Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 01:34 AM EDT

PDB ID	:	3K5O
Title	:	Crystal structure of E.coli Pol II
Authors	:	Yang, W.; Wang, F.
Deposited on	:	2009-10-07
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

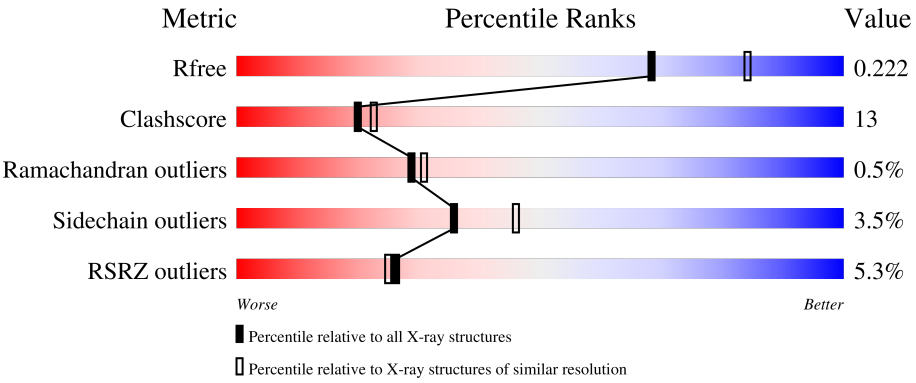
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 >=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	786	5% 77% 19%
1	B	786	5% 71% 21% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12674 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 polymerase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	0	0
			6137	3918	1087	1109	23			
1	B	744	Total	C	N	O	S	0	0	0
			6015	3847	1056	1089	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P21189
A	-1	PRO	-	expression tag	UNP P21189
A	0	HIS	-	expression tag	UNP P21189
A	335	ASN	ASP	engineered mutation	UNP P21189
B	-2	GLY	-	expression tag	UNP P21189
B	-1	PRO	-	expression tag	UNP P21189
B	0	HIS	-	expression tag	UNP P21189
B	335	ASN	ASP	engineered mutation	UNP P21189

- Molecule 2 is water.

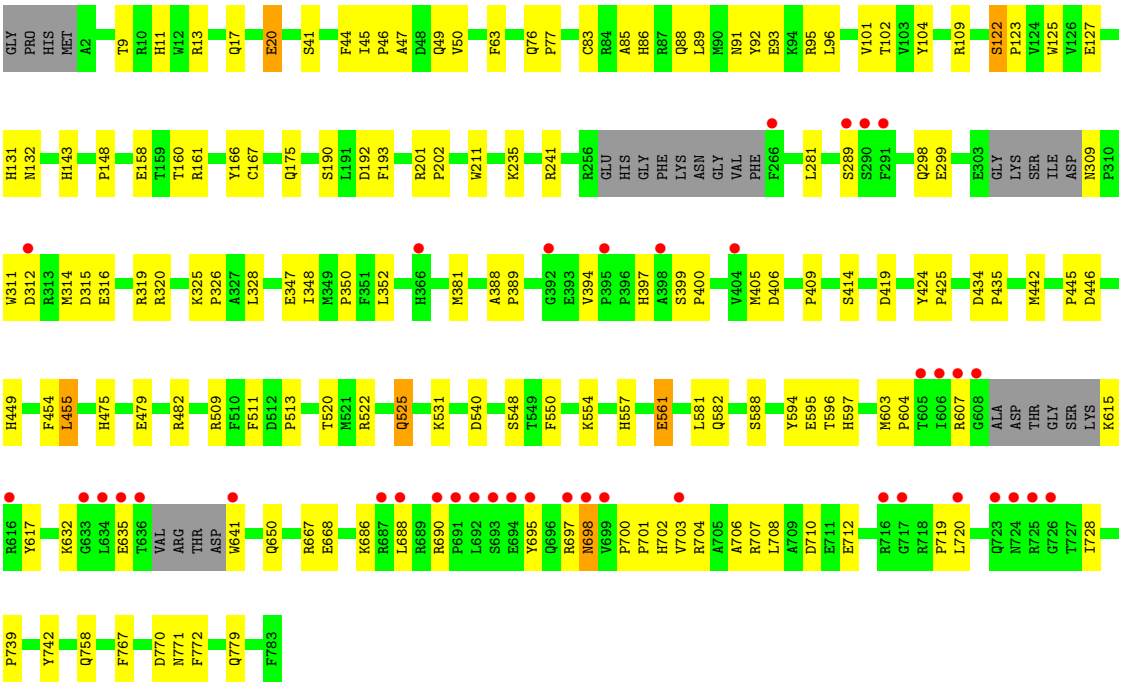
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	250	Total	O	0	0
			250	250		
2	B	272	Total	O	0	0
			272	272		

3 Residue-property plots (i)

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.

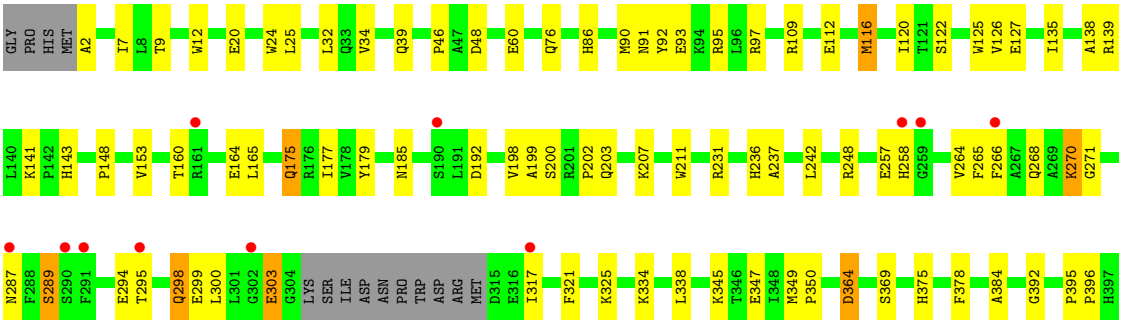
• Molecule 1: DNA polymerase II

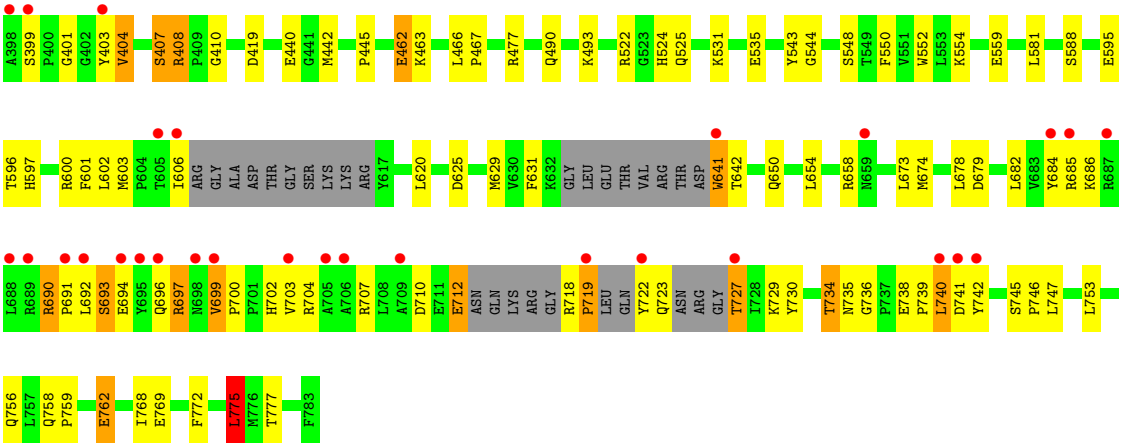
Chain A:



• Molecule 1: DNA polymerase II

Chain B:




A398 S399 P400 G401 G402 Y403 V404 S407 R408 P409 G410 D419 E440 G441 M442 P445 E462 K463 L466 P467 R477 Q490 K493 R522 G523 H524 Q525 K531 E535 Y543 G544 S548 T549 F550 V551 W552 L553 K554 E559 L581 S588 E595
T596 H597 R600 F601 L602 M603 P604 T605 I606 ARG GLY ALA ASP THR GLY SER LYS LYS ARG Y617 L620 D625 M629 V630 F631 K632 GLY LEU GLU THR VAL ARG THR ASP W641 T642 Q650 L654 R658 M659 L673 M674 L678 D679 L682 V683 Y684 R685 K686 R687
L688 R689 R690 P691 L692 S693 E694 Y695 Q696 R697 N698 V699 P700 P701 H702 V703 R704 A705 A706 R707 L708 A709 D710 E711 E712 ASN GLN LYS ARG GLY R718 P719 LEU GLN Y722 Q723 ASN ARG GLY T727 I728 K729 Y730 T734 N735 G736 P737 E738 P739 L740 D741 Y742 S745 P746 L747 L753
Q756 L757 Q758 P759 E762 I768 E769 F772 L775 M776 T777 F783

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.85Å 116.82Å 163.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 47.52 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 91.1 (47.52-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.223 0.218 , 0.222	Depositor DCC
R_{free} test set	2225 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12674	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7531e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.40	0/6299	0.69	0/8546
1	B	0.40	0/6175	0.71	4/8376 (0.0%)
All	All	0.40	0/12474	0.70	4/16922 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	734	THR	N-CA-C	-6.39	93.75	111.00
1	B	775	LEU	CA-CB-CG	5.90	128.87	115.30
1	B	408	ARG	N-CA-C	-5.28	96.75	111.00
1	B	736	GLY	N-CA-C	5.14	125.95	113.10

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	6137	0	5992	114	0
1	B	6015	0	5849	191	0
2	A	250	0	0	3	0
2	B	272	0	0	8	0
All	All	12674	0	11841	302	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 (302) 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:522:ARG:NH1	1:A:525:GLN:HE22	1.49	1.10
1:A:522:ARG:HH11	1:A:525:GLN:NE2	1.56	1.02
1:B:674:MET:HE3	1:B:753:LEU:HD22	1.40	1.01
1:A:311:TRP:CZ2	1:B:696:GLN:HB2	2.00	0.95
1:B:258:HIS:HD2	1:B:266:PHE:HD2	1.10	0.95
1:A:49:GLN:HE22	1:A:102:THR:H	1.04	0.95
1:B:685:ARG:HD2	1:B:727:THR:HG21	1.53	0.91
1:B:692:LEU:O	1:B:693:SER:HB3	1.70	0.91
1:B:258:HIS:HD2	1:B:266:PHE:CD2	1.89	0.90
1:B:116:MET:HE1	1:B:378:PHE:CG	2.08	0.89
1:A:712:GLU:HG2	1:A:742:TYR:CD1	2.11	0.86
1:A:49:GLN:NE2	1:A:102:THR:H	1.75	0.85
1:B:685:ARG:CD	1:B:727:THR:HG21	2.07	0.84
1:B:674:MET:HE1	1:B:753:LEU:HB2	1.60	0.83
1:B:674:MET:CE	1:B:753:LEU:HB2	2.10	0.82
1:B:199:ALA:H	1:B:203:GLN:NE2	1.77	0.82
1:A:522:ARG:HH11	1:A:525:GLN:HE22	0.86	0.81
1:B:258:HIS:CD2	1:B:266:PHE:HD2	1.97	0.80
1:A:83:CYS:HB3	1:A:88:GLN:HE21	1.47	0.80
1:B:93:GLU:O	1:B:97:ARG:HG2	1.82	0.80
1:B:758:GLN:HG3	1:B:772:PHE:CD2	2.16	0.80
1:B:477:ARG:HE	1:B:493:LYS:HB2	1.45	0.79
1:B:642:THR:H	1:B:756:GLN:HE22	1.27	0.78
1:B:116:MET:CE	1:B:378:PHE:HB2	2.16	0.76
1:B:294:GLU:O	1:B:298:GLN:HG2	1.85	0.76
1:A:49:GLN:HE22	1:A:102:THR:N	1.83	0.75
1:A:91:ASN:HB2	2:A:1051:HOH:O	1.87	0.75
1:A:85:ALA:O	1:A:88:GLN:HG2	1.87	0.75
1:B:699:VAL:CG1	1:B:704:ARG:HG3	2.17	0.73
1:B:745:SER:HB3	1:B:746:PRO:HD2	1.70	0.72
1:A:311:TRP:CE2	1:B:696:GLN:HB2	2.25	0.72
1:A:389:PRO:O	1:A:509:ARG:HD3	1.89	0.72
1:B:629:MET:HE1	1:B:654:LEU:HB2	1.73	0.71
1:B:696:GLN:HG2	1:B:697:ARG:H	1.56	0.71
1:B:116:MET:HE2	1:B:378:PHE:HB2	1.73	0.70
1:B:654:LEU:O	1:B:658:ARG:HG3	1.92	0.70
1:A:710:ASP:HB3	1:A:720:LEU:HD22	1.74	0.70
1:B:375:HIS:HD2	2:B:808:HOH:O	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:MET:HE1	1:B:378:PHE:CB	2.22	0.69
1:B:722:TYR:HE1	1:B:727:THR:O	1.74	0.69
1:B:642:THR:H	1:B:756:GLN:NE2	1.90	0.68
1:B:258:HIS:CD2	1:B:266:PHE:CD2	2.78	0.68
1:A:758:GLN:HG3	1:A:772:PHE:CD2	2.28	0.68
1:B:160:THR:CG2	1:B:164:GLU:HB2	2.23	0.68
1:A:309:ASN:OD1	1:A:719:PRO:HG2	1.94	0.67
1:B:175:GLN:NE2	1:B:211:TRP:HE1	1.92	0.67
1:A:131:HIS:CE1	1:A:132:ASN:ND2	2.63	0.66
1:A:540:ASP:OD1	1:A:554:LYS:HE3	1.97	0.65
1:B:768:ILE:O	1:B:769:GLU:HB2	1.97	0.64
1:B:700:PRO:HD2	1:B:703:VAL:CG2	2.27	0.64
1:A:615:LYS:HG3	1:A:615:LYS:O	1.97	0.64
1:B:772:PHE:O	1:B:775:LEU:HD22	1.97	0.64
1:A:581:LEU:HD12	1:A:588:SER:HB2	1.79	0.64
1:B:303:GLU:HG3	1:B:303:GLU:O	1.96	0.64
1:B:693:SER:HA	1:B:707:ARG:HH21	1.63	0.63
1:B:699:VAL:HG11	1:B:704:ARG:HG3	1.79	0.63
1:B:522:ARG:HH22	1:B:525:GLN:HE22	1.45	0.63
1:A:405:MET:CE	1:A:531:LYS:HE3	2.29	0.63
1:B:696:GLN:CG	1:B:697:ARG:H	2.11	0.63
1:B:674:MET:HE3	1:B:753:LEU:CD2	2.23	0.62
1:B:762:GLU:OE1	1:B:772:PHE:HB3	2.00	0.62
1:A:394:VAL:HG11	1:A:511:PHE:O	2.00	0.62
1:B:2:ALA:HB2	1:B:127:GLU:HG2	1.82	0.62
1:B:175:GLN:HE22	1:B:177:ILE:HG22	1.63	0.62
1:B:86:HIS:CE1	1:B:90:MET:CE	2.82	0.62
1:B:559:GLU:OE1	1:B:597:HIS:HD2	1.83	0.62
1:B:699:VAL:HG12	1:B:704:ARG:HG3	1.82	0.61
1:A:131:HIS:CE1	1:A:132:ASN:HD21	2.19	0.61
1:B:734:THR:O	1:B:735:ASN:HB2	1.99	0.61
1:B:116:MET:HE1	1:B:378:PHE:CD1	2.35	0.61
1:A:635:GLU:HG2	1:A:641:TRP:CD2	2.36	0.60
1:B:740:LEU:HD12	1:B:740:LEU:O	2.01	0.60
1:A:706:ALA:HA	1:A:728:ILE:CD1	2.32	0.60
1:B:522:ARG:NH2	1:B:525:GLN:NE2	2.50	0.60
1:B:679:ASP:HA	1:B:682:LEU:HD22	1.84	0.59
1:B:692:LEU:O	1:B:693:SER:CB	2.46	0.59
1:B:696:GLN:CG	1:B:697:ARG:N	2.66	0.59
1:B:650:GLN:HB3	2:B:1187:HOH:O	2.03	0.59
1:B:522:ARG:NH2	1:B:525:GLN:HE22	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ALA:H	1:B:203:GLN:HE22	1.50	0.58
1:A:706:ALA:HA	1:A:728:ILE:HD12	1.85	0.58
1:B:34:VAL:HG13	1:B:138:ALA:CB	2.34	0.58
1:B:364:ASP:OD1	1:B:364:ASP:N	2.36	0.58
1:B:758:GLN:HG3	1:B:772:PHE:HD2	1.66	0.58
1:B:32:LEU:HD21	1:B:135:ILE:CD1	2.34	0.58
1:B:718:ARG:CA	1:B:719:PRO:C	2.71	0.58
1:B:739:PRO:HG2	1:B:741:ASP:O	2.03	0.58
1:B:691:PRO:HG2	1:B:694:GLU:OE1	2.04	0.57
1:B:192:ASP:OD1	1:B:192:ASP:C	2.42	0.57
1:A:388:ALA:HB1	1:A:509:ARG:HD2	1.85	0.57
1:B:198:VAL:HB	1:B:203:GLN:HE21	1.69	0.57
1:B:685:ARG:CG	1:B:727:THR:CG2	2.82	0.57
1:A:49:GLN:NE2	1:A:101:VAL:HA	2.20	0.57
1:A:442:MET:O	1:A:445:PRO:HD3	2.04	0.57
1:B:690:ARG:HD2	1:B:694:GLU:HG2	1.86	0.57
1:A:316:GLU:OE2	1:A:319:ARG:NH1	2.37	0.57
1:B:127:GLU:OE1	1:B:139:ARG:NH1	2.39	0.56
1:A:49:GLN:HE21	1:A:101:VAL:HA	1.70	0.56
1:A:86:HIS:HE1	1:A:109:ARG:NH1	2.02	0.56
1:A:697:ARG:O	1:A:698:ASN:C	2.44	0.56
1:B:34:VAL:HG22	1:B:135:ILE:HB	1.86	0.56
1:B:758:GLN:HB3	1:B:759:PRO:HD3	1.88	0.56
1:B:32:LEU:HD21	1:B:135:ILE:HD12	1.88	0.56
1:B:384:ALA:O	1:B:463:LYS:HE3	2.06	0.56
1:A:400:PRO:HB2	1:A:520:THR:HG21	1.87	0.56
1:B:641:TRP:HA	1:B:641:TRP:CE3	2.40	0.56
1:A:13:ARG:NE	1:A:20:GLU:OE2	2.35	0.55
1:A:686:LYS:HD3	1:A:702:HIS:CG	2.41	0.55
1:A:309:ASN:HD22	1:A:312:ASP:H	1.54	0.55
1:B:629:MET:HE1	1:B:654:LEU:CB	2.35	0.55
1:B:642:THR:HG23	1:B:756:GLN:NE2	2.22	0.55
1:A:557:HIS:HD2	1:A:561:GLU:OE2	1.89	0.55
1:B:641:TRP:HA	1:B:641:TRP:HE3	1.71	0.55
1:A:617:TYR:CZ	1:A:632:LYS:HG3	2.43	0.54
1:A:706:ALA:CA	1:A:728:ILE:CD1	2.85	0.54
1:B:710:ASP:C	1:B:712:GLU:N	2.60	0.54
1:B:160:THR:HG23	1:B:164:GLU:HB2	1.89	0.54
1:B:718:ARG:N	1:B:719:PRO:C	2.61	0.54
1:A:47:ALA:O	1:A:50:VAL:HG23	2.08	0.54
1:A:712:GLU:HG2	1:A:742:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:CE1	1:B:90:MET:HE3	2.44	0.53
1:B:86:HIS:ND1	1:B:90:MET:HE1	2.23	0.53
1:A:394:VAL:O	1:A:394:VAL:HG13	2.07	0.53
1:B:125:TRP:HB2	1:B:141:LYS:HG2	1.90	0.53
1:B:407:SER:HB2	1:B:606:ILE:HB	1.89	0.53
1:B:700:PRO:HD2	1:B:703:VAL:HB	1.90	0.53
1:A:175:GLN:NE2	1:A:211:TRP:HZ2	2.06	0.52
1:A:405:MET:HE3	1:A:531:LYS:HE3	1.91	0.52
1:A:522:ARG:NH1	1:A:525:GLN:NE2	2.29	0.52
1:A:85:ALA:HB3	1:A:88:GLN:CD	2.30	0.52
1:A:557:HIS:CD2	1:A:561:GLU:OE2	2.63	0.52
1:B:347:GLU:O	1:B:350:PRO:HD2	2.10	0.51
1:A:690:ARG:HB2	1:A:695:TYR:CE2	2.46	0.51
1:B:442:MET:O	1:B:445:PRO:HD3	2.11	0.51
1:B:477:ARG:NE	1:B:493:LYS:HB2	2.19	0.51
1:B:686:LYS:HE2	1:B:702:HIS:CE1	2.46	0.51
1:A:454:PHE:HB3	1:A:455:LEU:CD1	2.41	0.51
1:A:603:MET:HE2	1:A:604:PRO:O	2.12	0.50
1:B:334:LYS:HE3	1:B:338:LEU:HD13	1.93	0.50
1:A:201:ARG:HB2	1:A:202:PRO:HD3	1.93	0.50
1:A:315:ASP:OD2	1:B:697:ARG:NH2	2.44	0.50
1:A:700:PRO:HG2	1:A:703:VAL:CG2	2.41	0.50
1:B:710:ASP:O	1:B:712:GLU:N	2.44	0.50
1:B:112:GLU:O	1:B:116:MET:HB2	2.11	0.50
1:B:2:ALA:HA	1:B:126:VAL:O	2.12	0.50
1:B:440:GLU:HG3	1:B:463:LYS:HD3	1.93	0.50
1:B:700:PRO:HD2	1:B:703:VAL:HG21	1.92	0.50
1:A:690:ARG:HD2	1:A:695:TYR:CZ	2.47	0.49
1:B:710:ASP:C	1:B:712:GLU:H	2.15	0.49
1:A:381:MET:HE1	1:A:388:ALA:HB2	1.95	0.49
1:B:86:HIS:CE1	1:B:109:ARG:NH1	2.81	0.49
1:B:730:TYR:HB2	1:B:738:GLU:O	2.12	0.49
1:B:629:MET:HG2	1:B:631:PHE:CZ	2.47	0.49
1:B:601:PHE:HE2	1:B:603:MET:HE2	1.77	0.49
1:B:543:TYR:HB2	1:B:603:MET:HE3	1.94	0.49
1:B:289:SER:HB3	1:B:299:GLU:OE2	2.13	0.49
1:A:701:PRO:HA	1:A:704:ARG:HG2	1.95	0.48
1:B:674:MET:HE3	1:B:753:LEU:HB2	1.93	0.48
1:A:63:PHE:CD1	1:A:63:PHE:C	2.86	0.48
1:A:122:SER:HB2	1:A:123:PRO:HD3	1.95	0.48
1:B:248:ARG:NH1	1:B:271:GLY:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:HE1	1:B:109:ARG:NH1	2.11	0.48
1:A:347:GLU:O	1:A:350:PRO:HD2	2.14	0.48
1:A:397:HIS:HB2	1:A:513:PRO:HB3	1.95	0.48
1:B:629:MET:CE	1:B:654:LEU:HB2	2.43	0.48
1:A:160:THR:HG22	1:A:166:TYR:CZ	2.49	0.48
1:B:200:SER:HB2	1:B:202:PRO:HD2	1.96	0.48
1:B:295:THR:HA	1:B:298:GLN:CG	2.44	0.48
1:B:403:TYR:HB2	1:B:524:HIS:CD2	2.49	0.48
1:B:700:PRO:HD2	1:B:703:VAL:CB	2.44	0.48
1:B:734:THR:CG2	1:B:746:PRO:HG2	2.44	0.48
1:A:175:GLN:NE2	1:A:175:GLN:O	2.48	0.47
1:A:289:SER:HB3	1:A:299:GLU:OE2	2.14	0.47
1:A:596:THR:HG22	1:A:597:HIS:N	2.28	0.47
1:B:462:GLU:HB2	2:B:1275:HOH:O	2.14	0.47
1:A:45:ILE:HG22	1:A:46:PRO:O	2.14	0.47
1:B:410:GLY:O	1:B:602:LEU:HD12	2.15	0.47
1:B:347:GLU:C	1:B:350:PRO:HD2	2.35	0.47
1:B:690:ARG:CB	1:B:691:PRO:CD	2.92	0.47
1:B:39:GLN:HG2	2:B:1039:HOH:O	2.15	0.47
1:B:419:ASP:HB3	1:B:548:SER:OG	2.14	0.47
1:B:685:ARG:CG	1:B:727:THR:HG23	2.45	0.47
1:A:399:SER:HA	1:A:400:PRO:HD3	1.78	0.47
1:A:455:LEU:N	1:A:455:LEU:HD12	2.30	0.47
1:B:522:ARG:HH21	1:B:525:GLN:CD	2.17	0.47
1:B:685:ARG:HD2	1:B:727:THR:CG2	2.36	0.47
1:A:175:GLN:HB3	2:A:1133:HOH:O	2.14	0.46
1:A:550:PHE:N	1:A:550:PHE:CD2	2.83	0.46
1:B:257:GLU:HB2	1:B:265:PHE:CE1	2.51	0.46
1:B:401:GLY:O	1:B:524:HIS:NE2	2.47	0.46
1:A:690:ARG:HD2	1:A:695:TYR:CE1	2.50	0.46
1:B:91:ASN:HD21	1:B:95:ARG:HH11	1.63	0.46
1:B:550:PHE:N	1:B:550:PHE:CD2	2.84	0.46
1:A:475:HIS:HD2	2:A:999:HOH:O	1.98	0.46
1:B:199:ALA:N	1:B:203:GLN:NE2	2.56	0.46
1:A:89:LEU:O	1:A:93:GLU:HG3	2.16	0.46
1:A:158:GLU:HB2	1:A:167:CYS:SG	2.56	0.46
1:A:594:TYR:OH	1:A:597:HIS:HB2	2.16	0.46
1:B:91:ASN:ND2	1:B:95:ARG:HH11	2.14	0.46
1:A:770:ASP:OD1	1:A:771:ASN:N	2.46	0.46
1:B:160:THR:HG21	1:B:164:GLU:HB2	1.95	0.46
1:A:309:ASN:HB3	1:A:312:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HA	1:A:235:LYS:HD3	1.63	0.45
1:B:46:PRO:HB3	1:B:76:GLN:HG2	1.98	0.45
1:B:349:MET:HB2	1:B:350:PRO:HD3	1.97	0.45
1:B:300:LEU:HG	1:B:345:LYS:HG2	1.98	0.45
1:B:544:GLY:HA2	1:B:548:SER:O	2.16	0.45
1:B:595:GLU:HG3	2:B:1061:HOH:O	2.15	0.45
1:A:419:ASP:OD2	1:A:595:GLU:OE1	2.35	0.45
1:A:706:ALA:CA	1:A:728:ILE:HD12	2.47	0.45
1:B:581:LEU:HD12	1:B:588:SER:HB2	1.99	0.45
1:B:741:ASP:O	1:B:742:TYR:CD2	2.70	0.45
1:B:298:GLN:HB3	1:B:303:GLU:O	2.16	0.45
1:B:741:ASP:O	1:B:742:TYR:CB	2.63	0.45
1:B:179:TYR:CE1	1:B:207:LYS:HE2	2.52	0.45
1:B:7:ILE:HG12	1:B:25:LEU:CD2	2.46	0.45
1:B:258:HIS:O	1:B:264:VAL:HG22	2.17	0.45
1:A:406:ASP:OD1	1:A:607:ARG:HA	2.17	0.44
1:B:684:TYR:O	1:B:729:LYS:HA	2.17	0.44
1:A:434:ASP:OD1	1:A:435:PRO:HD2	2.18	0.44
1:A:419:ASP:HB3	1:A:548:SER:OG	2.18	0.44
1:B:120:ILE:O	1:B:375:HIS:HE1	2.00	0.44
1:B:600:ARG:HB2	1:B:620:LEU:HB3	2.00	0.44
1:B:678:LEU:O	1:B:682:LEU:HD13	2.17	0.44
1:B:691:PRO:HD2	1:B:694:GLU:HB2	2.00	0.44
1:A:455:LEU:CD1	1:A:455:LEU:N	2.81	0.44
1:A:479:GLU:OE2	1:A:482:ARG:NH2	2.50	0.44
1:A:325:LYS:N	1:A:326:PRO:CD	2.80	0.44
1:B:237:ALA:HB1	1:B:242:LEU:O	2.18	0.44
1:A:424:TYR:HB2	1:A:425:PRO:HD3	2.00	0.44
1:B:699:VAL:HA	1:B:700:PRO:HD3	1.78	0.44
1:B:673:LEU:HD23	1:B:674:MET:CE	2.47	0.44
1:B:24:TRP:HE1	1:B:270:LYS:HE3	1.83	0.43
1:B:403:TYR:HB2	1:B:524:HIS:HD2	1.83	0.43
1:B:531:LYS:O	1:B:535:GLU:HG3	2.17	0.43
1:B:690:ARG:HB3	1:B:691:PRO:CD	2.48	0.43
1:B:522:ARG:NH2	1:B:525:GLN:OE1	2.47	0.43
1:B:231:ARG:HG2	1:B:231:ARG:HH11	1.83	0.43
1:B:395:PRO:HA	1:B:396:PRO:HD2	1.92	0.43
1:A:320:ARG:HB3	1:A:328:LEU:HB2	2.00	0.43
1:B:408:ARG:HE	1:B:408:ARG:HB3	1.67	0.43
1:B:596:THR:HG22	1:B:597:HIS:N	2.33	0.43
1:A:161:ARG:HG3	1:A:314:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:OG	1:A:86:HIS:HD2	2.02	0.43
1:A:131:HIS:ND1	1:A:132:ASN:ND2	2.66	0.43
1:A:348:ILE:O	1:A:352:LEU:HG	2.19	0.43
1:A:690:ARG:HB2	1:A:695:TYR:CZ	2.54	0.43
1:B:86:HIS:CE1	1:B:109:ARG:HD3	2.53	0.43
1:B:97:ARG:NE	2:B:1132:HOH:O	2.52	0.43
1:B:153:VAL:O	1:B:153:VAL:HG13	2.19	0.43
1:A:76:GLN:HA	1:A:77:PRO:HD3	1.92	0.42
1:B:165:LEU:HB2	1:B:236:HIS:NE2	2.33	0.42
1:B:629:MET:CE	1:B:654:LEU:HD13	2.49	0.42
1:B:741:ASP:O	1:B:742:TYR:HB2	2.19	0.42
1:A:690:ARG:HG3	1:A:690:ARG:HH11	1.84	0.42
1:B:691:PRO:HA	1:B:723:GLN:O	2.19	0.42
1:B:48:ASP:H	1:B:76:GLN:NE2	2.18	0.42
1:B:334:LYS:HA	1:B:334:LYS:HD2	1.81	0.42
1:B:403:TYR:O	1:B:404:VAL:CG2	2.68	0.42
1:B:629:MET:HE2	1:B:654:LEU:HD13	2.00	0.42
1:A:405:MET:CE	1:A:531:LYS:CE	2.97	0.42
1:B:86:HIS:CE1	1:B:90:MET:HE1	2.55	0.42
1:B:287:ASN:ND2	1:B:287:ASN:H	2.17	0.42
1:B:86:HIS:CE1	1:B:109:ARG:HH11	2.37	0.42
1:B:125:TRP:CE2	1:B:143:HIS:CD2	3.07	0.42
1:A:241:ARG:HA	1:A:241:ARG:HD2	1.85	0.42
1:B:185:ASN:OD1	1:B:185:ASN:C	2.58	0.42
1:A:44:PHE:HB2	1:A:104:TYR:HB2	2.00	0.42
1:B:466:LEU:N	1:B:467:PRO:CD	2.83	0.42
1:B:699:VAL:HG11	1:B:704:ARG:CG	2.46	0.42
1:A:9:THR:OG1	1:A:11:HIS:HE1	2.02	0.41
1:B:9:THR:HA	2:B:838:HOH:O	2.19	0.41
1:A:86:HIS:CE1	1:A:109:ARG:NH1	2.86	0.41
1:A:92:TYR:O	1:A:96:LEU:HG	2.21	0.41
1:B:34:VAL:HG21	1:B:126:VAL:HG21	2.02	0.41
1:B:673:LEU:HD23	1:B:674:MET:HE2	2.01	0.41
1:B:321:PHE:CE1	1:B:325:LYS:HE2	2.56	0.41
1:A:289:SER:CB	1:A:299:GLU:OE2	2.69	0.41
1:B:543:TYR:CG	1:B:544:GLY:N	2.88	0.41
1:A:522:ARG:HD3	1:A:522:ARG:HA	1.88	0.41
1:B:294:GLU:H	1:B:294:GLU:CD	2.23	0.41
1:B:522:ARG:NH2	1:B:525:GLN:CD	2.74	0.41
1:A:700:PRO:HG2	1:A:703:VAL:HG23	2.02	0.41
1:A:739:PRO:HG2	1:A:742:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASP:OD1	1:A:449:HIS:HD2	2.04	0.41
1:A:667:ARG:HB3	1:A:779:GLN:OE1	2.20	0.41
1:A:706:ALA:HB2	1:A:728:ILE:CD1	2.51	0.41
1:B:32:LEU:HD21	1:B:135:ILE:HD11	2.03	0.41
1:B:543:TYR:HB2	1:B:603:MET:CE	2.50	0.41
1:B:552:TRP:CE2	1:B:554:LYS:HA	2.56	0.40
1:B:60:GLU:HB3	1:B:92:TYR:OH	2.22	0.40
1:B:86:HIS:ND1	1:B:90:MET:CE	2.82	0.40
1:A:125:TRP:CE2	1:A:143:HIS:CD2	3.08	0.40
1:A:668:GLU:OE1	1:A:668:GLU:HA	2.22	0.40
1:B:12:TRP:HA	1:B:20:GLU:O	2.21	0.40
1:A:85:ALA:HB3	1:A:88:GLN:CG	2.51	0.40
1:A:193:PHE:CD2	1:A:193:PHE:N	2.89	0.40
1:B:392:GLY:HA2	2:B:1106:HOH:O	2.20	0.40
1:A:309:ASN:CG	1:A:719:PRO:HG2	2.41	0.40
1:A:409:PRO:HB2	1:A:767:PHE:CZ	2.56	0.40
1:B:685:ARG:HG3	1:B:727:THR:CG2	2.51	0.40
1:B:693:SER:O	1:B:693:SER:OG	2.39	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	748/786 (95%)	733 (98%)	12 (2%)	3 (0%)	34	37
1	B	730/786 (93%)	709 (97%)	17 (2%)	4 (0%)	29	31
All	All	1478/1572 (94%)	1442 (98%)	29 (2%)	7 (0%)	29	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	693	SER
1	A	698	ASN
1	B	122	SER
1	B	699	VAL
1	A	122	SER
1	A	414	SER
1	B	404	VAL

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	642/672 (96%)	625 (97%)	17 (3%)	46	58
1	B	629/672 (94%)	602 (96%)	27 (4%)	29	36
All	All	1271/1344 (95%)	1227 (96%)	44 (4%)	36	46

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	20	GLU
1	A	95	ARG
1	A	127	GLU
1	A	148	PRO
1	A	190	SER
1	A	192	ASP
1	A	281	LEU
1	A	298	GLN
1	A	455	LEU
1	A	525	GLN
1	A	561	GLU
1	A	582	GLN
1	A	650	GLN
1	A	688	LEU
1	A	707	ARG
1	A	708	LEU

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Mol	Chain	Res	Type
1	B	116	MET
1	B	148	PRO
1	B	175	GLN
1	B	268	GLN
1	B	270	LYS
1	B	289	SER
1	B	298	GLN
1	B	303	GLU
1	B	317	ILE
1	B	364	ASP
1	B	369	SER
1	B	399	SER
1	B	407	SER
1	B	462	GLU
1	B	490	GLN
1	B	625	ASP
1	B	641	TRP
1	B	690	ARG
1	B	697	ARG
1	B	712	GLU
1	B	719	PRO
1	B	727	THR
1	B	740	LEU
1	B	747	LEU
1	B	762	GLU
1	B	775	LEU
1	B	777	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	11	HIS
1	A	33	GLN
1	A	39	GLN
1	A	49	GLN
1	A	86	HIS
1	A	88	GLN
1	A	131	HIS
1	A	132	ASN
1	A	332	ASN
1	A	449	HIS

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Mol	Chain	Res	Type
1	A	475	HIS
1	A	497	ASN
1	A	525	GLN
1	A	557	HIS
1	A	571	GLN
1	A	584	GLN
1	A	649	GLN
1	A	735	ASN
1	A	756	GLN
1	B	76	GLN
1	B	86	HIS
1	B	91	ASN
1	B	137	ASN
1	B	175	GLN
1	B	203	GLN
1	B	258	HIS
1	B	287	ASN
1	B	375	HIS
1	B	390	ASN
1	B	597	HIS
1	B	735	ASN
1	B	756	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 monosaccharides in this entry.

5.6 Ligand geometry

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^{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	758/786 (96%)	0.09	39 (5%)	28	26	18, 35, 65, 85	0
1	B	744/786 (94%)	0.13	40 (5%)	25	24	17, 36, 67, 81	0
All	All	1502/1572 (95%)	0.11	79 (5%)	26	25	17, 36, 66, 85	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	709	ALA	6.8
1	A	398	ALA	5.8
1	A	636	THR	5.1
1	A	697	ARG	5.1
1	A	698	ASN	4.9
1	A	633	GLY	4.8
1	B	706	ALA	4.7
1	B	291	PHE	4.7
1	B	287	ASN	4.6
1	B	641	TRP	4.4
1	A	703	VAL	4.3
1	B	705	ALA	4.2
1	A	726	GLY	4.2
1	A	366	HIS	4.2
1	B	398	ALA	4.0
1	B	302	GLY	3.8
1	B	740	LEU	3.8
1	B	694	GLU	3.8
1	A	607	ARG	3.7
1	B	687	ARG	3.7
1	A	724	ASN	3.7
1	A	289	SER	3.6
1	B	719	PRO	3.6
1	A	699	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	720	LEU	3.6
1	A	687	ARG	3.5
1	A	693	SER	3.4
1	B	722	TYR	3.4
1	A	694	GLU	3.4
1	A	291	PHE	3.3
1	B	606	ILE	3.3
1	A	690	ARG	3.2
1	A	717	GLY	3.2
1	B	691	PRO	3.2
1	A	266	PHE	3.2
1	A	392	GLY	3.2
1	A	641	TRP	3.2
1	B	605	THR	3.1
1	A	290	SER	3.1
1	A	692	LEU	3.1
1	A	634	LEU	3.1
1	B	692	LEU	3.1
1	A	312	ASP	3.0
1	B	727	THR	3.0
1	B	258	HIS	2.9
1	A	635	GLU	2.8
1	B	742	TYR	2.8
1	B	161	ARG	2.8
1	B	685	ARG	2.7
1	B	403	TYR	2.7
1	B	703	VAL	2.7
1	B	259	GLY	2.7
1	B	698	ASN	2.7
1	B	290	SER	2.6
1	B	688	LEU	2.6
1	A	395	PRO	2.6
1	A	608	GLY	2.6
1	B	399	SER	2.6
1	B	317	ILE	2.6
1	A	688	LEU	2.6
1	A	691	PRO	2.6
1	A	606	ILE	2.6
1	A	716	ARG	2.4
1	B	190	SER	2.4
1	B	695	TYR	2.4
1	B	741	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	616	ARG	2.4
1	B	295	THR	2.3
1	A	725	ARG	2.3
1	A	404	VAL	2.3
1	B	696	GLN	2.2
1	B	699	VAL	2.2
1	A	605	THR	2.2
1	B	659	ASN	2.1
1	B	689	ARG	2.1
1	B	684	TYR	2.1
1	A	695	TYR	2.1
1	B	266	PHE	2.1
1	A	723	GLN	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 monosaccharides 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.