



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:12 AM UTC

PDB ID : 3E2E / pdb\_00003e2e  
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)

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

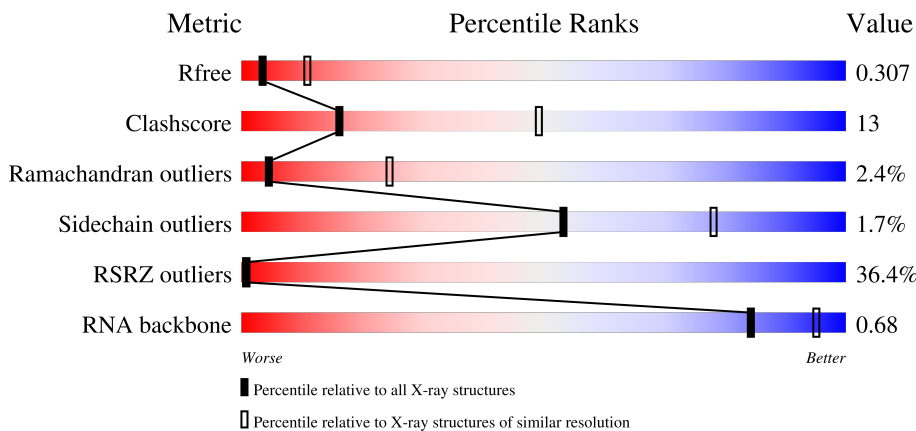
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	889	
2	R	7	
3	T	33	
4	N	33	

## 2 Entry composition

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
			Total	C	N	O	S			
1	A	832	6589	4206	1139	1207	37	0	0	0

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 mutation	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
			Total	C	N	O	P			
2	R	7	153	69	32	46	6	0	0	0

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

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

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

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

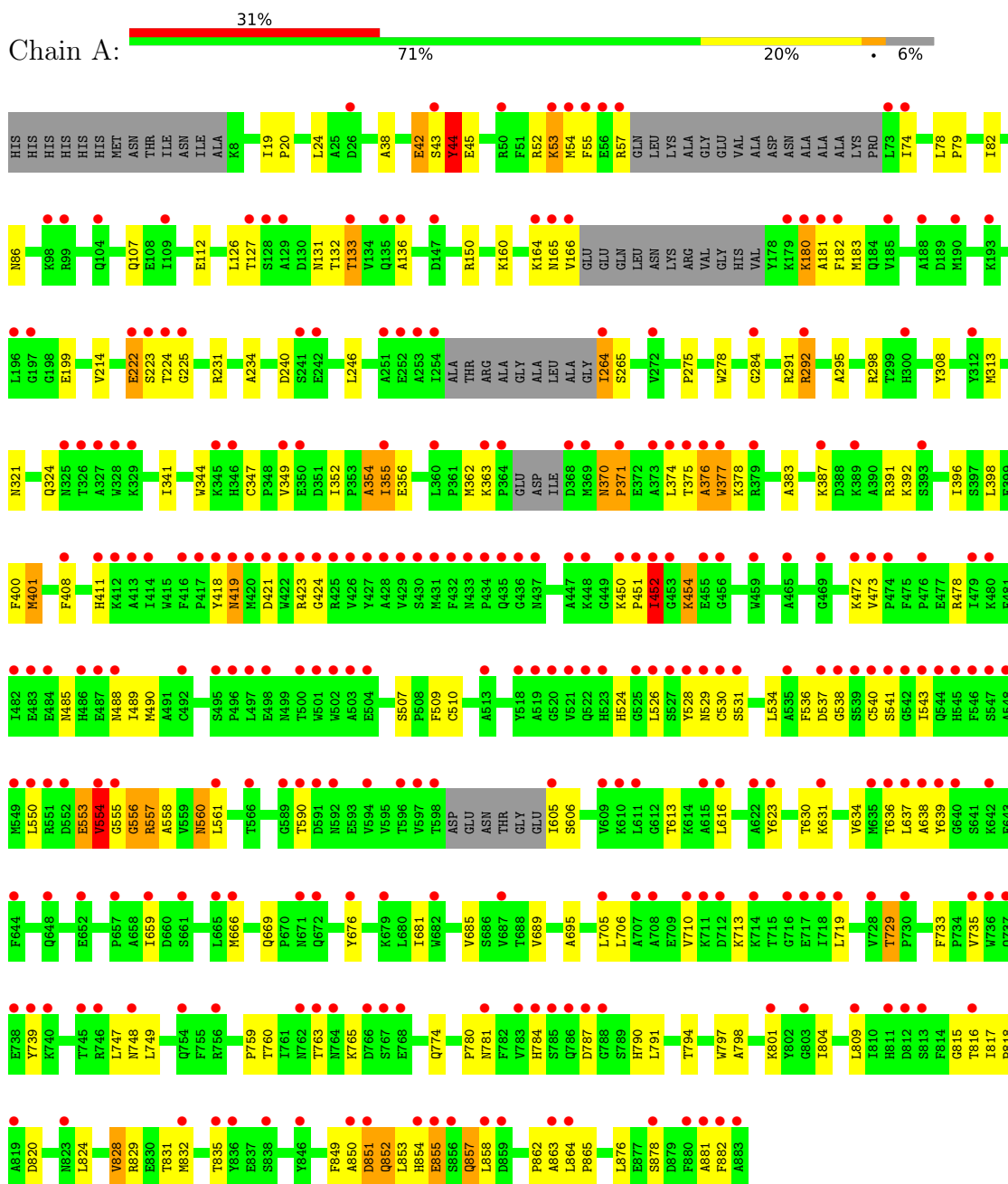
- Molecule 5 is water.

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

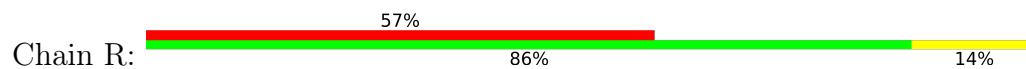
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

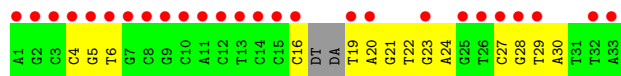
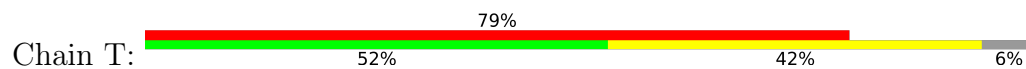
- Molecule 1: DNA-directed RNA polymerase



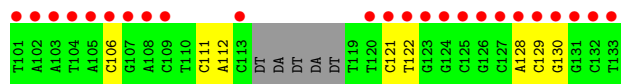
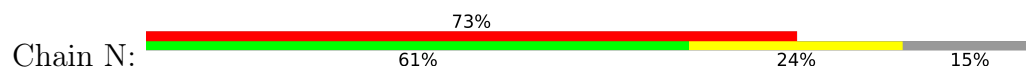
- Molecule 2: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*UP\*G)-3')



- Molecule 3: DNA (31-MER)



- Molecule 4: DNA (28-MER)



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.01Å 81.01Å 358.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.80 – 3.00 37.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.80-3.00) 98.4 (37.80-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.01Å)	Xtrriage
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 (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 86.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	8013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.44	1/6738 (0.0%)	0.95	24/9109 (0.3%)
2	R	0.40	0/172	0.75	0/269
3	T	0.22	0/707	0.70	0/1086
4	N	0.23	0/631	0.77	0/969
All	All	0.41	1/8248 (0.0%)	0.91	24/11433 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	ILE	CA-CB	5.43	1.56	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	SER	N-CA-C	10.68	129.88	114.39
1	A	553	GLU	N-CA-C	10.56	122.37	111.07
1	A	553	GLU	CA-C-N	8.10	136.28	121.70
1	A	553	GLU	C-N-CA	8.10	136.28	121.70
1	A	43	SER	CA-C-N	8.09	136.25	121.70
1	A	43	SER	C-N-CA	8.09	136.25	121.70
1	A	560	ASN	N-CA-C	5.82	119.95	112.86
1	A	370	ASN	CA-C-N	5.60	126.84	119.84
1	A	370	ASN	C-N-CA	5.60	126.84	119.84
1	A	857	GLN	N-CA-C	-5.59	105.75	113.18
1	A	669	GLN	CA-C-N	5.53	124.73	118.97
1	A	669	GLN	C-N-CA	5.53	124.73	118.97
1	A	553	GLU	CA-C-O	-5.25	115.31	120.82
1	A	264	ILE	CA-C-N	5.19	131.04	121.70
1	A	264	ILE	C-N-CA	5.19	131.04	121.70
1	A	44	TYR	N-CA-C	5.17	125.46	111.00
1	A	53	LYS	CA-C-N	5.16	130.99	121.70
1	A	53	LYS	C-N-CA	5.16	130.99	121.70
1	A	376	ALA	CA-C-N	5.16	130.99	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ALA	C-N-CA	5.16	130.99	121.70
1	A	354	ALA	CA-C-N	5.15	130.97	121.70
1	A	354	ALA	C-N-CA	5.15	130.97	121.70
1	A	554	VAL	N-CA-CB	5.11	120.18	111.50
1	A	558	ALA	N-CA-C	-5.11	105.80	112.23

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	181	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	200	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 (200) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:850:ALA:HA	1:A:851:ASP:C	1.98	0.87
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: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
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
1:A:739:TYR:H	1:A:774:GLN:NE2	1.95	0.65
2:R:1:G:C4	3:T:19:DT:H5''	2.32	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:507:SER:HB3	1:A:510:CYS:HB2	1.80	0.62
1:A:556:GLY:CA	1:A:557:ARG:CB	2.77	0.62
1:A:224:THR:N	1:A:225:GLY:HA2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:GLU:H	1:A:223:SER:C	2.09	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:291:ARG:O	1:A:292:ARG:HB3	2.03	0.58
1:A:850:ALA:HA	1:A:851:ASP:O	2.02	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:O	1:A:472:LYS:HG2	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
1:A:710:VAL:HG11	1:A:719:LEU:H	1.71	0.56
1:A:829:ARG:NH2	5:A:907:HOH:O	2.38	0.56
1:A:180:LYS:HE3	1:A:183:MET:HG2	1.88	0.56
1:A:20:PRO:O	1:A:24:LEU:HB2	2.06	0.55
3:T:22:DT:H2'	3:T:23:DG:C8	2.42	0.55
4:N:121:DC:H4'	4:N:122:DT:OP1	2.07	0.55
1:A:729:THR:CG2	1:A:733:PHE:HB3	2.37	0.55
1:A:308:TYR:HD2	1:A:313:MET:HE1	1.71	0.54
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:400:PHE:HD1	1:A:401:MET:HE3	1.71	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:222:GLU:N	1:A:223:SER:C	2.66	0.53
1:A:560:ASN:O	1:A:881:ALA:HB2	2.08	0.53
1:A:383:ALA:O	1:A:387:LYS:HG3	2.09	0.53
1:A:424:GLY:HA3	5:A:897:HOH:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:126:LEU:HD13	1:A:246:LEU:HB2	1.92	0.52
2:R:1:G:C4	3:T:19:DT:C5'	2.93	0.52
1:A:524:HIS:HB2	1:A:528:TYR:HB2	1.92	0.52
1:A:862:PRO:HB2	1:A:863:ALA:CB	2.40	0.51
3:T:20:DA:H8	3:T:20:DA:O5'	1.93	0.51
1:A:739:TYR:H	1:A:774:GLN:HE21	1.57	0.51
1:A:180:LYS:HG2	1:A:182:PHE:HD1	1.76	0.51
1:A:862:PRO:HB2	1:A:863:ALA:CA	2.41	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:637:LEU:C	1:A:639:TYR:H	2.19	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
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:54:MET:HE1	1:A:127:THR:HG21	1.95	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:374:LEU:C	1:A:376:ALA:HB2	2.40	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:706:LEU:HD11	1:A:849:PHE:HB2	1.97	0.47
1:A:798:ALA:HB1	1:A:804:ILE:HD12	1.96	0.47
1:A:536:PHE:HB3	1:A:882:PHE:HB3	1.96	0.46
1:A:107:GLN:HB2	5:A:938:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:CYS:SG	1:A:349:VAL:HG22	2.56	0.46
3:T:16:DC:H2''	3:T:19:DT:O4	2.16	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:223:SER:HA	1:A:224:THR:HA	1.70	0.45
1:A:278:TRP:CD2	1:A:284:GLY:HA3	2.52	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:165:ASN:HA	1:A:166:VAL:HA	1.67	0.45
1:A:376:ALA:CB	1:A:377:TRP:HB2	2.45	0.45
1:A:790:HIS:NE2	1:A:832:MET:HB2	2.32	0.45
2:R:1:G:C2	3:T:19:DT:H5'	2.52	0.45
1:A:489:ILE:HG22	1:A:490:MET:N	2.32	0.45
1:A:824:LEU:O	1:A:828:VAL:HG22	2.17	0.45
3:T:20:DA:O5'	3:T:20:DA:C8	2.70	0.45
4:N:129:DC:H2''	4:N:130:DG:C8	2.52	0.45
1:A:82:ILE:HD13	1:A:112:GLU:HG3	1.98	0.44
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:231:ARG:HE	1:A:234:ALA:HB2	1.83	0.43
1:A:760:THR:O	3:T:20:DA:C2'	2.65	0.43
1:A:278:TRP:NE1	1:A:324:GLN:HE22	2.16	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:160:LYS:O	1:A:164:LYS:HG3	2.19	0.43
1:A:451:PRO:CA	1:A:452:ILE:HB	2.45	0.43
1:A:324:GLN:HA	1:A:418:TYR:CD1	2.52	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
3:T:19:DT:H3'	3:T:20:DA:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:555:GLY:O	1:A:556:GLY:C	2.63	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:540:CYS:O	1:A:541:SER:C	2.63	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
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:74:ILE:HG13	5:A:903:HOH:O	2.20	0.40
1:A:452:ILE:HG23	5:A:933:HOH: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
1	A	820/889 (92%)	738 (90%)	62 (8%)	20 (2%)	4 24

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
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%)	681 (98%)	12 (2%)	53 78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TYR

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Mol	Chain	Res	Type
1	A	133	THR
1	A	401	MET
1	A	419	ASN
1	A	452	ILE
1	A	473	VAL
1	A	554	VAL
1	A	659	ILE
1	A	729	THR
1	A	735	VAL
1	A	828	VAL
1	A	858	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	41	HIS
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	463	HIS
1	A	522	GLN
1	A	544	GLN
1	A	649	GLN
1	A	669	GLN
1	A	697	ASN
1	A	726	HIS
1	A	774	GLN
1	A	781	ASN
1	A	786	GLN
1	A	811	HIS
1	A	823	ASN
1	A	857	GLN

### 5.3.3 RNA

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 oligosaccharides 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	832/889 (93%)	1.77	273 (32%) <b>1</b> <b>1</b>	30, 100, 101, 102	0
2	R	7/7 (100%)	2.90	4 (57%) <b>0</b> <b>0</b>	99, 100, 100, 101	0
3	T	31/33 (93%)	2.57	26 (83%) <b>0</b> <b>0</b>	97, 100, 101, 102	0
4	N	28/33 (84%)	2.84	24 (85%) <b>0</b> <b>0</b>	99, 100, 101, 101	0
All	All	898/962 (93%)	1.84	327 (36%) <b>1</b> <b>1</b>	30, 100, 101, 102	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	ASN	5.7
1	A	165	ASN	5.4
2	R	7	G	5.2
1	A	423	ARG	5.2
1	A	422	TRP	4.9
1	A	424	GLY	4.9
1	A	418	TYR	4.8
1	A	850	ALA	4.8
4	N	129	DC	4.7
1	A	882	PHE	4.7
1	A	421	ASP	4.7
1	A	425	ARG	4.7
1	A	766	ASP	4.6
1	A	53	LYS	4.5
1	A	538	GLY	4.4
1	A	429	VAL	4.4
3	T	12	DC	4.3
4	N	124	DG	4.3
1	A	855	GLU	4.3
2	R	1	G	4.3
1	A	545	HIS	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	417	PRO	4.2
1	A	548	ALA	4.2
1	A	433	ASN	4.2
1	A	883	ALA	4.2
1	A	166	VAL	4.1
1	A	420	MET	4.1
1	A	541	SER	4.1
4	N	106	DC	4.0
1	A	251	ALA	4.0
4	N	105	DA	4.0
1	A	147	ASP	3.9
1	A	522	GLN	3.9
1	A	57	ARG	3.8
3	T	11	DA	3.8
4	N	101	DT	3.8
1	A	374	LEU	3.8
1	A	540	CYS	3.7
1	A	665	LEU	3.7
1	A	426	VAL	3.7
1	A	459	TRP	3.7
3	T	1	DA	3.6
4	N	122	DT	3.6
1	A	529	ASN	3.6
1	A	537	ASP	3.6
1	A	451	PRO	3.6
1	A	544	GLN	3.5
1	A	56	GLU	3.5
1	A	346	HIS	3.5
1	A	555	GLY	3.5
1	A	264	ILE	3.5
1	A	427	TYR	3.5
1	A	542	GLY	3.5
1	A	495	SER	3.5
1	A	718	ILE	3.4
1	A	739	TYR	3.4
2	R	6	U	3.4
1	A	164	LYS	3.4
1	A	711	LYS	3.4
1	A	784	HIS	3.4
3	T	16	DC	3.4
1	A	128	SER	3.3
1	A	413	ALA	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	549	MET	3.3
1	A	631	LYS	3.3
1	A	224	THR	3.3
4	N	130	DG	3.3
1	A	430	SER	3.3
1	A	492	CYS	3.3
1	A	863	ALA	3.3
4	N	120	DT	3.3
3	T	9	DG	3.3
3	T	19	DT	3.3
1	A	222	GLU	3.3
1	A	638	ALA	3.3
1	A	710	VAL	3.2
3	T	13	DT	3.2
1	A	355	ILE	3.2
3	T	23	DG	3.2
1	A	325	ASN	3.2
1	A	550	LEU	3.2
4	N	113	DC	3.2
1	A	448	LYS	3.2
1	A	589	GLY	3.2
1	A	487	GLU	3.2
1	A	546	PHE	3.2
1	A	623	TYR	3.2
1	A	543	ILE	3.2
1	A	786	GLN	3.2
1	A	594	VAL	3.1
1	A	846	TYR	3.1
1	A	74	ILE	3.1
4	N	103	DA	3.1
1	A	104	GLN	3.1
1	A	552	ASP	3.1
1	A	498	GLU	3.1
1	A	326	THR	3.1
1	A	223	SER	3.1
1	A	787	ASP	3.1
1	A	411	HIS	3.1
1	A	547	SER	3.1
1	A	728	VAL	3.1
1	A	748	ASN	3.0
1	A	864	LEU	3.0
1	A	597	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	785	SER	3.0
4	N	128	DA	3.0
1	A	486	HIS	3.0
1	A	881	ALA	3.0
1	A	364	PRO	3.0
1	A	519	ALA	3.0
1	A	472	LYS	3.0
1	A	416	PHE	3.0
1	A	254	ILE	3.0
1	A	196	LEU	3.0
3	T	4	DC	3.0
1	A	54	MET	3.0
1	A	635	MET	3.0
1	A	528	TYR	2.9
4	N	107	DG	2.9
4	N	131	DG	2.9
1	A	300	HIS	2.9
1	A	605	ILE	2.9
1	A	639	TYR	2.9
1	A	714	LYS	2.9
1	A	622	ALA	2.9
2	R	2	G	2.9
1	A	539	SER	2.9
1	A	763	THR	2.9
1	A	738	GLU	2.9
1	A	764	ASN	2.9
1	A	859	ASP	2.8
1	A	371	PRO	2.8
1	A	730	PRO	2.8
1	A	811	HIS	2.8
1	A	181	ALA	2.8
1	A	408	PHE	2.8
1	A	496	PRO	2.8
4	N	121	DC	2.8
1	A	436	GLY	2.8
1	A	661	SER	2.8
1	A	856	SER	2.8
1	A	591	ASP	2.8
1	A	716	GLY	2.7
1	A	813	SER	2.7
1	A	480	LYS	2.7
4	N	127	DC	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	616	LEU	2.7
1	A	55	PHE	2.7
1	A	717	GLU	2.7
1	A	518	TYR	2.7
3	T	33	DA	2.7
1	A	432	PHE	2.7
1	A	502	TRP	2.7
1	A	373	ALA	2.7
3	T	5	DG	2.7
3	T	7	DG	2.7
1	A	193	LYS	2.7
1	A	642	LYS	2.7
1	A	835	THR	2.6
1	A	523	HIS	2.6
1	A	225	GLY	2.6
1	A	788	GLY	2.6
3	T	6	DT	2.6
1	A	615	ALA	2.6
1	A	637	LEU	2.6
1	A	708	ALA	2.6
1	A	854	HIS	2.6
1	A	644	PHE	2.6
1	A	435	GLN	2.6
1	A	596	THR	2.6
1	A	682	TRP	2.6
4	N	123	DG	2.6
1	A	109	ILE	2.6
1	A	666	MET	2.6
1	A	488	ASN	2.6
1	A	640	GLY	2.6
1	A	350	GLU	2.6
1	A	136	ALA	2.6
1	A	272	VAL	2.6
1	A	469	GLY	2.6
1	A	671	ASN	2.6
1	A	179	LYS	2.6
1	A	431	MET	2.5
1	A	185	VAL	2.5
3	T	2	DG	2.5
1	A	483	GLU	2.5
1	A	369	MET	2.5
1	A	838	SER	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	479	ILE	2.5
1	A	878	SER	2.5
1	A	26	ASP	2.5
1	A	434	PRO	2.5
3	T	25	DG	2.5
4	N	126	DG	2.5
1	A	513	ALA	2.5
1	A	127	THR	2.5
1	A	412	LYS	2.5
1	A	312	TYR	2.5
1	A	43	SER	2.4
1	A	504	GLU	2.4
1	A	611	LEU	2.4
3	T	20	DA	2.4
1	A	482	ILE	2.4
1	A	527	SER	2.4
1	A	768	GLU	2.4
1	A	99	ARG	2.4
1	A	812	ASP	2.4
1	A	474	PRO	2.4
4	N	125	DC	2.4
1	A	672	GLN	2.4
1	A	762	ASN	2.4
1	A	754	GLN	2.4
4	N	104	DT	2.4
1	A	500	THR	2.4
1	A	836	TYR	2.4
1	A	610	LYS	2.4
1	A	551	ARG	2.4
4	N	102	DA	2.4
1	A	349	VAL	2.4
1	A	687	VAL	2.4
1	A	453	GLY	2.3
1	A	745	THR	2.3
1	A	705	LEU	2.3
1	A	393	SER	2.3
1	A	345	LYS	2.3
1	A	819	ALA	2.3
1	A	497	LEU	2.3
1	A	521	VAL	2.3
1	A	554	VAL	2.3
1	A	476	PRO	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	452	ILE	2.3
3	T	26	DT	2.3
1	A	636	THR	2.3
1	A	609	VAL	2.3
1	A	801	LYS	2.3
1	A	803	GLY	2.3
4	N	133	DT	2.3
1	A	880	PHE	2.3
1	A	135	GLN	2.3
1	A	368	ASP	2.3
1	A	719	LEU	2.3
1	A	241	SER	2.3
1	A	676	TYR	2.3
1	A	180	LYS	2.3
3	T	3	DC	2.3
1	A	456	GLY	2.2
1	A	520	GLY	2.2
1	A	858	LEU	2.2
1	A	377	TRP	2.2
1	A	98	LYS	2.2
1	A	679	LYS	2.2
1	A	767	SER	2.2
1	A	473	VAL	2.2
3	T	14	DC	2.2
1	A	129	ALA	2.2
1	A	253	ALA	2.2
1	A	428	ALA	2.2
1	A	376	ALA	2.2
1	A	447	ALA	2.2
1	A	535	ALA	2.2
1	A	387	LYS	2.2
1	A	740	LYS	2.2
4	N	109	DC	2.2
1	A	531	SER	2.2
1	A	648	GLN	2.2
1	A	484	GLU	2.2
1	A	832	MET	2.2
1	A	197	GLY	2.2
1	A	657	PRO	2.2
1	A	375	THR	2.2
1	A	598	THR	2.2
1	A	735	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	783	VAL	2.2
1	A	659	ILE	2.2
1	A	242	GLU	2.2
1	A	652	GLU	2.2
1	A	389	LYS	2.1
1	A	188	ALA	2.1
1	A	781	ASN	2.1
3	T	28	DG	2.1
1	A	182	PHE	2.1
1	A	530	CYS	2.1
1	A	133	THR	2.1
1	A	73	LEU	2.1
1	A	329	LYS	2.1
1	A	190	MET	2.1
1	A	292	ARG	2.1
1	A	379	ARG	2.1
1	A	737	GLN	2.1
3	T	10	DC	2.1
1	A	437	ASN	2.1
1	A	501	TRP	2.1
1	A	712	ASP	2.1
1	A	566	THR	2.1
1	A	809	LEU	2.1
4	N	108	DA	2.1
3	T	29	DT	2.1
1	A	592	ASN	2.1
1	A	328	TRP	2.1
1	A	363	LYS	2.1
1	A	746	ARG	2.1
1	A	284	GLY	2.1
1	A	525	GLY	2.1
1	A	823	ASN	2.1
1	A	50	ARG	2.1
1	A	360	LEU	2.1
3	T	27	DC	2.1
1	A	816	THR	2.1
1	A	503	ALA	2.1
1	A	252	GLU	2.1
3	T	32	DT	2.0
1	A	756	ARG	2.0
1	A	327	ALA	2.0
1	A	465	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	T	8	DC	2.0
4	N	132	DC	2.0
1	A	455	GLU	2.0
1	A	414	ILE	2.0
1	A	736	TRP	2.0
1	A	590	THR	2.0
1	A	707	ALA	2.0
1	A	851	ASP	2.0
1	A	450	LYS	2.0
3	T	15	DC	2.0
1	A	526	LEU	2.0
1	A	561	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 oligosaccharides 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.