



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1X9W
Title : T7 DNA polymerase in complex with a primer/template DNA containing a disordered N-2 aminofluorene on the template, crystallized with dideoxy-ATP as the incoming nucleotide.
Authors : Dutta, S.; Li, Y.; Johnson, D.; Dzantiev, L.; Richardson, C.C.; Romano, L.J.; Ellenberger, T.
Deposited on : 2004-08-24
Resolution : 2.30 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

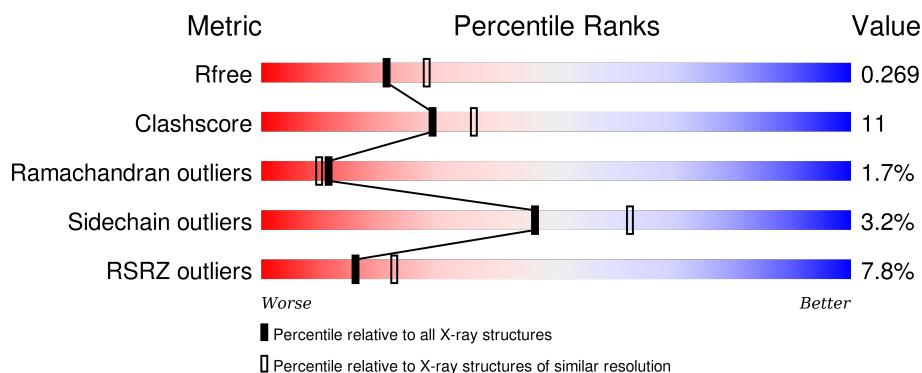
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	C	22	<div> <div>9%</div> <div>23% 14% 9% 5% 50%</div> </div>
2	D	26	<div> <div>4%</div> <div>19% 23% 58%</div> </div>
3	A	698	<div> <div>6%</div> <div>75% 19% . .</div> </div>
4	B	108	<div> <div>13%</div> <div>62% 35% .</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6567 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*T*GP*GP*T*AP*GP*TP*GP*TP*GP*AP*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	11	Total	C	N	O	P	0	0	0
			225	110	43	63	9			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(AFG)*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	11	Total	C	N	O	P	0	0	0
			216	105	39	62	10			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	673	Total	C	N	O	S	0	0	0
			5222	3324	905	969	24			

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	C	N	O	S	0	0	0
			783	506	122	152	3			

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

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

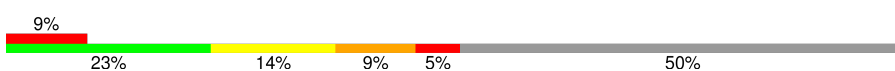
- Molecule 6 is water.

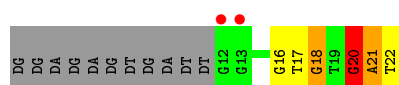
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	103	Total 103	O 103	0	0
6	B	7	Total 7	O 7	0	0
6	C	4	Total 4	O 4	0	0
6	D	6	Total 6	O 6	0	0

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.

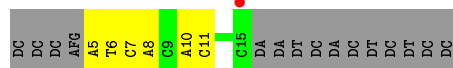
- Molecule 1: 5'-D(*GP*GP*AP*GP*AP*GP*TP*GP*AP*TP*T*GP*GP*T*AP*GP*TP*GP*TP*GP*AP*(2DT))-3'

Chain C: 




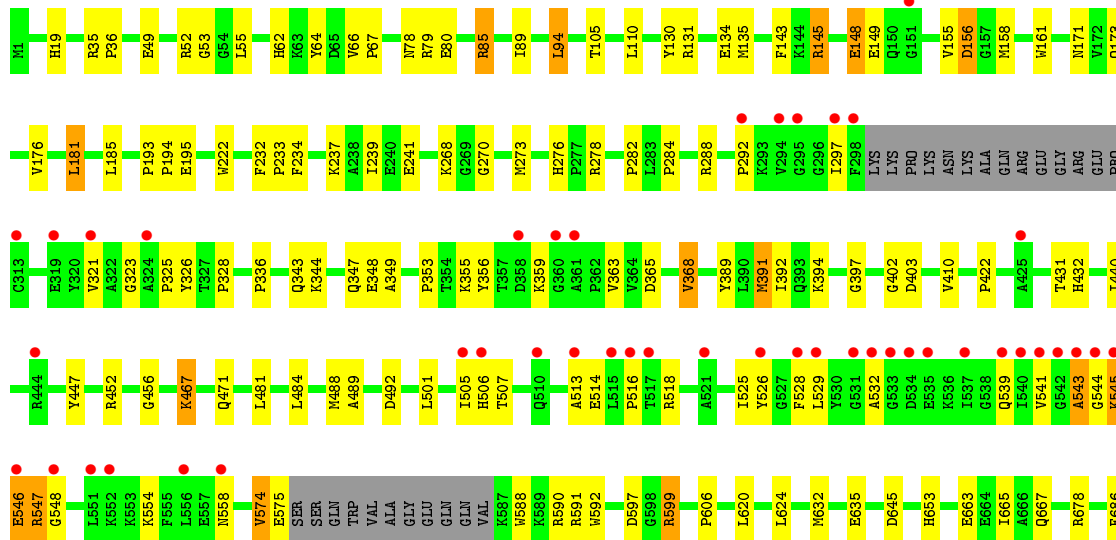
- Molecule 2: 5'-D(*CP*CP*CP*(AFG)*AP*TP*CP*AP*CP*AP*CP*TP*AP*CP*CP*AP*AP*TP*CP*AP*CP*TP*CP*TP*CP*C)-3'

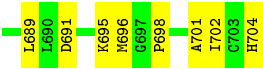
Chain D: 



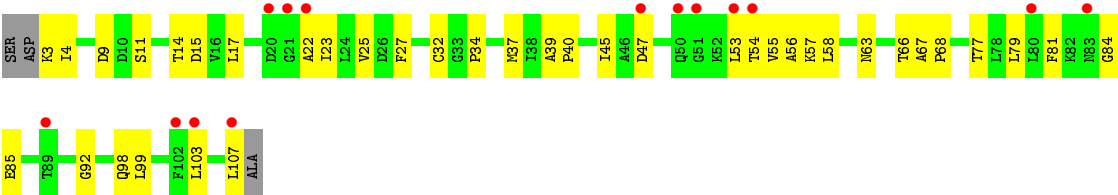
- Molecule 3: DNA polymerase

Chain A: 





● Molecule 4: Thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.94Å 213.56Å 52.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.68 – 2.30 47.68 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.68-2.30) 93.5 (47.68-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.258 0.242 , 0.269	Depositor DCC
R_{free} test set	2503 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 50967 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

5.1 Standard geometry

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

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	0.40	0/231	0.82	1/355 (0.3%)
2	D	0.46	0/241	0.88	0/368
3	A	0.36	0/5351	0.58	0/7264
4	B	0.32	0/798	0.58	0/1088
All	All	0.36	0/6621	0.60	1/9075 (0.0%)

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	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	DG	N9-C1'-C2'	-5.02	103.05	112.60

There are no chirality outliers.

All (5) 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

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Mol	Chain	Res	Type	Group
2	D	5	DA	Sidechain
2	D	6	DT	Sidechain

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	C	225	0	127	17	0
2	D	216	0	125	3	0
3	A	5222	0	4963	105	0
4	B	783	0	767	24	0
5	A	1	0	0	0	0
6	A	103	0	0	2	0
6	B	7	0	0	1	0
6	C	4	0	0	0	0
6	D	6	0	0	0	0
All	All	6567	0	5982	142	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 11.

All (142) 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'	1.33	1.09
4:B:23:ILE:HD13	4:B:54:THR:HB	1.59	0.84
1:C:22:2DT:C6	1:C:22:2DT:H5'	2.14	0.76
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.69	0.73
1:C:21:DA:H2'	1:C:22:2DT:H73	1.70	0.73
1:C:21:DA:H2''	1:C:22:2DT:C5'	2.19	0.73
3:A:632:MET:HA	3:A:635:GLU:HG2	1.73	0.71
1:C:21:DA:H2''	1:C:22:2DT:H5''	1.75	0.68
3:A:145:ARG:O	3:A:149:GLU:HG3	1.94	0.68
1:C:17:DT:H2''	1:C:18:DG:H5'	1.74	0.67
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.75	0.66
3:A:507:THR:HG23	3:A:518:ARG:HE	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:365:ASP:OD1	3:A:368:VAL:HG12	1.94	0.66
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.78	0.66
3:A:505:ILE:HD12	3:A:506:HIS:N	2.10	0.66
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.78	0.65
3:A:501:LEU:CD2	3:A:689:LEU:HB3	2.27	0.65
1:C:16:DG:H2''	1:C:17:DT:H5'	1.79	0.64
3:A:344:LYS:O	3:A:348:GLU:HG3	1.96	0.64
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.39	0.62
3:A:270:GLY:HA3	3:A:288:ARG:HB2	1.82	0.62
3:A:507:THR:CG2	3:A:518:ARG:HE	2.12	0.62
3:A:276:HIS:CD2	3:A:278:ARG:H	2.17	0.62
3:A:365:ASP:H	3:A:368:VAL:CG1	2.11	0.61
3:A:55:LEU:HD13	3:A:89:ILE:HD11	1.81	0.61
3:A:391:MET:HE2	3:A:392:ILE:HA	1.82	0.61
4:B:4:ILE:HG21	4:B:57:LYS:HG3	1.83	0.61
3:A:391:MET:HE2	3:A:392:ILE:HD13	1.82	0.60
3:A:546:GLU:O	3:A:548:GLY:N	2.34	0.60
3:A:481:LEU:HD23	3:A:529:LEU:HD11	1.85	0.59
2:D:8:DA:H4'	3:A:432:HIS:O	2.03	0.58
3:A:131:ARG:O	3:A:135:MET:HG2	2.03	0.58
3:A:501:LEU:HD21	3:A:689:LEU:HB3	1.86	0.57
3:A:355:LYS:HE2	3:A:363:VAL:HG21	1.87	0.57
1:C:20:DG:H5'	3:A:394:LYS:NZ	2.20	0.57
3:A:233:PRO:HB2	3:A:456:GLY:O	2.05	0.56
3:A:525:ILE:HG23	3:A:526:TYR:N	2.20	0.56
3:A:506:HIS:HB2	3:A:518:ARG:CZ	2.36	0.56
3:A:173:GLN:O	3:A:176:VAL:HG22	2.06	0.56
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.41	0.56
3:A:64:TYR:O	3:A:67:PRO:HD2	2.05	0.55
3:A:19:HIS:O	3:A:36:PRO:HD3	2.06	0.55
3:A:323:GLY:O	3:A:325:PRO:HD3	2.08	0.54
1:C:21:DA:H2''	1:C:22:2DT:H5'	1.90	0.54
1:C:20:DG:H5'	3:A:394:LYS:HZ3	1.73	0.53
3:A:284:PRO:HA	3:A:288:ARG:HH22	1.74	0.52
3:A:663:GLU:HG2	3:A:696:MET:SD	2.50	0.52
3:A:292:PRO:HG3	6:B:4089:HOH:O	2.10	0.51
4:B:37:MET:O	4:B:40:PRO:HD2	2.11	0.51
3:A:695:LYS:NZ	3:A:704:HIS:C	2.64	0.51
4:B:3:LYS:HG3	4:B:47:ASP:OD1	2.11	0.51
3:A:276:HIS:HD2	3:A:278:ARG:H	1.58	0.51
3:A:273:MET:CE	3:A:284:PRO:HG3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:22:ALA:HB1	4:B:53:LEU:HD12	1.93	0.51
3:A:49:GLU:CD	3:A:52:ARG:HH12	2.14	0.50
3:A:49:GLU:HA	3:A:52:ARG:NH1	2.27	0.50
3:A:452:ARG:HB3	3:A:701:ALA:HB2	1.93	0.50
3:A:158:MET:HA	3:A:161:TRP:CD2	2.45	0.50
1:C:16:DG:H2''	1:C:17:DT:C5'	2.42	0.49
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.93	0.49
3:A:79:ARG:HG2	3:A:80:GLU:N	2.26	0.49
3:A:410:VAL:HG23	3:A:410:VAL:O	2.13	0.49
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.94	0.49
3:A:353:PRO:HB2	3:A:356:TYR:CZ	2.48	0.49
1:C:17:DT:H2''	1:C:18:DG:C5'	2.42	0.49
3:A:546:GLU:O	3:A:547:ARG:C	2.51	0.49
3:A:597:ASP:OD1	3:A:599:ARG:CD	2.61	0.48
1:C:17:DT:H1'	1:C:18:DG:H5''	1.95	0.48
3:A:237:LYS:O	3:A:241:GLU:HG3	2.13	0.48
3:A:505:ILE:HD12	3:A:506:HIS:H	1.77	0.48
3:A:590:ARG:HD3	3:A:592:TRP:CE2	2.48	0.48
3:A:148:GLU:N	3:A:148:GLU:OE2	2.46	0.48
3:A:155:VAL:O	3:A:156:ASP:C	2.50	0.48
4:B:22:ALA:HB3	4:B:53:LEU:HA	1.96	0.48
4:B:58:LEU:HD21	4:B:66:THR:HB	1.96	0.48
4:B:103:LEU:O	4:B:107:LEU:HD13	2.14	0.48
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.14	0.47
3:A:484:LEU:O	3:A:488:MET:HG2	2.14	0.47
1:C:20:DG:H2''	1:C:21:DA:H5'	1.97	0.47
3:A:347:GLN:C	3:A:349:ALA:H	2.17	0.47
3:A:525:ILE:CG2	3:A:526:TYR:N	2.77	0.47
3:A:489:ALA:HA	3:A:492:ASP:OD1	2.14	0.47
3:A:588:TRP:CH2	3:A:606:PRO:HG3	2.50	0.47
4:B:79:LEU:HB3	4:B:81:PHE:CE1	2.50	0.47
3:A:343:GLN:OE1	3:A:347:GLN:NE2	2.48	0.47
1:C:21:DA:H5''	3:A:440:ILE:O	2.16	0.46
3:A:158:MET:HA	3:A:161:TRP:CE2	2.51	0.46
4:B:17:LEU:HA	4:B:84:GLY:HA2	1.97	0.46
3:A:667:GLN:HG3	3:A:696:MET:CE	2.46	0.46
3:A:49:GLU:OE1	3:A:52:ARG:NH1	2.41	0.46
3:A:588:TRP:CD2	3:A:591:ARG:HD2	2.50	0.46
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.16	0.46
4:B:27:PHE:CE1	4:B:79:LEU:HD22	2.51	0.46
3:A:591:ARG:O	3:A:591:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.51	0.46
1:C:20:DG:H2"	1:C:21:DA:C5'	2.46	0.45
3:A:268:LYS:O	3:A:328:PRO:HB2	2.16	0.45
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.98	0.45
4:B:67:ALA:HB3	4:B:68:PRO:HD3	1.97	0.45
4:B:11:SER:O	4:B:15:ASP:HB2	2.17	0.45
3:A:698:PRO:CG	3:A:702:ILE:HD12	2.47	0.45
3:A:513:ALA:O	3:A:514:GLU:HB2	2.17	0.45
2:D:7:DC:H4'	3:A:431:THR:HG22	1.98	0.45
4:B:4:ILE:HG23	4:B:55:VAL:O	2.18	0.44
3:A:574:VAL:HB	3:A:575:GLU:H	1.62	0.44
3:A:53:GLY:HA2	6:A:4063:HOH:O	2.18	0.44
3:A:698:PRO:HD2	3:A:702:ILE:HD12	1.98	0.44
4:B:25:VAL:HA	4:B:56:ALA:O	2.18	0.44
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.53	0.44
3:A:667:GLN:HG3	3:A:696:MET:HE1	1.99	0.43
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.84	0.43
3:A:391:MET:HE1	3:A:447:TYR:CD2	2.52	0.43
3:A:282:PRO:C	3:A:284:PRO:HD3	2.38	0.43
3:A:391:MET:HE3	3:A:391:MET:O	2.19	0.43
3:A:347:GLN:C	3:A:349:ALA:N	2.72	0.43
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.99	0.43
3:A:467:LYS:HD2	3:A:467:LYS:HA	1.90	0.43
3:A:554:LYS:O	3:A:558:ASN:ND2	2.51	0.42
3:A:181:LEU:HD22	3:A:185:LEU:HD11	2.01	0.42
3:A:501:LEU:HD12	3:A:501:LEU:N	2.34	0.42
3:A:422:PRO:HB2	6:A:4025:HOH:O	2.20	0.42
3:A:543:ALA:O	3:A:545:LYS:N	2.52	0.42
4:B:34:PRO:O	4:B:37:MET:HB2	2.20	0.42
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.55	0.42
3:A:143:PHE:CE2	3:A:158:MET:HG3	2.55	0.42
3:A:105:THR:HB	3:A:110:LEU:O	2.20	0.41
3:A:528:PHE:HD1	3:A:529:LEU:HD23	1.85	0.41
3:A:282:PRO:O	3:A:284:PRO:HD3	2.21	0.41
3:A:234:PHE:CD2	3:A:410:VAL:CG1	3.03	0.41
3:A:321:VAL:HG11	4:B:98:GLN:NE2	2.35	0.41
2:D:10:DA:H2"	2:D:11:DC:C6	2.55	0.41
3:A:155:VAL:HG12	3:A:156:ASP:N	2.35	0.41
3:A:678:ARG:NH1	3:A:691:ASP:OD1	2.54	0.41
4:B:9:ASP:OD1	4:B:63:ASN:HB3	2.21	0.41
3:A:326:TYR:HB3	4:B:92:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:LEU:HD22	3:A:689:LEU:HB3	1.99	0.41
3:A:698:PRO:HG2	3:A:702:ILE:HD12	2.03	0.41
1:C:16:DG:H1'	1:C:17:DT:H5''	2.02	0.40
3:A:546:GLU:C	3:A:548:GLY:N	2.75	0.40
3:A:397:GLY:O	3:A:402:GLY:HA3	2.21	0.40
3:A:506:HIS:HB2	3:A:518:ARG:NH2	2.35	0.40
4:B:81:PHE:HA	4:B:85:GLU:O	2.21	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	
3	A	667/698 (96%)	634 (95%)	20 (3%)	13 (2%)	10	8
4	B	103/108 (95%)	96 (93%)	7 (7%)	0	100	100
All	All	770/806 (96%)	730 (95%)	27 (4%)	13 (2%)	11	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	544	GLY
3	A	547	ARG
3	A	359	LYS
3	A	516	PRO
3	A	539	GLN
3	A	543	ALA
3	A	545	LYS
3	A	541	VAL
3	A	546	GLU
3	A	653	HIS

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Mol	Chain	Res	Type
3	A	297	ILE
3	A	532	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	518/579 (90%)	500 (96%)	18 (4%)	43	58
4	B	80/87 (92%)	79 (99%)	1 (1%)	76	87
All	All	598/666 (90%)	579 (97%)	19 (3%)	46	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	62	HIS
3	A	78	ASN
3	A	85	ARG
3	A	94	LEU
3	A	145	ARG
3	A	148	GLU
3	A	171	ASN
3	A	181	LEU
3	A	195	GLU
3	A	232	PHE
3	A	368	VAL
3	A	391	MET
3	A	403	ASP
3	A	467	LYS
3	A	574	VAL
3	A	599	ARG
3	A	624	LEU
3	A	686	PHE
4	B	14	THR

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

Mol	Chain	Res	Type
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
4	B	50	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	1.41	3 (27%)	12,28,31	5.02	4 (33%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	22	2DT	C6-C5	-2.07	1.34	1.40
1	C	22	2DT	C6-N1	2.57	1.38	1.35
1	C	22	2DT	C4-N3	3.09	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	22	2DT	C5-C4-N3	-8.97	115.15	125.14
1	C	22	2DT	O4'-C4'-C5'	-3.89	103.81	109.54
1	C	22	2DT	C5M-C5-C6	2.20	123.05	118.62
1	C	22	2DT	C4-N3-C2	14.05	127.39	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	22	2DT	6	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

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	C	10/22 (45%)	0.47	2 (20%) 1 2	34, 44, 72, 75	0
2	D	11/26 (42%)	0.35	1 (9%) 11 17	26, 38, 62, 72	0
3	A	673/698 (96%)	0.35	45 (6%) 21 29	16, 30, 63, 70	0
4	B	105/108 (97%)	0.64	14 (13%) 4 7	28, 43, 58, 62	0
All	All	799/854 (93%)	0.39	62 (7%) 16 22	16, 33, 62, 75	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	294	VAL	7.9
4	B	20	ASP	7.4
3	A	313	CYS	5.5
3	A	298	PHE	5.4
3	A	532	ALA	5.1
3	A	535	GLU	5.0
3	A	533	GLY	4.7
3	A	531	GLY	4.7
4	B	21	GLY	4.5
3	A	543	ALA	4.3
4	B	107	LEU	4.2
4	B	22	ALA	4.2
3	A	541	VAL	4.1
2	D	15	DC	4.0
4	B	103	LEU	3.8
3	A	526	TYR	3.8
3	A	521	ALA	3.6
4	B	83	ASN	3.5
3	A	540	ILE	3.3
3	A	360	GLY	3.3
3	A	151	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	506	HIS	3.2
3	A	516	PRO	3.2
3	A	513	ALA	3.2
4	B	53	LEU	3.2
3	A	528	PHE	3.0
4	B	89	THR	3.0
3	A	292	PRO	3.0
3	A	515	LEU	3.0
3	A	297	ILE	2.9
3	A	544	GLY	2.8
3	A	548	GLY	2.8
3	A	510	GLN	2.8
3	A	551	LEU	2.7
3	A	295	GLY	2.7
3	A	529	LEU	2.7
3	A	542	GLY	2.7
3	A	505	ILE	2.6
1	C	12	DG	2.5
3	A	534	ASP	2.5
3	A	546	GLU	2.5
4	B	54	THR	2.5
3	A	517	THR	2.4
1	C	13	DG	2.4
3	A	556	LEU	2.4
4	B	50	GLN	2.4
3	A	361	ALA	2.3
3	A	539	GLN	2.3
4	B	51	GLY	2.3
3	A	319	GLU	2.3
3	A	444	ARG	2.3
3	A	558	ASN	2.3
4	B	47	ASP	2.2
3	A	321	VAL	2.2
3	A	552	LYS	2.2
4	B	102	PHE	2.2
3	A	537	ILE	2.2
4	B	80	LEU	2.2
3	A	425	ALA	2.1
3	A	545	LYS	2.1
3	A	324	ALA	2.0
3	A	358	ASP	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
1	2DT	C	22	19/20	0.97	0.16	-	32,33,34,35	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	0.86	0.45	-	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.