Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:32 AM GMT

PDB ID	:	3IRH
Title	:	Structure of an Enterococcus Faecalis HD-domain protein complexed with dGTP and dATP
Authors	:	Vorontsov, I.I.; Minasov, G.; Shuvalova, L.; Brunzelle, J.S.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-08-24
Resolution	:	2.40 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:

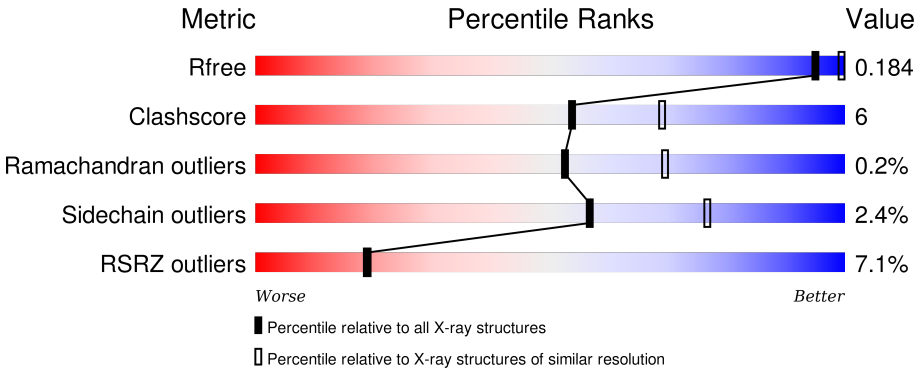
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	480	6% 79% 14% • 6%
1	B	480	8% 76% 16% • 7%
1	C	480	6% 81% 14% 5%
1	D	480	6% 75% 15% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTP	D	459	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15380 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 HD domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	3	0
			3735	2392	637	694	12			
1	B	445	Total	C	N	O	S	0	5	0
			3694	2362	631	688	13			
1	C	454	Total	C	N	O	S	0	2	0
			3757	2406	640	698	13			
1	D	434	Total	C	N	O	S	0	5	0
			3597	2302	611	672	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q836G9
A	-22	HIS	-	expression tag	UNP Q836G9
A	-21	HIS	-	expression tag	UNP Q836G9
A	-20	HIS	-	expression tag	UNP Q836G9
A	-19	HIS	-	expression tag	UNP Q836G9
A	-18	HIS	-	expression tag	UNP Q836G9
A	-17	HIS	-	expression tag	UNP Q836G9
A	-16	SER	-	expression tag	UNP Q836G9
A	-15	SER	-	expression tag	UNP Q836G9
A	-14	GLY	-	expression tag	UNP Q836G9
A	-13	VAL	-	expression tag	UNP Q836G9
A	-12	ASP	-	expression tag	UNP Q836G9
A	-11	LEU	-	expression tag	UNP Q836G9
A	-10	GLY	-	expression tag	UNP Q836G9
A	-9	THR	-	expression tag	UNP Q836G9
A	-8	GLU	-	expression tag	UNP Q836G9
A	-7	ASN	-	expression tag	UNP Q836G9
A	-6	LEU	-	expression tag	UNP Q836G9
A	-5	TYR	-	expression tag	UNP Q836G9
A	-4	PHE	-	expression tag	UNP Q836G9
A	-3	GLN	-	expression tag	UNP Q836G9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q836G9
A	-1	ASN	-	expression tag	UNP Q836G9
A	0	ALA	-	expression tag	UNP Q836G9
B	-23	MET	-	expression tag	UNP Q836G9
B	-22	HIS	-	expression tag	UNP Q836G9
B	-21	HIS	-	expression tag	UNP Q836G9
B	-20	HIS	-	expression tag	UNP Q836G9
B	-19	HIS	-	expression tag	UNP Q836G9
B	-18	HIS	-	expression tag	UNP Q836G9
B	-17	HIS	-	expression tag	UNP Q836G9
B	-16	SER	-	expression tag	UNP Q836G9
B	-15	SER	-	expression tag	UNP Q836G9
B	-14	GLY	-	expression tag	UNP Q836G9
B	-13	VAL	-	expression tag	UNP Q836G9
B	-12	ASP	-	expression tag	UNP Q836G9
B	-11	LEU	-	expression tag	UNP Q836G9
B	-10	GLY	-	expression tag	UNP Q836G9
B	-9	THR	-	expression tag	UNP Q836G9
B	-8	GLU	-	expression tag	UNP Q836G9
B	-7	ASN	-	expression tag	UNP Q836G9
B	-6	LEU	-	expression tag	UNP Q836G9
B	-5	TYR	-	expression tag	UNP Q836G9
B	-4	PHE	-	expression tag	UNP Q836G9
B	-3	GLN	-	expression tag	UNP Q836G9
B	-2	SER	-	expression tag	UNP Q836G9
B	-1	ASN	-	expression tag	UNP Q836G9
B	0	ALA	-	expression tag	UNP Q836G9
C	-23	MET	-	expression tag	UNP Q836G9
C	-22	HIS	-	expression tag	UNP Q836G9
C	-21	HIS	-	expression tag	UNP Q836G9
C	-20	HIS	-	expression tag	UNP Q836G9
C	-19	HIS	-	expression tag	UNP Q836G9
C	-18	HIS	-	expression tag	UNP Q836G9
C	-17	HIS	-	expression tag	UNP Q836G9
C	-16	SER	-	expression tag	UNP Q836G9
C	-15	SER	-	expression tag	UNP Q836G9
C	-14	GLY	-	expression tag	UNP Q836G9
C	-13	VAL	-	expression tag	UNP Q836G9
C	-12	ASP	-	expression tag	UNP Q836G9
C	-11	LEU	-	expression tag	UNP Q836G9
C	-10	GLY	-	expression tag	UNP Q836G9
C	-9	THR	-	expression tag	UNP Q836G9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q836G9
C	-7	ASN	-	expression tag	UNP Q836G9
C	-6	LEU	-	expression tag	UNP Q836G9
C	-5	TYR	-	expression tag	UNP Q836G9
C	-4	PHE	-	expression tag	UNP Q836G9
C	-3	GLN	-	expression tag	UNP Q836G9
C	-2	SER	-	expression tag	UNP Q836G9
C	-1	ASN	-	expression tag	UNP Q836G9
C	0	ALA	-	expression tag	UNP Q836G9
D	-23	MET	-	expression tag	UNP Q836G9
D	-22	HIS	-	expression tag	UNP Q836G9
D	-21	HIS	-	expression tag	UNP Q836G9
D	-20	HIS	-	expression tag	UNP Q836G9
D	-19	HIS	-	expression tag	UNP Q836G9
D	-18	HIS	-	expression tag	UNP Q836G9
D	-17	HIS	-	expression tag	UNP Q836G9
D	-16	SER	-	expression tag	UNP Q836G9
D	-15	SER	-	expression tag	UNP Q836G9
D	-14	GLY	-	expression tag	UNP Q836G9
D	-13	VAL	-	expression tag	UNP Q836G9
D	-12	ASP	-	expression tag	UNP Q836G9
D	-11	LEU	-	expression tag	UNP Q836G9
D	-10	GLY	-	expression tag	UNP Q836G9
D	-9	THR	-	expression tag	UNP Q836G9
D	-8	GLU	-	expression tag	UNP Q836G9
D	-7	ASN	-	expression tag	UNP Q836G9
D	-6	LEU	-	expression tag	UNP Q836G9
D	-5	TYR	-	expression tag	UNP Q836G9
D	-4	PHE	-	expression tag	UNP Q836G9
D	-3	GLN	-	expression tag	UNP Q836G9
D	-2	SER	-	expression tag	UNP Q836G9
D	-1	ASN	-	expression tag	UNP Q836G9
D	0	ALA	-	expression tag	UNP Q836G9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

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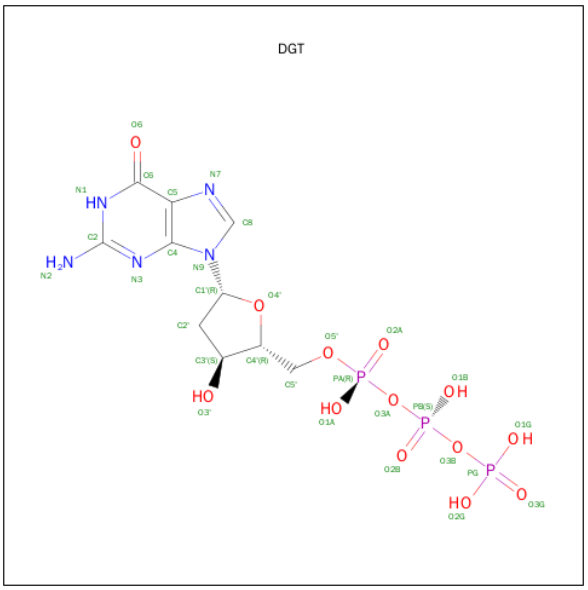
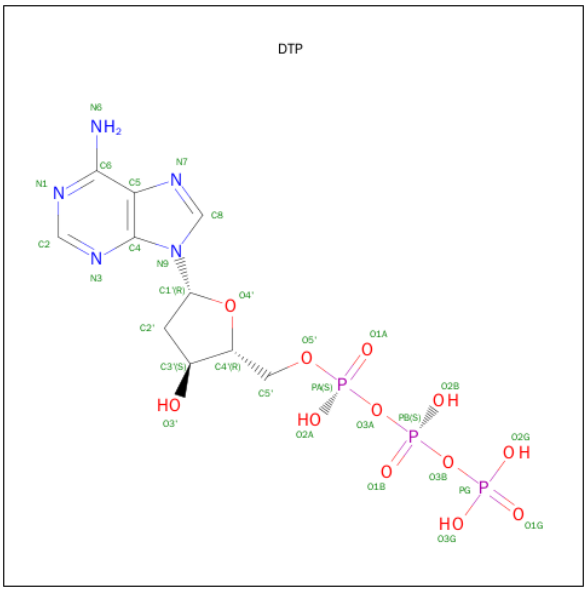
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Ca 1 1	0	0

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

- 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	B	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 water.

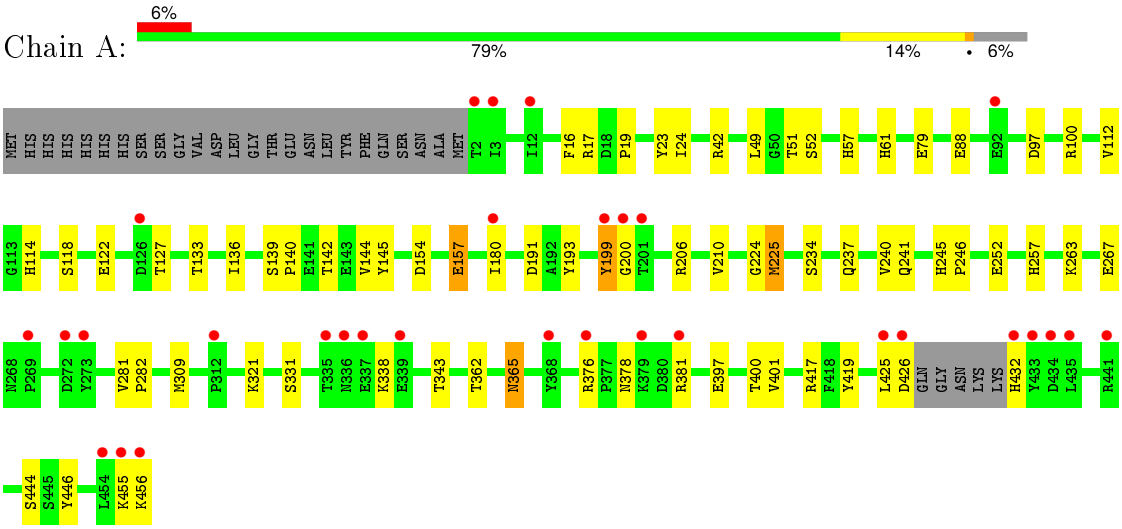
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		
5	B	111	Total	O	0	0
			111	111		
5	C	100	Total	O	0	0
			100	100		
5	D	104	Total	O	0	0
			104	104		

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.

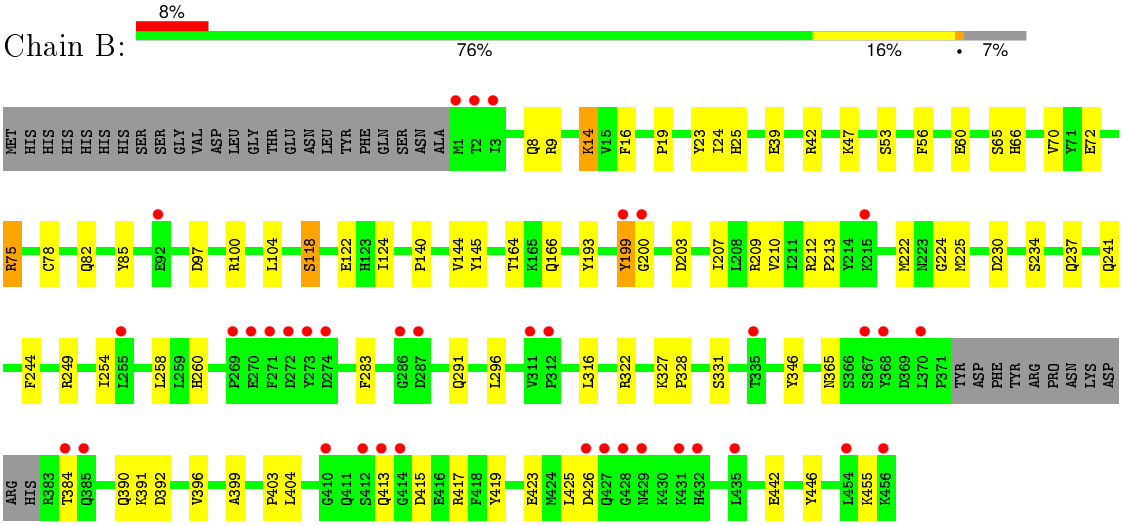
- Molecule 1: HD domain protein

Chain A:



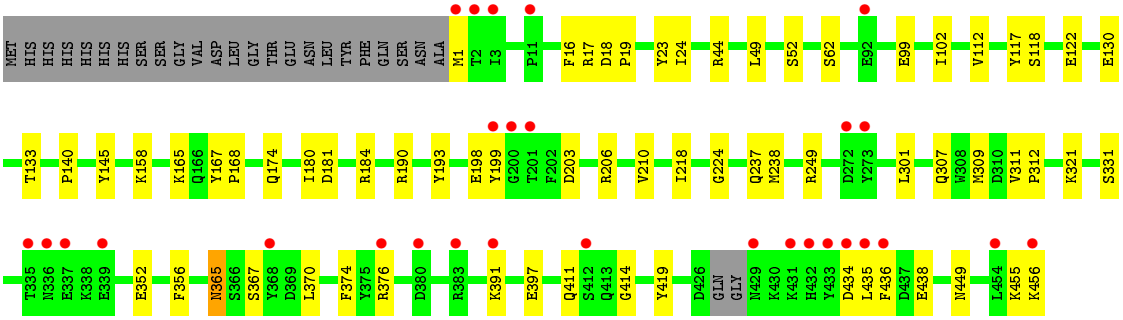
- Molecule 1: HD domain protein

Chain B:

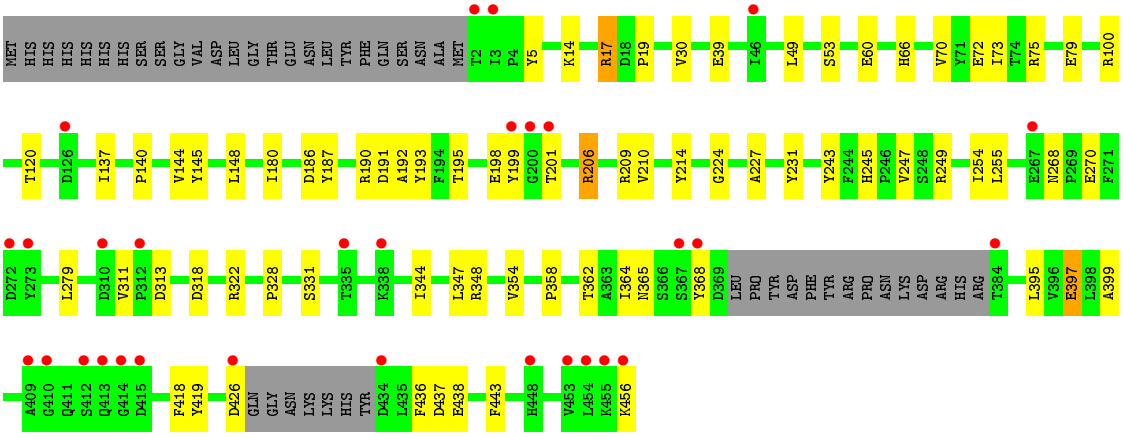


- Molecule 1: HD domain protein

Chain C:



- Molecule 1: HD domain protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.25Å 188.66Å 67.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.40) 99.2 (29.85-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.244 0.187 , 0.184	Depositor DCC
R_{free} test set	3759 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 75107 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15380	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.99% 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: CA, DTP, DGT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/3828	0.57	0/5183
1	B	0.49	0/3782	0.60	0/5118
1	C	0.48	0/3850	0.58	0/5211
1	D	0.48	0/3684	0.60	1/4985 (0.0%)
All	All	0.48	0/15144	0.59	1/20497 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	17	ARG	NE-CZ-NH2	-5.01	117.79	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	3735	0	3640	47	0
1	B	3694	0	3617	53	0
1	C	3757	0	3670	47	0
1	D	3597	0	3518	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	2	0
4	B	30	0	12	0	0
4	D	30	0	12	3	0
5	A	94	0	0	1	0
5	B	111	0	0	0	0
5	C	100	0	0	1	0
5	D	104	0	0	2	0
All	All	15380	0	14517	191	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 6.

All (191) 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:198:GLU:HG2	1:D:201:THR:HG23	1.21	1.20
1:B:237:GLN:HG3	5:C:461:HOH:O	1.71	0.90
1:B:249:ARG:HD2	1:B:365:ASN:HD21	1.37	0.89
1:D:198:GLU:HG2	1:D:201:THR:CG2	2.02	0.89
1:A:309:MET:HE3	1:A:321:LYS:HA	1.56	0.85
1:D:249:ARG:HD2	1:D:365:ASN:HD21	1.45	0.81
1:D:210:VAL:HG11	1:D:224:GLY:HA3	1.61	0.81
1:B:423:GLU:HA	1:B:426:ASP:HB2	1.62	0.81
1:A:365:ASN:HB2	1:A:419:TYR:HE1	1.45	0.79
1:D:198:GLU:CG	1:D:201:THR:HG23	2.11	0.76
1:B:140:PRO:HA	1:B:145:TYR:CD2	2.22	0.75
1:C:112:VAL:HG12	1:C:133:THR:HG23	1.68	0.74
1:A:309:MET:CE	1:A:321:LYS:HA	2.19	0.73
1:D:192:ALA:HB1	1:D:198:GLU:HA	1.70	0.73
1:C:203:ASP:OD2	1:C:206:ARG:HG3	1.89	0.72
1:B:210:VAL:HG11	1:B:224:GLY:HA3	1.70	0.72
1:C:181:ASP:OD2	1:C:184:ARG:HG3	1.89	0.71
1:B:249:ARG:HH11	1:B:365:ASN:ND2	1.88	0.71
1:C:62:SER:N	1:D:60:GLU:OE1	2.24	0.71
1:C:374:PHE:HB2	1:C:376:ARG:HH21	1.56	0.70
1:D:249:ARG:HD2	1:D:365:ASN:ND2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:HB3	1:B:104:LEU:HD21	1.75	0.69
1:B:222:MET:HE1	1:B:396:VAL:HG11	1.75	0.68
1:D:192:ALA:HB1	1:D:198:GLU:HG3	1.76	0.67
1:D:186:ASP:OD2	1:D:190:ARG:NH1	2.28	0.67
1:D:348:ARG:HE	1:D:362:THR:HG21	1.60	0.66
1:C:18:ASP:OD1	1:C:190:ARG:NH2	2.28	0.66
1:A:446:TYR:CE2	1:A:455:LYS:HB2	2.32	0.65
1:B:423:GLU:HA	1:B:426:ASP:CB	2.27	0.64
1:A:17:ARG:HE	1:C:206:ARG:NH1	1.95	0.64
1:D:79[A]:GLU:HG2	1:D:100[A]:ARG:NH2	2.13	0.64
1:A:210:VAL:HG11	1:A:224:GLY:HA3	1.80	0.63
1:C:17:ARG:HH22	1:D:199:TYR:HE1	1.46	0.63
1:A:199:TYR:HB3	1:A:237:GLN:HB3	1.80	0.63
1:B:39:GLU:HG2	1:B:144:VAL:HG23	1.80	0.63
1:B:203:ASP:OD2	1:D:17:ARG:NH2	2.27	0.63
1:A:240:VAL:HG23	1:A:241:GLN:HG3	1.80	0.62
1:C:140:PRO:HA	1:C:145:TYR:CD2	2.34	0.62
1:A:23:TYR:HE1	1:C:206:ARG:HG2	1.64	0.61
1:B:392:ASP:H	1:C:449:ASN:HD21	1.48	0.61
1:A:365:ASN:HB2	1:A:419:TYR:CE1	2.32	0.60
1:B:403:PRO:HD2	1:C:411:GLN:HE22	1.67	0.60
1:A:42[B]:ARG:NH2	1:A:112:VAL:O	2.32	0.58
1:C:249:ARG:HD3	1:C:370:LEU:HD11	1.85	0.58
1:B:222:MET:CE	1:B:396:VAL:HG11	2.33	0.57
1:D:397:GLU:HG3	1:D:399:ALA:H	1.69	0.57
1:C:365:ASN:C	1:C:365:ASN:HD22	2.08	0.57
1:D:322:ARG:NH2	5:D:479:HOH:O	2.29	0.57
1:C:16:PHE:HB2	1:C:24:ILE:HB	1.88	0.56
4:D:459:DTP:H5'1	4:D:459:DTP:H8	1.88	0.56
1:A:140:PRO:HA	1:A:145:TYR:CD2	2.40	0.56
1:A:16:PHE:HB2	1:A:24:ILE:HB	1.88	0.56
1:D:368:TYR:CE1	4:D:459:DTP:H2'2	2.41	0.55
1:B:249:ARG:HH11	1:B:365:ASN:HD21	1.53	0.55
1:D:72:GLU:OE1	1:D:75:ARG:NH1	2.39	0.55
1:A:122:GLU:HG2	1:A:127:THR:HG22	1.88	0.55
1:A:263:LYS:O	1:A:267:GLU:HG2	2.07	0.54
1:D:331:SER:HB3	1:D:419:TYR:CE2	2.42	0.54
1:D:19:PRO:HB2	1:D:193:TYR:CE2	2.43	0.54
1:D:140:PRO:HA	1:D:145:TYR:CD2	2.43	0.54
1:B:19:PRO:HB2	1:B:193:TYR:CE2	2.44	0.53
1:B:47:LYS:HD3	1:B:60:GLU:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:TYR:CE2	1:D:30:VAL:HG22	2.43	0.53
1:A:23:TYR:CE1	1:C:206:ARG:HG2	2.44	0.53
1:C:210:VAL:HG11	1:C:224:GLY:HA3	1.91	0.53
1:A:343:THR:OG1	1:A:456:LYS:OXT	2.23	0.53
1:D:268:ASN:OD1	1:D:270:GLU:HG2	2.08	0.53
1:D:311:VAL:HG12	1:D:313:ASP:H	1.74	0.53
1:D:254:ILE:CD1	1:D:328:PRO:HA	2.40	0.52
1:D:186:ASP:OD1	1:D:190:ARG:NH1	2.42	0.52
1:D:79[A]:GLU:HG2	1:D:100[A]:ARG:HH22	1.74	0.51
1:C:455:LYS:O	1:C:456:LYS:C	2.48	0.51
1:A:142:THR:HG22	1:A:145:TYR:H	1.74	0.51
1:B:322:ARG:HG2	1:B:327:LYS:HB2	1.93	0.51
1:C:331:SER:HB3	1:C:419:TYR:CE2	2.46	0.50
1:B:39:GLU:HG2	1:B:144:VAL:CG2	2.42	0.50
1:B:230:ASP:OD1	1:C:237:GLN:CD	2.50	0.50
1:D:362:THR:CG2	1:D:418:PHE:CE1	2.95	0.50
1:C:44:ARG:NH1	1:D:53:SER:O	2.44	0.50
1:D:247:VAL:HG21	3:D:458:DGT:H5'	1.93	0.49
1:C:49:LEU:HB3	1:C:52:SER:HB2	1.94	0.49
1:C:307:GLN:HE22	1:D:279:LEU:HD21	1.77	0.49
1:A:51:THR:OG1	1:A:252[B]:GLU:HG3	2.11	0.49
1:D:243:TYR:CD2	4:D:459:DTP:H1'	2.48	0.49
1:B:212[A]:ARG:HG2	1:B:213:PRO:HD2	1.92	0.49
1:C:367:SER:OG	1:C:414:GLY:HA2	2.11	0.49
1:A:331:SER:OG	1:A:417:ARG:NH1	2.45	0.49
1:D:348:ARG:HH21	1:D:362:THR:HG22	1.78	0.49
1:C:102:ILE:HD11	1:C:158:LYS:HB3	1.94	0.49
1:D:254:ILE:HD11	1:D:328:PRO:HA	1.95	0.48
1:D:245:HIS:HD2	1:D:247:VAL:H	1.61	0.48
1:A:397:GLU:O	1:A:400:THR:HB	2.13	0.48
1:C:309:MET:HE3	1:C:321:LYS:HE2	1.94	0.48
1:D:120:THR:HG21	1:D:255:LEU:HG	1.95	0.48
1:D:75:ARG:NH2	1:D:79[A]:GLU:OE2	2.46	0.48
1:A:200:GLY:HA2	1:A:234:SER:HB3	1.96	0.48
1:B:392:ASP:N	1:C:449:ASN:HD21	2.12	0.48
1:B:249:ARG:NH2	1:B:415:ASP:OD2	2.45	0.47
1:D:348:ARG:HE	1:D:362:THR:CG2	2.25	0.47
1:D:362:THR:HA	1:D:419:TYR:O	2.14	0.47
1:B:283:PHE:CE2	1:B:296:LEU:HD11	2.49	0.47
1:A:61:HIS:HE1	1:A:191:ASP:OD1	1.97	0.47
1:D:362:THR:HG23	1:D:418:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ALA:CB	1:D:198:GLU:HG3	2.43	0.47
1:A:97:ASP:OD2	1:A:100:ARG:NH1	2.47	0.47
1:C:19:PRO:HB2	1:C:193:TYR:CE2	2.50	0.47
1:C:331:SER:HB3	1:C:419:TYR:CD2	2.50	0.47
1:B:124:ILE:HD12	1:B:260:HIS:HB2	1.97	0.47
1:A:112:VAL:HG12	1:A:133:THR:HG23	1.95	0.47
1:A:365:ASN:CB	1:A:419:TYR:HE1	2.22	0.47
1:B:25:HIS:HD2	1:B:72:GLU:OE2	1.99	0.46
1:B:75:ARG:HB3	1:B:104:LEU:CD2	2.44	0.46
1:D:39:GLU:HG2	1:D:144:VAL:HG23	1.96	0.46
1:D:186:ASP:CG	1:D:190:ARG:NH1	2.69	0.46
3:A:458:DGT:O2B	1:B:14:LYS:NZ	2.48	0.46
1:D:249:ARG:HH11	1:D:365:ASN:ND2	2.14	0.46
1:A:365:ASN:HD22	1:A:365:ASN:HA	1.56	0.46
1:A:154:ASP:O	1:A:157:GLU:HG3	2.15	0.46
1:A:79:GLU:OE2	1:A:100:ARG:NH2	2.48	0.46
1:C:435:LEU:HA	1:C:438:GLU:HB2	1.98	0.46
1:D:331:SER:HB3	1:D:419:TYR:CD2	2.50	0.46
1:C:99:GLU:O	1:C:102:ILE:HG22	2.16	0.45
1:B:331:SER:HB3	1:B:419:TYR:CE2	2.51	0.45
1:A:142:THR:CG2	1:A:144:VAL:HB	2.46	0.45
1:B:85:TYR:OH	1:B:212[B]:ARG:CZ	2.65	0.45
1:D:214:TYR:CE1	1:D:395:LEU:HD11	2.52	0.45
1:B:346:TYR:OH	1:B:442:GLU:OE2	2.21	0.45
1:A:19:PRO:HB2	1:A:193:TYR:CE2	2.52	0.45
1:A:61:HIS:H	1:A:61:HIS:CD2	2.33	0.44
1:B:200:GLY:HA2	1:B:234:SER:HB3	1.98	0.44
1:A:118:SER:O	1:A:122:GLU:HG3	2.17	0.44
1:B:254:ILE:CD1	1:B:328:PRO:HA	2.48	0.44
1:B:78:CYS:HB3	1:B:100:ARG:HD2	2.00	0.44
1:D:331:SER:HA	1:D:418:PHE:O	2.18	0.44
1:B:66:HIS:O	1:B:70:VAL:HG23	2.18	0.44
1:D:358:PRO:O	1:D:362:THR:HB	2.18	0.43
1:B:82:GLN:OE1	1:B:97:ASP:HB2	2.17	0.43
1:B:16:PHE:HB2	1:B:24:ILE:HB	2.00	0.43
1:D:137:ILE:HG23	1:D:148:LEU:CD1	2.48	0.43
1:B:53:SER:HA	1:B:56:PHE:O	2.19	0.43
1:D:180:ILE:HG12	1:D:231:TYR:CE2	2.53	0.43
1:C:118:SER:O	1:C:122:GLU:HG3	2.18	0.43
1:A:206:ARG:HG3	1:C:23:TYR:HE1	1.83	0.43
1:C:434:ASP:C	1:C:436:PHE:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LYS:HB2	1:C:449:ASN:HD22	1.83	0.43
1:C:44:ARG:NH2	3:D:458:DGT:N7	2.67	0.43
1:D:347:LEU:HD22	1:D:443:PHE:CD1	2.54	0.43
1:D:49:LEU:HA	1:D:49:LEU:HD23	1.77	0.43
1:A:57:HIS:HD2	1:B:65:SER:HB3	1.84	0.43
1:B:384:THR:HG21	1:B:399:ALA:HB2	2.01	0.43
1:B:118:SER:O	1:B:122:GLU:HG3	2.19	0.43
1:D:100[B]:ARG:NH2	5:D:461:HOH:O	2.23	0.42
1:D:245:HIS:CD2	1:D:247:VAL:H	2.35	0.42
1:C:352:GLU:HA	1:C:356:PHE:O	2.19	0.42
1:D:344:ILE:HD13	1:D:364:ILE:HD11	2.01	0.42
1:A:17:ARG:NE	1:C:206:ARG:NH1	2.65	0.42
1:D:354:VAL:O	1:D:354:VAL:CG1	2.68	0.42
1:C:311:VAL:HA	1:C:312:PRO:HD3	1.92	0.42
1:D:318:ASP:O	1:D:322:ARG:HG3	2.19	0.42
1:B:164:THR:CB	1:B:166:GLN:HE21	2.32	0.42
1:A:17:ARG:HG2	1:C:206:ARG:HH22	1.83	0.42
1:B:199:TYR:HD1	1:B:241:GLN:HE22	1.68	0.42
1:A:49:LEU:HB3	1:A:52:SER:HB2	2.02	0.42
1:D:73:ILE:HD12	1:D:186:ASP:HB2	2.02	0.41
1:B:392:ASP:H	1:C:449:ASN:ND2	2.14	0.41
1:C:199:TYR:HB2	1:C:238:MET:SD	2.60	0.41
1:B:244:PHE:CE2	1:B:413:GLN:HB2	2.55	0.41
1:A:136:ILE:O	1:A:142:THR:HG21	2.20	0.41
1:B:258:LEU:HD12	1:B:316:LEU:HD12	2.03	0.41
1:B:404:LEU:HD12	1:C:411:GLN:HG2	2.01	0.41
1:C:174:GLN:NE2	1:C:218:ILE:H	2.19	0.41
1:A:378:ASN:HB3	1:A:381:ARG:HB2	2.02	0.41
1:B:331:SER:OG	1:B:417:ARG:HD3	2.20	0.41
1:A:88:GLU:HG3	5:A:537:HOH:O	2.21	0.41
1:C:117:TYR:HD1	1:C:301:LEU:HD12	1.86	0.41
1:B:423:GLU:CA	1:B:426:ASP:HB2	2.42	0.41
1:D:348:ARG:NE	1:D:362:THR:HG21	2.29	0.41
1:A:139:SER:HA	1:A:140:PRO:HD3	1.93	0.41
1:A:245:HIS:HA	1:A:246:PRO:HD3	1.87	0.41
1:B:446:TYR:CE2	1:B:455:LYS:HB2	2.55	0.41
1:D:206:ARG:HE	1:D:227:ALA:HB2	1.86	0.41
1:A:257:HIS:HE1	1:A:362:THR:O	2.04	0.40
1:A:114:HIS:HD2	1:A:118:SER:OG	2.05	0.40
1:D:66:HIS:O	1:D:70:VAL:HG23	2.21	0.40
1:A:281:VAL:N	1:A:282:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ASP:C	1:C:436:PHE:N	2.75	0.40
1:B:209:ARG:HA	1:B:209:ARG:HD3	1.86	0.40
1:A:225:MET:O	1:A:225:MET:HG3	2.19	0.40
1:B:23:TYR:OH	1:D:209[B]:ARG:NH2	2.54	0.40
1:D:191:ASP:O	1:D:195:THR:HG23	2.22	0.40
1:C:167:TYR:CD1	1:C:168:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/480 (94%)	428 (95%)	20 (4%)	1 (0%)	52	69
1	B	446/480 (93%)	429 (96%)	16 (4%)	1 (0%)	52	69
1	C	452/480 (94%)	434 (96%)	17 (4%)	1 (0%)	52	69
1	D	433/480 (90%)	418 (96%)	15 (4%)	0	100	100
All	All	1780/1920 (93%)	1709 (96%)	68 (4%)	3 (0%)	52	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	GLN
1	C	180	ILE
1	A	180	ILE

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	407/430 (95%)	396 (97%)	11 (3%)	52 73
1	B	403/430 (94%)	392 (97%)	11 (3%)	52 73
1	C	410/430 (95%)	403 (98%)	7 (2%)	68 85
1	D	393/430 (91%)	384 (98%)	9 (2%)	58 78
All	All	1613/1720 (94%)	1575 (98%)	38 (2%)	57 76

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	GLU
1	A	199	TYR
1	A	225	MET
1	A	338	LYS
1	A	365	ASN
1	A	376	ARG
1	A	401	VAL
1	A	425	LEU
1	A	426	ASP
1	A	432	HIS
1	A	444	SER
1	B	9	ARG
1	B	14	LYS
1	B	42	ARG
1	B	75	ARG
1	B	118	SER
1	B	199	TYR
1	B	207	ILE
1	B	225	MET
1	B	291	GLN
1	B	390	GLN
1	B	425	LEU
1	C	1	MET
1	C	130	GLU
1	C	165	LYS
1	C	198	GLU
1	C	365	ASN
1	C	391	LYS
1	C	397	GLU
1	D	14	LYS

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Mol	Chain	Res	Type
1	D	187	TYR
1	D	206	ARG
1	D	397	GLU
1	D	426	ASP
1	D	436	PHE
1	D	437	ASP
1	D	438	GLU
1	D	456	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	28	HIS
1	A	61	HIS
1	A	114	HIS
1	A	241	GLN
1	A	365	ASN
1	A	448	HIS
1	B	25	HIS
1	B	28	HIS
1	B	114	HIS
1	B	123	HIS
1	B	166	GLN
1	B	241	GLN
1	B	365	ASN
1	B	427	GLN
1	B	449	ASN
1	C	28	HIS
1	C	48	GLN
1	C	114	HIS
1	C	174	GLN
1	C	307	GLN
1	C	365	ASN
1	C	449	ASN
1	D	8	GLN
1	D	25	HIS
1	D	48	GLN
1	D	129	HIS
1	D	179	GLN
1	D	245	HIS
1	D	257	HIS

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Mol	Chain	Res	Type
1	D	365	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	DGT	A	458	-	25,33,33	1.08	2 (8%)	35,52,52	1.55	5 (14%)
3	DGT	B	458	-	25,33,33	1.18	2 (8%)	35,52,52	1.63	6 (17%)
4	DTP	B	459	-	24,32,32	2.75	7 (29%)	32,50,50	2.34	7 (21%)
3	DGT	C	458	-	25,33,33	1.17	2 (8%)	35,52,52	1.78	8 (22%)
3	DGT	D	458	-	25,33,33	1.14	2 (8%)	35,52,52	1.61	5 (14%)
4	DTP	D	459	-	24,32,32	2.71	7 (29%)	32,50,50	2.29	4 (12%)

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
3	DGT	A	458	-	-	0/18/34/34	0/3/3/3
3	DGT	B	458	-	-	0/18/34/34	0/3/3/3
4	DTP	B	459	-	-	0/18/34/34	0/3/3/3
3	DGT	C	458	-	-	0/18/34/34	0/3/3/3
3	DGT	D	458	-	-	0/18/34/34	0/3/3/3
4	DTP	D	459	-	-	0/18/34/34	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	459	DTP	PA-O1A	2.30	1.59	1.51
4	D	459	DTP	PA-O1A	2.36	1.59	1.51
4	B	459	DTP	PB-O1B	2.37	1.59	1.51
4	D	459	DTP	PB-O1B	2.40	1.59	1.51
4	B	459	DTP	PG-O1G	2.50	1.59	1.51
4	D	459	DTP	PG-O1G	2.62	1.59	1.51
3	C	458	DGT	C5-C4	3.05	1.47	1.40
3	A	458	DGT	C5-C4	3.06	1.47	1.40
3	B	458	DGT	C5-C4	3.45	1.48	1.40
3	D	458	DGT	C5-C4	3.48	1.48	1.40
3	A	458	DGT	C6-C5	3.54	1.48	1.41
3	D	458	DGT	C6-C5	3.68	1.48	1.41
3	B	458	DGT	C6-C5	3.77	1.48	1.41
3	C	458	DGT	C6-C5	3.82	1.48	1.41
4	D	459	DTP	PA-O2A	5.56	1.78	1.54
4	D	459	DTP	PB-O2B	5.57	1.78	1.54
4	B	459	DTP	PA-O2A	5.65	1.79	1.54
4	B	459	DTP	PB-O2B	5.68	1.79	1.54
4	D	459	DTP	PG-O3G	6.68	1.78	1.54
4	D	459	DTP	PG-O2G	6.72	1.78	1.54
4	B	459	DTP	PG-O2G	6.79	1.79	1.54
4	B	459	DTP	PG-O3G	6.85	1.79	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	459	DTP	N3-C2-N1	-10.64	120.75	128.89
4	D	459	DTP	N3-C2-N1	-10.63	120.75	128.89
4	D	459	DTP	PA-O3A-PB	-4.08	121.28	132.73
3	C	458	DGT	C6-C5-C4	-3.84	116.30	120.90
3	D	458	DGT	C6-C5-C4	-3.84	116.31	120.90
3	B	458	DGT	C5-C6-N1	-3.80	118.40	123.59
3	C	458	DGT	N3-C2-N1	-3.70	121.81	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	459	DTP	PA-O3A-PB	-3.65	122.47	132.73
3	A	458	DGT	C5-C6-N1	-3.60	118.67	123.59
3	C	458	DGT	C5-C6-N1	-3.53	118.77	123.59
3	A	458	DGT	C6-C5-C4	-3.52	116.69	120.90
3	D	458	DGT	C5-C6-N1	-3.51	118.79	123.59
4	D	459	DTP	PB-O3B-PG	-3.47	121.04	132.67
4	B	459	DTP	PB-O3B-PG	-3.45	121.11	132.67
3	B	458	DGT	C6-C5-C4	-3.41	116.82	120.90
3	C	458	DGT	PB-O3B-PG	-3.33	121.50	132.67
3	B	458	DGT	N3-C2-N1	-3.30	122.42	127.44
3	D	458	DGT	N3-C2-N1	-3.24	122.52	127.44
3	A	458	DGT	N3-C2-N1	-3.14	122.67	127.44
3	D	458	DGT	PB-O3B-PG	-2.62	123.89	132.67
3	C	458	DGT	C4-C5-N7	-2.56	107.12	109.48
3	B	458	DGT	PB-O3B-PG	-2.48	124.35	132.67
3	B	458	DGT	C4-C5-N7	-2.43	107.24	109.48
4	B	459	DTP	C2'-C1'-N9	-2.31	108.54	114.16
3	A	458	DGT	PA-O3A-PB	-2.24	126.43	132.73
3	C	458	DGT	PA-O3A-PB	-2.09	126.86	132.73
4	B	459	DTP	C4-C5-N7	-2.07	107.57	109.48
4	B	459	DTP	C2'-C3'-C4'	2.08	107.09	102.77
4	B	459	DTP	O4'-C1'-N9	2.18	111.49	107.72
3	C	458	DGT	N2-C2-N1	2.22	120.88	117.20
4	D	459	DTP	O4'-C1'-N9	2.33	111.76	107.72
3	A	458	DGT	C6-N1-C2	4.32	121.93	115.94
3	D	458	DGT	C6-N1-C2	4.41	122.05	115.94
3	C	458	DGT	C6-N1-C2	4.43	122.08	115.94
3	B	458	DGT	C6-N1-C2	4.73	122.50	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	458	DGT	1	0
3	D	458	DGT	2	0
4	D	459	DTP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	450/480 (93%)	0.35	31 (6%)	20	19	30, 39, 52, 64	0
1	B	445/480 (92%)	0.46	37 (8%)	14	14	29, 39, 53, 70	4 (0%)
1	C	454/480 (94%)	0.29	29 (6%)	23	23	30, 39, 52, 64	0
1	D	434/480 (90%)	0.37	30 (6%)	20	19	29, 39, 53, 66	2 (0%)
All	All	1783/1920 (92%)	0.37	127 (7%)	19	19	29, 39, 53, 70	6 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	9.4
1	B	199	TYR	7.0
1	C	435	LEU	7.0
1	B	435	LEU	6.4
1	A	432	HIS	6.3
1	D	384	THR	6.3
1	B	273	TYR	5.9
1	C	2	THR	5.8
1	D	414	GLY	5.7
1	B	412	SER	5.4
1	D	199	TYR	5.3
1	A	433	TYR	5.1
1	C	456	LYS	4.9
1	A	434	ASP	4.8
1	C	3	ILE	4.8
1	A	454	LEU	4.8
1	B	200	GLY	4.7
1	B	271	PHE	4.6
1	D	455	LYS	4.6
1	D	2	THR	4.6
1	D	410	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	199	TYR	4.5
1	B	432	HIS	4.5
1	D	368	TYR	4.4
1	D	200	GLY	4.3
1	A	456	LYS	4.3
1	B	272	ASP	4.3
1	B	370	LEU	4.3
1	D	367	SER	4.2
1	B	2	THR	4.1
1	C	429	ASN	4.1
1	B	287	ASP	4.1
1	B	413	GLN	4.0
1	D	413	GLN	4.0
1	A	368	TYR	3.9
1	D	272	ASP	3.9
1	A	273	TYR	3.9
1	C	432	HIS	3.9
1	A	3	ILE	3.8
1	C	201	THR	3.8
1	A	200	GLY	3.8
1	C	431	LYS	3.8
1	B	335	THR	3.7
1	D	273	TYR	3.7
1	C	1	MET	3.7
1	A	435	LEU	3.7
1	B	410	GLY	3.6
1	C	380	ASP	3.6
1	A	2	THR	3.6
1	B	311	VAL	3.5
1	B	456	LYS	3.5
1	C	391	LYS	3.5
1	D	453	VAL	3.5
1	B	429	ASN	3.4
1	C	272	ASP	3.3
1	B	431	LYS	3.2
1	B	426	ASP	3.2
1	D	415	ASP	3.2
1	C	436	PHE	3.2
1	C	11	PRO	3.1
1	D	409	ALA	3.1
1	B	312	PRO	3.0
1	A	441	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLU	3.0
1	A	426	ASP	3.0
1	D	338	LYS	3.0
1	D	454	LEU	3.0
1	C	199	TYR	3.0
1	B	454	LEU	2.9
1	C	337	GLU	2.9
1	B	385	GLN	2.8
1	C	335	THR	2.8
1	C	200	GLY	2.8
1	D	201	THR	2.8
1	B	427	GLN	2.8
1	C	339	GLU	2.8
1	D	267	GLU	2.8
1	D	126	ASP	2.7
1	C	454	LEU	2.7
1	A	269	PRO	2.7
1	A	455	LYS	2.7
1	A	381	ARG	2.7
1	A	376	ARG	2.7
1	D	456	LYS	2.6
1	A	180	ILE	2.6
1	B	3	ILE	2.6
1	C	434	ASP	2.6
1	B	368	TYR	2.6
1	B	215	LYS	2.6
1	C	376	ARG	2.6
1	A	12	ILE	2.6
1	B	274	ASP	2.5
1	C	368	TYR	2.5
1	B	367	SER	2.5
1	A	312	PRO	2.5
1	C	92	GLU	2.4
1	A	336	ASN	2.4
1	C	336	ASN	2.4
1	D	335	THR	2.4
1	B	414	GLY	2.4
1	C	433	TYR	2.4
1	D	434	ASP	2.4
1	B	428	GLY	2.3
1	D	448	HIS	2.3
1	A	335	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	269	PRO	2.3
1	C	383	ARG	2.3
1	A	339	GLU	2.2
1	B	384	THR	2.2
1	D	312	PRO	2.2
1	B	255	LEU	2.2
1	A	126	ASP	2.2
1	C	273	TYR	2.2
1	A	379	LYS	2.1
1	B	270	GLU	2.1
1	D	412	SER	2.1
1	D	426	ASP	2.1
1	D	3	ILE	2.1
1	D	310	ASP	2.1
1	A	337	GLU	2.1
1	C	412	SER	2.1
1	B	286	GLY	2.0
1	B	92	GLU	2.0
1	A	425	LEU	2.0
1	A	272	ASP	2.0
1	D	46	ILE	2.0
1	A	201	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
4	DTP	D	459	30/30	0.65	0.34	2.54	67,68,86,87	30
4	DTP	B	459	30/30	0.74	0.29	2.00	55,58,73,74	30
3	DGT	C	458	31/31	0.95	0.20	1.48	28,34,61,63	0
3	DGT	A	458	31/31	0.95	0.13	-0.56	28,36,67,68	0
3	DGT	B	458	31/31	0.95	0.13	-0.78	33,41,66,68	0
3	DGT	D	458	31/31	0.93	0.13	-1.20	33,44,69,71	0
2	CA	C	457	1/1	0.97	0.06	-3.45	35,35,35,35	0
2	CA	D	457	1/1	0.98	0.06	-5.59	34,34,34,34	0
2	CA	A	457	1/1	0.98	0.05	-7.14	31,31,31,31	0
2	CA	B	457	1/1	0.99	0.04	-10.88	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.