



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2016 – 10:40 PM EDT

PDB ID : 4TO3
Title : Structural basis of cellular dNTP regulation, SAMHD1-dGTP-dGTP-dCTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.20 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

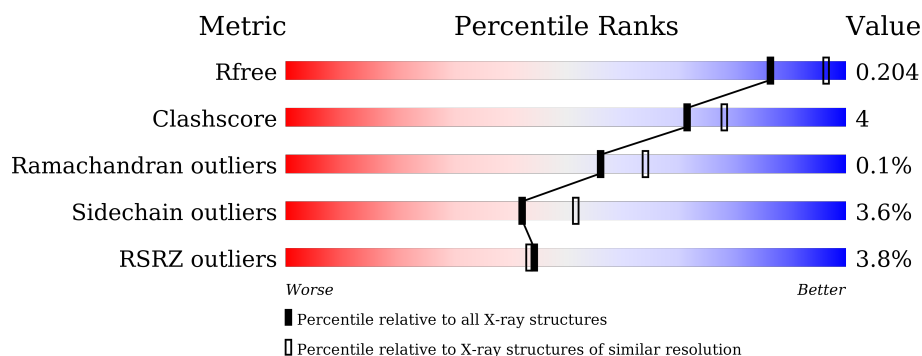
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	514	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
1	C	514	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>6%</div> </div> </div>
1	D	514	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16708 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.

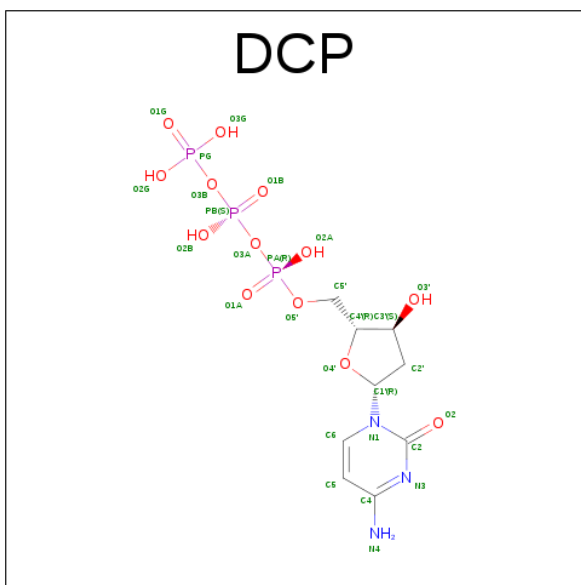
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	3	0
			3963	2537	690	715	21			
1	B	481	Total	C	N	O	S	0	3	0
			3962	2536	689	716	21			
1	C	481	Total	C	N	O	S	0	2	0
			3953	2531	687	714	21			
1	D	481	Total	C	N	O	S	0	4	0
			3972	2542	691	718	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
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 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).

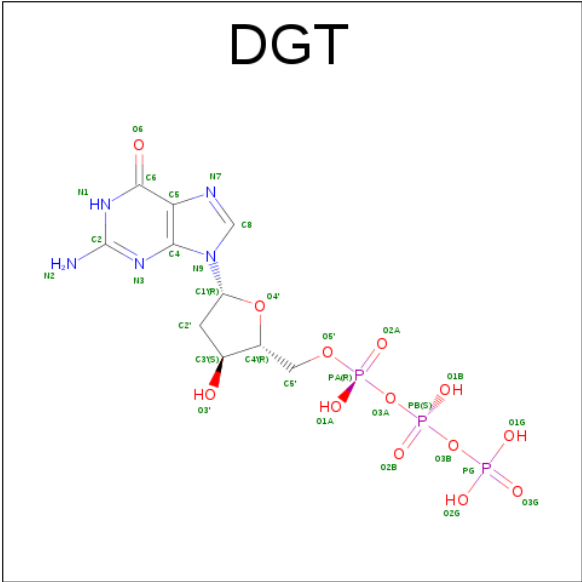


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	B	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	C	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	D	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

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

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

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

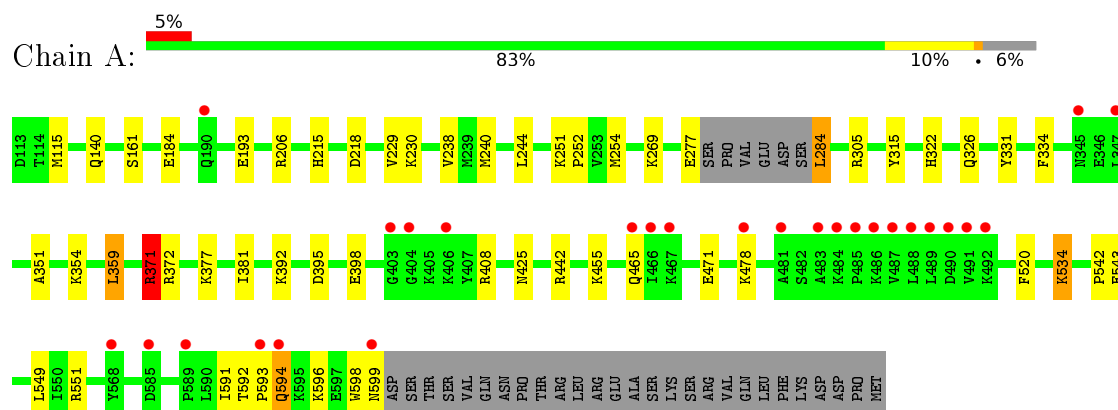
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	130	Total	O	0	0
			130	130		
5	C	91	Total	O	0	0
			91	91		
5	D	159	Total	O	0	0
			159	159		

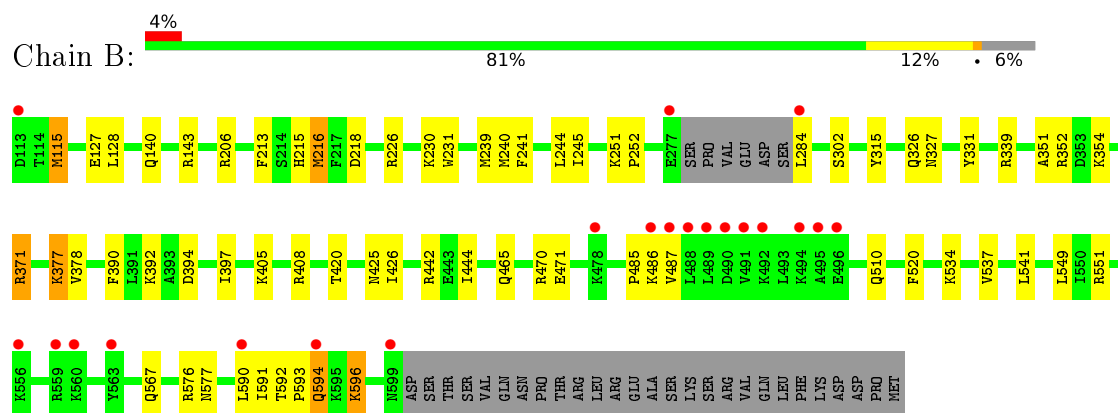
3 Residue-property plots

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.

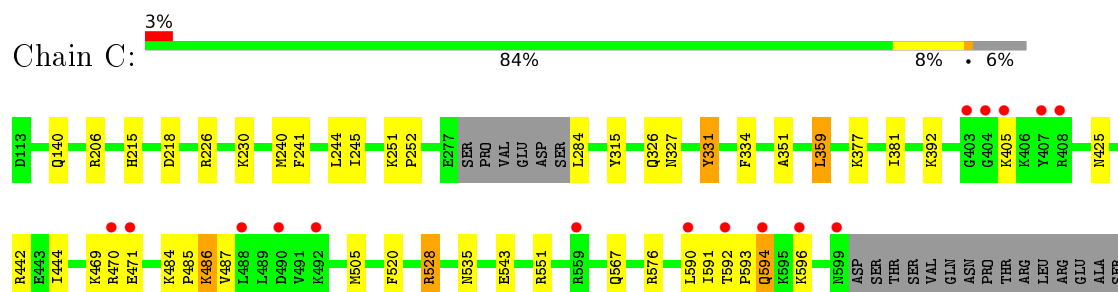
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

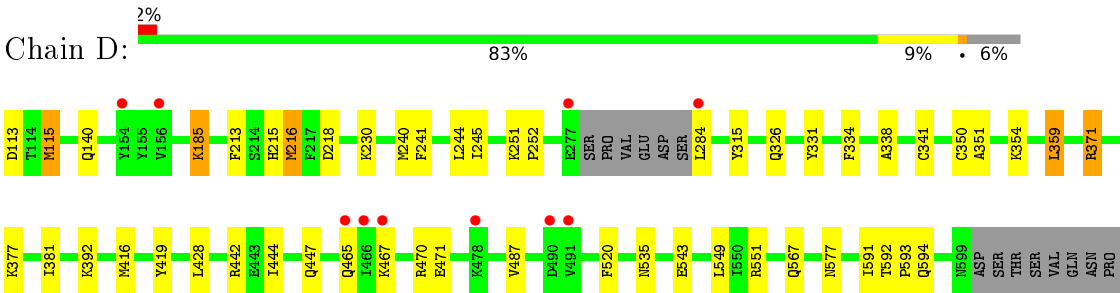


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



LYS
SER
ARG
VAL
GLN
LEU
PHE
LYS
ASP
ASP
PRO
MET

● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.41Å 146.03Å 98.11Å 90.00° 114.52° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 39.31 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.2 (40.00-2.20) 96.2 (39.31-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.168 , 0.204 0.173 , 0.204	Depositor DCC
R_{free} test set	5486 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16708	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DGT, DCP

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	0.78	1/4057 (0.0%)	0.85	10/5476 (0.2%)
1	B	0.76	0/4055	0.83	8/5473 (0.1%)
1	C	0.74	0/4046	0.82	9/5461 (0.2%)
1	D	0.80	0/4066	0.85	2/5488 (0.0%)
All	All	0.77	1/16224 (0.0%)	0.84	29/21898 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	SER	CB-OG	8.30	1.53	1.42

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	LYS	CD-CE-NZ	8.60	131.47	111.70
1	C	551	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	C	442	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	B	576	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	A	254	MET	CG-SD-CE	6.61	110.78	100.20
1	A	442	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	442	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	305	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	A	371	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	C	551	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	551	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	551	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	D	442	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	551	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	D	551	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	C	226	ARG	NE-CZ-NH2	5.48	123.04	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	551	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	C	528	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	C	528	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	371	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	206	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	206	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	284	LEU	CA-CB-CG	5.23	127.34	115.30
1	B	226	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	206	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	576	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	C	505	MET	CG-SD-CE	5.05	108.28	100.20
1	B	352	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	3963	0	3943	32	0
1	B	3962	0	3944	41	0
1	C	3953	0	3937	27	0
1	D	3972	0	3948	43	0
2	A	28	0	12	1	0
2	B	28	0	12	5	0
2	C	28	0	12	0	0
2	D	28	0	12	1	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	62	0	24	0	0
4	B	93	0	36	0	0
4	C	31	0	12	0	0
4	D	62	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	110	0	0	3	0
5	B	130	0	0	2	0
5	C	91	0	0	1	0
5	D	159	0	0	5	0
All	All	16708	0	15916	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (138) 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:240:MET:HG2	1:D:416:MET:CE	1.89	1.02
1:D:240:MET:HG2	1:D:416:MET:HE1	1.40	1.00
1:D:240:MET:SD	1:D:416:MET:CE	2.51	0.98
1:D:240:MET:SD	1:D:416:MET:HE2	2.06	0.95
1:D:371:ARG:HG3	1:D:371:ARG:HH21	1.32	0.92
1:D:240:MET:CG	1:D:416:MET:CE	2.54	0.85
1:D:371:ARG:CG	1:D:371:ARG:HH21	1.95	0.80
1:D:240:MET:CG	1:D:416:MET:HE1	2.11	0.79
1:D:467:LYS:HD3	5:D:891:HOH:O	1.82	0.78
1:D:240:MET:CG	1:D:416:MET:HE2	2.16	0.76
1:B:140:GLN:HG3	1:B:240:MET:HE1	1.71	0.72
1:B:534:LYS:O	1:B:537:VAL:HG22	1.90	0.72
2:A:701:DCP:N3	5:A:908:HOH:O	2.22	0.71
1:D:371:ARG:NH2	5:D:879:HOH:O	2.22	0.70
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.73	0.70
1:C:140:GLN:HG3	1:C:240:MET:HE1	1.73	0.69
1:A:140:GLN:HG3	1:A:240:MET:HE1	1.72	0.69
1:D:240:MET:HG2	1:D:416:MET:HE2	1.74	0.68
2:B:701:DCP:N3	5:B:930:HOH:O	2.26	0.67
1:B:140:GLN:CG	1:B:240:MET:HE1	2.25	0.67
1:D:140:GLN:HG3	1:D:240:MET:HE1	1.76	0.66
1:A:140:GLN:CG	1:A:240:MET:HE1	2.26	0.65
1:B:534:LYS:O	1:B:537:VAL:CG2	2.45	0.65
1:D:535:ASN:OD1	1:D:535:ASN:N	2.29	0.65
1:C:535:ASN:N	1:C:535:ASN:OD1	2.31	0.64
1:D:140:GLN:CG	1:D:240:MET:HE1	2.28	0.64
1:C:140:GLN:CG	1:C:240:MET:HE1	2.27	0.63
1:B:231:TRP:HZ3	1:B:239:MET:CE	2.11	0.63
1:B:215:HIS:NE2	2:B:701:DCP:O2A	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331[B]:TYR:C	1:A:331[B]:TYR:CD1	2.73	0.61
1:D:213:PHE:HB2	1:D:216:MET:HG2	1.82	0.61
1:B:215:HIS:CE1	2:B:701:DCP:O2A	2.54	0.61
1:B:213:PHE:HB2	1:B:216:MET:HG2	1.81	0.60
1:D:331[B]:TYR:C	1:D:331[B]:TYR:CD1	2.76	0.59
1:B:115[A]:MET:HE2	1:B:127:GLU:HB3	1.84	0.59
1:C:331[A]:TYR:C	1:C:331[A]:TYR:CD1	2.76	0.58
1:B:327:ASN:O	1:D:326:GLN:HG2	2.03	0.57
1:C:485:PRO:O	1:C:486:LYS:HB2	2.05	0.57
1:B:231:TRP:CZ3	1:B:239:MET:CE	2.88	0.57
1:C:392:LYS:HE2	1:C:444:ILE:HD11	1.87	0.57
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.36	0.57
1:B:331[B]:TYR:C	1:B:331[B]:TYR:CD1	2.78	0.56
1:A:326:GLN:HG2	1:C:327:ASN:O	2.04	0.56
1:B:115[A]:MET:HG3	1:B:128:LEU:O	2.05	0.56
1:A:534:LYS:HE3	1:A:542:PRO:O	2.06	0.55
1:C:469:LYS:HD2	1:C:471:GLU:OE2	2.06	0.55
1:A:371:ARG:NH1	1:A:549:LEU:HD21	2.22	0.55
1:D:487:VAL:HG21	1:D:567:GLN:HG3	1.88	0.55
1:B:390:PHE:CZ	1:B:426:ILE:CG2	2.90	0.55
1:B:231:TRP:HZ3	1:B:239:MET:HE1	1.71	0.54
1:B:392:LYS:HE2	1:B:444:ILE:HD11	1.89	0.54
1:A:543:GLU:HG3	1:C:543:GLU:HG3	1.90	0.53
2:B:701:DCP:H5	5:B:886:HOH:O	2.08	0.53
1:A:115[B]:MET:C	1:A:115[B]:MET:SD	2.88	0.52
1:D:447:GLN:HG3	5:D:933:HOH:O	2.09	0.52
1:D:392:LYS:HE2	1:D:444:ILE:HD11	1.90	0.51
1:A:322:HIS:HE1	5:A:845:HOH:O	1.92	0.51
1:B:591:ILE:O	1:B:594:GLN:HG2	2.10	0.51
1:B:371:ARG:NH2	1:B:549:LEU:HD21	2.26	0.50
1:B:485:PRO:O	1:B:486:LYS:HB2	2.11	0.49
1:A:251:LYS:HB2	1:A:252:PRO:HD3	1.95	0.49
1:B:231:TRP:CZ3	1:B:239:MET:HE3	2.48	0.49
1:B:215:HIS:HE2	2:B:701:DCP:PA	2.36	0.49
1:B:390:PHE:CZ	1:B:426:ILE:HG23	2.48	0.48
1:A:543:GLU:HG2	1:C:543:GLU:HG2	1.95	0.48
1:C:251:LYS:HB2	1:C:252:PRO:HD3	1.95	0.48
1:A:543:GLU:CG	1:C:543:GLU:CG	2.91	0.48
1:B:251:LYS:HB2	1:B:252:PRO:HD3	1.96	0.47
1:C:244:LEU:HD23	1:C:244:LEU:C	2.34	0.47
1:A:229:VAL:HG12	1:A:230:LYS:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:HG13	1:A:269:LYS:HE2	1.96	0.47
1:A:395:ASP:OD1	1:A:408:ARG:NH1	2.48	0.47
1:A:455:LYS:CE	5:A:886:HOH:O	2.62	0.47
1:B:213:PHE:CB	1:B:216:MET:HG2	2.45	0.47
1:C:592:THR:N	1:C:593:PRO:CD	2.78	0.46
1:B:394:ASP:O	1:B:408:ARG:HD2	2.15	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.15	0.46
1:D:251:LYS:HB2	1:D:252:PRO:HD3	1.98	0.46
1:A:398:GLU:O	1:A:398:GLU:HG3	2.16	0.46
1:A:591:ILE:O	1:A:594:GLN:HG2	2.16	0.46
1:D:591:ILE:O	1:D:594:GLN:HG2	2.16	0.45
1:D:115[A]:MET:SD	1:D:115[A]:MET:C	2.94	0.45
2:D:703:DCP:H5'1	5:D:854:HOH:O	2.16	0.45
1:A:592:THR:N	1:A:593:PRO:CD	2.80	0.45
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.45
1:C:484:LYS:HD2	1:C:484:LYS:HA	1.81	0.44
1:D:416:MET:HE1	1:D:419:TYR:HD2	1.82	0.44
1:B:351:ALA:O	1:B:520:PHE:HA	2.17	0.44
1:D:215:HIS:HA	1:D:218:ASP:OD1	2.17	0.44
1:A:215:HIS:HA	1:A:218:ASP:OD1	2.16	0.44
1:C:334:PHE:CE2	1:C:359:LEU:HD11	2.52	0.44
1:B:215:HIS:HA	1:B:218:ASP:OD1	2.17	0.44
1:B:487:VAL:HG11	1:B:567:GLN:HG3	1.99	0.44
1:D:213:PHE:CB	1:D:216:MET:HG2	2.45	0.44
1:B:592:THR:N	1:B:593:PRO:CD	2.81	0.43
1:D:244:LEU:HD23	1:D:244:LEU:C	2.38	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.18	0.43
1:A:240:MET:HE2	1:A:240:MET:HB3	1.83	0.43
1:B:231:TRP:HZ3	1:B:239:MET:HE3	1.79	0.43
1:C:240:MET:HE2	1:C:240:MET:HB3	1.85	0.43
1:C:215:HIS:HA	1:C:218:ASP:OD1	2.19	0.43
1:A:543:GLU:HG2	1:C:543:GLU:CG	2.49	0.43
1:D:416:MET:HE3	1:D:416:MET:HA	2.02	0.42
1:A:372:ARG:HG2	5:C:890:HOH:O	2.19	0.42
1:D:416:MET:HE3	1:D:419:TYR:HB3	2.01	0.42
1:B:244:LEU:C	1:B:244:LEU:HD23	2.39	0.42
1:D:334:PHE:CE2	1:D:359:LEU:HD11	2.53	0.42
1:B:241:PHE:O	1:B:245:ILE:HG12	2.20	0.42
1:C:591:ILE:O	1:C:594:GLN:HG2	2.20	0.42
1:D:240:MET:HB3	1:D:240:MET:HE2	1.80	0.42
1:D:185:LYS:HE3	1:D:338:ALA:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLU:CG	1:C:543:GLU:HG3	2.50	0.42
1:B:534:LYS:O	1:B:537:VAL:HG23	2.20	0.42
1:B:596:LYS:HD2	1:B:596:LYS:HA	1.77	0.42
1:A:334:PHE:CE2	1:A:359:LEU:HD11	2.54	0.41
1:D:371:ARG:NH1	1:D:549:LEU:HD21	2.35	0.41
1:B:377:LYS:HG2	1:B:378:VAL:N	2.35	0.41
1:B:487:VAL:HG23	1:B:590:LEU:HD12	2.02	0.41
1:A:244:LEU:HD23	1:A:244:LEU:C	2.40	0.41
1:D:592:THR:N	1:D:593:PRO:CD	2.83	0.41
1:B:143:ARG:HD2	1:B:420:THR:HA	2.01	0.41
1:C:487:VAL:HG11	1:C:567:GLN:HG3	2.02	0.41
1:A:425:ASN:HB2	1:D:428:LEU:HD13	2.02	0.41
1:C:241:PHE:O	1:C:245:ILE:HG12	2.20	0.41
1:B:537:VAL:HG23	1:B:541:LEU:CD1	2.50	0.41
1:D:381:ILE:HA	1:D:381:ILE:HD12	1.95	0.41
1:B:231:TRP:CZ3	1:B:239:MET:HE1	2.52	0.41
1:D:341:CYS:HB2	1:D:350:CYS:SG	2.61	0.41
1:D:371:ARG:HG3	1:D:371:ARG:NH2	2.15	0.41
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.90	0.40
1:D:241:PHE:O	1:D:245:ILE:HG12	2.20	0.40
1:D:371:ARG:CG	1:D:371:ARG:NH2	2.66	0.40
1:A:140:GLN:CG	1:A:240:MET:CE	2.98	0.40
1:A:398:GLU:O	1:A:398:GLU:CG	2.69	0.40
1:A:598:TRP:O	1:A:599:ASN:HB2	2.22	0.40
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.91	0.40
1:C:487:VAL:HG23	1:C:590:LEU:HD12	2.02	0.40
1:D:447:GLN:CG	5:D:933:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	480/514 (93%)	473 (98%)	7 (2%)	0	100	100
1	B	480/514 (93%)	470 (98%)	10 (2%)	0	100	100
1	C	479/514 (93%)	471 (98%)	7 (2%)	1 (0%)	52	59
1	D	481/514 (94%)	474 (98%)	7 (2%)	0	100	100
All	All	1920/2056 (93%)	1888 (98%)	31 (2%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	LYS

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	430/459 (94%)	415 (96%)	15 (4%)	43	53
1	B	430/459 (94%)	411 (96%)	19 (4%)	35	42
1	C	429/459 (94%)	416 (97%)	13 (3%)	48	60
1	D	431/459 (94%)	414 (96%)	17 (4%)	39	48
All	All	1720/1836 (94%)	1656 (96%)	64 (4%)	42	50

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	193	GLU
1	A	277	GLU
1	A	284	LEU
1	A	315	TYR
1	A	354	LYS
1	A	359	LEU
1	A	371	ARG
1	A	377	LYS
1	A	465	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	471	GLU
1	A	478	LYS
1	A	534	LYS
1	A	594	GLN
1	A	596	LYS
1	B	115[A]	MET
1	B	115[B]	MET
1	B	216	MET
1	B	230	LYS
1	B	284	LEU
1	B	302	SER
1	B	315	TYR
1	B	326	GLN
1	B	339	ARG
1	B	354	LYS
1	B	377	LYS
1	B	405	LYS
1	B	465	GLN
1	B	470	ARG
1	B	471	GLU
1	B	510	GLN
1	B	577	ASN
1	B	594	GLN
1	B	596	LYS
1	C	230	LYS
1	C	284	LEU
1	C	315	TYR
1	C	326	GLN
1	C	331[A]	TYR
1	C	331[B]	TYR
1	C	359	LEU
1	C	377	LYS
1	C	405	LYS
1	C	470	ARG
1	C	528	ARG
1	C	594	GLN
1	C	596	LYS
1	D	113	ASP
1	D	115[A]	MET
1	D	115[B]	MET
1	D	185	LYS
1	D	216	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	230	LYS
1	D	284	LEU
1	D	315	TYR
1	D	354	LYS
1	D	359	LEU
1	D	371	ARG
1	D	377	LYS
1	D	465	GLN
1	D	470	ARG
1	D	471	GLU
1	D	543	GLU
1	D	577	ASN

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

Mol	Chain	Res	Type
1	A	425	ASN
1	B	425	ASN
1	C	425	ASN
1	D	425	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 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	DCP	A	701	3	22,29,29	0.88	0	28,45,45	1.44	3 (10%)
4	DGT	A	703	3	25,33,33	1.00	1 (4%)	29,52,52	1.62	6 (20%)
4	DGT	A	704	3	25,33,33	1.10	2 (8%)	29,52,52	2.10	6 (20%)
2	DCP	B	701	3	22,29,29	1.11	3 (13%)	28,45,45	1.55	4 (14%)
4	DGT	B	703	3	25,33,33	1.53	4 (16%)	29,52,52	2.28	5 (17%)
4	DGT	B	704	3	25,33,33	1.47	4 (16%)	29,52,52	2.48	9 (31%)
4	DGT	B	705	3	25,33,33	1.30	3 (12%)	29,52,52	2.09	6 (20%)
4	DGT	C	701	3	25,33,33	1.16	3 (12%)	29,52,52	2.40	9 (31%)
2	DCP	C	703	3	22,29,29	0.97	1 (4%)	28,45,45	1.07	2 (7%)
4	DGT	D	702	3	25,33,33	1.10	2 (8%)	29,52,52	1.99	7 (24%)
2	DCP	D	703	3	22,29,29	1.29	1 (4%)	28,45,45	1.32	2 (7%)
4	DGT	D	705	3	25,33,33	1.08	2 (8%)	29,52,52	1.95	6 (20%)

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	DCP	A	701	3	-	0/18/34/34	0/2/2/2
4	DGT	A	703	3	-	0/18/34/34	0/3/3/3
4	DGT	A	704	3	-	0/18/34/34	0/3/3/3
2	DCP	B	701	3	-	0/18/34/34	0/2/2/2
4	DGT	B	703	3	-	0/18/34/34	0/3/3/3
4	DGT	B	704	3	-	0/18/34/34	0/3/3/3
4	DGT	B	705	3	-	0/18/34/34	0/3/3/3
4	DGT	C	701	3	-	0/18/34/34	0/3/3/3
2	DCP	C	703	3	-	0/18/34/34	0/2/2/2
4	DGT	D	702	3	-	0/18/34/34	0/3/3/3
2	DCP	D	703	3	-	0/18/34/34	0/2/2/2
4	DGT	D	705	3	-	0/18/34/34	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	DCP	C2-N3	-3.46	1.31	1.38
4	D	705	DGT	PB-O1B	-2.86	1.42	1.55
4	B	704	DGT	PB-O1B	-2.52	1.44	1.55
4	B	703	DGT	PA-O2A	-2.34	1.42	1.51
4	D	702	DGT	PG-O2G	-2.32	1.46	1.54
4	B	705	DGT	PG-O2G	-2.28	1.46	1.54
4	D	705	DGT	PG-O2G	-2.21	1.47	1.54
4	D	702	DGT	PB-O2B	-2.09	1.43	1.51
2	C	703	DCP	O4'-C4'	-2.03	1.40	1.45
4	C	701	DGT	PA-O1A	-2.02	1.46	1.55
4	B	704	DGT	PA-O1A	-2.01	1.46	1.55
4	B	703	DGT	PB-O1B	-2.00	1.46	1.55
2	B	701	DCP	PA-O5'	2.03	1.67	1.59
2	B	701	DCP	O3'-C3'	2.04	1.47	1.43
2	B	701	DCP	C6-C5	2.08	1.42	1.38
4	A	704	DGT	C6-C5	2.17	1.45	1.41
4	B	705	DGT	C8-N7	2.23	1.39	1.34
4	C	701	DGT	C5-C4	2.70	1.46	1.40
4	B	705	DGT	C5-C4	2.88	1.47	1.40
4	A	704	DGT	C5-C4	2.89	1.47	1.40
4	C	701	DGT	C6-C5	2.92	1.47	1.41
4	B	704	DGT	C5-C4	2.98	1.47	1.40
4	A	703	DGT	C6-C5	3.08	1.47	1.41
4	B	703	DGT	C5-C4	3.82	1.49	1.40
4	B	704	DGT	C6-C5	4.44	1.50	1.41
4	B	703	DGT	C6-C5	4.60	1.50	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	DGT	C5-C6-N1	-6.54	114.97	123.52
4	B	704	DGT	C5-C6-N1	-6.53	114.98	123.52
4	B	705	DGT	C5-C6-N1	-5.83	115.90	123.52
4	C	701	DGT	C1'-N9-C4	-5.19	119.48	127.07
4	A	704	DGT	C5-C6-N1	-4.71	117.36	123.52
4	C	701	DGT	C6-C5-C4	-4.27	115.98	120.86
4	C	701	DGT	C5-C6-N1	-4.21	118.01	123.52
4	D	702	DGT	N3-C2-N1	-4.17	121.89	127.56
4	A	703	DGT	C6-C5-C4	-4.14	116.12	120.86
4	D	705	DGT	C5-C6-N1	-4.02	118.27	123.52
4	A	704	DGT	C6-C5-C4	-4.00	116.29	120.86
4	B	705	DGT	C1'-N9-C4	-3.98	121.25	127.07
4	D	702	DGT	C6-C5-C4	-3.97	116.32	120.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	DGT	N3-C2-N1	-3.85	122.31	127.56
4	A	704	DGT	C1'-N9-C4	-3.75	121.59	127.07
4	D	702	DGT	C1'-N9-C4	-3.62	121.79	127.07
4	D	705	DGT	C6-C5-C4	-3.61	116.73	120.86
4	D	702	DGT	C5-C6-N1	-3.49	118.95	123.52
4	B	705	DGT	C6-C5-C4	-3.39	116.99	120.86
4	B	704	DGT	C6-C5-C4	-3.21	117.18	120.86
4	C	701	DGT	N3-C2-N1	-2.89	123.62	127.56
4	B	703	DGT	N3-C2-N1	-2.86	123.67	127.56
4	C	701	DGT	O4'-C1'-N9	-2.86	102.72	107.71
4	D	705	DGT	N3-C2-N1	-2.82	123.72	127.56
4	A	703	DGT	C5-C6-N1	-2.69	120.01	123.52
4	D	702	DGT	O4'-C1'-N9	-2.61	103.16	107.71
4	A	704	DGT	N3-C2-N1	-2.52	124.12	127.56
4	B	703	DGT	C6-C5-C4	-2.43	118.08	120.86
4	B	704	DGT	O1B-PB-O3A	-2.24	95.69	105.27
4	B	704	DGT	O4'-C1'-N9	-2.08	104.08	107.71
4	B	705	DGT	O4'-C1'-N9	-2.05	104.14	107.71
4	B	704	DGT	O1B-PB-O2B	2.17	123.85	112.56
4	D	705	DGT	C2'-C1'-N9	2.30	119.81	114.14
4	A	703	DGT	O1B-PB-O3B	2.30	115.14	105.27
2	B	701	DCP	O2A-PA-O1A	2.33	124.67	112.56
4	D	702	DGT	O2G-PG-O1G	2.47	116.50	107.44
4	A	703	DGT	O2G-PG-O3G	2.48	118.71	110.63
2	D	703	DCP	O3G-PG-O2G	2.48	116.56	107.44
4	C	701	DGT	C2'-C1'-N9	2.50	120.30	114.14
2	C	703	DCP	O3G-PG-O2G	2.56	116.83	107.44
2	A	701	DCP	O3G-PG-O2G	2.57	116.89	107.44
4	C	701	DGT	O2G-PG-O1G	2.61	117.02	107.44
4	C	701	DGT	O1A-PA-O2A	2.62	126.22	112.56
4	A	703	DGT	O2G-PG-O1G	2.73	117.45	107.44
2	B	701	DCP	O3G-PG-O2G	2.76	117.57	107.44
4	B	705	DGT	O2G-PG-O1G	2.81	117.77	107.44
4	B	704	DGT	O2G-PG-O1G	2.87	117.98	107.44
4	B	704	DGT	O2G-PG-O3G	2.95	120.25	110.63
4	A	704	DGT	O1B-PB-O2B	3.15	128.97	112.56
2	A	701	DCP	O4'-C1'-N1	3.22	113.34	107.71
2	C	703	DCP	O4'-C1'-N1	3.31	113.49	107.71
4	B	703	DGT	O2G-PG-O3G	3.42	121.79	110.63
4	A	703	DGT	C6-N1-C2	3.48	119.97	115.88
4	D	705	DGT	O2G-PG-O3G	3.75	122.86	110.63
2	B	701	DCP	O4'-C1'-N1	3.83	114.41	107.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	DCP	C6-C5-C4	4.68	119.27	117.44
2	A	701	DCP	C6-C5-C4	4.69	119.27	117.44
2	D	703	DCP	O4'-C1'-N1	4.83	116.15	107.71
4	D	702	DGT	C6-N1-C2	4.93	121.66	115.88
4	D	705	DGT	C6-N1-C2	5.24	122.03	115.88
4	B	705	DGT	C6-N1-C2	5.73	122.60	115.88
4	A	704	DGT	C6-N1-C2	5.82	122.70	115.88
4	C	701	DGT	C6-N1-C2	6.42	123.40	115.88
4	B	704	DGT	C6-N1-C2	7.76	124.97	115.88
4	B	703	DGT	C6-N1-C2	7.95	125.20	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	DCP	1	0
2	B	701	DCP	5	0
2	D	703	DCP	1	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, 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	481/514 (93%)	0.00	27 (5%)	28 27	30, 55, 92, 132	0
1	B	481/514 (93%)	0.01	21 (4%)	38 37	30, 55, 88, 121	0
1	C	481/514 (93%)	-0.08	16 (3%)	50 49	33, 58, 88, 117	0
1	D	481/514 (93%)	-0.13	10 (2%)	67 65	27, 47, 80, 115	0
All	All	1924/2056 (93%)	-0.05	74 (3%)	44 43	27, 53, 88, 132	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	VAL	6.3
1	C	488	LEU	5.6
1	B	488	LEU	5.2
1	C	490	ASP	5.2
1	A	487	VAL	4.9
1	A	488	LEU	4.8
1	B	490	ASP	4.6
1	A	489	LEU	4.5
1	D	466	ILE	4.5
1	B	489	LEU	4.5
1	C	596	LYS	4.4
1	A	490	ASP	4.3
1	B	492	LYS	4.2
1	A	403	GLY	4.2
1	D	465	GLN	4.2
1	B	599	ASN	4.1
1	A	486	LYS	4.0
1	C	599	ASN	3.8
1	A	491	VAL	3.7
1	A	599	ASN	3.7
1	A	466	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	481	ALA	3.6
1	C	590	LEU	3.6
1	B	491	VAL	3.4
1	A	406	LYS	3.3
1	B	560	LYS	3.2
1	D	478	LYS	3.2
1	A	485	PRO	3.1
1	D	491	VAL	3.1
1	A	467	LYS	3.1
1	B	486	LYS	3.1
1	C	405	LYS	3.0
1	C	403	GLY	3.0
1	B	284	LEU	3.0
1	A	483	ALA	2.9
1	A	589	PRO	2.9
1	B	496	GLU	2.8
1	A	345	ASN	2.8
1	B	590	LEU	2.8
1	D	490	ASP	2.8
1	C	471	GLU	2.7
1	C	592	THR	2.7
1	C	404	GLY	2.6
1	D	284	LEU	2.6
1	A	593	PRO	2.5
1	B	113	ASP	2.5
1	C	408	ARG	2.5
1	A	347	LEU	2.5
1	A	492	LYS	2.4
1	A	404	GLY	2.4
1	B	494	LYS	2.4
1	B	559	ARG	2.3
1	B	594	GLN	2.3
1	D	467	LYS	2.3
1	C	492	LYS	2.3
1	A	190	GLN	2.3
1	B	277	GLU	2.3
1	C	594	GLN	2.3
1	C	470	ARG	2.2
1	A	594	GLN	2.2
1	B	556	LYS	2.2
1	C	407	TYR	2.2
1	A	484	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	478	LYS	2.2
1	B	495	ALA	2.2
1	B	563	TYR	2.1
1	A	465	GLN	2.1
1	D	277	GLU	2.1
1	A	478	LYS	2.1
1	A	568	TYR	2.1
1	D	154	TYR	2.1
1	A	585	ASP	2.0
1	C	559	ARG	2.0
1	D	156	VAL	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
4	DGT	B	705	31/31	0.99	0.18	0.06	30,34,40,41	0
4	DGT	D	705	31/31	0.99	0.16	-0.16	28,33,39,43	0
4	DGT	B	704	31/31	0.98	0.14	-0.29	37,41,46,49	0
4	DGT	D	702	31/31	0.99	0.13	-0.39	32,37,41,44	0
4	DGT	A	704	31/31	0.99	0.14	-0.42	31,36,43,46	0
4	DGT	C	701	31/31	0.98	0.12	-0.45	30,35,42,44	0
4	DGT	A	703	31/31	0.98	0.14	-0.50	33,36,42,46	0
2	DCP	D	703	28/28	0.94	0.12	-0.69	32,41,69,76	0
4	DGT	B	703	31/31	0.99	0.15	-0.74	35,39,45,50	0
2	DCP	C	703	28/28	0.95	0.09	-0.83	41,55,80,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DCP	A	701	28/28	0.94	0.09	-1.14	39,51,84,89	0
2	DCP	B	701	28/28	0.95	0.09	-1.58	32,49,77,78	0
3	MG	D	701	1/1	0.94	0.12	-	38,38,38,38	0
3	MG	D	704	1/1	0.76	0.10	-	81,81,81,81	0
3	MG	A	706	1/1	0.96	0.10	-	33,33,33,33	0
3	MG	C	704	1/1	0.95	0.07	-	85,85,85,85	0
3	MG	A	702	1/1	0.95	0.10	-	112,112,112,112	0
3	MG	B	702	1/1	0.94	0.10	-	80,80,80,80	0
3	MG	A	705	1/1	0.95	0.08	-	43,43,43,43	0
3	MG	C	702	1/1	0.98	0.10	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.