Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:28 PM GMT

PDB ID	:	1X9M
Title	:	T7 DNA polymerase in complex with an N-2-acetylaminofluorene-adducted DNA
Authors	:	Dutta, S.; Li, Y.; Johnson, D.; Dzantiev, L.; Richardson, C.C.; Romano, L.J.; Ellenberger, T.
Deposited on	:	2004-08-23
Resolution	:	2.10 Å(reported)

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

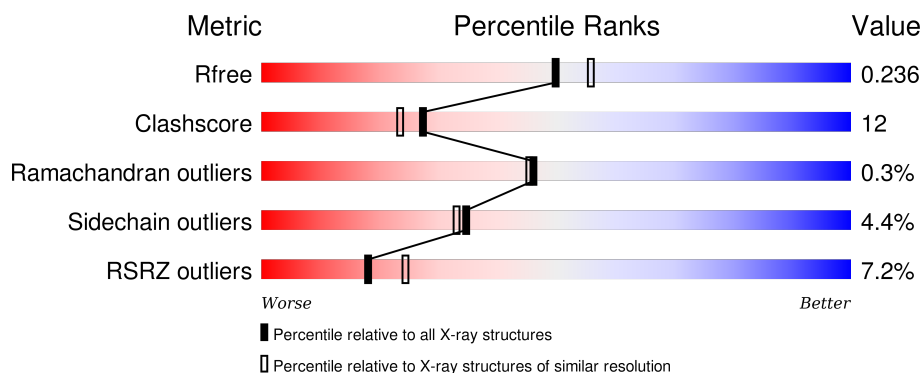|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		12
Ramachandran outliers		0.3%
Sidechain outliers		4.4%
RSRZ outliers		7.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	C	22	5% / 14% 18% 14% 55%
2	D	26	4% / 27% 8% 12% 54%
3	A	698	6% / 74% 21% · ·
4	B	108	11% / 69% 26% · ·

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
1	2DT	C	22	-	-	X	-
5	MG	A	3001	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6824 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 DNA chain called 5'-D(*GP*GP*AP*GP*AP*GP*TP*GP*AP*TP*TP*G P*GP*TP*AP*GP*TP*GP*TP*GP*AP*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	10	Total 209	C 100	N 38	O 61	P 10	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(8FG)P*AP*TP*CP*AP*CP*AP*CP *TP*AP*CP*CP*AP*AP*TP*CP*AP*CP*TP*CP*TP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total 258	C 130	N 45	O 71	P 12	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	675	Total 5251	C 3355	N 917	O 955	S 24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP P00581
A	?	-	ARG	DELETION	UNP P00581
A	?	-	PHE	DELETION	UNP P00581
A	?	-	GLY	DELETION	UNP P00581
A	?	-	SER	DELETION	UNP P00581
A	?	-	HIS	DELETION	UNP P00581

- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total 790	C 514	N 129	O 144	S 3	0	0	0

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

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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	266	Total O 266 266	0	0
6	B	15	Total O 15 15	0	0
6	C	11	Total O 11 11	0	0
6	D	23	Total O 23 23	0	0

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.
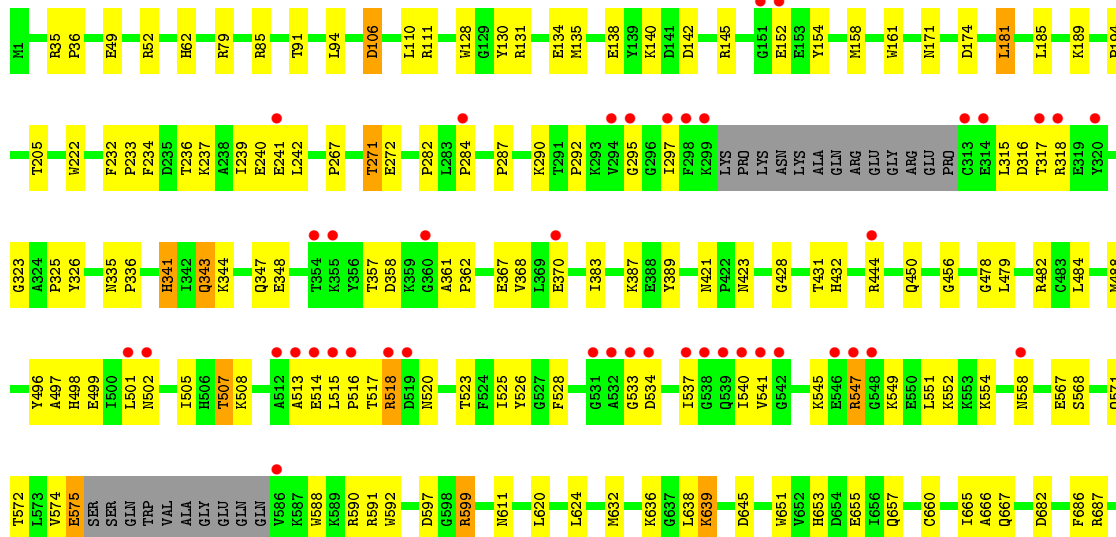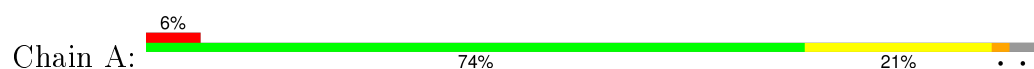
- Molecule 1: 5'-D(*GP*GP*AP*GP*AP*GP*TP*GP*AP*TP*TP*GP*GP*TP*AP*GP*TP* GP*TP*GP*AP*(2DT))-3'
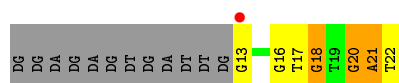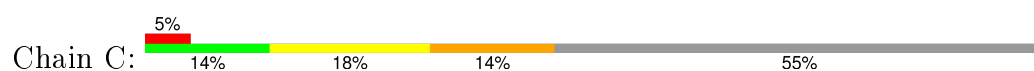
- Molecule 2: 5'-D(*CP*CP*CP*(8FG)P*AP*TP*CP*AP*CP*AP*CP*TP*AP*CP*CP*AP*A P*TP*CP*AP*CP*TP*CP*TP*CP*C)-3'
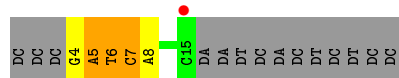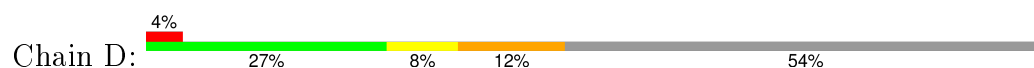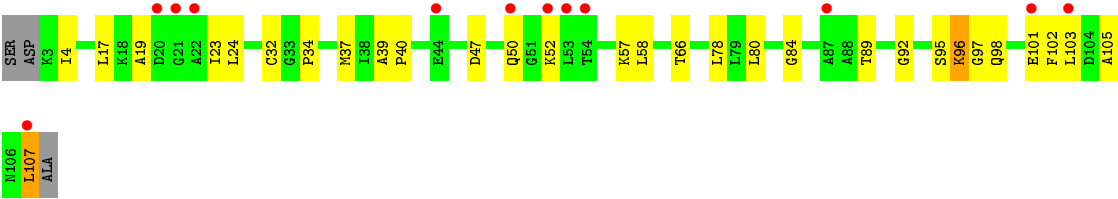

- Molecule 3: DNA polymerase

K695 M696 H704

• **Molecule 4: Thioredoxin 1**

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.11Å 212.31Å 52.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.10 47.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.3 (47.38-2.10) 94.4 (47.38-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.61 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.236 0.212 , 0.236	Depositor DCC
R_{free} test set	3239 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 65243 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2DT, MG, 8FG

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	C	0.52	0/213	0.87	0/328
2	D	0.53	0/244	0.99	0/372
3	A	0.39	0/5380	0.60	0/7299
4	B	0.33	0/805	0.59	0/1092
All	All	0.40	0/6642	0.63	0/9091

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
2	D	0	3
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	18	DG	Sidechain
1	C	20	DG	Sidechain
1	C	21	DA	Sidechain
2	D	5	DA	Sidechain
2	D	6	DT	Sidechain
2	D	7	DC	Sidechain

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	C	209	0	115	21	0
2	D	258	0	146	7	0
3	A	5251	0	5084	110	1
4	B	790	0	808	25	0
5	A	1	0	0	0	0
6	A	266	0	0	4	0
6	B	15	0	0	1	0
6	C	11	0	0	0	0
6	D	23	0	0	0	0
All	All	6824	0	6153	151	1

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 12.

All (151) 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:C:22:2DT:H6	1:C:22:2DT:H5'	1.30	1.14
1:C:21:DA:H2"	1:C:22:2DT:H5"	1.22	1.12
3:A:271:THR:HG22	3:A:290:LYS:HG2	1.53	0.90
4:B:19:ALA:HB3	4:B:23:ILE:HD11	1.57	0.84
1:C:17:DT:H2"	1:C:18:DG:H5"	1.57	0.83
1:C:21:DA:H2"	1:C:22:2DT:C5'	2.07	0.83
1:C:17:DT:H2"	1:C:18:DG:C5'	2.13	0.79
3:A:297:ILE:HG13	4:B:101:GLU:HG3	1.67	0.77
3:A:496:TYR:CE1	3:A:505:ILE:HD11	2.21	0.76
3:A:335:ASN:H	3:A:341:HIS:HD2	1.32	0.76
3:A:316:ASP:OD2	3:A:318:ARG:HG3	1.87	0.75
3:A:517:THR:H	3:A:520:ASN:HD22	1.35	0.75
3:A:496:TYR:CZ	3:A:505:ILE:HD11	2.24	0.73
4:B:19:ALA:CB	4:B:23:ILE:HD11	2.20	0.71
4:B:96:LYS:NZ	4:B:96:LYS:HB2	2.06	0.71
1:C:22:2DT:C6	1:C:22:2DT:H5'	2.17	0.70
3:A:317:THR:HG22	3:A:317:THR:O	1.90	0.69
1:C:17:DT:C2'	1:C:18:DG:H5"	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:507:THR:HG23	3:A:518:ARG:HG3	1.76	0.67
2:D:6:DT:H2"	2:D:7:DC:H5'	1.76	0.67
1:C:20:DG:H2"	1:C:21:DA:H5'	1.75	0.67
3:A:271:THR:HG23	3:A:272:GLU:H	1.60	0.67
4:B:52:LYS:NZ	4:B:107:LEU:HB3	2.12	0.65
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.33	0.64
1:C:16:DG:H2"	1:C:17:DT:C5'	2.28	0.64
4:B:96:LYS:HB2	4:B:96:LYS:HZ3	1.63	0.63
3:A:49:GLU:HA	3:A:52:ARG:NH1	2.13	0.63
3:A:106:ASP:OD1	3:A:110:LEU:HG	1.97	0.63
3:A:423:ASN:HD21	3:A:428:GLY:HA2	1.65	0.62
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.80	0.62
3:A:423:ASN:ND2	3:A:428:GLY:HA2	2.14	0.61
3:A:498:HIS:CE1	3:A:502:ASN:HD22	2.19	0.61
1:C:17:DT:P	3:A:357:THR:HG21	2.41	0.60
3:A:588:TRP:CD1	3:A:591:ARG:NH1	2.69	0.60
1:C:16:DG:H2"	1:C:17:DT:H5'	1.83	0.60
3:A:537:ILE:HG13	3:A:552:LYS:HE3	1.81	0.60
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.37	0.59
3:A:79:ARG:HD3	6:A:4226:HOH:O	2.01	0.59
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.84	0.58
3:A:499:GLU:HG2	3:A:508:LYS:HD2	1.85	0.58
1:C:21:DA:C2'	1:C:22:2DT:H5"	2.15	0.58
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.38	0.57
3:A:91:THR:HB	3:A:181:LEU:HD13	1.86	0.57
3:A:343:GLN:OE1	3:A:347:GLN:NE2	2.37	0.57
3:A:344:LYS:O	3:A:348:GLU:HG3	2.05	0.57
1:C:13:DG:H3'	3:A:111:ARG:NH1	2.20	0.56
2:D:5:DA:OP2	3:A:611:ASN:ND2	2.37	0.56
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.88	0.56
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.88	0.56
4:B:52:LYS:HZ1	4:B:107:LEU:HB3	1.72	0.55
3:A:236:THR:O	3:A:240:GLU:HG3	2.06	0.55
3:A:515:LEU:HD21	3:A:551:LEU:HD13	1.88	0.55
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.48	0.54
3:A:128:TRP:HZ3	3:A:131:ARG:NH1	2.06	0.54
3:A:367:GLU:HG3	3:A:368:VAL:N	2.24	0.53
3:A:537:ILE:O	3:A:540:ILE:HG22	2.07	0.53
3:A:357:THR:HG22	3:A:358:ASP:N	2.23	0.53
3:A:297:ILE:HD12	4:B:102:PHE:HB2	1.91	0.52
1:C:20:DG:H2"	1:C:21:DA:C5'	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:292:PRO:HG2	6:B:4026:HOH:O	2.09	0.52
3:A:290:LYS:NZ	3:A:290:LYS:HB3	2.24	0.52
3:A:568:SER:O	3:A:572:THR:HG23	2.10	0.52
3:A:574:VAL:HG12	3:A:575:GLU:N	2.25	0.52
2:D:6:DT:H2"	2:D:7:DC:C5'	2.40	0.52
3:A:189:LYS:HG2	3:A:194:PRO:HG3	1.91	0.52
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.40	0.51
3:A:597:ASP:OD1	3:A:599:ARG:CD	2.59	0.51
2:D:8:DA:H4'	3:A:432:HIS:O	2.11	0.50
3:A:282:PRO:C	3:A:284:PRO:HD3	2.31	0.50
3:A:295:GLY:HA2	3:A:318:ARG:NH2	2.27	0.50
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.12	0.50
3:A:547:ARG:O	3:A:551:LEU:HG	2.12	0.49
4:B:95:SER:OG	4:B:98:GLN:HG3	2.12	0.49
2:D:7:DC:H4'	3:A:431:THR:HG22	1.93	0.49
3:A:131:ARG:O	3:A:135:MET:HG2	2.12	0.49
3:A:498:HIS:CE1	3:A:502:ASN:ND2	2.80	0.49
3:A:517:THR:OG1	3:A:520:ASN:ND2	2.44	0.49
3:A:145:ARG:HH11	3:A:145:ARG:HG3	1.78	0.49
3:A:233:PRO:HB2	3:A:456:GLY:O	2.12	0.49
3:A:52:ARG:NH2	6:A:4272:HOH:O	2.45	0.49
3:A:267:PRO:HB3	3:A:287:PRO:HB3	1.95	0.49
3:A:242:LEU:HD13	3:A:450:GLN:NE2	2.28	0.49
4:B:19:ALA:HB3	4:B:23:ILE:CD1	2.35	0.48
3:A:537:ILE:HG13	3:A:552:LYS:CE	2.43	0.48
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.95	0.47
3:A:383:ILE:O	3:A:387:LYS:HG3	2.14	0.47
3:A:632:MET:O	3:A:636:LYS:HG3	2.13	0.47
3:A:554:LYS:HD2	3:A:558:ASN:HD21	1.79	0.47
1:C:22:2DT:C5'	1:C:22:2DT:H6	2.22	0.47
4:B:97:GLY:O	4:B:101:GLU:HG2	2.14	0.47
3:A:545:LYS:O	3:A:549:LYS:N	2.46	0.47
3:A:484:LEU:O	3:A:488:MET:HG2	2.14	0.47
1:C:21:DA:H2'	1:C:22:2DT:H73	1.97	0.46
4:B:4:ILE:HG21	4:B:57:LYS:HG3	1.96	0.46
4:B:52:LYS:HZ2	4:B:107:LEU:HB3	1.81	0.46
4:B:47:ASP:O	4:B:50:GLN:NE2	2.48	0.46
3:A:523:THR:HG21	3:A:540:ILE:HD13	1.97	0.45
3:A:478:GLY:O	3:A:482:ARG:HG3	2.16	0.45
3:A:590:ARG:HD3	3:A:592:TRP:CZ2	2.52	0.45
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:357:THR:HG22	3:A:358:ASP:H	1.80	0.45
3:A:525:ILE:CG2	3:A:526:TYR:N	2.79	0.45
3:A:444:ARG:HD3	3:A:444:ARG:HA	1.86	0.45
3:A:638:LEU:N	3:A:638:LEU:HD12	2.31	0.45
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.99	0.45
1:C:17:DT:H2"	1:C:18:DG:H5'	1.94	0.45
3:A:432:HIS:HD2	6:A:4029:HOH:O	2.00	0.45
1:C:16:DG:H2"	1:C:17:DT:H5"	1.98	0.44
4:B:103:LEU:O	4:B:107:LEU:HD22	2.18	0.44
3:A:158:MET:HA	3:A:161:TRP:CE2	2.52	0.44
3:A:638:LEU:N	3:A:638:LEU:CD1	2.81	0.44
1:C:13:DG:H3'	3:A:111:ARG:HH11	1.82	0.44
3:A:660:CYS:SG	3:A:666:ALA:HA	2.58	0.44
3:A:271:THR:HG23	3:A:272:GLU:N	2.31	0.43
3:A:367:GLU:HG3	3:A:368:VAL:H	1.82	0.43
3:A:335:ASN:H	3:A:341:HIS:CD2	2.22	0.43
3:A:639:LYS:HE3	6:A:4207:HOH:O	2.18	0.43
3:A:432:HIS:CD2	3:A:432:HIS:N	2.86	0.43
3:A:533:GLY:O	3:A:537:ILE:HG12	2.19	0.43
4:B:37:MET:O	4:B:40:PRO:HD2	2.18	0.43
3:A:326:TYR:HB3	4:B:92:GLY:HA2	2.00	0.42
3:A:696:MET:HE2	3:A:696:MET:HB2	1.84	0.42
4:B:58:LEU:HD21	4:B:66:THR:HB	2.00	0.42
3:A:497:ALA:O	3:A:501:LEU:HG	2.20	0.42
3:A:297:ILE:HG13	4:B:101:GLU:CG	2.45	0.42
3:A:237:LYS:O	3:A:241:GLU:HG3	2.19	0.42
4:B:17:LEU:HA	4:B:84:GLY:HA2	2.02	0.42
3:A:567:GLU:O	3:A:571:GLN:HG3	2.19	0.42
3:A:323:GLY:O	3:A:325:PRO:HD3	2.19	0.42
3:A:282:PRO:O	3:A:284:PRO:HD3	2.20	0.41
3:A:540:ILE:HG23	3:A:541:VAL:HG13	2.02	0.41
3:A:432:HIS:HE1	3:A:651:TRP:O	2.03	0.41
3:A:695:LYS:HD2	3:A:704:HIS:O	2.20	0.41
3:A:181:LEU:HD22	3:A:185:LEU:HD11	2.02	0.41
3:A:343:GLN:HE21	3:A:343:GLN:HB3	1.55	0.41
3:A:514:GLU:HG2	3:A:554:LYS:HG2	2.01	0.41
3:A:140:LYS:HE3	3:A:154:TYR:OH	2.20	0.41
2:D:4:8FG:H2"	2:D:5:DA:OP2	2.20	0.41
3:A:655:GLU:OE1	3:A:657:GLN:NE2	2.54	0.41
3:A:525:ILE:HG23	3:A:526:TYR:N	2.35	0.41
1:C:16:DG:C2'	1:C:17:DT:H5"	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:24:LEU:HD11	4:B:78:LEU:HB3	2.02	0.41
2:D:4:8FG:C39	3:A:528:PHE:HB3	2.51	0.40
3:A:138:GLU:O	3:A:142:ASP:OD1	2.39	0.40
3:A:361:ALA:HA	3:A:362:PRO:HD3	1.95	0.40
3:A:423:ASN:HD21	3:A:599:ARG:NH2	2.19	0.40
3:A:574:VAL:CG1	3:A:575:GLU:N	2.84	0.40
3:A:515:LEU:HA	3:A:516:PRO:HD3	1.84	0.40
1:C:16:DG:H1'	1:C:17:DT:H5"	2.04	0.40
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.20	0.40
4:B:50:GLN:C	4:B:52:LYS:H	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:205:THR:OG1	3:A:687:ARG:NH2[2_655]	2.14	0.06

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	
3	A	669/698 (96%)	642 (96%)	25 (4%)	2 (0%)	46	45
4	B	103/108 (95%)	102 (99%)	1 (1%)	0	100	100
All	All	772/806 (96%)	744 (96%)	26 (3%)	2 (0%)	46	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	513	ALA
3	A	653	HIS

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	
3	A	527/579 (91%)	504 (96%)	23 (4%)	35	33
4	B	81/87 (93%)	77 (95%)	4 (5%)	31	28
All	All	608/666 (91%)	581 (96%)	27 (4%)	35	33

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	62	HIS
3	A	106	ASP
3	A	152	GLU
3	A	171	ASN
3	A	174	ASP
3	A	181	LEU
3	A	232	PHE
3	A	271	THR
3	A	341	HIS
3	A	343	GLN
3	A	370	GLU
3	A	479	LEU
3	A	507	THR
3	A	518	ARG
3	A	534	ASP
3	A	547	ARG
3	A	575	GLU
3	A	599	ARG
3	A	624	LEU
3	A	639	LYS
3	A	667	GLN
3	A	682	ASP
3	A	686	PHE
4	B	80	LEU
4	B	89	THR
4	B	96	LYS
4	B	107	LEU

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

Mol	Chain	Res	Type
3	A	78	ASN
3	A	150	GLN
3	A	227	GLN
3	A	266	GLN
3	A	341	HIS
3	A	343	GLN
3	A	347	GLN
3	A	423	ASN
3	A	432	HIS
3	A	450	GLN
3	A	498	HIS
3	A	502	ASN
3	A	510	GLN
3	A	520	ASN
3	A	667	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#|Z| > 2$
1	2DT	C	22	1,2	11,20,21	1.47	3 (27%)	12,28,31	5.01	4 (33%)
2	8FG	D	4	2	36,44,45	4.04	21 (58%)	48,66,69	2.01	11 (22%)

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
1	2DT	C	22	1,2	-	0/3/18/19	0/2/2/2
2	8FG	D	4	2	-	0/11/41/42	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	8FG	C32-N29	-2.90	1.40	1.44
2	D	4	8FG	C39-C35	-2.58	1.39	1.46
1	C	22	2DT	C6-C5	-2.22	1.34	1.40
2	D	4	8FG	C42-C41	2.54	1.44	1.38
2	D	4	8FG	C42-C43	2.56	1.44	1.38
1	C	22	2DT	C6-N1	2.63	1.38	1.35
2	D	4	8FG	C33-C34	3.12	1.45	1.39
2	D	4	8FG	C41-C40	3.14	1.45	1.38
1	C	22	2DT	C4-N3	3.15	1.39	1.33
2	D	4	8FG	C30-N29	3.28	1.44	1.38
2	D	4	8FG	C40-C38	3.78	1.46	1.39
2	D	4	8FG	C36-C35	4.07	1.46	1.39
2	D	4	8FG	C43-C39	4.25	1.47	1.39
2	D	4	8FG	C33-C32	4.55	1.47	1.39
2	D	4	8FG	C35-C34	4.59	1.48	1.40
2	D	4	8FG	C36-C31	4.69	1.47	1.38
2	D	4	8FG	C31-C32	4.72	1.48	1.39
2	D	4	8FG	C6-N1	4.77	1.42	1.33
2	D	4	8FG	C39-C38	4.94	1.49	1.40
2	D	4	8FG	C8-N7	5.46	1.41	1.34
2	D	4	8FG	C2-N1	7.37	1.48	1.35
2	D	4	8FG	C6-C5	7.94	1.57	1.41
2	D	4	8FG	C4-N3	8.37	1.48	1.35
2	D	4	8FG	C8-N29	10.81	1.54	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	22	2DT	C5-C4-N3	-8.86	115.28	125.14
2	D	4	8FG	C5-C6-N1	-5.35	116.27	123.59
2	D	4	8FG	N3-C2-N1	-4.65	120.37	127.44
2	D	4	8FG	C32-N29-C8	-3.77	112.03	120.96
1	C	22	2DT	O4'-C4'-C5'	-3.36	104.59	109.54
2	D	4	8FG	C6-C5-C4	-3.02	117.29	120.90
2	D	4	8FG	O44-C30-C45	-2.74	112.28	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	8FG	C38-C37-C34	-2.45	99.14	102.74
1	C	22	2DT	C5M-C5-C6	2.20	123.04	118.62
2	D	4	8FG	N2-C2-N1	2.23	120.90	117.20
2	D	4	8FG	C32-N29-C30	3.32	126.06	120.95
2	D	4	8FG	C4-C5-N7	4.31	113.33	109.55
2	D	4	8FG	C6-N1-C2	5.04	122.94	115.94
2	D	4	8FG	C45-C30-N29	5.11	126.85	117.83
1	C	22	2DT	C4-N3-C2	14.21	127.53	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	22	2DT	7	0
2	D	4	8FG	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	C	9/22 (40%)	0.30	1 (11%)	7	10	27, 33, 71, 86	0
2	D	11/26 (42%)	0.45	1 (9%)	11	16	19, 31, 63, 81	0
3	A	675/698 (96%)	0.43	44 (6%)	22	29	14, 29, 60, 76	0
4	B	105/108 (97%)	0.73	12 (11%)	7	9	25, 38, 55, 63	0
All	All	800/854 (93%)	0.47	58 (7%)	18	24	14, 31, 60, 86	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	532	ALA	7.9
3	A	294	VAL	7.3
3	A	586	VAL	5.0
3	A	298	PHE	4.8
4	B	103	LEU	4.4
4	B	21	GLY	4.2
3	A	354	THR	4.2
3	A	313	CYS	4.1
4	B	107	LEU	3.9
3	A	540	ILE	3.8
3	A	534	ASP	3.7
3	A	537	ILE	3.7
3	A	314	GLU	3.6
3	A	548	GLY	3.5
3	A	515	LEU	3.5
4	B	53	LEU	3.4
3	A	539	GLN	3.3
3	A	152	GLU	3.2
3	A	297	ILE	3.1
3	A	704	HIS	3.0
3	A	546	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	15	DC	3.0
3	A	547	ARG	3.0
3	A	444	ARG	2.9
4	B	20	ASP	2.8
3	A	518	ARG	2.8
3	A	519	ASP	2.8
3	A	541	VAL	2.8
3	A	295	GLY	2.7
3	A	513	ALA	2.7
3	A	531	GLY	2.6
3	A	514	GLU	2.5
3	A	318	ARG	2.5
4	B	87	ALA	2.5
3	A	501	LEU	2.5
4	B	50	GLN	2.5
4	B	22	ALA	2.4
3	A	299	LYS	2.4
4	B	44	GLU	2.4
4	B	101	GLU	2.4
3	A	533	GLY	2.4
3	A	355	LYS	2.4
3	A	360	GLY	2.3
3	A	542	GLY	2.2
3	A	502	ASN	2.2
3	A	151	GLY	2.2
1	C	13	DG	2.2
3	A	538	GLY	2.2
3	A	512	ALA	2.2
3	A	516	PRO	2.1
3	A	320	TYR	2.1
4	B	52	LYS	2.1
3	A	317	THR	2.1
3	A	241	GLU	2.1
3	A	558	ASN	2.1
3	A	284	PRO	2.0
3	A	370	GLU	2.0
4	B	54	THR	2.0

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	8FG	D	4	39/40	0.76	0.28	-	44,54,68,68	0
1	2DT	C	22	19/20	0.95	0.17	-	28,31,34,35	0

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
5	MG	A	3001	1/1	0.79	0.28	8.46	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.