Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 10:24 AM EDT

PDB ID	:	3PKQ
Title	:	Q83D Variant of S. Enterica RmlA with dGTP
Authors	:	Chang, A.; Moretti, R.; Bingman, C.A.; Thorson, J.S.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2010-11-11
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 (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:

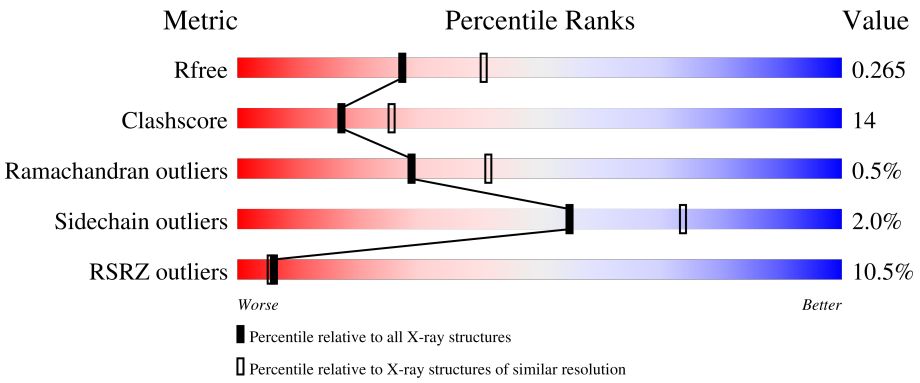
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	292	2% 76% 21% • •
1	B	292	4% 72% 25% • •
1	C	292	16% 71% 25% • •
1	D	292	19% 72% 23% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	294	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9278 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.

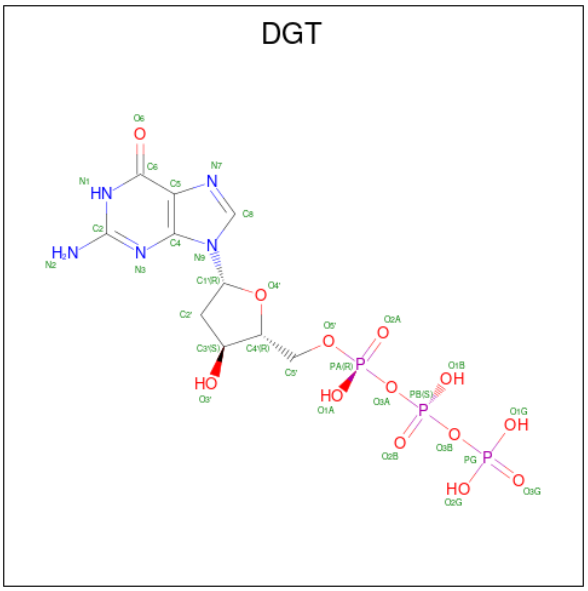
- Molecule 1 is a protein called Glucose-1-phosphate thymidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2251	1440	372	428	11	0	3	0
1	B	286	2259	1446	374	427	12	0	3	0
1	C	284	2221	1424	367	419	11	0	0	0
1	D	278	2172	1394	358	409	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ASP	GLN	engineered mutation	UNP P26393
B	83	ASP	GLN	engineered mutation	UNP P26393
C	83	ASP	GLN	engineered mutation	UNP P26393
D	83	ASP	GLN	engineered mutation	UNP P26393

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

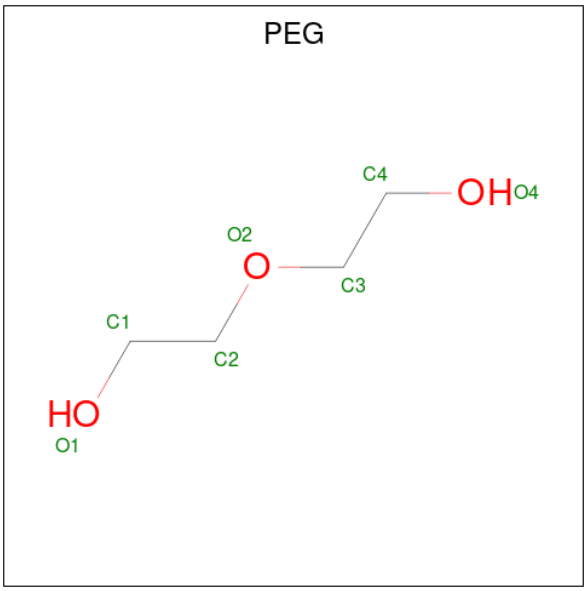


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0
2	B	1	31	10	5	13	3	0	0
2	C	1	31	10	5	13	3	0	0
2	D	1	31	10	5	13	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	2	2	2	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

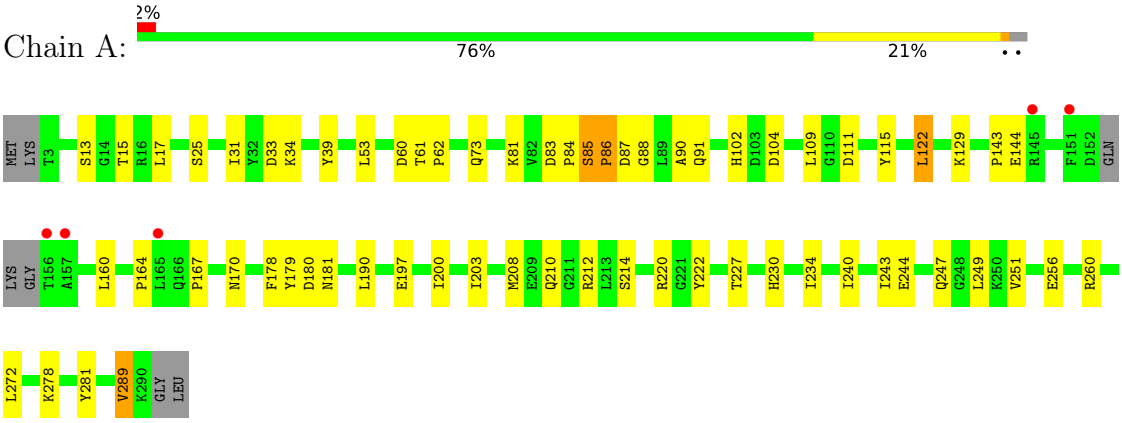
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	98	Total O 98 98	0	0
5	B	83	Total O 83 83	0	0
5	C	28	Total O 28 28	0	0
5	D	16	Total O 16 16	0	0

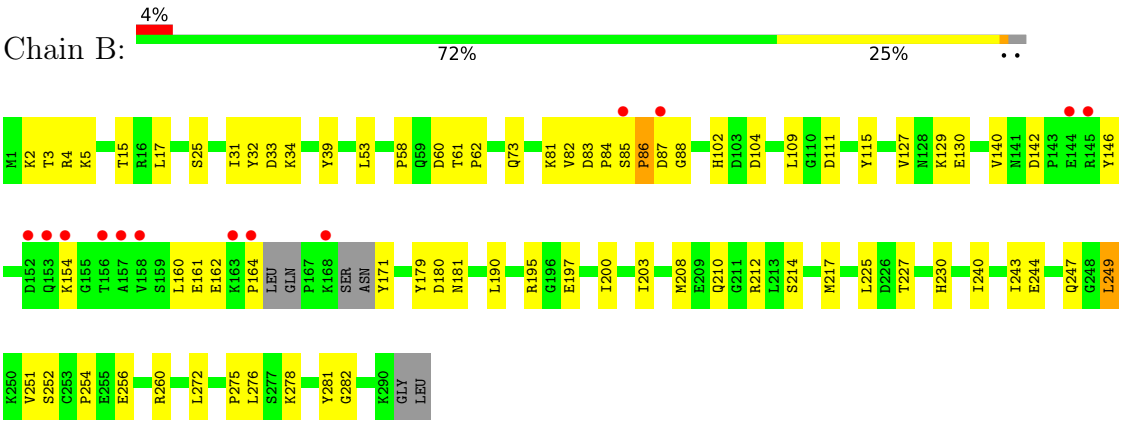
3 Residue-property plots (i)

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.

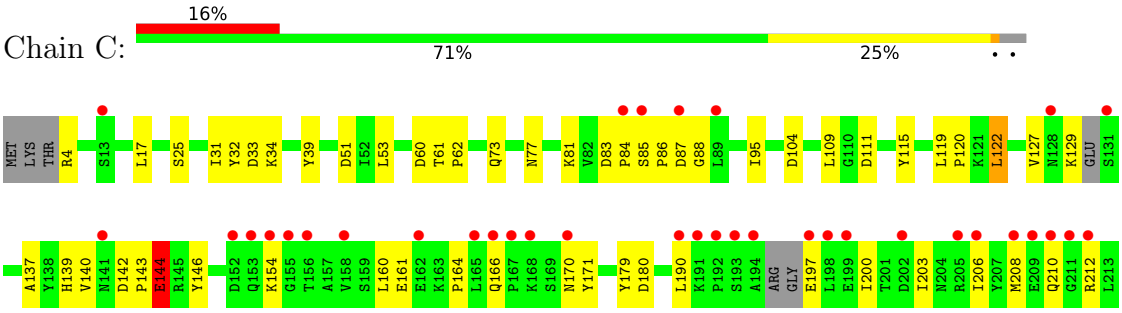
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

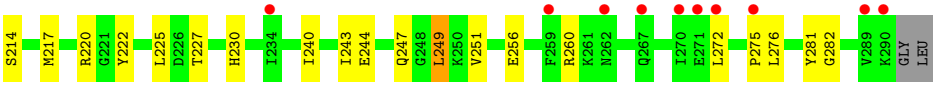


• Molecule 1: Glucose-1-phosphate thymidylyltransferase



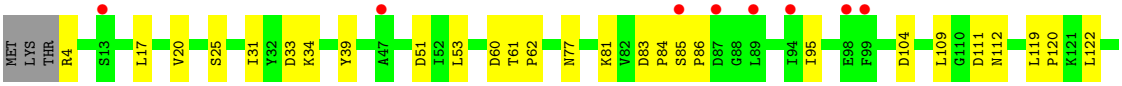
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

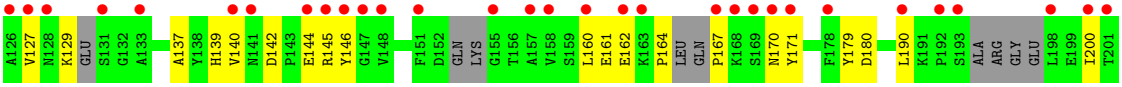


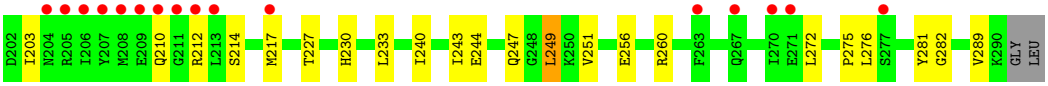


- Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	109.40Å 109.40Å 110.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.71 – 2.40 44.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.71-2.40) 97.4 (44.71-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.212 , 0.271 0.207 , 0.265	Depositor DCC
R_{free} test set	2516 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,-l,-k 0.014 for -h,l,k 0.013 for l,-k,h 0.026 for -l,-k,-h 0.064 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9278	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: DGT, MG, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.53	0/2298	0.60	0/3113
1	B	0.48	0/2305	0.57	0/3116
1	C	0.39	0/2266	0.57	2/3066 (0.1%)
1	D	0.37	0/2215	0.56	0/2994
All	All	0.45	0/9084	0.58	2/12289 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	144	GLU	CA-CB-CG	5.55	125.62	113.40
1	C	225	LEU	CA-CB-CG	5.29	127.46	115.30

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	2251	0	2243	75	0
1	B	2259	0	2262	78	0
1	C	2221	0	2222	68	0
1	D	2172	0	2170	54	0
2	A	31	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	12	2	0
2	C	31	0	12	1	0
2	D	31	0	12	2	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	20	6	0
4	C	7	0	10	3	0
5	A	98	0	0	3	0
5	B	83	0	0	7	0
5	C	28	0	0	1	0
5	D	16	0	0	3	0
All	All	9278	0	8975	251	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 14.

All (251) 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:86[B]:PRO:HB2	1:B:87[B]:ASP:HA	1.27	1.15
1:C:87:ASP:HB3	1:C:197:GLU:HG3	1.17	1.09
1:C:33:ASP:HB2	1:D:230:HIS:ND1	1.77	1.00
1:B:86[B]:PRO:HB2	1:B:87[B]:ASP:CA	1.93	0.99
1:D:142:ASP:HB2	1:D:144:GLU:OE2	1.62	0.98
1:A:87[A]:ASP:HB3	1:A:197:GLU:HG3	1.46	0.95
1:A:200:ILE:HB	5:A:380:HOH:O	1.67	0.93
1:A:234:ILE:HB	4:A:294:PEG:H11	1.48	0.92
1:A:33:ASP:HB2	1:B:230:HIS:ND1	1.84	0.91
1:A:230:HIS:ND1	1:B:33:ASP:HB2	1.87	0.90
1:C:33:ASP:CB	1:D:230:HIS:ND1	2.36	0.88
1:A:87[B]:ASP:HB3	1:A:197:GLU:HG3	1.53	0.88
1:C:87:ASP:HB3	1:C:197:GLU:CG	2.04	0.87
1:A:88:GLY:N	1:A:197:GLU:HG2	1.90	0.86
1:B:88:GLY:N	1:B:197:GLU:HG2	1.91	0.85
1:A:33:ASP:CB	1:B:230:HIS:ND1	2.40	0.85
1:B:247:GLN:NE2	1:C:115:TYR:HE2	1.76	0.82
4:C:293:PEG:H41	1:D:233:LEU:HD23	1.61	0.82
1:C:88:GLY:N	1:C:197:GLU:HG2	1.95	0.81
1:B:247:GLN:NE2	1:C:115:TYR:CE2	2.50	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86[B]:PRO:CB	1:A:87[B]:ASP:HA	2.12	0.79
1:A:230:HIS:ND1	1:B:33:ASP:CB	2.46	0.79
1:B:115:TYR:HE2	1:C:247:GLN:NE2	1.83	0.77
1:B:86[B]:PRO:HD3	2:B:500:DGT:O6	1.85	0.76
1:A:86[B]:PRO:HD2	2:A:500:DGT:O6	1.86	0.75
1:C:230:HIS:ND1	1:D:33:ASP:HB2	2.03	0.74
1:A:86[B]:PRO:HB3	1:A:87[B]:ASP:C	2.08	0.73
1:B:115:TYR:CE2	1:C:247:GLN:NE2	2.57	0.73
1:A:86[B]:PRO:HB3	1:A:88:GLY:N	2.04	0.73
1:C:33:ASP:HB2	1:D:230:HIS:CE1	2.24	0.73
1:A:86[B]:PRO:CB	1:A:87[B]:ASP:CA	2.66	0.72
1:A:87[B]:ASP:HB3	1:A:197:GLU:CG	2.19	0.72
1:A:87[A]:ASP:HB3	1:A:197:GLU:CG	2.20	0.71
1:B:87[B]:ASP:HB3	1:B:197:GLU:HG3	1.73	0.71
1:B:85[A]:SER:N	1:B:86[A]:PRO:HD3	2.05	0.70
1:B:86[B]:PRO:CB	1:B:87[B]:ASP:CA	2.71	0.69
1:B:247:GLN:HE22	1:C:115:TYR:HE2	1.42	0.67
1:D:142:ASP:CB	1:D:144:GLU:OE2	2.38	0.67
1:B:86[B]:PRO:HB3	1:B:88:GLY:N	2.10	0.66
1:B:86[B]:PRO:CB	1:B:88:GLY:N	2.57	0.66
1:A:115:TYR:HE2	1:D:247:GLN:NE2	1.94	0.65
1:A:33:ASP:HB2	1:B:230:HIS:CE1	2.31	0.65
1:A:86[B]:PRO:HB3	1:A:87[B]:ASP:CA	2.27	0.65
1:B:115:TYR:HE2	1:C:247:GLN:HE22	1.45	0.65
1:A:86[B]:PRO:HB3	1:A:87[B]:ASP:HA	1.81	0.63
1:A:234:ILE:CB	4:A:294:PEG:H11	2.24	0.62
1:A:230:HIS:CE1	1:B:33:ASP:HB2	2.34	0.62
1:C:32:TYR:O	4:C:293:PEG:H42	2.00	0.62
1:B:58:PRO:HA	1:B:82:VAL:HG11	1.81	0.62
1:C:85:SER:N	1:C:86:PRO:HD3	2.14	0.61
1:C:144:GLU:CD	1:C:144:GLU:H	2.03	0.61
1:A:86[B]:PRO:HB2	1:A:87[B]:ASP:HA	1.81	0.61
1:D:85:SER:N	1:D:86:PRO:HD3	2.15	0.61
1:A:84:PRO:C	1:A:86[A]:PRO:HD3	2.21	0.61
1:B:84:PRO:O	1:B:85[B]:SER:HB2	2.02	0.60
1:A:86[B]:PRO:HG2	2:A:500:DGT:O6	2.02	0.59
1:D:109:LEU:HB3	2:D:500:DGT:H4'	1.85	0.58
1:C:230:HIS:ND1	1:D:33:ASP:CB	2.66	0.58
1:B:86[B]:PRO:HB2	1:B:88:GLY:N	2.19	0.57
1:B:243:ILE:HG23	1:B:247:GLN:OE1	2.03	0.57
1:A:15:THR:HB	5:B:358:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASP:C	1:D:85:SER:H	2.07	0.57
1:C:83:ASP:C	1:C:85:SER:H	2.08	0.56
1:B:249:LEU:HB3	1:C:220:ARG:HG3	1.87	0.56
1:B:160:LEU:HD12	1:B:208:MET:HE2	1.87	0.56
1:D:210:GLN:OE1	1:D:212:ARG:HD3	2.06	0.56
1:B:61:THR:OG1	1:B:82:VAL:HG22	2.06	0.56
1:C:34:LYS:HE2	1:C:251:VAL:O	2.05	0.56
1:A:115:TYR:CE2	1:D:247:GLN:NE2	2.73	0.55
1:C:144:GLU:OE1	1:C:144:GLU:N	2.38	0.55
1:C:210:GLN:OE1	1:C:212:ARG:HD3	2.06	0.55
1:C:109:LEU:HB3	2:C:500:DGT:H4'	1.87	0.55
1:A:17:LEU:HD23	1:A:230:HIS:HD2	1.71	0.55
1:B:142:ASP:OD1	1:B:142:ASP:N	2.39	0.55
1:D:17:LEU:HD23	1:D:230:HIS:HD2	1.72	0.55
1:D:144:GLU:OE1	1:D:144:GLU:N	2.30	0.55
1:C:160:LEU:HD12	1:C:208:MET:HE2	1.89	0.54
4:A:294:PEG:H12	1:B:32:TYR:HA	1.89	0.54
1:B:109:LEU:HB3	2:B:500:DGT:H4'	1.88	0.54
1:C:142:ASP:N	1:C:142:ASP:OD1	2.40	0.54
1:D:256:GLU:O	1:D:260:ARG:HG2	2.07	0.54
1:C:17:LEU:HD23	1:C:230:HIS:HD2	1.73	0.54
1:B:2:LYS:HG2	5:B:319:HOH:O	2.07	0.54
1:B:225:LEU:CD2	5:B:366:HOH:O	2.55	0.54
1:C:53:LEU:HD11	1:C:81:LYS:HG3	1.90	0.54
1:D:167:PRO:CD	5:D:308:HOH:O	2.56	0.54
1:A:179:TYR:O	4:A:293:PEG:H31	2.07	0.54
1:A:210:GLN:OE1	1:A:212:ARG:HD3	2.08	0.53
1:B:87[B]:ASP:HB3	1:B:197:GLU:CG	2.38	0.53
1:D:53:LEU:HD11	1:D:81:LYS:HG3	1.91	0.53
1:A:53:LEU:HD11	1:A:81:LYS:HG3	1.90	0.53
1:A:86[B]:PRO:CD	2:A:500:DGT:O6	2.53	0.53
1:C:32:TYR:HA	4:C:293:PEG:H31	1.90	0.53
1:D:111:ASP:HB2	1:D:227:THR:OG1	2.08	0.53
1:B:111:ASP:HB2	1:B:227:THR:OG1	2.09	0.53
1:C:111:ASP:HB2	1:C:227:THR:OG1	2.09	0.53
1:A:85[B]:SER:O	1:A:86[B]:PRO:O	2.27	0.53
1:B:17:LEU:HD23	1:B:230:HIS:HD2	1.73	0.53
1:B:87[A]:ASP:HB3	1:B:197:GLU:HG3	1.90	0.53
1:D:142:ASP:OD1	1:D:142:ASP:N	2.42	0.53
1:B:86[B]:PRO:HB2	1:B:87[B]:ASP:C	2.28	0.53
1:B:256:GLU:O	1:B:260:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LYS:HE2	1:D:251:VAL:O	2.09	0.52
1:B:210:GLN:OE1	1:B:212:ARG:HD3	2.09	0.52
1:A:111:ASP:HB2	1:A:227:THR:OG1	2.08	0.52
1:B:243:ILE:CD1	1:C:243:ILE:HD11	2.40	0.52
1:A:160:LEU:HD12	1:A:208:MET:HE2	1.92	0.52
1:B:225:LEU:HD23	5:B:366:HOH:O	2.09	0.52
1:D:171:TYR:HE2	1:D:217:MET:HG3	1.75	0.52
1:C:256:GLU:O	1:C:260:ARG:HG2	2.09	0.52
1:B:195:ARG:NH1	1:B:197:GLU:OE1	2.43	0.52
1:A:256:GLU:O	1:A:260:ARG:HG2	2.11	0.51
1:B:84:PRO:C	1:B:86[A]:PRO:HD3	2.30	0.51
1:D:25:SER:HB2	1:D:60:ASP:CG	2.30	0.51
1:B:86[B]:PRO:CB	1:B:87[B]:ASP:C	2.79	0.51
1:D:167:PRO:HD3	5:D:308:HOH:O	2.12	0.50
1:A:178:PHE:HB3	4:A:293:PEG:H32	1.91	0.50
1:B:58:PRO:CA	1:B:82:VAL:HG11	2.40	0.50
1:A:220:ARG:HG3	1:D:249:LEU:HB3	1.93	0.50
1:B:25:SER:HB2	1:B:60:ASP:CG	2.31	0.50
1:B:102:HIS:HA	1:B:181:ASN:ND2	2.26	0.50
1:B:171:TYR:HE2	1:B:217:MET:HG3	1.77	0.50
1:A:129:LYS:HE3	1:A:214:SER:OG	2.13	0.49
1:B:85[A]:SER:N	1:B:86[A]:PRO:CD	2.74	0.49
1:B:84:PRO:O	1:B:85[B]:SER:CB	2.57	0.49
1:B:243:ILE:CD1	1:C:243:ILE:CD1	2.91	0.49
1:D:190:LEU:HD22	1:D:203:ILE:HG13	1.94	0.49
1:A:109:LEU:HB3	2:A:500:DGT:H4'	1.94	0.49
1:A:234:ILE:HB	4:A:294:PEG:C1	2.33	0.49
1:C:171:TYR:HE2	1:C:217:MET:HG3	1.78	0.48
1:D:84:PRO:C	1:D:86:PRO:HD3	2.33	0.48
1:C:119:LEU:HB3	1:C:120:PRO:HD3	1.95	0.48
1:A:122:LEU:HD22	1:A:222:TYR:OH	2.14	0.48
1:C:243:ILE:HG23	1:C:247:GLN:OE1	2.13	0.48
1:A:34:LYS:HE2	1:A:251:VAL:O	2.14	0.48
1:D:31:ILE:HB	1:D:39:TYR:CE1	2.48	0.48
1:B:179:TYR:OH	1:B:200:ILE:HD11	2.13	0.48
1:C:31:ILE:HB	1:C:39:TYR:CE1	2.50	0.47
1:A:86[B]:PRO:CG	2:A:500:DGT:O6	2.62	0.47
1:D:272:LEU:O	1:D:275:PRO:HD2	2.13	0.47
1:A:289:VAL:O	1:A:289:VAL:HG13	2.13	0.47
1:B:243:ILE:HD11	1:C:243:ILE:CD1	2.44	0.47
1:D:240:ILE:O	1:D:244:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ILE:HG23	1:D:247:GLN:OE1	2.14	0.47
1:D:249:LEU:HD23	1:D:249:LEU:H	1.79	0.47
1:A:25:SER:HB2	1:A:60:ASP:CG	2.34	0.47
1:C:230:HIS:O	5:C:314:HOH:O	2.20	0.47
1:A:61:THR:HB	1:A:62:PRO:HD3	1.96	0.47
1:A:85[A]:SER:N	1:A:86[A]:PRO:HD3	2.30	0.47
1:C:25:SER:HB2	1:C:60:ASP:CG	2.34	0.47
1:C:190:LEU:HD22	1:C:203:ILE:HG13	1.95	0.47
1:C:272:LEU:O	1:C:275:PRO:HD2	2.14	0.47
1:C:84:PRO:C	1:C:86:PRO:HD3	2.33	0.47
1:B:3:THR:HB	1:B:5:LYS:HE3	1.97	0.47
1:A:164:PRO:HG2	1:A:167:PRO:HB3	1.97	0.47
1:D:161:GLU:O	1:D:164:PRO:HD3	2.15	0.47
1:B:53:LEU:HD11	1:B:81:LYS:HG3	1.96	0.46
1:A:86[B]:PRO:HD2	2:A:500:DGT:C6	2.44	0.46
1:C:164:PRO:C	1:C:166:GLN:N	2.66	0.46
1:B:2:LYS:HE3	5:B:354:HOH:O	2.16	0.46
1:A:83:ASP:OD2	1:A:86[B]:PRO:HD3	2.16	0.46
1:B:34:LYS:HE2	1:B:251:VAL:O	2.16	0.46
1:B:190:LEU:HD22	1:B:203:ILE:HG13	1.97	0.46
1:C:164:PRO:HB2	1:C:166:GLN:C	2.36	0.46
1:B:61:THR:HB	1:B:62:PRO:HD3	1.97	0.46
1:B:140:VAL:HG11	1:B:146:TYR:CE2	2.51	0.46
1:A:85[A]:SER:N	1:A:86[A]:PRO:CD	2.79	0.45
1:C:61:THR:HB	1:C:62:PRO:HD3	1.97	0.45
1:A:17:LEU:CD2	1:A:230:HIS:HD2	2.30	0.45
1:C:179:TYR:OH	1:C:200:ILE:HD11	2.16	0.45
1:A:73:GLN:HB2	1:A:272:LEU:HD21	1.98	0.45
1:C:240:ILE:O	1:C:244:GLU:HG3	2.17	0.45
1:D:81:LYS:HD3	1:D:95:ILE:HG22	1.99	0.45
1:D:179:TYR:OH	1:D:200:ILE:HD11	2.17	0.45
1:A:243:ILE:HG23	1:A:247:GLN:OE1	2.16	0.45
1:B:104:ASP:OD1	1:B:180:ASP:HA	2.17	0.45
1:C:122:LEU:HD22	1:C:222:TYR:OH	2.17	0.45
1:B:83:ASP:HA	1:B:84:PRO:HD3	1.81	0.45
1:C:249:LEU:H	1:C:249:LEU:HD23	1.82	0.44
1:A:144:GLU:CD	1:A:144:GLU:H	2.21	0.44
1:D:4:ARG:CZ	1:D:127:VAL:HG11	2.48	0.44
1:D:104:ASP:OD1	1:D:180:ASP:HA	2.16	0.44
1:A:31:ILE:HB	1:A:39:TYR:CE1	2.52	0.44
1:D:61:THR:HB	1:D:62:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85[B]:SER:HA	1:A:86[B]:PRO:HD2	1.67	0.44
1:B:252:SER:O	1:B:254:PRO:HD3	2.17	0.44
1:C:104:ASP:OD1	1:C:180:ASP:HA	2.17	0.44
1:A:83:ASP:HA	1:A:84:PRO:HD3	1.81	0.44
1:A:102:HIS:HA	1:A:181:ASN:ND2	2.31	0.44
1:D:140:VAL:HG11	1:D:146:TYR:CE2	2.52	0.44
1:C:206:ILE:O	1:C:210:GLN:HG3	2.17	0.44
1:D:137:ALA:HB1	1:D:171:TYR:HB3	2.00	0.44
1:A:86[B]:PRO:CB	1:A:87[B]:ASP:C	2.82	0.43
1:B:87[A]:ASP:HB3	1:B:197:GLU:CG	2.48	0.43
1:D:109:LEU:HD13	2:D:500:DGT:H5'A	2.00	0.43
1:D:129:LYS:HE3	1:D:214:SER:OG	2.18	0.43
1:A:17:LEU:HD23	1:A:230:HIS:CD2	2.53	0.43
1:A:278:LYS:HB2	5:A:302:HOH:O	2.18	0.43
1:D:119:LEU:HB3	1:D:120:PRO:HD3	2.01	0.43
1:C:73:GLN:HB2	1:C:272:LEU:HD21	2.00	0.43
1:C:276:LEU:O	1:C:282:GLY:HA3	2.18	0.43
1:D:51:ASP:OD2	1:D:77:ASN:HB3	2.19	0.43
1:B:73:GLN:HB2	1:B:272:LEU:HD21	2.01	0.43
1:B:278:LYS:HB2	5:B:299:HOH:O	2.19	0.43
1:C:140:VAL:HG11	1:C:146:TYR:CE2	2.54	0.43
1:A:104:ASP:OD1	1:A:180:ASP:HA	2.19	0.43
1:A:179:TYR:OH	1:A:200:ILE:HD11	2.19	0.43
1:A:190:LEU:HD22	1:A:203:ILE:HG13	2.00	0.42
1:B:31:ILE:HB	1:B:39:TYR:CE1	2.53	0.42
1:C:33:ASP:OD1	1:C:34:LYS:NZ	2.47	0.42
1:D:139:HIS:CE1	1:D:170:ASN:HB3	2.54	0.42
1:C:139:HIS:CE1	1:C:170:ASN:HB3	2.53	0.42
1:C:83:ASP:OD2	1:C:85:SER:HA	2.19	0.42
1:C:85:SER:N	1:C:86:PRO:CD	2.82	0.42
1:C:137:ALA:HB1	1:C:171:TYR:HB3	2.02	0.42
1:C:87:ASP:C	1:C:197:GLU:HG2	2.39	0.42
1:C:129:LYS:HE3	1:C:214:SER:OG	2.19	0.42
1:B:276:LEU:O	1:B:282:GLY:HA3	2.19	0.42
1:A:90:ALA:HB1	1:A:203:ILE:HD12	2.02	0.42
1:D:276:LEU:O	1:D:282:GLY:HA3	2.19	0.42
1:A:83:ASP:C	1:A:85[B]:SER:H	2.22	0.42
1:C:51:ASP:OD2	1:C:77:ASN:HB3	2.20	0.42
1:B:225:LEU:HD22	5:B:366:HOH:O	2.20	0.42
1:D:144:GLU:HG2	1:D:145:ARG:HG2	2.01	0.42
1:D:83:ASP:OD2	1:D:85:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLU:O	1:C:164:PRO:HD3	2.18	0.41
5:A:372:HOH:O	1:B:15:THR:HB	2.19	0.41
1:A:143:PRO:HG3	1:A:170:ASN:HA	2.03	0.41
1:B:272:LEU:O	1:B:275:PRO:HD2	2.21	0.41
1:B:4:ARG:CZ	1:B:127:VAL:HG11	2.51	0.41
1:D:83:ASP:HA	1:D:84:PRO:HD3	1.82	0.41
1:A:86[A]:PRO:HB2	1:A:91:GLN:OE1	2.20	0.41
1:B:247:GLN:HB2	1:B:249:LEU:CD1	2.51	0.41
1:C:81:LYS:HD3	1:C:95:ILE:HG22	2.02	0.41
1:B:129:LYS:HE3	1:B:214:SER:OG	2.21	0.41
1:D:167:PRO:HD2	5:D:308:HOH:O	2.18	0.41
1:C:4:ARG:CZ	1:C:127:VAL:HG11	2.51	0.41
1:B:161:GLU:O	1:B:164:PRO:HD3	2.20	0.40
1:B:240:ILE:O	1:B:244:GLU:HG3	2.21	0.40
1:C:83:ASP:HA	1:C:84:PRO:HD3	1.82	0.40
1:C:143:PRO:HG3	1:C:170:ASN:HA	2.03	0.40
1:D:17:LEU:O	1:D:20:VAL:HG22	2.21	0.40
1:D:144:GLU:H	1:D:144:GLU:CD	2.18	0.40
1:A:83:ASP:C	1:A:85[A]:SER:H	2.24	0.40
1:C:247:GLN:HB2	1:C:249:LEU:CD2	2.51	0.40
1:D:17:LEU:HD23	1:D:230:HIS:CD2	2.54	0.40
1:A:13:SER:CB	1:A:15:THR:HG23	2.52	0.40
1:A:240:ILE:O	1:A:244:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	284/292 (97%)	275 (97%)	5 (2%)	4 (1%)	11 15
1	B	283/292 (97%)	269 (95%)	11 (4%)	3 (1%)	14 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	278/292 (95%)	265 (95%)	13 (5%)	0	100	100
1	D	268/292 (92%)	255 (95%)	12 (4%)	1 (0%)	34	48
All	All	1113/1168 (95%)	1064 (96%)	41 (4%)	8 (1%)	29	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86[A]	PRO
1	A	86[B]	PRO
1	B	86[A]	PRO
1	B	86[B]	PRO
1	A	85[A]	SER
1	A	85[B]	SER
1	D	162	GLU
1	B	162	GLU

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	243/245 (99%)	239 (98%)	4 (2%)	62	79
1	B	243/245 (99%)	239 (98%)	4 (2%)	62	79
1	C	239/245 (98%)	234 (98%)	5 (2%)	53	72
1	D	234/245 (96%)	228 (97%)	6 (3%)	46	66
All	All	959/980 (98%)	940 (98%)	19 (2%)	55	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	249	LEU
1	A	281	TYR
1	A	289	VAL

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Mol	Chain	Res	Type
1	B	130	GLU
1	B	154	LYS
1	B	249	LEU
1	B	281	TYR
1	C	122	LEU
1	C	144	GLU
1	C	154	LYS
1	C	249	LEU
1	C	281	TYR
1	D	112	ASN
1	D	122	LEU
1	D	160	LEU
1	D	249	LEU
1	D	281	TYR
1	D	289	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	B	27	GLN
1	C	27	GLN
1	D	27	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 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
4	PEG	C	293	-	6,6,6	0.50	0	5,5,5	0.24	0
2	DGT	B	500	3	26,33,33	0.85	1 (3%)	32,52,52	1.33	6 (18%)
2	DGT	D	500	3	26,33,33	0.80	1 (3%)	32,52,52	1.35	6 (18%)
2	DGT	A	500	3	26,33,33	0.80	0	32,52,52	1.43	5 (15%)
4	PEG	A	294	-	6,6,6	0.69	0	5,5,5	0.29	0
2	DGT	C	500	3	26,33,33	0.79	0	32,52,52	1.34	5 (15%)
4	PEG	A	293	-	6,6,6	0.54	0	5,5,5	0.67	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
4	PEG	C	293	-	-	2/4/4/4	-
2	DGT	B	500	3	-	5/18/34/34	0/3/3/3
2	DGT	D	500	3	-	6/18/34/34	0/3/3/3
2	DGT	A	500	3	-	6/18/34/34	0/3/3/3
4	PEG	A	294	-	-	2/4/4/4	-
2	DGT	C	500	3	-	6/18/34/34	0/3/3/3
4	PEG	A	293	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	DGT	C6-N1	-2.22	1.34	1.37
2	D	500	DGT	C6-N1	-2.21	1.34	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	DGT	PB-O3B-PG	-3.20	121.85	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	DGT	PB-O3B-PG	-3.11	122.17	132.83
2	A	500	DGT	PB-O3B-PG	-3.05	122.35	132.83
2	A	500	DGT	O6-C6-C5	-2.73	119.04	124.37
2	A	500	DGT	PA-O3A-PB	-2.68	123.62	132.83
2	B	500	DGT	PB-O3B-PG	-2.66	123.69	132.83
2	A	500	DGT	C2'-C1'-N9	-2.64	108.19	114.27
2	B	500	DGT	C2'-C1'-N9	-2.58	108.31	114.27
2	D	500	DGT	C2'-C1'-N9	-2.52	108.46	114.27
2	D	500	DGT	PA-O3A-PB	-2.47	124.33	132.83
2	C	500	DGT	PA-O3A-PB	-2.44	124.45	132.83
2	C	500	DGT	C5-C6-N1	2.41	118.21	113.95
2	B	500	DGT	PA-O3A-PB	-2.41	124.54	132.83
2	B	500	DGT	C5-C6-N1	2.37	118.14	113.95
2	B	500	DGT	C8-N7-C5	2.33	107.44	102.99
2	A	500	DGT	C5-C6-N1	2.32	118.06	113.95
2	C	500	DGT	C2'-C1'-N9	-2.32	108.92	114.27
2	C	500	DGT	O6-C6-C5	-2.30	119.88	124.37
2	D	500	DGT	C5-C6-N1	2.28	117.98	113.95
2	B	500	DGT	O6-C6-C5	-2.25	119.97	124.37
2	D	500	DGT	C8-N7-C5	2.25	107.27	102.99
2	D	500	DGT	O6-C6-C5	-2.12	120.23	124.37

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	DGT	C5'-O5'-PA-O1A
2	A	500	DGT	C5'-O5'-PA-O2A
2	A	500	DGT	O4'-C4'-C5'-O5'
2	B	500	DGT	C5'-O5'-PA-O1A
2	B	500	DGT	C5'-O5'-PA-O2A
2	B	500	DGT	O4'-C4'-C5'-O5'
2	C	500	DGT	C5'-O5'-PA-O1A
2	C	500	DGT	C5'-O5'-PA-O2A
2	C	500	DGT	O4'-C4'-C5'-O5'
2	D	500	DGT	C5'-O5'-PA-O1A
2	D	500	DGT	C5'-O5'-PA-O2A
2	D	500	DGT	O4'-C4'-C5'-O5'
2	A	500	DGT	C3'-C4'-C5'-O5'
2	B	500	DGT	C3'-C4'-C5'-O5'
2	C	500	DGT	C3'-C4'-C5'-O5'
2	D	500	DGT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	294	PEG	O2-C3-C4-O4
4	A	293	PEG	O1-C1-C2-O2
4	C	293	PEG	C4-C3-O2-C2
4	A	294	PEG	O1-C1-C2-O2
4	C	293	PEG	O1-C1-C2-O2
2	A	500	DGT	C5'-O5'-PA-O3A
2	B	500	DGT	C5'-O5'-PA-O3A
2	C	500	DGT	C5'-O5'-PA-O3A
2	D	500	DGT	C5'-O5'-PA-O3A
2	A	500	DGT	PG-O3B-PB-O1B
2	C	500	DGT	PG-O3B-PB-O1B
2	D	500	DGT	PG-O3B-PB-O1B

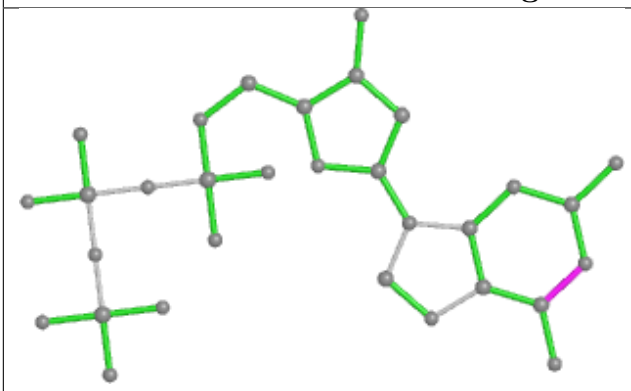
There are no ring outliers.

7 monomers are involved in 20 short contacts:

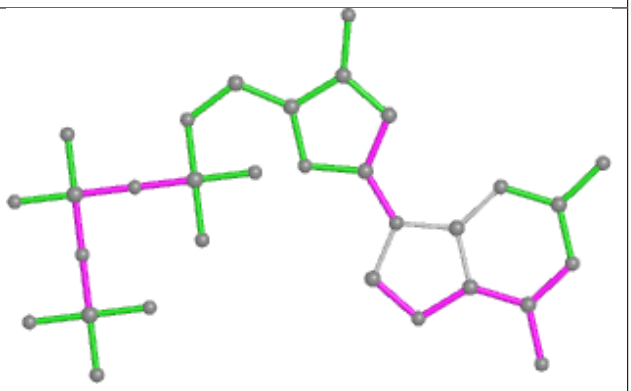
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	293	PEG	3	0
2	B	500	DGT	2	0
2	D	500	DGT	2	0
2	A	500	DGT	6	0
4	A	294	PEG	4	0
2	C	500	DGT	1	0
4	A	293	PEG	2	0

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.

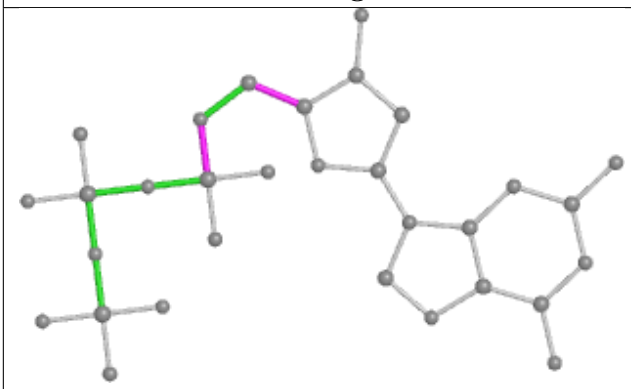
Ligand DGT B 500



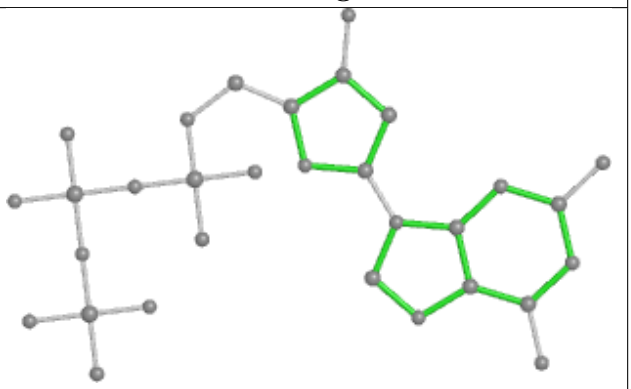
Bond lengths



Bond angles

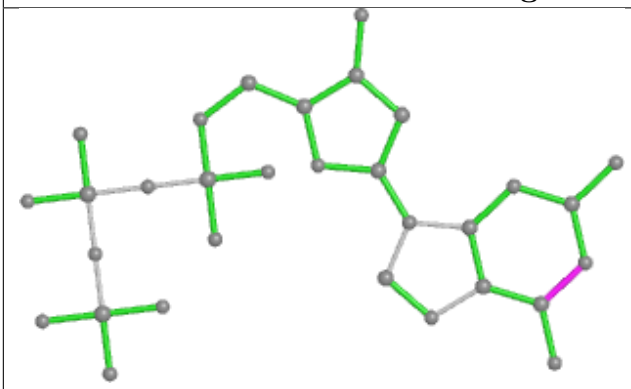


Torsions

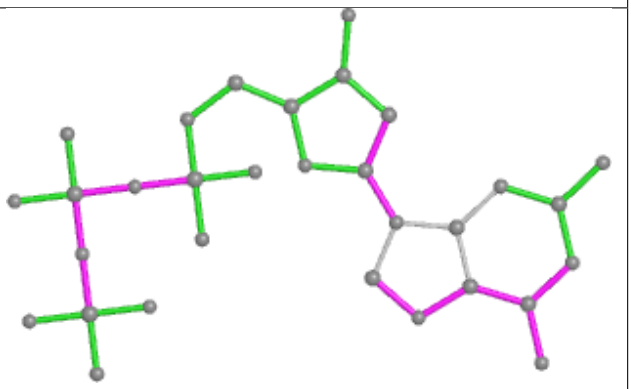


Rings

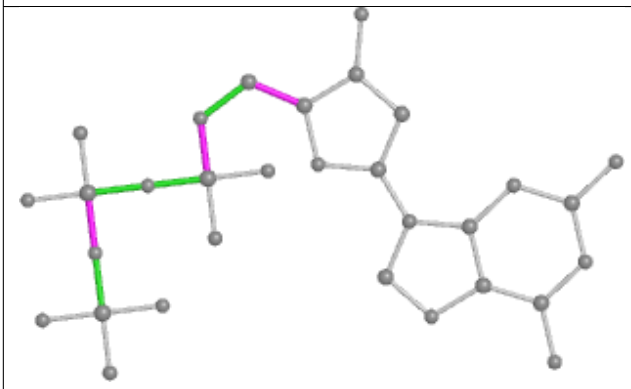
Ligand DGT D 500



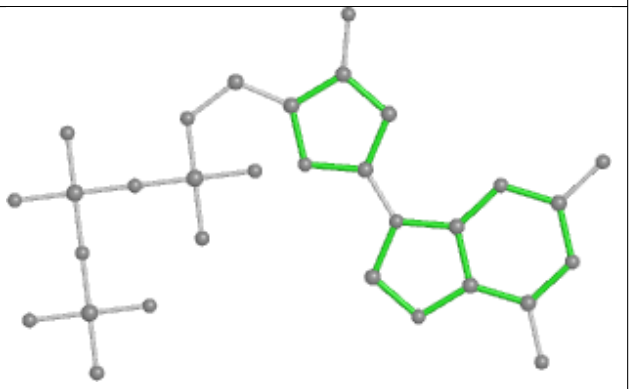
Bond lengths



Bond angles

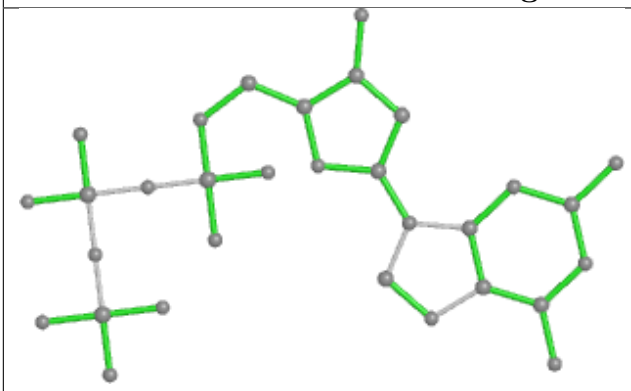


Torsions

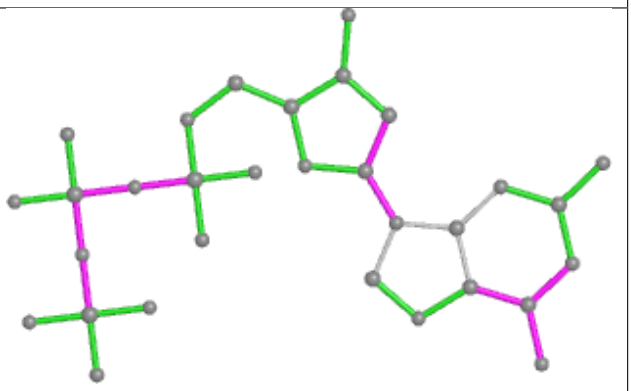


Rings

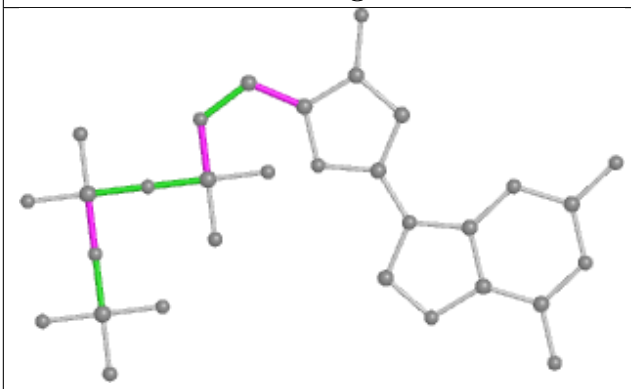
Ligand DGT A 500



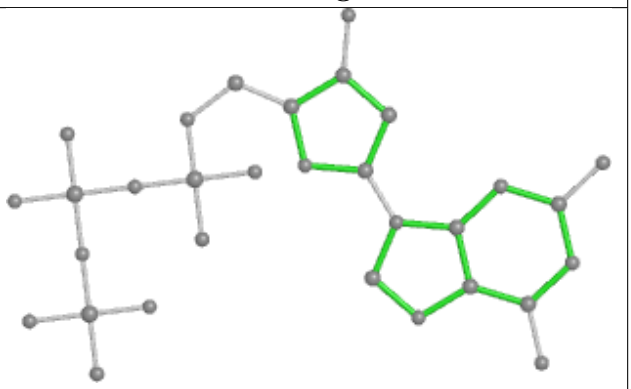
Bond lengths



Bond angles

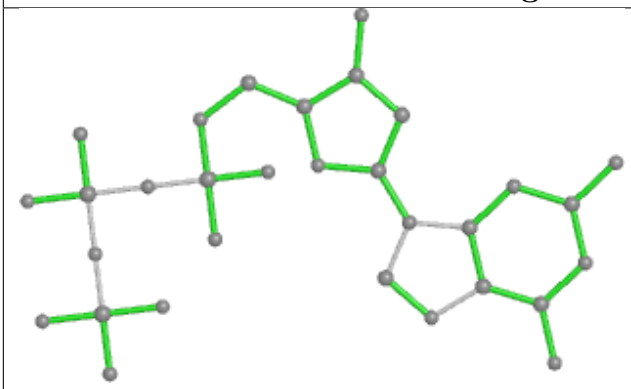


Torsions

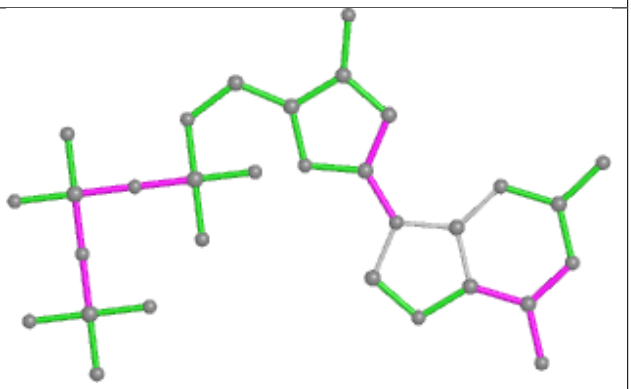


Rings

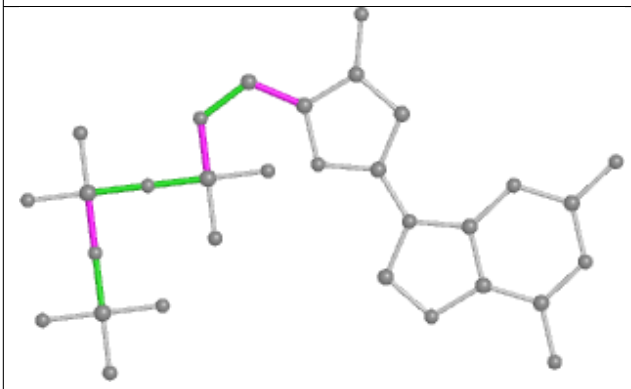
Ligand DGT C 500



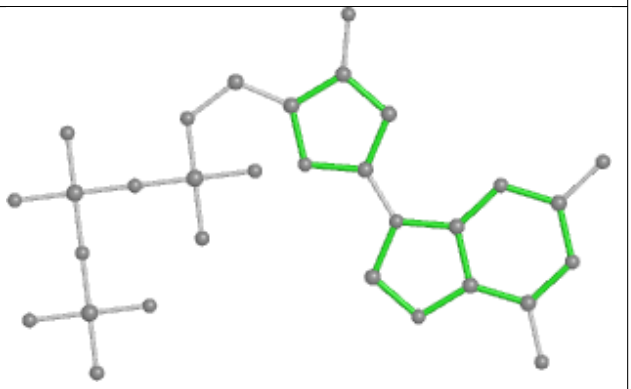
Bond lengths



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 (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	285/292 (97%)	-0.01	5 (1%)	68	66	20, 43, 86, 115	0
1	B	286/292 (97%)	0.08	13 (4%)	33	31	22, 44, 102, 138	0
1	C	284/292 (97%)	0.69	46 (16%)	1	1	28, 59, 110, 162	0
1	D	278/292 (95%)	0.86	55 (19%)	1	0	28, 62, 105, 160	0
All	All	1133/1168 (97%)	0.40	119 (10%)	6	5	20, 52, 102, 162	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	8.5
1	C	198	LEU	6.6
1	C	194	ALA	6.2
1	D	163	LYS	5.9
1	C	87	ASP	5.9
1	D	89	LEU	5.5
1	C	154	LYS	5.5
1	C	289	VAL	5.2
1	A	151	PHE	5.2
1	D	198	LEU	5.0
1	D	147	GLY	5.0
1	D	87	ASP	4.7
1	D	160	LEU	4.6
1	D	85	SER	4.5
1	C	156	THR	4.5
1	C	155	GLY	4.4
1	B	153	GLN	4.4
1	D	145	ARG	4.3
1	C	193	SER	4.3
1	D	170	ASN	4.1
1	A	156	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	99	PHE	4.1
1	B	156	THR	4.1
1	C	191	LYS	4.0
1	D	146	TYR	3.9
1	D	131	SER	3.8
1	C	153	GLN	3.8
1	C	272	LEU	3.8
1	C	158	VAL	3.8
1	D	267	GLN	3.8
1	D	171	TYR	3.7
1	D	213	LEU	3.7
1	D	200	ILE	3.6
1	D	211	GLY	3.6
1	C	165	LEU	3.6
1	B	154	LYS	3.6
1	D	151	PHE	3.6
1	D	127	VAL	3.5
1	C	197	GLU	3.4
1	D	155	GLY	3.3
1	D	208	MET	3.3
1	D	169	SER	3.3
1	D	217	MET	3.3
1	D	148	VAL	3.2
1	C	267	GLN	3.2
1	D	158	VAL	3.2
1	B	157	ALA	3.2
1	C	152	ASP	3.1
1	C	166	GLN	3.1
1	D	144	GLU	3.0
1	C	131	SER	2.9
1	B	163	LYS	2.9
1	C	212	ARG	2.9
1	D	277	SER	2.9
1	D	178	PHE	2.9
1	D	263	PHE	2.9
1	D	270	ILE	2.9
1	D	206	ILE	2.9
1	D	162	GLU	2.8
1	D	140	VAL	2.8
1	C	190	LEU	2.8
1	C	271	GLU	2.8
1	C	208	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	13	SER	2.7
1	C	202	ASP	2.7
1	B	164	PRO	2.7
1	C	211	GLY	2.7
1	C	192	PRO	2.6
1	B	152	ASP	2.6
1	C	209	GLU	2.6
1	D	212	ARG	2.6
1	D	210	GLN	2.6
1	B	144	GLU	2.6
1	C	84	PRO	2.5
1	D	128	ASN	2.5
1	B	145	ARG	2.5
1	D	98	GLU	2.5
1	D	271	GLU	2.5
1	D	193	SER	2.5
1	C	210	GLN	2.5
1	D	167	PRO	2.5
1	A	165	LEU	2.5
1	B	158	VAL	2.4
1	B	168	LYS	2.4
1	D	209	GLU	2.4
1	D	190	LEU	2.4
1	D	205	ARG	2.3
1	C	162	GLU	2.3
1	C	290	LYS	2.3
1	D	201	THR	2.3
1	C	141	ASN	2.3
1	D	168	LYS	2.3
1	B	87[A]	ASP	2.3
1	C	128	ASN	2.3
1	C	262	ASN	2.3
1	C	89	LEU	2.3
1	C	170	ASN	2.3
1	D	204	ASN	2.3
1	D	133	ALA	2.2
1	A	145	ARG	2.2
1	D	94	ILE	2.2
1	D	192	PRO	2.2
1	C	275	PRO	2.1
1	C	199	GLU	2.1
1	C	85	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	207	TYR	2.1
1	C	270	ILE	2.1
1	C	13	SER	2.1
1	D	47	ALA	2.1
1	C	168	LYS	2.1
1	D	141	ASN	2.1
1	D	157	ALA	2.1
1	C	206	ILE	2.1
1	B	85[A]	SER	2.1
1	C	205	ARG	2.1
1	C	234	ILE	2.1
1	C	259	PHE	2.1
1	D	126	ALA	2.0
1	C	167	PRO	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	B	501	1/1	0.48	0.27	75,75,75,75	0
3	MG	C	501	1/1	0.70	0.28	64,64,64,64	0
3	MG	A	501	1/1	0.76	0.25	77,77,77,77	0
4	PEG	A	293	7/7	0.81	0.21	46,52,61,72	0
3	MG	D	502	1/1	0.82	0.22	73,73,73,73	0
4	PEG	C	293	7/7	0.82	0.34	48,67,78,93	0
3	MG	B	502	1/1	0.85	0.13	64,64,64,64	0
2	DGT	C	500	31/31	0.86	0.19	47,75,101,104	31
2	DGT	A	500	31/31	0.87	0.22	34,65,102,108	31

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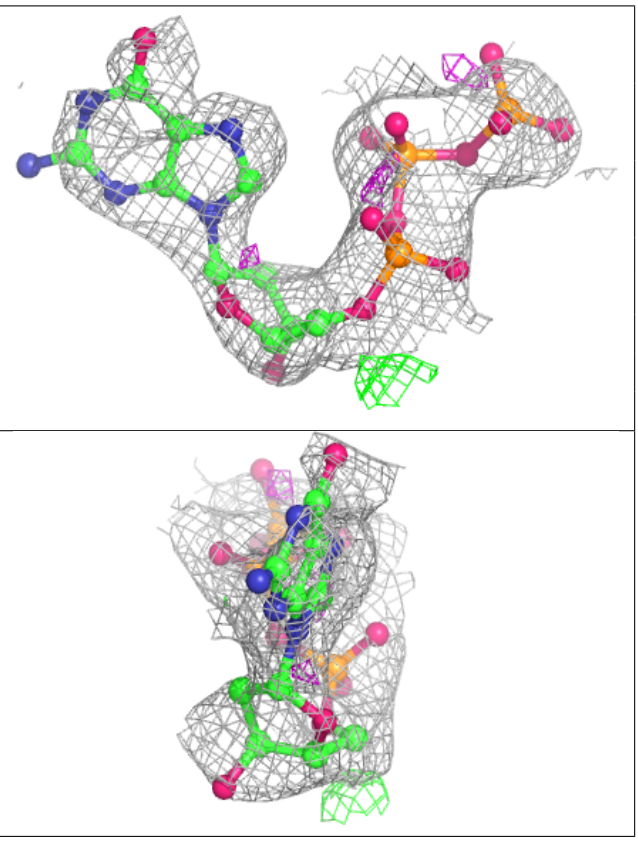
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	A	294	7/7	0.89	0.26	27,58,72,99	0
2	DGT	D	500	31/31	0.93	0.17	47,72,92,113	31
2	DGT	B	500	31/31	0.95	0.12	36,69,89,104	31

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.

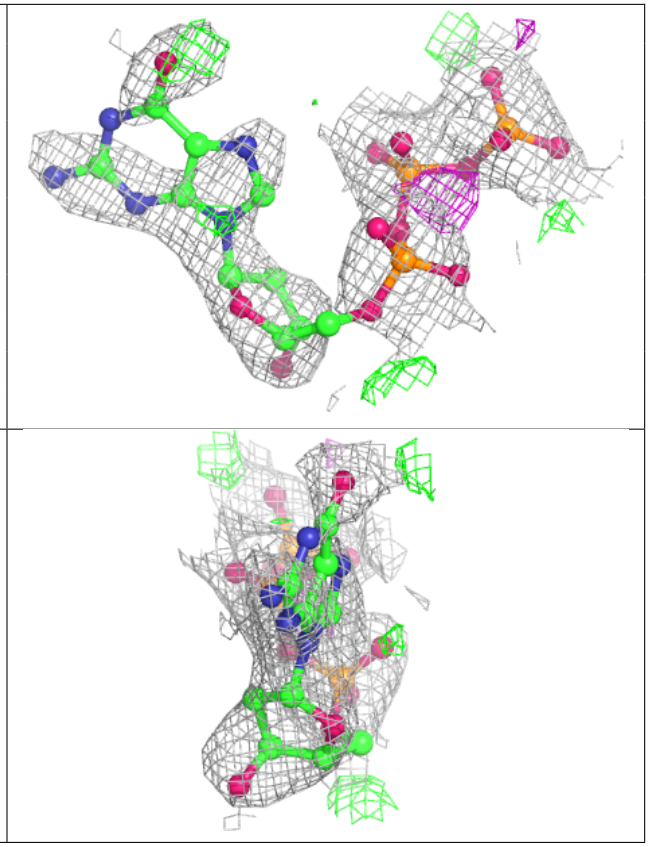
Electron density around DGT C 500:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



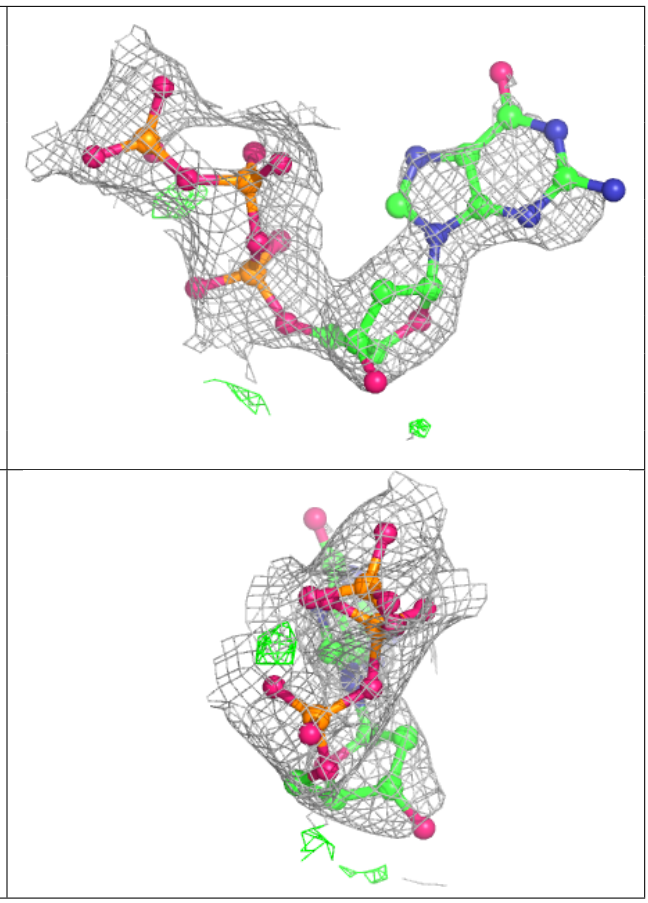
Electron density around DGT A 500:

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



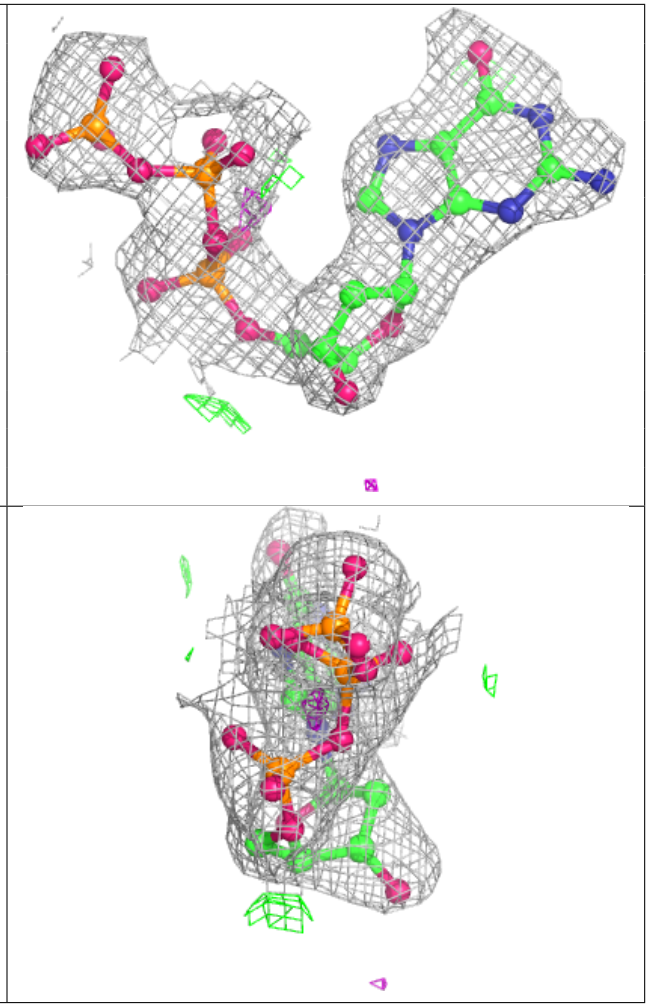
Electron density around DGT D 500:

$2mF_o$-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 500:

$2mF_o$-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.