Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:21 pm BST

PDB ID	:	5KHN
Title	:	Crystal structures of the Burkholderia multivorans hopanoid transporter HpnN
Authors	:	Su, C.-C.; Yu, E.W.
Deposited on	:	2016-06-15
Resolution	:	3.44 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 ①) were used in the production of this report:

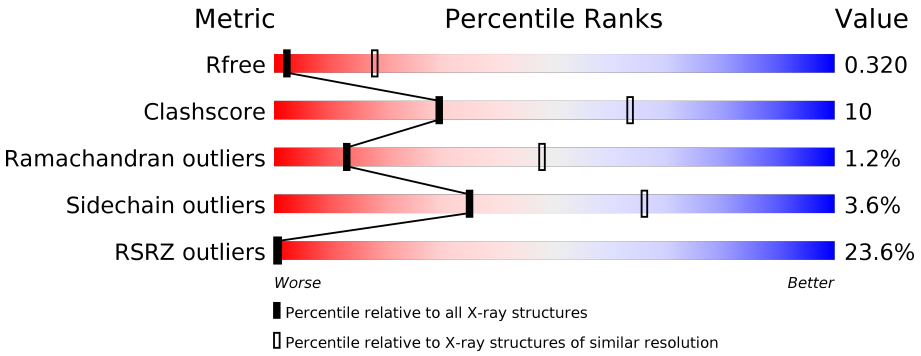
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.44 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

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	883	23% 69% 26%
1	B	883	22% 73% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12612 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 RND transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	848	Total	C	N	O	S	0	0	0
			6303	4069	1080	1136	18			
1	A	848	Total	C	N	O	S	0	0	0
			6309	4073	1081	1137	18			

There are 18 discrepancies between the modelled and reference sequences:

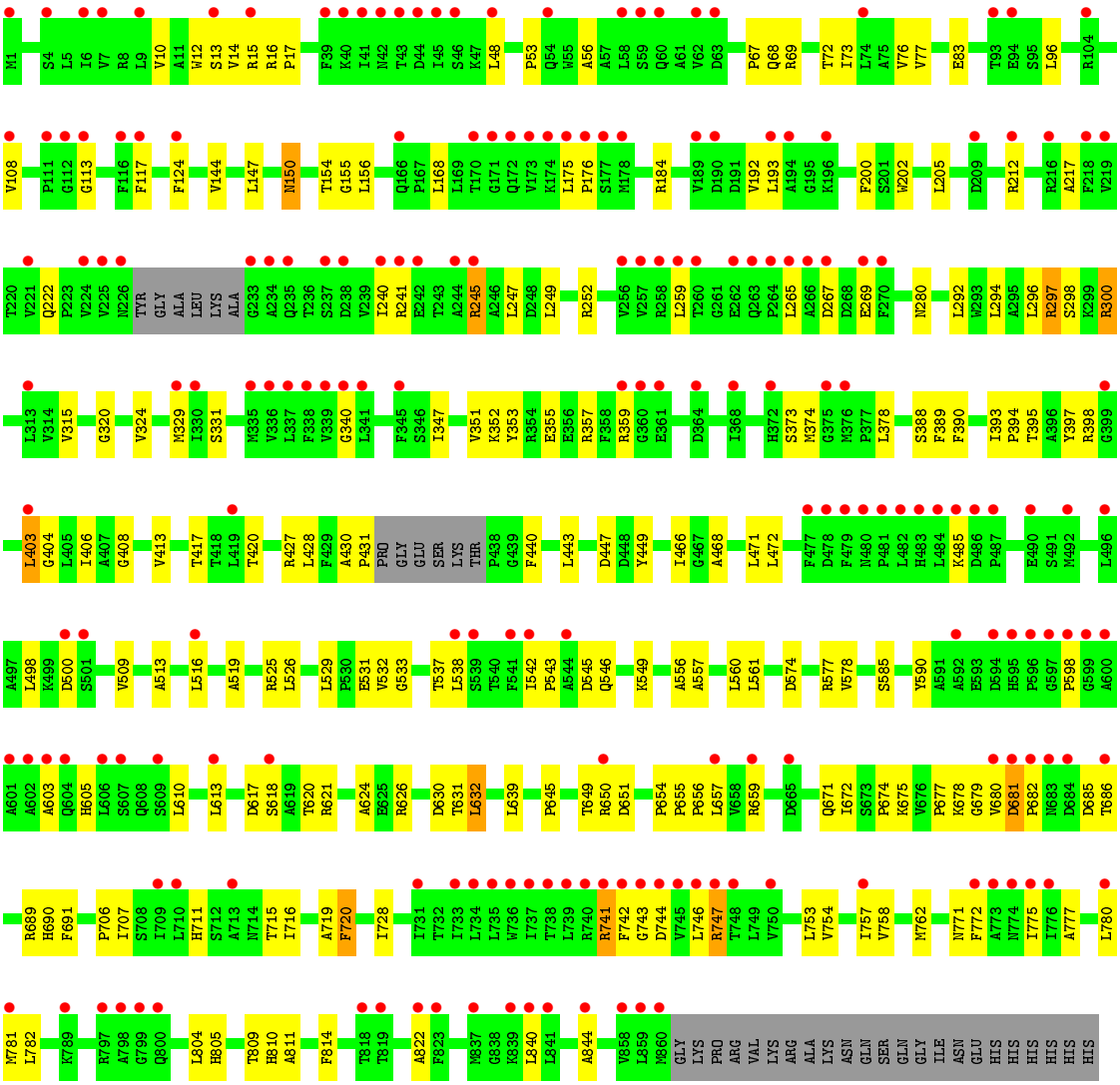
Chain	Residue	Modelled	Actual	Comment	Reference
B	360	GLY	ASP	engineered mutation	UNP A0A1B4TSD3
B	362	ALA	ARG	engineered mutation	UNP A0A1B4TSD3
B	365	ALA	HIS	engineered mutation	UNP A0A1B4TSD3
B	878	HIS	-	expression tag	UNP A0A1B4TSD3
B	879	HIS	-	expression tag	UNP A0A1B4TSD3
B	880	HIS	-	expression tag	UNP A0A1B4TSD3
B	881	HIS	-	expression tag	UNP A0A1B4TSD3
B	882	HIS	-	expression tag	UNP A0A1B4TSD3
B	883	HIS	-	expression tag	UNP A0A1B4TSD3
A	360	GLY	ASP	engineered mutation	UNP A0A1B4TSD3
A	362	ALA	ARG	engineered mutation	UNP A0A1B4TSD3
A	365	ALA	HIS	engineered mutation	UNP A0A1B4TSD3
A	878	HIS	-	expression tag	UNP A0A1B4TSD3
A	879	HIS	-	expression tag	UNP A0A1B4TSD3
A	880	HIS	-	expression tag	UNP A0A1B4TSD3
A	881	HIS	-	expression tag	UNP A0A1B4TSD3
A	882	HIS	-	expression tag	UNP A0A1B4TSD3
A	883	HIS	-	expression tag	UNP A0A1B4TSD3

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.

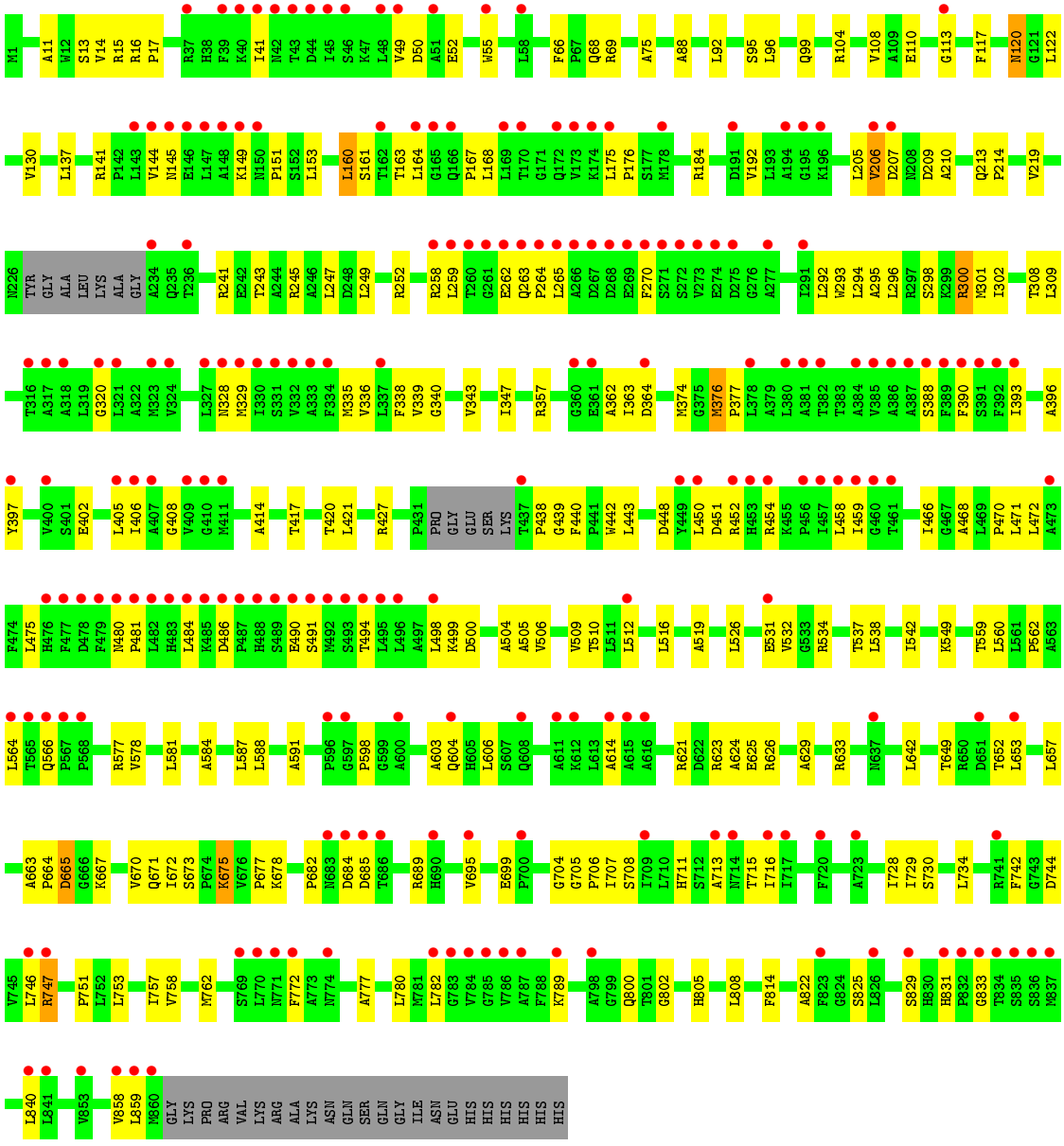
- Molecule 1: RND transporter

Chain B:



- Molecule 1: RND transporter

Chain A:


M1 A11 W12 S13 V14 R15 R16 P17 R37 H38 F39 K40 I41 N42 T43 D44 I45 S46 K47 L48 V49 D50 A51 E52 W55 L58 F66 P67 Q68 R69 A75 A88 L92 S95 L96 Q99 R104 V108 A109 E110 G113 F117 N120 G121 L122
V130 L137 R141 P142 L143 V144 N145 E146 L147 A148 K149 N150 P151 S152 L153 L160 S161 T162 T163 L164 G165 Q166 P167 L168 L169 T170 G171 Q172 V173 K174 L175 P176 S177 M178 R184 D191 V192 L193 A194 G195 K196 L205 V206 D207 N208 D209 A210 Q213 P214 V219
N226 TYR GLY ALA LEU LYS ALA GLY A234 Q235 T236 R241 E242 T243 A244 R245 A246 L247 D248 L249 R252 R258 L259 T260 G261 E262 Q263 P264 L265 A266 D267 D268 E269 F270 S271 S272 V273 E274 D275 G276 A277 I291 L292 W293 L294 A295 L296 R297 S298 K299 R300 M301 I302 T308 L309
T316 A317 A318 L319 G320 L321 A322 M323 V324 L327 N328 M329 I330 S331 V332 A333 F334 M335 V336 L337 F338 V339 G340 V343 I347 R357 G360 E361 A362 I363 D364 M374 G375 M376 P377 L378 A379 L380 A381 T382 T383 A384 V385 A386 A387 S388 F389 F390 S391 F392 I393 A396
Y397 V400 S401 E402 L405 I406 A407 G408 V409 G410 N411 A414 T417 T420 L421 R427 P431 PRO GLY GLU SER LYS T437 P438 G439 F440 P441 W442 L443 D448 Y449 L450 D451 R452 H453 R454 K455 P456 I457 L458 I459 G460 T461 I466 G467 A468 L469 P470 L471 L472 A473
F474 L475 H476 F477 D478 F479 N480 P481 L482 H483 L484 K485 D486 P487 H488 S489 E490 S491 N492 S493 T494 L495 L496 A497 L498 K499 D500 A504 A505 V506 V509 T510 L511 L512 L516 A519 L526 E531 V532 G533 R534 T537 L538 I542 K549 T559 L560 L561 P562 A563
L564 T565 Q566 P567 P568 R577 V578 L581 A584 L587 L588 A591 P596 G597 P598 G599 A600 A603 Q604 H605 L606 S607 Q608 A611 K612 L613 A614 A615 A616 R621 D622 R623 A624 E625 R626 A629 R633 N637 L642 T649 K650 D651 T652 L653 L657
A663 P664 D665 G666 K667 V670 Q671 I672 S673 P674 K675 V676 P677 K678 P682 N683 D684 D685 T686 R689 H690 V695 E699 P700 G704 G705 P706 I707 S708 I709 L710 H711 S712 A713 N714 T715 I716 I717 F720 A723 I728 I729 S730 L734 R741 F742 G743 D744
V745 L746 R747 P751 L752 L753 I757 V758 M762 S769 L770 N771 F772 A773 N774 A777 L780 M781 L782 G783 V784 G785 V786 A787 F788 K789 A798 G799 Q800 T801 G802 H805 L808 F814 A822 F823 G824 S825 L826 S829 H830 H831 P832 G833 T834 S835 S836 M837
L840 L841 W853 V858 L859 M860 GLY LYS PRO ARG VAL LYS ARG ALA LYS ASN GLN SER GLN GLY ILE ASN GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.91Å 129.55Å 111.73Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	93.80 – 3.44 93.80 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.6 (93.80-3.44) 99.7 (93.80-3.44)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.283 , 0.319 0.285 , 0.320	Depositor DCC
R_{free} test set	1928 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	124.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.378 for l,-k,h	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	12612	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	0.24	0/6443	0.42	0/8814
1	B	0.27	1/6437 (0.0%)	0.43	0/8804
All	All	0.25	1/12880 (0.0%)	0.43	0/17618

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	ASN	C-N	5.30	1.44	1.34

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	6309	0	6537	138	1
1	B	6303	0	6528	115	1
All	All	12612	0	13065	244	1

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 10.

All (244) 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:B:685:ASP:HB2	1:B:689:ARG:HD3	1.64	0.79
1:B:83:GLU:HG3	1:B:631:THR:HG23	1.69	0.74
1:B:300:ARG:H	1:B:300:ARG:HD2	1.52	0.73
1:B:351:VAL:HG11	1:B:811:ALA:HB2	1.70	0.73
1:A:685:ASP:HB2	1:A:689:ARG:HD3	1.72	0.72
1:A:292:LEU:HD22	1:A:302:ILE:HG23	1.72	0.71
1:A:484:LEU:HB2	1:A:833:GLY:HA2	1.74	0.69
1:A:50:ASP:HB2	1:A:396:ALA:HB1	1.75	0.68
1:B:753:LEU:HD13	1:A:466:ILE:HG12	1.75	0.68
1:A:728:ILE:HD12	1:A:729:ILE:HG13	1.76	0.68
1:A:440:PHE:O	1:A:805:HIS:NE2	2.22	0.67
1:A:328:ASN:ND2	1:A:402:GLU:OE1	2.28	0.67
1:B:331:SER:HA	1:B:403:LEU:HB2	1.75	0.67
1:B:352:LYS:HE2	1:B:373:SER:OG	1.95	0.67
1:B:69:ARG:NH2	1:B:671:GLN:OE1	2.28	0.66
1:A:751:PRO:HB2	1:A:789:LYS:HE3	1.77	0.66
1:A:728:ILE:HG23	1:A:782:LEU:HD13	1.77	0.66
1:B:472:LEU:HD13	1:A:472:LEU:HD13	1.77	0.65
1:B:340:GLY:HA3	1:B:822:ALA:HB2	1.79	0.65
1:B:777:ALA:HB3	1:B:840:LEU:HD12	1.78	0.64
1:B:76:VAL:HG11	1:B:498:LEU:HD11	1.79	0.63
1:B:681:ASP:N	1:B:681:ASP:OD1	2.28	0.63
1:B:388:SER:HB3	1:B:780:LEU:HA	1.81	0.63
1:A:164:LEU:HD13	1:A:588:LEU:HG	1.81	0.62
1:A:340:GLY:HA3	1:A:822:ALA:HB2	1.82	0.62
1:B:546:GLN:HB3	1:B:549:LYS:HG2	1.80	0.62
1:A:468:ALA:HB1	1:A:471:LEU:HD12	1.81	0.62
1:A:728:ILE:HD12	1:A:729:ILE:N	2.14	0.62
1:A:663:ALA:O	1:A:665:ASP:N	2.33	0.61
1:B:150:ASN:HB3	1:B:155:GLY:HA3	1.83	0.61
1:B:192:VAL:HG11	1:B:624:ALA:HB2	1.83	0.60
1:B:156:LEU:HD21	1:B:632:LEU:HD12	1.82	0.60
1:A:92:LEU:HD12	1:A:219:VAL:HG11	1.84	0.60
1:B:526:LEU:HD13	1:B:672:ILE:HG12	1.84	0.60
1:B:247:LEU:O	1:B:249:LEU:N	2.31	0.60
1:A:509:VAL:HG13	1:A:706:PRO:HD2	1.84	0.59
1:A:137:LEU:HB3	1:A:560:LEU:HD11	1.84	0.59
1:A:649:THR:H	1:A:652:THR:HG1	1.50	0.59
1:A:458:LEU:HD11	1:A:858:VAL:HG23	1.85	0.59
1:B:509:VAL:HG13	1:B:706:PRO:HD2	1.84	0.59
1:A:130:VAL:HG21	1:A:549:LYS:HD3	1.86	0.58
1:A:777:ALA:HB3	1:A:840:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:THR:HG22	1:B:222:GLN:HG2	1.86	0.58
1:B:516:LEU:HD11	1:B:538:LEU:HB3	1.85	0.58
1:A:192:VAL:O	1:A:623:ARG:NH1	2.37	0.57
1:B:144:VAL:HG11	1:B:560:LEU:HD13	1.86	0.57
1:B:617:ASP:OD1	1:B:618:SER:N	2.35	0.57
1:B:324:VAL:HG21	1:B:406:ILE:HD11	1.87	0.57
1:B:675:LYS:HE3	1:A:678:LYS:HG3	1.85	0.57
1:A:122:LEU:HB2	1:A:642:LEU:HG	1.87	0.57
1:A:364:ASP:OD2	1:A:427:ARG:NH1	2.38	0.56
1:A:388:SER:HB3	1:A:780:LEU:HA	1.86	0.56
1:A:308:THR:HG22	1:A:421:LEU:HD22	1.86	0.56
1:B:557:ALA:HB1	1:B:561:LEU:HD12	1.86	0.56
1:A:163:THR:HA	1:A:167:PRO:HG2	1.88	0.55
1:B:48:LEU:O	1:B:398:ARG:N	2.40	0.55
1:B:202:TRP:HD1	1:B:631:THR:HG22	1.72	0.55
1:B:626:ARG:HA	1:B:630:ASP:HB2	1.89	0.54
1:A:176:PRO:HB3	1:A:598:PRO:HG2	1.89	0.54
1:A:184:ARG:HD3	1:A:205:LEU:HG	1.89	0.54
1:A:293:TRP:HD1	1:A:302:ILE:HD11	1.71	0.54
1:A:265:LEU:HD12	1:A:491:SER:OG	2.08	0.54
1:B:675:LYS:O	1:B:677:PRO:HD3	2.08	0.53
1:A:298:SER:HB2	1:A:300:ARG:HD2	1.91	0.53
1:B:757:ILE:HD11	1:A:757:ILE:HD11	1.91	0.53
1:A:560:LEU:O	1:A:564:LEU:N	2.42	0.53
1:B:685:ASP:HB2	1:B:689:ARG:HH11	1.73	0.53
1:A:526:LEU:HD21	1:A:699:GLU:HG2	1.91	0.53
1:B:674:PRO:HB3	1:B:691:PHE:CG	2.44	0.53
1:A:292:LEU:HG	1:A:347:ILE:HD11	1.89	0.53
1:A:534:ARG:HB3	1:A:673:SER:HB3	1.91	0.53
1:B:73:ILE:HD11	1:B:240:ILE:HD12	1.91	0.53
1:A:510:THR:HG22	1:A:671:GLN:HG2	1.91	0.52
1:A:343:VAL:HG12	1:A:347:ILE:HG12	1.91	0.52
1:A:744:ASP:HA	1:A:747:ARG:HB2	1.91	0.52
1:A:713:ALA:HA	1:A:772:PHE:HE2	1.74	0.52
1:B:77:VAL:HB	1:B:217:ALA:HB3	1.92	0.52
1:A:376:MET:HG2	1:A:377:PRO:HD3	1.92	0.52
1:A:258:ARG:HB3	1:A:494:THR:HG21	1.91	0.52
1:B:147:LEU:HD22	1:B:632:LEU:HD11	1.90	0.52
1:B:351:VAL:CG1	1:B:811:ALA:HB2	2.39	0.52
1:A:130:VAL:HG11	1:A:549:LYS:HB3	1.93	0.51
1:A:393:ILE:HD11	1:A:405:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLU:O	1:A:629:ALA:N	2.41	0.51
1:B:716:ILE:HG21	1:B:772:PHE:HD1	1.74	0.51
1:A:512:LEU:HD11	1:A:667:LYS:HB3	1.92	0.51
1:A:578:VAL:HG13	1:A:614:ALA:HB1	1.93	0.51
1:A:711:HIS:O	1:A:715:THR:OG1	2.23	0.51
1:B:292:LEU:HD23	1:B:347:ILE:HD11	1.92	0.51
1:A:145:ASN:O	1:A:149:LYS:HG3	2.11	0.51
1:B:678:LYS:HB3	1:A:675:LYS:HD3	1.93	0.51
1:A:113:GLY:HA2	1:A:117:PHE:HB2	1.92	0.51
1:A:11:ALA:HA	1:A:14:VAL:HG12	1.91	0.51
1:A:175:LEU:HD11	1:A:603:ALA:HB2	1.93	0.51
1:A:141:ARG:HD3	1:A:559:THR:HB	1.92	0.51
1:A:504:ALA:O	1:A:506:VAL:N	2.43	0.51
1:B:649:THR:HG22	1:B:651:ASP:H	1.75	0.50
1:B:193:LEU:HD21	1:B:613:LEU:HA	1.93	0.50
1:B:585:SER:HB2	1:B:610:LEU:HB3	1.93	0.50
1:B:720:PHE:HZ	1:A:470:PRO:HB3	1.77	0.49
1:A:99:GLN:HE22	1:A:243:THR:HG22	1.78	0.49
1:A:161:SER:HB3	1:A:584:ALA:HA	1.95	0.49
1:B:113:GLY:HA2	1:B:117:PHE:HB2	1.95	0.49
1:B:13:SER:OG	1:B:420:THR:O	2.30	0.49
1:A:537:THR:HG22	1:A:538:LEU:H	1.78	0.49
1:A:753:LEU:O	1:A:757:ILE:HG13	2.12	0.49
1:B:355:GLU:O	1:B:359:ARG:N	2.46	0.49
1:B:574:ASP:OD1	1:B:621:ARG:NH1	2.46	0.49
1:A:75:ALA:HB3	1:A:219:VAL:HG13	1.94	0.49
1:A:296:LEU:O	1:A:296:LEU:HD12	2.13	0.49
1:A:300:ARG:HD2	1:A:300:ARG:H	1.77	0.49
1:A:581:LEU:HB3	1:A:614:ALA:HB2	1.94	0.49
1:B:468:ALA:HB1	1:B:471:LEU:HD12	1.94	0.49
1:B:294:LEU:HB3	1:B:814:PHE:CE1	2.49	0.48
1:B:758:VAL:O	1:B:762:MET:HG2	2.14	0.48
1:A:192:VAL:HG11	1:A:624:ALA:HB2	1.96	0.48
1:B:212:ARG:CZ	1:B:500:ASP:HB3	2.44	0.48
1:A:531:GLU:OE1	1:A:531:GLU:N	2.46	0.48
1:A:695:VAL:HG13	1:A:707:ILE:HD11	1.95	0.48
1:A:294:LEU:HB3	1:A:814:PHE:CE1	2.48	0.48
1:A:357:ARG:HH11	1:A:362:ALA:HA	1.79	0.48
1:A:161:SER:HB2	1:A:587:LEU:HD12	1.96	0.48
1:B:809:THR:HG23	1:B:810:HIS:ND1	2.29	0.47
1:B:53:PRO:HA	1:B:56:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:PRO:HD2	1:B:657:LEU:HD22	1.95	0.47
1:B:685:ASP:O	1:B:689:ARG:HB2	2.14	0.47
1:A:320:GLY:HA3	1:A:406:ILE:HG23	1.96	0.47
1:A:704:GLY:H	1:A:708:SER:HB2	1.80	0.47
1:B:395:THR:HB	1:B:719:ALA:HB1	1.96	0.47
1:B:545:ASP:N	1:B:545:ASP:OD1	2.48	0.47
1:B:440:PHE:O	1:B:805:HIS:NE2	2.48	0.46
1:B:754:VAL:O	1:B:758:VAL:HG23	2.15	0.46
1:B:443:LEU:HD12	1:B:804:LEU:HB3	1.97	0.46
1:A:206:VAL:HG12	1:A:207:ASP:N	2.31	0.46
1:B:241:ARG:O	1:B:245:ARG:HB2	2.15	0.46
1:B:96:LEU:HB3	1:B:108:VAL:HG21	1.98	0.46
1:B:154:THR:HG22	1:B:577:ARG:HA	1.97	0.46
1:B:374:MET:HB3	1:B:378:LEU:HD13	1.97	0.46
1:B:200:PHE:O	1:B:631:THR:HG21	2.14	0.46
1:B:728:ILE:HG12	1:B:782:LEU:HD13	1.97	0.46
1:B:781:MET:HG3	1:B:844:ALA:HB1	1.97	0.46
1:A:153:LEU:HD22	1:A:581:LEU:HD11	1.98	0.46
1:A:509:VAL:HG11	1:A:707:ILE:HG13	1.98	0.46
1:B:746:LEU:HB2	1:A:459:ILE:HD11	1.98	0.45
1:A:308:THR:HB	1:A:417:THR:HG22	1.98	0.45
1:A:588:LEU:HD13	1:A:606:LEU:HB3	1.98	0.45
1:B:617:ASP:HB3	1:B:620:THR:HG22	1.99	0.45
1:B:771:ASN:O	1:B:775:ILE:HB	2.16	0.45
1:A:99:GLN:HG2	1:A:104:ARG:HH11	1.80	0.45
1:A:730:SER:O	1:A:734:LEU:HB2	2.17	0.45
1:B:393:ILE:HB	1:B:394:PRO:HD3	1.98	0.45
1:B:556:ALA:O	1:B:560:LEU:HB2	2.16	0.45
1:A:829:SER:O	1:A:831:HIS:N	2.35	0.45
1:A:15:ARG:NH1	1:A:16:ARG:HH21	2.15	0.45
1:A:95:SER:OG	1:A:247:LEU:HD11	2.16	0.45
1:A:160:LEU:HD22	1:A:164:LEU:HD11	1.99	0.45
1:A:499:LYS:HD3	1:A:682:PRO:HD3	1.98	0.45
1:A:241:ARG:NH2	1:A:259:LEU:HD11	2.32	0.45
1:A:96:LEU:HB3	1:A:108:VAL:HG21	1.99	0.45
1:B:14:VAL:HG12	1:B:15:ARG:H	1.82	0.45
1:B:176:PRO:HB3	1:B:598:PRO:HG2	1.97	0.45
1:B:720:PHE:CZ	1:B:775:ILE:HG13	2.52	0.45
1:A:728:ILE:HD12	1:A:729:ILE:H	1.80	0.45
1:B:578:VAL:HG23	1:B:621:ARG:NH2	2.31	0.45
1:B:12:TRP:CD1	1:B:16:ARG:HD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:VAL:HG23	1:A:672:ILE:HD12	1.97	0.44
1:B:805:HIS:O	1:B:809:THR:HG22	2.17	0.44
1:A:450:LEU:HA	1:A:450:LEU:HD12	1.87	0.44
1:A:675:LYS:O	1:A:677:PRO:HD3	2.17	0.44
1:B:654:PRO:HB2	1:B:656:PRO:HD2	2.00	0.44
1:B:677:PRO:HA	1:A:677:PRO:HB2	2.00	0.44
1:A:69:ARG:NH1	1:A:671:GLN:OE1	2.48	0.44
1:A:88:ALA:HB1	1:A:249:LEU:HD12	1.98	0.44
1:B:124:PHE:CD2	1:B:543:PRO:HB3	2.53	0.44
1:B:269:GLU:OE1	1:B:485:LYS:HE3	2.18	0.44
1:A:390:PHE:CE1	1:A:408:GLY:HA3	2.53	0.44
1:A:13:SER:OG	1:A:420:THR:O	2.36	0.44
1:A:450:LEU:O	1:A:454:ARG:N	2.51	0.44
1:A:577:ARG:HD2	1:A:621:ARG:HH21	1.83	0.44
1:A:300:ARG:CD	1:A:300:ARG:H	2.31	0.44
1:A:448:ASP:O	1:A:452:ARG:HB2	2.17	0.44
1:A:747:ARG:HG3	1:A:859:LEU:HA	1.99	0.44
1:A:509:VAL:HG12	1:A:705:GLY:H	1.82	0.43
1:B:17:PRO:HB2	1:B:428:LEU:HD11	2.00	0.43
1:B:542:ILE:HD11	1:B:650:ARG:HG2	2.00	0.43
1:A:562:PRO:O	1:A:566:GLN:NE2	2.51	0.43
1:A:519:ALA:HB1	1:A:670:VAL:HG22	2.00	0.43
1:B:466:ILE:HG12	1:A:753:LEU:HD13	1.99	0.43
1:A:110:GLU:HA	1:A:219:VAL:HA	2.00	0.43
1:A:338:PHE:CE2	1:A:414:ALA:HB2	2.53	0.43
1:B:753:LEU:O	1:B:757:ILE:HG13	2.18	0.43
1:A:153:LEU:HD12	1:A:625:GLU:HB2	2.00	0.43
1:B:741:ARG:NH1	1:B:741:ARG:HA	2.34	0.43
1:A:494:THR:O	1:A:498:LEU:HG	2.19	0.43
1:B:443:LEU:O	1:B:447:ASP:HB2	2.19	0.43
1:A:168:LEU:HD22	1:A:591:ALA:HB1	2.00	0.43
1:B:390:PHE:CE1	1:B:408:GLY:HA3	2.54	0.43
1:A:532:VAL:HG13	1:A:672:ILE:HG23	2.00	0.43
1:B:10:VAL:O	1:B:14:VAL:HG23	2.19	0.43
1:B:413:VAL:O	1:B:417:THR:OG1	2.34	0.42
1:B:743:GLY:O	1:B:747:ARG:HD3	2.19	0.42
1:A:758:VAL:O	1:A:762:MET:HG2	2.19	0.42
1:A:298:SER:OG	1:A:301:MET:HB2	2.19	0.42
1:B:744:ASP:HA	1:B:747:ARG:HB2	2.00	0.42
1:A:263:GLN:N	1:A:264:PRO:HD2	2.34	0.42
1:A:151:PRO:HG2	1:A:633:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HB2	1:B:205:LEU:HD21	2.01	0.42
1:A:336:VAL:HG11	1:A:825:SER:HB3	2.02	0.42
1:A:542:ILE:HD11	1:A:653:LEU:HD11	2.01	0.42
1:B:357:ARG:NH2	1:B:431:PRO:O	2.38	0.42
1:A:309:LEU:HD21	1:A:339:VAL:HG13	2.02	0.42
1:B:686:THR:O	1:B:690:HIS:ND1	2.53	0.42
1:B:720:PHE:CE1	1:B:775:ILE:HG13	2.55	0.42
1:A:209:ASP:OD1	1:A:210:ALA:N	2.53	0.42
1:A:49:VAL:HB	1:A:716:ILE:HD11	2.01	0.42
1:A:500:ASP:OD1	1:A:500:ASP:N	2.53	0.42
1:B:17:PRO:HG2	1:B:428:LEU:HD21	2.02	0.42
1:A:120:ASN:N	1:A:120:ASN:OD1	2.53	0.41
1:A:440:PHE:CE2	1:A:808:LEU:HD12	2.55	0.41
1:B:509:VAL:HG11	1:B:707:ILE:HG13	2.02	0.41
1:B:655:PRO:N	1:B:656:PRO:HD2	2.35	0.41
1:A:144:VAL:HG11	1:A:560:LEU:HD22	2.03	0.41
1:A:480:ASN:HA	1:A:481:PRO:HD3	1.96	0.41
1:B:513:ALA:HB3	1:B:519:ALA:HB2	2.03	0.41
1:B:529:LEU:HB2	1:B:532:VAL:CG2	2.51	0.41
1:A:41:ILE:HG21	1:A:270:PHE:CZ	2.56	0.41
1:B:175:LEU:HD11	1:B:603:ALA:HB2	2.03	0.41
1:A:516:LEU:HD11	1:A:538:LEU:HB3	2.02	0.41
1:B:711:HIS:O	1:B:715:THR:HG22	2.20	0.41
1:A:213:GLN:HB2	1:A:214:PRO:HD3	2.02	0.41
1:A:481:PRO:O	1:A:484:LEU:HD23	2.21	0.41
1:A:758:VAL:O	1:A:762:MET:N	2.51	0.41
1:A:66:PHE:HB3	1:A:68:GLN:NE2	2.36	0.41
1:A:443:LEU:HB2	1:A:805:HIS:CE1	2.56	0.41
1:B:296:LEU:O	1:B:298:SER:N	2.54	0.41
1:B:389:PHE:HB3	1:B:404:GLY:HA2	2.03	0.40
1:B:315:VAL:HG23	1:B:413:VAL:HG11	2.04	0.40
1:A:728:ILE:HG13	1:A:728:ILE:H	1.69	0.40
1:B:240:ILE:HB	1:B:259:LEU:HD21	2.03	0.40
1:B:320:GLY:O	1:B:324:VAL:HG22	2.21	0.40
1:B:529:LEU:HB2	1:B:532:VAL:HG23	2.03	0.40
1:A:15:ARG:O	1:A:17:PRO:HD3	2.22	0.40
1:B:537:THR:HG22	1:B:538:LEU:H	1.86	0.40
1:B:67:PRO:HD2	1:B:659:ARG:HH21	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:TYR:OH	1:A:451:ASP:OD2[1_554]	2.14	0.06

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	842/883 (95%)	774 (92%)	56 (7%)	12 (1%)	11	44
1	B	842/883 (95%)	778 (92%)	56 (7%)	8 (1%)	15	52
All	All	1684/1766 (95%)	1552 (92%)	112 (7%)	20 (1%)	13	48

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	ARG
1	A	665	ASP
1	B	679	GLY
1	A	206	VAL
1	A	802	GLY
1	B	741	ARG
1	A	295	ALA
1	A	505	ALA
1	A	664	PRO
1	A	675	LYS
1	B	430	ALA
1	A	363	ILE
1	A	475	LEU
1	A	438	PRO
1	A	439	GLY
1	A	486	ASP
1	B	645	PRO
1	B	680	VAL
1	B	682	PRO
1	B	533	GLY

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	661/690 (96%)	638 (96%)	23 (4%)	36	67
1	B	659/690 (96%)	635 (96%)	24 (4%)	35	66
All	All	1320/1380 (96%)	1273 (96%)	47 (4%)	35	66

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	GLN
1	B	168	LEU
1	B	245	ARG
1	B	252	ARG
1	B	265	LEU
1	B	267	ASP
1	B	280	ASN
1	B	297	ARG
1	B	300	ARG
1	B	329	MET
1	B	353	TYR
1	B	397	TYR
1	B	403	LEU
1	B	427	ARG
1	B	449	TYR
1	B	525	ARG
1	B	531	GLU
1	B	605	HIS
1	B	632	LEU
1	B	639	LEU
1	B	681	ASP
1	B	720	PHE
1	B	742	PHE
1	B	747	ARG
1	A	52	GLU
1	A	55	TRP
1	A	120	ASN

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Mol	Chain	Res	Type
1	A	160	LEU
1	A	245	ARG
1	A	252	ARG
1	A	262	GLU
1	A	300	ARG
1	A	329	MET
1	A	335	MET
1	A	374	MET
1	A	376	MET
1	A	397	TYR
1	A	442	TRP
1	A	490	GLU
1	A	604	GLN
1	A	626	ARG
1	A	657	LEU
1	A	684	ASP
1	A	742	PHE
1	A	746	LEU
1	A	747	ARG
1	A	800	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	848/883 (96%)	1.44	204 (24%)	0	1	71, 125, 165, 201	0
1	B	848/883 (96%)	1.25	197 (23%)	0	1	77, 127, 165, 204	0
All	All	1696/1766 (96%)	1.35	401 (23%)	0	1	71, 126, 165, 204	0

All (401) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	597	GLY	28.0
1	B	44	ASP	24.9
1	A	272	SER	23.0
1	A	267	ASP	19.8
1	B	43	THR	19.1
1	A	271	SER	19.0
1	A	480	ASN	18.5
1	A	478	ASP	17.9
1	B	598	PRO	16.3
1	A	483	HIS	16.1
1	A	269	GLU	15.9
1	B	596	PRO	15.8
1	A	479	PHE	15.5
1	B	45	ILE	14.9
1	A	484	LEU	14.3
1	A	273	VAL	14.1
1	A	266	ALA	13.3
1	A	263	GLN	12.9
1	A	482	LEU	12.6
1	B	241	ARG	12.5
1	A	265	LEU	11.9
1	A	772	PHE	11.8
1	A	44	ASP	11.8
1	A	270	PHE	11.6

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Mol	Chain	Res	Type	RSRZ
1	A	264	PRO	11.4
1	A	860	MET	11.4
1	A	769	SER	11.3
1	B	741	ARG	11.0
1	A	43	THR	11.0
1	A	274	GLU	10.8
1	A	333	ALA	10.6
1	A	783	GLY	10.5
1	B	173	VAL	10.4
1	A	481	PRO	10.3
1	A	770	LEU	10.2
1	B	329	MET	10.0
1	B	745	VAL	10.0
1	A	268	ASP	9.9
1	A	41	ILE	9.9
1	A	489	SER	9.8
1	B	600	ALA	9.5
1	A	42	ASN	9.5
1	A	485	LYS	9.3
1	B	174	LYS	9.3
1	A	334	PHE	9.3
1	A	145	ASN	9.2
1	A	207	ASP	9.1
1	A	490	GLU	9.1
1	A	453	HIS	8.9
1	A	456	PRO	8.7
1	B	41	ILE	8.5
1	A	388	SER	8.4
1	A	492	MET	8.4
1	A	685	ASP	8.2
1	A	391	SER	8.1
1	A	859	LEU	8.1
1	B	108	VAL	8.1
1	A	385	VAL	8.1
1	A	324	VAL	8.0
1	A	384	ALA	8.0
1	B	740	ARG	8.0
1	B	175	LEU	8.0
1	A	261	GLY	7.8
1	A	831	HIS	7.7
1	A	487	PRO	7.7
1	A	488	HIS	7.6

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Mol	Chain	Res	Type	RSRZ
1	B	486	ASP	7.5
1	A	392	PHE	7.5
1	A	683	ASN	7.4
1	A	321	LEU	7.2
1	B	330	ILE	7.2
1	B	209	ASP	7.0
1	A	491	SER	7.0
1	A	386	ALA	6.9
1	B	372	HIS	6.8
1	A	486	ASP	6.8
1	B	485	LYS	6.8
1	B	360	GLY	6.7
1	B	860	MET	6.7
1	B	746	LEU	6.7
1	B	603	ALA	6.7
1	B	602	ALA	6.6
1	A	45	ILE	6.5
1	B	224	VAL	6.5
1	B	193	LEU	6.4
1	A	149	LYS	6.4
1	A	686	THR	6.4
1	B	859	LEU	6.3
1	A	382	THR	6.3
1	A	720	PHE	6.2
1	A	858	VAL	6.2
1	B	737	ILE	6.1
1	A	457	ILE	6.1
1	A	771	ASN	6.0
1	B	492	MET	6.0
1	A	317	ALA	5.9
1	A	493	SER	5.9
1	B	42	ASN	5.9
1	A	826	LEU	5.9
1	B	480	ASN	5.8
1	B	483	HIS	5.8
1	A	194	ALA	5.7
1	B	54	GLN	5.7
1	A	832	PRO	5.7
1	A	716	ILE	5.7
1	B	683	ASN	5.7
1	A	567	PRO	5.6
1	A	332	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	736	TRP	5.6
1	B	744	ASP	5.5
1	A	840	LEU	5.5
1	A	381	ALA	5.5
1	A	327	LEU	5.5
1	B	490	GLU	5.4
1	A	148	ALA	5.4
1	A	48	LEU	5.3
1	B	172	GLN	5.3
1	B	269	GLU	5.3
1	A	411	MET	5.2
1	A	360	GLY	5.2
1	B	257	VAL	5.2
1	B	682	PRO	5.2
1	A	196	LYS	5.2
1	A	51	ALA	5.2
1	B	63	ASP	5.1
1	B	684	ASP	5.1
1	B	748	THR	5.0
1	B	58	LEU	5.0
1	A	833	GLY	5.0
1	A	604	GLN	5.0
1	A	774	ASN	4.9
1	A	174	LYS	4.9
1	A	234	ALA	4.8
1	B	361	GLU	4.8
1	B	601	ALA	4.8
1	B	1	MET	4.8
1	B	376	MET	4.7
1	B	212	ARG	4.7
1	B	46	SER	4.7
1	B	256	VAL	4.7
1	A	717	ILE	4.7
1	B	177	SER	4.6
1	A	329	MET	4.6
1	A	786	VAL	4.6
1	B	592	ALA	4.5
1	B	595	HIS	4.5
1	A	166	GLN	4.4
1	A	454	ARG	4.4
1	B	242	GLU	4.4
1	B	604	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	337	LEU	4.4
1	B	487	PRO	4.4
1	A	320	GLY	4.4
1	B	837	MET	4.4
1	A	713	ALA	4.3
1	B	62	VAL	4.3
1	A	364	ASP	4.3
1	B	797	ARG	4.3
1	A	709	ILE	4.3
1	B	742	PHE	4.3
1	B	196	LYS	4.3
1	B	650	ARG	4.3
1	A	49	VAL	4.3
1	B	341	LEU	4.3
1	B	234	ALA	4.3
1	A	653	LEU	4.3
1	A	165	GLY	4.2
1	B	117	PHE	4.2
1	B	13	SER	4.2
1	B	6	ILE	4.2
1	A	40	LYS	4.2
1	A	837	MET	4.2
1	B	176	PRO	4.2
1	A	787	ALA	4.2
1	B	170	THR	4.2
1	B	237	SER	4.2
1	B	709	ILE	4.1
1	A	170	THR	4.1
1	A	690	HIS	4.1
1	A	39	PHE	4.1
1	A	406	ILE	4.1
1	A	389	PHE	4.0
1	A	615	ALA	4.0
1	A	785	GLY	4.0
1	A	259	LEU	4.0
1	A	150	ASN	4.0
1	B	178	MET	4.0
1	A	143	LEU	4.0
1	A	564	LEU	4.0
1	B	479	PHE	3.9
1	B	39	PHE	3.9
1	A	714	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	858	VAL	3.9
1	B	9	LEU	3.9
1	B	15	ARG	3.9
1	B	113	GLY	3.9
1	B	238	ASP	3.9
1	A	597	GLY	3.8
1	A	512	LEU	3.8
1	B	111	PRO	3.8
1	A	175	LEU	3.8
1	B	266	ALA	3.8
1	B	710	LEU	3.8
1	B	747	ARG	3.8
1	B	776	ILE	3.8
1	A	608	GLN	3.8
1	A	616	ALA	3.8
1	A	498	LEU	3.7
1	B	774	ASN	3.7
1	B	171	GLY	3.7
1	A	113	GLY	3.7
1	B	478	ASP	3.7
1	B	218	PHE	3.7
1	B	665	ASP	3.6
1	B	263	GLN	3.6
1	B	599	GLY	3.6
1	A	380	LEU	3.6
1	B	264	PRO	3.6
1	B	258	ARG	3.6
1	B	419	LEU	3.6
1	A	596	PRO	3.6
1	B	613	LEU	3.6
1	A	637	ASN	3.5
1	A	147	LEU	3.5
1	B	124	PHE	3.5
1	A	452	ARG	3.5
1	A	789	LYS	3.5
1	A	146	GLU	3.4
1	A	473	ALA	3.4
1	A	55	TRP	3.4
1	B	74	LEU	3.4
1	A	566	GLN	3.4
1	B	4	SER	3.4
1	B	190	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	481	PRO	3.4
1	B	59	SER	3.4
1	B	609	SER	3.4
1	A	853	VAL	3.4
1	B	482	LEU	3.4
1	A	260	THR	3.4
1	B	840	LEU	3.4
1	B	48	LEU	3.3
1	B	260	THR	3.3
1	A	784	VAL	3.3
1	A	836	SER	3.3
1	A	829	SER	3.3
1	B	259	LEU	3.3
1	A	195	GLY	3.3
1	A	612	LYS	3.3
1	A	275	ASP	3.3
1	A	614	ALA	3.3
1	A	236	THR	3.3
1	B	336	VAL	3.3
1	A	172	GLN	3.2
1	A	258	ARG	3.2
1	A	495	LEU	3.2
1	A	700	PRO	3.2
1	B	823	PHE	3.2
1	B	484	LEU	3.2
1	A	262	GLU	3.2
1	B	112	GLY	3.2
1	B	244	ALA	3.2
1	A	460	GLY	3.2
1	A	496	LEU	3.2
1	A	695	VAL	3.2
1	A	437	THR	3.1
1	A	328	ASN	3.1
1	A	409	VAL	3.1
1	A	169	LEU	3.1
1	B	839	LYS	3.1
1	B	775	ILE	3.1
1	B	40	LYS	3.1
1	B	743	GLY	3.1
1	B	240	ILE	3.1
1	A	565	THR	3.0
1	A	458	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	844	ALA	3.0
1	B	233	GLY	3.0
1	A	361	GLU	3.0
1	A	835	SER	3.0
1	A	834	THR	3.0
1	B	606	LEU	2.9
1	B	798	ALA	2.9
1	B	116	PHE	2.9
1	A	651	ASP	2.9
1	B	731	ILE	2.9
1	B	750	VAL	2.9
1	B	681	ASP	2.9
1	A	407	ALA	2.9
1	A	144	VAL	2.9
1	B	773	ALA	2.8
1	A	798	ALA	2.8
1	B	500	ASP	2.8
1	B	339	VAL	2.8
1	B	541	PHE	2.8
1	B	781	MET	2.8
1	A	461	THR	2.8
1	A	397	TYR	2.8
1	B	772	PHE	2.8
1	B	335	MET	2.8
1	B	262	GLU	2.7
1	B	686	THR	2.7
1	B	340	GLY	2.7
1	B	194	ALA	2.7
1	A	316	THR	2.7
1	A	390	PHE	2.7
1	B	477	PHE	2.7
1	B	368	ILE	2.7
1	A	449	TYR	2.7
1	B	538	LEU	2.7
1	B	364	ASP	2.7
1	B	337	LEU	2.7
1	A	477	PHE	2.7
1	A	531	GLU	2.7
1	A	330	ILE	2.7
1	A	318	ALA	2.7
1	B	739	LEU	2.6
1	A	46	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	800	GLN	2.6
1	B	216	ARG	2.6
1	B	496	LEU	2.5
1	B	789	LYS	2.5
1	B	60	GLN	2.5
1	B	542	ILE	2.5
1	B	618	SER	2.5
1	A	611	ALA	2.5
1	B	375	GLY	2.5
1	B	270	PHE	2.5
1	B	780	LEU	2.5
1	B	818	THR	2.5
1	A	162	THR	2.5
1	A	684	ASP	2.5
1	B	501	SER	2.4
1	A	206	VAL	2.4
1	B	93	THR	2.4
1	A	277	ALA	2.4
1	B	657	LEU	2.4
1	A	58	LEU	2.4
1	A	405	LEU	2.4
1	A	331	SER	2.4
1	A	476	HIS	2.4
1	A	323	MET	2.4
1	B	226	ASN	2.4
1	A	741	ARG	2.4
1	B	104	ARG	2.3
1	B	399	GLY	2.3
1	A	378	LEU	2.3
1	A	782	LEU	2.3
1	A	191	ASP	2.3
1	A	291	ILE	2.3
1	B	189	VAL	2.3
1	A	494	THR	2.3
1	B	841	LEU	2.3
1	A	746	LEU	2.3
1	A	823	PHE	2.3
1	B	94	GLU	2.3
1	B	221	VAL	2.3
1	B	594	ASP	2.3
1	B	219	VAL	2.3
1	B	733	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	539	SER	2.3
1	A	410	GLY	2.2
1	B	265	LEU	2.2
1	B	359	ARG	2.2
1	A	37	ARG	2.2
1	A	600	ALA	2.2
1	A	400	VAL	2.2
1	A	747	ARG	2.2
1	B	819	THR	2.2
1	B	267	ASP	2.2
1	B	713	ALA	2.2
1	B	544	ALA	2.2
1	B	166	GLN	2.2
1	B	822	ALA	2.2
1	A	568	PRO	2.2
1	B	403	LEU	2.1
1	B	738	THR	2.1
1	B	7	VAL	2.1
1	B	757	ILE	2.1
1	A	393	ILE	2.1
1	B	516	LEU	2.1
1	B	235	GLN	2.1
1	A	450	LEU	2.1
1	B	345	PHE	2.1
1	A	387	ALA	2.1
1	B	680	VAL	2.1
1	A	173	VAL	2.1
1	B	734	LEU	2.1
1	A	164	LEU	2.1
1	A	459	ILE	2.1
1	B	799	GLY	2.1
1	B	607	SER	2.1
1	B	338	PHE	2.0
1	B	225	VAL	2.0
1	A	178	MET	2.0
1	A	723	ALA	2.0
1	B	245	ARG	2.0
1	B	659	ARG	2.0
1	B	735	LEU	2.0
1	A	841	LEU	2.0
1	B	313	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.