Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:34 am BST

PDB ID	:	1Q32
Title	:	Crystal Structure Analysis of the Yeast Tyrosyl-DNA Phosphodiesterase
Authors	:	He, X.; Babaoglu, K.; Price, A.; Nitiss, K.C.; Nitiss, J.L.; White, S.W.
Deposited on	:	2003-07-28
Resolution	:	2.03 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
https://www.wwpdb.org/validation/2017/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:

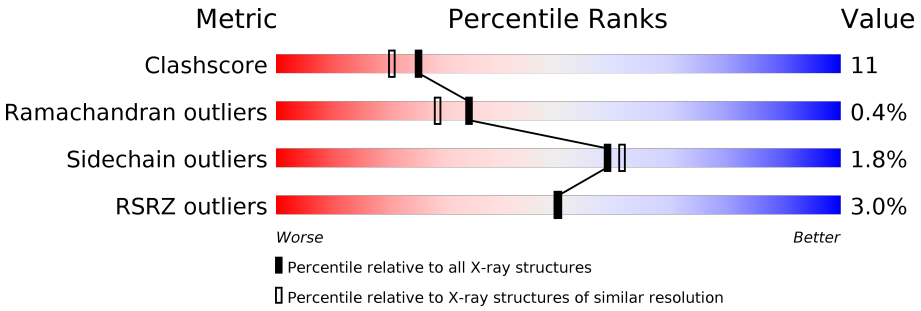
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.03 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))
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 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 <=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	544	2% 60% 16% • 23%
1	B	544	% 60% 16% • 23%
1	C	544	% 62% 14% • 23%
1	D	544	5% 59% 16% • 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14518 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 tyrosyl-DNA phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3429	2223	567	619	20			
1	B	420	Total	C	N	O	S	0	0	0
			3426	2221	568	617	20			
1	C	417	Total	C	N	O	S	0	0	0
			3408	2212	563	613	20			
1	D	415	Total	C	N	O	S	0	0	0
			3393	2203	559	611	20			

- Molecule 2 is water.

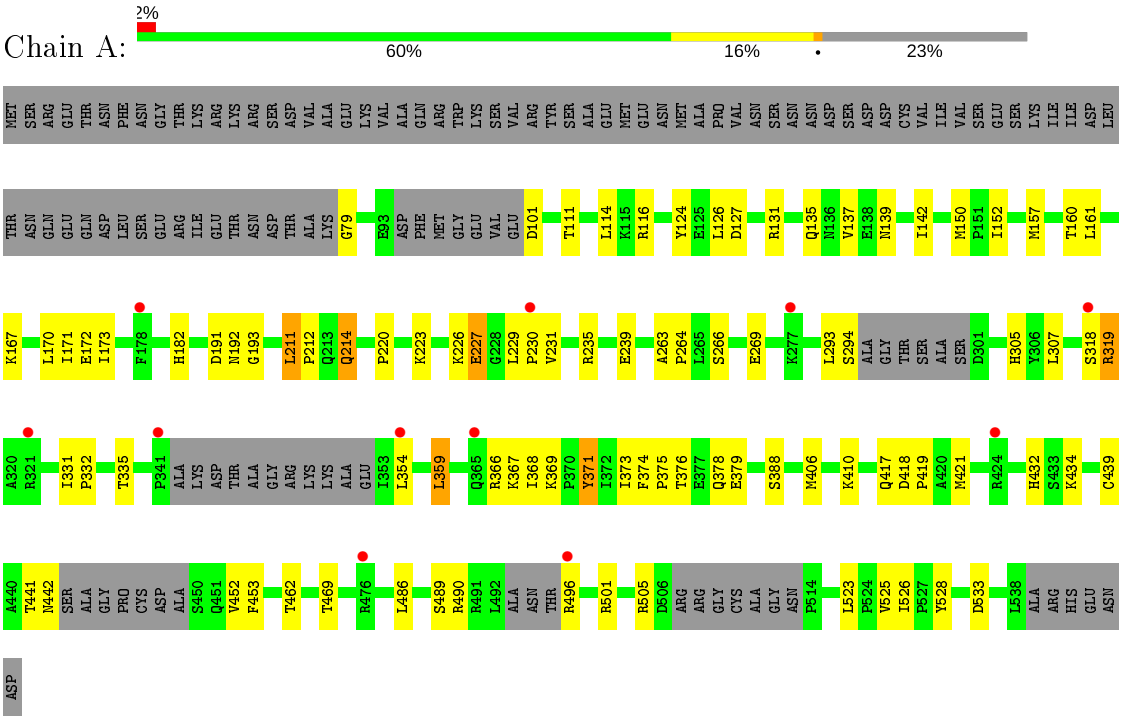
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	220	Total	O	0	0
			220	220		
2	B	264	Total	O	0	0
			264	264		
2	C	231	Total	O	0	0
			231	231		
2	D	147	Total	O	0	0
			147	147		

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 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.

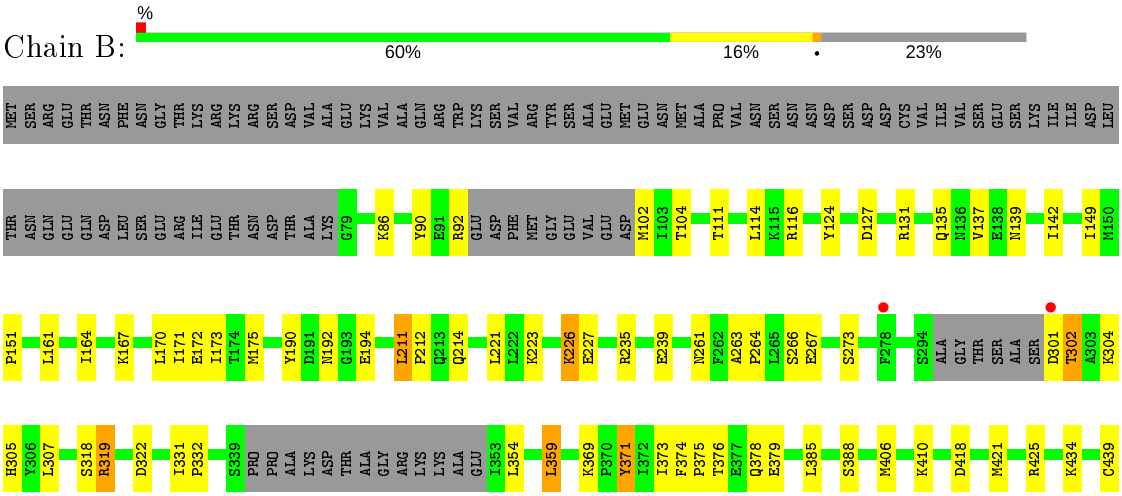
- Molecule 1: tyrosyl-DNA phosphodiesterase

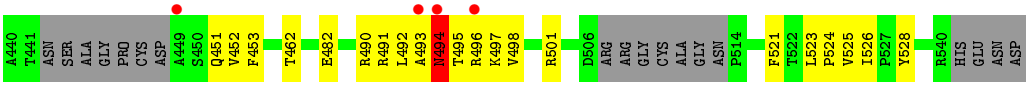
Chain A:



- Molecule 1: tyrosyl-DNA phosphodiesterase

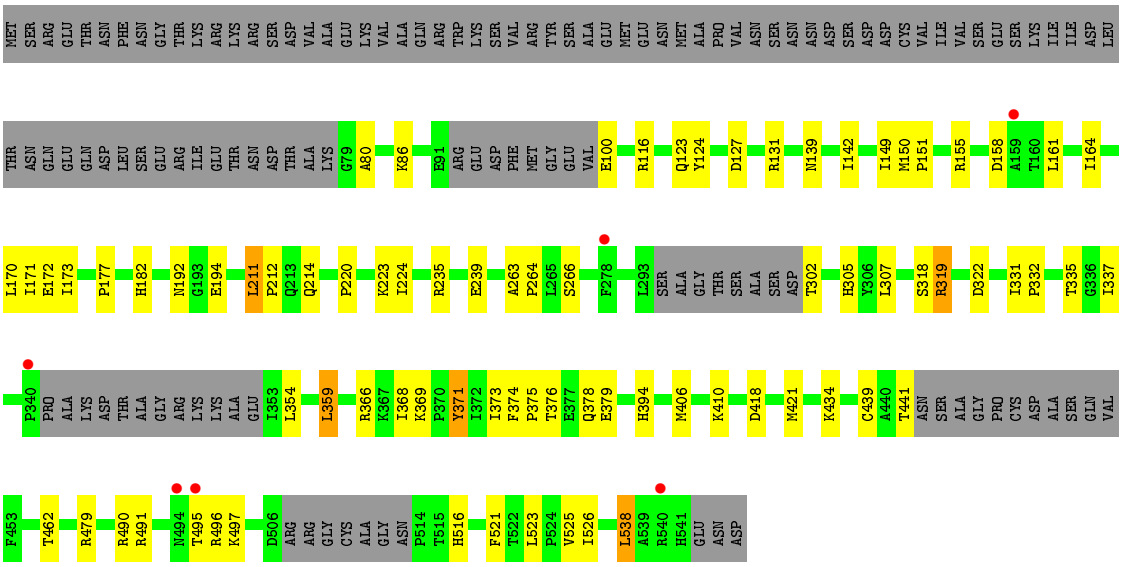
Chain B:





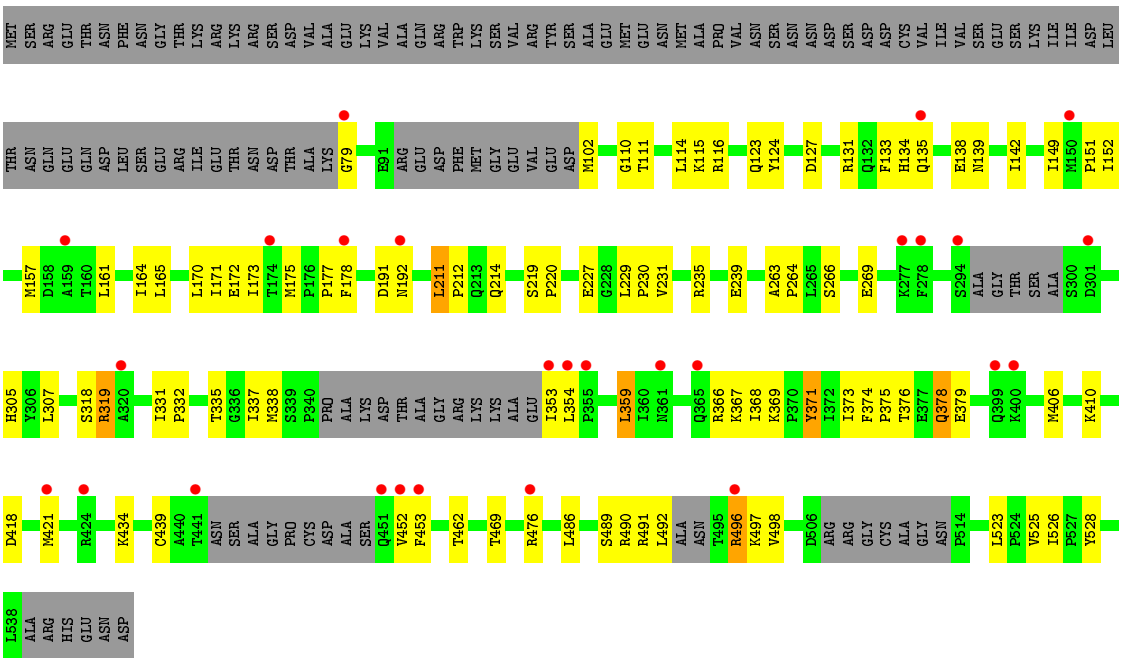
• Molecule 1: tyrosyl-DNA phosphodiesterase

Chain C:



• Molecule 1: tyrosyl-DNA phosphodiesterase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.16Å 82.21Å 98.44Å 89.39° 85.81° 67.12°	Depositor
Resolution (Å)	30.00 – 2.03 39.64 – 1.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.03) 80.1 (39.64-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.28 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.241 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14518	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.36	0/3516	0.61	0/4752
1	B	0.36	0/3512	0.61	0/4747
1	C	0.36	0/3496	0.61	0/4727
1	D	0.35	0/3479	0.60	0/4702
All	All	0.36	0/14003	0.61	0/18928

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	3429	0	3432	75	0
1	B	3426	0	3435	80	0
1	C	3408	0	3410	62	0
1	D	3393	0	3403	76	0
2	A	220	0	0	10	0
2	B	264	0	0	9	0
2	C	231	0	0	11	0
2	D	147	0	0	8	0
All	All	14518	0	13680	293	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 (293) 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:152:ILE:HG21	1:A:157:MET:HE3	1.36	1.05
1:D:319:ARG:H	1:D:319:ARG:NE	1.63	0.96
1:A:319:ARG:NE	1:A:319:ARG:H	1.62	0.95
1:C:319:ARG:H	1:C:319:ARG:NE	1.63	0.95
1:B:319:ARG:NE	1:B:319:ARG:H	1.63	0.95
1:A:319:ARG:HE	1:A:319:ARG:N	1.67	0.93
1:C:319:ARG:N	1:C:319:ARG:HE	1.68	0.92
1:D:319:ARG:N	1:D:319:ARG:HE	1.68	0.91
1:B:226:LYS:HD3	1:B:226:LYS:H	1.34	0.90
1:B:319:ARG:HE	1:B:319:ARG:N	1.68	0.90
1:D:318:SER:HB2	1:D:319:ARG:HH21	1.40	0.87
1:B:318:SER:HB2	1:B:319:ARG:HH21	1.40	0.87
1:A:318:SER:HB2	1:A:319:ARG:HH21	1.40	0.86
1:C:318:SER:HB2	1:C:319:ARG:HH21	1.39	0.86
1:B:226:LYS:CD	1:B:226:LYS:H	1.92	0.81
1:D:231:VAL:CG1	1:D:266:SER:HA	2.10	0.80
1:C:192:ASN:HB2	2:C:743:HOH:O	1.82	0.79
1:A:211:LEU:HB2	1:A:212:PRO:HD3	1.65	0.79
1:D:319:ARG:H	1:D:319:ARG:HE	0.82	0.77
1:B:524:PRO:HG2	2:B:769:HOH:O	1.84	0.76
1:A:441:THR:O	1:A:442:ASN:HB2	1.82	0.76
1:B:211:LEU:HB2	1:B:212:PRO:HD3	1.66	0.75
1:A:231:VAL:HG13	1:A:266:SER:HA	1.68	0.75
1:D:211:LEU:HB2	1:D:212:PRO:HD3	1.67	0.75
1:C:211:LEU:HB2	1:C:212:PRO:HD3	1.67	0.75
1:A:231:VAL:CG1	1:A:266:SER:HA	2.15	0.74
1:A:319:ARG:HE	1:A:319:ARG:H	0.82	0.73
1:C:496:ARG:N	1:C:496:ARG:HD2	2.04	0.72
1:B:319:ARG:HE	1:B:319:ARG:H	0.83	0.72
1:C:354:LEU:HB2	1:C:359:LEU:HD13	1.73	0.71
1:A:354:LEU:HB2	1:A:359:LEU:HD13	1.72	0.71
1:D:354:LEU:HB2	1:D:359:LEU:HD13	1.72	0.71
1:A:152:ILE:CG2	1:A:157:MET:HE3	2.19	0.70
1:B:354:LEU:HB2	1:B:359:LEU:HD13	1.73	0.70
1:C:302:THR:HB	1:C:441:THR:OG1	1.92	0.69
1:B:406:MET:SD	2:B:742:HOH:O	2.50	0.69
1:C:319:ARG:H	1:C:319:ARG:HE	0.82	0.69
1:D:231:VAL:HG11	1:D:266:SER:HA	1.75	0.68
1:B:496:ARG:O	1:B:497:LYS:HD3	1.94	0.67
1:D:490:ARG:HG2	1:D:496:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:MET:N	2:D:553:HOH:O	2.30	0.64
1:A:229:LEU:HD23	1:A:230:PRO:CD	2.28	0.64
1:A:182:HIS:NE2	2:A:609:HOH:O	2.29	0.64
1:D:123:GLN:HG2	2:D:686:HOH:O	1.96	0.64
1:B:494:ASN:O	1:B:495:THR:HG23	1.98	0.63
1:A:469:THR:HG23	2:A:689:HOH:O	2.00	0.62
1:D:229:LEU:HD12	1:D:230:PRO:HD2	1.82	0.62
1:A:131:ARG:CZ	1:A:161:LEU:HD11	2.30	0.62
1:B:127:ASP:O	1:B:131:ARG:HG3	2.00	0.62
1:B:111:THR:HG23	1:B:114:LEU:HB2	1.81	0.62
1:B:226:LYS:HD3	1:B:226:LYS:N	2.09	0.61
1:A:231:VAL:HG12	2:A:564:HOH:O	1.99	0.61
1:A:293:LEU:O	1:A:294:SER:HB2	2.00	0.61
1:C:127:ASP:O	1:C:131:ARG:HG3	2.01	0.61
1:B:301:ASP:O	1:B:302:THR:HB	2.01	0.61
1:B:111:THR:HG21	1:B:190:TYR:HE2	1.66	0.61
1:A:127:ASP:O	1:A:131:ARG:HG3	2.01	0.60
1:D:127:ASP:O	1:D:131:ARG:HG3	2.01	0.60
1:A:229:LEU:HD23	1:A:230:PRO:HD2	1.83	0.60
1:A:496:ARG:HG3	2:A:750:HOH:O	2.01	0.60
1:B:192:ASN:HD21	1:B:194:GLU:CD	2.05	0.60
1:D:192:ASN:N	2:D:555:HOH:O	2.33	0.59
1:D:165:LEU:O	1:D:165:LEU:HD23	2.02	0.59
1:A:131:ARG:NH1	1:A:161:LEU:HD11	2.17	0.59
1:A:376:THR:OG1	1:A:379:GLU:HG3	2.03	0.59
1:A:137:VAL:O	1:A:167:LYS:HD3	2.02	0.59
1:D:376:THR:OG1	1:D:379:GLU:HG3	2.02	0.59
1:B:322:ASP:O	1:B:406:MET:HE1	2.03	0.59
1:C:490:ARG:NH1	1:C:490:ARG:HB3	2.18	0.59
1:B:92:ARG:HD3	2:B:790:HOH:O	2.04	0.58
1:A:294:SER:HB2	1:A:490:ARG:HD3	1.83	0.58
1:A:533:ASP:OD1	2:A:619:HOH:O	2.17	0.58
1:D:231:VAL:HG13	1:D:266:SER:HA	1.84	0.58
1:B:490:ARG:NH1	1:B:490:ARG:HB3	2.19	0.57
1:C:177:PRO:O	1:C:479:ARG:NH2	2.32	0.57
1:C:182:HIS:NE2	2:C:626:HOH:O	2.32	0.57
1:A:490:ARG:HB3	1:A:490:ARG:NH1	2.19	0.57
1:D:490:ARG:NH1	1:D:490:ARG:HB3	2.19	0.57
1:D:476:ARG:HG2	2:D:673:HOH:O	2.04	0.57
1:C:149:ILE:O	1:C:151:PRO:HD3	2.04	0.57
1:C:161:LEU:HA	1:C:164:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD23	1:A:230:PRO:N	2.21	0.56
1:C:223:LYS:HD3	1:C:224:ILE:N	2.20	0.56
1:B:434:LYS:HB2	1:B:462:THR:O	2.06	0.56
1:B:124:TYR:CZ	1:B:142:ILE:HG23	2.41	0.56
1:D:231:VAL:HG12	2:D:613:HOH:O	2.06	0.56
1:C:131:ARG:HD2	2:C:766:HOH:O	2.05	0.55
1:B:175:MET:HA	1:B:175:MET:HE2	1.87	0.55
1:D:235:ARG:O	1:D:239:GLU:HG3	2.07	0.55
1:B:235:ARG:O	1:B:239:GLU:HG3	2.06	0.55
1:D:134:HIS:CE1	1:D:135:GLN:HG2	2.42	0.55
1:A:505:ARG:NH1	2:A:673:HOH:O	2.39	0.55
1:B:376:THR:OG1	1:B:379:GLU:HG3	2.07	0.55
1:A:235:ARG:O	1:A:239:GLU:HG3	2.07	0.54
1:C:235:ARG:O	1:C:239:GLU:HG3	2.07	0.54
1:C:394:HIS:CD2	1:C:538:LEU:HD12	2.43	0.54
1:A:231:VAL:HG11	1:A:266:SER:HA	1.90	0.54
1:A:434:LYS:HB2	1:A:462:THR:O	2.07	0.54
1:C:376:THR:OG1	1:C:379:GLU:HG3	2.07	0.54
1:C:421:MET:HG3	2:C:751:HOH:O	2.07	0.54
1:B:223:LYS:HG3	2:B:703:HOH:O	2.07	0.54
1:D:418:ASP:HA	1:D:526:ILE:CD1	2.38	0.54
1:A:124:TYR:CZ	1:A:142:ILE:HG23	2.43	0.53
1:C:373:ILE:CD1	1:C:525:VAL:HG11	2.38	0.53
1:D:170:LEU:HD12	1:D:171:ILE:N	2.23	0.53
1:C:116:ARG:HG3	1:C:139:ASN:HD22	1.73	0.53
1:C:124:TYR:CZ	1:C:142:ILE:HG23	2.45	0.53
1:D:124:TYR:CZ	1:D:142:ILE:HG23	2.44	0.53
1:D:373:ILE:CD1	1:D:525:VAL:HG11	2.39	0.53
1:A:170:LEU:HD12	1:A:171:ILE:N	2.24	0.52
1:B:161:LEU:HA	1:B:164:ILE:HG22	1.91	0.52
1:A:116:ARG:HE	1:A:139:ASN:ND2	2.08	0.52
1:C:170:LEU:HD12	1:C:171:ILE:N	2.26	0.51
1:C:192:ASN:HD21	1:C:194:GLU:CD	2.11	0.51
1:D:489:SER:HB3	1:D:496:ARG:NH2	2.25	0.51
1:A:452:VAL:O	1:A:453:PHE:HB2	2.11	0.51
1:D:418:ASP:HA	1:D:526:ILE:HD12	1.91	0.51
1:B:170:LEU:HD12	1:B:171:ILE:N	2.25	0.51
1:D:111:THR:HG23	1:D:114:LEU:HB2	1.93	0.51
1:B:410:LYS:HE3	2:B:753:HOH:O	2.11	0.51
1:C:418:ASP:HA	1:C:526:ILE:HD12	1.93	0.51
1:B:116:ARG:HE	1:B:139:ASN:ND2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLN:HG2	2:C:709:HOH:O	2.11	0.50
1:D:476:ARG:HD3	2:D:651:HOH:O	2.12	0.50
1:A:101:ASP:HB3	2:A:610:HOH:O	2.11	0.50
1:A:373:ILE:CD1	1:A:525:VAL:HG11	2.42	0.50
1:D:452:VAL:O	1:D:453:PHE:HB2	2.10	0.50
1:C:373:ILE:HD11	1:C:525:VAL:HG11	1.93	0.50
1:D:421:MET:HE1	1:D:523:LEU:O	2.12	0.50
1:A:418:ASP:HA	1:A:526:ILE:HD12	1.94	0.50
1:A:79:GLY:HA2	1:A:220:PRO:HB3	1.93	0.50
1:B:452:VAL:O	1:B:453:PHE:HB2	2.12	0.50
1:A:501:ARG:HD2	2:A:620:HOH:O	2.12	0.50
1:B:116:ARG:HG3	1:B:139:ASN:HD22	1.76	0.50
1:C:369:LYS:HD3	1:C:371:TYR:OH	2.12	0.50
1:D:133:PHE:HB2	1:D:164:ILE:CD1	2.42	0.50
1:D:335:THR:HG21	1:D:368:ILE:HD13	1.94	0.50
1:A:111:THR:HG23	1:A:114:LEU:HB2	1.94	0.49
1:A:193:GLY:O	1:A:223:LYS:HA	2.12	0.49
1:A:406:MET:O	1:A:410:LYS:HB2	2.11	0.49
1:D:434:LYS:HB2	1:D:462:THR:O	2.12	0.49
1:A:369:LYS:HD3	1:A:371:TYR:OH	2.13	0.49
1:A:421:MET:HE1	1:A:523:LEU:O	2.12	0.49
1:B:369:LYS:HD3	1:B:371:TYR:OH	2.13	0.49
1:A:173:ILE:N	1:A:173:ILE:HD12	2.28	0.49
1:B:418:ASP:HA	1:B:526:ILE:HD12	1.95	0.49
1:C:223:LYS:HD2	1:C:224:ILE:O	2.13	0.49
1:B:373:ILE:CD1	1:B:525:VAL:HG11	2.43	0.49
1:C:173:ILE:HD12	1:C:173:ILE:N	2.27	0.49
1:C:479:ARG:HD2	2:C:706:HOH:O	2.11	0.49
1:A:418:ASP:HA	1:A:526:ILE:CD1	2.42	0.49
1:B:173:ILE:HD12	1:B:173:ILE:N	2.28	0.48
1:B:406:MET:O	1:B:410:LYS:HB2	2.12	0.48
1:B:421:MET:HE1	1:B:523:LEU:O	2.13	0.48
1:B:418:ASP:HA	1:B:526:ILE:CD1	2.43	0.48
1:D:173:ILE:HD12	1:D:173:ILE:N	2.28	0.48
1:D:338:MET:CE	1:D:353:ILE:HA	2.44	0.48
1:A:305:HIS:HB2	1:A:439:CYS:HB3	1.95	0.48
1:C:305:HIS:HB2	1:C:439:CYS:HB3	1.95	0.48
1:D:369:LYS:HD3	1:D:371:TYR:OH	2.13	0.48
1:A:496:ARG:HG2	1:A:496:ARG:O	2.12	0.48
1:C:223:LYS:HD3	1:C:224:ILE:H	1.77	0.48
1:C:322:ASP:O	1:C:406:MET:HE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:MET:O	1:C:410:LYS:HB2	2.14	0.48
1:A:126:LEU:HB2	1:A:150:MET:O	2.13	0.48
1:B:322:ASP:HB2	1:B:406:MET:HE3	1.95	0.48
1:C:418:ASP:HA	1:C:526:ILE:CD1	2.43	0.48
1:D:406:MET:O	1:D:410:LYS:HB2	2.13	0.48
1:C:150:MET:HE2	2:C:730:HOH:O	2.12	0.47
1:D:116:ARG:HE	1:D:139:ASN:ND2	2.12	0.47
1:C:80:ALA:N	1:C:220:PRO:HG3	2.30	0.47
1:C:496:ARG:O	1:C:497:LYS:HD3	2.14	0.47
1:D:115:LYS:HG3	1:D:138:GLU:OE2	2.14	0.47
1:D:305:HIS:HB2	1:D:439:CYS:HB3	1.95	0.47
1:D:307:LEU:HD23	1:D:307:LEU:C	2.35	0.47
1:C:434:LYS:HB2	1:C:462:THR:O	2.15	0.47
1:A:135:GLN:NE2	1:A:160:THR:HG23	2.30	0.47
1:B:376:THR:HG22	1:B:528:TYR:CZ	2.50	0.47
1:B:302:THR:HG23	1:B:304:LYS:NZ	2.31	0.46
1:C:335:THR:HG21	1:C:368:ILE:HD13	1.98	0.46
1:D:149:ILE:O	1:D:151:PRO:HD3	2.16	0.46
1:B:137:VAL:O	1:B:167:LYS:HD3	2.16	0.46
1:C:123:GLN:HB3	2:C:730:HOH:O	2.14	0.46
1:D:376:THR:HG22	1:D:528:TYR:CZ	2.51	0.46
1:A:293:LEU:O	1:A:294:SER:CB	2.64	0.46
1:B:102:MET:HA	2:B:606:HOH:O	2.16	0.46
1:D:219:SER:HB2	1:D:220:PRO:HD2	1.97	0.46
1:D:373:ILE:HD11	1:D:525:VAL:HG11	1.98	0.46
1:A:157:MET:CE	1:A:161:LEU:HB3	2.47	0.45
1:A:307:LEU:HD23	1:A:307:LEU:C	2.35	0.45
1:B:307:LEU:C	1:B:307:LEU:HD23	2.37	0.45
1:C:155:ARG:HG2	2:C:735:HOH:O	2.15	0.45
1:D:266:SER:O	1:D:491:ARG:NH2	2.47	0.45
1:D:79:GLY:HA2	1:D:220:PRO:HB3	1.98	0.45
1:D:496:ARG:HA	1:D:496:ARG:NE	2.30	0.45
1:A:335:THR:HG21	1:A:368:ILE:HD13	1.99	0.45
1:B:263:ALA:HB3	1:B:264:PRO:HD3	1.99	0.45
1:A:191:ASP:O	1:A:192:ASN:HB2	2.17	0.45
1:C:263:ALA:HB3	1:C:264:PRO:HD3	1.99	0.45
1:C:307:LEU:C	1:C:307:LEU:HD23	2.37	0.45
1:B:175:MET:CE	1:B:175:MET:HA	2.45	0.45
1:A:111:THR:CG2	1:A:114:LEU:HB2	2.46	0.45
1:B:149:ILE:O	1:B:151:PRO:HD3	2.17	0.45
1:B:267:GLU:OE2	1:B:493:ALA:N	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:HIS:HB2	1:B:439:CYS:HB3	1.98	0.44
1:D:338:MET:HE1	1:D:353:ILE:HA	1.99	0.44
1:D:421:MET:HG3	2:D:569:HOH:O	2.15	0.44
1:D:227:GLU:OE2	1:D:230:PRO:HG3	2.17	0.44
1:B:161:LEU:O	1:B:164:ILE:HG22	2.16	0.44
1:B:493:ALA:O	1:B:495:THR:N	2.50	0.44
1:B:302:THR:CG2	1:B:304:LYS:NZ	2.80	0.44
1:B:192:ASN:OD1	1:B:194:GLU:HG3	2.18	0.44
1:B:90:TYR:O	1:B:425:ARG:HD2	2.17	0.44
1:C:495:THR:HG21	1:C:516:HIS:CE1	2.52	0.44
1:A:376:THR:HG22	1:A:528:TYR:CZ	2.52	0.44
1:B:373:ILE:HD11	1:B:525:VAL:HG11	1.99	0.44
1:B:194:GLU:OE2	1:B:221:LEU:HD21	2.18	0.43
1:C:172:GLU:C	1:C:173:ILE:HD12	2.38	0.43
1:C:421:MET:HE1	1:C:523:LEU:O	2.18	0.43
1:A:211:LEU:HD13	1:A:388:SER:HB3	2.01	0.43
1:A:489:SER:HB3	1:A:496:ARG:O	2.17	0.43
1:B:211:LEU:HD22	1:B:385:LEU:HD13	1.99	0.43
1:A:263:ALA:HB3	1:A:264:PRO:HD3	2.01	0.43
1:A:269:GLU:HB2	1:A:486:LEU:HB3	2.01	0.43
1:B:86:LYS:HB3	1:B:104:THR:HG22	1.99	0.43
1:D:492:LEU:HD11	1:D:498:VAL:HG22	2.00	0.43
1:B:374:PHE:CG	1:B:375:PRO:HD2	2.53	0.43
1:B:170:LEU:HD12	1:B:171:ILE:H	1.83	0.43
1:C:192:ASN:O	1:C:223:LYS:NZ	2.50	0.43
1:D:170:LEU:HD12	1:D:171:ILE:H	1.82	0.43
1:A:172:GLU:C	1:A:173:ILE:HD12	2.39	0.43
1:C:337:ILE:HG12	1:C:366:ARG:NE	2.34	0.43
1:D:263:ALA:HB3	1:D:264:PRO:HD3	2.01	0.43
1:D:337:ILE:HG12	1:D:366:ARG:NE	2.34	0.43
1:D:376:THR:HG1	1:D:379:GLU:HG3	1.83	0.43
1:A:374:PHE:CG	1:A:375:PRO:HD2	2.54	0.43
1:D:172:GLU:C	1:D:173:ILE:HD12	2.39	0.42
1:D:489:SER:HB3	1:D:496:ARG:O	2.18	0.42
1:D:374:PHE:CG	1:D:375:PRO:HD2	2.54	0.42
2:A:724:HOH:O	1:D:177:PRO:HG2	2.18	0.42
1:C:322:ASP:HB2	1:C:406:MET:HE3	2.02	0.42
1:D:496:ARG:O	1:D:497:LYS:HD3	2.19	0.42
1:A:373:ILE:HD11	1:A:525:VAL:HG11	2.00	0.42
1:B:172:GLU:C	1:B:173:ILE:HD12	2.40	0.42
1:B:226:LYS:H	1:B:226:LYS:CE	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLN:HG3	2:B:698:HOH:O	2.19	0.42
1:A:223:LYS:HG2	2:A:615:HOH:O	2.20	0.42
1:C:359:LEU:HA	1:C:359:LEU:HD12	1.91	0.42
1:D:152:ILE:HB	1:D:157:MET:CE	2.50	0.42
1:D:331:ILE:HB	1:D:332:PRO:HD3	2.02	0.42
1:A:157:MET:HE1	1:A:161:LEU:HB3	2.02	0.42
1:B:301:ASP:O	1:B:302:THR:CB	2.67	0.42
1:C:521:PHE:HB3	2:C:567:HOH:O	2.19	0.42
1:D:161:LEU:O	1:D:165:LEU:HB2	2.19	0.42
1:D:116:ARG:HE	1:D:139:ASN:HD22	1.67	0.42
1:B:111:THR:CG2	1:B:114:LEU:HB2	2.50	0.42
1:A:417:GLN:O	1:A:419:PRO:HD3	2.20	0.41
1:B:273:SER:HB2	1:B:482:GLU:HB2	2.01	0.41
1:B:331:ILE:HB	1:B:332:PRO:HD3	2.03	0.41
1:C:158:ASP:OD2	1:C:158:ASP:C	2.59	0.41
1:D:378:GLN:HB3	1:D:378:GLN:HE21	1.67	0.41
1:D:110:GLY:O	1:D:134:HIS:HB2	2.19	0.41
1:A:331:ILE:HB	1:A:332:PRO:HD3	2.02	0.41
1:A:214:GLN:NE2	1:A:432:HIS:HB3	2.36	0.41
1:C:331:ILE:HB	1:C:332:PRO:HD3	2.02	0.41
1:C:266:SER:O	1:C:491:ARG:NH2	2.52	0.41
1:A:211:LEU:HB2	1:A:212:PRO:CD	2.45	0.41
1:B:495:THR:O	1:B:496:ARG:HD3	2.21	0.41
1:A:127:ASP:HB3	1:A:152:ILE:HG12	2.03	0.41
1:D:366:ARG:O	1:D:367:LYS:HB2	2.20	0.41
1:A:170:LEU:HD12	1:A:171:ILE:H	1.85	0.41
1:A:227:GLU:CD	1:A:227:GLU:H	2.24	0.41
1:B:211:LEU:HD13	1:B:388:SER:HB3	2.01	0.41
1:C:374:PHE:CG	1:C:375:PRO:HD2	2.56	0.41
1:B:227:GLU:HA	1:B:261:ASN:ND2	2.36	0.40
1:B:266:SER:O	1:B:491:ARG:NH2	2.51	0.40
1:B:495:THR:C	1:B:496:ARG:HD3	2.41	0.40
1:B:501:ARG:HD2	2:B:671:HOH:O	2.22	0.40
1:D:178:PHE:CE2	1:D:469:THR:HG21	2.56	0.40
1:B:116:ARG:HE	1:B:139:ASN:HD22	1.69	0.40
1:B:301:ASP:HB3	1:B:302:THR:H	1.70	0.40
1:B:492:LEU:HD11	1:B:498:VAL:HG22	2.03	0.40
1:D:211:LEU:HB2	1:D:212:PRO:CD	2.47	0.40
1:C:100:GLU:N	2:C:761:HOH:O	2.54	0.40
1:D:173:ILE:HG22	1:D:175:MET:HG3	2.03	0.40
1:D:269:GLU:HB2	1:D:486:LEU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LYS:HE3	1:B:86:LYS:HB2	1.94	0.40
1:C:479:ARG:HH11	1:C:479:ARG:HG2	1.87	0.40
1:D:102:MET:HA	2:D:562:HOH:O	2.21	0.40
1:D:123:GLN:HB3	1:D:123:GLN:HE21	1.70	0.40
1:A:366:ARG:O	1:A:367:LYS:HB2	2.21	0.40
1:B:521:PHE:HB3	2:B:546:HOH:O	2.22	0.40
1:C:86:LYS:HE3	1:C:86:LYS:HB2	1.93	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	405/544 (74%)	389 (96%)	15 (4%)	1 (0%)	47	43
1	B	408/544 (75%)	391 (96%)	14 (3%)	3 (1%)	22	15
1	C	405/544 (74%)	392 (97%)	12 (3%)	1 (0%)	47	43
1	D	401/544 (74%)	383 (96%)	16 (4%)	2 (0%)	29	22
All	All	1619/2176 (74%)	1555 (96%)	57 (4%)	7 (0%)	34	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	302	THR
1	B	494	ASN
1	D	191	ASP
1	B	211	LEU
1	A	211	LEU
1	C	211	LEU
1	D	211	LEU

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	388/491 (79%)	381 (98%)	7 (2%)	59	61
1	B	385/491 (78%)	377 (98%)	8 (2%)	53	55
1	C	383/491 (78%)	377 (98%)	6 (2%)	62	66
1	D	384/491 (78%)	378 (98%)	6 (2%)	62	66
All	All	1540/1964 (78%)	1513 (98%)	27 (2%)	59	61

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

Mol	Chain	Res	Type
1	A	214	GLN
1	A	226	LYS
1	A	227	GLU
1	A	319	ARG
1	A	359	LEU
1	A	371	TYR
1	A	378	GLN
1	B	214	GLN
1	B	226	LYS
1	B	319	ARG
1	B	359	LEU
1	B	371	TYR
1	B	378	GLN
1	B	451	GLN
1	B	494	ASN
1	C	214	GLN
1	C	319	ARG
1	C	359	LEU
1	C	371	TYR
1	C	378	GLN
1	C	538	LEU
1	D	214	GLN
1	D	319	ARG
1	D	359	LEU

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Mol	Chain	Res	Type
1	D	371	TYR
1	D	378	GLN
1	D	496	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	139	ASN
1	A	214	GLN
1	A	242	ASN
1	A	288	ASN
1	A	309	GLN
1	A	378	GLN
1	A	468	GLN
1	B	123	GLN
1	B	136	ASN
1	B	139	ASN
1	B	214	GLN
1	B	242	ASN
1	B	288	ASN
1	B	309	GLN
1	B	357	ASN
1	B	378	GLN
1	B	451	GLN
1	B	468	GLN
1	B	494	ASN
1	C	123	GLN
1	C	139	ASN
1	C	214	GLN
1	C	242	ASN
1	C	288	ASN
1	C	309	GLN
1	C	378	GLN
1	C	394	HIS
1	C	468	GLN
1	C	494	ASN
1	D	123	GLN
1	D	139	ASN
1	D	214	GLN
1	D	242	ASN
1	D	288	ASN

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Mol	Chain	Res	Type
1	D	309	GLN
1	D	378	GLN
1	D	468	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	419/544 (77%)	-0.07	11 (2%) 56 55	20, 37, 59, 70	0
1	B	420/544 (77%)	-0.14	6 (1%) 75 74	19, 35, 58, 73	0
1	C	417/544 (76%)	-0.14	6 (1%) 75 74	19, 36, 59, 74	0
1	D	415/544 (76%)	0.07	27 (6%) 18 18	24, 40, 62, 78	0
All	All	1671/2176 (76%)	-0.07	50 (2%) 50 50	19, 37, 60, 78	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	PHE	7.5
1	D	301	ASP	4.8
1	D	453	PHE	4.4
1	D	496	ARG	4.2
1	B	493	ALA	4.1
1	D	451	GLN	3.7
1	A	496	ARG	3.6
1	B	494	ASN	3.6
1	B	278	PHE	3.5
1	B	449	ALA	3.4
1	D	354	LEU	3.4
1	C	340	PRO	3.3
1	B	496	ARG	3.3
1	D	361	ASN	3.2
1	A	318	SER	3.2
1	D	365	GLN	3.1
1	D	278	PHE	3.0
1	D	353	ILE	3.0
1	D	400	LYS	2.8
1	A	354	LEU	2.8
1	A	341	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	476	ARG	2.8
1	D	424	ARG	2.8
1	D	320	ALA	2.7
1	C	494	ASN	2.6
1	D	452	VAL	2.6
1	D	192	ASN	2.6
1	A	178	PHE	2.5
1	A	230	PRO	2.5
1	D	399	GLN	2.5
1	D	277	LYS	2.5
1	A	321	ARG	2.5
1	D	79	GLY	2.5
1	D	135	GLN	2.4
1	D	421	MET	2.4
1	D	476	ARG	2.4
1	B	301	ASP	2.3
1	C	159	ALA	2.2
1	D	441	THR	2.2
1	D	159	ALA	2.2
1	A	424	ARG	2.2
1	D	355	PRO	2.2
1	C	495	THR	2.1
1	C	540	ARG	2.1
1	A	365	GLN	2.1
1	D	294	SER	2.1
1	C	278	PHE	2.1
1	D	150	MET	2.0
1	D	174	THR	2.0
1	A	277	LYS	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.