Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:34 PM GMT

PDB ID	:	4TO6
Title	:	Structure basis of cellular dNTP regulation, SAMHD1-dGTP-dATP-dTTP/dGTP complex
Authors	:	Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on	:	2014-06-05
Resolution	:	2.33 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

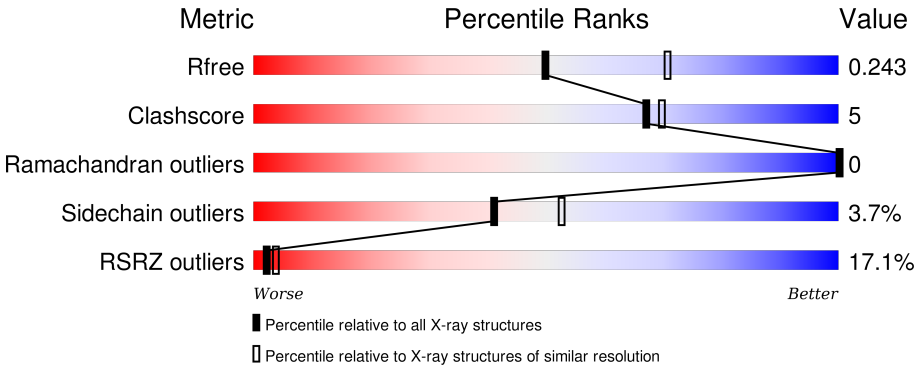
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	8% 82% 10% • 7%
1	B	514	11% 83% 10% • 7%
1	C	514	24% 82% 11% • 7%
1	D	514	22% 82% 10% • 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16098 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.

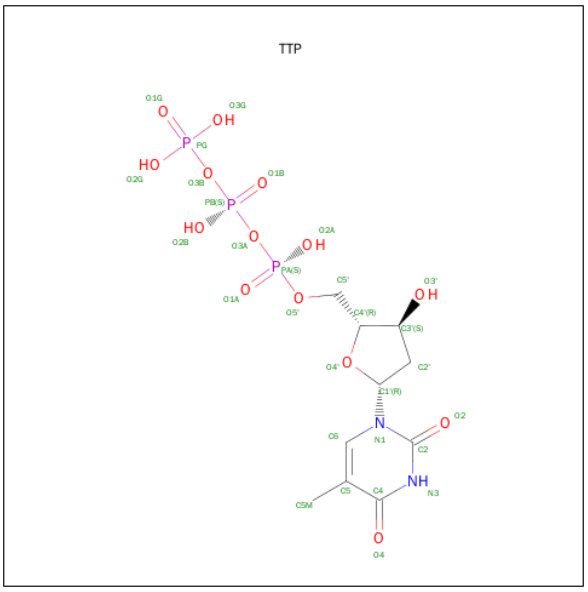
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	B	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	C	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	D	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			

There are 8 discrepancies between the modelled and reference sequences:

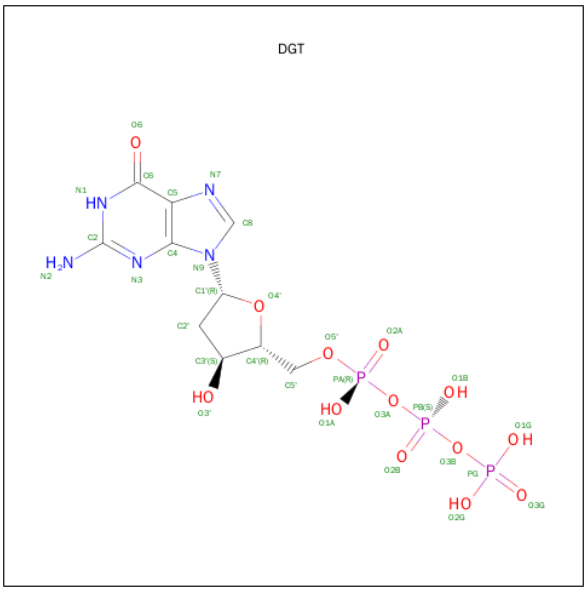
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation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

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



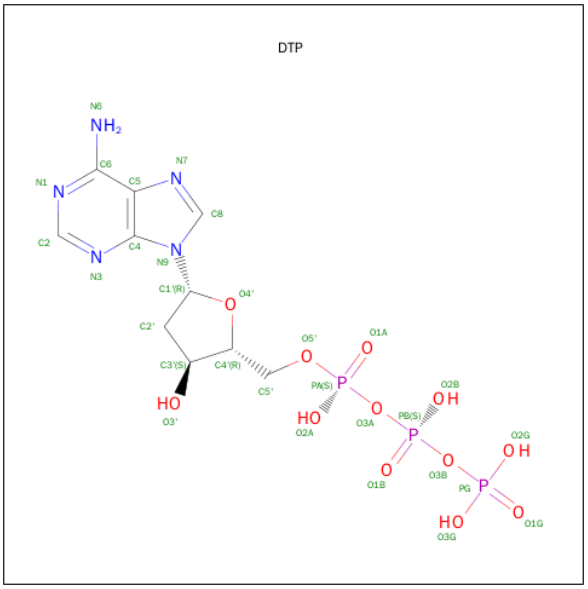
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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



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

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



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

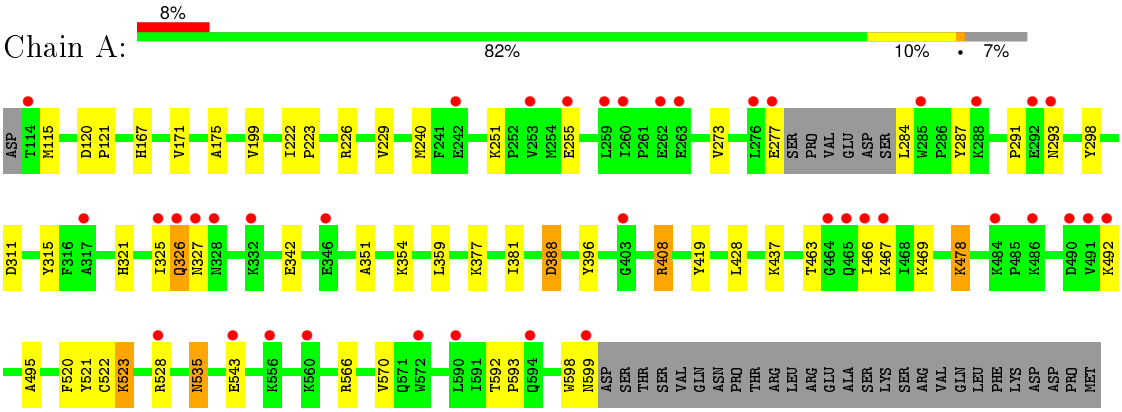
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	16	Total O 16 16	0	0
6	B	4	Total O 4 4	0	0
6	C	5	Total O 5 5	0	0
6	D	7	Total O 7 7	0	0

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.

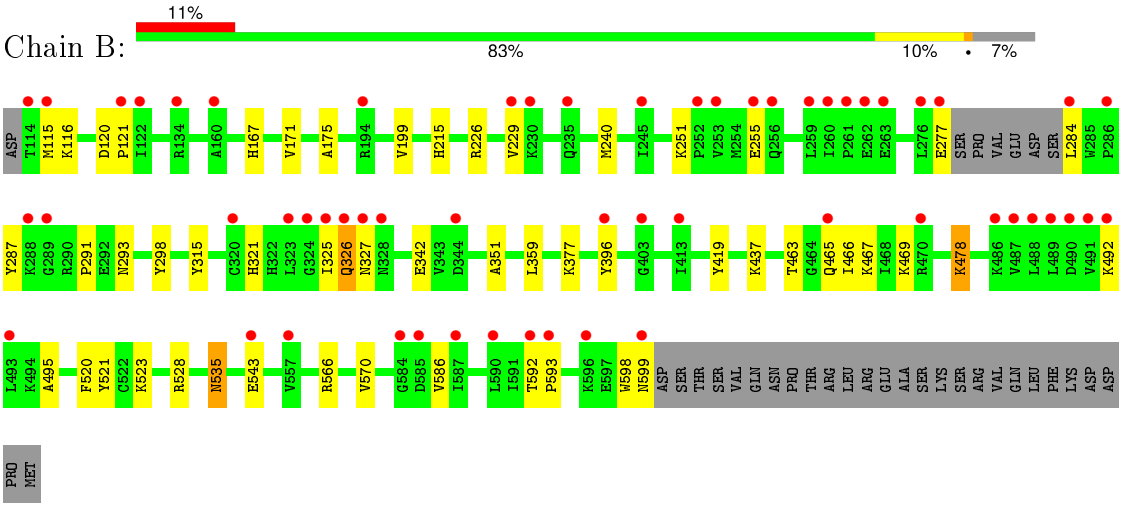
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



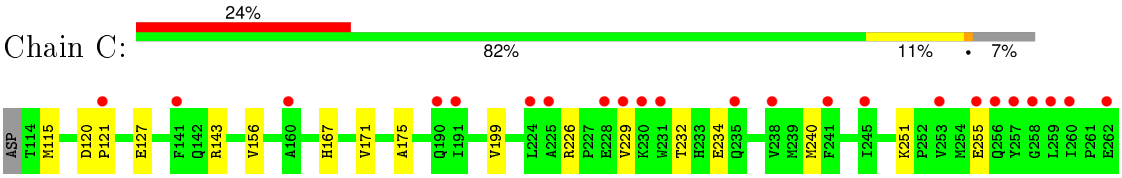
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

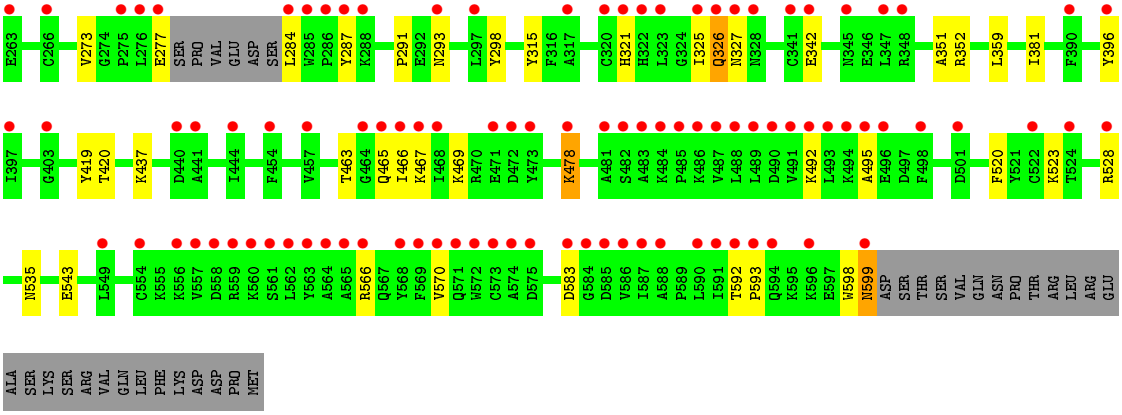
Chain B:



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

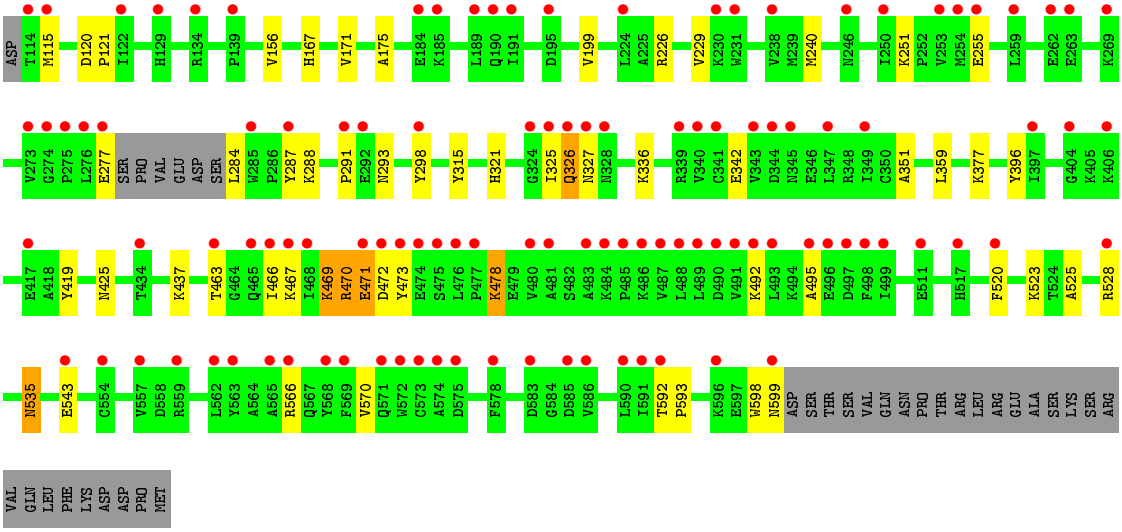
Chain C:





• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.59Å 140.81Å 96.90Å 90.00° 114.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.33 47.89 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.33) 99.4 (47.89-2.33)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.225 , 0.244 0.226 , 0.243	Depositor DCC
R_{free} test set	4268 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	58.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.1	EDS
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 85116 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16098	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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, TTP, 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	0.62	0/4017	0.72	3/5422 (0.1%)
1	B	0.57	0/4017	0.69	0/5422
1	C	0.57	0/4017	0.69	0/5422
1	D	0.56	0/4017	0.68	0/5422
All	All	0.58	0/16068	0.69	3/21688 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	408	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	388	ASP	CB-CG-OD1	5.52	123.27	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3925	0	3917	37	1
1	B	3925	0	3917	34	2
1	C	3925	0	3917	35	1
1	D	3925	0	3917	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	13	1	0
2	B	29	0	13	1	0
2	D	29	0	13	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	62	0	24	5	0
3	D	31	0	12	2	0
4	A	30	0	12	1	0
4	B	30	0	12	2	0
4	C	30	0	12	3	0
4	D	30	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	16	0	0	1	0
6	B	4	0	0	0	0
6	C	5	0	0	0	0
6	D	7	0	0	1	0
All	All	16098	0	15815	154	2

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 5.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LYS:HE3	1:D:470:ARG:N	1.62	1.15
1:C:598:TRP:O	1:C:599:ASN:HB2	1.49	1.10
1:D:469:LYS:NZ	1:D:469:LYS:HA	1.73	1.03
1:D:470:ARG:HA	1:D:473:TYR:CE2	1.94	1.03
1:D:469:LYS:HE3	1:D:470:ARG:H	0.86	1.02
1:B:116:LYS:NZ	3:C:704:DGT:O3G	2.02	0.92
1:D:470:ARG:NH1	1:D:471:GLU:HB3	1.87	0.90
1:D:470:ARG:HA	1:D:473:TYR:CZ	2.11	0.86
1:D:469:LYS:HZ2	1:D:469:LYS:HA	1.39	0.85
1:D:469:LYS:HB3	1:D:471:GLU:OE2	1.76	0.84
1:D:469:LYS:CE	1:D:470:ARG:H	1.82	0.84
1:A:523:LYS:NZ	3:C:704:DGT:O1G	2.10	0.83
1:D:470:ARG:NH1	1:D:471:GLU:CB	2.42	0.83
1:C:598:TRP:O	1:C:599:ASN:CB	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ARG:NH1	1:D:471:GLU:CA	2.47	0.78
1:D:470:ARG:CZ	1:D:471:GLU:HB3	2.15	0.77
1:B:326:GLN:HG2	1:D:326:GLN:HE21	1.51	0.76
1:B:326:GLN:HE21	1:D:326:GLN:HG2	1.51	0.75
1:D:469:LYS:CE	1:D:470:ARG:HG3	2.21	0.69
1:D:470:ARG:HA	1:D:473:TYR:CD2	2.27	0.69
1:D:469:LYS:CE	1:D:469:LYS:HA	2.22	0.68
1:D:469:LYS:HE2	1:D:470:ARG:HG3	1.75	0.68
1:D:470:ARG:NH1	1:D:471:GLU:HA	2.11	0.65
1:D:470:ARG:CA	1:D:473:TYR:CE2	2.78	0.64
1:A:354:LYS:NZ	4:A:703:DTP:O1A	2.30	0.63
1:A:521:TYR:O	1:A:521:TYR:CD1	2.52	0.63
1:D:469:LYS:HD3	1:D:470:ARG:HD3	1.79	0.63
1:D:470:ARG:HH11	1:D:471:GLU:HA	1.61	0.62
1:D:471:GLU:OE2	1:D:471:GLU:N	2.32	0.62
1:A:326:GLN:HE21	1:C:326:GLN:HG2	1.64	0.61
1:A:326:GLN:HG2	1:C:326:GLN:HE21	1.64	0.61
1:D:469:LYS:CA	1:D:469:LYS:CE	2.79	0.61
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.02	0.60
1:B:521:TYR:O	1:B:521:TYR:CD1	2.53	0.60
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.02	0.59
1:D:470:ARG:NE	1:D:471:GLU:N	2.50	0.59
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.84	0.59
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.02	0.59
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.02	0.59
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.01	0.59
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.03	0.59
1:D:471:GLU:CD	1:D:472:ASP:OD1	2.41	0.58
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.03	0.58
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.03	0.58
1:C:463:THR:O	1:C:466:ILE:HG12	2.04	0.57
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.86	0.57
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.87	0.57
1:B:463:THR:O	1:B:466:ILE:HG12	2.05	0.56
1:A:463:THR:O	1:A:466:ILE:HG12	2.04	0.56
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.88	0.56
1:D:463:THR:O	1:D:466:ILE:HG12	2.05	0.56
1:D:175:ALA:HB1	1:D:199:VAL:HG12	1.87	0.56
1:A:522:CYS:SG	1:C:583:ASP:HB3	2.47	0.55
1:A:521:TYR:C	1:A:521:TYR:CD1	2.80	0.55
1:B:521:TYR:C	1:B:521:TYR:CD1	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:TYR:O	6:A:812:HOH:O	2.18	0.54
1:D:469:LYS:HE3	1:D:470:ARG:HG3	1.89	0.54
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.44	0.53
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.43	0.53
1:B:226:ARG:O	1:B:229:VAL:HG12	2.09	0.53
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.44	0.52
1:C:226:ARG:O	1:C:229:VAL:HG12	2.10	0.52
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.44	0.52
1:A:377:LYS:NZ	4:C:701:DTP:O1B	2.43	0.52
1:D:226:ARG:O	1:D:229:VAL:HG12	2.09	0.52
1:C:566:ARG:O	1:C:570:VAL:HG23	2.10	0.51
1:D:470:ARG:HB3	1:D:473:TYR:CE2	2.45	0.51
1:D:470:ARG:CZ	1:D:471:GLU:N	2.73	0.51
1:B:566:ARG:O	1:B:570:VAL:HG23	2.10	0.51
1:A:226:ARG:O	1:A:229:VAL:HG12	2.11	0.50
1:D:566:ARG:O	1:D:570:VAL:HG23	2.11	0.50
1:A:566:ARG:O	1:A:570:VAL:HG23	2.11	0.50
1:B:543:GLU:HG2	1:D:543:GLU:HG2	1.92	0.50
1:C:156:VAL:O	3:C:704:DGT:H8	2.12	0.49
1:D:288:LYS:NZ	6:D:801:HOH:O	2.38	0.49
3:C:703:DGT:O1A	3:C:703:DGT:O1B	2.30	0.48
1:C:325:ILE:HG22	1:C:326:GLN:N	2.29	0.48
1:A:251:LYS:O	1:A:255:GLU:HG3	2.14	0.48
4:B:704:DTP:O1B	3:D:704:DGT:H5'A	2.13	0.48
1:B:251:LYS:O	1:B:255:GLU:HG3	2.14	0.48
1:D:469:LYS:HA	1:D:469:LYS:HZ1	1.69	0.47
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:C:167:HIS:O	1:C:171:VAL:HG23	2.14	0.47
1:A:167:HIS:O	1:A:171:VAL:HG23	2.14	0.47
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.97	0.47
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.47
1:A:535:ASN:OD1	1:A:535:ASN:N	2.46	0.47
1:D:287:TYR:CD1	1:D:298:TYR:CE1	3.02	0.47
1:D:251:LYS:O	1:D:255:GLU:HG3	2.15	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:A:327:ASN:O	1:C:326:GLN:HB3	2.14	0.47
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.96	0.47
1:D:471:GLU:OE2	1:D:472:ASP:N	2.47	0.47
1:C:352:ARG:NH2	4:C:701:DTP:O1G	2.44	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:D:167:HIS:O	1:D:171:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:HIS:O	1:B:171:VAL:HG23	2.15	0.46
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.97	0.46
1:B:326:GLN:HB3	1:D:327:ASN:O	2.16	0.46
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.46
1:B:586:VAL:HG11	1:D:525:ALA:HB3	1.98	0.46
1:C:592:THR:N	1:C:593:PRO:CD	2.79	0.46
1:C:287:TYR:CD1	1:C:298:TYR:CE1	3.04	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.46
1:A:325:ILE:HG22	1:A:326:GLN:N	2.30	0.46
1:A:311:ASP:OD2	2:A:701:TTP:O1A	2.34	0.46
1:C:325:ILE:CG2	1:C:326:GLN:N	2.79	0.45
1:A:326:GLN:HG2	1:C:326:GLN:HG2	1.97	0.45
1:C:251:LYS:O	1:C:255:GLU:HG3	2.15	0.45
1:A:326:GLN:HB3	1:C:327:ASN:O	2.17	0.45
1:A:287:TYR:CD1	1:A:298:TYR:CE1	3.04	0.45
1:B:586:VAL:CG1	1:D:525:ALA:HB3	2.46	0.45
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.98	0.45
1:B:326:GLN:HG2	1:D:326:GLN:HG2	1.98	0.45
1:D:535:ASN:OD1	1:D:535:ASN:N	2.47	0.45
1:B:325:ILE:HG22	1:B:326:GLN:N	2.31	0.45
1:A:522:CYS:SG	1:C:583:ASP:CB	3.05	0.45
1:D:240:MET:CE	1:D:419:TYR:HD2	2.31	0.44
1:D:325:ILE:HG22	1:D:326:GLN:N	2.31	0.44
1:B:287:TYR:CD1	1:B:298:TYR:CE1	3.05	0.44
1:A:325:ILE:CG2	1:A:326:GLN:N	2.80	0.44
1:D:469:LYS:CA	1:D:469:LYS:HE3	2.47	0.44
1:B:325:ILE:CG2	1:B:326:GLN:N	2.81	0.44
1:B:535:ASN:OD1	1:B:535:ASN:N	2.47	0.44
1:C:352:ARG:HH22	4:C:701:DTP:PG	2.40	0.44
1:D:351:ALA:O	1:D:520:PHE:HA	2.18	0.43
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.06	0.43
1:C:351:ALA:O	1:C:520:PHE:HA	2.18	0.43
1:A:598:TRP:O	1:A:599:ASN:HB2	2.19	0.43
1:D:156:VAL:O	3:D:704:DGT:H8	2.18	0.43
1:A:240:MET:CE	1:A:419:TYR:HD2	2.32	0.43
1:C:143:ARG:HD2	1:C:420:THR:HA	2.01	0.43
1:B:321:HIS:CE1	1:C:321:HIS:CE1	3.06	0.43
1:C:240:MET:CE	1:C:419:TYR:HD2	2.32	0.42
1:D:469:LYS:CA	1:D:469:LYS:HZ2	2.23	0.42
1:D:325:ILE:CG2	1:D:326:GLN:N	2.82	0.42
1:C:381:ILE:HA	1:C:381:ILE:HD12	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ARG:CB	1:D:473:TYR:CE2	3.02	0.42
1:B:327:ASN:O	1:D:326:GLN:HB3	2.20	0.42
3:C:704:DGT:H2'A	3:C:704:DGT:N3	2.35	0.42
1:C:232:THR:HB	1:C:234:GLU:OE1	2.20	0.41
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.41
1:C:127:GLU:HG3	1:D:336:LYS:HE3	2.02	0.41
1:B:215:HIS:CD2	2:B:701:TTP:C6	3.08	0.41
1:A:222:ILE:HB	1:A:223:PRO:HD3	2.03	0.41
1:B:598:TRP:O	1:B:599:ASN:HB2	2.20	0.41
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.88	0.41
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.02	0.41
1:C:478:LYS:HD2	1:C:478:LYS:H	1.85	0.41
4:B:704:DTP:O2B	1:D:377:LYS:NZ	2.54	0.40
1:B:543:GLU:CG	1:D:543:GLU:CG	2.99	0.40
1:D:478:LYS:H	1:D:478:LYS:HD2	1.86	0.40
1:B:240:MET:CE	1:B:419:TYR:HD2	2.34	0.40
1:B:377:LYS:NZ	4:D:702:DTP:O2B	2.55	0.40

All (2) 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:408:ARG:NH2	1:B:478:LYS:CG[1_454]	1.86	0.34
1:B:543:GLU:O	1:C:465:GLN:OE1[1_655]	2.07	0.13

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	476/514 (93%)	470 (99%)	6 (1%)	0	100	100
1	B	476/514 (93%)	469 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	476/514 (93%)	470 (99%)	6 (1%)	0	100	100
1	D	476/514 (93%)	471 (99%)	5 (1%)	0	100	100
All	All	1904/2056 (93%)	1880 (99%)	24 (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	426/459 (93%)	410 (96%)	16 (4%)	40	51
1	B	426/459 (93%)	411 (96%)	15 (4%)	43	55
1	C	426/459 (93%)	410 (96%)	16 (4%)	40	51
1	D	426/459 (93%)	410 (96%)	16 (4%)	40	51
All	All	1704/1836 (93%)	1641 (96%)	63 (4%)	41	53

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU
1	A	315	TYR
1	A	326	GLN
1	A	342	GLU
1	A	359	LEU
1	A	388	ASP
1	A	467	LYS
1	A	469	LYS
1	A	478	LYS
1	A	492	LYS
1	A	523	LYS

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Mol	Chain	Res	Type
1	A	528	ARG
1	A	535	ASN
1	B	115	MET
1	B	277	GLU
1	B	284	LEU
1	B	315	TYR
1	B	326	GLN
1	B	342	GLU
1	B	359	LEU
1	B	465	GLN
1	B	467	LYS
1	B	469	LYS
1	B	478	LYS
1	B	492	LYS
1	B	523	LYS
1	B	528	ARG
1	B	535	ASN
1	C	115	MET
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	315	TYR
1	C	326	GLN
1	C	342	GLU
1	C	359	LEU
1	C	467	LYS
1	C	469	LYS
1	C	478	LYS
1	C	492	LYS
1	C	523	LYS
1	C	528	ARG
1	C	535	ASN
1	C	599	ASN
1	D	115	MET
1	D	277	GLU
1	D	284	LEU
1	D	315	TYR
1	D	326	GLN
1	D	342	GLU
1	D	359	LEU
1	D	467	LYS
1	D	469	LYS

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Mol	Chain	Res	Type
1	D	470	ARG
1	D	471	GLU
1	D	478	LYS
1	D	492	LYS
1	D	523	LYS
1	D	528	ARG
1	D	535	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	243	HIS
1	A	326	GLN
1	A	364	HIS
1	B	235	GLN
1	B	243	HIS
1	B	326	GLN
1	C	215	HIS
1	C	235	GLN
1	C	243	HIS
1	C	322	HIS
1	C	326	GLN
1	D	235	GLN
1	D	243	HIS
1	D	326	GLN

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 (i)

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	TTP	A	701	-	21,30,30	0.71	0	31,47,47	2.00	6 (19%)
3	DGT	A	702	5	25,33,33	1.09	2 (8%)	35,52,52	2.37	10 (28%)
4	DTP	A	703	5	24,32,32	1.15	3 (12%)	32,50,50	2.46	7 (21%)
2	TTP	B	701	-	21,30,30	0.65	0	31,47,47	2.13	7 (22%)
3	DGT	B	702	5	25,33,33	1.11	3 (12%)	35,52,52	1.97	7 (20%)
4	DTP	B	704	5	24,32,32	1.05	1 (4%)	32,50,50	2.44	8 (25%)
4	DTP	C	701	5	24,32,32	1.07	2 (8%)	32,50,50	2.20	7 (21%)
3	DGT	C	703	-	25,33,33	1.46	2 (8%)	35,52,52	2.03	10 (28%)
3	DGT	C	704	5	25,33,33	1.12	2 (8%)	35,52,52	1.85	9 (25%)
4	DTP	D	702	5	24,32,32	1.18	2 (8%)	32,50,50	1.85	5 (15%)
2	TTP	D	703	-	21,30,30	0.62	0	31,47,47	2.07	5 (16%)
3	DGT	D	704	5	25,33,33	1.20	2 (8%)	35,52,52	2.33	14 (40%)

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	TTP	A	701	-	-	0/18/34/34	0/2/2/2
3	DGT	A	702	5	-	0/18/34/34	0/3/3/3
4	DTP	A	703	5	-	0/18/34/34	0/3/3/3
2	TTP	B	701	-	-	0/18/34/34	0/2/2/2
3	DGT	B	702	5	-	0/18/34/34	0/3/3/3
4	DTP	B	704	5	-	0/18/34/34	0/3/3/3
4	DTP	C	701	5	-	0/18/34/34	0/3/3/3
3	DGT	C	703	-	-	0/18/34/34	0/3/3/3
3	DGT	C	704	5	-	0/18/34/34	0/3/3/3
4	DTP	D	702	5	-	0/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTP	D	703	-	-	0/18/34/34	0/2/2/2
3	DGT	D	704	5	-	0/18/34/34	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	DTP	O4'-C4'	-2.11	1.40	1.45
3	B	702	DGT	C4-N3	-2.02	1.32	1.35
4	D	702	DTP	C5-C4	2.06	1.45	1.40
4	A	703	DTP	C5-C4	2.17	1.45	1.40
4	D	702	DTP	C2-N3	2.18	1.36	1.32
3	C	704	DGT	C5-C4	2.29	1.45	1.40
4	A	703	DTP	C2-N3	2.31	1.36	1.32
3	B	702	DGT	C5-C4	2.60	1.46	1.40
4	B	704	DTP	C5-C4	2.66	1.46	1.40
4	C	701	DTP	C2-N3	2.69	1.37	1.32
3	A	702	DGT	C6-C5	2.83	1.46	1.41
3	B	702	DGT	C6-C5	2.95	1.47	1.41
3	A	702	DGT	C5-C4	2.97	1.47	1.40
3	D	704	DGT	C6-C5	3.00	1.47	1.41
4	C	701	DTP	C5-C4	3.06	1.47	1.40
3	D	704	DGT	C5-C4	3.23	1.47	1.40
3	C	704	DGT	C6-C5	3.51	1.48	1.41
3	C	703	DGT	C5-C4	3.85	1.49	1.40
3	C	703	DGT	C6-C5	4.77	1.50	1.41

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	704	DTP	N3-C2-N1	-10.76	120.65	128.89
4	A	703	DTP	N3-C2-N1	-10.46	120.89	128.89
4	C	701	DTP	N3-C2-N1	-9.09	121.94	128.89
4	D	702	DTP	N3-C2-N1	-6.71	123.76	128.89
3	A	702	DGT	C5-C6-N1	-5.69	115.81	123.59
3	A	702	DGT	PA-O3A-PB	-5.54	117.19	132.73
2	D	703	TTP	PB-O3A-PA	-5.52	117.23	132.73
3	B	702	DGT	PA-O3A-PB	-5.48	117.33	132.73
2	A	701	TTP	C5-C4-N3	-5.40	119.12	125.14
2	B	701	TTP	C5-C4-N3	-5.36	119.17	125.14
2	D	703	TTP	PB-O3B-PG	-5.20	115.25	132.67
3	D	704	DGT	O3A-PA-O5'	-5.03	89.60	102.94
3	D	704	DGT	C5-C6-N1	-4.70	117.16	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	703	DGT	PA-O3A-PB	-4.70	119.53	132.73
2	B	701	TTP	PB-O3A-PA	-4.58	119.87	132.73
2	A	701	TTP	PB-O3A-PA	-4.52	120.05	132.73
3	A	702	DGT	C4-C5-N7	-4.43	105.40	109.48
3	C	703	DGT	PB-O3B-PG	-4.36	118.05	132.67
4	D	702	DTP	C4-C5-N7	-4.29	105.54	109.48
2	D	703	TTP	C5-C4-N3	-4.23	120.42	125.14
2	B	701	TTP	PB-O3B-PG	-4.15	118.75	132.67
3	D	704	DGT	PB-O3B-PG	-4.12	118.87	132.67
3	C	704	DGT	PA-O3A-PB	-4.09	121.25	132.73
3	B	702	DGT	C6-C5-C4	-3.99	116.13	120.90
2	A	701	TTP	PB-O3B-PG	-3.87	119.69	132.67
4	A	703	DTP	PB-O3B-PG	-3.79	119.96	132.67
4	A	703	DTP	PA-O3A-PB	-3.75	122.19	132.73
3	C	703	DGT	C5-C6-N1	-3.75	118.46	123.59
3	C	703	DGT	C6-C5-C4	-3.73	116.44	120.90
3	C	704	DGT	N3-C2-N1	-3.73	121.77	127.44
3	C	704	DGT	C6-C5-C4	-3.70	116.47	120.90
3	B	702	DGT	N3-C2-N1	-3.68	121.83	127.44
4	C	701	DTP	PA-O3A-PB	-3.65	122.48	132.73
4	B	704	DTP	PB-O3B-PG	-3.62	120.52	132.67
4	B	704	DTP	PA-O3A-PB	-3.61	122.59	132.73
3	A	702	DGT	O5'-PA-O2A	-3.51	96.00	109.62
3	C	704	DGT	PB-O3B-PG	-3.50	120.92	132.67
4	C	701	DTP	PB-O3B-PG	-3.43	121.17	132.67
3	B	702	DGT	C5-C6-N1	-3.43	118.90	123.59
4	A	703	DTP	C4-C5-N7	-3.41	106.34	109.48
3	D	704	DGT	PA-O3A-PB	-3.29	123.48	132.73
3	C	704	DGT	C5-C6-N1	-3.24	119.16	123.59
3	C	704	DGT	C4-C5-N7	-3.23	106.50	109.48
3	A	702	DGT	PB-O3B-PG	-3.21	121.89	132.67
3	D	704	DGT	C4-C5-N7	-3.20	106.54	109.48
3	C	703	DGT	C4-C5-N7	-3.18	106.55	109.48
3	D	704	DGT	N3-C2-N1	-2.96	122.94	127.44
4	D	702	DTP	PB-O3B-PG	-2.90	122.94	132.67
3	B	702	DGT	PB-O3B-PG	-2.88	123.00	132.67
3	D	704	DGT	C6-C5-C4	-2.87	117.46	120.90
4	B	704	DTP	C4-C5-N7	-2.64	107.05	109.48
3	A	702	DGT	N3-C2-N1	-2.62	123.46	127.44
3	C	703	DGT	N3-C2-N1	-2.61	123.47	127.44
4	C	701	DTP	C4-C5-N7	-2.44	107.23	109.48
4	B	704	DTP	C1'-N9-C4	-2.26	123.32	127.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	702	DTP	PA-O3A-PB	-2.18	126.60	132.73
3	D	704	DGT	O4'-C1'-C2'	-2.10	102.09	106.27
3	C	703	DGT	O2G-PG-O3B	-2.06	95.74	105.09
3	D	704	DGT	O1A-PA-O2A	2.02	123.46	112.53
3	C	704	DGT	N2-C2-N1	2.04	120.58	117.20
2	A	701	TTP	O2B-PB-O1B	2.04	123.60	112.53
4	B	704	DTP	O2G-PG-O1G	2.09	117.31	110.58
3	D	704	DGT	C3'-C2'-C1'	2.10	107.45	102.40
4	B	704	DTP	C2'-C3'-C4'	2.14	107.21	102.77
3	D	704	DGT	O1A-PA-O3A	2.19	115.02	105.09
2	B	701	TTP	O3G-PG-O2G	2.19	115.74	107.38
3	A	702	DGT	O1A-PA-O2A	2.21	124.49	112.53
4	A	703	DTP	O2A-PA-O3A	2.22	115.17	105.09
4	C	701	DTP	O2G-PG-O1G	2.24	117.78	110.58
2	B	701	TTP	C2'-C3'-C4'	2.27	107.48	102.77
4	C	701	DTP	C2-N1-C6	2.35	122.97	118.77
3	D	704	DGT	O4'-C1'-N9	2.41	111.89	107.72
4	D	702	DTP	O3G-PG-O2G	2.42	116.58	107.38
4	C	701	DTP	O3G-PG-O1G	2.46	118.49	110.58
3	C	704	DGT	O2G-PG-O1G	2.57	117.18	107.38
4	A	703	DTP	C2'-C3'-C4'	2.63	108.23	102.77
3	C	703	DGT	C2'-C3'-C4'	2.69	108.34	102.77
4	A	703	DTP	O3G-PG-O2G	2.80	118.04	107.38
2	A	701	TTP	O3G-PG-O2G	2.80	118.05	107.38
2	B	701	TTP	C5M-C5-C4	2.84	123.71	120.05
3	A	702	DGT	O1B-PB-O3A	3.06	118.99	105.09
2	D	703	TTP	O3G-PG-O2G	3.14	119.35	107.38
3	C	703	DGT	O2G-PG-O1G	3.19	119.53	107.38
4	B	704	DTP	C2-N1-C6	3.27	124.61	118.77
3	B	702	DGT	O2G-PG-O3G	3.36	121.41	110.58
3	C	704	DGT	C6-N1-C2	3.94	121.41	115.94
3	D	704	DGT	O2G-PG-O1G	4.16	123.22	107.38
3	A	702	DGT	O1G-PG-O3G	4.20	124.09	110.58
3	C	703	DGT	C6-N1-C2	4.30	121.91	115.94
3	B	702	DGT	C6-N1-C2	4.64	122.38	115.94
2	D	703	TTP	C4-N3-C2	5.10	119.65	115.25
3	D	704	DGT	C6-N1-C2	5.21	123.17	115.94
2	A	701	TTP	C4-N3-C2	5.23	119.76	115.25
3	A	702	DGT	C6-N1-C2	5.31	123.31	115.94
2	B	701	TTP	C4-N3-C2	5.96	120.40	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	480/514 (93%)	0.65	39 (8%) 15 23	29, 59, 94, 136	0
1	B	480/514 (93%)	0.89	57 (11%) 6 10	33, 66, 103, 133	0
1	C	480/514 (93%)	1.39	122 (25%) 1 2	35, 80, 129, 171	0
1	D	480/514 (93%)	1.37	111 (23%) 1 2	33, 77, 134, 176	0
All	All	1920/2056 (93%)	1.08	329 (17%) 2 4	29, 70, 119, 176	0

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	489	LEU	14.7
1	D	489	LEU	12.6
1	D	562	LEU	11.8
1	C	496	GLU	10.3
1	C	488	LEU	10.2
1	C	486	LYS	9.7
1	D	590	LEU	8.4
1	D	490	ASP	8.4
1	D	491	VAL	8.0
1	D	466	ILE	7.9
1	B	488	LEU	7.9
1	D	274	GLY	7.3
1	D	487	VAL	7.3
1	D	465	GLN	6.6
1	C	285	TRP	6.6
1	D	493	LEU	6.5
1	D	481	ALA	6.4
1	C	498	PHE	6.4
1	D	592	THR	6.0
1	C	557	VAL	6.0
1	D	488	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	466	ILE	5.9
1	D	473	TYR	5.9
1	B	599	ASN	5.7
1	D	497	ASP	5.7
1	C	263	GLU	5.6
1	B	489	LEU	5.6
1	C	255	GLU	5.6
1	D	599	ASN	5.5
1	C	590	LEU	5.5
1	D	345	ASN	5.4
1	C	584	GLY	5.4
1	B	487	VAL	5.4
1	D	486	LYS	5.3
1	B	276	LEU	5.2
1	B	262	GLU	5.2
1	A	466	ILE	5.1
1	B	277	GLU	5.1
1	C	478	LYS	5.1
1	D	472	ASP	5.1
1	D	287	TYR	5.0
1	C	403	GLY	5.0
1	C	276	LEU	4.9
1	C	483	ALA	4.9
1	D	573	CYS	4.8
1	C	284	LEU	4.8
1	D	483	ALA	4.8
1	D	563	TYR	4.7
1	D	568	TYR	4.7
1	D	275	PRO	4.7
1	C	554	CYS	4.7
1	B	490	ASP	4.7
1	D	476	LEU	4.6
1	B	326	GLN	4.6
1	D	586	VAL	4.6
1	D	277	GLU	4.5
1	C	586	VAL	4.5
1	B	229	VAL	4.5
1	C	465	GLN	4.4
1	C	592	THR	4.4
1	C	253	VAL	4.4
1	C	563	TYR	4.4
1	C	341	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	467	LYS	4.3
1	A	255	GLU	4.3
1	C	495	ALA	4.3
1	D	326	GLN	4.3
1	A	260	ILE	4.2
1	B	587	ILE	4.2
1	D	569	PHE	4.2
1	D	496	GLU	4.1
1	B	253	VAL	4.1
1	B	328	ASN	4.1
1	B	492	LYS	4.1
1	C	484	LYS	4.0
1	D	273	VAL	4.0
1	D	498	PHE	4.0
1	C	561	SER	4.0
1	C	596	LYS	4.0
1	B	590	LEU	4.0
1	C	573	CYS	4.0
1	D	263	GLU	4.0
1	C	473	TYR	4.0
1	C	568	TYR	4.0
1	C	493	LEU	4.0
1	C	490	ASP	3.9
1	C	594	GLN	3.9
1	B	596	LYS	3.9
1	A	263	GLU	3.9
1	C	258	GLY	3.9
1	C	562	LEU	3.8
1	C	228	GLU	3.8
1	D	596	LYS	3.8
1	D	492	LYS	3.8
1	C	591	ILE	3.8
1	C	275	PRO	3.8
1	D	468	ILE	3.7
1	C	287	TYR	3.7
1	C	326	GLN	3.7
1	C	558	ASP	3.7
1	B	230	LYS	3.6
1	C	231	TRP	3.6
1	D	189	LEU	3.6
1	D	191	ILE	3.6
1	D	480	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	114	THR	3.6
1	A	560	LYS	3.6
1	C	565	ALA	3.6
1	D	115	MET	3.6
1	C	293	ASN	3.6
1	B	557	VAL	3.5
1	D	528	ARG	3.5
1	C	571	GLN	3.5
1	D	485	PRO	3.5
1	B	396	TYR	3.5
1	A	543	GLU	3.5
1	D	511	GLU	3.5
1	D	475	SER	3.4
1	A	277	GLU	3.4
1	D	572	TRP	3.4
1	C	570	VAL	3.4
1	D	471	GLU	3.4
1	C	191	ILE	3.4
1	B	134	ARG	3.4
1	A	590	LEU	3.4
1	C	467	LYS	3.4
1	D	554	CYS	3.4
1	B	263	GLU	3.3
1	B	592	THR	3.3
1	A	486	LYS	3.3
1	D	591	ILE	3.3
1	A	327	ASN	3.3
1	C	494	LYS	3.3
1	C	345	ASN	3.2
1	B	260	ILE	3.2
1	A	465	GLN	3.2
1	B	327	ASN	3.2
1	C	572	TRP	3.2
1	B	288	LYS	3.2
1	D	575	ASP	3.2
1	B	284	LEU	3.2
1	C	593	PRO	3.2
1	C	347	LEU	3.2
1	A	490	ASP	3.2
1	A	114	THR	3.2
1	C	492	LYS	3.1
1	D	292	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	254	MET	3.1
1	B	491	VAL	3.1
1	D	578	PHE	3.1
1	C	560	LYS	3.1
1	C	440	ASP	3.1
1	C	262	GLU	3.1
1	C	569	PHE	3.1
1	D	495	ALA	3.0
1	C	241	PHE	3.0
1	D	543	GLU	3.0
1	B	325	ILE	3.0
1	D	565	ALA	3.0
1	D	253	VAL	3.0
1	C	396	TYR	3.0
1	C	564	ALA	3.0
1	D	190	GLN	3.0
1	C	277	GLU	3.0
1	C	491	VAL	3.0
1	C	390	PHE	3.0
1	C	556	LYS	3.0
1	C	444	ILE	3.0
1	C	259	LEU	3.0
1	D	259	LEU	3.0
1	D	276	LEU	3.0
1	D	585	ASP	2.9
1	A	325	ILE	2.9
1	C	325	ILE	2.9
1	A	259	LEU	2.9
1	A	262	GLU	2.9
1	D	477	PRO	2.9
1	C	472	ASP	2.9
1	D	463	THR	2.8
1	A	556	LYS	2.8
1	D	559	ARG	2.8
1	C	471	GLU	2.8
1	D	255	GLU	2.8
1	C	454	PHE	2.8
1	C	468	ILE	2.8
1	C	588	ALA	2.8
1	A	285	TRP	2.8
1	D	557	VAL	2.7
1	B	585	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	297	LEU	2.7
1	C	587	ILE	2.7
1	B	252	PRO	2.7
1	C	528	ARG	2.7
1	A	464	GLY	2.7
1	B	261	PRO	2.7
1	C	225	ALA	2.7
1	C	441	ALA	2.7
1	B	289	GLY	2.7
1	A	328	ASN	2.7
1	C	230	LYS	2.7
1	A	253	VAL	2.7
1	C	238	VAL	2.7
1	C	266	CYS	2.7
1	D	327	ASN	2.6
1	A	332	LYS	2.6
1	C	575	ASP	2.6
1	B	320	CYS	2.6
1	B	543	GLU	2.6
1	A	484	LYS	2.6
1	C	260	ILE	2.6
1	A	326	GLN	2.6
1	A	288	LYS	2.6
1	C	566	ARG	2.6
1	A	293	ASN	2.6
1	B	413	ILE	2.5
1	C	501	ASP	2.5
1	B	593	PRO	2.5
1	C	485	PRO	2.5
1	C	327	ASN	2.5
1	D	285	TRP	2.5
1	D	574	ALA	2.5
1	B	323	LEU	2.5
1	D	122	ILE	2.5
1	D	230	LYS	2.5
1	B	470	ARG	2.5
1	C	574	ALA	2.5
1	C	288	LYS	2.5
1	D	224	LEU	2.5
1	A	594	GLN	2.5
1	D	484	LYS	2.4
1	A	292	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	235	GLN	2.4
1	D	417	GLU	2.4
1	D	325	ILE	2.4
1	C	559	ARG	2.4
1	C	224	LEU	2.4
1	A	491	VAL	2.4
1	C	141	PHE	2.4
1	C	585	ASP	2.4
1	C	257	TYR	2.4
1	C	397	ILE	2.4
1	A	346	GLU	2.4
1	D	114	THR	2.4
1	C	245	ILE	2.4
1	A	599	ASN	2.3
1	B	324	GLY	2.3
1	B	584	GLY	2.3
1	C	487	VAL	2.3
1	D	520	PHE	2.3
1	A	242	GLU	2.3
1	A	492	LYS	2.3
1	A	572	TRP	2.3
1	D	129	HIS	2.3
1	C	160	ALA	2.3
1	C	464	GLY	2.3
1	D	340	VAL	2.3
1	B	121	PRO	2.3
1	D	499	ILE	2.3
1	D	566	ARG	2.3
1	C	190	GLN	2.3
1	C	457	VAL	2.3
1	B	259	LEU	2.3
1	C	342	GLU	2.3
1	D	347	LEU	2.3
1	C	481	ALA	2.2
1	D	238	VAL	2.2
1	D	269	LYS	2.2
1	D	298	TYR	2.2
1	D	184	GLU	2.2
1	C	348	ARG	2.2
1	D	571	GLN	2.2
1	B	160	ALA	2.2
1	D	397	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	517	HIS	2.2
1	B	486	LYS	2.2
1	D	328	ASN	2.2
1	D	583	ASP	2.2
1	D	185	LYS	2.2
1	C	322	HIS	2.2
1	C	524	THR	2.2
1	D	434	THR	2.2
1	B	122	ILE	2.2
1	B	194	ARG	2.2
1	D	339	ARG	2.2
1	C	235	GLN	2.2
1	A	276	LEU	2.2
1	C	549	LEU	2.2
1	C	320	CYS	2.2
1	C	482	SER	2.2
1	C	599	ASN	2.2
1	D	349	ILE	2.1
1	B	493	LEU	2.1
1	C	317	ALA	2.1
1	D	324	GLY	2.1
1	C	229	VAL	2.1
1	B	344	ASP	2.1
1	C	583	ASP	2.1
1	D	344	ASP	2.1
1	A	317	ALA	2.1
1	B	256	GLN	2.1
1	D	474	GLU	2.1
1	C	286	PRO	2.1
1	B	255	GLU	2.1
1	C	256	GLN	2.1
1	C	323	LEU	2.1
1	D	404	GLY	2.1
1	D	246	ASN	2.1
1	B	286	PRO	2.1
1	B	115	MET	2.1
1	A	403	GLY	2.1
1	A	467	LYS	2.1
1	D	134	ARG	2.1
1	C	321	HIS	2.1
1	C	522	CYS	2.1
1	C	328	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	465	GLN	2.1
1	D	291	PRO	2.1
1	D	406	LYS	2.1
1	D	343	VAL	2.1
1	D	195	ASP	2.0
1	D	231	TRP	2.0
1	D	139	PRO	2.0
1	B	245	ILE	2.0
1	A	528	ARG	2.0
1	D	341	CYS	2.0
1	D	262	GLU	2.0
1	C	121	PRO	2.0
1	B	403	GLY	2.0
1	D	250	ILE	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
3	DGT	C	703	31/31	0.86	0.18	0.30	66,83,98,110	0
4	DTP	D	702	30/30	0.98	0.15	-0.73	32,39,42,44	0
2	TTP	A	701	29/29	0.92	0.14	-0.79	37,55,81,89	0
2	TTP	D	703	29/29	0.92	0.15	-0.88	58,73,91,100	0
3	DGT	B	702	31/31	0.97	0.13	-0.96	39,44,49,49	0
3	DGT	D	704	31/31	0.97	0.14	-0.97	37,41,50,51	0
4	DTP	C	701	30/30	0.98	0.16	-1.00	33,36,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	DTP	B	704	30/30	0.98	0.15	-1.07	34,39,46,49	0
3	DGT	C	704	31/31	0.97	0.13	-1.11	47,54,69,71	0
4	DTP	A	703	30/30	0.98	0.14	-1.23	42,45,56,56	0
2	TTP	B	701	29/29	0.94	0.13	-1.40	58,68,79,81	0
3	DGT	A	702	31/31	0.97	0.13	-1.41	38,43,49,52	0
5	MG	B	703	1/1	0.98	0.10	-	55,55,55,55	0
5	MG	A	704	1/1	0.86	0.09	-	59,59,59,59	0
5	MG	C	702	1/1	0.99	0.09	-	47,47,47,47	0
5	MG	D	701	1/1	0.95	0.10	-	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.