Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 PM GMT

PDB ID	:	4TNY
Title	:	Structural basis of cellular dNTP regulation, SAMHD1-dGTP-dATP-dGTP complex
Authors	:	Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on	:	2014-06-05
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

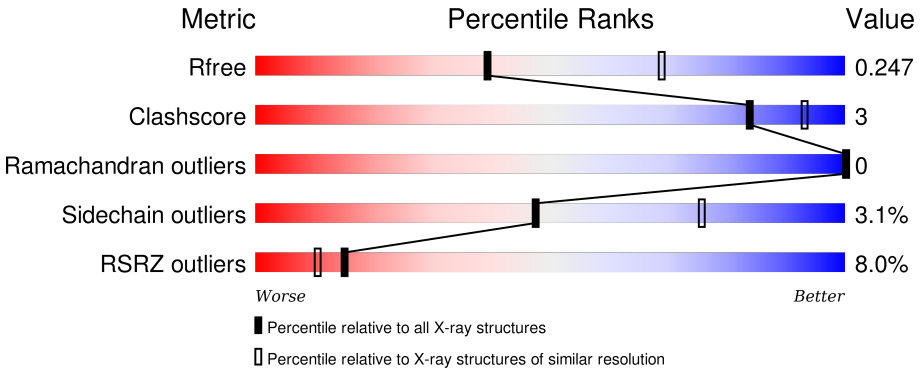
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	514	3% 86% 7% • 6%
1	B	514	5% 86% 7% • 6%
1	C	514	9% 85% 8% • 6%
1	D	514	13% 84% 8% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16275 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.

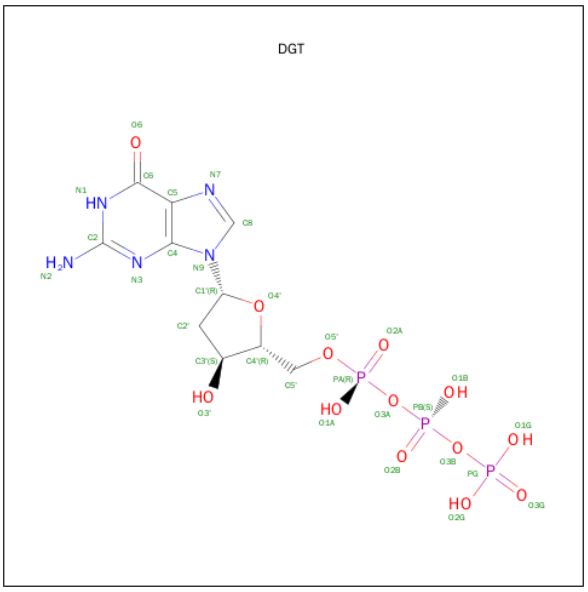
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	C	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	B	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	D	481	Total	C	N	O	S	0	4	0
			3966	2535	691	719	21			

There are 8 discrepancies between the modelled and reference sequences:

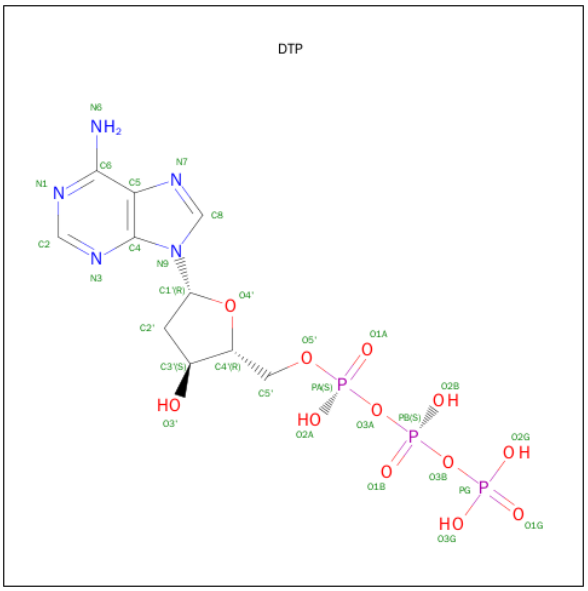
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- 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
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		

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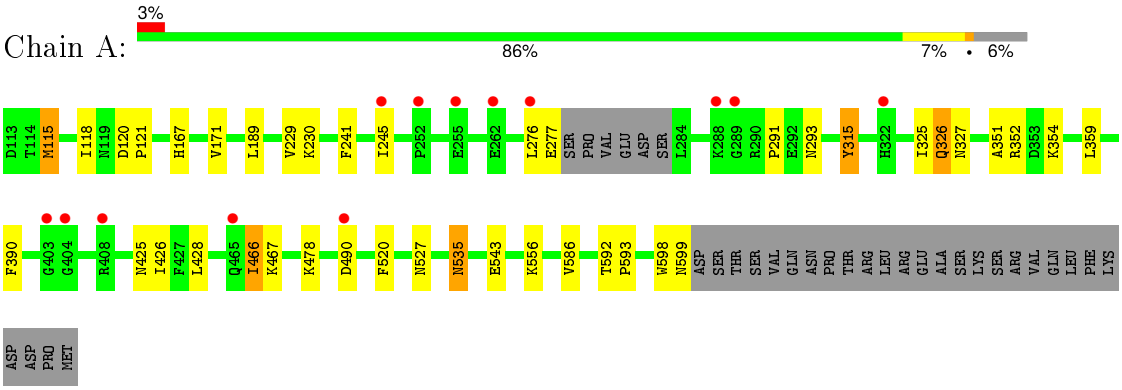
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	3	Total O 3 3	0	0
5	B	1	Total O 1 1	0	0
5	D	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

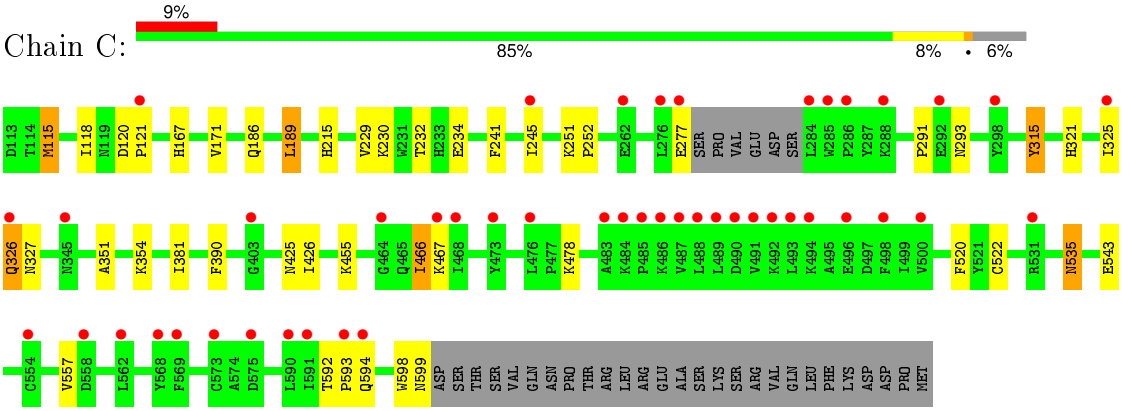
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



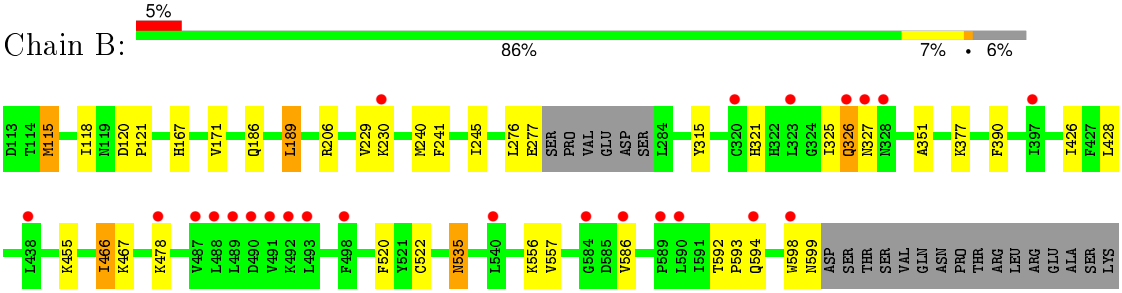
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

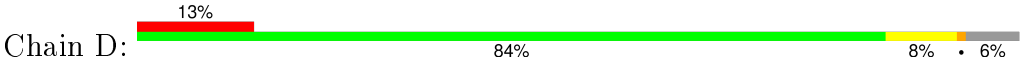
Chain B:

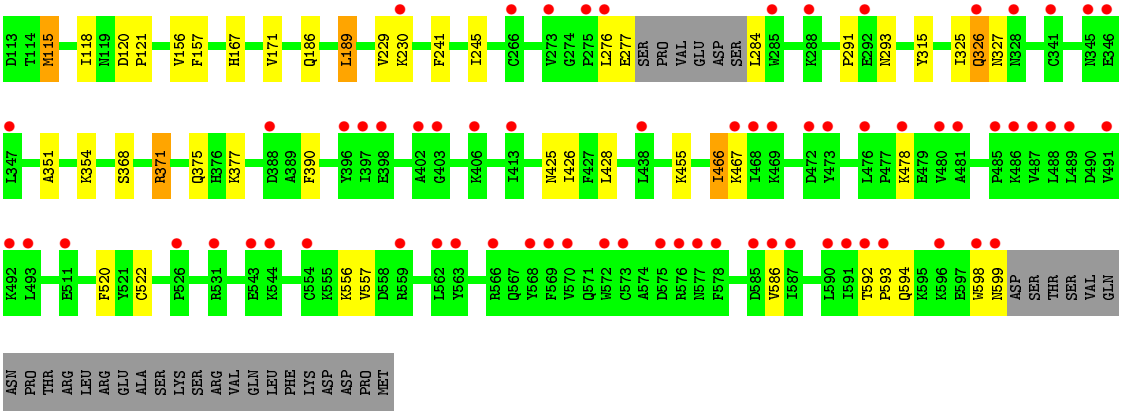


SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:





ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.25Å 141.87Å 98.33Å 90.00° 116.38° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.69 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.60) 98.8 (48.69-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.214 , 0.244 0.220 , 0.247	Depositor DCC
R_{free} test set	3295 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.8	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 65672 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16275	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.63	0/4067	0.71	0/5490
1	B	0.61	0/4067	0.70	0/5490
1	C	0.60	0/4067	0.71	0/5490
1	D	0.58	0/4059	0.70	0/5479
All	All	0.61	0/16260	0.71	0/21949

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Peptide
1	B	276	LEU	Peptide
1	D	276	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3974	0	3944	24	1
1	B	3974	0	3944	23	0
1	C	3974	0	3944	30	0
1	D	3966	0	3939	26	0
2	A	31	0	12	2	0
2	B	62	0	24	1	0
2	C	62	0	24	4	0
2	D	93	0	36	8	0
3	A	30	0	12	2	0
3	B	30	0	12	2	0
3	C	30	0	12	2	0
3	D	30	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	16275	0	15915	98	1

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 3.

All (98) 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:377:LYS:NZ	3:D:703:DTP:O2B	2.09	0.85
1:A:535:ASN:N	1:A:535:ASN:OD1	2.21	0.71
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.32	0.68
1:B:535:ASN:OD1	1:B:535:ASN:N	2.22	0.66
1:C:535:ASN:N	1:C:535:ASN:OD1	2.21	0.66
2:D:704:DGT:O3G	2:D:704:DGT:PA	2.54	0.66
1:C:390:PHE:CE2	1:C:426:ILE:HD11	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LYS:NZ	3:C:701:DTP:O1A	2.32	0.60
1:D:390:PHE:CE2	1:D:426:ILE:HD11	2.37	0.60
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.00	0.60
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.37	0.59
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.03	0.57
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.39	0.57
1:B:206:ARG:NH2	2:B:702:DGT:O2B	2.34	0.57
1:D:466:ILE:HD13	1:D:466:ILE:N	2.21	0.56
1:A:327:ASN:O	1:C:326:GLN:HG2	2.06	0.56
1:B:598:TRP:O	1:B:599:ASN:HB2	2.07	0.55
1:C:598:TRP:O	1:C:599:ASN:HB2	2.06	0.55
1:B:326:GLN:HG2	1:D:327:ASN:O	2.07	0.54
1:A:326:GLN:HG2	1:C:327:ASN:O	2.07	0.54
1:B:466:ILE:N	1:B:466:ILE:HD13	2.23	0.54
1:C:215:HIS:NE2	2:C:702:DGT:O2A	2.40	0.54
1:D:598:TRP:O	1:D:599:ASN:HB2	2.08	0.54
1:A:598:TRP:O	1:A:599:ASN:HB2	2.07	0.54
1:C:466:ILE:N	1:C:466:ILE:HD13	2.22	0.53
3:B:704:DTP:O2B	1:D:377:LYS:NZ	2.32	0.53
2:C:702:DGT:H4'	2:C:702:DGT:O1A	2.09	0.53
1:A:466:ILE:N	1:A:466:ILE:HD13	2.24	0.52
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.12	0.50
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.93	0.49
1:B:586:VAL:HG11	1:D:522[A]:CYS:SG	2.53	0.49
1:D:598:TRP:O	1:D:599:ASN:CB	2.62	0.48
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.95	0.48
1:D:351:ALA:O	1:D:520:PHE:HA	2.13	0.48
1:A:315:TYR:CD1	2:A:701:DGT:H3'	2.47	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.48
1:B:327:ASN:O	1:D:326:GLN:HG2	2.13	0.48
1:C:351:ALA:O	1:C:520:PHE:HA	2.14	0.48
1:A:598:TRP:O	1:A:599:ASN:CB	2.61	0.48
1:D:241:PHE:O	1:D:245:ILE:HG12	2.14	0.48
2:D:704:DGT:O1A	2:D:704:DGT:PG	2.72	0.47
1:B:598:TRP:O	1:B:599:ASN:CB	2.61	0.47
1:C:598:TRP:O	1:C:599:ASN:CB	2.61	0.47
1:B:241:PHE:O	1:B:245:ILE:HG12	2.14	0.47
1:C:241:PHE:O	1:C:245:ILE:HG12	2.14	0.47
1:A:354:LYS:NZ	3:A:702:DTP:O1A	2.42	0.47
1:A:315:TYR:CE2	2:A:701:DGT:H5'	2.48	0.47
1:A:241:PHE:O	1:A:245:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:HIS:O	1:D:171:VAL:HG23	2.15	0.47
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.14	0.47
1:A:167:HIS:O	1:A:171:VAL:HG23	2.16	0.46
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.46
1:C:167:HIS:O	1:C:171:VAL:HG23	2.16	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.46
1:B:167:HIS:O	1:B:171:VAL:HG23	2.15	0.46
1:D:156:VAL:O	2:D:705:DGT:H8	2.16	0.46
1:A:543:GLU:HG2	1:C:543:GLU:HG2	1.98	0.45
1:B:592:THR:N	1:B:593:PRO:CD	2.80	0.45
1:B:229:VAL:HG12	1:B:230:LYS:N	2.32	0.45
1:C:592:THR:N	1:C:593:PRO:CD	2.80	0.45
1:C:229:VAL:HG12	1:C:230:LYS:N	2.32	0.45
1:C:115:MET:SD	1:C:115:MET:C	2.96	0.45
1:B:115:MET:C	1:B:115:MET:SD	2.94	0.45
2:D:705:DGT:H3'	2:D:705:DGT:PA	2.57	0.44
1:D:592:THR:N	1:D:593:PRO:CD	2.80	0.44
1:D:115:MET:SD	1:D:115:MET:C	2.96	0.44
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.89	0.44
1:A:115:MET:C	1:A:115:MET:SD	2.95	0.44
1:A:229:VAL:HG12	1:A:230:LYS:N	2.33	0.44
1:D:229:VAL:HG12	1:D:230:LYS:N	2.32	0.44
3:C:701:DTP:O1B	2:D:702:DGT:H5'A	2.18	0.44
1:D:455:LYS:HG2	1:D:557:VAL:HG12	2.00	0.43
1:D:186:GLN:HB2	1:D:189:LEU:HD22	2.00	0.43
1:D:368:SER:HA	1:D:371:ARG:HD2	1.99	0.43
2:D:704:DGT:O1A	2:D:704:DGT:O1G	2.36	0.43
1:C:455:LYS:HG2	1:C:557:VAL:HG12	2.00	0.43
1:B:455:LYS:HG2	1:B:557:VAL:HG12	2.01	0.43
1:B:230:LYS:HA	1:B:230:LYS:HD2	1.88	0.43
1:C:230:LYS:HD2	1:C:230:LYS:HA	1.85	0.43
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.19	0.42
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.59	0.42
1:B:186:GLN:HB2	1:B:189:LEU:HD22	2.00	0.42
1:C:186:GLN:HB2	1:C:189:LEU:HD22	2.01	0.42
2:D:705:DGT:H2'A	2:D:705:DGT:N3	2.34	0.42
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.00	0.42
1:C:425:ASN:HB2	1:B:428:LEU:HD13	2.01	0.42
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.20	0.42
1:C:390:PHE:CE2	1:C:426:ILE:CD1	3.03	0.41
2:C:702:DGT:O1B	2:C:702:DGT:O3G	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HH22	3:A:702:DTP:PG	2.44	0.41
3:B:704:DTP:H2'1	1:D:157:PHE:CE2	2.56	0.41
1:C:315:TYR:CE2	2:C:702:DGT:H5'	2.56	0.41
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.21	0.41
1:D:375:GLN:NE2	2:D:704:DGT:O6	2.45	0.41
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.09	0.40
1:D:354:LYS:NZ	3:D:703:DTP:O1A	2.53	0.40
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.03	0.40
1:C:232:THR:HB	1:C:234:GLU:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ASP:OD1	1:A:527:ASN:O[2_545]	2.17	0.03

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	482/514 (94%)	476 (99%)	6 (1%)	0	100	100
1	B	482/514 (94%)	477 (99%)	5 (1%)	0	100	100
1	C	482/514 (94%)	475 (98%)	7 (2%)	0	100	100
1	D	481/514 (94%)	476 (99%)	5 (1%)	0	100	100
All	All	1927/2056 (94%)	1904 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	432/459 (94%)	419 (97%)	13 (3%)	48	76
1	B	432/459 (94%)	418 (97%)	14 (3%)	46	74
1	C	432/459 (94%)	420 (97%)	12 (3%)	51	78
1	D	431/459 (94%)	417 (97%)	14 (3%)	46	74
All	All	1727/1836 (94%)	1674 (97%)	53 (3%)	47	76

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	118	ILE
1	A	189	LEU
1	A	277	GLU
1	A	315	TYR
1	A	325	ILE
1	A	326	GLN
1	A	359	LEU
1	A	466	ILE
1	A	467	LYS
1	A	478	LYS
1	A	535	ASN
1	A	556	LYS
1	C	115	MET
1	C	118	ILE
1	C	189	LEU
1	C	277	GLU
1	C	315	TYR
1	C	325	ILE
1	C	326	GLN
1	C	466	ILE
1	C	467	LYS
1	C	478	LYS
1	C	535	ASN

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Mol	Chain	Res	Type
1	C	594	GLN
1	B	115	MET
1	B	118	ILE
1	B	189	LEU
1	B	240	MET
1	B	277	GLU
1	B	315	TYR
1	B	325	ILE
1	B	326	GLN
1	B	466	ILE
1	B	467	LYS
1	B	478	LYS
1	B	535	ASN
1	B	556	LYS
1	B	594	GLN
1	D	115	MET
1	D	118	ILE
1	D	189	LEU
1	D	277	GLU
1	D	284	LEU
1	D	315	TYR
1	D	325	ILE
1	D	326	GLN
1	D	371	ARG
1	D	466	ILE
1	D	467	LYS
1	D	478	LYS
1	D	556	LYS
1	D	594	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	A	425	ASN
1	C	364	HIS
1	C	425	ASN
1	B	364	HIS
1	B	425	ASN
1	D	364	HIS
1	D	425	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DGT	A	701	-	25,33,33	1.46	3 (12%)	35,52,52	2.06	11 (31%)
3	DTP	A	702	4	24,32,32	0.92	1 (4%)	32,50,50	2.82	11 (34%)
2	DGT	B	702	-	25,33,33	1.43	3 (12%)	35,52,52	2.19	11 (31%)
2	DGT	B	703	4	25,33,33	1.29	2 (8%)	35,52,52	1.97	10 (28%)
3	DTP	B	704	4	24,32,32	0.85	1 (4%)	32,50,50	2.66	8 (25%)
3	DTP	C	701	4	24,32,32	1.06	2 (8%)	32,50,50	2.06	7 (21%)
2	DGT	C	702	-	25,33,33	1.30	2 (8%)	35,52,52	1.98	9 (25%)
2	DGT	C	703	4	25,33,33	0.94	2 (8%)	35,52,52	1.73	6 (17%)
2	DGT	D	702	4	25,33,33	0.94	0	35,52,52	1.83	9 (25%)
3	DTP	D	703	4	24,32,32	1.02	2 (8%)	32,50,50	2.01	7 (21%)
2	DGT	D	704	-	25,33,33	1.36	2 (8%)	35,52,52	2.09	10 (28%)
2	DGT	D	705	4	25,33,33	1.13	2 (8%)	35,52,52	1.85	6 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	A	701	-	-	0/18/34/34	0/3/3/3
3	DTP	A	702	4	-	0/18/34/34	0/3/3/3
2	DGT	B	702	-	-	0/18/34/34	0/3/3/3
2	DGT	B	703	4	-	0/18/34/34	0/3/3/3
3	DTP	B	704	4	-	0/18/34/34	0/3/3/3
3	DTP	C	701	4	-	0/18/34/34	0/3/3/3
2	DGT	C	702	-	-	0/18/34/34	0/3/3/3
2	DGT	C	703	4	-	0/18/34/34	0/3/3/3
2	DGT	D	702	4	-	0/18/34/34	0/3/3/3
3	DTP	D	703	4	-	0/18/34/34	0/3/3/3
2	DGT	D	704	-	-	0/18/34/34	0/3/3/3
2	DGT	D	705	4	-	0/18/34/34	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	DGT	O4'-C4'	-2.64	1.38	1.45
3	D	703	DTP	O4'-C4'	-2.38	1.39	1.45
2	B	702	DGT	C8-N7	2.04	1.38	1.34
3	C	701	DTP	C5-C4	2.05	1.45	1.40
3	C	701	DTP	C2-N3	2.12	1.35	1.32
3	D	703	DTP	C5-C4	2.19	1.45	1.40
2	C	703	DGT	C6-C5	2.32	1.45	1.41
3	A	702	DTP	C5-C4	2.40	1.45	1.40
3	B	704	DTP	C5-C4	2.59	1.46	1.40
2	C	703	DGT	C5-C4	2.91	1.47	1.40
2	D	705	DGT	C6-C5	2.94	1.47	1.41
2	D	704	DGT	C5-C4	3.37	1.48	1.40
2	C	702	DGT	C5-C4	3.38	1.48	1.40
2	B	703	DGT	C5-C4	3.44	1.48	1.40
2	D	705	DGT	C5-C4	3.52	1.48	1.40
2	B	702	DGT	C5-C4	3.75	1.49	1.40
2	A	701	DGT	C6-C5	3.80	1.48	1.41
2	A	701	DGT	C5-C4	3.91	1.49	1.40
2	B	703	DGT	C6-C5	3.93	1.49	1.41
2	B	702	DGT	C6-C5	3.97	1.49	1.41
2	C	702	DGT	C6-C5	4.10	1.49	1.41
2	D	704	DGT	C6-C5	4.51	1.50	1.41

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	DTP	N3-C2-N1	-11.65	119.97	128.89
3	B	704	DTP	N3-C2-N1	-10.34	120.98	128.89
3	D	703	DTP	N3-C2-N1	-7.79	122.93	128.89
3	C	701	DTP	N3-C2-N1	-6.50	123.92	128.89
2	B	702	DGT	PA-O3A-PB	-5.16	118.24	132.73
2	A	701	DGT	PA-O3A-PB	-5.03	118.60	132.73
2	C	703	DGT	PA-O3A-PB	-4.99	118.73	132.73
2	D	704	DGT	PA-O3A-PB	-4.95	118.84	132.73
3	B	704	DTP	PB-O3B-PG	-4.71	116.86	132.67
2	D	705	DGT	PA-O3A-PB	-4.67	119.61	132.73
2	C	702	DGT	PA-O3A-PB	-4.64	119.70	132.73
2	B	703	DGT	C5-C6-N1	-4.62	117.27	123.59
2	B	703	DGT	PA-O3A-PB	-4.61	119.78	132.73
2	A	701	DGT	C5-C6-N1	-4.59	117.31	123.59
3	B	704	DTP	C4-C5-N7	-4.59	105.25	109.48
2	C	702	DGT	PB-O3B-PG	-4.58	117.31	132.67
3	C	701	DTP	C4-C5-N7	-4.49	105.35	109.48
2	D	704	DGT	PB-O3B-PG	-4.37	118.02	132.67
2	D	705	DGT	C6-C5-C4	-4.36	115.69	120.90
2	B	702	DGT	C5-C6-N1	-4.27	117.75	123.59
2	B	702	DGT	C6-C5-C4	-4.24	115.83	120.90
2	D	702	DGT	PA-O3A-PB	-4.21	120.91	132.73
2	C	702	DGT	C5-C6-N1	-4.05	118.05	123.59
2	D	704	DGT	C6-C5-C4	-4.02	116.09	120.90
3	A	702	DTP	C1'-N9-C4	-3.99	120.39	127.16
3	C	701	DTP	O5'-PA-O1A	-3.91	94.45	109.62
2	D	704	DGT	C4-C5-N7	-3.89	105.90	109.48
2	A	701	DGT	PB-O3B-PG	-3.82	119.87	132.67
2	A	701	DGT	C6-C5-C4	-3.77	116.39	120.90
2	B	703	DGT	C4-C5-N7	-3.71	106.06	109.48
2	C	703	DGT	C5-C6-N1	-3.66	118.58	123.59
2	D	702	DGT	C5-C6-N1	-3.64	118.62	123.59
3	A	702	DTP	O5'-PA-O1A	-3.64	95.50	109.62
3	B	704	DTP	PA-O3A-PB	-3.46	123.02	132.73
3	B	704	DTP	C1'-N9-C4	-3.46	121.30	127.16
2	C	702	DGT	C4-C5-N7	-3.45	106.30	109.48
2	D	705	DGT	N3-C2-N1	-3.44	122.20	127.44
2	D	705	DGT	PB-O3B-PG	-3.42	121.21	132.67
3	D	703	DTP	C4-C5-N7	-3.39	106.36	109.48
3	C	701	DTP	PA-O3A-PB	-3.38	123.23	132.73
2	D	704	DGT	C5-C6-N1	-3.38	118.97	123.59
2	C	702	DGT	C6-C5-C4	-3.33	116.92	120.90
2	D	705	DGT	C5-C6-N1	-3.17	119.26	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	702	DGT	C4-C5-N7	-3.16	106.57	109.48
2	B	702	DGT	N3-C2-N1	-3.15	122.65	127.44
2	D	704	DGT	C1'-N9-C4	-3.04	122.00	127.16
2	D	702	DGT	N3-C2-N1	-3.02	122.84	127.44
2	C	703	DGT	C6-C5-C4	-3.02	117.29	120.90
2	D	702	DGT	C6-C5-C4	-3.01	117.30	120.90
3	A	702	DTP	C4-C5-N7	-2.97	106.75	109.48
3	A	702	DTP	PA-O3A-PB	-2.95	124.45	132.73
3	B	704	DTP	O5'-PA-O1A	-2.94	98.22	109.62
2	B	702	DGT	C1'-N9-C4	-2.85	122.32	127.16
2	B	702	DGT	PB-O3B-PG	-2.82	123.21	132.67
2	C	703	DGT	PB-O3B-PG	-2.75	123.43	132.67
2	C	703	DGT	N3-C2-N1	-2.75	123.26	127.44
2	A	701	DGT	C1'-N9-C4	-2.71	122.56	127.16
2	D	704	DGT	N3-C2-N1	-2.70	123.33	127.44
2	B	703	DGT	PB-O3B-PG	-2.70	123.62	132.67
3	A	702	DTP	PB-O3B-PG	-2.63	123.83	132.67
3	A	702	DTP	O4'-C1'-N9	-2.52	103.35	107.72
3	C	701	DTP	PB-O3B-PG	-2.52	124.22	132.67
2	D	702	DGT	PB-O3B-PG	-2.51	124.24	132.67
2	A	701	DGT	C4-C5-N7	-2.47	107.21	109.48
2	C	702	DGT	N3-C2-N1	-2.39	123.81	127.44
3	D	703	DTP	PB-O3B-PG	-2.32	124.88	132.67
2	A	701	DGT	N3-C2-N1	-2.31	123.92	127.44
2	D	702	DGT	C4-C5-N7	-2.30	107.36	109.48
2	B	703	DGT	N3-C2-N1	-2.30	123.95	127.44
2	B	703	DGT	O3A-PA-O5'	-2.26	96.95	102.94
3	D	703	DTP	PA-O3A-PB	-2.25	126.42	132.73
2	B	703	DGT	C6-C5-C4	-2.07	118.43	120.90
3	C	701	DTP	O3'-C3'-C4'	-2.02	101.88	110.05
2	D	702	DGT	O1B-PB-O3A	2.02	114.24	105.09
2	D	704	DGT	O1G-PG-O3G	2.02	117.08	110.58
3	B	704	DTP	O2A-PA-O1A	2.04	123.56	112.53
3	D	703	DTP	O2B-PB-O1B	2.04	123.61	112.53
2	B	703	DGT	O1B-PB-O3B	2.05	114.38	105.09
3	A	702	DTP	O2A-PA-O3A	2.09	114.59	105.09
2	A	701	DGT	N2-C2-N1	2.13	120.72	117.20
2	B	703	DGT	O1G-PG-O3G	2.21	117.71	110.58
2	A	701	DGT	O2G-PG-O1G	2.28	116.07	107.38
2	C	702	DGT	O4'-C1'-N9	2.32	111.73	107.72
2	C	702	DGT	O1G-PG-O3G	2.32	118.06	110.58
2	A	701	DGT	O4'-C1'-N9	2.37	111.82	107.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	DTP	O3A-PA-O5'	2.46	109.46	102.94
2	B	702	DGT	O2G-PG-O3G	2.54	118.75	110.58
2	D	702	DGT	O1G-PG-O3G	2.61	118.98	110.58
2	B	702	DGT	N2-C2-N1	2.69	121.65	117.20
3	D	703	DTP	C2'-C3'-C4'	2.75	108.47	102.77
3	C	701	DTP	O3G-PG-O1G	2.79	119.56	110.58
2	D	704	DGT	O4'-C1'-N9	2.84	112.64	107.72
3	D	703	DTP	O3G-PG-O1G	3.07	120.47	110.58
3	A	702	DTP	O2G-PG-O1G	3.08	120.49	110.58
2	B	702	DGT	O4'-C1'-N9	3.55	113.87	107.72
3	B	704	DTP	C2-N1-C6	3.70	125.38	118.77
2	D	704	DGT	C6-N1-C2	4.01	121.50	115.94
3	A	702	DTP	C2-N1-C6	4.03	125.97	118.77
2	C	703	DGT	C6-N1-C2	4.32	121.93	115.94
2	C	702	DGT	C6-N1-C2	4.33	121.95	115.94
2	D	702	DGT	C6-N1-C2	4.51	122.19	115.94
2	A	701	DGT	C6-N1-C2	4.51	122.20	115.94
2	B	703	DGT	C6-N1-C2	4.55	122.26	115.94
2	D	705	DGT	C6-N1-C2	4.58	122.30	115.94
2	B	702	DGT	C6-N1-C2	5.09	123.01	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	DGT	2	0
3	A	702	DTP	2	0
2	B	702	DGT	1	0
3	B	704	DTP	2	0
3	C	701	DTP	2	0
2	C	702	DGT	4	0
2	D	702	DGT	1	0
3	D	703	DTP	2	0
2	D	704	DGT	4	0
2	D	705	DGT	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	481/514 (93%)	0.15	13 (2%)	58	51	35, 63, 104, 133	0
1	B	481/514 (93%)	0.41	24 (4%)	32	26	37, 75, 119, 156	0
1	C	481/514 (93%)	0.47	47 (9%)	10	6	36, 74, 121, 156	0
1	D	481/514 (93%)	0.89	69 (14%)	4	2	41, 100, 169, 208	0
All	All	1924/2056 (93%)	0.48	153 (7%)	15	10	35, 76, 139, 208	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	599	ASN	7.0
1	B	490	ASP	6.9
1	D	562	LEU	6.5
1	D	569	PHE	6.5
1	C	489	LEU	6.4
1	C	488	LEU	5.9
1	D	480	VAL	5.8
1	D	488	LEU	5.6
1	D	585	ASP	5.5
1	C	491	VAL	5.5
1	D	554	CYS	5.4
1	D	481	ALA	5.3
1	D	592	THR	5.3
1	D	487	VAL	5.2
1	D	476	LEU	5.2
1	C	493	LEU	5.1
1	C	490	ASP	4.9
1	D	570	VAL	4.8
1	D	493	LEU	4.7
1	D	478	LYS	4.5
1	D	341	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	573	CYS	4.4
1	D	572	TRP	4.4
1	D	586	VAL	4.3
1	D	397	ILE	4.2
1	D	347	LEU	4.2
1	D	485	PRO	4.2
1	D	587	ILE	4.2
1	B	540	LEU	4.1
1	D	402	ALA	4.1
1	D	563	TYR	4.1
1	D	276	LEU	4.0
1	D	345	ASN	4.0
1	C	492	LYS	4.0
1	B	488	LEU	4.0
1	D	590	LEU	3.9
1	B	590	LEU	3.8
1	D	593	PRO	3.8
1	D	468	ILE	3.8
1	D	489	LEU	3.6
1	A	245	ILE	3.6
1	B	397	ILE	3.6
1	B	491	VAL	3.6
1	C	284	LEU	3.6
1	D	467	LYS	3.5
1	D	469	LYS	3.5
1	D	472	ASP	3.5
1	D	403	GLY	3.4
1	B	492	LYS	3.4
1	D	531	ARG	3.4
1	C	286	PRO	3.4
1	A	262	GLU	3.4
1	C	568	TYR	3.3
1	C	468	ILE	3.3
1	D	396	TYR	3.3
1	D	273	VAL	3.3
1	A	252	PRO	3.3
1	B	489	LEU	3.2
1	D	473	TYR	3.2
1	A	255	GLU	3.2
1	B	328	ASN	3.2
1	C	486	LYS	3.2
1	D	388[A]	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	594	GLN	3.1
1	C	403	GLY	3.0
1	C	487	VAL	3.0
1	D	285	TRP	3.0
1	C	467	LYS	3.0
1	D	511[A]	GLU	3.0
1	D	591	ILE	3.0
1	C	277	GLU	2.9
1	B	598	TRP	2.8
1	D	559	ARG	2.8
1	C	562	LEU	2.8
1	B	230	LYS	2.8
1	C	498	PHE	2.8
1	D	230	LYS	2.8
1	D	266	CYS	2.8
1	D	526	PRO	2.8
1	C	288	LYS	2.7
1	C	575	ASP	2.7
1	B	589	PRO	2.7
1	C	494	LYS	2.7
1	D	328	ASN	2.7
1	C	473	TYR	2.7
1	C	484	LYS	2.7
1	D	406	LYS	2.6
1	C	345	ASN	2.6
1	C	262	GLU	2.6
1	B	478	LYS	2.6
1	C	569	PHE	2.6
1	D	578	PHE	2.6
1	D	346	GLU	2.6
1	C	476	LEU	2.6
1	A	490	ASP	2.6
1	C	245	ILE	2.6
1	C	531	ARG	2.5
1	D	576	ARG	2.5
1	C	121	PRO	2.5
1	A	276	LEU	2.5
1	C	326	GLN	2.5
1	B	498	PHE	2.5
1	C	554	CYS	2.5
1	D	596	LYS	2.5
1	C	285	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	590	LEU	2.4
1	B	586	VAL	2.4
1	B	326	GLN	2.4
1	B	584	GLY	2.4
1	C	573	CYS	2.4
1	B	327	ASN	2.4
1	D	288	LYS	2.4
1	C	593	PRO	2.4
1	B	320	CYS	2.4
1	C	485	PRO	2.3
1	D	568	TYR	2.3
1	C	483	ALA	2.3
1	C	496	GLU	2.3
1	C	298	TYR	2.3
1	D	543	GLU	2.3
1	D	275	PRO	2.3
1	B	493	LEU	2.2
1	A	403	GLY	2.2
1	D	438	LEU	2.2
1	D	575	ASP	2.2
1	D	577	ASN	2.2
1	C	464	GLY	2.2
1	B	594	GLN	2.2
1	C	500	VAL	2.2
1	D	491	VAL	2.2
1	A	408	ARG	2.2
1	D	544	LYS	2.2
1	C	292	GLU	2.2
1	C	558	ASP	2.1
1	A	288	LYS	2.1
1	A	465	GLN	2.1
1	C	325	ILE	2.1
1	D	292	GLU	2.1
1	C	276	LEU	2.1
1	C	591	ILE	2.1
1	A	289	GLY	2.1
1	D	398	GLU	2.1
1	D	486	LYS	2.1
1	D	326	GLN	2.1
1	A	404	GLY	2.1
1	B	323	LEU	2.0
1	B	487	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	413	ILE	2.0
1	D	598	TRP	2.0
1	A	322	HIS	2.0
1	D	492	LYS	2.0
1	B	438	LEU	2.0
1	D	566	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	DGT	B	702	31/31	0.90	0.15	-0.93	41,57,111,116	0
3	DTP	C	701	30/30	0.98	0.14	-1.59	24,27,33,34	0
2	DGT	B	703	31/31	0.94	0.11	-1.77	24,30,34,36	0
2	DGT	D	704	31/31	0.89	0.15	-1.78	47,54,88,94	0
2	DGT	C	702	31/31	0.93	0.13	-1.80	45,58,92,100	0
2	DGT	A	701	31/31	0.93	0.13	-1.85	36,58,89,98	0
3	DTP	D	703	30/30	0.97	0.12	-1.96	23,29,34,36	0
2	DGT	C	703	31/31	0.95	0.11	-2.05	25,27,34,34	0
2	DGT	D	705	31/31	0.92	0.13	-2.08	25,28,30,35	0
3	DTP	A	702	30/30	0.98	0.10	-2.30	23,27,33,34	0
3	DTP	B	704	30/30	0.96	0.10	-2.67	20,24,34,37	0
2	DGT	D	702	31/31	0.97	0.10	-2.90	21,27,30,35	0
4	MG	A	703	1/1	0.68	0.10	-	28,28,28,28	0
4	MG	D	701	1/1	0.97	0.05	-	30,30,30,30	0
4	MG	C	704	1/1	0.71	0.07	-	45,45,45,45	0
4	MG	B	701	1/1	0.95	0.05	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.