



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:41 AM GMT

PDB ID : 3MR3
Title : Human DNA polymerase eta - DNA ternary complex with the 3'T of a CPD in the active site (TT1)
Authors : Biertumpfel, C.; Zhao, Y.; Ramon-Maiques, S.; Gregory, M.T.; Lee, J.Y.; Yang, W.
Deposited on : 2010-04-28
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

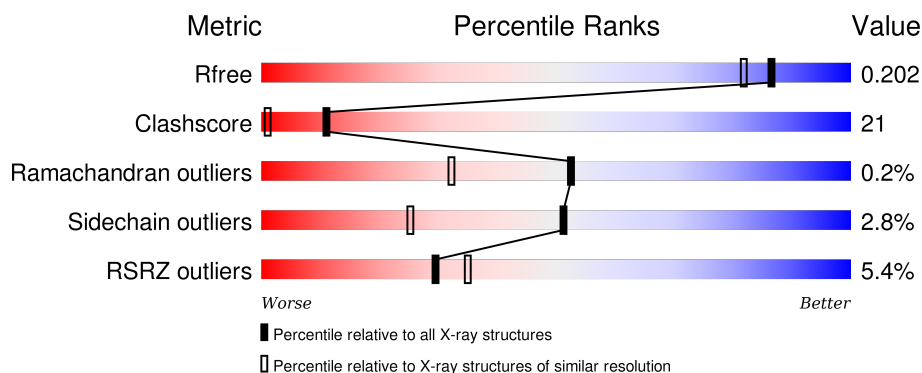
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	435	<div> <div>5%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
2	T	11	<div> <div>82%</div> <div>18%</div> </div>
3	P	9	<div> <div>11%</div> <div>78%</div> <div>11%</div> <div>11%</div> </div>

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	DZ4	A	442	-	-	X	X
6	GOL	A	436	-	-	-	X
6	GOL	A	437	-	-	-	X
6	GOL	A	438	-	-	X	X
6	GOL	A	440	-	-	-	X
6	GOL	A	441	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4528 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 DNA polymerase eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	40	0
			3584	2251	653	653	27			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q9Y253
A	-1	PRO	-	EXPRESSION TAG	UNP Q9Y253
A	0	HIS	-	EXPRESSION TAG	UNP Q9Y253

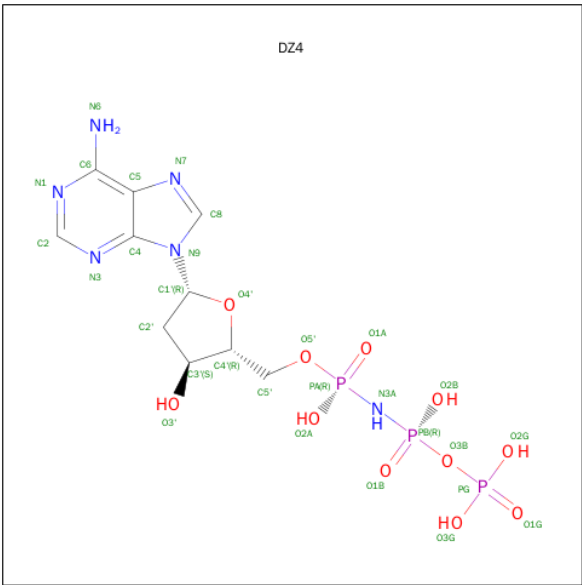
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*(TTD)P*AP*TP*GP*AP*CP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	11	Total	C	N	O	P	0	1	1
			254	126	43	74	11			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*GP*CP*GP*TP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	P	0	0	0
			180	87	33	52	8			

- Molecule 4 is 2'-DEOXY-5'-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)P HOSPHORYL]AMINO}PHOSPHORYL]ADENOSINE (three-letter code: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃).

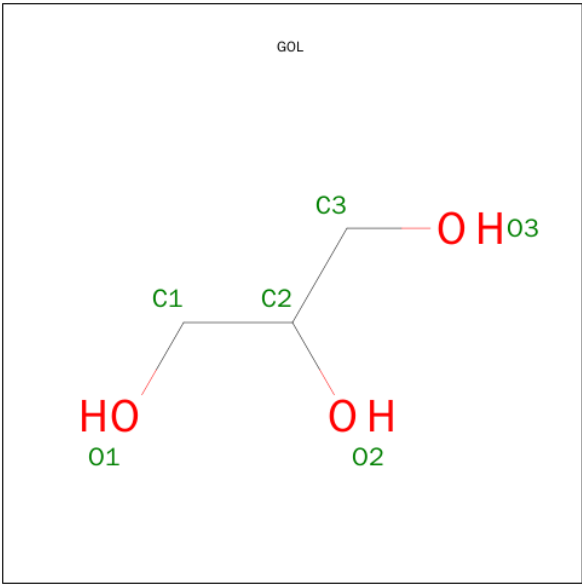


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	A	1	Total	C	N			0	0
			11	6	5				

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0

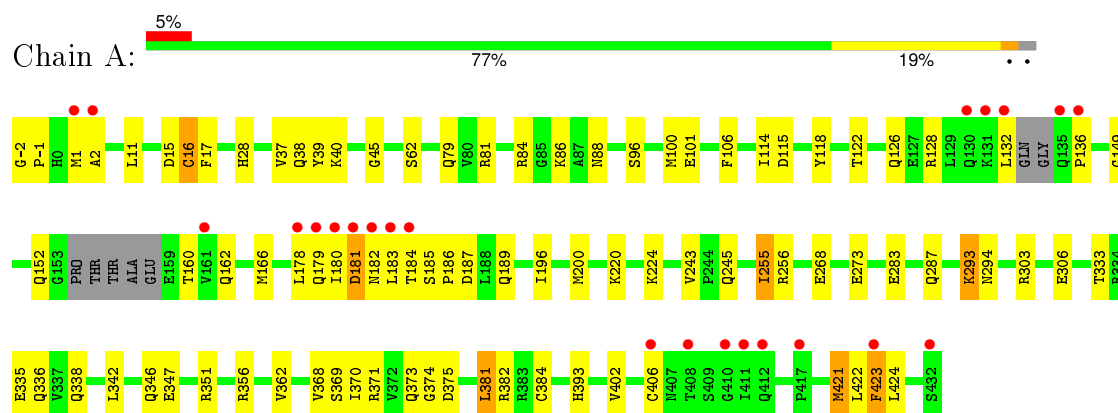
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	368	Total O 368 368	0	0
7	T	30	Total O 30 30	0	0
7	P	33	Total O 33 33	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA polymerase eta



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	98.24Å 98.24Å 82.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.05 – 1.75 37.05 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.05-1.75) 99.5 (37.05-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.75Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.188 , 0.205 0.187 , 0.202	Depositor DCC
R_{free} test set	3499 reflections (8.37%)	DCC
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.8	EDS
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45282 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4528	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, DZ4, TTD

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	0.46	0/3798	0.66	0/5113
2	T	0.73	0/207	1.01	1/316 (0.3%)
3	P	0.64	0/201	1.06	1/308 (0.3%)
All	All	0.48	0/4206	0.71	2/5737 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	DC	C1'-O4'-C4'	-8.02	102.08	110.10
2	T	8	DC	C1'-O4'-C4'	-5.83	104.27	110.10

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	3584	0	3657	163	0
2	T	254	0	149	1	0
3	P	180	0	102	4	0
4	A	41	0	16	9	0
5	A	2	0	0	0	0
6	A	36	0	46	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	368	0	0	23	0
7	P	33	0	0	1	0
7	T	30	0	0	1	0
All	All	4528	0	3970	170	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 21.

All (170) 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:A:160:THR:CB	1:A:166[B]:MET:HE1	1.71	1.18
1:A:180[B]:ILE:HG21	1:A:182[B]:ASN:ND2	1.63	1.11
1:A:160:THR:HB	1:A:166[B]:MET:HE1	1.09	1.07
1:A:180[B]:ILE:HG21	1:A:182[B]:ASN:CG	1.80	1.01
1:A:303:ARG:HA	6:A:441:GOL:H2	1.42	1.00
1:A:11[C]:LEU:HD12	1:A:118:TYR:CE2	1.97	0.99
1:A:11[B]:LEU:HD21	1:A:224[B]:LYS:HD3	1.45	0.96
1:A:180[B]:ILE:CG2	1:A:182[B]:ASN:CG	2.38	0.92
1:A:96:SER:HB2	1:A:114[B]:ILE:CD1	1.98	0.92
1:A:184[B]:THR:HB	1:A:186:PRO:HD2	1.52	0.91
1:A:384:CYS:SG	3:P:1:DC:H5'	2.11	0.91
1:A:160:THR:HB	1:A:166[B]:MET:CE	1.99	0.89
1:A:160:THR:CG2	1:A:166[B]:MET:HE1	2.04	0.87
1:A:160:THR:CB	1:A:166[B]:MET:CE	2.52	0.87
1:A:136:PRO:HA	1:A:180[A]:ILE:HD12	1.54	0.87
1:A:160:THR:HG22	1:A:166[B]:MET:CE	2.05	0.87
1:A:11[B]:LEU:CD2	1:A:224[B]:LYS:HD3	2.06	0.85
1:A:11[C]:LEU:HD12	1:A:118:TYR:CZ	2.11	0.85
1:A:160:THR:HG22	1:A:166[B]:MET:HE2	1.59	0.84
1:A:180[B]:ILE:HG22	1:A:182[B]:ASN:H	1.44	0.82
1:A:160:THR:CG2	1:A:166[B]:MET:CE	2.58	0.81
1:A:293[A]:LYS:HG2	4:A:442:DZ4:H8	1.62	0.81
1:A:96:SER:HB2	1:A:114[B]:ILE:HD13	1.62	0.79
4:A:442:DZ4:C6	7:A:798:HOH:O	2.32	0.78
1:A:178[B]:LEU:HD23	1:A:183[B]:LEU:CD1	2.15	0.77
1:A:39[A]:TYR:O	1:A:45:GLY:HA2	1.85	0.77
1:A:178[B]:LEU:HD23	1:A:183[B]:LEU:HD12	1.67	0.77
6:A:440:GOL:H12	7:A:460:HOH:O	1.84	0.77
1:A:40[A]:LYS:HG3	1:A:79:GLN:NE2	1.99	0.76
1:A:351[B]:ARG:HG2	1:A:351[B]:ARG:HH21	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180[B]:ILE:O	1:A:181[B]:ASP:HB3	1.87	0.73
1:A:86[B]:LYS:HB2	1:A:86[B]:LYS:NZ	2.04	0.72
1:A:371[B]:ARG:NH2	1:A:373:GLN:HA	2.05	0.72
1:A:28:HIS:HA	6:A:438:GOL:H31	1.69	0.72
1:A:371[B]:ARG:HH21	1:A:373:GLN:HA	1.54	0.71
1:A:185[B]:SER:HB3	1:A:186:PRO:HD3	1.71	0.71
1:A:303:ARG:O	6:A:441:GOL:H11	1.92	0.70
1:A:183[B]:LEU:HD22	1:A:187:ASP:OD2	1.92	0.70
1:A:179[A]:GLN:HG2	1:A:179[A]:GLN:O	1.91	0.70
1:A:421[B]:MET:HE3	1:A:422:LEU:CA	2.24	0.68
1:A:421[B]:MET:HE3	1:A:422:LEU:N	2.09	0.68
3:P:1:DC:N4	7:P:365:HOH:O	2.26	0.67
1:A:220:LYS:HB3	1:A:256[A]:ARG:HH12	1.60	0.66
4:A:442:DZ4:N6	7:A:798:HOH:O	2.28	0.66
1:A:81[B]:ARG:HH11	1:A:88:ASN:HD21	1.43	0.66
1:A:2:ALA:HB1	7:A:555:HOH:O	1.95	0.66
1:A:333:THR:OG1	1:A:336:GLN:HB2	1.96	0.66
1:A:81[B]:ARG:NH1	1:A:88:ASN:HD21	1.93	0.66
1:A:245[A]:GLN:NE2	7:A:778:HOH:O	2.29	0.65
1:A:96:SER:HB2	1:A:114[B]:ILE:HD11	1.76	0.65
1:A:180[B]:ILE:HG22	1:A:182[B]:ASN:N	2.11	0.65
6:A:436:GOL:H32	7:A:595:HOH:O	1.96	0.65
1:A:96:SER:CB	1:A:114[B]:ILE:HD13	2.27	0.65
1:A:180[B]:ILE:O	1:A:181[B]:ASP:CB	2.46	0.64
1:A:342:LEU:HD21	6:A:439:GOL:H2	1.81	0.63
1:A:245[A]:GLN:HG3	7:A:801:HOH:O	1.98	0.63
1:A:86[B]:LYS:HB2	1:A:86[B]:LYS:HZ3	1.62	0.63
1:A:245[B]:GLN:HG3	7:A:801:HOH:O	1.98	0.63
1:A:181[A]:ASP:OD1	1:A:182[A]:ASN:N	2.31	0.63
1:A:122:THR:O	1:A:126:GLN:HG2	1.99	0.63
1:A:28:HIS:ND1	6:A:438:GOL:C3	2.62	0.62
1:A:293[A]:LYS:CG	4:A:442:DZ4:H8	2.30	0.62
1:A:381:LEU:HD23	1:A:381:LEU:O	2.00	0.62
1:A:293[A]:LYS:HD2	1:A:294:ASN:N	2.15	0.61
1:A:162:GLN:HG2	7:A:538:HOH:O	1.98	0.61
1:A:180[A]:ILE:CG2	7:A:758:HOH:O	2.48	0.60
1:A:303:ARG:HA	6:A:441:GOL:C2	2.24	0.60
1:A:185[B]:SER:N	1:A:186:PRO:CD	2.65	0.60
1:A:421[B]:MET:HE3	1:A:422:LEU:C	2.23	0.59
1:A:40[B]:LYS:HG2	1:A:79:GLN:NE2	2.18	0.58
1:A:86[B]:LYS:NZ	7:A:740:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181[A]:ASP:C	1:A:181[A]:ASP:OD1	2.41	0.58
1:A:243:VAL:HG12	6:A:441:GOL:C3	2.33	0.58
1:A:243:VAL:HG12	6:A:441:GOL:H31	1.85	0.57
1:A:184[B]:THR:HG21	7:A:629:HOH:O	2.03	0.57
1:A:189:GLN:NE2	7:A:800:HOH:O	2.38	0.57
1:A:393:HIS:CE1	6:A:439:GOL:HO2	2.20	0.57
1:A:368:VAL:HG11	1:A:402:VAL:HG23	1.87	0.57
1:A:294:ASN:OD1	4:A:442:DZ4:N7	2.37	0.57
1:A:335:GLU:OE2	1:A:338:GLN:NE2	2.39	0.56
1:A:179[A]:GLN:CG	1:A:179[A]:GLN:O	2.54	0.56
1:A:28:HIS:ND1	6:A:438:GOL:H31	2.19	0.56
1:A:184[B]:THR:CB	1:A:186:PRO:HD2	2.32	0.56
1:A:293[A]:LYS:HD3	4:A:442:DZ4:C8	2.35	0.56
1:A:2:ALA:HB1	7:A:791:HOH:O	2.05	0.56
1:A:293[A]:LYS:CE	2:T:10:DC:OP1	2.54	0.56
1:A:255:ILE:N	1:A:255:ILE:HD13	2.21	0.55
1:A:28:HIS:CD2	6:A:437:GOL:O3	2.61	0.54
1:A:28:HIS:ND1	6:A:438:GOL:H32	2.23	0.54
1:A:368:VAL:HG11	1:A:402:VAL:CG2	2.38	0.54
1:A:179[A]:GLN:NE2	1:A:185[A]:SER:OG	2.42	0.53
1:A:342:LEU:CD2	6:A:439:GOL:H2	2.39	0.53
1:A:371[B]:ARG:HH21	1:A:373:GLN:CA	2.21	0.53
1:A:39[A]:TYR:O	1:A:45:GLY:CA	2.56	0.53
1:A:15:ASP:O	1:A:16:CYS:C	2.48	0.52
1:A:293[A]:LYS:CD	4:A:442:DZ4:H8	2.39	0.52
1:A:180[B]:ILE:O	1:A:180[B]:ILE:HG23	2.08	0.52
1:A:11[B]:LEU:CD2	1:A:224[B]:LYS:CD	2.84	0.52
1:A:136:PRO:HA	1:A:180[A]:ILE:CD1	2.34	0.51
1:A:62:SER:HA	7:T:71:HOH:O	2.10	0.51
1:A:2:ALA:CB	7:A:791:HOH:O	2.58	0.51
1:A:11[B]:LEU:HD22	1:A:118:TYR:CE2	2.46	0.50
1:A:356:ARG:HD3	1:A:362:VAL:HG12	1.94	0.50
1:A:370:ILE:HG12	1:A:381:LEU:HD22	1.93	0.50
1:A:371[B]:ARG:CZ	1:A:375:ASP:O	2.60	0.49
1:A:369:SER:HB3	1:A:423:PHE:HB3	1.94	0.49
1:A:38:GLN:O	1:A:39[B]:TYR:HB2	2.11	0.49
1:A:181[B]:ASP:O	1:A:181[B]:ASP:OD1	2.29	0.49
1:A:101:GLU:OE1	6:A:440:GOL:O1	2.28	0.49
1:A:185[B]:SER:N	1:A:186:PRO:HD2	2.27	0.49
1:A:178[B]:LEU:HD23	1:A:183[B]:LEU:HD13	1.92	0.48
1:A:106:PHE:CG	1:A:200[A]:MET:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37[B]:VAL:CG1	1:A:45:GLY:HA3	2.43	0.48
1:A:81[B]:ARG:NH1	1:A:88:ASN:ND2	2.61	0.48
1:A:149:GLY:O	1:A:152[B]:GLN:HG3	2.13	0.48
1:A:179[A]:GLN:NE2	1:A:185[A]:SER:CB	2.77	0.48
1:A:2:ALA:HA	7:A:791:HOH:O	2.13	0.48
4:A:442:DZ4:C5	7:A:798:HOH:O	2.60	0.48
1:A:351[B]:ARG:CG	1:A:351[B]:ARG:HH21	2.21	0.48
1:A:81[B]:ARG:HH11	1:A:88:ASN:ND2	2.09	0.48
1:A:-2:GLY:N	1:A:-1:PRO:HD2	2.28	0.48
1:A:381:LEU:HD23	1:A:381:LEU:C	2.33	0.48
1:A:370:ILE:CD1	1:A:381:LEU:HD22	2.43	0.48
1:A:384:CYS:SG	3:P:1:DC:C5'	2.94	0.47
1:A:37[C]:VAL:CG2	1:A:45:GLY:HA3	2.44	0.47
1:A:382[C]:ARG:NH1	7:A:767:HOH:O	2.48	0.47
1:A:342:LEU:O	1:A:346:GLN:HG3	2.16	0.46
1:A:185[A]:SER:O	1:A:189:GLN:HG3	2.16	0.46
1:A:185[B]:SER:O	1:A:189:GLN:HG3	2.16	0.46
1:A:106:PHE:CD2	1:A:200[A]:MET:HG2	2.51	0.45
1:A:382[B]:ARG:NH2	3:P:3:DG:OP2	2.49	0.45
1:A:1:MET:HE3	7:A:735:HOH:O	2.15	0.45
1:A:128:ARG:HG3	1:A:132:LEU:HD13	1.97	0.45
1:A:96:SER:O	1:A:100:MET:HG2	2.15	0.45
6:A:440:GOL:C1	7:A:460:HOH:O	2.52	0.45
1:A:62:SER:OG	1:A:62:SER:O	2.32	0.45
1:A:243:VAL:HG12	6:A:441:GOL:H32	1.99	0.44
1:A:37[B]:VAL:HG12	1:A:38:GLN:N	2.32	0.44
1:A:180[B]:ILE:CG2	1:A:182[B]:ASN:OD1	2.65	0.44
1:A:371[B]:ARG:NH2	1:A:374:GLY:H	2.15	0.44
1:A:84[B]:ARG:CZ	1:A:347:GLU:HB2	2.48	0.44
1:A:423:PHE:HD1	1:A:424:LEU:N	2.17	0.43
1:A:273:GLU:HG2	7:A:795:HOH:O	2.18	0.43
1:A:180[B]:ILE:CG2	1:A:182[B]:ASN:CB	2.97	0.42
1:A:303:ARG:C	6:A:441:GOL:H11	2.39	0.42
1:A:160:THR:HA	1:A:166[B]:MET:HE3	2.00	0.42
1:A:11[B]:LEU:HD23	1:A:224[B]:LYS:CD	2.50	0.42
1:A:283:GLU:O	1:A:287:GLN:HG3	2.19	0.42
1:A:179[A]:GLN:CD	1:A:179[A]:GLN:H	2.23	0.42
1:A:81[B]:ARG:HE	1:A:88:ASN:ND2	2.18	0.41
1:A:293[A]:LYS:CD	4:A:442:DZ4:C8	2.98	0.41
1:A:17:PHE:HE2	1:A:114[B]:ILE:HD12	1.85	0.41
1:A:37[C]:VAL:HG22	1:A:38:GLN:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:CB	1:A:114[B]:ILE:CD1	2.84	0.41
1:A:2:ALA:CA	7:A:791:HOH:O	2.68	0.41
1:A:196:ILE:O	1:A:200[A]:MET:HG3	2.21	0.41
1:A:45:GLY:HA2	7:A:584:HOH:O	2.20	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	469/435 (108%)	462 (98%)	6 (1%)	1 (0%)	52 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	CYS

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	408/372 (110%)	395 (97%)	13 (3%)	46 20

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ASP
1	A	181[A]	ASP
1	A	181[B]	ASP
1	A	255	ILE
1	A	268	GLU
1	A	293[A]	LYS
1	A	293[B]	LYS
1	A	306	GLU
1	A	381	LEU
1	A	406	CYS
1	A	421[A]	MET
1	A	421[B]	MET
1	A	423	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	28	HIS
1	A	79	GLN
1	A	88	ASN
1	A	189	GLN
1	A	338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	TTD	T	3[A]	-	40,45,46	1.55	9 (22%)	58,74,77	3.25	24 (41%)
2	TTD	T	3[B]	-	40,45,46	1.89	10 (25%)	58,74,77	3.21	25 (43%)

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	TTD	T	3[A]	-	-	0/22/109/110	0/3/6/6
2	TTD	T	3[B]	-	-	0/22/109/110	0/3/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	3[B]	TTD	C5-C4	-3.55	1.44	1.51
2	T	3[A]	TTD	C5T-C4T	-3.08	1.45	1.51
2	T	3[A]	TTD	C5-C4	-2.93	1.45	1.51
2	T	3[B]	TTD	C5'-C4R	-2.48	1.43	1.51
2	T	3[B]	TTD	PB-O5P	-2.09	1.43	1.51
2	T	3[A]	TTD	PB-O5P	-2.09	1.43	1.51
2	T	3[B]	TTD	C5-C6	-2.00	1.52	1.55
2	T	3[B]	TTD	C1'-N1	2.19	1.48	1.45
2	T	3[A]	TTD	C1R-N1T	2.20	1.48	1.45
2	T	3[A]	TTD	O4T-C4T	2.33	1.27	1.22
2	T	3[A]	TTD	C1'-N1	2.33	1.48	1.45
2	T	3[B]	TTD	C5A-C5	2.34	1.58	1.53
2	T	3[A]	TTD	C4-N3	2.36	1.41	1.37
2	T	3[A]	TTD	C5A-C5	2.53	1.58	1.53
2	T	3[B]	TTD	C4-N3	3.01	1.42	1.37
2	T	3[B]	TTD	O4T-C4T	3.33	1.28	1.22
2	T	3[A]	TTD	C5T-C6T	3.66	1.59	1.55
2	T	3[B]	TTD	C5T-C6T	4.62	1.60	1.55
2	T	3[B]	TTD	C1R-N1T	5.30	1.52	1.45

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	3[B]	TTD	O4-C4-C5	-8.06	116.35	122.92
2	T	3[B]	TTD	O4T-C4T-C5T	-7.95	116.44	122.92
2	T	3[A]	TTD	O4T-C4T-C5T	-7.40	116.89	122.92
2	T	3[A]	TTD	C5T-C6T-N1T	-6.59	106.37	115.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	3[A]	TTD	O4-C4-C5	-5.71	118.27	122.92
2	T	3[B]	TTD	C5T-C6T-N1T	-5.64	107.71	115.70
2	T	3[A]	TTD	C5T-C6T-C6	-5.56	79.87	89.27
2	T	3[A]	TTD	C5T-C5-C6	-4.38	82.82	88.37
2	T	3[A]	TTD	C4T-N3T-C2T	-4.30	119.10	126.84
2	T	3[B]	TTD	C4T-N3T-C2T	-4.01	119.63	126.84
2	T	3[B]	TTD	C5T-C6T-C6	-3.64	83.13	89.27
2	T	3[A]	TTD	O2-C2-N1	-2.76	119.19	123.36
2	T	3[A]	TTD	C3R-C2'-C1'	-2.69	97.54	103.04
2	T	3[B]	TTD	C5A-C5-C6	-2.62	106.17	114.32
2	T	3[B]	TTD	C6-C5-C4	-2.47	107.21	114.27
2	T	3[B]	TTD	O3R-PB-O5P	-2.37	100.11	109.46
2	T	3[A]	TTD	O3R-PB-O5P	-2.37	100.11	109.46
2	T	3[B]	TTD	O4'-C4R-C5'	-2.34	100.94	109.32
2	T	3[A]	TTD	O4'-C4R-C5'	-2.33	101.00	109.32
2	T	3[A]	TTD	O4T-C4T-N3T	-2.23	116.73	120.50
2	T	3[A]	TTD	C5-C5T-C4T	-2.22	105.52	113.09
2	T	3[A]	TTD	C6-C5-C4	-2.18	108.05	114.27
2	T	3[B]	TTD	O2-C2-N1	-2.13	120.14	123.36
2	T	3[B]	TTD	O2T-C2T-N1T	-2.11	120.19	123.36
2	T	3[A]	TTD	C5A-C5-C6	-2.01	108.06	114.32
2	T	3[B]	TTD	C3R-C2'-C1'	-2.01	98.94	103.04
2	T	3[B]	TTD	C5-C5T-C6T	2.14	91.07	88.37
2	T	3[B]	TTD	O3'-C3'-C2R	2.20	118.04	110.74
2	T	3[B]	TTD	N3-C2-N1	2.26	119.09	116.82
2	T	3[B]	TTD	C5'-C4R-C3R	2.33	120.10	114.46
2	T	3[A]	TTD	C5'-C4R-C3R	2.44	120.37	114.46
2	T	3[B]	TTD	N3T-C2T-N1T	2.45	119.28	116.82
2	T	3[B]	TTD	C5-C6-C6T	2.45	93.42	89.27
2	T	3[A]	TTD	C2R-C1R-N1T	2.58	119.18	115.64
2	T	3[B]	TTD	C5M-C5T-C4T	2.88	112.52	108.41
2	T	3[A]	TTD	C5-C6-C6T	3.18	94.64	89.27
2	T	3[A]	TTD	N3-C2-N1	3.24	120.07	116.82
2	T	3[B]	TTD	C5T-C5-C4	3.63	125.47	113.09
2	T	3[A]	TTD	C5-C5T-C6T	3.88	93.28	88.37
2	T	3[B]	TTD	C2R-C1R-N1T	4.10	121.27	115.64
2	T	3[B]	TTD	C5A-C5-C4	4.24	114.47	108.41
2	T	3[A]	TTD	C5M-C5T-C4T	4.36	114.64	108.41
2	T	3[A]	TTD	C5T-C5-C4	4.85	129.63	113.09
2	T	3[B]	TTD	C5-C4-N3	4.92	120.29	116.01
2	T	3[A]	TTD	C5-C4-N3	7.16	122.23	116.01
2	T	3[A]	TTD	C5-C6-N1	7.56	126.41	115.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	3[B]	TTD	C5T-C4T-N3T	9.92	124.62	116.01
2	T	3[B]	TTD	C5-C6-N1	11.06	131.38	115.70
2	T	3[A]	TTD	C5T-C4T-N3T	11.92	126.36	116.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
4	DZ4	A	433	5	27,32,32	6.38	18 (66%)	32,50,50	2.33	12 (37%)
6	GOL	A	436	-	5,5,5	1.45	1 (20%)	5,5,5	3.41	4 (80%)
6	GOL	A	437	-	5,5,5	0.35	0	5,5,5	0.49	0
6	GOL	A	438	-	5,5,5	0.94	0	5,5,5	1.12	1 (20%)
6	GOL	A	439	-	5,5,5	1.25	1 (20%)	5,5,5	2.15	3 (60%)
6	GOL	A	440	-	5,5,5	3.10	2 (40%)	5,5,5	2.87	2 (40%)
6	GOL	A	441	-	5,5,5	0.73	0	5,5,5	1.19	0
4	DZ4	A	442	-	9,12,32	2.86	7 (77%)	6,17,50	3.26	3 (50%)

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
4	DZ4	A	433	5	-	0/13/34/34	0/3/3/3
6	GOL	A	436	-	-	0/4/4/4	0/0/0/0
6	GOL	A	437	-	-	0/4/4/4	0/0/0/0
6	GOL	A	438	-	-	0/4/4/4	0/0/0/0
6	GOL	A	439	-	-	0/4/4/4	0/0/0/0
6	GOL	A	440	-	-	0/4/4/4	0/0/0/0
6	GOL	A	441	-	-	0/4/4/4	0/0/0/0
4	DZ4	A	442	-	-	0/0/0/34	0/2/2/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	433	DZ4	PA-O1A	-21.42	1.21	1.46
4	A	433	DZ4	PB-O1B	-16.31	1.27	1.46
4	A	433	DZ4	PB-O2B	-10.51	1.27	1.56
4	A	433	DZ4	PG-O1G	-7.27	1.27	1.51
4	A	433	DZ4	PG-O2G	-5.09	1.36	1.54
4	A	433	DZ4	PG-O3G	-4.99	1.36	1.54
4	A	442	DZ4	C8-N7	-4.89	1.25	1.34
4	A	433	DZ4	O3'-C3'	-4.82	1.32	1.43
4	A	433	DZ4	PA-O2A	-4.56	1.44	1.56
4	A	433	DZ4	O4'-C4'	-4.54	1.34	1.45
6	A	440	GOL	C3-C2	-4.19	1.36	1.52
4	A	433	DZ4	C8-N7	-4.06	1.26	1.34
4	A	433	DZ4	C2-N3	-3.79	1.25	1.32
4	A	442	DZ4	C5-N7	-3.70	1.26	1.39
4	A	442	DZ4	C2-N3	-3.69	1.25	1.32
4	A	433	DZ4	O4'-C1'	-3.39	1.34	1.42
4	A	433	DZ4	C6-N6	-3.29	1.24	1.34
4	A	433	DZ4	C5-N7	-2.89	1.29	1.39
4	A	442	DZ4	C6-N6	-2.62	1.26	1.34
4	A	442	DZ4	C5-C4	2.03	1.45	1.40
6	A	439	GOL	O1-C1	2.04	1.51	1.42
4	A	442	DZ4	C2-N1	2.26	1.38	1.33
4	A	442	DZ4	C4-N3	2.36	1.39	1.35
4	A	433	DZ4	C5'-C4'	2.37	1.59	1.51
4	A	433	DZ4	C2-N1	2.39	1.38	1.33
4	A	433	DZ4	PB-N3A	2.60	1.70	1.63
4	A	433	DZ4	C4-N3	2.63	1.39	1.35
6	A	436	GOL	O3-C3	3.16	1.56	1.42
6	A	440	GOL	O2-C2	5.30	1.59	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	433	DZ4	N3-C2-N1	-7.15	123.42	128.89
4	A	442	DZ4	N3-C2-N1	-6.63	123.82	128.89
6	A	436	GOL	C3-C2-C1	-3.89	95.85	111.12
4	A	433	DZ4	O1B-PB-N3A	-3.86	105.97	111.90
6	A	440	GOL	O2-C2-C1	-3.15	94.22	108.65
4	A	433	DZ4	C2'-C3'-C4'	-3.07	96.40	102.77
4	A	442	DZ4	C4-C5-N7	-2.71	106.99	109.48
4	A	433	DZ4	C4-C5-N7	-2.51	107.17	109.48
6	A	436	GOL	O3-C3-C2	-2.29	99.07	110.18
6	A	439	GOL	C3-C2-C1	-2.14	102.72	111.12
4	A	433	DZ4	PG-O3B-PB	-2.13	125.52	132.67
6	A	438	GOL	O2-C2-C1	-2.06	99.20	108.65
4	A	433	DZ4	O1A-PA-N3A	-2.03	108.78	111.90
4	A	433	DZ4	O2B-PB-O1B	2.06	114.30	110.00
4	A	433	DZ4	O5'-C5'-C4'	2.12	116.92	109.12
6	A	439	GOL	O2-C2-C1	2.32	119.27	108.65
4	A	433	DZ4	O4'-C1'-N9	2.40	111.88	107.72
4	A	433	DZ4	O3'-C3'-C2'	2.43	118.79	110.74
4	A	433	DZ4	N6-C6-N1	2.79	125.20	119.20
4	A	442	DZ4	N6-C6-N1	2.88	125.38	119.20
6	A	439	GOL	O2-C2-C3	3.16	123.14	108.65
6	A	436	GOL	O2-C2-C3	3.91	126.60	108.65
6	A	436	GOL	O2-C2-C1	4.72	130.30	108.65
6	A	440	GOL	O2-C2-C3	5.31	132.99	108.65
4	A	433	DZ4	O2A-PA-O1A	5.41	121.29	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	436	GOL	1	0
6	A	437	GOL	1	0
6	A	438	GOL	4	0
6	A	439	GOL	3	0
6	A	440	GOL	3	0
6	A	441	GOL	7	0
4	A	442	DZ4	9	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	428/435 (98%)	0.00	23 (5%) 29 35	7, 17, 38, 52	0
2	T	10/11 (90%)	-0.31	0 100 100	14, 20, 44, 53	0
3	P	9/9 (100%)	-0.05	1 (11%) 7 9	14, 20, 30, 44	0
All	All	447/455 (98%)	-0.01	24 (5%) 29 35	7, 17, 39, 53	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	LEU	4.9
1	A	410	GLY	4.9
1	A	183[A]	LEU	4.8
1	A	411	ILE	4.8
1	A	412	GLN	4.7
1	A	180[A]	ILE	4.1
3	P	1	DC	4.0
1	A	182[A]	ASN	3.8
1	A	417	PRO	3.4
1	A	130	GLN	3.0
1	A	131	LYS	3.0
1	A	432	SER	2.9
1	A	408	THR	2.8
1	A	135	GLN	2.6
1	A	423	PHE	2.6
1	A	181[A]	ASP	2.5
1	A	161	VAL	2.5
1	A	1	MET	2.3
1	A	184[A]	THR	2.3
1	A	406	CYS	2.2
1	A	136	PRO	2.1
1	A	2	ALA	2.1
1	A	179[A]	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	178[A]	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TTD	T	3[B]	40/41	0.90	0.14	-	15,23,60,60	28
2	TTD	T	3[A]	40/41	0.90	0.14	-	9,22,60,60	28

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
6	GOL	A	441	6/6	0.86	0.30	23.04	28,33,33,35	0
6	GOL	A	436	6/6	0.83	0.18	11.79	17,22,25,27	0
6	GOL	A	440	6/6	0.84	0.34	11.21	48,49,50,50	0
6	GOL	A	437	6/6	0.84	0.20	8.03	35,36,36,36	0
4	DZ4	A	442	11/30	0.79	0.38	4.74	31,36,38,38	0
6	GOL	A	438	6/6	0.81	0.20	3.08	52,52,52,53	0
5	MG	A	435	1/1	0.99	0.08	-0.14	9,9,9,9	0
4	DZ4	A	433	30/30	0.98	0.06	-0.58	6,9,12,13	0
5	MG	A	434	1/1	0.99	0.04	-2.93	9,9,9,9	0
6	GOL	A	439	6/6	0.64	0.17	-	52,52,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.