W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:17 AM GMT

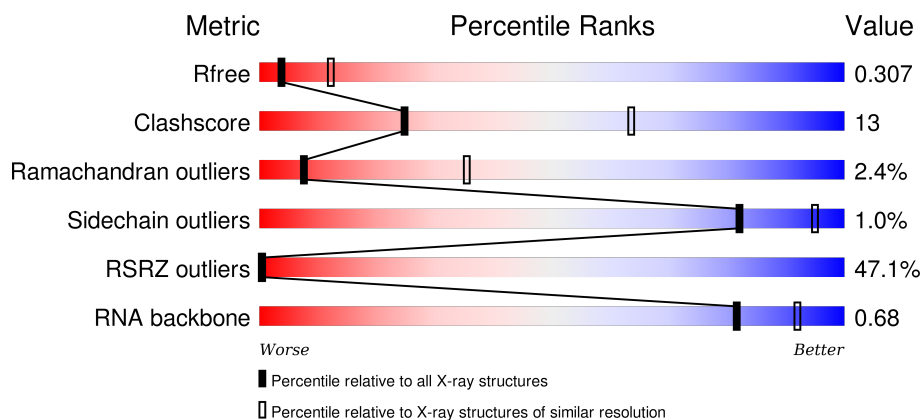|		
PDB ID	:	3E2E
Title	:	Crystal Structure of an Intermediate Complex of T7 RNAP and 7nt of RNA
Authors	:	Durniak, K.J.; Bailey, S.; Steitz, T.A.
Deposited on	:	2008-08-05
Resolution	:	3.00 Å(reported)

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 3.00 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		0.307
Clashscore		13
Ramachandran outliers		2.4%
Sidechain outliers		1.0%
RSRZ outliers		47.1%
RNA backbone		0.68

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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	889	40% / 72% 19% · 6%
2	R	7	100% / 86% 14%
3	T	33	94% / 52% 39% · 6%
4	N	33	82% / 55% 24% 6% 15%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8013 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-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6589	4206	1139	1207	37			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P00573
A	-4	HIS	-	EXPRESSION TAG	UNP P00573
A	-3	HIS	-	EXPRESSION TAG	UNP P00573
A	-2	HIS	-	EXPRESSION TAG	UNP P00573
A	-1	HIS	-	EXPRESSION TAG	UNP P00573
A	0	HIS	-	EXPRESSION TAG	UNP P00573
A	266	LEU	PRO	ENGINEERED	UNP P00573

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*GP*UP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	7	Total	C	N	O	P	0	0	0
			153	69	32	46	6			

- Molecule 3 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	31	Total	C	N	O	P	0	0	0
			633	301	113	188	31			

- Molecule 4 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	28	Total	C	N	O	P	0	0	0
			565	271	101	166	27			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total 64	O 64	0	0
5	N	5	Total 5	O 5	0	0
5	R	1	Total 1	O 1	0	0
5	T	3	Total 3	O 3	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-directed RNA polymerase

W796 W797 A798 K801 Y802 G803 I804 L809 S813 F814 G815 T816 I817 P818 A819 D820 A821 A822 N823 L824 V828 R829 E830 T831 M832 T835 Y836 E837 S838 C839 D840 Y846 D847 Q848 F849 A850 D851 Q852 L853 H854 E855 S856 Q857 L858 D859 K860 M861 P862 A863 L864 P865 A866 N869

L870 R873 D874 I875 L876 E877 S878 D879 F880 A881 F882 A883

- Molecule 2: RNA (5'-R(*GP*GP*GP*AP*GP*UP*G)-3')

Chain R:

100%

86%   14%

G1 G2 G3 A4 G5 U6 G7

- Molecule 3: DNA (31-MER)

Chain T:

94%

52%   39%   • 6%

A1 G2 C3 C4 G5 T6 G7 C8 G9 C10 A11 C12 T13 C14 C15 C16 DT DA T19 A20 G21 T22 G23 A24 G25 T26 C27 G28 T29 A30 T31 T32 A33

- Molecule 4: DNA (28-MER)

Chain N:

82%

55%   24%   6%   15%

T101 A102 A103 T104 A105 C106 G107 A108 C109 T110 C111 A112 C113 DT DA DT DA DT T119 T120 C121 T122 G123 G124 C125 G126 C127 A128 C129 G130 G131 C132 T133
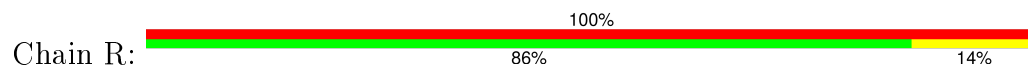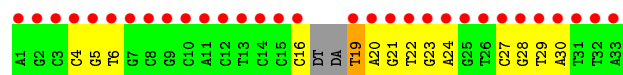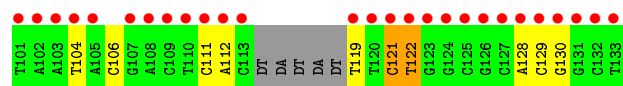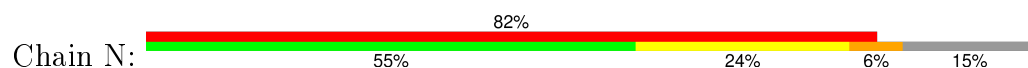
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	81.01Å 81.01Å 358.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.80 – 3.00 37.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.80-3.00) 98.5 (37.79-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.31 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.292 0.251 , 0.307	Depositor DCC
R_{free} test set	1330 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 85.3	EDS
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 26097 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	8013	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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)

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	0.34	0/6738	0.58	4/9109 (0.0%)
2	R	0.65	0/172	1.12	0/269
3	T	0.63	0/707	1.24	1/1086 (0.1%)
4	N	0.65	0/631	1.33	4/969 (0.4%)
All	All	0.41	0/8248	0.77	9/11433 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	19	DT	O4'-C1'-N1	8.94	114.26	108.00
4	N	122	DT	O4'-C1'-N1	7.05	112.93	108.00
1	A	43	SER	N-CA-C	6.99	129.88	111.00
4	N	121	DC	P-O3'-C3'	6.39	127.37	119.70
4	N	104	DT	C1'-O4'-C4'	-6.28	103.82	110.10
4	N	119	DT	O4'-C4'-C3'	-6.05	102.08	104.50
1	A	553	GLU	C-N-CA	5.83	136.28	121.70
1	A	43	SER	C-N-CA	5.82	136.25	121.70
1	A	44	TYR	N-CA-C	5.36	125.46	111.00

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	6589	0	6558	176	0
2	R	153	0	75	4	0
3	T	633	0	351	19	0
4	N	565	0	315	5	0
5	A	64	0	0	9	0
5	N	5	0	0	0	0
5	R	1	0	0	0	0
5	T	3	0	0	1	0
All	All	8013	0	7299	195	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 13.

All (195) 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:376:ALA:HB3	1:A:377:TRP:CB	1.72	1.19
1:A:553:GLU:CG	1:A:554:VAL:HG23	1.87	1.04
1:A:354:ALA:CA	1:A:355:ILE:HG12	1.88	1.04
1:A:131:ASN:HB3	1:A:132:THR:HA	1.06	1.03
1:A:354:ALA:HA	1:A:355:ILE:CG1	1.87	1.03
1:A:354:ALA:HB1	1:A:356:GLU:H	1.24	1.00
1:A:553:GLU:HG3	1:A:554:VAL:HG23	1.40	1.00
1:A:354:ALA:HA	1:A:355:ILE:HG12	1.01	1.00
1:A:131:ASN:CB	1:A:132:THR:HA	1.92	0.98
1:A:376:ALA:HB3	1:A:377:TRP:HB3	0.98	0.97
1:A:376:ALA:CB	1:A:377:TRP:HB3	1.94	0.96
1:A:451:PRO:HA	1:A:452:ILE:CB	1.99	0.93
1:A:451:PRO:HA	1:A:452:ILE:CG1	1.99	0.93
1:A:882:PHE:HA	5:A:907:HOH:O	1.69	0.92
1:A:556:GLY:HA3	1:A:557:ARG:HB2	1.51	0.91
3:T:19:DT:H2"	3:T:20:DA:OP1	1.69	0.89
1:A:370:ASN:HB2	1:A:371:PRO:HD2	1.55	0.89
1:A:131:ASN:HB3	1:A:132:THR:CA	2.00	0.85
1:A:349:VAL:CG2	1:A:352:ILE:HG12	2.06	0.85
1:A:850:ALA:HA	1:A:851:ASP:C	1.98	0.82
1:A:53:LYS:HB3	1:A:54:MET:HB2	1.63	0.79
1:A:556:GLY:HA3	1:A:557:ARG:CB	2.13	0.79
1:A:278:TRP:H	1:A:321:ASN:HD21	1.31	0.79
1:A:376:ALA:CB	1:A:377:TRP:CB	2.56	0.78
1:A:553:GLU:HG2	1:A:554:VAL:HG23	1.69	0.75
1:A:863:ALA:HB3	1:A:864:LEU:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:PRO:HA	1:A:452:ILE:HB	1.70	0.73
1:A:354:ALA:HB3	1:A:391:ARG:HE	1.52	0.73
1:A:222:GLU:HB3	1:A:223:SER:HB3	1.68	0.73
1:A:354:ALA:HB1	1:A:356:GLU:N	2.03	0.72
1:A:451:PRO:HA	1:A:452:ILE:HG13	1.71	0.71
1:A:864:LEU:HD12	1:A:865:PRO:HD2	1.73	0.70
1:A:553:GLU:HG3	1:A:554:VAL:CG2	2.20	0.70
1:A:349:VAL:HG23	1:A:352:ILE:HG12	1.73	0.69
1:A:816:THR:HG22	1:A:817:ILE:N	2.08	0.69
1:A:710:VAL:HG21	1:A:719:LEU:HB2	1.76	0.68
1:A:550:LEU:HD11	1:A:695:ALA:HB2	1.75	0.68
1:A:784:HIS:HA	1:A:787:ASP:OD1	1.95	0.67
1:A:862:PRO:HB2	1:A:863:ALA:HB2	1.78	0.66
1:A:816:THR:HG22	1:A:817:ILE:H	1.60	0.65
1:A:375:THR:OG1	1:A:376:ALA:HA	1.97	0.65
2:R:1:G:C4	3:T:19:DT:H5"	2.32	0.65
1:A:739:TYR:H	1:A:774:GLN:NE2	1.95	0.65
1:A:452:ILE:HD11	1:A:529:ASN:HA	1.79	0.64
2:R:1:G:C5	3:T:19:DT:H5"	2.34	0.62
1:A:556:GLY:CA	1:A:557:ARG:CB	2.77	0.62
1:A:507:SER:HB3	1:A:510:CYS:HB2	1.80	0.62
1:A:224:THR:N	1:A:225:GLY:HA2	2.15	0.61
1:A:150:ARG:HH22	1:A:199:GLU:HB3	1.66	0.60
1:A:52:ARG:HA	1:A:55:PHE:HB2	1.84	0.59
1:A:180:LYS:HB3	1:A:181:ALA:HA	1.83	0.59
1:A:748:ASN:HB3	4:N:106:DC:H2"	1.84	0.59
1:A:489:ILE:HG22	1:A:490:MET:H	1.68	0.59
1:A:850:ALA:HA	1:A:851:ASP:O	2.02	0.58
1:A:291:ARG:O	1:A:292:ARG:HB3	2.03	0.58
1:A:452:ILE:CD1	1:A:529:ASN:HA	2.34	0.58
1:A:376:ALA:H	1:A:378:LYS:N	2.01	0.58
1:A:472:LYS:HG2	1:A:472:LYS:O	2.04	0.58
1:A:278:TRP:H	1:A:321:ASN:ND2	1.99	0.57
1:A:729:THR:HG22	1:A:733:PHE:HB3	1.86	0.57
1:A:710:VAL:HG11	1:A:719:LEU:N	2.19	0.57
1:A:863:ALA:HB3	1:A:864:LEU:CA	2.34	0.57
3:T:6:DT:H3	4:N:128:DA:H61	1.53	0.56
1:A:352:ILE:HD12	1:A:398:LEU:HD11	1.86	0.56
1:A:804:ILE:HG12	1:A:820:ASP:HB3	1.87	0.56
1:A:349:VAL:HG21	1:A:352:ILE:HG12	1.83	0.56
4:N:111:DC:H2"	4:N:112:DA:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ARG:NH2	5:A:907:HOH:O	2.38	0.56
1:A:710:VAL:HG11	1:A:719:LEU:H	1.71	0.56
1:A:180:LYS:HE3	1:A:183:MET:HG2	1.88	0.56
1:A:222:GLU:H	1:A:223:SER:C	2.09	0.55
1:A:20:PRO:O	1:A:24:LEU:HB2	2.06	0.55
4:N:121:DC:H4'	4:N:122:DT:OP1	2.07	0.55
3:T:22:DT:H2'	3:T:23:DG:C8	2.42	0.55
1:A:729:THR:CG2	1:A:733:PHE:HB3	2.37	0.55
1:A:224:THR:H	1:A:225:GLY:HA2	1.71	0.54
1:A:324:GLN:HA	1:A:418:TYR:HD1	1.72	0.54
1:A:760:THR:O	3:T:20:DA:H2'	2.08	0.54
1:A:639:TYR:HB3	1:A:780:PRO:HB3	1.89	0.54
1:A:681:ILE:O	1:A:685:VAL:HG12	2.08	0.54
1:A:560:ASN:O	1:A:881:ALA:HB2	2.08	0.53
1:A:424:GLY:HA3	5:A:897:HOH:O	2.08	0.53
1:A:383:ALA:O	1:A:387:LYS:HG3	2.09	0.53
1:A:408:PHE:HA	1:A:411:HIS:CD2	2.43	0.53
1:A:291:ARG:O	1:A:292:ARG:CB	2.57	0.53
1:A:375:THR:O	1:A:378:LYS:HB2	2.08	0.53
1:A:763:THR:HG22	1:A:765:LYS:H	1.73	0.53
1:A:180:LYS:HA	1:A:182:PHE:N	2.25	0.52
1:A:423:ARG:HH11	1:A:781:ASN:HD22	1.56	0.52
1:A:53:LYS:CB	1:A:54:MET:HB2	2.38	0.52
2:R:1:G:C4	3:T:19:DT:C5'	2.93	0.52
1:A:126:LEU:HD13	1:A:246:LEU:HB2	1.92	0.52
1:A:524:HIS:HB2	1:A:528:TYR:HB2	1.92	0.52
3:T:20:DA:O5'	3:T:20:DA:H8	1.93	0.51
1:A:862:PRO:HB2	1:A:863:ALA:CB	2.40	0.51
1:A:739:TYR:H	1:A:774:GLN:HE21	1.57	0.51
1:A:862:PRO:HB2	1:A:863:ALA:CA	2.41	0.51
1:A:180:LYS:HG2	1:A:182:PHE:HD1	1.76	0.51
1:A:264:ILE:N	1:A:265:SER:HB3	2.25	0.51
1:A:705:LEU:HB3	1:A:857:GLN:HE21	1.76	0.51
1:A:324:GLN:HE21	1:A:418:TYR:H	1.58	0.51
1:A:851:ASP:O	1:A:853:LEU:N	2.44	0.50
3:T:4:DC:H6	5:T:36:HOH:O	1.94	0.50
1:A:531:SER:HA	1:A:817:ILE:HG22	1.94	0.50
1:A:133:THR:HG23	1:A:136:ALA:HB2	1.93	0.50
1:A:537:ASP:O	1:A:882:PHE:HB2	2.12	0.49
1:A:362:MET:H	1:A:377:TRP:HE1	1.60	0.49
1:A:214:VAL:HG11	1:A:749:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ARG:NH1	1:A:878:SER:O	2.45	0.49
1:A:543:ILE:HD13	1:A:689:VAL:HG11	1.94	0.49
1:A:341:ILE:HD11	1:A:509:PHE:CZ	2.47	0.49
1:A:222:GLU:N	1:A:223:SER:C	2.66	0.49
1:A:376:ALA:H	1:A:378:LYS:H	1.61	0.48
1:A:747:LEU:HB2	1:A:759:PRO:HD2	1.96	0.48
1:A:816:THR:CG2	1:A:817:ILE:N	2.76	0.48
1:A:538:GLY:HA2	5:A:887:HOH:O	2.13	0.48
1:A:421:ASP:O	1:A:423:ARG:O	2.32	0.47
1:A:298:ARG:HH21	1:A:419:ASN:HB2	1.79	0.47
1:A:454:LYS:H	1:A:526:LEU:HD22	1.80	0.47
1:A:829:ARG:HB2	1:A:876:LEU:HD23	1.97	0.47
1:A:831:THR:O	1:A:835:THR:HG23	2.15	0.47
1:A:798:ALA:HB1	1:A:804:ILE:HD12	1.96	0.47
1:A:706:LEU:HD11	1:A:849:PHE:HB2	1.97	0.47
1:A:536:PHE:HB3	1:A:882:PHE:HB3	1.96	0.46
1:A:133:THR:HG23	1:A:136:ALA:CB	2.45	0.46
1:A:623:TYR:HB2	1:A:666:MET:SD	2.54	0.46
1:A:107:GLN:HB2	5:A:938:HOH:O	2.15	0.46
1:A:637:LEU:C	1:A:639:TYR:H	2.19	0.46
3:T:16:DC:H2"	3:T:19:DT:O4	2.16	0.46
1:A:347:CYS:SG	1:A:349:VAL:HG22	2.56	0.46
1:A:864:LEU:HD12	1:A:865:PRO:CD	2.44	0.46
1:A:530:CYS:SG	1:A:818:PRO:HG2	2.56	0.45
1:A:354:ALA:CB	1:A:355:ILE:HG12	2.42	0.45
1:A:794:THR:OG1	1:A:831:THR:HG21	2.15	0.45
1:A:278:TRP:CD2	1:A:284:GLY:HA3	2.52	0.45
1:A:223:SER:HA	1:A:224:THR:HA	1.70	0.45
1:A:854:HIS:O	1:A:855:GLU:HB2	2.16	0.45
1:A:816:THR:CG2	1:A:817:ILE:H	2.27	0.45
1:A:131:ASN:CB	1:A:132:THR:CA	2.76	0.45
1:A:376:ALA:CB	1:A:377:TRP:HB2	2.45	0.45
2:R:1:G:C2	3:T:19:DT:H5'	2.52	0.45
1:A:400:PHE:HD1	1:A:401:MET:HE2	1.82	0.45
1:A:790:HIS:NE2	1:A:832:MET:HB2	2.32	0.45
1:A:165:ASN:HA	1:A:166:VAL:HA	1.67	0.45
3:T:20:DA:C8	3:T:20:DA:O5'	2.70	0.45
1:A:489:ILE:HG22	1:A:490:MET:N	2.32	0.45
4:N:129:DC:H2"	4:N:130:DG:C8	2.52	0.45
1:A:824:LEU:O	1:A:828:VAL:HG22	2.17	0.45
1:A:82:ILE:HD13	1:A:112:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:LEU:HD21	1:A:809:LEU:HD13	1.99	0.44
1:A:797:TRP:CZ2	1:A:801:LYS:HD2	2.52	0.44
3:T:23:DG:H2"	3:T:24:DA:C8	2.53	0.44
1:A:376:ALA:N	1:A:378:LYS:H	2.15	0.44
1:A:534:LEU:O	1:A:815:GLY:HA2	2.18	0.44
1:A:354:ALA:CB	1:A:356:GLU:H	2.12	0.44
1:A:760:THR:O	3:T:20:DA:C2'	2.65	0.43
1:A:231:ARG:HE	1:A:234:ALA:HB2	1.83	0.43
3:T:4:DC:H2"	3:T:5:DG:C8	2.52	0.43
1:A:392:LYS:O	1:A:396:ILE:HG12	2.19	0.43
1:A:849:PHE:O	1:A:852:GLN:HB2	2.18	0.43
1:A:705:LEU:O	1:A:857:GLN:NE2	2.52	0.43
1:A:451:PRO:CA	1:A:452:ILE:HB	2.45	0.43
1:A:160:LYS:O	1:A:164:LYS:HG3	2.19	0.43
1:A:324:GLN:HA	1:A:418:TYR:CD1	2.52	0.43
3:T:19:DT:H3'	3:T:20:DA:H5'	2.00	0.43
1:A:53:LYS:O	1:A:57:ARG:HB3	2.19	0.43
1:A:605:ILE:HA	1:A:606:SER:HA	1.77	0.43
1:A:485:ASN:HB3	1:A:488:ASN:HB2	2.00	0.42
1:A:590:THR:HB	1:A:613:THR:H	1.84	0.42
1:A:616:LEU:HD13	1:A:676:TYR:HB2	2.00	0.42
1:A:374:LEU:C	1:A:376:ALA:HB2	2.40	0.42
3:T:27:DC:H2"	3:T:28:DG:C8	2.54	0.42
1:A:862:PRO:HB2	1:A:863:ALA:HA	2.02	0.42
1:A:344:TRP:O	1:A:355:ILE:HD12	2.19	0.42
1:A:354:ALA:HA	1:A:355:ILE:CB	2.46	0.42
1:A:295:ALA:O	1:A:419:ASN:ND2	2.53	0.42
1:A:556:GLY:O	1:A:561:LEU:HB2	2.19	0.42
1:A:636:THR:HA	1:A:639:TYR:HD2	1.84	0.42
1:A:355:ILE:HA	5:A:918:HOH:O	2.19	0.41
1:A:478:ARG:HH12	1:A:882:PHE:HZ	1.67	0.41
3:T:29:DT:H2"	3:T:30:DA:C8	2.55	0.41
1:A:42:GLU:HA	1:A:45:GLU:HB2	2.03	0.41
1:A:450:LYS:O	1:A:452:ILE:HG13	2.21	0.41
1:A:78:LEU:N	1:A:79:PRO:HD2	2.35	0.41
1:A:452:ILE:HG22	1:A:526:LEU:O	2.20	0.41
1:A:38:ALA:O	1:A:42:GLU:HB2	2.21	0.41
1:A:630:THR:O	1:A:634:VAL:HG23	2.21	0.41
1:A:451:PRO:HA	1:A:452:ILE:CD1	2.49	0.40
1:A:240:ASP:O	3:T:21:DG:H2"	2.21	0.40
1:A:53:LYS:HB3	1:A:54:MET:CB	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:NH1	5:A:940:HOH:O	2.54	0.40
1:A:275:PRO:HG2	1:A:324:GLN:HG2	2.03	0.40
1:A:86:ASN:HD22	1:A:86:ASN:HA	1.74	0.40
1:A:452:ILE:HG23	5:A:933:HOH:O	2.21	0.40
1:A:74:ILE:HG13	5:A:903: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	820/889 (92%)	738 (90%)	62 (8%)	20 (2%)	7	35

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	A	371	PRO
1	A	452	ILE
1	A	554	VAL
1	A	557	ARG
1	A	851	ASP
1	A	852	GLN
1	A	42	GLU
1	A	180	LYS
1	A	556	GLY
1	A	855	GLU
1	A	222	GLU
1	A	377	TRP
1	A	454	LYS
1	A	44	TYR
1	A	638	ALA

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Mol	Chain	Res	Type
1	A	713	LYS
1	A	355	ILE
1	A	631	LYS
1	A	363	LYS

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	693/735 (94%)	686 (99%)	7 (1%)	82	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TYR
1	A	133	THR
1	A	419	ASN
1	A	452	ILE
1	A	735	VAL
1	A	828	VAL
1	A	858	LEU

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

Mol	Chain	Res	Type
1	A	22	ASN
1	A	86	ASN
1	A	269	GLN
1	A	321	ASN
1	A	324	GLN
1	A	410	ASN
1	A	419	ASN
1	A	522	GLN
1	A	697	ASN
1	A	774	GLN

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Mol	Chain	Res	Type
1	A	781	ASN
1	A	786	GLN
1	A	811	HIS
1	A	823	ASN
1	A	857	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	6/7 (85%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	A	832/889 (93%)	2.15	358 (43%)	0	0	30, 100, 101, 102	0
2	R	7/7 (100%)	5.67	7 (100%)	0	0	99, 100, 100, 101	0
3	T	31/33 (93%)	3.97	31 (100%)	0	0	97, 100, 101, 102	0
4	N	28/33 (84%)	4.49	27 (96%)	0	0	99, 100, 101, 101	0
All	All	898/962 (93%)	2.31	423 (47%)	0	0	30, 100, 101, 102	0

All (423) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	1	G	13.4
1	A	131	ASN	8.8
4	N	120	DT	8.6
1	A	716	GLY	8.2
1	A	598	THR	8.1
1	A	357	ARG	7.9
1	A	374	LEU	7.8
1	A	646	PHE	7.8
1	A	527	SER	7.7
4	N	128	DA	7.6
1	A	223	SER	7.5
1	A	385	TYR	7.4
1	A	224	THR	7.2
4	N	121	DC	7.2
1	A	714	LYS	7.1
1	A	128	SER	7.1
1	A	241	SER	7.1
1	A	375	THR	7.0
1	A	369	MET	7.0
1	A	715	THR	6.9
3	T	5	DG	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	6.8
1	A	597	VAL	6.7
1	A	222	GLU	6.7
1	A	325	ASN	6.4
1	A	671	ASN	6.4
1	A	54	MET	6.4
4	N	125	DC	6.3
1	A	230	HIS	6.2
1	A	130	ASP	6.2
1	A	479	ILE	6.1
2	R	7	G	6.1
3	T	3	DC	6.1
1	A	638	ALA	6.0
3	T	9	DG	6.0
4	N	130	DG	6.0
1	A	10	ASP	6.0
1	A	265	SER	6.0
1	A	596	THR	5.8
1	A	523	HIS	5.8
1	A	353	PRO	5.7
1	A	526	LEU	5.6
1	A	591	ASP	5.6
4	N	129	DC	5.6
4	N	126	DG	5.5
3	T	33	DA	5.4
4	N	127	DC	5.4
1	A	376	ALA	5.2
1	A	358	GLU	5.2
3	T	2	DG	5.2
1	A	98	LYS	5.2
3	T	19	DT	5.2
1	A	364	PRO	5.2
1	A	99	ARG	5.1
1	A	489	ILE	5.1
2	R	3	G	5.1
1	A	518	TYR	5.1
1	A	605	ILE	5.1
1	A	299	THR	5.0
1	A	312	TYR	5.0
1	A	252	GLU	5.0
3	T	29	DT	5.0
3	T	1	DA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	879	ASP	4.9
1	A	568	GLN	4.9
1	A	346	HIS	4.9
4	N	119	DT	4.9
3	T	20	DA	4.9
1	A	382	ALA	4.9
4	N	123	DG	4.8
1	A	393	SER	4.8
1	A	78	LEU	4.7
1	A	311	VAL	4.7
4	N	101	DT	4.7
4	N	122	DT	4.7
1	A	354	ALA	4.7
1	A	710	VAL	4.7
4	N	111	DC	4.6
4	N	131	DG	4.6
4	N	104	DT	4.6
1	A	181	ALA	4.6
2	R	6	U	4.6
1	A	623	TYR	4.6
1	A	381	ALA	4.5
1	A	506	ASP	4.5
3	T	15	DC	4.5
2	R	2	G	4.5
4	N	132	DC	4.4
1	A	764	ASN	4.3
1	A	348	PRO	4.3
1	A	582	LEU	4.3
1	A	355	ILE	4.3
1	A	573	ILE	4.3
1	A	41	HIS	4.3
1	A	370	ASN	4.3
1	A	127	THR	4.3
3	T	6	DT	4.3
1	A	878	SER	4.2
1	A	488	ASN	4.2
1	A	449	GLY	4.2
3	T	26	DT	4.2
1	A	473	VAL	4.1
1	A	165	ASN	4.1
1	A	239	GLN	4.1
1	A	371	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	588	ASN	4.1
3	T	11	DA	4.1
1	A	390	ALA	4.1
1	A	253	ALA	4.1
1	A	797	TRP	4.1
1	A	52	ARG	4.0
4	N	124	DG	4.0
1	A	344	TRP	4.0
1	A	851	ASP	4.0
1	A	639	TYR	4.0
1	A	574	VAL	4.0
1	A	482	ILE	3.9
3	T	8	DC	3.9
1	A	762	ASN	3.9
1	A	667	PHE	3.9
3	T	4	DC	3.9
1	A	593	GLU	3.9
1	A	615	ALA	3.9
1	A	567	VAL	3.9
1	A	711	LYS	3.9
1	A	566	THR	3.8
1	A	249	GLU	3.8
1	A	555	GLY	3.8
1	A	560	ASN	3.8
1	A	132	THR	3.8
1	A	373	ALA	3.8
1	A	608	LYS	3.8
1	A	589	GLY	3.8
1	A	345	LYS	3.8
4	N	112	DA	3.7
1	A	721	LYS	3.7
1	A	499	ASN	3.7
1	A	279	THR	3.7
1	A	869	ASN	3.7
1	A	476	PRO	3.7
4	N	102	DA	3.6
1	A	511	PHE	3.6
1	A	360	LEU	3.6
1	A	76	THR	3.6
1	A	465	ALA	3.6
1	A	459	TRP	3.6
1	A	564	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	522	GLN	3.6
1	A	388	ASP	3.6
1	A	343	LYS	3.6
1	A	837	GLU	3.6
1	A	380	ALA	3.6
3	T	13	DT	3.5
1	A	389	LYS	3.5
3	T	21	DG	3.5
1	A	865	PRO	3.5
1	A	81	MET	3.5
3	T	28	DG	3.5
1	A	519	ALA	3.5
4	N	103	DA	3.5
3	T	22	DT	3.5
4	N	105	DA	3.5
1	A	502	TRP	3.5
1	A	835	THR	3.5
1	A	487	GLU	3.5
3	T	23	DG	3.5
1	A	644	PHE	3.5
1	A	347	CYS	3.5
1	A	447	ALA	3.4
1	A	554	VAL	3.4
3	T	24	DA	3.4
1	A	513	ALA	3.4
1	A	575	ALA	3.4
1	A	883	ALA	3.4
1	A	139	SER	3.4
1	A	492	CYS	3.4
1	A	668	THR	3.4
1	A	719	LEU	3.4
1	A	565	GLU	3.4
1	A	90	GLU	3.4
1	A	803	GLY	3.3
1	A	818	PRO	3.3
1	A	468	ALA	3.3
1	A	720	ARG	3.3
1	A	647	ARG	3.3
1	A	819	ALA	3.3
1	A	361	PRO	3.3
4	N	133	DT	3.3
1	A	517	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	859	ASP	3.3
1	A	578	VAL	3.2
1	A	813	SER	3.2
3	T	32	DT	3.2
2	R	5	G	3.2
1	A	251	ALA	3.2
1	A	505	GLN	3.2
1	A	28	TYR	3.2
1	A	765	LYS	3.2
1	A	744	GLN	3.2
3	T	10	DC	3.2
1	A	654	THR	3.2
1	A	779	ALA	3.2
1	A	552	ASP	3.2
1	A	607	GLU	3.2
3	T	7	DG	3.1
1	A	570	ILE	3.1
1	A	480	LYS	3.1
1	A	756	ARG	3.1
1	A	616	LEU	3.1
1	A	448	LYS	3.1
1	A	846	TYR	3.1
1	A	451	PRO	3.1
1	A	362	MET	3.1
1	A	79	PRO	3.1
3	T	16	DC	3.1
1	A	661	SER	3.1
1	A	326	THR	3.1
1	A	406	ASN	3.1
1	A	769	ILE	3.1
1	A	180	LYS	3.0
1	A	824	LEU	3.0
1	A	583	GLN	3.0
1	A	660	ASP	3.0
3	T	25	DG	3.0
1	A	232	GLN	3.0
1	A	157	LEU	3.0
1	A	396	ILE	3.0
1	A	768	GLU	3.0
1	A	236	VAL	3.0
1	A	539	SER	3.0
3	T	30	DA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	766	ASP	3.0
1	A	738	GLU	3.0
1	A	590	THR	3.0
1	A	771	ALA	3.0
1	A	453	GLY	3.0
1	A	562	LEU	2.9
1	A	640	GLY	2.9
1	A	717	GLU	2.9
1	A	563	PRO	2.9
1	A	551	ARG	2.9
1	A	561	LEU	2.9
1	A	676	TYR	2.9
1	A	197	GLY	2.9
1	A	94	ALA	2.9
1	A	51	PHE	2.9
1	A	543	ILE	2.9
1	A	57	ARG	2.9
1	A	752	LEU	2.9
1	A	770	ASP	2.9
1	A	466	ASN	2.9
1	A	379	ARG	2.9
1	A	491	ALA	2.9
1	A	240	ASP	2.9
1	A	352	ILE	2.8
1	A	778	ILE	2.8
2	R	4	A	2.8
1	A	725	VAL	2.8
1	A	189	ASP	2.8
1	A	472	LYS	2.8
1	A	277	PRO	2.8
1	A	104	GLN	2.8
1	A	190	MET	2.8
1	A	635	MET	2.8
1	A	718	ILE	2.8
1	A	498	GLU	2.8
4	N	113	DC	2.8
1	A	484	GLU	2.8
1	A	556	GLY	2.8
1	A	613	THR	2.8
1	A	780	PRO	2.8
1	A	278	TRP	2.7
1	A	630	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	627	ARG	2.7
1	A	49	ALA	2.7
1	A	202	SER	2.7
1	A	531	SER	2.7
1	A	823	ASN	2.7
1	A	359	GLU	2.7
1	A	342	THR	2.7
1	A	88	TRP	2.7
1	A	742	PRO	2.7
1	A	416	PHE	2.7
1	A	368	ASP	2.7
1	A	724	ALA	2.6
1	A	433	ASN	2.6
1	A	755	PHE	2.6
1	A	77	LEU	2.6
1	A	483	GLU	2.6
1	A	75	THR	2.6
1	A	247	ALA	2.6
4	N	108	DA	2.6
1	A	739	TYR	2.6
1	A	141	ILE	2.6
1	A	397	SER	2.6
1	A	507	SER	2.6
1	A	836	TYR	2.6
1	A	275	PRO	2.6
3	T	27	DC	2.6
1	A	100	PRO	2.6
4	N	107	DG	2.6
1	A	486	HIS	2.6
1	A	525	GLY	2.6
1	A	828	VAL	2.5
1	A	145	ILE	2.5
1	A	880	PHE	2.5
1	A	93	LYS	2.5
1	A	50	ARG	2.5
1	A	184	GLN	2.5
1	A	30	GLU	2.5
1	A	553	GLU	2.5
1	A	97	GLY	2.5
1	A	785	SER	2.5
1	A	166	VAL	2.5
1	A	327	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	43	SER	2.5
1	A	378	LYS	2.5
1	A	349	VAL	2.5
4	N	109	DC	2.5
1	A	298	ARG	2.5
1	A	873	ARG	2.5
1	A	861	MET	2.5
1	A	242	GLU	2.5
1	A	455	GLU	2.5
1	A	413	ALA	2.5
1	A	85	ILE	2.5
1	A	763	THR	2.5
1	A	109	ILE	2.5
3	T	31	DT	2.5
1	A	620	TRP	2.5
1	A	464	GLY	2.4
1	A	786	GLN	2.4
1	A	633	SER	2.4
1	A	537	ASP	2.4
1	A	83	ALA	2.4
1	A	713	LYS	2.4
1	A	866	ALA	2.4
1	A	882	PHE	2.4
1	A	478	ARG	2.4
1	A	383	ALA	2.4
1	A	577	LYS	2.4
1	A	670	PRO	2.4
1	A	187	GLU	2.4
1	A	862	PRO	2.4
1	A	287	TRP	2.4
1	A	46	MET	2.4
1	A	331	ASN	2.4
1	A	300	HIS	2.4
1	A	581	ILE	2.4
1	A	781	ASN	2.3
1	A	9	ASN	2.3
1	A	363	LYS	2.3
1	A	23	THR	2.3
1	A	821	ALA	2.3
1	A	875	ILE	2.3
1	A	571	TYR	2.3
1	A	595	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
4	N	110	DT	2.3
1	A	541	SER	2.3
1	A	264	ILE	2.3
1	A	533	PRO	2.3
1	A	73	LEU	2.3
1	A	45	GLU	2.3
1	A	310	ASP	2.3
1	A	458	TYR	2.3
1	A	579	ASN	2.2
1	A	286	TYR	2.2
1	A	650	VAL	2.2
1	A	129	ALA	2.2
1	A	643	GLU	2.2
1	A	412	LYS	2.2
1	A	391	ARG	2.2
1	A	847	ASP	2.2
1	A	529	ASN	2.2
1	A	87	ASP	2.2
1	A	774	GLN	2.2
1	A	703	ALA	2.2
1	A	860	LYS	2.2
1	A	426	VAL	2.2
1	A	351	ASP	2.2
1	A	411	HIS	2.2
1	A	795	VAL	2.2
1	A	584	ALA	2.2
1	A	108	GLU	2.2
1	A	870	LEU	2.2
1	A	254	ILE	2.2
1	A	672	GLN	2.1
1	A	500	THR	2.1
1	A	542	GLY	2.1
1	A	674	ALA	2.1
1	A	686	SER	2.1
1	A	22	ASN	2.1
1	A	55	PHE	2.1
3	T	12	DC	2.1
1	A	772	HIS	2.1
1	A	274	PRO	2.1
1	A	816	THR	2.1
1	A	839	CYS	2.1
1	A	105	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	838	SER	2.1
1	A	648	GLN	2.1
1	A	659	ILE	2.1
1	A	524	HIS	2.1
1	A	559	VAL	2.1
1	A	250	TYR	2.1
1	A	637	LEU	2.1
1	A	272	VAL	2.1
1	A	504	GLU	2.1
1	A	754	GLN	2.1
3	T	14	DC	2.1
1	A	53	LYS	2.1
1	A	881	ALA	2.1
1	A	150	ARG	2.0
1	A	328	TRP	2.0
1	A	164	LYS	2.0
1	A	494	LYS	2.0
1	A	840	ASP	2.0
1	A	15	GLU	2.0
1	A	409	ALA	2.0
1	A	621	LEU	2.0
1	A	731	ASP	2.0
1	A	457	TYR	2.0
1	A	266	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.