:D:354:VAL:CG1	2.68	0.42
1:B:164:THR:CB	1:B:166:GLN:HE21	2.32	0.42
1:D:318:ASP:O	1:D:322:ARG:HG3	2.19	0.42
1:A:17:ARG:HG2	1:C:206:ARG:HH22	1.83	0.42
1:B:199:TYR:HD1	1:B:241:GLN:HE22	1.68	0.42
1:A:49:LEU:HB3	1:A:52:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:PHE:CE2	1:B:413:GLN:HB2	2.55	0.41
1:B:392:ASP:H	1:C:449:ASN:ND2	2.14	0.41
1:C:199:TYR:HB2	1:C:238:MET:SD	2.60	0.41
1:D:73:ILE:HD12	1:D:186:ASP:HB2	2.02	0.41
1:A:136:ILE:O	1:A:142:THR:HG21	2.20	0.41
1:B:258:LEU:HD12	1:B:316:LEU:HD12	2.03	0.41
1:B:404:LEU:HD12	1:C:411:GLN:HG2	2.01	0.41
1:C:174:GLN:NE2	1:C:218:ILE:H	2.19	0.41
1:A:378:ASN:HB3	1:A:381:ARG:HB2	2.02	0.41
1:A:88:GLU:HG3	5:A:537:HOH:O	2.21	0.41
1:B:331:SER:OG	1:B:417:ARG:HD3	2.20	0.41
1:C:117:TYR:HD1	1:C:301:LEU:HD12	1.86	0.41
1:A:139:SER:HA	1:A:140:PRO:HD3	1.93	0.41
1:A:245:HIS:HA	1:A:246:PRO:HD3	1.87	0.41
1:B:423:GLU:CA	1:B:426:ASP:HB2	2.42	0.41
1:B:446:TYR:CE2	1:B:455:LYS:HB2	2.55	0.41
1:D:348:ARG:NE	1:D:362:THR:HG21	2.29	0.41
1:D:206:ARG:HE	1:D:227:ALA:HB2	1.86	0.41
1:A:257:HIS:HE1	1:A:362:THR:O	2.04	0.40
1:B:309:MET:HE3	1:B:321:LYS:HG3	2.02	0.40
1:A:114:HIS:HD2	1:A:118:SER:OG	2.05	0.40
1:D:66:HIS:O	1:D:70:VAL:HG23	2.21	0.40
1:A:281:VAL:N	1:A:282:PRO:HD2	2.36	0.40
1:B:23:TYR:OH	1:D:209[B]:ARG:NH2	2.54	0.40
1:B:209:ARG:HD3	1:B:209:ARG:HA	1.86	0.40
1:C:167:TYR:CD1	1:C:168:PRO:HD2	2.57	0.40
1:D:191:ASP:O	1:D:195:THR:HG23	2.22	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	449/480 (94%)	428 (95%)	20 (4%)	1 (0%)	43	58
1	B	446/480 (93%)	429 (96%)	16 (4%)	1 (0%)	43	58
1	C	452/480 (94%)	434 (96%)	17 (4%)	1 (0%)	43	58
1	D	433/480 (90%)	418 (96%)	15 (4%)	0	100	100
All	All	1780/1920 (93%)	1709 (96%)	68 (4%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	GLN
1	C	180	ILE
1	A	180	ILE

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	407/430 (95%)	394 (97%)	13 (3%)	34	56
1	B	403/430 (94%)	390 (97%)	13 (3%)	34	56
1	C	410/430 (95%)	401 (98%)	9 (2%)	45	67
1	D	393/430 (91%)	383 (98%)	10 (2%)	42	64
All	All	1613/1720 (94%)	1568 (97%)	45 (3%)	38	60

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	127	THR
1	A	157	GLU
1	A	199	TYR
1	A	225	MET
1	A	337	GLU
1	A	338	LYS
1	A	365	ASN

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Mol	Chain	Res	Type
1	A	401	VAL
1	A	411	GLN
1	A	425	LEU
1	A	432	HIS
1	A	444	SER
1	B	9	ARG
1	B	14	LYS
1	B	39	GLU
1	B	42	ARG
1	B	75	ARG
1	B	118	SER
1	B	199	TYR
1	B	207	ILE
1	B	225	MET
1	B	291	GLN
1	B	390	GLN
1	B	425	LEU
1	B	452	LEU
1	C	1	MET
1	C	27	GLN
1	C	130	GLU
1	C	198	GLU
1	C	207	ILE
1	C	365	ASN
1	C	397	GLU
1	C	423	GLU
1	C	438	GLU
1	D	14	LYS
1	D	39	GLU
1	D	88	GLU
1	D	179	GLN
1	D	206	ARG
1	D	367	SER
1	D	397	GLU
1	D	401	VAL
1	D	436	PHE
1	D	456	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS

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Mol	Chain	Res	Type
1	A	29	GLN
1	A	48	GLN
1	A	57	HIS
1	A	61	HIS
1	A	114	HIS
1	A	166	GLN
1	A	276	GLN
1	A	291	GLN
1	A	365	ASN
1	A	385	GLN
1	A	448	HIS
1	B	25	HIS
1	B	28	HIS
1	B	48	GLN
1	B	114	HIS
1	B	123	HIS
1	B	135	GLN
1	B	166	GLN
1	B	223	ASN
1	B	237	GLN
1	B	365	ASN
1	B	385	GLN
1	B	432	HIS
1	B	449	ASN
1	C	48	GLN
1	C	57	HIS
1	C	114	HIS
1	C	174	GLN
1	C	223	ASN
1	C	307	GLN
1	C	365	ASN
1	C	411	GLN
1	C	449	ASN
1	D	8	GLN
1	D	25	HIS
1	D	129	HIS
1	D	179	GLN
1	D	241	GLN
1	D	245	HIS
1	D	257	HIS
1	D	291	GLN
1	D	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 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
3	DGT	B	458	-	32,33,33	1.19	3 (9%)	48,52,52	1.79	7 (14%)
3	DGT	A	458	-	32,33,33	1.17	3 (9%)	48,52,52	1.74	6 (12%)
3	DGT	D	458	-	32,33,33	1.24	4 (12%)	48,52,52	1.78	6 (12%)
3	DGT	C	458	-	32,33,33	1.30	3 (9%)	48,52,52	1.81	7 (14%)
4	DTP	D	459	-	31,32,32	2.47	11 (35%)	46,50,50	1.78	8 (17%)
4	DTP	B	459	-	31,32,32	2.52	9 (29%)	46,50,50	1.85	10 (21%)

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	B	458	-	-	3/22/34/34	0/3/3/3
3	DGT	A	458	-	-	8/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DGT	D	458	-	-	6/22/34/34	0/3/3/3
3	DGT	C	458	-	-	4/22/34/34	0/3/3/3
4	DTP	D	459	-	-	3/22/34/34	0/3/3/3
4	DTP	B	459	-	-	6/22/34/34	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	459	DTP	PG-O3G	6.59	1.79	1.54
4	B	459	DTP	PG-O2G	6.54	1.79	1.54
4	D	459	DTP	PG-O2G	6.47	1.78	1.54
4	D	459	DTP	PG-O3G	6.44	1.78	1.54
4	B	459	DTP	PB-O2B	5.15	1.79	1.55
4	B	459	DTP	PA-O2A	5.12	1.79	1.55
4	D	459	DTP	PB-O2B	5.05	1.78	1.55
4	D	459	DTP	PA-O2A	5.04	1.78	1.55
3	D	458	DGT	C5-C4	3.49	1.48	1.38
3	B	458	DGT	C5-C4	3.46	1.48	1.38
3	A	458	DGT	C5-C4	3.15	1.47	1.38
3	C	458	DGT	C5-C4	3.15	1.47	1.38
3	C	458	DGT	PB-O3A	3.09	1.62	1.59
4	D	459	DTP	PG-O1G	3.00	1.59	1.50
3	C	458	DGT	PA-O3A	2.90	1.62	1.59
4	B	459	DTP	PG-O1G	2.87	1.59	1.50
4	B	459	DTP	PB-O3A	2.82	1.62	1.59
3	D	458	DGT	PB-O3B	2.65	1.62	1.59
4	D	459	DTP	PB-O1B	2.63	1.59	1.50
4	B	459	DTP	PB-O1B	2.61	1.59	1.50
4	D	459	DTP	PA-O1A	2.59	1.59	1.50
3	D	458	DGT	PA-O3A	2.53	1.62	1.59
4	B	459	DTP	PA-O1A	2.52	1.59	1.50
4	B	459	DTP	PB-O3B	2.37	1.62	1.59
3	A	458	DGT	C5-N7	-2.33	1.34	1.39
3	D	458	DGT	PB-O3A	2.26	1.61	1.59
3	A	458	DGT	PB-O3A	2.24	1.61	1.59
4	D	459	DTP	PB-O3B	2.23	1.61	1.59
4	D	459	DTP	PB-O3A	2.18	1.61	1.59
4	D	459	DTP	C5-N7	-2.12	1.35	1.39
3	B	458	DGT	C6-N1	-2.11	1.34	1.38
3	B	458	DGT	PA-O3A	2.10	1.61	1.59
4	D	459	DTP	C8-N7	2.02	1.35	1.31

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	458	DGT	C5-C4-N3	-6.07	118.73	128.39
3	D	458	DGT	C5-C4-N3	-5.86	119.06	128.39
3	C	458	DGT	C5-C4-N3	-5.72	119.28	128.39
4	D	459	DTP	C5-C4-N3	-5.68	118.89	126.72
3	A	458	DGT	C5-C4-N3	-5.63	119.43	128.39
3	C	458	DGT	C2-N3-C4	5.49	121.76	112.30
4	B	459	DTP	C5-C4-N3	-5.30	119.42	126.72
3	D	458	DGT	C2-N3-C4	5.20	121.26	112.30
4	B	459	DTP	N3-C2-N1	-5.17	120.75	128.58
4	D	459	DTP	N3-C2-N1	-5.17	120.75	128.58
3	B	458	DGT	C2-N3-C4	5.12	121.13	112.30
3	B	458	DGT	N9-C4-N3	4.98	135.91	125.95
3	A	458	DGT	C2-N3-C4	4.82	120.61	112.30
3	D	458	DGT	N9-C4-N3	4.79	135.53	125.95
3	A	458	DGT	N9-C4-N3	4.79	135.53	125.95
3	C	458	DGT	N9-C4-N3	4.35	134.65	125.95
4	D	459	DTP	N3-C4-N9	3.81	133.64	127.17
4	D	459	DTP	C2-N3-C4	3.80	121.10	111.83
4	B	459	DTP	C2-N3-C4	3.75	120.99	111.83
4	B	459	DTP	N3-C4-N9	3.49	133.10	127.17
3	C	458	DGT	C6-C5-N7	3.46	136.58	130.29
3	A	458	DGT	O6-C6-C5	-3.41	117.54	126.53
4	B	459	DTP	N9-C8-N7	-3.40	109.11	113.94
3	D	458	DGT	C6-C5-N7	3.16	136.05	130.29
3	B	458	DGT	C6-C5-N7	3.10	135.94	130.29
4	D	459	DTP	N9-C8-N7	-2.92	109.79	113.94
3	A	458	DGT	C6-C5-N7	2.75	135.29	130.29
3	D	458	DGT	O6-C6-C5	-2.74	119.31	126.53
3	C	458	DGT	O6-C6-C5	-2.68	119.45	126.53
4	B	459	DTP	C4-C5-N7	-2.63	107.57	110.58
4	B	459	DTP	C2'-C1'-N9	-2.59	108.54	114.63
4	B	459	DTP	C4-N9-C8	2.58	108.45	105.74
4	B	459	DTP	C5-N7-C8	2.51	107.39	103.45
3	B	458	DGT	O6-C6-C5	-2.37	120.28	126.53
4	D	459	DTP	C5-N7-C8	2.25	106.99	103.45
3	C	458	DGT	C4-C5-N7	-2.24	107.12	110.67
4	D	459	DTP	C4-C5-N7	-2.24	108.02	110.58
3	D	458	DGT	C5-C6-N1	2.18	118.79	113.25
3	C	458	DGT	C5-C6-N1	2.17	118.77	113.25
3	B	458	DGT	C4-C5-N7	-2.16	107.24	110.67
3	A	458	DGT	C5-C6-N1	2.13	118.67	113.25
4	B	459	DTP	C2'-C3'-C4'	2.11	107.09	102.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	459	DTP	O4'-C1'-N9	2.11	111.76	107.96
3	B	458	DGT	C5-C6-N1	2.02	118.40	113.25

There are no chirality outliers.

All (30) torsion outliers are listed below:

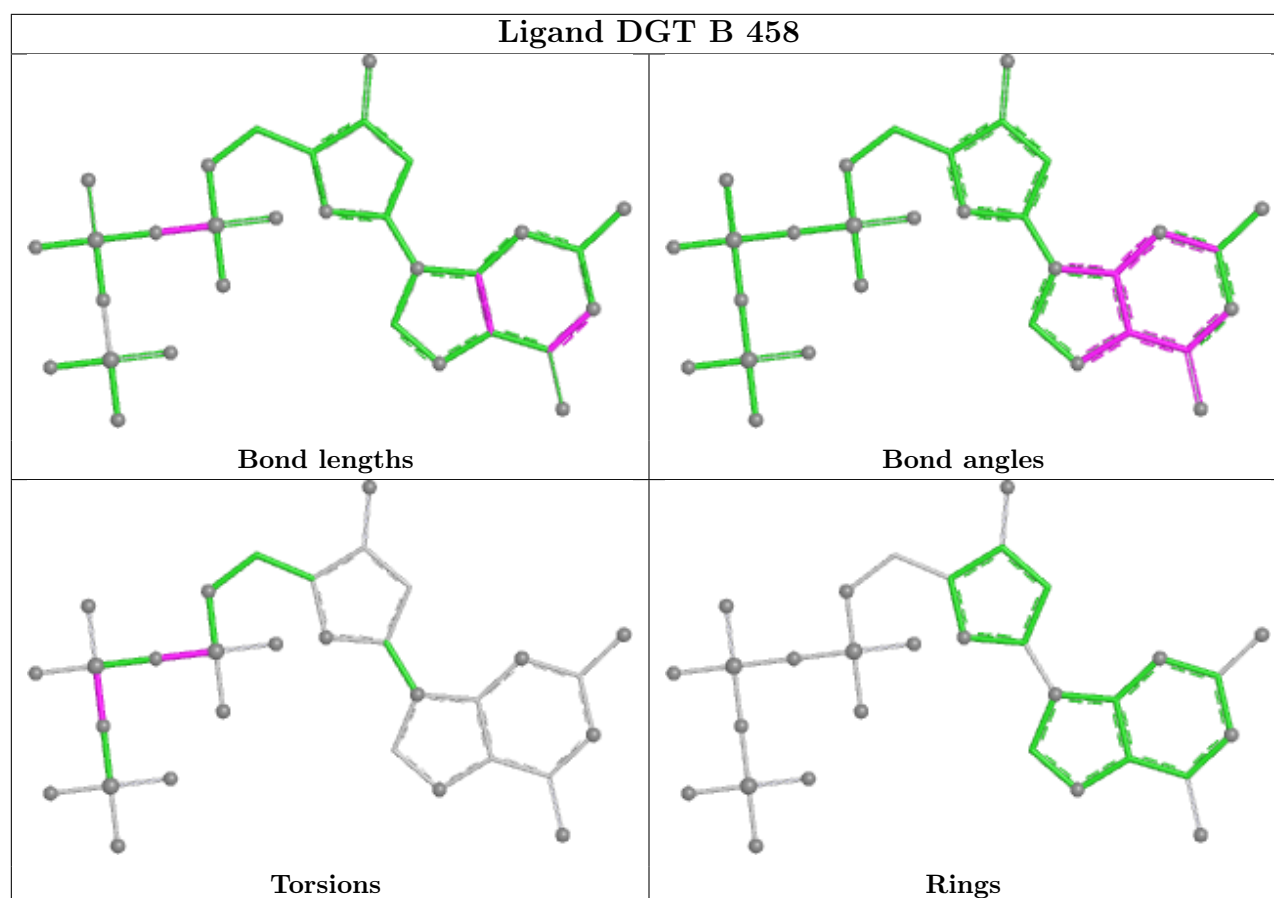
Mol	Chain	Res	Type	Atoms
3	A	458	DGT	PB-O3B-PG-O1G
3	A	458	DGT	C5'-O5'-PA-O3A
3	A	458	DGT	C5'-O5'-PA-O1A
3	A	458	DGT	C5'-O5'-PA-O2A
3	D	458	DGT	PB-O3B-PG-O1G
3	D	458	DGT	C5'-O5'-PA-O3A
3	D	458	DGT	C5'-O5'-PA-O1A
3	C	458	DGT	O4'-C4'-C5'-O5'
3	C	458	DGT	C3'-C4'-C5'-O5'
4	B	459	DTP	O4'-C4'-C5'-O5'
4	B	459	DTP	C3'-C4'-C5'-O5'
4	D	459	DTP	C2'-C1'-N9-C4
4	D	459	DTP	O4'-C1'-N9-C4
3	A	458	DGT	O4'-C4'-C5'-O5'
3	D	458	DGT	C5'-O5'-PA-O2A
3	C	458	DGT	PB-O3A-PA-O2A
4	B	459	DTP	PG-O3B-PB-O2B
4	B	459	DTP	PA-O3A-PB-O2B
4	D	459	DTP	O4'-C4'-C5'-O5'
3	B	458	DGT	PB-O3A-PA-O1A
3	B	458	DGT	PB-O3A-PA-O2A
3	A	458	DGT	PB-O3B-PG-O3G
3	A	458	DGT	PB-O3B-PG-O2G
3	D	458	DGT	PB-O3B-PG-O2G
3	C	458	DGT	PB-O3A-PA-O1A
3	D	458	DGT	PB-O3A-PA-O1A
4	B	459	DTP	PG-O3B-PB-O1B
3	A	458	DGT	C3'-C4'-C5'-O5'
3	B	458	DGT	PG-O3B-PB-O1B
4	B	459	DTP	PA-O3A-PB-O1B

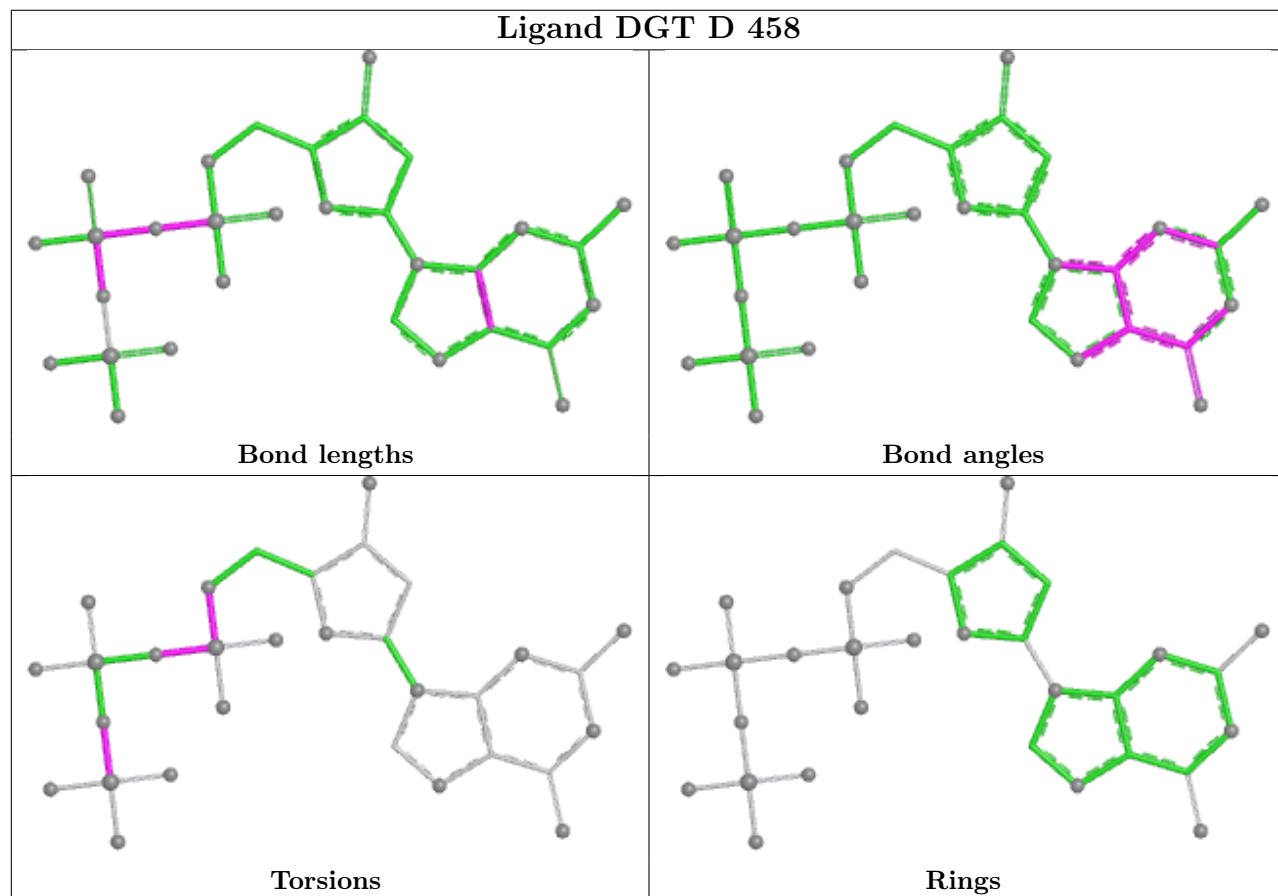
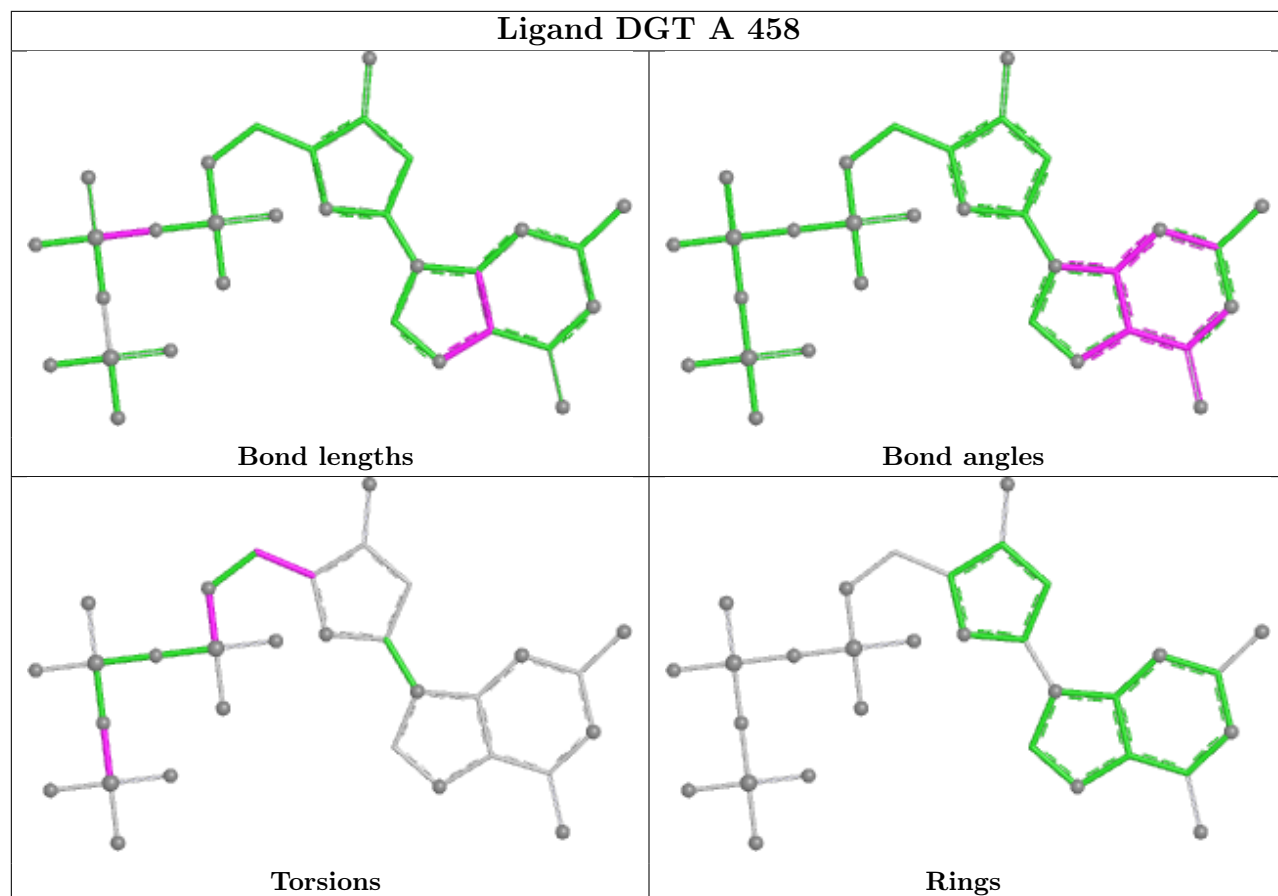
There are no ring outliers.

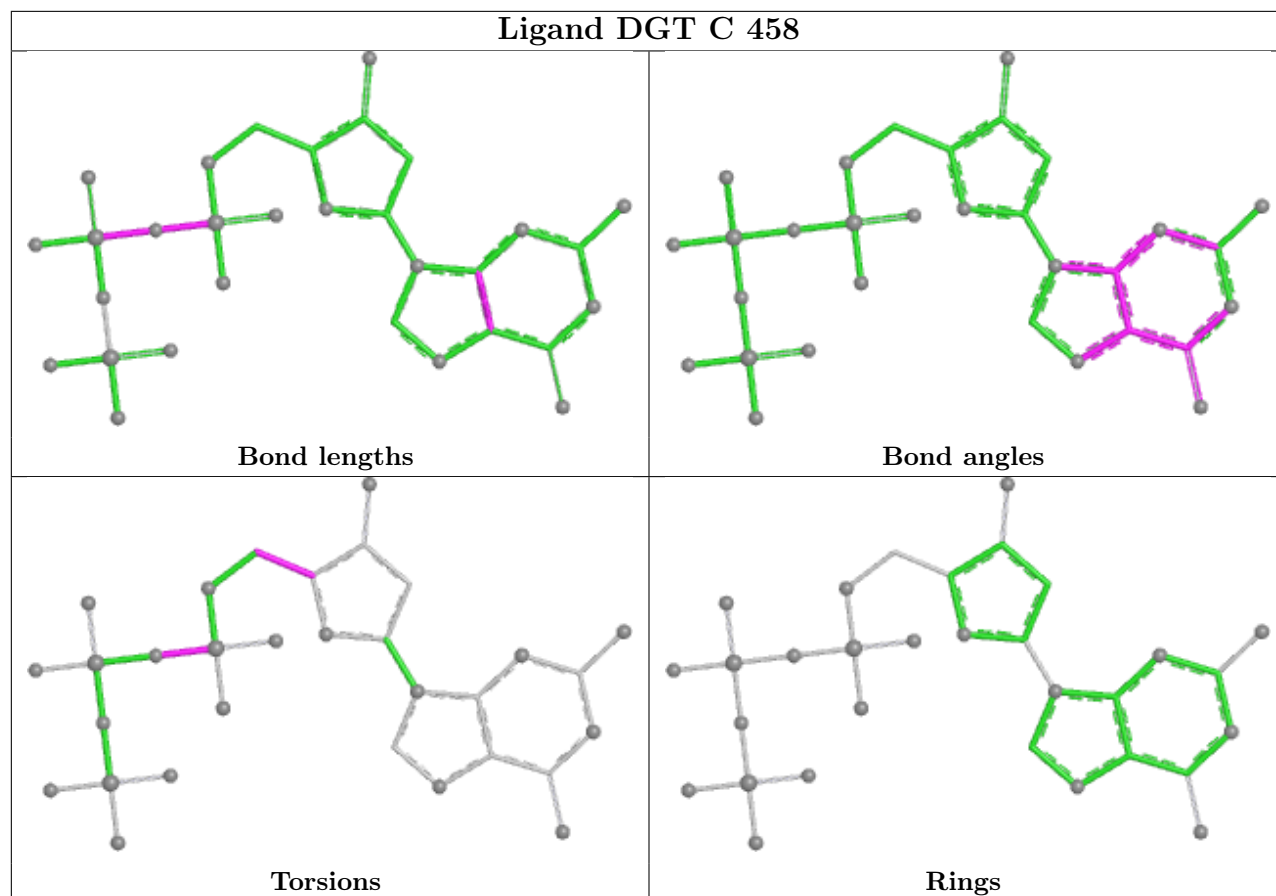
3 monomers are involved in 6 short contacts:

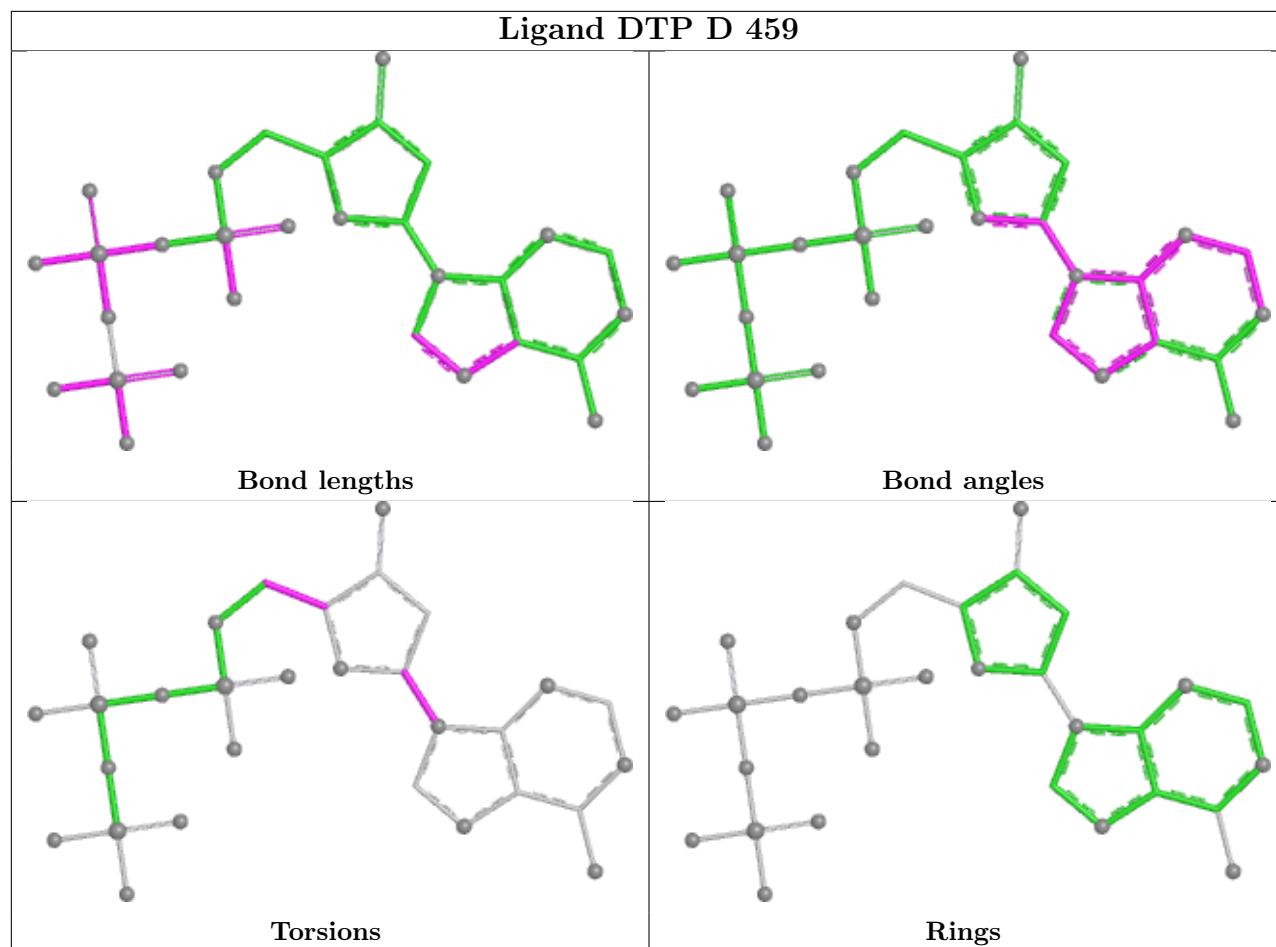
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	458	DGT	1	0
3	D	458	DGT	2	0
4	D	459	DTP	3	0

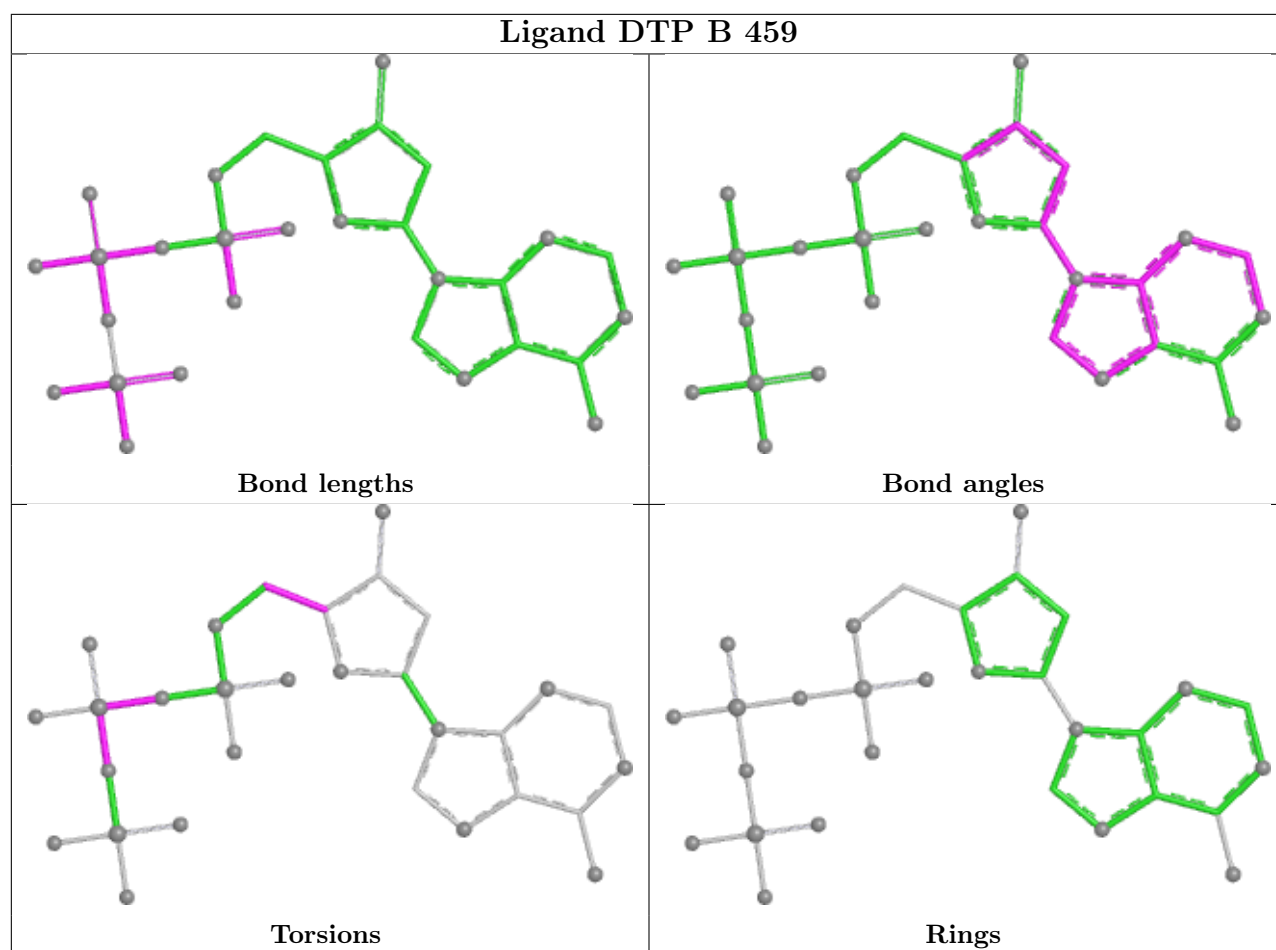
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	450/480 (93%)	0.06	6 (1%) 75 71	17, 39, 52, 64	3 (0%)
1	B	445/480 (92%)	0.11	13 (2%) 53 50	19, 38, 52, 70	9 (2%)
1	C	454/480 (94%)	0.11	3 (0%) 84 81	16, 39, 52, 64	2 (0%)
1	D	434/480 (90%)	0.12	14 (3%) 50 46	17, 39, 52, 64	7 (1%)
All	All	1783/1920 (92%)	0.10	36 (2%) 65 60	16, 39, 52, 70	21 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	4.6
1	B	199	TYR	4.5
1	A	200	GLY	4.1
1	C	435	LEU	4.1
1	D	199	TYR	3.9
1	C	199	TYR	3.5
1	B	371	PRO	3.4
1	B	410	GLY	3.3
1	D	200	GLY	3.1
1	D	368	TYR	3.0
1	B	426	ASP	3.0
1	C	200	GLY	2.8
1	A	199	TYR	2.7
1	B	435	LEU	2.7
1	D	410	GLY	2.5
1	D	367	SER	2.5
1	D	369	ASP	2.5
1	B	429	ASN	2.5
1	B	1	MET	2.5
1	D	404	LEU	2.4
1	A	273	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	414	GLY	2.3
1	B	335	THR	2.3
1	D	201	THR	2.2
1	D	384	THR	2.2
1	A	228	VAL	2.2
1	A	412	SER	2.2
1	D	405	VAL	2.2
1	D	366	SER	2.2
1	D	198	GLU	2.1
1	D	406	ALA	2.0
1	D	60	GLU	2.0
1	B	201	THR	2.0
1	B	273	TYR	2.0
1	B	367	SER	2.0
1	B	389	MET	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.

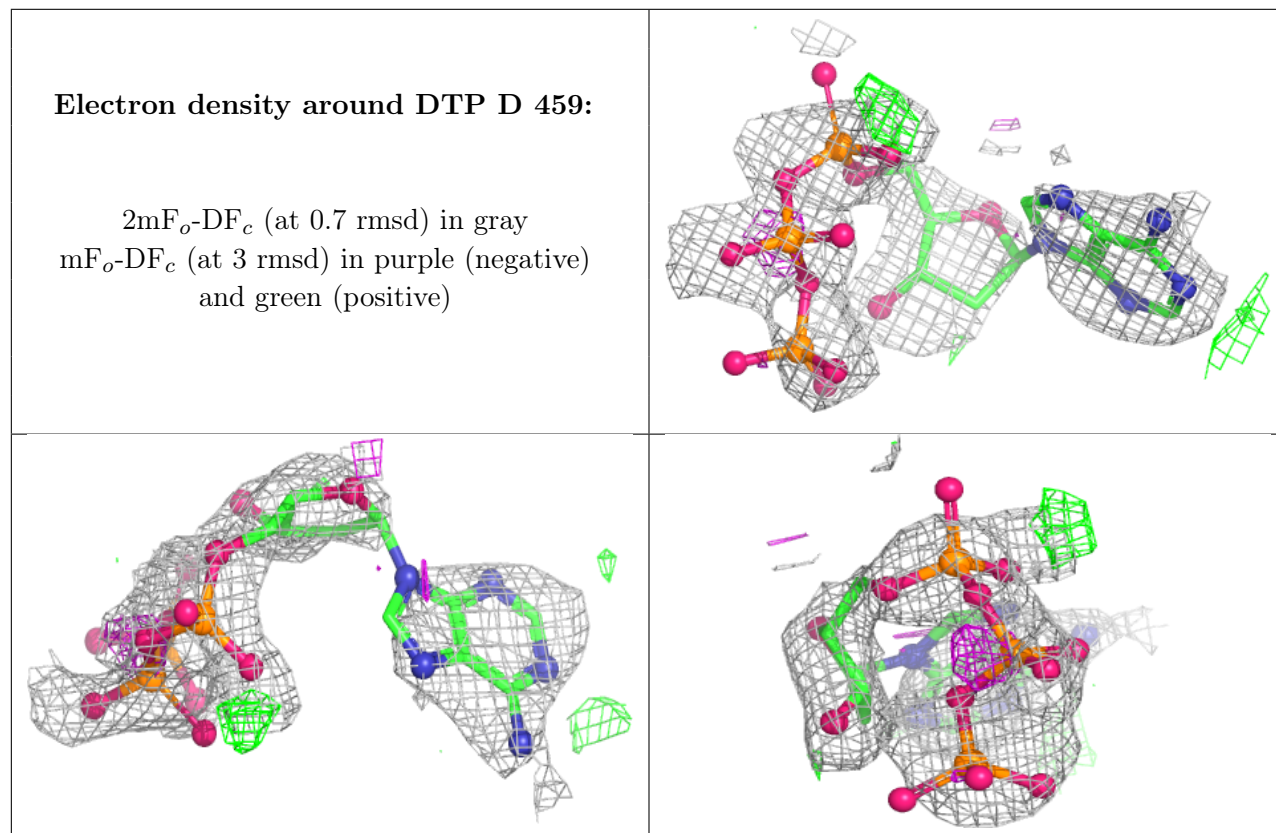
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DTP	D	459	30/30	0.73	0.18	67,68,86,87	30
4	DTP	B	459	30/30	0.78	0.17	55,58,73,74	30
3	DGT	D	458	31/31	0.89	0.10	33,44,69,71	0
3	DGT	B	458	31/31	0.90	0.10	33,41,66,68	0
3	DGT	C	458	31/31	0.92	0.10	28,34,61,63	0
3	DGT	A	458	31/31	0.92	0.10	28,36,67,68	0
2	CA	C	457	1/1	0.98	0.12	35,35,35,35	0
2	CA	A	457	1/1	0.99	0.13	31,31,31,31	0

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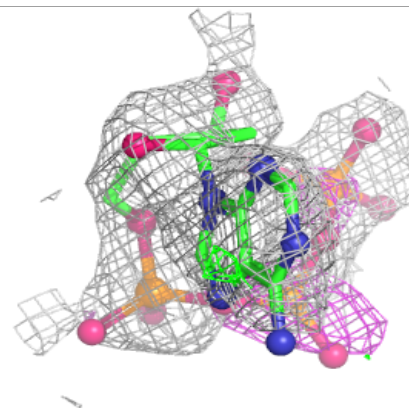
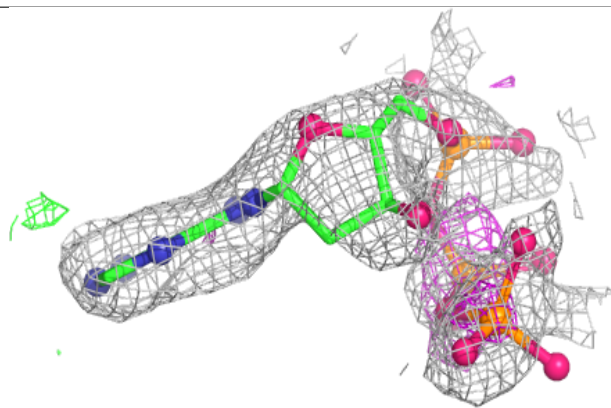
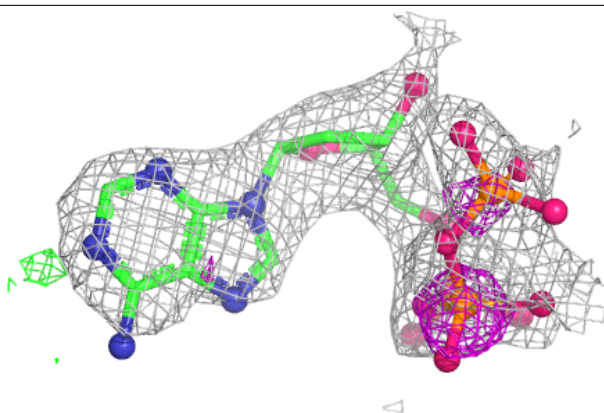
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	457	1/1	0.99	0.13	34,34,34,34	0
2	CA	B	457	1/1	1.00	0.11	29,29,29,29	0

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.

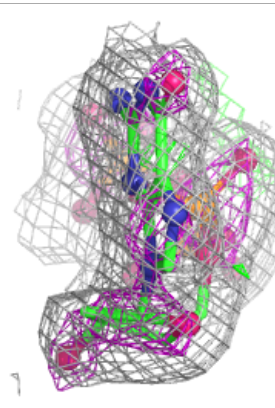
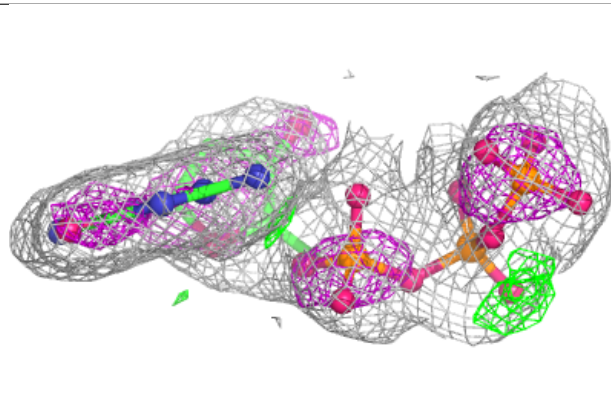
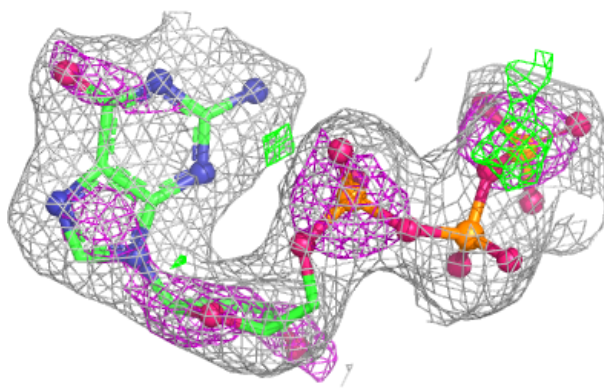


Electron density around DTP B 459:

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

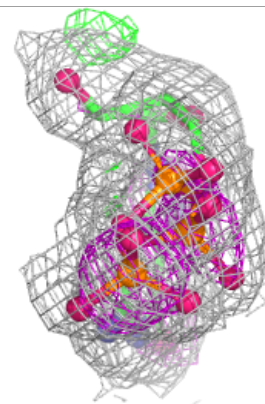
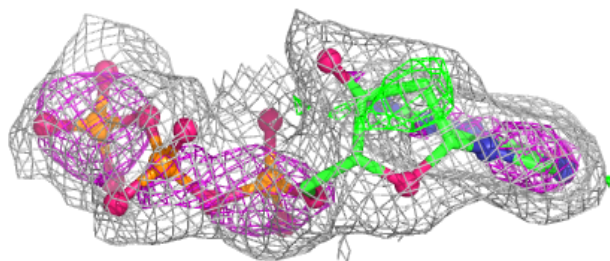
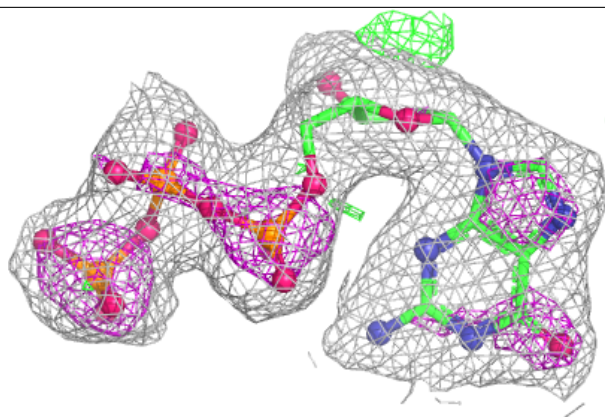
**Electron density around DGT D 458:**

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



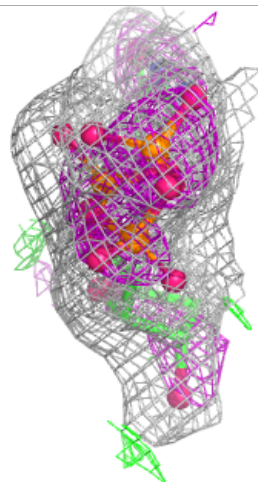
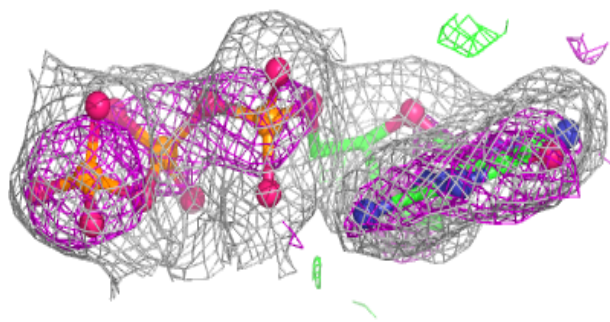
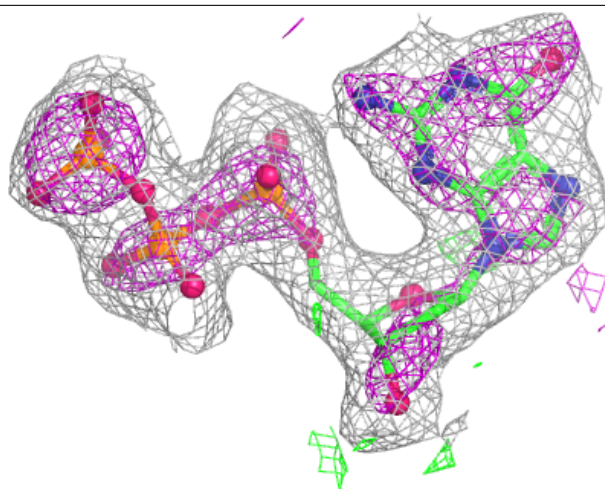
Electron density around DGT B 458:

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



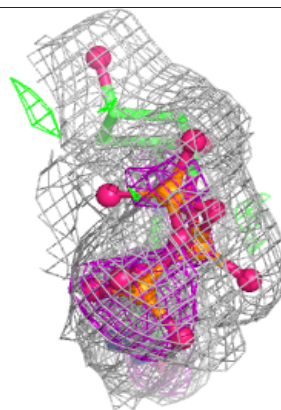
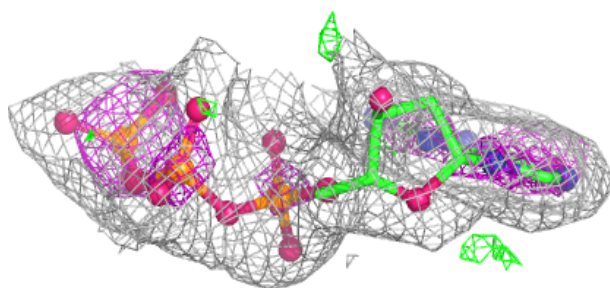
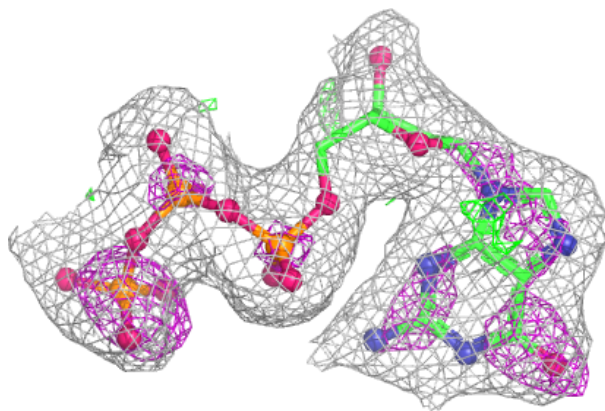
Electron density around DGT C 458:

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



Electron density around DGT A 458:

$2mF_o-DF_c$ (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.