Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 10:16 AM EST

PDB ID	:	3F2B
Title	:	DNA Polymerase PolC from Geobacillus kaustophilus complex with DNA, dGTP, Mg and Zn
Authors	:	Davies, D.R.; Evans, R.J.; Bullard, J.M.; Christensen, J.; Green, L.S.; Guiles, J.W.; Ribble, W.K.; Janjic, N.; Jarvis, T.C.
Deposited on	:	2008-10-29
Resolution	:	2.39 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:

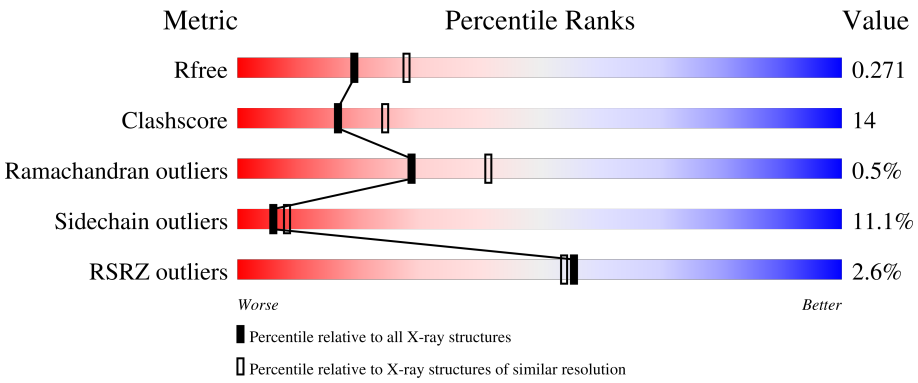
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	1041	2%; 70%; 21%; • 5%
2	P	17	6%; 18%; 47%; 12%; 24%
3	T	22	5%; 36%; 36%; 9%; 18%

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
7	DGT	A	1456	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8591 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 DNA-directed DNA polymerase III alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7815	4973	1324	1482	36	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	expression tag	UNP Q5L0J3
A	425	GLY	-	linker	UNP Q5L0J3
A	426	SER	-	linker	UNP Q5L0J3
A	427	GLY	-	linker	UNP Q5L0J3
A	428	SER	-	linker	UNP Q5L0J3
A	429	GLY	-	linker	UNP Q5L0J3
A	1445	SER	-	expression tag	UNP Q5L0J3
A	1446	GLY	-	expression tag	UNP Q5L0J3
A	1447	GLY	-	expression tag	UNP Q5L0J3
A	1448	HIS	-	expression tag	UNP Q5L0J3
A	1449	HIS	-	expression tag	UNP Q5L0J3
A	1450	HIS	-	expression tag	UNP Q5L0J3
A	1451	HIS	-	expression tag	UNP Q5L0J3
A	1452	HIS	-	expression tag	UNP Q5L0J3
A	1453	HIS	-	expression tag	UNP Q5L0J3
A	1454	HIS	-	expression tag	UNP Q5L0J3
A	1455	HIS	-	expression tag	UNP Q5L0J3

- Molecule 2 is a DNA chain called 5'-D(*DCP*DAP*DGP*DTP*DGP*DAP*DGP*DAP*DCP*DGP*DGP*DGP*DCP*DAP*DAP*DCP*DC)-3'.

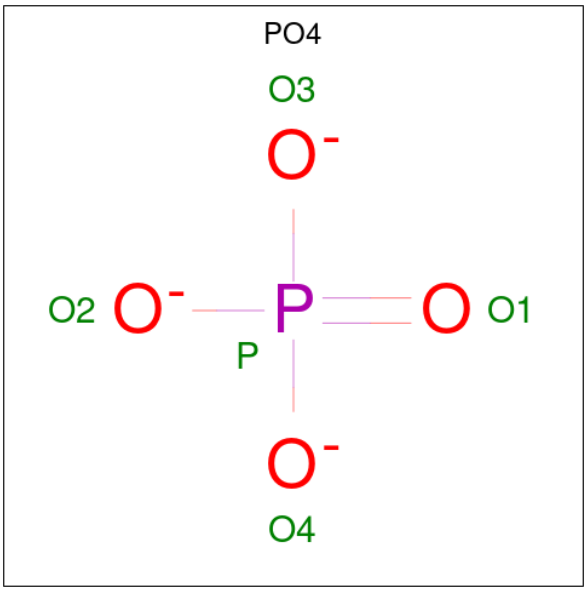
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	13	269	126	57	73	13	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*DAP*DTP*DAP*DAP*DCP*DGP*DGP*DTP*D

TP*DGP*DCP*DCP*DCP*DGP*DTP*DCP*DTP*DCP*DAP*DCP*DTP*DG)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	18	362	174	63	108	17	0	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
4	A	1	5	4	1		0	0
			Total	O	P			
4	A	1	5	4	1		0	0
			Total	O	P			
4	A	1	5	4	1		0	0

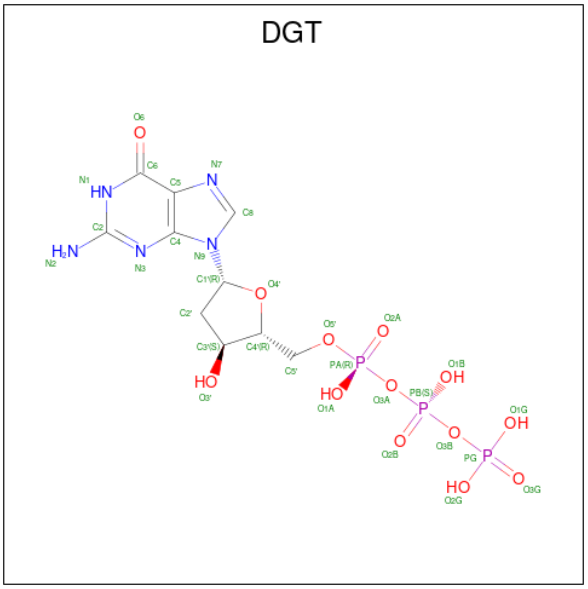
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	3	3	3	0	0

- Molecule 7 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		
7	A	1	31	10	5	13	3	0	0

- Molecule 8 is water.

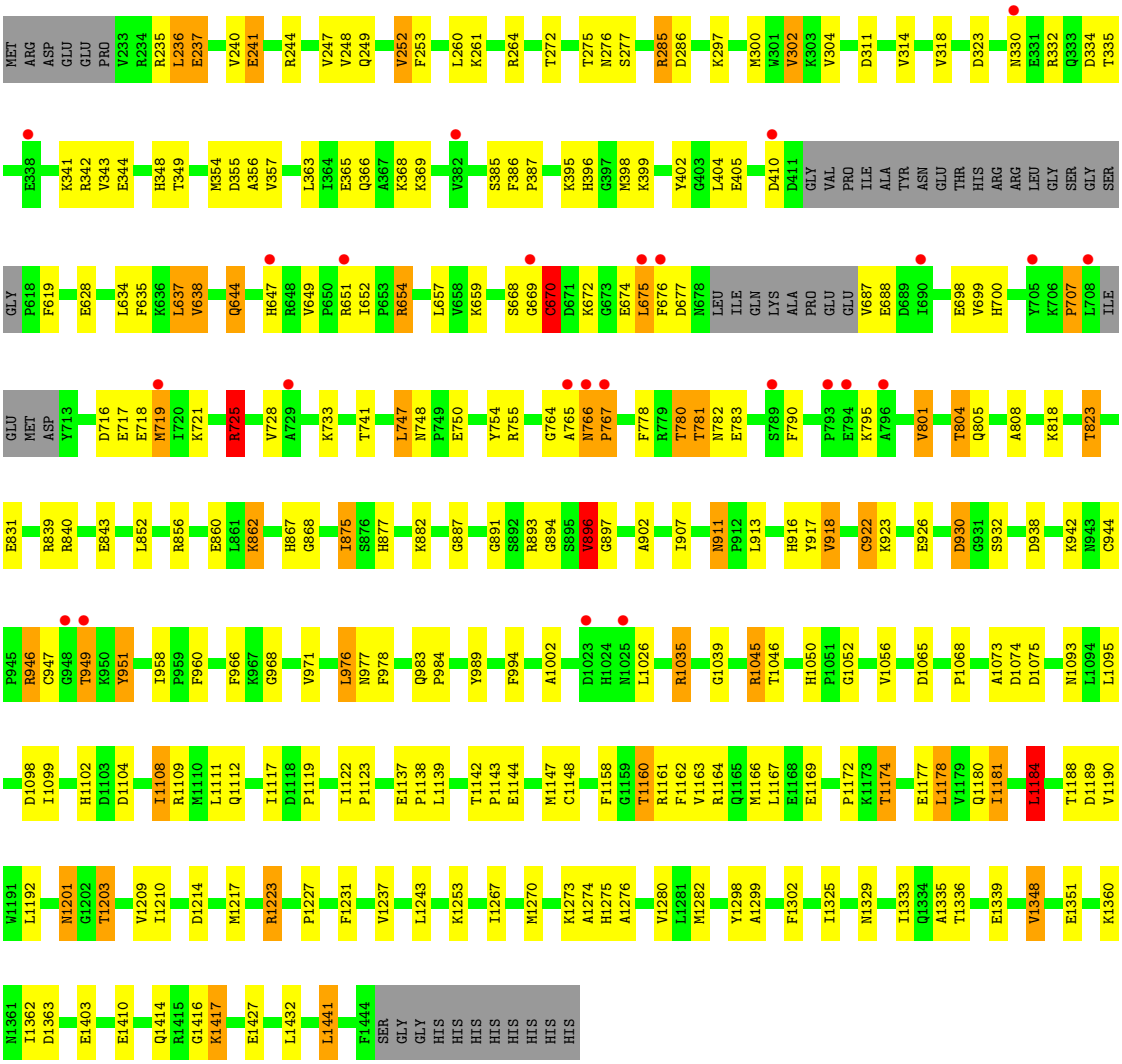
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	84	84	84	0	0
			Total	O		
8	P	4	4	4	0	0
			Total	O		
8	T	7	7	7	0	0

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: DNA-directed DNA polymerase III alpha chain

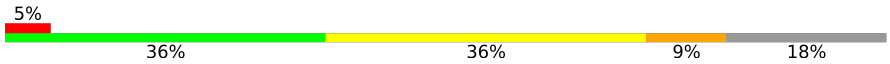
Chain A: 2% 70% 21% 5%

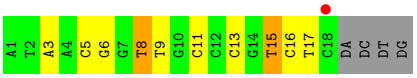


• Molecule 2: 5'-D(*DCP*DAP*DGP*DTP*DGP*DAP*DGP*DAP*DCP*DGP*DGP*DGP*DCP*DAP*DAP*DCP*DC)-3'

Chain P:

• Molecule 3: 5'-D(*DAP*DTP*DAP*DAP*DCP*DGP*DGP*DTP*DTP*DGP*DCP*DCP*DCP*DGP*DTP*DCP*DTP*DCP*DAP*DCP*DTP*DG)-3'

Chain T: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	116.17Å 140.79Å 184.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.52 – 2.39 43.51 – 2.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.52-2.39) 99.6 (43.51-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.228 , 0.273 0.226 , 0.271	Depositor DCC
R_{free} test set	3017 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8591	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, PO4, MG, ZN

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	0.60	6/7979 (0.1%)	0.73	8/10798 (0.1%)
2	P	1.25	0/303	2.00	14/465 (3.0%)
3	T	1.49	5/404 (1.2%)	2.17	24/621 (3.9%)
All	All	0.70	11/8686 (0.1%)	0.94	46/11884 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	8	DT	C4'-O4'	-9.95	1.35	1.45
1	A	688	GLU	CG-CD	7.21	1.62	1.51
1	A	717	GLU	CD-OE1	6.43	1.32	1.25
1	A	718	GLU	CD-OE1	-6.32	1.18	1.25
3	T	13	DC	N1-C2	5.80	1.46	1.40
1	A	718	GLU	CG-CD	5.66	1.60	1.51
3	T	8	DT	O4'-C1'	-5.52	1.35	1.42
1	A	719	MET	SD-CE	5.50	2.08	1.77
3	T	13	DC	C4-C5	5.43	1.47	1.43
1	A	670	CYS	CB-SG	-5.33	1.73	1.81
3	T	16	DC	N1-C2	5.28	1.45	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	8	DT	O4'-C1'-N1	16.10	119.27	108.00
2	P	16	DC	O4'-C1'-N1	15.11	118.57	108.00
3	T	8	DT	N1-C1'-C2'	-13.02	87.87	112.60
3	T	15	DT	P-O3'-C3'	8.73	130.17	119.70
2	P	17	DC	N3-C4-N4	-8.48	112.06	118.00
3	T	13	DC	C6-N1-C2	8.13	123.55	120.30
3	T	17	DT	O4'-C1'-N1	7.53	113.27	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	17	DT	C6-C5-C7	-7.40	118.46	122.90
3	T	13	DC	C5-C6-N1	-7.27	117.37	121.00
2	P	13	DC	C5-C4-N4	-7.16	115.19	120.20
3	T	16	DC	P-O3'-C3'	6.95	128.04	119.70
3	T	17	DT	C4-C5-C7	6.93	123.16	119.00
3	T	16	DC	N1-C2-O2	6.75	122.95	118.90
2	P	17	DC	O4'-C1'-N1	-6.72	103.29	108.00
3	T	13	DC	N3-C4-C5	6.59	124.54	121.90
3	T	8	DT	O5'-P-OP2	-6.49	99.86	105.70
3	T	13	DC	C2-N3-C4	-6.38	116.71	119.90
3	T	5	DC	O4'-C1'-N1	-6.37	103.54	108.00
3	T	8	DT	C5-C4-O4	-6.37	120.44	124.90
2	P	17	DC	C5-C4-N4	6.36	124.65	120.20
2	P	8	DA	P-O3'-C3'	-6.29	112.16	119.70
1	A	896	VAL	CB-CA-C	-6.16	99.70	111.40
3	T	3	DA	O4'-C1'-N9	-6.09	103.73	108.00
2	P	5	DG	P-O3'-C3'	6.06	126.98	119.70
3	T	13	DC	N1-C2-O2	5.96	122.47	118.90
3	T	15	DT	C6-C5-C7	-5.96	119.33	122.90
1	A	1441	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	718	GLU	OE1-CD-OE2	-5.86	116.27	123.30
3	T	15	DT	C4-C5-C7	5.79	122.47	119.00
3	T	8	DT	C5'-C4'-C3'	5.67	124.30	114.10
2	P	16	DC	P-O3'-C3'	5.64	126.46	119.70
2	P	12	DG	O4'-C1'-N9	5.63	111.94	108.00
2	P	13	DC	N3-C2-O2	5.57	125.80	121.90
1	A	1184	LEU	CB-CG-CD1	-5.54	101.58	111.00
2	P	17	DC	N1-C1'-C2'	5.53	123.11	112.60
3	T	9	DT	O4'-C1'-N1	-5.52	104.13	108.00
1	A	725	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	P	13	DC	N1-C2-O2	-5.27	115.74	118.90
1	A	1201	ASN	CB-CA-C	-5.15	100.10	110.40
2	P	13	DC	N3-C4-N4	5.13	121.59	118.00
3	T	8	DT	N3-C4-O4	5.10	122.96	119.90
2	P	15	DA	P-O3'-C3'	5.08	125.79	119.70
1	A	976	LEU	CA-CB-CG	5.06	126.94	115.30
3	T	11	DC	P-O3'-C3'	5.03	125.74	119.70
3	T	16	DC	N3-C2-O2	-5.02	118.38	121.90
1	A	716	ASP	CB-CG-OD1	5.01	122.81	118.30

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	7815	0	7742	225	0
2	P	269	0	142	4	0
3	T	362	0	205	4	0
4	A	15	0	0	0	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	31	0	12	9	0
8	A	84	0	0	4	0
8	P	4	0	0	0	0
8	T	7	0	0	0	0
All	All	8591	0	8101	235	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 (235) 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:A:719:MET:SD	1:A:719:MET:CE	2.08	1.39
1:A:947:CYS:SG	1:A:949:THR:OG1	1.96	1.21
1:A:946:ARG:HG3	1:A:946:ARG:HH11	1.04	1.18
1:A:966:PHE:HE2	1:A:1217:MET:HE2	1.09	1.10
7:A:1456:DGT:H5'A	7:A:1456:DGT:H8	1.34	1.10
1:A:342:ARG:HB2	1:A:781:THR:HB	1.31	1.07
1:A:1147:MET:HE1	1:A:1325:ILE:HG21	1.36	1.07
1:A:877:HIS:CA	1:A:907:ILE:HD11	1.84	1.06
1:A:877:HIS:HA	1:A:907:ILE:HD11	1.30	1.06
1:A:1217:MET:HE3	1:A:1231:PHE:HB2	1.34	1.06
1:A:1217:MET:CE	1:A:1231:PHE:HB2	1.85	1.06
1:A:946:ARG:HH11	1:A:946:ARG:CG	1.71	1.03
1:A:966:PHE:HE2	1:A:1217:MET:CE	1.71	1.03
1:A:1201:ASN:HB3	1:A:1203:THR:HG22	1.41	1.02
1:A:669:GLY:HA2	1:A:698:GLU:HB2	1.39	1.01
1:A:966:PHE:CE2	1:A:1217:MET:HE2	1.96	1.00
7:A:1456:DGT:H8	7:A:1456:DGT:C5'	1.90	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HG2	1:A:275:THR:HB	1.43	0.99
1:A:946:ARG:HG3	1:A:946:ARG:NH1	1.72	0.98
1:A:1160:THR:HG21	3:T:6:DG:OP1	1.67	0.95
1:A:365:GLU:HG2	1:A:396:HIS:CE1	2.02	0.94
1:A:1282:MET:HE1	8:A:78:HOH:O	1.68	0.94
1:A:1201:ASN:CB	1:A:1203:THR:HG22	1.97	0.94
1:A:780:THR:HG22	1:A:783:GLU:HG2	1.49	0.93
1:A:669:GLY:HA2	1:A:698:GLU:CB	1.98	0.93
1:A:1160:THR:HG22	1:A:1163:VAL:H	1.35	0.91
1:A:877:HIS:HA	1:A:907:ILE:CD1	2.01	0.90
1:A:1102:HIS:HA	3:T:8:DT:H5"	1.53	0.89
1:A:335:THR:H	1:A:782:ASN:ND2	1.72	0.88
7:A:1456:DGT:H5'A	2:P:17:DC:H2'	1.56	0.87
1:A:669:GLY:CA	1:A:698:GLU:HB2	2.06	0.85
1:A:780:THR:HG22	1:A:783:GLU:H	1.42	0.84
1:A:966:PHE:CE2	1:A:1217:MET:CE	2.59	0.84
1:A:1142:THR:HG22	1:A:1144:GLU:H	1.41	0.84
1:A:896:VAL:HG22	8:A:86:HOH:O	1.78	0.83
1:A:237:GLU:HG2	1:A:275:THR:CB	2.07	0.83
1:A:801:VAL:O	1:A:805:GLN:HB2	1.77	0.83
1:A:342:ARG:CB	1:A:781:THR:HB	2.08	0.82
1:A:343:VAL:H	1:A:804:THR:CG2	1.93	0.82
1:A:1102:HIS:HD2	1:A:1104:ASP:H	1.27	0.82
1:A:343:VAL:H	1:A:804:THR:HG21	1.45	0.81
1:A:1142:THR:HG22	1:A:1144:GLU:N	1.95	0.81
1:A:334:ASP:OD2	1:A:781:THR:HG22	1.80	0.81
1:A:1217:MET:HE3	1:A:1231:PHE:CB	2.10	0.80
1:A:654:ARG:NH1	1:A:674:GLU:OE2	2.19	0.76
1:A:938:ASP:OD1	1:A:1174:THR:HG23	1.86	0.75
7:A:1456:DGT:H5'A	7:A:1456:DGT:C8	2.14	0.75
1:A:644:GLN:H	1:A:644:GLN:HE21	1.31	0.75
1:A:1102:HIS:CD2	1:A:1104:ASP:H	2.04	0.74
1:A:877:HIS:N	1:A:907:ILE:HD11	2.02	0.73
1:A:1201:ASN:CB	1:A:1203:THR:CG2	2.66	0.72
1:A:1045:ARG:CG	1:A:1046:THR:HG23	2.20	0.71
1:A:1045:ARG:HG3	1:A:1046:THR:HG23	1.73	0.71
1:A:1217:MET:HE1	1:A:1231:PHE:HB2	1.70	0.71
7:A:1456:DGT:C5'	7:A:1456:DGT:C8	2.69	0.70
1:A:368:LYS:HA	1:A:398:MET:HE1	1.73	0.69
1:A:1201:ASN:HB2	1:A:1203:THR:CG2	2.24	0.68
1:A:911:ASN:HD22	1:A:911:ASN:C	1.97	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:GLN:HE21	1:A:644:GLN:N	1.94	0.66
1:A:368:LYS:HA	1:A:398:MET:CE	2.26	0.65
7:A:1456:DGT:H8	7:A:1456:DGT:H5'	1.78	0.65
1:A:780:THR:CG2	1:A:783:GLU:H	2.09	0.64
1:A:946:ARG:CG	1:A:946:ARG:NH1	2.43	0.64
1:A:1174:THR:HG22	1:A:1177:GLU:H	1.62	0.63
1:A:1137:GLU:HB3	1:A:1138:PRO:HD3	1.80	0.62
1:A:764:GLY:O	1:A:767:PRO:CD	2.48	0.62
1:A:1102:HIS:CD2	1:A:1104:ASP:HB2	2.35	0.62
1:A:942:LYS:O	1:A:951:TYR:HB2	1.99	0.61
1:A:365:GLU:CG	1:A:396:HIS:CE1	2.82	0.61
1:A:1158:PHE:HA	1:A:1163:VAL:HG11	1.83	0.61
1:A:1403:GLU:O	1:A:1403:GLU:HG3	2.01	0.61
1:A:1102:HIS:HA	3:T:8:DT:C5'	2.29	0.60
1:A:1201:ASN:HB2	1:A:1203:THR:HG22	1.81	0.60
1:A:1201:ASN:HD22	1:A:1203:THR:HG21	1.66	0.59
1:A:1210:ILE:CG2	1:A:1270:MET:CE	2.80	0.59
1:A:675:LEU:HD23	1:A:676:PHE:H	1.68	0.58
1:A:765:ALA:C	1:A:767:PRO:HD2	2.23	0.58
1:A:368:LYS:HB2	1:A:398:MET:HE3	1.84	0.58
1:A:856:ARG:O	1:A:860:GLU:HB2	2.03	0.58
1:A:277:SER:OG	1:A:1035:ARG:HG2	2.04	0.58
1:A:354:MET:HE3	1:A:1045:ARG:HB2	1.85	0.58
1:A:237:GLU:CG	1:A:275:THR:HB	2.28	0.57
1:A:911:ASN:ND2	1:A:913:LEU:H	2.02	0.57
1:A:818:LYS:HE2	1:A:1065:ASP:O	2.06	0.56
1:A:766:ASN:N	1:A:767:PRO:HD2	2.19	0.56
1:A:1045:ARG:HG2	1:A:1046:THR:HG23	1.88	0.56
1:A:1142:THR:CG2	1:A:1144:GLU:H	2.17	0.56
1:A:244:ARG:HH11	1:A:244:ARG:HB2	1.70	0.56
1:A:668:SER:HB2	1:A:675:LEU:HD22	1.87	0.56
1:A:780:THR:HG22	1:A:783:GLU:CG	2.30	0.56
1:A:1302:PHE:CZ	1:A:1348:VAL:HG22	2.41	0.55
1:A:1108:ILE:HD11	1:A:1119:PRO:CB	2.36	0.55
1:A:1181:ILE:HA	1:A:1184:LEU:HD11	1.88	0.55
1:A:342:ARG:NH2	1:A:344:GLU:OE1	2.37	0.55
1:A:1108:ILE:HD11	1:A:1119:PRO:CG	2.37	0.55
1:A:1148:CYS:SG	1:A:1164:ARG:HD3	2.46	0.55
1:A:365:GLU:HG2	1:A:396:HIS:HE1	1.67	0.55
1:A:675:LEU:HD23	1:A:676:PHE:N	2.22	0.54
1:A:1217:MET:HE3	1:A:1231:PHE:CA	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLN:HG2	1:A:747:LEU:HD21	1.89	0.54
1:A:1045:ARG:HG3	1:A:1045:ARG:O	2.05	0.54
1:A:236:LEU:HD23	1:A:277:SER:HA	1.90	0.54
1:A:1108:ILE:HG13	1:A:1108:ILE:O	2.05	0.54
2:P:5:DG:H1'	2:P:6:DA:C8	2.43	0.54
1:A:1210:ILE:CG2	1:A:1270:MET:HE3	2.38	0.53
1:A:839:ARG:O	1:A:843:GLU:HG2	2.08	0.53
1:A:1093:ASN:ND2	8:A:24:HOH:O	2.41	0.53
1:A:1073:ALA:O	1:A:1074:ASP:HB2	2.08	0.53
1:A:917:TYR:HB3	1:A:951:TYR:CD1	2.44	0.53
1:A:1336:THR:HG23	1:A:1339:GLU:OE1	2.09	0.53
1:A:342:ARG:HB2	1:A:781:THR:CB	2.21	0.53
1:A:1108:ILE:CD1	1:A:1119:PRO:CB	2.87	0.53
1:A:764:GLY:O	1:A:767:PRO:HD3	2.10	0.52
1:A:647:HIS:HD2	1:A:651:ARG:NH2	2.08	0.52
1:A:780:THR:CG2	1:A:783:GLU:HG2	2.30	0.52
1:A:1137:GLU:CB	1:A:1138:PRO:HD3	2.40	0.51
1:A:1117:ILE:O	1:A:1119:PRO:HD3	2.11	0.51
1:A:669:GLY:N	1:A:698:GLU:HB2	2.24	0.51
1:A:334:ASP:OD1	1:A:341:LYS:NZ	2.37	0.50
1:A:1166:MET:HE1	1:A:1184:LEU:CD1	2.41	0.50
1:A:1210:ILE:HG22	1:A:1270:MET:CE	2.40	0.50
1:A:343:VAL:HB	1:A:804:THR:HG23	1.93	0.50
1:A:966:PHE:CE2	1:A:1217:MET:HE1	2.47	0.50
1:A:930:ASP:HB2	1:A:932:SER:OG	2.12	0.50
1:A:911:ASN:C	1:A:911:ASN:ND2	2.65	0.50
1:A:922:CYS:O	1:A:923:LYS:HB2	2.12	0.49
1:A:721:LYS:HE3	1:A:790:PHE:CG	2.47	0.49
1:A:725:ARG:NH1	1:A:790:PHE:HD2	2.10	0.49
2:P:10:DG:H2"	2:P:11:DG:OP2	2.11	0.49
1:A:1108:ILE:HD12	1:A:1119:PRO:HB3	1.95	0.49
1:A:891:GLY:O	1:A:977:ASN:HB2	2.13	0.49
1:A:368:LYS:CA	1:A:398:MET:CE	2.90	0.49
1:A:1188:THR:O	1:A:1189:ASP:HB2	2.13	0.49
1:A:634:LEU:O	1:A:638:VAL:HG12	2.13	0.48
1:A:725:ARG:NH1	1:A:790:PHE:CD2	2.80	0.48
1:A:882:LYS:HD2	1:A:989:TYR:CD2	2.48	0.48
1:A:635:PHE:HA	1:A:1068:PRO:HG3	1.95	0.48
1:A:916:HIS:HD2	1:A:918:VAL:HG22	1.78	0.48
1:A:1181:ILE:HA	1:A:1184:LEU:CD1	2.43	0.48
1:A:1210:ILE:CG2	1:A:1270:MET:HE1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:CA	1:A:398:MET:HE3	2.43	0.48
1:A:399:LYS:NZ	1:A:808:ALA:O	2.46	0.48
1:A:728:VAL:HG13	1:A:795:LYS:HE3	1.96	0.48
1:A:368:LYS:HD3	1:A:398:MET:HE2	1.95	0.48
1:A:1075:ASP:C	1:A:1075:ASP:OD1	2.52	0.48
1:A:237:GLU:HG2	1:A:275:THR:OG1	2.13	0.47
1:A:335:THR:H	1:A:782:ASN:HD21	1.56	0.47
1:A:386:PHE:HB2	1:A:387:PRO:HD3	1.95	0.47
1:A:343:VAL:H	1:A:804:THR:HG23	1.73	0.47
1:A:1161:ARG:HH12	1:A:1329:ASN:HD21	1.62	0.47
1:A:860:GLU:HG2	1:A:960:PHE:CE1	2.49	0.47
1:A:240:VAL:HG23	1:A:241:GLU:HG3	1.95	0.47
1:A:1166:MET:HE1	1:A:1184:LEU:HD13	1.97	0.47
1:A:1403:GLU:O	1:A:1403:GLU:CG	2.61	0.47
1:A:1416:GLY:O	1:A:1417:LYS:HB2	2.13	0.46
1:A:235:ARG:HG3	1:A:235:ARG:HH11	1.81	0.46
1:A:766:ASN:N	1:A:767:PRO:CD	2.78	0.46
1:A:634:LEU:O	1:A:638:VAL:CG1	2.64	0.46
1:A:1298:TYR:OH	1:A:1351:GLU:OE1	2.29	0.46
1:A:1276:ALA:O	1:A:1280:VAL:HG23	2.15	0.46
1:A:1102:HIS:HD2	1:A:1104:ASP:HB2	1.81	0.46
3:T:15:DT:H6	3:T:15:DT:H2'	1.58	0.46
1:A:252:VAL:HG13	1:A:300:MET:O	2.16	0.46
1:A:719:MET:CE	1:A:719:MET:CG	2.94	0.45
1:A:966:PHE:CZ	1:A:1227:PRO:HB3	2.52	0.45
1:A:958:ILE:HG12	1:A:1273:LYS:HD2	1.99	0.45
1:A:1102:HIS:HD2	1:A:1104:ASP:N	2.05	0.45
1:A:355:ASP:O	1:A:755:ARG:HD3	2.16	0.45
1:A:700:HIS:HD2	1:A:741:THR:O	1.99	0.45
1:A:1201:ASN:HB2	1:A:1203:THR:HG23	1.98	0.45
1:A:983:GLN:HB3	1:A:984:PRO:HD3	1.99	0.45
1:A:1201:ASN:HD22	1:A:1203:THR:CG2	2.30	0.44
1:A:1363:ASP:OD1	1:A:1363:ASP:C	2.56	0.44
1:A:897:GLY:HA3	1:A:1274:ALA:HB1	1.98	0.44
1:A:747:LEU:HD13	1:A:748:ASN:ND2	2.33	0.44
1:A:335:THR:N	1:A:782:ASN:ND2	2.54	0.44
1:A:355:ASP:O	1:A:755:ARG:CD	2.65	0.44
1:A:944:CYS:C	1:A:946:ARG:H	2.21	0.44
1:A:1190:VAL:HG22	1:A:1267:ILE:HG23	1.98	0.44
2:P:5:DG:H4'	2:P:6:DA:O5'	2.17	0.44
1:A:728:VAL:HG13	1:A:795:LYS:CE	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:GLY:HA2	7:A:1456:DGT:O3'	2.17	0.44
1:A:272:THR:HG23	1:A:272:THR:O	2.17	0.43
1:A:619:PHE:CD2	1:A:674:GLU:HB2	2.53	0.43
1:A:285:ARG:HE	1:A:285:ARG:HB2	1.69	0.43
1:A:1122:ILE:HA	1:A:1123:PRO:HD3	1.84	0.43
1:A:1275:HIS:CD2	7:A:1456:DGT:H2'	2.52	0.43
1:A:1160:THR:HG23	1:A:1162:PHE:H	1.83	0.43
1:A:634:LEU:HD23	1:A:634:LEU:HA	1.79	0.43
1:A:386:PHE:CZ	1:A:402:TYR:HB3	2.54	0.43
1:A:1161:ARG:NH1	1:A:1329:ASN:HD21	2.17	0.43
1:A:669:GLY:HA2	1:A:698:GLU:CD	2.40	0.43
1:A:1275:HIS:CE1	7:A:1456:DGT:H2'	2.53	0.43
1:A:253:PHE:CZ	1:A:1035:ARG:HB3	2.54	0.42
1:A:902:ALA:HB1	1:A:907:ILE:HG22	2.01	0.42
1:A:1137:GLU:HB3	1:A:1138:PRO:CD	2.49	0.42
1:A:348:HIS:HE1	1:A:405:GLU:OE2	2.01	0.42
1:A:244:ARG:HB2	1:A:244:ARG:NH1	2.35	0.42
1:A:823:THR:HB	8:A:54:HOH:O	2.19	0.42
1:A:1223:ARG:HA	1:A:1223:ARG:HD2	1.64	0.42
1:A:978:PHE:CE2	1:A:1099:ILE:HG23	2.54	0.42
1:A:1172:PRO:HB2	1:A:1178:LEU:HD13	2.02	0.42
1:A:248:VAL:CG1	1:A:249:GLN:N	2.83	0.42
1:A:368:LYS:HD3	1:A:398:MET:CE	2.50	0.42
1:A:780:THR:HG22	1:A:783:GLU:N	2.21	0.42
1:A:1184:LEU:HA	1:A:1190:VAL:HG11	2.02	0.42
1:A:754:TYR:CE1	1:A:1039:GLY:HA3	2.54	0.42
1:A:1143:PRO:HA	1:A:1148:CYS:O	2.20	0.42
1:A:386:PHE:CE2	1:A:402:TYR:HB3	2.55	0.42
1:A:1333:ILE:C	1:A:1335:ALA:H	2.23	0.42
1:A:860:GLU:CG	1:A:960:PHE:CE1	3.04	0.41
1:A:1112:GLN:HG3	1:A:1117:ILE:O	2.20	0.41
1:A:236:LEU:HB3	1:A:276:ASN:HB3	2.02	0.41
1:A:1160:THR:HG23	1:A:1161:ARG:N	2.35	0.41
1:A:911:ASN:HD22	1:A:913:LEU:H	1.68	0.41
1:A:1002:ALA:HB3	1:A:1050:HIS:CB	2.51	0.41
1:A:349:THR:O	1:A:356:ALA:HB3	2.20	0.41
1:A:368:LYS:CB	1:A:398:MET:HE3	2.48	0.41
1:A:766:ASN:C	1:A:766:ASN:HD22	2.23	0.41
1:A:311:ASP:HB3	1:A:314:VAL:HG12	2.01	0.41
1:A:302:VAL:CG1	1:A:304:VAL:HG23	2.50	0.41
1:A:875:ILE:HG12	1:A:994:PHE:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:ARG:HG3	1:A:1275:HIS:CE1	2.56	0.41
1:A:348:HIS:CE1	1:A:405:GLU:OE2	2.74	0.41
1:A:887:GLY:O	1:A:1109:ARG:HD2	2.21	0.41
1:A:804:THR:HG22	1:A:805:GLN:N	2.36	0.40
1:A:1298:TYR:O	1:A:1299:ALA:C	2.59	0.40
1:A:1410:GLU:O	1:A:1414:GLN:HG2	2.20	0.40
1:A:1210:ILE:HG21	1:A:1270:MET:HE1	2.02	0.40
1:A:637:LEU:HG	1:A:652:ILE:HD13	2.02	0.40
1:A:823:THR:HG21	1:A:868:GLY:HA3	2.02	0.40
1:A:867:HIS:NE2	1:A:968:GLY:HA3	2.37	0.40
1:A:917:TYR:HB3	1:A:951:TYR:CG	2.56	0.40
1:A:862:LYS:HB3	1:A:862:LYS:HE3	1.90	0.40
1:A:1095:LEU:HD23	1:A:1095:LEU:HA	1.87	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	986/1041 (95%)	932 (94%)	49 (5%)	5 (0%)	29 41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	670	CYS
1	A	767	PRO
1	A	330	ASN
1	A	1052	GLY
1	A	707	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	853/904 (94%)	758 (89%)	95 (11%)	6 8

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
1	A	237	GLU
1	A	241	GLU
1	A	247	VAL
1	A	252	VAL
1	A	260	LEU
1	A	261	LYS
1	A	264	ARG
1	A	285	ARG
1	A	286	ASP
1	A	297	LYS
1	A	302	VAL
1	A	318	VAL
1	A	323	ASP
1	A	332	ARG
1	A	357	VAL
1	A	363	LEU
1	A	369	LYS
1	A	385	SER
1	A	395	LYS
1	A	404	LEU
1	A	410	ASP
1	A	628	GLU
1	A	637	LEU
1	A	638	VAL
1	A	644	GLN
1	A	649	VAL
1	A	654	ARG
1	A	657	LEU
1	A	659	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	670	CYS
1	A	672	LYS
1	A	675	LEU
1	A	677	ASP
1	A	687	VAL
1	A	699	VAL
1	A	707	PRO
1	A	725	ARG
1	A	733	LYS
1	A	747	LEU
1	A	750	GLU
1	A	766	ASN
1	A	778	PHE
1	A	780	THR
1	A	781	THR
1	A	801	VAL
1	A	804	THR
1	A	823	THR
1	A	831	GLU
1	A	840	ARG
1	A	852	LEU
1	A	862	LYS
1	A	875	ILE
1	A	896	VAL
1	A	911	ASN
1	A	918	VAL
1	A	922	CYS
1	A	926	GLU
1	A	930	ASP
1	A	946	ARG
1	A	949	THR
1	A	951	TYR
1	A	971	VAL
1	A	976	LEU
1	A	1026	LEU
1	A	1035	ARG
1	A	1045	ARG
1	A	1056	VAL
1	A	1098	ASP
1	A	1108	ILE
1	A	1111	LEU
1	A	1139	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1160	THR
1	A	1167	LEU
1	A	1169	GLU
1	A	1174	THR
1	A	1178	LEU
1	A	1180	GLN
1	A	1181	ILE
1	A	1184	LEU
1	A	1192	LEU
1	A	1203	THR
1	A	1209	VAL
1	A	1214	ASP
1	A	1223	ARG
1	A	1237	VAL
1	A	1243	LEU
1	A	1253	LYS
1	A	1348	VAL
1	A	1360	LYS
1	A	1362	ILE
1	A	1417	LYS
1	A	1427	GLU
1	A	1432	LEU
1	A	1441	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	HIS
1	A	396	HIS
1	A	620	HIS
1	A	633	ASN
1	A	644	GLN
1	A	647	HIS
1	A	700	HIS
1	A	766	ASN
1	A	782	ASN
1	A	803	ASN
1	A	805	GLN
1	A	911	ASN
1	A	924	HIS
1	A	943	ASN
1	A	1093	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1102	HIS
1	A	1112	GLN
1	A	1180	GLN
1	A	1200	GLN
1	A	1201	ASN
1	A	1329	ASN
1	A	1439	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
7	DGT	A	1456	6	26,33,33	1.07	1 (3%)	32,52,52	1.89	7 (21%)
4	PO4	A	2	-	4,4,4	0.87	0	6,6,6	0.47	0
4	PO4	A	1	-	4,4,4	0.93	0	6,6,6	0.33	0
4	PO4	A	3	-	4,4,4	0.83	0	6,6,6	0.59	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
7	DGT	A	1456	6	-	7/18/34/34	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1456	DGT	C6-N1	-2.83	1.33	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1456	DGT	C2'-C1'-N9	-6.12	100.15	114.27
7	A	1456	DGT	C8-N7-C5	3.21	109.10	102.99
7	A	1456	DGT	O5'-PA-O2A	-3.03	97.21	109.07
7	A	1456	DGT	O4'-C4'-C5'	-2.72	100.42	109.37
7	A	1456	DGT	C5'-C4'-C3'	-2.51	100.00	114.74
7	A	1456	DGT	PB-O3B-PG	-2.50	124.25	132.83
7	A	1456	DGT	C5-C6-N1	2.17	117.78	113.95

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1456	DGT	PB-O3B-PG-O1G
7	A	1456	DGT	PB-O3B-PG-O2G
7	A	1456	DGT	O4'-C4'-C5'-O5'
7	A	1456	DGT	C3'-C4'-C5'-O5'
7	A	1456	DGT	PB-O3A-PA-O5'
7	A	1456	DGT	PA-O3A-PB-O1B
7	A	1456	DGT	PB-O3B-PG-O3G

There are no ring outliers.

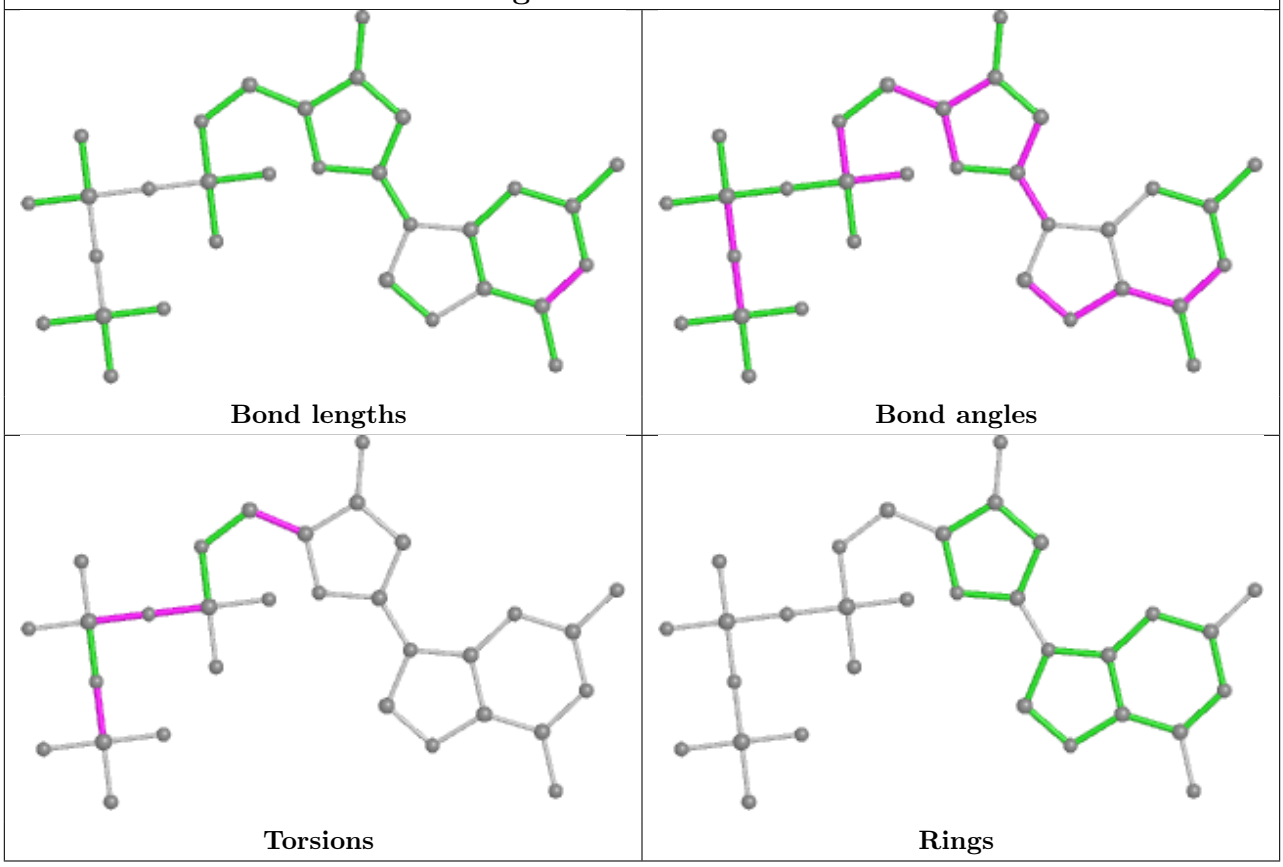
1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1456	DGT	9	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 1456



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	994/1041 (95%)	0.17	25 (2%)	57	55	29, 42, 58, 79	0
2	P	13/17 (76%)	0.38	1 (7%)	13	12	27, 43, 79, 89	0
3	T	18/22 (81%)	-0.01	1 (5%)	24	23	27, 43, 65, 69	0
All	All	1025/1080 (94%)	0.17	27 (2%)	56	54	27, 42, 59, 89	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	PRO	7.0
1	A	765	ALA	4.4
1	A	793	PRO	3.8
1	A	647	HIS	3.7
2	P	5	DG	3.5
1	A	676	PHE	3.4
1	A	675	LEU	3.3
1	A	796	ALA	3.2
1	A	766	ASN	2.9
1	A	338	GLU	2.6
1	A	708	LEU	2.5
1	A	330	ASN	2.4
1	A	1023	ASP	2.4
1	A	690	ILE	2.3
1	A	705	TYR	2.3
1	A	382	VAL	2.3
1	A	789	SER	2.2
1	A	1025	ASN	2.1
1	A	948	GLY	2.1
1	A	410	ASP	2.1
1	A	651	ARG	2.0
3	T	18	DC	2.0
1	A	719	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	949	THR	2.0
1	A	669	GLY	2.0
1	A	729	ALA	2.0
1	A	794	GLU	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)

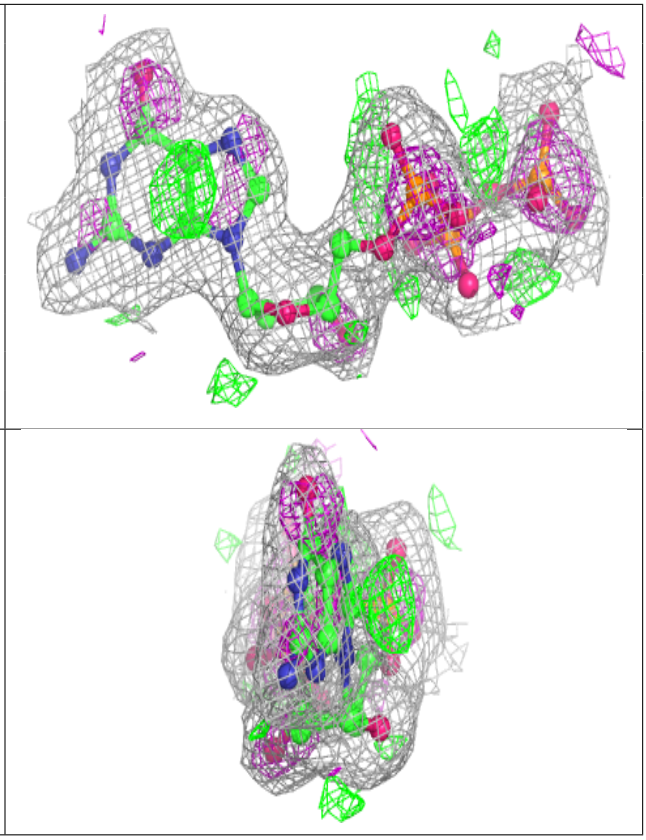
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	A	1	5/5	0.77	0.23	92,93,94,94	0
6	MG	A	6	1/1	0.80	0.11	61,61,61,61	0
4	PO4	A	2	5/5	0.82	0.30	123,123,123,123	0
4	PO4	A	3	5/5	0.87	0.35	97,97,97,97	0
6	MG	A	7	1/1	0.87	0.07	49,49,49,49	0
6	MG	A	5	1/1	0.94	0.04	24,24,24,24	0
5	ZN	A	4	1/1	0.95	0.05	73,73,73,73	0
7	DGT	A	1456	31/31	0.98	0.08	23,27,30,30	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 DGT A 1456:

$2mF_o$-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.