Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 06:01 pm BST

PDB ID	:	2Y9Y
Title	:	Chromatin Remodeling Factor ISW1a(del_ATPase)
Authors	:	Yamada, K.; Frouws, T.D.; Angst, B.; Fitzgerald, D.J.; DeLuca, C.; Schimmele, K.; Sargent, D.F.; Richmond, T.J.
Deposited on	:	2011-02-17
Resolution	:	3.25 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:

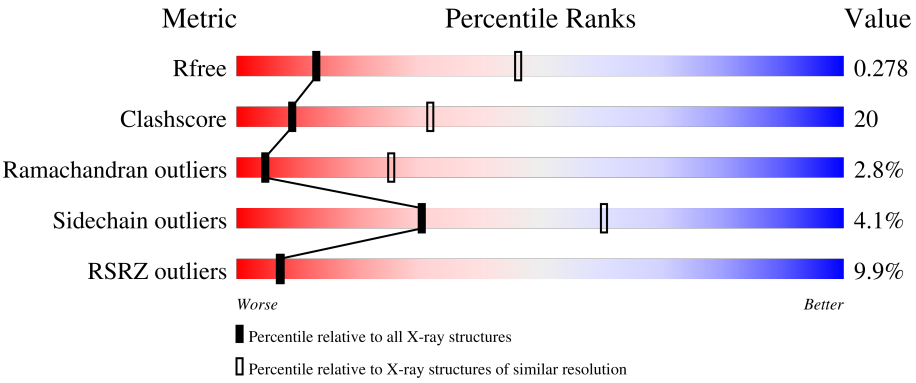
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	374	7% 48% 24% · 26%
2	B	624	9% 55% 36% · 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7170 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 IMITATION SWITCH PROTEIN 1 (DEL_ATPASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2317	1473	399	437	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	MET	-	expression tag	UNP P38144
A	815	GLN	LYS	engineered mutation	UNP P38144
A	844	LYS	ASP	engineered mutation	UNP P38144
A	848	GLN	GLU	engineered mutation	UNP P38144
A	851	GLN	LYS	engineered mutation	UNP P38144
A	853	GLU	GLN	engineered mutation	UNP P38144
A	1130	HIS	-	expression tag	UNP P38144
A	1131	HIS	-	expression tag	UNP P38144
A	1132	HIS	-	expression tag	UNP P38144
A	1133	HIS	-	expression tag	UNP P38144
A	1134	HIS	-	expression tag	UNP P38144
A	1135	HIS	-	expression tag	UNP P38144

- Molecule 2 is a protein called ISWI ONE COMPLEX PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	592	Total	C	N	O	S	0	0	0
			4853	3123	818	897	15			

There are 2 discrepancies between the modelled and reference sequences:

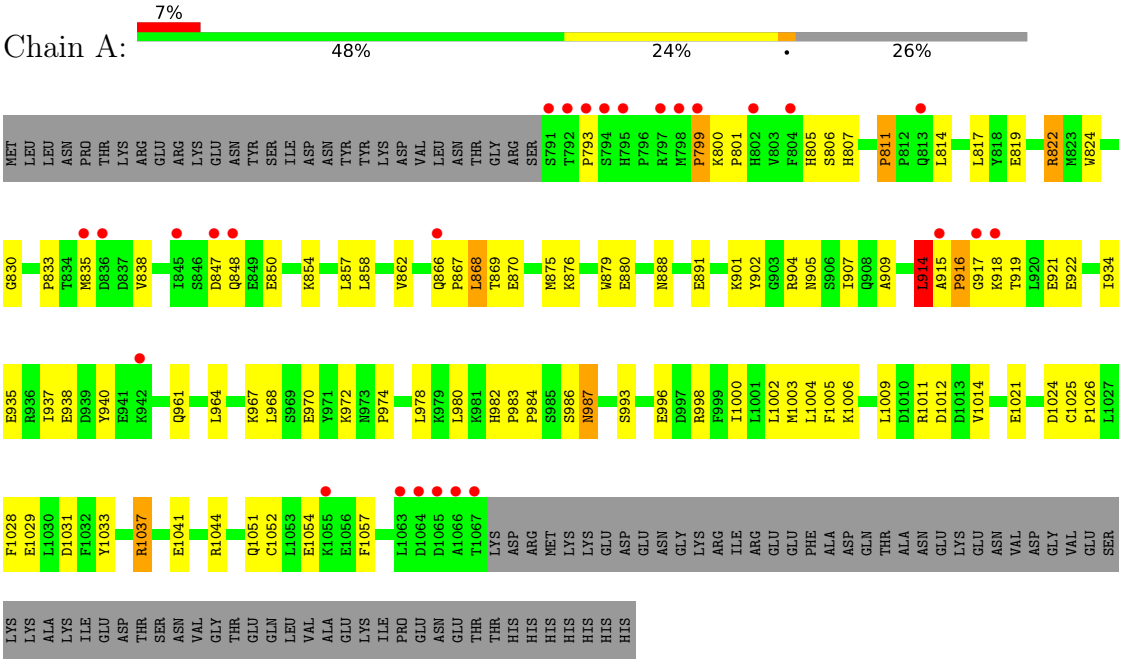
Chain	Residue	Modelled	Actual	Comment	Reference
B	126	MET	-	expression tag	UNP P43596
B	682	LYS	ASN	engineered mutation	UNP P43596

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.

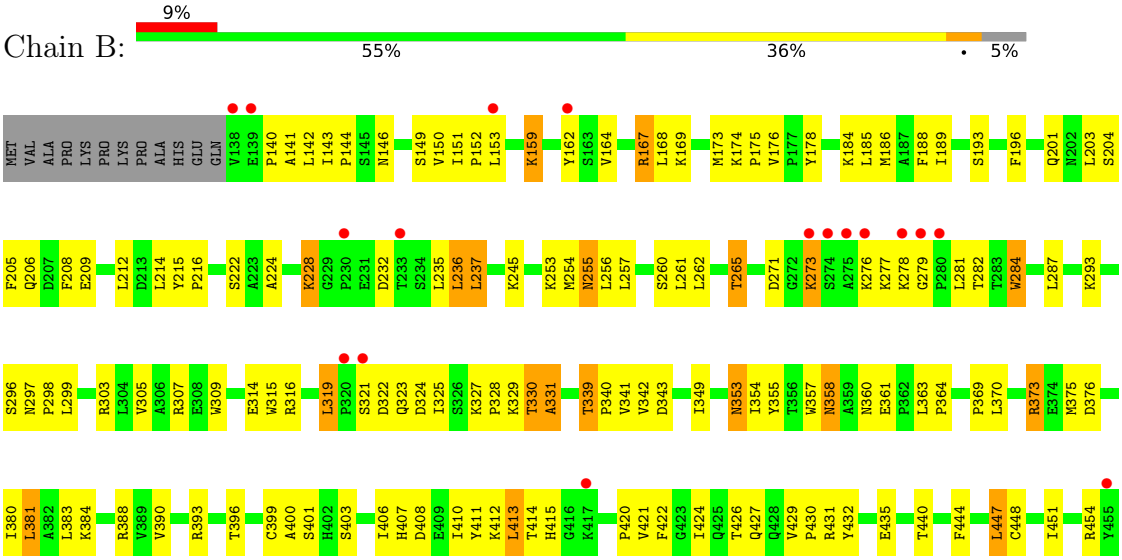
• Molecule 1: IMITATION SWITCH PROTEIN 1 (DEL_ATPASE)

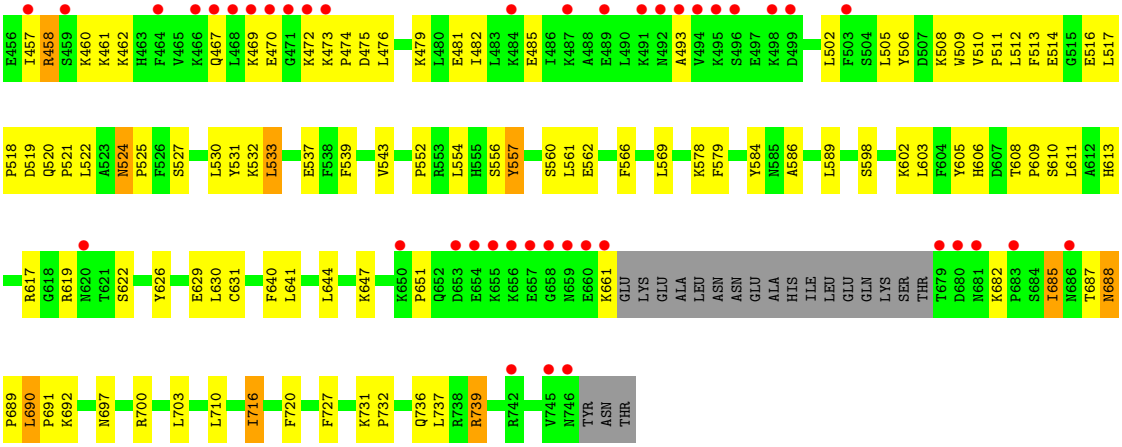
Chain A:



• Molecule 2: ISWI ONE COMPLEX PROTEIN 3

Chain B:




E456 I457 R458 S459 K460 K461 K462 H463 F464 V465 K466 Q467 L468 K469 E470 G471 K472 K473 P474 D475 L476 K479 L480 E481 I482 L483 K484 E485 I486 K487 A488 E489 L490 K491 N492 A493 V494 K495 S496 E497 K498 D499 L502 F503 S504 L505 Y506 D507 K508 W509 V510 P511 L512 F513 E514 G515 E516 L517
P518 D519 Q520 P521 L522 A523 N524 P525 F526 S527 L530 Y531 K532 L533 E537 F538 F539 V543 P552 R553 L554 H555 S556 Y557 S560 L561 E562 F566 L569 K578 F579 Y584 N585 A586 L589 S598 K602 L603 F604 Y605 H606 D607 T608 P609 S610 L611 A612 H613
R617 G618 R619 N620 T621 S622 Y626 E629 L630 C631 F640 L641 L644 K647 K650 P651 Q652 D653 E654 K655 K656 E657 G658 N659 E660 K661 GLU LYS GLU ALA LEU ASN ASN GLU ALA HIS ILE LEU GLU GLN LYS SER THR T679 D680 N681 K682 P683 S684 I685 N686 T687 N688
P689 L690 P691 K692 N697 R700 L703 L710 I716 F720 F727 K731 P732 Q736 L737 R738 R739 R742 V745 N746 TYR ASN THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	206.97Å 206.97Å 215.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.87 – 3.25 29.87 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.87-3.25) 100.0 (29.87-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.93 (at 3.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.283 , 0.296 0.276 , 0.278	Depositor DCC
R_{free} test set	1381 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	120.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 97.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å^2)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	0.21	0/2368	0.35	0/3186
2	B	0.21	0/4974	0.35	0/6723
All	All	0.21	0/7342	0.35	0/9909

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	2317	0	2300	87	0
2	B	4853	0	4857	204	0
All	All	7170	0	7157	287	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 20.

All (287) 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)
2:B:327:LYS:HB2	2:B:328:PRO:HD3	1.50	0.91
1:A:918:LYS:HB2	1:A:922:GLU:HG3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:LYS:HA	2:B:296:SER:HB3	1.54	0.87
2:B:339:THR:HB	2:B:340:PRO:HD3	1.61	0.83
2:B:413:LEU:HD22	2:B:533:LEU:HB2	1.58	0.83
1:A:937:ILE:HG21	1:A:940:TYR:HB3	1.60	0.82
2:B:690:LEU:HB3	2:B:691:PRO:HD3	1.60	0.82
2:B:152:PRO:HG3	2:B:431:ARG:HD2	1.62	0.80
2:B:237:LEU:H	2:B:237:LEU:HD23	1.46	0.79
2:B:164:VAL:HG22	2:B:609:PRO:HB2	1.61	0.79
2:B:153:LEU:H	2:B:153:LEU:HD23	1.50	0.77
2:B:381:LEU:HD12	2:B:381:LEU:H	1.51	0.76
2:B:554:LEU:H	2:B:598:SER:HB2	1.51	0.76
2:B:255:ASN:HD21	2:B:380:ILE:H	1.34	0.75
1:A:805:HIS:CD2	1:A:806:SER:H	2.04	0.75
2:B:324:ASP:HA	2:B:330:THR:HG21	1.68	0.74
2:B:373:ARG:H	2:B:373:ARG:HD3	1.51	0.74
2:B:144:PRO:HB2	2:B:421:VAL:HG21	1.68	0.73
2:B:150:VAL:HB	2:B:525:PRO:HG3	1.71	0.73
2:B:260:SER:HA	2:B:282:THR:HG21	1.72	0.71
1:A:974:PRO:O	1:A:998:ARG:HD2	1.92	0.70
1:A:805:HIS:CG	1:A:806:SER:H	2.09	0.70
2:B:316:ARG:HD2	2:B:360:ASN:HB3	1.71	0.70
2:B:167:ARG:H	2:B:167:ARG:HD3	1.56	0.70
2:B:149:SER:HB2	2:B:519:ASP:HB3	1.73	0.70
1:A:905:ASN:HD21	2:B:343:ASP:HB3	1.55	0.69
1:A:993:SER:HB3	1:A:996:GLU:HG3	1.75	0.69
2:B:509:TRP:HB3	2:B:513:PHE:HE2	1.58	0.69
2:B:150:VAL:HG12	2:B:431:ARG:H	1.58	0.69
1:A:983:PRO:HA	1:A:1052:CYS:HB3	1.76	0.67
1:A:934:ILE:O	1:A:937:ILE:HG12	1.93	0.67
1:A:1041:GLU:HG2	1:A:1044:ARG:HH21	1.60	0.66
2:B:393:ARG:O	2:B:396:THR:HG22	1.96	0.66
1:A:915:ALA:N	1:A:916:PRO:HD3	2.11	0.66
2:B:150:VAL:HA	2:B:431:ARG:HB2	1.76	0.66
2:B:228:LYS:HE3	2:B:228:LYS:HA	1.77	0.66
2:B:255:ASN:HB3	2:B:287:LEU:HD11	1.77	0.65
1:A:1003:MET:SD	1:A:1021:GLU:HG2	2.37	0.65
1:A:967:LYS:HD3	1:A:1057:PHE:CE2	2.32	0.64
2:B:451:ILE:HD12	2:B:512:LEU:HD22	1.79	0.64
2:B:426:THR:HG23	2:B:427:GLN:HG3	1.80	0.63
2:B:186:MET:HE1	2:B:205:PHE:HD2	1.63	0.63
2:B:586:ALA:HA	2:B:589:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:PRO:HB3	1:A:879:TRP:CE3	2.34	0.62
2:B:403:SER:HB3	2:B:406:ILE:HG12	1.82	0.62
2:B:358:ASN:HD22	2:B:358:ASN:H	1.47	0.62
1:A:811:PRO:HB3	1:A:879:TRP:HE3	1.65	0.61
2:B:315:TRP:O	2:B:363:LEU:HB2	2.00	0.61
2:B:641:LEU:HD21	2:B:710:LEU:HB2	1.80	0.61
2:B:341:VAL:HG22	2:B:343:ASP:H	1.65	0.61
1:A:814:LEU:HD23	1:A:817:LEU:HD12	1.82	0.60
2:B:353:ASN:HD22	2:B:353:ASN:N	2.00	0.60
2:B:557:TYR:HA	2:B:561:LEU:HD11	1.82	0.60
1:A:875:MET:HB3	1:A:879:TRP:HE1	1.66	0.60
2:B:159:LYS:NZ	2:B:159:LYS:HB3	2.15	0.60
1:A:974:PRO:HB2	1:A:1002:LEU:HD21	1.82	0.60
1:A:914:LEU:HD12	1:A:915:ALA:H	1.67	0.59
2:B:256:LEU:HD22	2:B:284:TRP:CD1	2.37	0.59
2:B:475:ASP:O	2:B:479:LYS:HG3	2.03	0.59
1:A:1006:LYS:HA	1:A:1006:LYS:HE3	1.85	0.58
2:B:578:LYS:HD3	2:B:584:TYR:CE1	2.38	0.58
2:B:556:SER:HA	2:B:566:PHE:CD2	2.39	0.58
2:B:697:ASN:HA	2:B:700:ARG:NE	2.19	0.58
1:A:807:HIS:CG	1:A:807:HIS:O	2.57	0.57
1:A:914:LEU:CD1	1:A:915:ALA:H	2.17	0.57
2:B:150:VAL:O	2:B:430:PRO:HA	2.04	0.57
1:A:967:LYS:HD3	1:A:1057:PHE:HE2	1.68	0.57
2:B:358:ASN:H	2:B:358:ASN:ND2	2.01	0.57
2:B:384:LYS:O	2:B:388:ARG:HG3	2.03	0.57
2:B:661:LYS:HA	2:B:661:LYS:HE2	1.86	0.57
2:B:261:LEU:O	2:B:265:THR:HG22	2.05	0.57
1:A:888:ASN:HB2	1:A:891:GLU:HG3	1.86	0.57
2:B:151:ILE:HD11	2:B:525:PRO:HB3	1.87	0.56
2:B:510:VAL:HB	2:B:511:PRO:HD3	1.87	0.56
2:B:458:ARG:HB2	2:B:461:LYS:HB3	1.87	0.56
2:B:516:GLU:HB3	2:B:517:LEU:HD12	1.87	0.56
2:B:400:ALA:HA	2:B:406:ILE:HD11	1.87	0.56
2:B:454:ARG:HH21	2:B:516:GLU:HG3	1.70	0.56
2:B:411:TYR:HA	2:B:414:THR:HG22	1.88	0.55
2:B:193:SER:HB2	2:B:201:GLN:NE2	2.20	0.55
1:A:875:MET:HB3	1:A:879:TRP:NE1	2.22	0.55
2:B:407:HIS:O	2:B:410:ILE:HG13	2.07	0.55
2:B:476:LEU:HA	2:B:479:LYS:HD2	1.88	0.55
1:A:983:PRO:CA	1:A:1052:CYS:HB3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:GLN:HE21	1:A:1009:LEU:HG	1.72	0.54
2:B:152:PRO:HD2	2:B:429:VAL:O	2.07	0.54
2:B:630:LEU:HD13	2:B:640:PHE:CZ	2.41	0.54
2:B:153:LEU:H	2:B:153:LEU:CD2	2.20	0.54
1:A:800:LYS:HB3	1:A:822:ARG:HE	1.73	0.54
1:A:987:ASN:N	1:A:987:ASN:HD22	2.05	0.54
2:B:245:LYS:O	2:B:245:LYS:HD3	2.08	0.54
2:B:447:LEU:HD22	2:B:513:PHE:HE1	1.71	0.54
1:A:1011:ARG:HG3	1:A:1012:ASP:OD1	2.08	0.54
1:A:937:ILE:HD13	1:A:940:TYR:HB3	1.90	0.54
2:B:732:PRO:HB3	2:B:737:LEU:HD13	1.90	0.53
2:B:739:ARG:NH1	2:B:739:ARG:HB2	2.23	0.53
1:A:833:PRO:HG2	1:A:858:LEU:HA	1.90	0.53
2:B:277:LYS:HE3	2:B:277:LYS:HA	1.91	0.53
1:A:866:GLN:HG3	1:A:867:PRO:HD2	1.91	0.53
2:B:473:LYS:N	2:B:474:PRO:CD	2.71	0.53
1:A:807:HIS:CD2	1:A:938:GLU:H	2.27	0.52
2:B:467:GLN:HE22	2:B:469:LYS:HB2	1.74	0.52
1:A:914:LEU:HB2	1:A:916:PRO:HG3	1.92	0.52
2:B:524:ASN:HB3	2:B:527:SER:OG	2.10	0.52
2:B:608:THR:OG1	2:B:609:PRO:HD3	2.09	0.52
2:B:140:PRO:HB3	2:B:457:ILE:HG12	1.91	0.52
2:B:212:LEU:HD12	2:B:254:MET:HG3	1.92	0.52
2:B:271:ASP:HB3	2:B:273:LYS:HE3	1.91	0.52
2:B:149:SER:HB2	2:B:519:ASP:CB	2.40	0.52
2:B:150:VAL:HG22	2:B:521:PRO:HA	1.92	0.52
2:B:167:ARG:H	2:B:167:ARG:CD	2.20	0.52
1:A:838:VAL:HG11	1:A:854:LYS:HE2	1.92	0.51
2:B:543:VAL:HG11	2:B:703:LEU:HG	1.92	0.51
1:A:907:ILE:HD11	2:B:342:VAL:HB	1.91	0.51
2:B:647:LYS:HD2	2:B:647:LYS:N	2.26	0.51
2:B:413:LEU:HD11	2:B:532:LYS:HD3	1.91	0.51
2:B:505:LEU:HB3	2:B:509:TRP:CD1	2.45	0.51
2:B:481:GLU:O	2:B:485:GLU:HG2	2.11	0.51
2:B:552:PRO:HD2	2:B:602:LYS:O	2.11	0.51
2:B:579:PHE:CD1	2:B:716:ILE:HG12	2.45	0.51
2:B:691:PRO:HB3	2:B:700:ARG:NE	2.25	0.51
2:B:143:ILE:HD12	2:B:146:ASN:OD1	2.10	0.51
2:B:363:LEU:HG	2:B:364:PRO:HD2	1.93	0.51
1:A:993:SER:HB3	1:A:996:GLU:CG	2.41	0.51
2:B:448:CYS:HA	2:B:451:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:543:VAL:HG21	2:B:703:LEU:HD23	1.91	0.51
2:B:688:ASN:H	2:B:689:PRO:CD	2.24	0.50
2:B:329:LYS:HB3	2:B:357:TRP:NE1	2.27	0.50
2:B:401:SER:HA	2:B:407:HIS:HD2	1.77	0.50
2:B:532:LYS:HE3	2:B:557:TYR:CE1	2.46	0.50
1:A:819:GLU:HA	1:A:822:ARG:HD2	1.93	0.50
1:A:980:LEU:HB3	1:A:983:PRO:HG2	1.92	0.50
1:A:982:HIS:N	1:A:983:PRO:CD	2.74	0.50
2:B:189:ILE:HD11	2:B:257:LEU:HD21	1.92	0.50
2:B:209:GLU:HA	2:B:214:LEU:HB2	1.93	0.50
2:B:408:ASP:O	2:B:412:LYS:HG3	2.11	0.50
2:B:185:LEU:HD23	2:B:208:PHE:HE2	1.76	0.50
2:B:186:MET:HE1	2:B:205:PHE:CD2	2.45	0.50
2:B:321:SER:C	2:B:323:GLN:H	2.15	0.50
1:A:800:LYS:HD3	1:A:822:ARG:NH2	2.26	0.50
2:B:297:ASN:HB2	2:B:298:PRO:HD3	1.93	0.50
2:B:164:VAL:HG11	2:B:610:SER:OG	2.11	0.50
2:B:167:ARG:HB2	2:B:687:THR:OG1	2.11	0.50
2:B:691:PRO:HB3	2:B:700:ARG:HE	1.77	0.50
1:A:805:HIS:CG	1:A:806:SER:N	2.77	0.49
2:B:215:TYR:H	2:B:222:SER:HB2	1.77	0.49
2:B:327:LYS:HB2	2:B:328:PRO:CD	2.35	0.49
1:A:972:LYS:O	1:A:974:PRO:HD3	2.13	0.49
2:B:169:LYS:NZ	2:B:682:LYS:HD2	2.28	0.49
2:B:189:ILE:HD11	2:B:257:LEU:CD2	2.43	0.49
1:A:800:LYS:NZ	1:A:857:LEU:HB3	2.28	0.48
2:B:173:MET:HA	2:B:629:GLU:O	2.12	0.48
2:B:307:ARG:HG2	2:B:307:ARG:HH11	1.78	0.48
2:B:315:TRP:CD1	2:B:369:PRO:HG2	2.48	0.48
2:B:688:ASN:HB2	2:B:689:PRO:HD3	1.96	0.48
1:A:1037:ARG:HA	1:A:1037:ARG:NE	2.28	0.48
2:B:613:HIS:O	2:B:617:ARG:HG3	2.13	0.48
1:A:980:LEU:HB3	1:A:983:PRO:CG	2.43	0.48
2:B:460:LYS:HG3	2:B:462:LYS:HE2	1.96	0.48
2:B:319:LEU:N	2:B:319:LEU:HD23	2.27	0.48
2:B:358:ASN:ND2	2:B:358:ASN:N	2.61	0.48
2:B:262:LEU:HD13	2:B:298:PRO:HB2	1.94	0.48
2:B:305:VAL:HB	2:B:309:TRP:CE2	2.48	0.48
2:B:537:GLU:CD	2:B:537:GLU:H	2.17	0.48
2:B:159:LYS:HD3	2:B:609:PRO:HG3	1.96	0.48
2:B:185:LEU:HD23	2:B:208:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:TYR:HE1	2:B:522:LEU:HB3	1.78	0.48
2:B:176:VAL:HG22	2:B:216:PRO:HB3	1.95	0.48
2:B:316:ARG:CD	2:B:360:ASN:HB3	2.39	0.48
2:B:603:LEU:HB3	2:B:631:CYS:SG	2.54	0.48
1:A:914:LEU:HD13	1:A:916:PRO:HD3	1.95	0.47
2:B:440:THR:HG21	2:B:569:LEU:HG	1.97	0.47
2:B:537:GLU:C	2:B:539:PHE:H	2.18	0.47
1:A:876:LYS:O	1:A:880:GLU:HG2	2.15	0.47
1:A:918:LYS:HB2	1:A:922:GLU:CG	2.36	0.47
1:A:1028:PHE:HB3	1:A:1031:ASP:HB3	1.96	0.47
2:B:151:ILE:HG21	2:B:531:TYR:CD1	2.49	0.47
1:A:982:HIS:C	1:A:984:PRO:HD2	2.35	0.47
1:A:800:LYS:HB3	1:A:822:ARG:NE	2.30	0.46
1:A:983:PRO:CB	1:A:1052:CYS:HB3	2.45	0.46
1:A:901:LYS:HD2	1:A:1011:ARG:NE	2.30	0.46
2:B:524:ASN:C	2:B:524:ASN:HD22	2.17	0.46
2:B:424:ILE:HD12	2:B:424:ILE:N	2.29	0.46
1:A:1024:ASP:CG	2:B:316:ARG:HH22	2.18	0.46
2:B:152:PRO:CG	2:B:431:ARG:HD2	2.39	0.46
2:B:508:LYS:O	2:B:511:PRO:HD2	2.16	0.46
2:B:325:ILE:HB	2:B:328:PRO:HD2	1.97	0.46
1:A:935:GLU:O	1:A:937:ILE:HG13	2.15	0.46
2:B:470:GLU:HA	2:B:473:LYS:HE2	1.97	0.46
1:A:968:LEU:HD12	1:A:1005:PHE:CG	2.51	0.46
2:B:184:LYS:HD3	2:B:396:THR:HG21	1.97	0.46
2:B:204:SER:HA	2:B:598:SER:OG	2.16	0.46
2:B:509:TRP:HB3	2:B:513:PHE:CE2	2.45	0.46
2:B:212:LEU:CD1	2:B:254:MET:HG3	2.47	0.45
2:B:299:LEU:HD11	2:B:375:MET:HG2	1.98	0.45
2:B:373:ARG:H	2:B:373:ARG:CD	2.18	0.45
2:B:460:LYS:NZ	2:B:460:LYS:HB3	2.31	0.45
2:B:142:LEU:HD21	2:B:517:LEU:HG	1.98	0.45
1:A:1051:GLN:O	1:A:1054:GLU:HB3	2.16	0.45
2:B:142:LEU:HD23	2:B:143:ILE:N	2.31	0.45
2:B:373:ARG:HD3	2:B:373:ARG:N	2.27	0.45
1:A:858:LEU:O	1:A:862:VAL:HG23	2.16	0.45
2:B:414:THR:HG23	2:B:415:HIS:CD2	2.52	0.45
2:B:422:PHE:HE1	2:B:531:TYR:HE1	1.63	0.45
2:B:168:LEU:HD12	2:B:168:LEU:N	2.32	0.45
1:A:850:GLU:OE2	1:A:854:LYS:HE3	2.17	0.45
2:B:141:ALA:O	2:B:454:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:GLN:NE2	2:B:602:LYS:HG2	2.32	0.45
2:B:431:ARG:HG3	2:B:435:GLU:HG3	1.99	0.45
2:B:383:LEU:N	2:B:383:LEU:HD22	2.32	0.44
1:A:1012:ASP:O	1:A:1014:VAL:HG23	2.17	0.44
2:B:146:ASN:HD22	2:B:146:ASN:N	2.14	0.44
1:A:799:PRO:HB2	1:A:800:LYS:H	1.59	0.44
1:A:824:TRP:CE2	1:A:867:PRO:HD3	2.51	0.44
2:B:685:ILE:HG12	2:B:687:THR:HG22	2.00	0.44
2:B:321:SER:O	2:B:322:ASP:HB2	2.17	0.44
2:B:420:PRO:HG3	2:B:530:LEU:HD11	1.99	0.44
1:A:961:GLN:NE2	1:A:1009:LEU:HG	2.32	0.44
1:A:982:HIS:N	1:A:983:PRO:HD2	2.33	0.44
1:A:869:THR:HG22	1:A:870:GLU:N	2.32	0.44
1:A:800:LYS:N	1:A:801:PRO:HD3	2.32	0.44
2:B:236:LEU:O	2:B:236:LEU:HD22	2.18	0.44
2:B:212:LEU:HD12	2:B:212:LEU:N	2.33	0.43
2:B:319:LEU:HD23	2:B:319:LEU:H	1.82	0.43
1:A:919:THR:HG23	1:A:921:GLU:H	1.84	0.43
1:A:964:LEU:CD2	1:A:1005:PHE:HB2	2.48	0.43
2:B:606:HIS:CD2	2:B:608:THR:HG23	2.54	0.43
2:B:685:ILE:HD13	2:B:685:ILE:C	2.39	0.43
2:B:399:CYS:O	2:B:403:SER:HB3	2.19	0.43
2:B:506:TYR:CE1	2:B:522:LEU:HB3	2.54	0.43
2:B:554:LEU:H	2:B:598:SER:CB	2.26	0.43
2:B:151:ILE:HG13	2:B:531:TYR:CG	2.54	0.43
1:A:1025:CYS:HA	1:A:1026:PRO:HD3	1.79	0.43
2:B:186:MET:CE	2:B:552:PRO:HB3	2.48	0.43
2:B:512:LEU:HD23	2:B:512:LEU:C	2.39	0.43
2:B:716:ILE:HD12	2:B:720:PHE:CE2	2.53	0.43
2:B:174:LYS:HA	2:B:175:PRO:HD3	1.90	0.43
2:B:314:GLU:HG3	2:B:390:VAL:HG22	2.00	0.43
1:A:1026:PRO:O	1:A:1029:GLU:HB2	2.19	0.43
2:B:178:TYR:CZ	2:B:214:LEU:HB3	2.53	0.43
2:B:554:LEU:HB2	2:B:598:SER:HB2	1.99	0.43
2:B:153:LEU:HD23	2:B:153:LEU:N	2.27	0.42
2:B:224:ALA:HB3	2:B:235:LEU:HD22	2.00	0.42
2:B:330:THR:O	2:B:331:ALA:HB2	2.19	0.42
1:A:875:MET:HB3	1:A:879:TRP:CD1	2.54	0.42
2:B:265:THR:HB	2:B:399:CYS:HA	2.01	0.42
2:B:444:PHE:CE1	2:B:522:LEU:HD12	2.55	0.42
2:B:688:ASN:H	2:B:689:PRO:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:VAL:HG21	2:B:610:SER:OG	2.19	0.42
2:B:383:LEU:HD22	2:B:383:LEU:H	1.84	0.42
2:B:651:PRO:HG2	2:B:691:PRO:O	2.20	0.42
2:B:579:PHE:CE2	2:B:589:LEU:HD11	2.55	0.42
2:B:736:GLN:HA	2:B:739:ARG:HG2	2.01	0.42
2:B:560:SER:C	2:B:562:GLU:H	2.23	0.42
2:B:173:MET:HE2	2:B:630:LEU:CD2	2.50	0.41
2:B:410:ILE:C	2:B:410:ILE:HD12	2.40	0.41
1:A:902:TYR:CD1	1:A:909:ALA:HB1	2.55	0.41
2:B:188:PHE:HE2	2:B:196:PHE:HZ	1.68	0.41
1:A:807:HIS:CD2	1:A:938:GLU:HB2	2.55	0.41
1:A:866:GLN:CG	1:A:867:PRO:HD2	2.51	0.41
1:A:978:LEU:HB3	1:A:998:ARG:CD	2.50	0.41
2:B:432:TYR:CD2	2:B:569:LEU:HB2	2.55	0.41
2:B:505:LEU:HB3	2:B:509:TRP:NE1	2.35	0.41
2:B:203:LEU:HD21	2:B:253:LYS:HB3	2.03	0.41
2:B:522:LEU:HD23	2:B:522:LEU:HA	1.91	0.41
1:A:835:MET:HA	1:A:838:VAL:HG12	2.02	0.41
2:B:354:ILE:N	2:B:354:ILE:HD12	2.36	0.41
2:B:611:LEU:HD23	2:B:626:TYR:CZ	2.56	0.41
1:A:1033:TYR:O	1:A:1037:ARG:HD2	2.21	0.41
2:B:472:LYS:O	2:B:476:LEU:HG	2.21	0.41
1:A:847:ASP:HB3	1:A:848:GLN:H	1.70	0.41
1:A:968:LEU:C	1:A:970:GLU:H	2.24	0.41
2:B:150:VAL:CG1	2:B:431:ARG:H	2.30	0.41
2:B:329:LYS:HD2	2:B:355:TYR:CD2	2.56	0.41
1:A:867:PRO:O	1:A:868:LEU:C	2.58	0.41
1:A:916:PRO:HB2	1:A:917:GLY:H	1.56	0.41
1:A:1000:ILE:O	1:A:1004:LEU:HG	2.21	0.41
1:A:835:MET:HG3	1:A:854:LYS:NZ	2.35	0.40
2:B:482:ILE:HD12	2:B:512:LEU:HD12	2.02	0.40
2:B:731:LYS:N	2:B:731:LYS:HD2	2.36	0.40
1:A:983:PRO:N	1:A:984:PRO:CD	2.84	0.40
2:B:303:ARG:HG2	2:B:370:LEU:HD13	2.02	0.40
1:A:1037:ARG:HH12	2:B:410:ILE:HD11	1.87	0.40
2:B:279:GLY:O	2:B:281:LEU:HG	2.21	0.40
2:B:516:GLU:O	2:B:518:PRO:HD3	2.22	0.40
2:B:361:GLU:HA	2:B:361:GLU:OE1	2.21	0.40
2:B:506:TYR:O	2:B:510:VAL:HG23	2.22	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	275/374 (74%)	214 (78%)	52 (19%)	9 (3%)	4 22
2	B	588/624 (94%)	481 (82%)	92 (16%)	15 (3%)	5 27
All	All	863/998 (86%)	695 (80%)	144 (17%)	24 (3%)	5 25

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	799	PRO
1	A	916	PRO
1	A	904	ARG
1	A	793	PRO
2	B	162	TYR
2	B	232	ASP
2	B	331	ALA
2	B	339	THR
2	B	514	GLU
2	B	533	LEU
2	B	622	SER
2	B	690	LEU
2	B	692	LYS
1	A	868	LEU
1	A	914	LEU
2	B	376	ASP
1	A	830	GLY
1	A	986	SER
2	B	278	LYS
2	B	349	ILE
2	B	502	LEU
2	B	688	ASN
1	A	811	PRO
2	B	493	ALA

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	254/343 (74%)	250 (98%)	4 (2%)	62 79
2	B	543/571 (95%)	514 (95%)	29 (5%)	22 53
All	All	797/914 (87%)	764 (96%)	33 (4%)	30 60

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	822	ARG
1	A	914	LEU
1	A	987	ASN
1	A	1037	ARG
2	B	159	LYS
2	B	167	ARG
2	B	228	LYS
2	B	236	LEU
2	B	237	LEU
2	B	255	ASN
2	B	265	THR
2	B	273	LYS
2	B	276	LYS
2	B	284	TRP
2	B	319	LEU
2	B	330	THR
2	B	353	ASN
2	B	358	ASN
2	B	373	ARG
2	B	381	LEU
2	B	413	LEU
2	B	447	LEU
2	B	458	ARG
2	B	520	GLN
2	B	524	ASN
2	B	557	TYR
2	B	605	TYR

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Mol	Chain	Res	Type
2	B	619	ARG
2	B	644	LEU
2	B	685	ILE
2	B	716	ILE
2	B	727	PHE
2	B	739	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	805	HIS
1	A	807	HIS
1	A	808	GLN
1	A	863	ASN
1	A	905	ASN
1	A	908	GLN
1	A	961	GLN
1	A	973	ASN
1	A	987	ASN
2	B	160	ASN
2	B	172	ASN
2	B	220	ASN
2	B	255	ASN
2	B	318	GLN
2	B	335	GLN
2	B	353	ASN
2	B	358	ASN
2	B	407	HIS
2	B	415	HIS
2	B	524	ASN
2	B	536	GLN
2	B	582	ASN
2	B	592	ASN
2	B	595	GLN
2	B	652	GLN
2	B	659	ASN
2	B	681	ASN
2	B	688	ASN
2	B	726	GLN
2	B	736	GLN
2	B	743	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

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	277/374 (74%)	0.47	27 (9%)	7	8	91, 154, 262, 349	0
2	B	592/624 (94%)	0.51	59 (9%)	7	7	79, 132, 259, 319	0
All	All	869/998 (87%)	0.50	86 (9%)	7	7	79, 138, 261, 349	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	274	SER	11.4
2	B	139	GLU	9.9
2	B	469	LYS	8.9
2	B	275	ALA	8.3
2	B	470	GLU	8.2
2	B	494	VAL	8.0
1	A	798	MET	7.3
2	B	680	ASP	6.0
2	B	468	LEU	5.7
2	B	467	GLN	5.6
2	B	280	PRO	5.4
1	A	791	SER	5.2
1	A	799	PRO	5.1
2	B	681	ASN	5.1
2	B	659	ASN	4.9
2	B	495	LYS	4.9
2	B	457	ILE	4.8
2	B	493	ALA	4.6
1	A	847	ASP	4.6
2	B	503	PHE	4.5
1	A	836	ASP	4.4
1	A	794	SER	4.3
1	A	866	GLN	4.3
1	A	942	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	471	GLY	4.2
2	B	661	LYS	4.2
2	B	658	GLY	4.1
2	B	679	THR	4.1
2	B	491	LYS	4.1
1	A	918	LYS	4.0
2	B	273	LYS	4.0
2	B	472	LYS	4.0
2	B	660	GLU	3.9
2	B	653	ASP	3.8
2	B	320	PRO	3.8
1	A	1067	THR	3.7
2	B	655	LYS	3.5
2	B	746	ASN	3.5
2	B	656	LYS	3.5
2	B	496	SER	3.4
2	B	498	LYS	3.4
2	B	499	ASP	3.3
2	B	464	PHE	3.3
2	B	459	SER	3.3
2	B	276	LYS	3.2
1	A	802	HIS	3.2
2	B	466	LYS	3.2
1	A	795	HIS	3.2
1	A	1064	ASP	3.2
1	A	848	GLN	3.2
2	B	492	ASN	3.1
2	B	162	TYR	3.1
2	B	650	LYS	3.1
1	A	804	PHE	3.0
2	B	278	LYS	2.9
2	B	417	LYS	2.9
1	A	835	MET	2.9
1	A	792	THR	2.9
2	B	683	PRO	2.9
2	B	138	VAL	2.9
2	B	279	GLY	2.9
2	B	230	PRO	2.8
2	B	742	ARG	2.8
2	B	745	VAL	2.8
1	A	797	ARG	2.8
1	A	917	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1055	LYS	2.8
1	A	793	PRO	2.7
1	A	1066	ALA	2.7
2	B	620	ASN	2.6
2	B	686	ASN	2.6
2	B	654	GLU	2.5
2	B	489	GLU	2.5
2	B	484	LYS	2.5
2	B	487	LYS	2.5
2	B	153	LEU	2.4
1	A	845	ILE	2.4
2	B	321	SER	2.4
1	A	1065	ASP	2.4
1	A	915	ALA	2.3
2	B	473	LYS	2.2
2	B	657	GLU	2.2
1	A	813	GLN	2.2
2	B	455	TYR	2.1
2	B	233	THR	2.1
1	A	1063	LEU	2.1

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.