



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 09:28 PM EST

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 : unknown
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

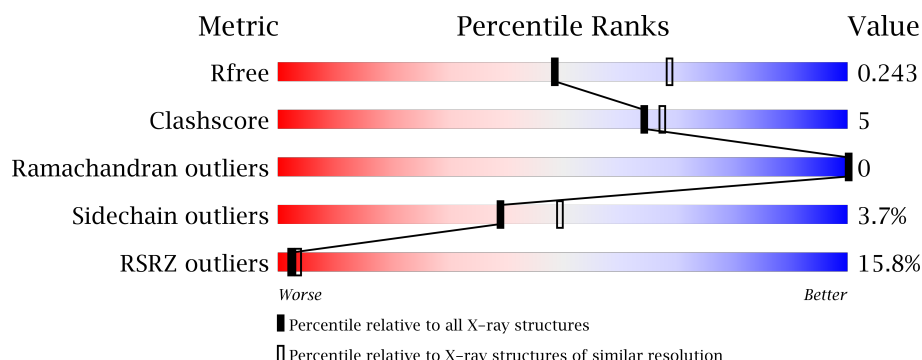
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>7%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>
1	B	514	<div> <div>10%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	C	514	<div> <div>22%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
1	D	514	<div> <div>19%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>

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.

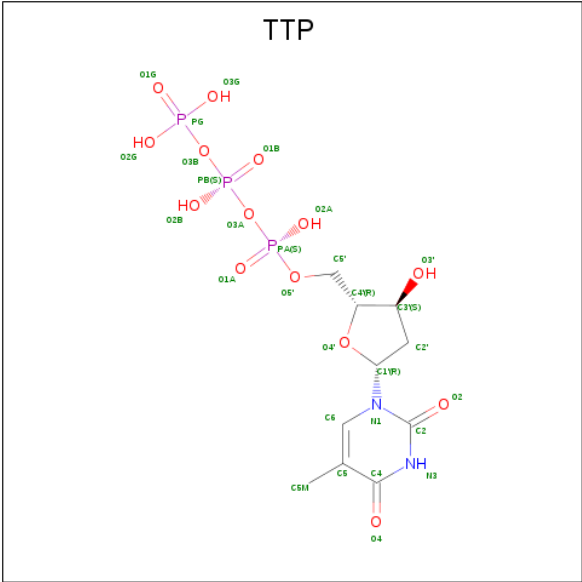
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

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:

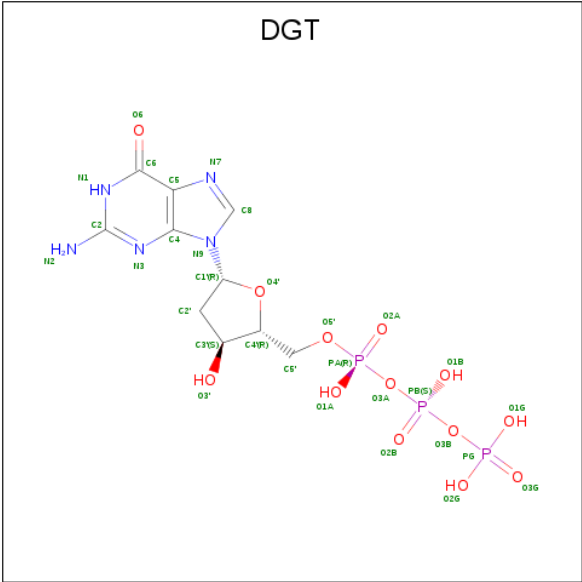
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	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: $C_{10}H_{17}N_2O_{14}P_3$).



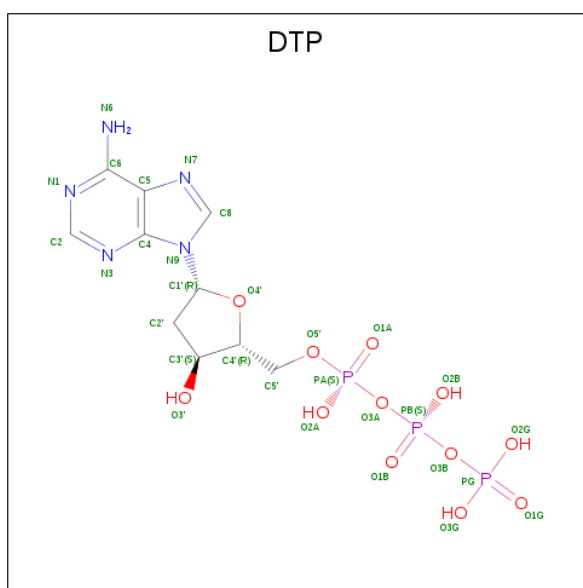
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

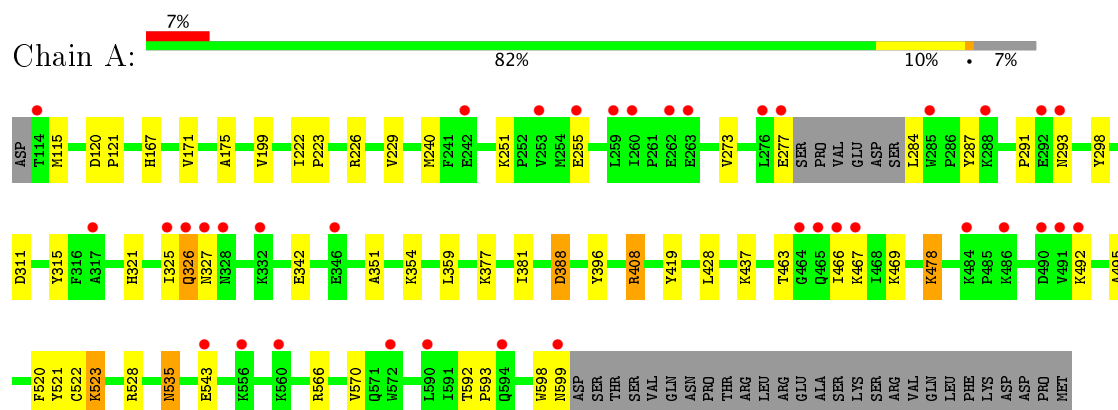
- Molecule 6 is water.

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

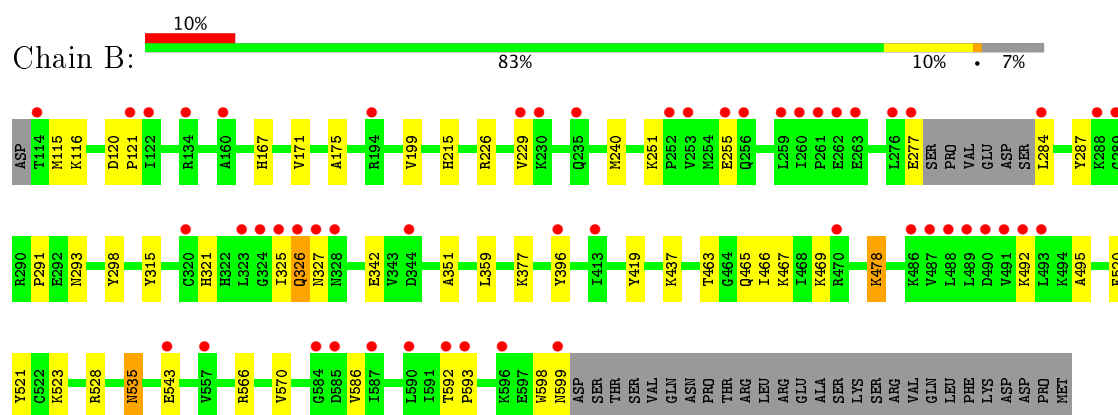
3 Residue-property plots [i](#)

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

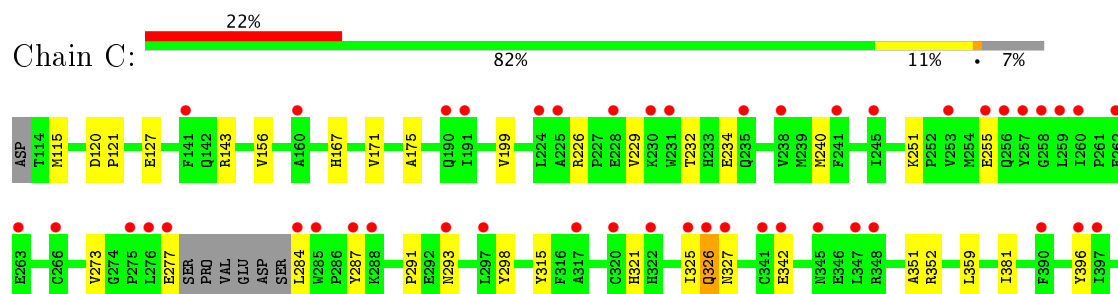
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

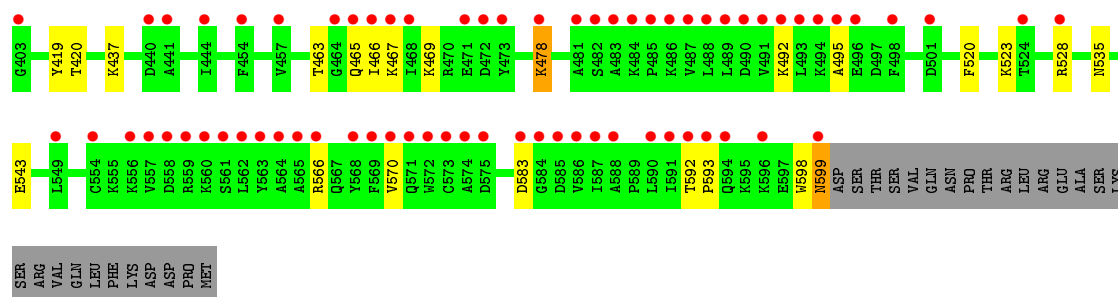


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



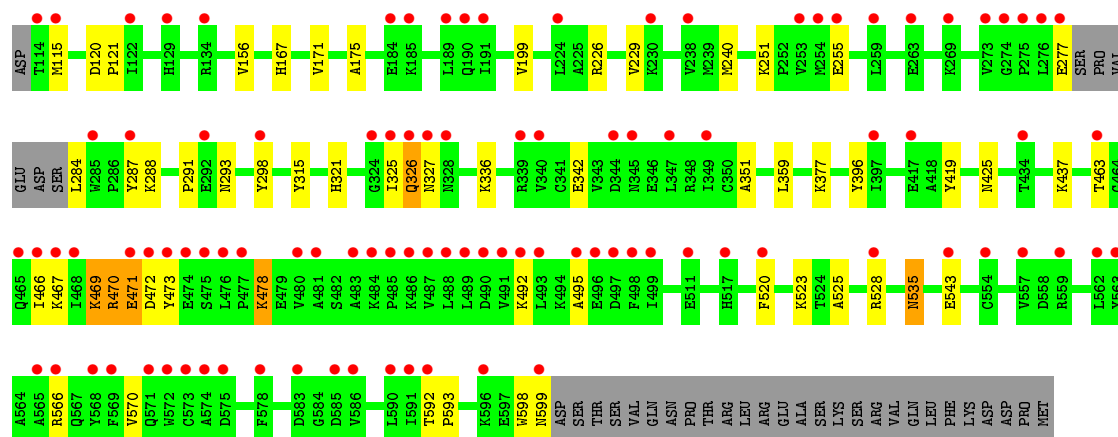
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D: 19% 82% 10% 7%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	4259 reflections (5.27%)	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
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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 [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	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:521:TYR:O	1:A:521:TYR:CD1	2.52	0.63
1:A:354:LYS:NZ	4:A:703:DTP:O1A	2.30	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:A:291:PRO:HG2	1:A:293:ASN:OD1	2.02	0.59
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.84	0.59
1:D:470:ARG:NE	1:D:471:GLU:N	2.50	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:A:175:ALA:HB1	1:A:199:VAL:HG12	1.86	0.57
1:C:463:THR:O	1:C:466:ILE:HG12	2.04	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:175:ALA:HB1	1:D:199:VAL:HG12	1.87	0.56
1:D:463:THR:O	1:D:466:ILE:HG12	2.05	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: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:D:469:LYS:HA	1:D:469:LYS:HZ1	1.69	0.47
1:A:167:HIS:O	1:A:171:VAL:HG23	2.14	0.47
1:A:535:ASN:N	1:A:535:ASN:OD1	2.46	0.47
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.47
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.97	0.47
1:D:251:LYS:O	1:D:255:GLU:HG3	2.15	0.47
1:D:287:TYR:CD1	1:D:298:TYR:CE1	3.02	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.96	0.47
1:A:327:ASN:O	1:C:326:GLN:HB3	2.14	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:C:352:ARG:NH2	4:C:701:DTP:O1G	2.44	0.47
1:D:471:GLU:OE2	1:D:472:ASP:N	2.47	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:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.46
1:C:287:TYR:CD1	1:C:298:TYR:CE1	3.04	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:251:LYS:O	1:C:255:GLU:HG3	2.15	0.45
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:A:287:TYR:CD1	1:A:298:TYR:CE1	3.04	0.45
1:A:326:GLN:HB3	1:C:327:ASN:O	2.17	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:B:287:TYR:CD1	1:B:298:TYR:CE1	3.05	0.44
1:D:325:ILE:HG22	1:D:326:GLN:N	2.31	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:A:598:TRP:O	1:A:599:ASN:HB2	2.19	0.43
1:C:351:ALA:O	1:C:520:PHE:HA	2.18	0.43
1:A:240:MET:CE	1:A:419:TYR:HD2	2.32	0.43
1:D:156:VAL:O	3:D:704:DGT:H8	2.18	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:C:381:ILE:HA	1:C:381:ILE:HD12	1.87	0.42
1:D:325:ILE:CG2	1:D:326:GLN:N	2.82	0.42
1:D:469:LYS:CA	1:D:469:LYS:HZ2	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ASN:O	1:D:326:GLN:HB3	2.20	0.42
1:D:470:ARG:CB	1:D:473:TYR:CE2	3.02	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:A:381:ILE:HA	1:A:381:ILE:HD12	1.88	0.41
1:B:598:TRP:O	1:B:599:ASN:HB2	2.20	0.41
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.02	0.41
1:C:478:LYS:H	1:C:478:LYS:HD2	1.85	0.41
4:B:704:DTP:O2B	1:D:377:LYS:NZ	2.54	0.40
1:D:478:LYS:H	1:D:478:LYS:HD2	1.86	0.40
1:B:543:GLU:CG	1:D:543:GLU:CG	2.99	0.40
1:B:377:LYS:NZ	4:D:702:DTP:O2B	2.55	0.40
1:B:240:MET:CE	1:B:419:TYR:HD2	2.34	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 ⓘ

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%)	38	48
1	B	426/459 (93%)	411 (96%)	15 (4%)	41	52
1	C	426/459 (93%)	410 (96%)	16 (4%)	38	48
1	D	426/459 (93%)	410 (96%)	16 (4%)	38	48
All	All	1704/1836 (93%)	1641 (96%)	63 (4%)	39	49

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

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	-	22,30,30	0.86	0	25,47,47	1.97	5 (20%)
3	DGT	A	702	5	26,33,33	1.10	2 (7%)	28,52,52	2.24	8 (28%)
4	DTP	A	703	5	26,32,32	1.15	3 (11%)	26,50,50	2.24	5 (19%)
2	TTP	B	701	-	22,30,30	0.78	0	25,47,47	2.11	6 (24%)
3	DGT	B	702	5	26,33,33	1.07	2 (7%)	28,52,52	2.11	6 (21%)
4	DTP	B	704	5	26,32,32	1.26	2 (7%)	26,50,50	2.20	4 (15%)
4	DTP	C	701	5	26,32,32	1.21	3 (11%)	26,50,50	2.05	6 (23%)
3	DGT	C	703	-	26,33,33	1.46	2 (7%)	28,52,52	1.99	8 (28%)
3	DGT	C	704	5	26,33,33	1.09	2 (7%)	28,52,52	2.13	8 (28%)
4	DTP	D	702	5	26,32,32	1.18	2 (7%)	26,50,50	1.72	3 (11%)
2	TTP	D	703	-	22,30,30	0.67	0	25,47,47	1.86	5 (20%)
3	DGT	D	704	5	26,33,33	1.25	3 (11%)	28,52,52	2.26	10 (35%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	DTP	O4'-C4'	-2.15	1.40	1.45
4	D	702	DTP	C5-C4	2.06	1.45	1.40
3	D	704	DGT	PG-O3B	2.17	1.63	1.60
4	A	703	DTP	C5-C4	2.17	1.45	1.40
3	C	704	DGT	C5-C4	2.29	1.45	1.40
4	D	702	DTP	C2-N3	2.32	1.36	1.32
4	A	703	DTP	C2-N3	2.45	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	2.86	1.37	1.32
3	A	702	DGT	C6-C5	2.92	1.46	1.41
3	A	702	DGT	C5-C4	2.97	1.47	1.40
3	B	702	DGT	C6-C5	3.04	1.47	1.41
4	C	701	DTP	PG-O3B	3.05	1.65	1.60
4	C	701	DTP	C5-C4	3.06	1.47	1.40
3	D	704	DGT	C6-C5	3.09	1.47	1.41
3	D	704	DGT	C5-C4	3.23	1.47	1.40
3	C	704	DGT	C6-C5	3.63	1.48	1.41
3	C	703	DGT	C5-C4	3.85	1.49	1.40
4	B	704	DTP	PG-O3B	4.02	1.66	1.60
3	C	703	DGT	C6-C5	4.97	1.50	1.41

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	DTP	N3-C2-N1	-9.42	120.65	128.86
4	A	703	DTP	N3-C2-N1	-9.15	120.89	128.86
4	C	701	DTP	N3-C2-N1	-7.95	121.94	128.86
4	D	702	DTP	N3-C2-N1	-5.86	123.76	128.86
2	A	701	TTP	C5-C4-N3	-5.55	119.12	125.24
2	B	701	TTP	C5-C4-N3	-5.50	119.17	125.24
3	A	702	DGT	C5-C6-N1	-5.39	115.81	123.48
3	B	702	DGT	C6-C5-C4	-4.74	116.13	120.84
3	D	704	DGT	C5-C6-N1	-4.44	117.16	123.48
3	C	703	DGT	C6-C5-C4	-4.43	116.44	120.84
3	C	704	DGT	C6-C5-C4	-4.40	116.47	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	TTP	C5-C4-N3	-4.37	120.42	125.24
3	A	702	DGT	C4-C5-N7	-4.15	105.40	109.41
4	D	702	DTP	C4-C5-N7	-4.01	105.54	109.41
3	C	704	DGT	N3-C2-N1	-3.90	121.77	127.46
3	B	702	DGT	N3-C2-N1	-3.85	121.83	127.46
3	C	703	DGT	C5-C6-N1	-3.53	118.46	123.48
3	D	704	DGT	C6-C5-C4	-3.40	117.46	120.84
2	D	703	TTP	C5-C6-N1	-3.36	118.51	122.15
2	A	701	TTP	C5-C6-N1	-3.35	118.53	122.15
3	A	702	DGT	O5'-PA-O2A	-3.28	96.00	109.25
3	B	702	DGT	C5-C6-N1	-3.22	118.90	123.48
4	C	701	DTP	O3B-PG-O1G	-3.21	91.70	111.44
4	A	703	DTP	C4-C5-N7	-3.18	106.34	109.41
3	D	704	DGT	N3-C2-N1	-3.09	122.94	127.46
3	C	704	DGT	C5-C6-N1	-3.04	119.16	123.48
3	C	704	DGT	C4-C5-N7	-3.01	106.50	109.41
3	D	704	DGT	C4-C5-N7	-2.97	106.54	109.41
3	C	703	DGT	C4-C5-N7	-2.96	106.55	109.41
3	A	702	DGT	N3-C2-N1	-2.74	123.46	127.46
3	C	703	DGT	N3-C2-N1	-2.73	123.47	127.46
2	B	701	TTP	C5-C6-N1	-2.56	119.38	122.15
4	B	704	DTP	C4-C5-N7	-2.45	107.05	109.41
4	C	701	DTP	C4-C5-N7	-2.25	107.23	109.41
3	D	704	DGT	O4'-C1'-C2'	-2.17	102.09	106.25
2	B	701	TTP	O3G-PG-O2G	2.01	115.74	107.61
4	C	701	DTP	O3G-PG-O1G	2.04	118.49	110.50
3	C	704	DGT	N2-C2-N1	2.09	120.58	117.24
4	B	704	DTP	C2'-C3'-C4'	2.10	107.21	102.73
2	D	703	TTP	O2B-PB-O1B	2.12	123.26	112.28
3	D	704	DGT	O1A-PA-O2A	2.16	123.46	112.28
2	A	701	TTP	O2B-PB-O1B	2.19	123.60	112.28
4	C	701	DTP	N6-C6-N1	2.19	123.10	118.77
4	A	703	DTP	N6-C6-N1	2.19	123.11	118.77
4	D	702	DTP	O3G-PG-O2G	2.22	116.58	107.61
2	B	701	TTP	C2'-C3'-C4'	2.23	107.48	102.73
3	A	702	DGT	O1A-PA-O2A	2.36	124.49	112.28
3	C	704	DGT	O2G-PG-O1G	2.37	117.18	107.61
4	C	701	DTP	C2-N1-C6	2.40	122.97	118.77
3	D	704	DGT	O4'-C1'-N9	2.44	111.89	107.78
4	A	703	DTP	C2'-C3'-C4'	2.58	108.23	102.73
4	A	703	DTP	O3G-PG-O2G	2.58	118.04	107.61
2	A	701	TTP	O3G-PG-O2G	2.59	118.05	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	DGT	C2'-C3'-C4'	2.64	108.34	102.73
3	B	702	DGT	O2G-PG-O3G	2.79	121.41	110.50
2	D	703	TTP	O3G-PG-O2G	2.91	119.35	107.61
3	C	703	DGT	O2G-PG-O1G	2.95	119.53	107.61
2	B	701	TTP	C5M-C5-C4	3.07	123.71	120.17
4	B	704	DTP	C2-N1-C6	3.34	124.61	118.77
3	A	702	DGT	C2-N3-C4	3.34	119.06	115.16
3	A	702	DGT	O1G-PG-O3G	3.47	124.09	110.50
3	C	704	DGT	C6-N1-C2	3.72	121.41	116.06
3	D	704	DGT	O2G-PG-O1G	3.87	123.22	107.61
3	C	703	DGT	C6-N1-C2	4.07	121.91	116.06
3	B	702	DGT	C6-N1-C2	4.40	122.38	116.06
3	C	703	DGT	C2-N3-C4	4.40	120.30	115.16
3	D	704	DGT	C2-N3-C4	4.48	120.40	115.16
3	D	704	DGT	C6-N1-C2	4.95	123.17	116.06
3	A	702	DGT	C6-N1-C2	5.04	123.31	116.06
3	B	702	DGT	C2-N3-C4	5.06	121.07	115.16
2	D	703	TTP	C4-N3-C2	5.14	119.65	115.16
2	A	701	TTP	C4-N3-C2	5.27	119.76	115.16
2	B	701	TTP	C4-N3-C2	5.99	120.40	115.16
3	C	704	DGT	C2-N3-C4	6.08	122.25	115.16

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 ⓘ

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, 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	480/514 (93%)	0.59	37 (7%) 14 21	29, 59, 94, 136	0
1	B	480/514 (93%)	0.81	52 (10%) 6 10	33, 66, 103, 133	0
1	C	480/514 (93%)	1.31	115 (23%) 1 1	35, 80, 129, 171	0
1	D	480/514 (93%)	1.28	100 (20%) 1 2	33, 77, 134, 176	0
All	All	1920/2056 (93%)	1.00	304 (15%) 2 3	29, 70, 119, 176	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	489	LEU	14.3
1	D	489	LEU	12.2
1	D	562	LEU	11.4
1	C	496	GLU	10.0
1	C	488	LEU	9.9
1	C	486	LYS	9.5
1	D	590	LEU	8.2
1	D	490	ASP	8.1
1	D	491	VAL	7.7
1	D	466	ILE	7.6
1	B	488	LEU	7.6
1	D	274	GLY	7.1
1	D	487	VAL	7.0
1	D	465	GLN	6.4
1	C	285	TRP	6.3
1	D	493	LEU	6.2
1	D	481	ALA	6.2
1	C	498	PHE	6.2
1	D	592	THR	5.8
1	C	557	VAL	5.8
1	D	488	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	473	TYR	5.7
1	C	466	ILE	5.7
1	B	599	ASN	5.5
1	D	497	ASP	5.5
1	C	263	GLU	5.5
1	C	255	GLU	5.4
1	B	489	LEU	5.4
1	D	599	ASN	5.3
1	C	590	LEU	5.3
1	D	345	ASN	5.3
1	C	584	GLY	5.2
1	D	486	LYS	5.2
1	B	487	VAL	5.1
1	B	262	GLU	5.0
1	C	478	LYS	5.0
1	B	277	GLU	5.0
1	B	276	LEU	5.0
1	D	472	ASP	4.9
1	A	466	ILE	4.9
1	D	287	TYR	4.9
1	C	403	GLY	4.8
1	C	276	LEU	4.8
1	C	483	ALA	4.7
1	D	563	TYR	4.6
1	C	284	LEU	4.6
1	D	573	CYS	4.6
1	D	483	ALA	4.6
1	D	568	TYR	4.6
1	D	275	PRO	4.5
1	B	490	ASP	4.5
1	B	326	GLN	4.5
1	D	476	LEU	4.5
1	C	554	CYS	4.4
1	D	277	GLU	4.4
1	D	586	VAL	4.4
1	C	586	VAL	4.3
1	C	465	GLN	4.3
1	B	229	VAL	4.3
1	C	563	TYR	4.2
1	D	467	LYS	4.2
1	C	592	THR	4.2
1	C	253	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLU	4.2
1	D	326	GLN	4.1
1	C	341	CYS	4.1
1	C	495	ALA	4.1
1	A	260	ILE	4.0
1	D	496	GLU	4.0
1	D	569	PHE	4.0
1	B	587	ILE	4.0
1	B	492	LYS	4.0
1	B	328	ASN	4.0
1	C	484	LYS	4.0
1	C	596	LYS	3.9
1	B	253	VAL	3.9
1	C	561	SER	3.9
1	D	263	GLU	3.9
1	D	498	PHE	3.9
1	B	590	LEU	3.9
1	C	473	TYR	3.9
1	C	568	TYR	3.9
1	D	273	VAL	3.9
1	C	493	LEU	3.8
1	C	573	CYS	3.8
1	C	594	GLN	3.8
1	C	490	ASP	3.8
1	B	596	LYS	3.8
1	A	263	GLU	3.8
1	D	596	LYS	3.7
1	C	228	GLU	3.7
1	D	492	LYS	3.7
1	C	258	GLY	3.7
1	C	562	LEU	3.7
1	C	591	ILE	3.6
1	C	275	PRO	3.6
1	C	287	TYR	3.6
1	B	230	LYS	3.6
1	C	326	GLN	3.6
1	D	468	ILE	3.5
1	C	558	ASP	3.5
1	A	560	LYS	3.5
1	C	231	TRP	3.5
1	D	189	LEU	3.5
1	D	191	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	114	THR	3.4
1	D	480	VAL	3.4
1	D	528	ARG	3.4
1	D	115	MET	3.4
1	C	565	ALA	3.4
1	C	571	GLN	3.4
1	C	293	ASN	3.4
1	B	396	TYR	3.4
1	D	485	PRO	3.4
1	B	557	VAL	3.4
1	A	543	GLU	3.3
1	D	511	GLU	3.3
1	A	277	GLU	3.3
1	D	475	SER	3.3
1	C	467	LYS	3.3
1	B	134	ARG	3.3
1	D	471	GLU	3.3
1	D	572	TRP	3.3
1	A	486	LYS	3.2
1	A	590	LEU	3.2
1	C	191	ILE	3.2
1	C	570	VAL	3.2
1	B	263	GLU	3.2
1	B	592	THR	3.2
1	D	554	CYS	3.2
1	C	494	LYS	3.2
1	A	327	ASN	3.1
1	A	465	GLN	3.1
1	D	591	ILE	3.1
1	B	288	LYS	3.1
1	C	345	ASN	3.1
1	B	327	ASN	3.1
1	B	260	ILE	3.1
1	C	572	TRP	3.1
1	D	575	ASP	3.1
1	B	284	LEU	3.1
1	C	492	LYS	3.1
1	C	593	PRO	3.1
1	C	347	LEU	3.0
1	A	490	ASP	3.0
1	D	292	GLU	3.0
1	A	114	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	254	MET	3.0
1	C	560	LYS	3.0
1	C	262	GLU	3.0
1	D	578	PHE	3.0
1	B	491	VAL	3.0
1	C	440	ASP	2.9
1	D	543	GLU	2.9
1	C	569	PHE	2.9
1	C	396	TYR	2.9
1	D	495	ALA	2.9
1	D	190	GLN	2.9
1	C	241	PHE	2.9
1	C	277	GLU	2.9
1	D	565	ALA	2.9
1	B	325	ILE	2.9
1	C	556	LYS	2.9
1	C	564	ALA	2.9
1	D	253	VAL	2.9
1	C	390	PHE	2.8
1	C	491	VAL	2.8
1	D	585	ASP	2.8
1	C	259	LEU	2.8
1	D	259	LEU	2.8
1	D	276	LEU	2.8
1	A	262	GLU	2.8
1	C	444	ILE	2.8
1	A	325	ILE	2.8
1	C	325	ILE	2.8
1	A	259	LEU	2.8
1	A	556	LYS	2.8
1	D	477	PRO	2.7
1	D	559	ARG	2.7
1	C	472	ASP	2.7
1	C	471	GLU	2.7
1	D	463	THR	2.7
1	D	255	GLU	2.7
1	C	528	ARG	2.6
1	C	454	PHE	2.6
1	B	585	ASP	2.6
1	A	285	TRP	2.6
1	C	468	ILE	2.6
1	C	588	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	297	LEU	2.6
1	B	252	PRO	2.6
1	C	587	ILE	2.6
1	C	230	LYS	2.6
1	D	557	VAL	2.6
1	A	464	GLY	2.6
1	B	261	PRO	2.6
1	B	289	GLY	2.6
1	C	225	ALA	2.6
1	C	441	ALA	2.6
1	A	328	ASN	2.6
1	A	332	LYS	2.6
1	D	327	ASN	2.5
1	B	543	GLU	2.5
1	A	253	VAL	2.5
1	A	484	LYS	2.5
1	C	238	VAL	2.5
1	A	288	LYS	2.5
1	C	575	ASP	2.5
1	C	266	CYS	2.5
1	A	326	GLN	2.5
1	C	566	ARG	2.5
1	A	293	ASN	2.5
1	B	320	CYS	2.5
1	C	260	ILE	2.5
1	C	501	ASP	2.4
1	D	230	LYS	2.4
1	B	413	ILE	2.4
1	C	327	ASN	2.4
1	B	593	PRO	2.4
1	C	485	PRO	2.4
1	B	470	ARG	2.4
1	C	288	LYS	2.4
1	D	285	TRP	2.4
1	D	484	LYS	2.4
1	D	574	ALA	2.4
1	A	594	GLN	2.4
1	B	323	LEU	2.4
1	A	292	GLU	2.4
1	B	235	GLN	2.4
1	D	417	GLU	2.4
1	D	122	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	574	ALA	2.3
1	D	224	LEU	2.3
1	C	559	ARG	2.3
1	D	325	ILE	2.3
1	A	346	GLU	2.3
1	C	585	ASP	2.3
1	C	224	LEU	2.3
1	C	257	TYR	2.3
1	C	141	PHE	2.3
1	A	491	VAL	2.3
1	A	492	LYS	2.3
1	C	397	ILE	2.3
1	D	114	THR	2.2
1	A	242	GLU	2.2
1	A	599	ASN	2.2
1	C	245	ILE	2.2
1	B	324	GLY	2.2
1	B	584	GLY	2.2
1	D	520	PHE	2.2
1	C	487	VAL	2.2
1	A	572	TRP	2.2
1	D	129	HIS	2.2
1	D	566	ARG	2.2
1	C	464	GLY	2.2
1	C	160	ALA	2.2
1	C	190	GLN	2.2
1	D	269	LYS	2.2
1	C	342	GLU	2.2
1	D	184	GLU	2.2
1	B	121	PRO	2.2
1	D	298	TYR	2.1
1	C	348	ARG	2.1
1	D	340	VAL	2.1
1	D	499	ILE	2.1
1	B	259	LEU	2.1
1	D	347	LEU	2.1
1	D	571	GLN	2.1
1	C	457	VAL	2.1
1	C	481	ALA	2.1
1	B	486	LYS	2.1
1	D	185	LYS	2.1
1	D	238	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	517	HIS	2.1
1	B	160	ALA	2.1
1	B	194	ARG	2.1
1	D	339	ARG	2.1
1	D	328	ASN	2.1
1	D	397	ILE	2.1
1	C	235	GLN	2.1
1	D	583	ASP	2.1
1	C	322	HIS	2.1
1	C	524	THR	2.1
1	C	599	ASN	2.1
1	D	434	THR	2.1
1	C	482	SER	2.1
1	A	276	LEU	2.0
1	B	122	ILE	2.0
1	C	549	LEU	2.0
1	D	474	GLU	2.0
1	B	256	GLN	2.0
1	B	493	LEU	2.0
1	D	349	ILE	2.0
1	B	255	GLU	2.0
1	C	256	GLN	2.0
1	D	324	GLY	2.0
1	C	317	ALA	2.0
1	B	344	ASP	2.0
1	C	583	ASP	2.0
1	D	344	ASP	2.0
1	A	467	LYS	2.0
1	C	320	CYS	2.0
1	D	134	ARG	2.0
1	A	317	ALA	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, 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	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
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.