



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 05:03 PM EDT

PDB ID : 5KHN
Title : Crystal structures of the Burkholderia multivorans hopanoid transporter HpnN
Authors : Su, C.-C.; Yu, E.W.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

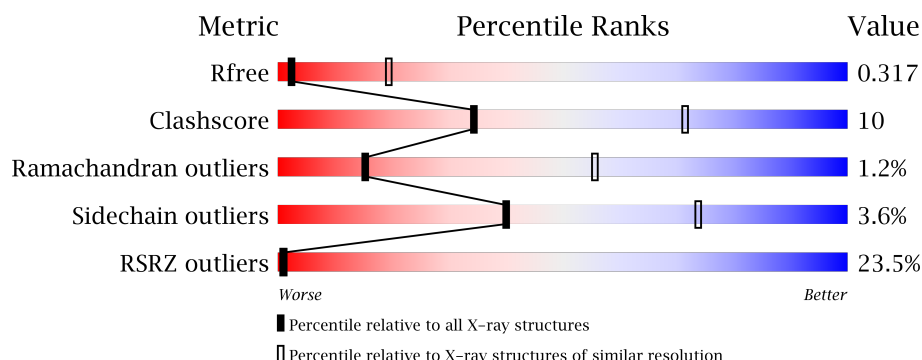
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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}	100719	1082 (3.52-3.36)
Clashscore	112137	1025 (3.50-3.38)
Ramachandran outliers	110173	1155 (3.52-3.36)
Sidechain outliers	110143	1156 (3.52-3.36)
RSRZ outliers	101464	1107 (3.52-3.36)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	883	
1	B	883	

2 Entry composition

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			

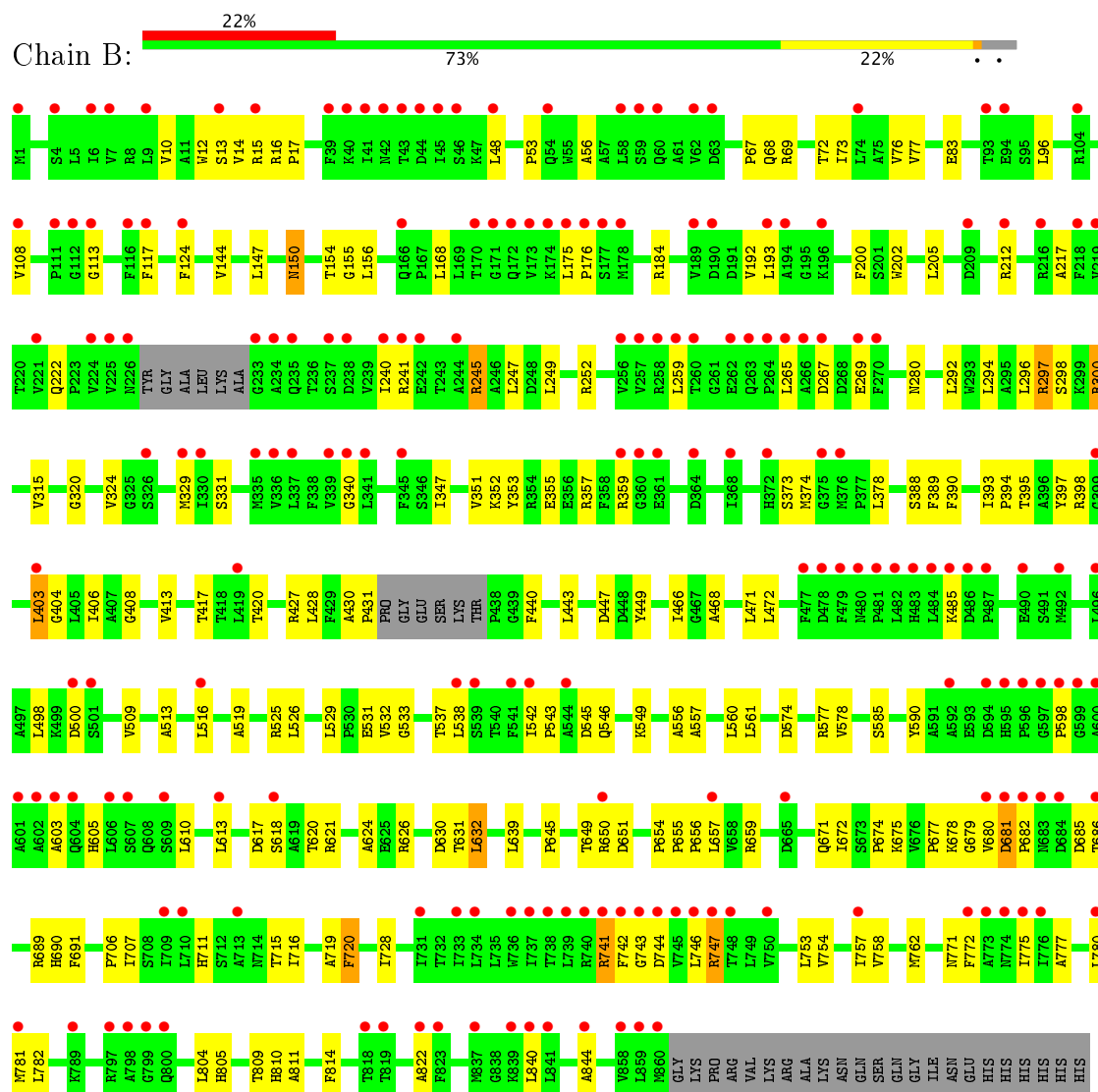
There are 18 discrepancies between the modelled and reference sequences:

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

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



• Molecule 1: RND transporter





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.283 , 0.319 0.283 , 0.317	Depositor DCC
R_{free} test set	1926 reflections (5.00%)	DCC
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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:681:ASP:N	1:B:681:ASP:OD1	2.28	0.63
1:B:76:VAL:HG11	1:B:498:LEU:HD11	1.79	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:675:LYS:HE3	1:A:678:LYS:HG3	1.85	0.57
1:B:324:VAL:HG21	1:B:406:ILE:HD11	1.87	0.57
1:A:122:LEU:HB2	1:A:642:LEU:HG	1.87	0.57
1:A:388:SER:HB3	1:A:780:LEU:HA	1.86	0.56
1:A:364:ASP:OD2	1:A:427:ARG:NH1	2.38	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:184:ARG:HD3	1:A:205:LEU:HG	1.89	0.54
1:A:176:PRO:HB3	1:A:598:PRO:HG2	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:296:LEU:O	1:A:296:LEU:HD12	2.13	0.49
1:A:75:ALA:HB3	1:A:219:VAL:HG13	1.94	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:161:SER:HB2	1:A:587:LEU:HD12	1.96	0.48
1:A:357:ARG:HH11	1:A:362:ALA:HA	1.79	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:374:MET:HB3	1:B:378:LEU:HD13	1.97	0.46
1:B:154:THR:HG22	1:B:577:ARG:HA	1.97	0.46
1:B:96:LEU:HB3	1:B:108:VAL:HG21	1.98	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:730:SER:O	1:A:734:LEU:HB2	2.17	0.45
1:A:99:GLN:HG2	1:A:104:ARG:HH11	1.80	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:96:LEU:HB3	1:A:108:VAL:HG21	1.99	0.45
1:A:241:ARG:NH2	1:A:259:LEU:HD11	2.32	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:88:ALA:HB1	1:A:249:LEU:HD12	1.98	0.44
1:A:69:ARG:NH1	1:A:671:GLN:OE1	2.48	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:500:ASP:OD1	1:A:500:ASP:N	2.53	0.42
1:A:49:VAL:HB	1:A:716:ILE:HD11	2.01	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%)	13	52
1	B	842/883 (95%)	778 (92%)	56 (7%)	8 (1%)	18	60
All	All	1684/1766 (95%)	1552 (92%)	112 (7%)	20 (1%)	15	55

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 ⓘ

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%)	41	75
1	B	659/690 (96%)	635 (96%)	24 (4%)	40	74
All	All	1320/1380 (96%)	1273 (96%)	47 (4%)	40	74

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 ⓘ

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, 95th 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	205 (24%)	1 1	71, 125, 165, 201	0
1	B	848/883 (96%)	1.25	193 (22%)	1 1	77, 127, 165, 204	0
All	All	1696/1766 (96%)	1.35	398 (23%)	1 1	71, 126, 165, 204	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	597	GLY	28.0
1	B	44	ASP	25.0
1	A	272	SER	23.2
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	18.0
1	B	598	PRO	16.4
1	A	483	HIS	16.1
1	A	269	GLU	15.9
1	B	596	PRO	15.8
1	A	479	PHE	15.6
1	B	45	ILE	14.9
1	A	484	LEU	14.3
1	A	273	VAL	14.2
1	A	266	ALA	13.2
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	11.7

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Mol	Chain	Res	Type	RSRZ
1	A	860	MET	11.4
1	A	769	SER	11.4
1	A	264	PRO	11.3
1	A	43	THR	11.1
1	B	741	ARG	11.0
1	A	274	GLU	11.0
1	A	333	ALA	10.6
1	A	783	GLY	10.4
1	A	481	PRO	10.4
1	B	173	VAL	10.3
1	A	770	LEU	10.3
1	B	329	MET	10.0
1	A	268	ASP	9.9
1	A	41	ILE	9.9
1	B	745	VAL	9.9
1	A	489	SER	9.7
1	B	600	ALA	9.6
1	A	42	ASN	9.5
1	A	485	LYS	9.4
1	B	174	LYS	9.3
1	A	207	ASP	9.3
1	A	334	PHE	9.2
1	A	145	ASN	9.1
1	A	490	GLU	9.0
1	A	453	HIS	8.9
1	A	456	PRO	8.6
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	8.2
1	A	324	VAL	8.1
1	A	859	LEU	8.1
1	B	740	ARG	8.0
1	B	108	VAL	8.0
1	B	175	LEU	8.0
1	A	385	VAL	8.0
1	A	384	ALA	7.9
1	A	831	HIS	7.8
1	A	261	GLY	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	7.6
1	A	392	PHE	7.6
1	A	683	ASN	7.3
1	A	321	LEU	7.3
1	B	330	ILE	7.2
1	B	209	ASP	7.2
1	A	491	SER	6.9
1	A	486	ASP	6.9
1	B	372	HIS	6.9
1	A	386	ALA	6.9
1	B	485	LYS	6.8
1	B	360	GLY	6.8
1	B	603	ALA	6.7
1	B	860	MET	6.7
1	B	602	ALA	6.6
1	B	746	LEU	6.6
1	A	45	ILE	6.6
1	B	224	VAL	6.5
1	B	193	LEU	6.4
1	A	149	LYS	6.4
1	A	686	THR	6.3
1	A	720	PHE	6.3
1	B	859	LEU	6.3
1	A	382	THR	6.2
1	A	771	ASN	6.1
1	A	858	VAL	6.1
1	B	737	ILE	6.1
1	A	457	ILE	6.0
1	B	492	MET	6.0
1	B	42	ASN	5.9
1	A	317	ALA	5.9
1	A	826	LEU	5.9
1	B	480	ASN	5.9
1	B	483	HIS	5.9
1	A	716	ILE	5.8
1	A	832	PRO	5.8
1	A	493	SER	5.8
1	A	194	ALA	5.7
1	B	54	GLN	5.7
1	B	683	ASN	5.7
1	A	332	VAL	5.6
1	A	567	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	736	TRP	5.5
1	B	744	ASP	5.5
1	A	840	LEU	5.5
1	A	327	LEU	5.5
1	A	148	ALA	5.4
1	A	48	LEU	5.4
1	A	381	ALA	5.4
1	B	269	GLU	5.3
1	B	490	GLU	5.3
1	A	360	GLY	5.3
1	A	51	ALA	5.2
1	B	172	GLN	5.2
1	A	196	LYS	5.2
1	A	411	MET	5.2
1	B	682	PRO	5.1
1	B	257	VAL	5.1
1	B	63	ASP	5.1
1	B	684	ASP	5.1
1	A	604	GLN	5.1
1	A	833	GLY	5.1
1	B	58	LEU	5.0
1	A	774	ASN	5.0
1	B	748	THR	4.9
1	B	361	GLU	4.9
1	A	174	LYS	4.9
1	B	1	MET	4.9
1	B	601	ALA	4.9
1	A	234	ALA	4.8
1	A	717	ILE	4.7
1	B	376	MET	4.7
1	B	46	SER	4.7
1	A	329	MET	4.7
1	B	177	SER	4.7
1	B	212	ARG	4.7
1	B	256	VAL	4.6
1	B	592	ALA	4.5
1	B	604	GLN	4.5
1	A	786	VAL	4.5
1	B	595	HIS	4.5
1	B	837	MET	4.4
1	B	487	PRO	4.4
1	A	320	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	454	ARG	4.4
1	A	337	LEU	4.4
1	A	713	ALA	4.4
1	A	166	GLN	4.4
1	A	364	ASP	4.4
1	A	49	VAL	4.3
1	B	797	ARG	4.3
1	B	242	GLU	4.3
1	A	653	LEU	4.3
1	A	709	ILE	4.3
1	B	650	ARG	4.3
1	B	62	VAL	4.3
1	B	742	PHE	4.3
1	B	196	LYS	4.3
1	B	117	PHE	4.2
1	B	341	LEU	4.2
1	A	40	LYS	4.2
1	A	165	GLY	4.2
1	A	837	MET	4.2
1	B	234	ALA	4.2
1	B	176	PRO	4.2
1	B	6	ILE	4.2
1	B	13	SER	4.2
1	B	709	ILE	4.1
1	A	39	PHE	4.1
1	A	615	ALA	4.1
1	A	690	HIS	4.1
1	B	237	SER	4.1
1	A	406	ILE	4.1
1	B	170	THR	4.1
1	A	787	ALA	4.1
1	A	150	ASN	4.0
1	A	389	PHE	4.0
1	A	170	THR	4.0
1	B	178	MET	4.0
1	B	479	PHE	4.0
1	A	143	LEU	4.0
1	A	714	ASN	4.0
1	A	564	LEU	4.0
1	A	259	LEU	3.9
1	B	39	PHE	3.9
1	A	597	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	785	GLY	3.9
1	A	175	LEU	3.9
1	B	15	ARG	3.9
1	B	113	GLY	3.9
1	B	9	LEU	3.8
1	B	266	ALA	3.8
1	B	858	VAL	3.8
1	A	616	ALA	3.8
1	B	710	LEU	3.8
1	A	608	GLN	3.8
1	B	776	ILE	3.8
1	B	111	PRO	3.8
1	B	747	ARG	3.8
1	B	238	ASP	3.8
1	A	512	LEU	3.7
1	B	478	ASP	3.7
1	B	774	ASN	3.7
1	A	113	GLY	3.7
1	B	599	GLY	3.7
1	A	498	LEU	3.7
1	B	263	GLN	3.6
1	A	596	PRO	3.6
1	B	218	PHE	3.6
1	B	171	GLY	3.6
1	B	264	PRO	3.6
1	B	613	LEU	3.6
1	A	637	ASN	3.6
1	B	665	ASP	3.6
1	B	419	LEU	3.6
1	A	147	LEU	3.6
1	A	380	LEU	3.6
1	B	124	PHE	3.6
1	B	258	ARG	3.5
1	A	452	ARG	3.5
1	A	146	GLU	3.4
1	A	473	ALA	3.5
1	B	4	SER	3.4
1	A	55	TRP	3.4
1	B	190	ASP	3.4
1	B	481	PRO	3.4
1	B	609	SER	3.4
1	B	840	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	48	LEU	3.4
1	B	482	LEU	3.4
1	A	829	SER	3.4
1	A	836	SER	3.4
1	A	789	LYS	3.4
1	A	275	ASP	3.4
1	A	566	GLN	3.4
1	A	853	VAL	3.4
1	B	59	SER	3.3
1	B	74	LEU	3.3
1	A	612	LYS	3.3
1	A	614	ALA	3.3
1	A	260	THR	3.3
1	A	195	GLY	3.3
1	B	260	THR	3.3
1	B	484	LEU	3.3
1	B	259	LEU	3.3
1	A	784	VAL	3.3
1	B	336	VAL	3.2
1	B	823	PHE	3.2
1	A	172	GLN	3.2
1	A	236	THR	3.2
1	A	258	ARG	3.2
1	A	328	ASN	3.2
1	B	112	GLY	3.2
1	A	262	GLU	3.2
1	A	700	PRO	3.2
1	A	495	LEU	3.1
1	B	839	LYS	3.1
1	A	437	THR	3.1
1	A	695	VAL	3.1
1	B	244	ALA	3.1
1	A	496	LEU	3.1
1	B	775	ILE	3.1
1	B	40	LYS	3.1
1	A	460	GLY	3.1
1	A	409	VAL	3.1
1	B	743	GLY	3.1
1	A	361	GLU	3.1
1	A	169	LEU	3.1
1	A	835	SER	3.0
1	A	834	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	798	ALA	3.0
1	B	844	ALA	3.0
1	A	565	THR	3.0
1	A	651	ASP	3.0
1	B	240	ILE	3.0
1	B	116	PHE	3.0
1	B	606	LEU	3.0
1	A	458	LEU	3.0
1	A	798	ALA	2.9
1	B	233	GLY	2.9
1	A	397	TYR	2.9
1	B	773	ALA	2.9
1	B	681	ASP	2.9
1	B	731	ILE	2.8
1	A	144	VAL	2.8
1	B	541	PHE	2.8
1	A	407	ALA	2.8
1	B	750	VAL	2.8
1	B	772	PHE	2.8
1	B	339	VAL	2.8
1	B	781	MET	2.8
1	B	335	MET	2.8
1	B	477	PHE	2.8
1	B	500	ASP	2.8
1	B	194	ALA	2.7
1	A	477	PHE	2.7
1	B	262	GLU	2.7
1	B	686	THR	2.7
1	A	390	PHE	2.7
1	A	330	ILE	2.7
1	B	364	ASP	2.7
1	A	316	THR	2.7
1	A	461	THR	2.7
1	B	368	ILE	2.7
1	B	538	LEU	2.7
1	B	340	GLY	2.7
1	A	46	SER	2.7
1	A	449	TYR	2.7
1	B	800	GLN	2.6
1	B	337	LEU	2.6
1	B	739	LEU	2.6
1	A	318	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	531	GLU	2.6
1	B	618	SER	2.6
1	B	542	ILE	2.6
1	B	216	ARG	2.6
1	A	611	ALA	2.5
1	B	496	LEU	2.5
1	B	789	LYS	2.5
1	B	60	GLN	2.5
1	A	206	VAL	2.5
1	B	375	GLY	2.5
1	B	270	PHE	2.5
1	B	780	LEU	2.5
1	A	162	THR	2.5
1	A	277	ALA	2.5
1	A	331	SER	2.5
1	A	476	HIS	2.5
1	A	405	LEU	2.4
1	B	657	LEU	2.4
1	A	684	ASP	2.4
1	A	323	MET	2.4
1	A	741	ARG	2.4
1	A	58	LEU	2.4
1	B	93	THR	2.4
1	B	818	THR	2.4
1	B	501	SER	2.4
1	B	399	GLY	2.4
1	B	226	ASN	2.3
1	A	191	ASP	2.3
1	B	189	VAL	2.3
1	B	594	ASP	2.3
1	B	841	LEU	2.3
1	A	782	LEU	2.3
1	B	94	GLU	2.3
1	B	539	SER	2.3
1	A	291	ILE	2.3
1	A	378	LEU	2.3
1	A	746	LEU	2.3
1	A	823	PHE	2.3
1	A	600	ALA	2.3
1	B	104	ARG	2.3
1	B	359	ARG	2.3
1	A	400	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	544	ALA	2.3
1	A	37	ARG	2.3
1	B	265	LEU	2.2
1	B	733	ILE	2.2
1	A	494	THR	2.2
1	B	713	ALA	2.2
1	B	221	VAL	2.2
1	B	219	VAL	2.2
1	B	267	ASP	2.2
1	A	410	GLY	2.2
1	A	747	ARG	2.2
1	A	568	PRO	2.2
1	B	822	ALA	2.2
1	B	819	THR	2.2
1	A	393	ILE	2.1
1	B	403	LEU	2.1
1	B	7	VAL	2.1
1	B	166	GLN	2.1
1	B	607	SER	2.1
1	B	738	THR	2.1
1	B	757	ILE	2.1
1	B	516	LEU	2.1
1	A	450	LEU	2.1
1	B	799	GLY	2.1
1	A	164	LEU	2.1
1	A	178	MET	2.1
1	A	173	VAL	2.1
1	B	345	PHE	2.1
1	A	387	ALA	2.0
1	B	235	GLN	2.0
1	B	225	VAL	2.0
1	A	723	ALA	2.0
1	B	734	LEU	2.0
1	A	459	ILE	2.0
1	B	680	VAL	2.0
1	B	326	SER	2.0
1	A	773	ALA	2.0
1	A	841	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 [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.