



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:56 AM EDT

PDB ID : 5KHN / pdb_00005khn
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

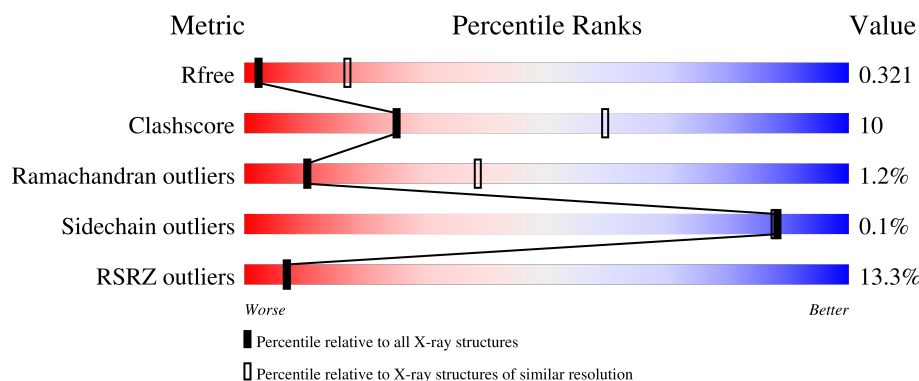
1 Overall quality at a glance

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}	180053	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (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 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 $\leq 5\%$. 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	14% 71% 24% .
1	B	883	11% 74% 22% .

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.

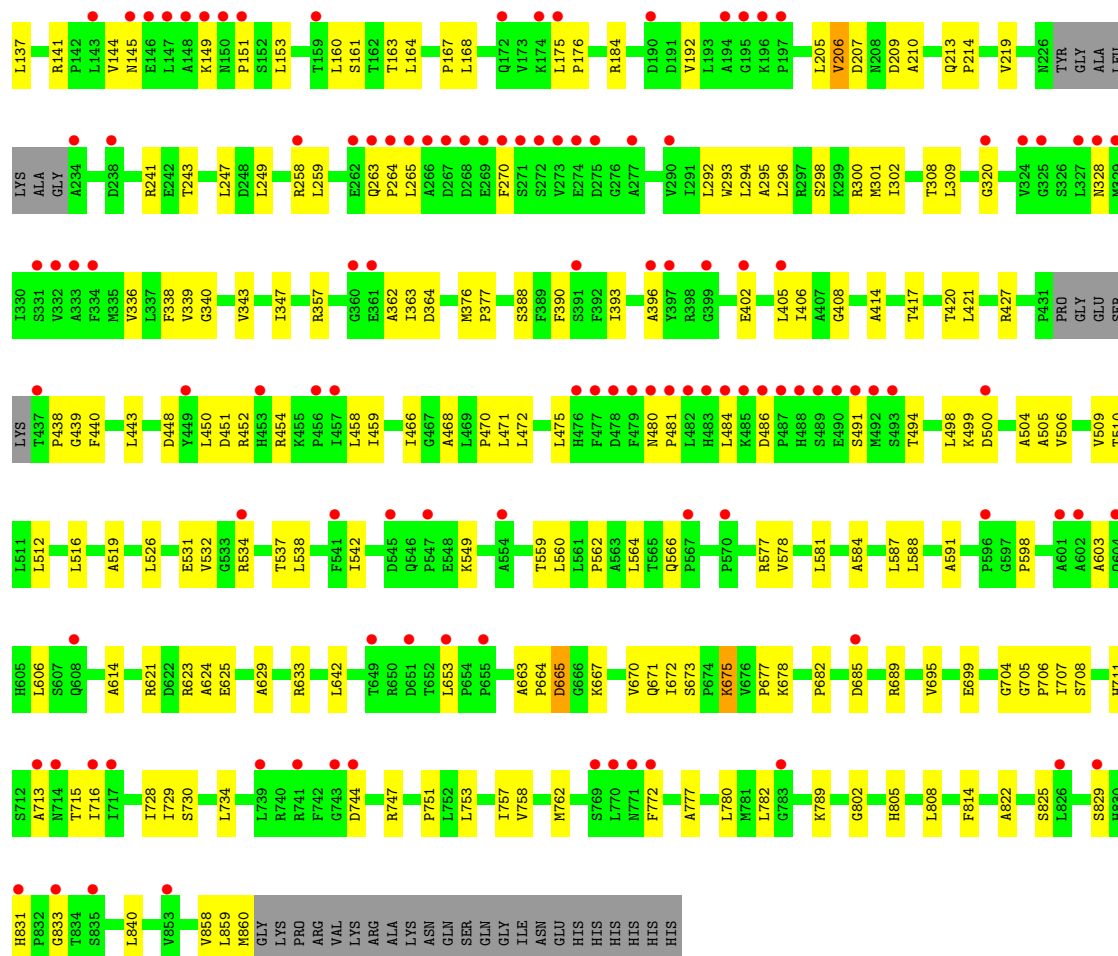
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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



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 0.290 , 0.321	Depositor DCC
R_{free} test set	1928 reflections (3.71%)	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)	0.28 , 239.6	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	0.13	0/6443	0.32	0/8814
1	B	0.17	0/6437	0.35	1/8804 (0.0%)
All	All	0.15	0/12880	0.34	1/17618 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	681	ASP	N-CA-C	5.72	116.61	109.57

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	139	1
1	B	6303	0	6528	120	1
All	All	12612	0	13065	250	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 (250) 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:B:753:LEU:HD13	1:A:466:ILE:HG12	1.75	0.68
1:A:50:ASP:HB2	1:A:396:ALA:HB1	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:OD1	1:B:681:ASP:N	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:B:150:ASN:HB3	1:B:155:GLY:HA3	1.83	0.61
1:A:663:ALA:O	1:A:665:ASP:N	2.33	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:B:526:LEU:HD13	1:B:672:ILE:HG12	1.84	0.60
1:A:92:LEU:HD12	1:A:219:VAL:HG11	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:B:509:VAL:HG13	1:B:706:PRO:HD2	1.84	0.59
1:A:458:LEU:HD11	1:A:858:VAL:HG23	1.85	0.59
1:B:442:TRP:CD1	1:B:442:TRP:H	2.20	0.58
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

Continued on next page...

Continued from previous page...

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:B:144:VAL:HG11	1:B:560:LEU:HD13	1.86	0.57
1:A:192:VAL:O	1:A:623:ARG:NH1	2.37	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:711:HIS:O	1:A:715:THR:OG1	2.23	0.56
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:B:757:ILE:HD11	1:A:757:ILE:HD11	1.91	0.53
1:A:298:SER:HB2	1:A:300:ARG:HD2	1.91	0.53
1:B:685:ASP:HB2	1:B:689:ARG:HH11	1.73	0.53
1:A:560:LEU:O	1:A:564:LEU:N	2.42	0.53
1:B:674:PRO:HB3	1:B:691:PHE:CG	2.44	0.53
1:A:526:LEU:HD21	1:A:699:GLU:HG2	1.91	0.53
1:B:73:ILE:HD11	1:B:240:ILE:HD12	1.91	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: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:B:77:VAL:HB	1:B:217:ALA:HB3	1.92	0.52
1:A:713:ALA:HA	1:A:772:PHE:HE2	1.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:ILE:HG21	1:B:772:PHE:HD1	1.74	0.51
1:A:393:ILE:HD11	1:A:405:LEU:HB2	1.91	0.51
1:A:625:GLU:O	1:A:629:ALA:N	2.41	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:B:292:LEU:HD23	1:B:347:ILE:HD11	1.92	0.51
1:B:678:LYS:HB3	1:A:675:LYS:HD3	1.93	0.51
1:A:145:ASN:O	1:A:149:LYS:HG3	2.11	0.51
1:A:11:ALA:HA	1:A:14:VAL:HG12	1.91	0.51
1:A:113:GLY:HA2	1:A:117:PHE:HB2	1.92	0.51
1:A:141:ARG:HD3	1:A:559:THR:HB	1.92	0.51
1:A:175:LEU:HD11	1:A:603:ALA:HB2	1.93	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:482:LEU:HG	1:B:492:MET:HE1	1.93	0.49
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:B:113:GLY:HA2	1:B:117:PHE:HB2	1.95	0.49
1:A:161:SER:HB3	1:A:584:ALA:HA	1.95	0.49
1:A:537:THR:HG22	1:A:538:LEU:H	1.78	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:753:LEU:O	1:A:757:ILE:HG13	2.12	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:B:468:ALA:HB1	1:B:471:LEU:HD12	1.94	0.49
1:A:581:LEU:HB3	1:A:614:ALA:HB2	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:294:LEU:HB3	1:A:814:PHE:CE1	2.48	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: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

Continued on next page...

Continued from previous page...

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:B:13:SER:OG	1:B:420:THR:O	2.30	0.47
1:B:395:THR:HB	1:B:719:ALA:HB1	1.96	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: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:B:241:ARG:O	1:B:245:ARG:HB2	2.15	0.46
1:A:206:VAL:HG12	1:A:207:ASP:N	2.31	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: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: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: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: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: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:B:14:VAL:HG12	1:B:15:ARG:H	1.82	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: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:B:578:VAL:HG23	1:B:621:ARG:NH2	2.31	0.45
1:A:728:ILE:HD12	1:A:729:ILE:H	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TRP:CD1	1:B:16:ARG:HD2	2.51	0.44
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:HD12	1:A:450:LEU:HA	1.87	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:675:LYS:O	1:A:677:PRO:HD3	2.17	0.44
1:A:860:MET:HE2	1:A:860:MET:HB3	1.87	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: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:A:13:SER:OG	1:A:420:THR:O	2.36	0.44
1:A:390:PHE:CE1	1:A:408:GLY:HA3	2.53	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:H	1:A:300:ARG:CD	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: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:509:VAL:HG12	1:A:705:GLY:H	1.82	0.43
1:A:562:PRO:O	1:A:566:GLN:NE2	2.51	0.43
1:B:466:ILE:HG12	1:A:753:LEU:HD13	1.99	0.43
1:A:519:ALA:HB1	1:A:670:VAL:HG22	2.00	0.43
1:B:753:LEU:O	1:B:757:ILE:HG13	2.18	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:335:MET:HE2	1:B:335:MET:HB3	1.86	0.43
1:A:153:LEU:HD12	1:A:625:GLU:HB2	2.00	0.43
1:B:741:ARG:HA	1:B:741:ARG:NH1	2.34	0.43
1:B:443:LEU:O	1:B:447:ASP:HB2	2.19	0.43
1:A:494:THR:O	1:A:498:LEU:HG	2.19	0.43
1:B:390:PHE:CE1	1:B:408:GLY:HA3	2.54	0.43
1:A:168:LEU:HD22	1:A:591:ALA:HB1	2.00	0.43
1:B:10:VAL:O	1:B:14:VAL:HG23	2.19	0.43
1:A:532:VAL:HG13	1:A:672:ILE:HG23	2.00	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:B:552:ALA:O	1:B:555:THR:OG1	2.31	0.42
1:A:758:VAL:O	1:A:762:MET:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:ASP:HA	1:B:747:ARG:HB2	2.00	0.42
1:A:298:SER:OG	1:A:301:MET:HB2	2.19	0.42
1:A:263:GLN:N	1:A:264:PRO:HD2	2.34	0.42
1:B:15:ARG:C	1:B:17:PRO:HD3	2.45	0.42
1:B:184:ARG:HB2	1:B:205:LEU:HD21	2.01	0.42
1:A:151:PRO:HG2	1:A:633:ARG:HH11	1.84	0.42
1:A:336:VAL:HG11	1:A:825:SER:HB3	2.02	0.42
1:B:357:ARG:NH2	1:B:431:PRO:O	2.38	0.42
1:A:542:ILE:HD11	1:A:653:LEU:HD11	2.01	0.42
1:A:675:LYS:C	1:A:677:PRO:HD3	2.44	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:309:LEU:HD21	1:A:339:VAL:HG13	2.02	0.42
1:B:17:PRO:HG2	1:B:428:LEU:HD21	2.02	0.42
1:A:49:VAL:HB	1:A:716:ILE:HD11	2.01	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:120:ASN:OD1	1:A:120:ASN:N	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:B:175:LEU:HD11	1:B:603:ALA:HB2	2.03	0.41
1:A:41:ILE:HG21	1:A:270:PHE:CZ	2.56	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:516:LEU:HD11	1:A:538:LEU:HB3	2.02	0.41
1:A:758:VAL:O	1:A:762:MET:N	2.51	0.41
1:B:296:LEU:O	1:B:298:SER:N	2.54	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:315:VAL:HG23	1:B:413:VAL:HG11	2.04	0.40
1:B:389:PHE:HB3	1:B:404:GLY:HA2	2.03	0.40
1:B:240:ILE:HB	1:B:259:LEU:HD21	2.03	0.40
1:A:728:ILE:H	1:A:728:ILE:HG13	1.69	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PRO:HD2	1:B:659:ARG:HH21	1.86	0.40
1:B:537:THR:HG22	1:B:538:LEU:H	1.86	0.40
1:A:15:ARG:O	1:A:17:PRO:HD3	2.22	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%)	9	35
1	B	842/883 (95%)	778 (92%)	56 (7%)	8 (1%)	12	42
All	All	1684/1766 (95%)	1552 (92%)	112 (7%)	20 (1%)	10	38

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	661 (100%)	0	100	100
1	B	659/690 (96%)	658 (100%)	1 (0%)	87	85
All	All	1320/1380 (96%)	1319 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	681	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	GLN
1	B	222	GLN
1	B	476	HIS
1	B	507	ASN
1	B	566	GLN
1	A	263	GLN
1	A	476	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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%)	0.68	126 (14%) 5 6	71, 125, 165, 201	0
1	B	848/883 (96%)	0.39	99 (11%) 9 8	77, 127, 165, 204	0
All	All	1696/1766 (96%)	0.54	225 (13%) 7 7	71, 126, 165, 204	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	SER	14.2
1	B	44	ASP	13.0
1	A	769	SER	12.0
1	A	489	SER	11.6
1	A	272	SER	11.5
1	A	478	ASP	10.6
1	A	483	HIS	9.6
1	A	273	VAL	9.5
1	A	479	PHE	9.4
1	B	740	ARG	9.2
1	A	267	ASP	8.9
1	A	268	ASP	8.8
1	A	491	SER	8.7
1	B	860	MET	8.7
1	B	226	ASN	8.2
1	B	241	ARG	8.2
1	B	596	PRO	8.1
1	B	741	ARG	7.9
1	A	274	GLU	7.9
1	A	651	ASP	7.9
1	A	608	GLN	7.6
1	A	263	GLN	7.5
1	A	490	GLU	7.4
1	A	269	GLU	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	7.4
1	B	172	GLN	7.4
1	A	482	LEU	7.3
1	A	481	PRO	7.2
1	B	483	HIS	7.1
1	A	43	THR	6.9
1	B	43	THR	6.8
1	A	266	ALA	6.7
1	A	741	ARG	6.7
1	B	63	ASP	6.7
1	A	360	GLY	6.6
1	A	480	ASN	6.5
1	B	209	ASP	6.3
1	A	488	HIS	6.3
1	B	45	ILE	6.2
1	A	265	LEU	6.2
1	A	146	GLU	6.1
1	A	772	PHE	6.1
1	B	597	GLY	6.0
1	B	39	PHE	5.8
1	A	831	HIS	5.8
1	A	456	PRO	5.8
1	A	270	PHE	5.7
1	B	650	ARG	5.7
1	B	478	ASP	5.5
1	A	148	ALA	5.5
1	B	800	GLN	5.5
1	B	737	ILE	5.5
1	B	329	MET	5.3
1	B	174	LYS	5.3
1	A	487	PRO	5.3
1	A	145	ASN	5.2
1	B	651	ASP	5.2
1	A	328	ASN	5.2
1	A	42	ASN	5.1
1	A	770	LEU	5.0
1	A	333	ALA	5.0
1	B	193	LEU	4.9
1	B	797	ARG	4.8
1	A	327	LEU	4.8
1	B	176	PRO	4.8
1	B	372	HIS	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	364	ASP	4.7
1	A	397	TYR	4.6
1	A	149	LYS	4.6
1	B	598	PRO	4.6
1	B	360	GLY	4.6
1	A	332	VAL	4.6
1	B	173	VAL	4.5
1	A	492	MET	4.4
1	B	773	ALA	4.4
1	A	744	ASP	4.4
1	A	602	ALA	4.4
1	A	150	ASN	4.4
1	A	713	ALA	4.3
1	B	263	GLN	4.3
1	B	41	ILE	4.3
1	A	829	SER	4.3
1	A	449	TYR	4.3
1	A	567	PRO	4.2
1	A	46	SER	4.1
1	A	604	GLN	4.1
1	A	477	PHE	4.1
1	A	717	ILE	4.1
1	A	195	GLY	4.1
1	A	534	ARG	4.0
1	A	49	VAL	4.0
1	A	771	ASN	4.0
1	B	539	SER	4.0
1	B	1	MET	3.9
1	A	112	GLY	3.9
1	A	486	ASP	3.8
1	A	143	LEU	3.8
1	A	596	PRO	3.7
1	A	194	ALA	3.7
1	A	234	ALA	3.7
1	B	827	TRP	3.7
1	B	11	ALA	3.7
1	B	289	PHE	3.7
1	A	329	MET	3.6
1	A	783	GLY	3.6
1	B	46	SER	3.6
1	A	41	ILE	3.6
1	A	324	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	269	GLU	3.6
1	A	457	ILE	3.6
1	A	264	PRO	3.6
1	A	826	LEU	3.6
1	B	837	MET	3.6
1	A	716	ILE	3.6
1	A	39	PHE	3.4
1	B	194	ALA	3.4
1	A	453	HIS	3.4
1	A	493	SER	3.4
1	A	147	LEU	3.4
1	B	736	TRP	3.4
1	B	485	LYS	3.3
1	A	290	VAL	3.3
1	B	538	LEU	3.3
1	B	745	VAL	3.3
1	A	547	PRO	3.3
1	A	172	GLN	3.2
1	B	798	ALA	3.2
1	A	685	ASP	3.2
1	B	175	LEU	3.2
1	A	275	ASP	3.2
1	A	51	ALA	3.2
1	A	601	ALA	3.2
1	A	320	GLY	3.2
1	A	151	PRO	3.1
1	A	258	ARG	3.1
1	B	54	GLN	3.1
1	A	196	LYS	3.1
1	B	744	ASP	3.1
1	B	604	GLN	3.1
1	B	490	GLU	3.1
1	B	541	PHE	3.1
1	B	190	ASP	3.1
1	B	601	ALA	3.0
1	A	331	SER	3.0
1	A	437	THR	3.0
1	B	603	ALA	3.0
1	B	60	GLN	3.0
1	B	224	VAL	2.9
1	A	325	GLY	2.9
1	B	6	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	174	LYS	2.9
1	B	600	ALA	2.9
1	B	678	LYS	2.9
1	A	485	LYS	2.9
1	B	767	GLY	2.9
1	B	255	ALA	2.9
1	B	365	ALA	2.8
1	B	487	PRO	2.8
1	B	124	PHE	2.8
1	A	833	GLY	2.8
1	B	368	ILE	2.8
1	A	541	PHE	2.8
1	A	175	LEU	2.8
1	B	262	GLU	2.8
1	B	330	ILE	2.7
1	B	839	LYS	2.7
1	A	277	ALA	2.7
1	B	542	ILE	2.7
1	A	402	GLU	2.7
1	B	482	LEU	2.7
1	B	117	PHE	2.7
1	B	79	ALA	2.7
1	B	484	LEU	2.7
1	B	477	PHE	2.6
1	A	653	LEU	2.6
1	B	4	SER	2.6
1	B	602	ALA	2.6
1	B	676	VAL	2.5
1	A	739	LEU	2.5
1	B	335	MET	2.5
1	B	42	ASN	2.4
1	A	190	ASP	2.4
1	B	361	GLU	2.4
1	A	391	SER	2.4
1	B	234	ALA	2.4
1	A	714	ASN	2.4
1	B	7	VAL	2.4
1	A	649	THR	2.3
1	A	476	HIS	2.3
1	A	835	SER	2.3
1	B	244	ALA	2.3
1	B	266	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	70	ASN	2.3
1	B	746	LEU	2.3
1	A	44	ASP	2.3
1	A	197	PRO	2.3
1	B	211	ALA	2.3
1	A	361	GLU	2.3
1	B	606	LEU	2.3
1	B	682	PRO	2.2
1	A	399	GLY	2.2
1	A	19	TRP	2.2
1	B	238	ASP	2.2
1	A	545	ASP	2.2
1	A	131	ALA	2.2
1	A	238	ASP	2.2
1	A	159	THR	2.2
1	B	169	LEU	2.2
1	B	47	LYS	2.1
1	A	396	ALA	2.1
1	A	570	PRO	2.1
1	A	334	PHE	2.1
1	B	544	ALA	2.1
1	A	500	ASP	2.1
1	B	859	LEU	2.1
1	B	328	ASN	2.1
1	A	554	ALA	2.1
1	A	262	GLU	2.1
1	A	655	PRO	2.1
1	A	405	LEU	2.0
1	B	362	ALA	2.0
1	B	258	ARG	2.0
1	A	48	LEU	2.0
1	A	743	GLY	2.0
1	A	853	VAL	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 oligosaccharides 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.