



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:40 AM UTC

PDB ID : 5KHS / pdb_00005khs
Title : Crystal structures of the Burkholderia multivorans hopanoid transporter HpnN
Authors : Su, C.-C.; Yu, E.W.
Deposited on : 2016-06-15
Resolution : 3.76 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

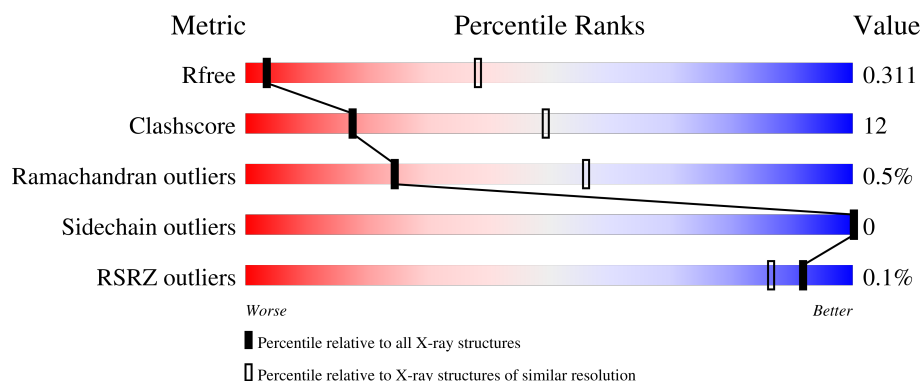
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.76 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	 69% 28% .
1	B	883	 72% 25% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12679 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 Putative RND superfamily efflux pump membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	853	Total	C	N	O	S	0	0	0
			6342	4094	1087	1143	18			
1	A	852	Total	C	N	O	S	0	0	0
			6337	4091	1086	1142	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	360	GLY	ASP	engineered mutation	UNP A0A0H3KP92
B	362	ALA	ARG	engineered mutation	UNP A0A0H3KP92
B	365	ALA	HIS	engineered mutation	UNP A0A0H3KP92
B	878	HIS	-	expression tag	UNP A0A0H3KP92
B	879	HIS	-	expression tag	UNP A0A0H3KP92
B	880	HIS	-	expression tag	UNP A0A0H3KP92
B	881	HIS	-	expression tag	UNP A0A0H3KP92
B	882	HIS	-	expression tag	UNP A0A0H3KP92
B	883	HIS	-	expression tag	UNP A0A0H3KP92
A	360	GLY	ASP	engineered mutation	UNP A0A0H3KP92
A	362	ALA	ARG	engineered mutation	UNP A0A0H3KP92
A	365	ALA	HIS	engineered mutation	UNP A0A0H3KP92
A	878	HIS	-	expression tag	UNP A0A0H3KP92
A	879	HIS	-	expression tag	UNP A0A0H3KP92
A	880	HIS	-	expression tag	UNP A0A0H3KP92
A	881	HIS	-	expression tag	UNP A0A0H3KP92
A	882	HIS	-	expression tag	UNP A0A0H3KP92
A	883	HIS	-	expression tag	UNP A0A0H3KP92

LYS	G375	L459	P598	I717
PRO	A376	G460		S718
ARG	P377	T461	L606	A719
VAL		L462	S607	F720
LYS	T383			
ARG		I466	L610	I728
ALA	F390		A614	
LYS		P470		L734
ASN	I393	L471	D617	
GLN	P394	L472	S618	T738
SER	T395			L739
GLN	A396	N480	R626	
GLY	Y397	P481		R747
ILE	R398	L482	A641	
ASN		H483		P751
ASN	S401	L484	T648	
GLU	E402	K485	T649	I757
HIS	L403			
HIS	G404	M492	T652	I776
HIS	L405	S493	L653	A777
HIS	I406	T494	P654	
HIS	A407	K499	P655	L782
HIS	G408	D500	P656	
		S501	L657	V786
	L419			
	T420	A504	A663	K789
	L421	A505	P664	
	L422	V506		W796
	P423	N507	L669	
	A424	D508	V670	H805
	L425	V509	Q671	
	L426	T510	I672	L808
	R427			
	L428	S515	P677	
	F429	L516		A811
		A517	V680	V812
	A430	D518	D681	L813
	P431		P682	L814
	PRO		N683	S815
	GLY		D684	
	GLU	L526	D685	T818
	LYS	V532	T686	
	SER		M687	T821
	THR	T537		A822
	PRO	L538	A692	
	G439			S825
	F440	F541		
	P441	I542	V695	S829
	W442	P543	H830	
	L443		H831	
			E699	
		Q546		W837
	D447		I703	
		L560	G704	
	L450		G705	L840
	D451	L581	P706	
		S585	I707	Q856
	R454		S712	P857
	K455	L588		V858
	P456			L859
	I457			M860
	L458			GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.16Å 143.37Å 112.66Å 90.00° 114.10° 90.00°	Depositor
Resolution (Å)	83.57 – 3.76 83.57 – 3.76	Depositor EDS
% Data completeness (in resolution range)	83.0 (83.57-3.76) 82.8 (83.57-3.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.78Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.263 , 0.307 0.266 , 0.311	Depositor DCC
R_{free} test set	1390 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	1.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.387 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12679	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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	0/6472	0.33	0/8852
1	B	0.15	0/6477	0.34	0/8859
All	All	0.14	0/12949	0.34	0/17711

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 [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	6337	0	6566	173	1
1	B	6342	0	6571	154	1
All	All	12679	0	13137	320	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 12.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:HG2	1:A:485:LYS:HE3	1.48	0.95
1:B:269:GLU:HB2	1:B:485:LYS:HZ1	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PRO:HA	1:B:549:LYS:HE2	1.60	0.82
1:A:751:PRO:HG3	1:A:859:LEU:HD13	1.65	0.78
1:A:395:THR:HG21	1:A:719:ALA:HA	1.65	0.76
1:A:751:PRO:HB2	1:A:789:LYS:HE3	1.67	0.74
1:B:616:ALA:HB3	1:B:620:THR:HG21	1.72	0.72
1:B:777:ALA:HB3	1:B:840:LEU:HD12	1.73	0.70
1:B:300:ARG:H	1:B:300:ARG:HD2	1.56	0.69
1:A:808:LEU:HD23	1:A:813:LEU:HD21	1.75	0.69
1:A:276:GLY:O	1:A:280:ASN:N	2.23	0.68
1:A:66:PHE:HE2	1:A:669:LEU:HB3	1.59	0.68
1:B:549:LYS:HD2	1:B:549:LYS:N	2.08	0.68
1:B:74:LEU:HD21	1:B:218:PHE:HB3	1.77	0.67
1:A:47:LYS:HE3	1:A:328:ASN:HB3	1.77	0.67
1:B:193:LEU:HD21	1:B:613:LEU:HA	1.77	0.67
1:B:76:VAL:HG11	1:B:498:LEU:HD11	1.77	0.66
1:A:150:ASN:HB2	1:A:155:GLY:HA3	1.77	0.66
1:B:447:ASP:OD2	1:B:805:HIS:ND1	2.30	0.65
1:A:355:GLU:OE1	1:A:359:ARG:NH1	2.29	0.65
1:B:108:VAL:HG13	1:B:221:VAL:HG12	1.78	0.65
1:B:472:LEU:HD13	1:A:472:LEU:HD13	1.78	0.65
1:B:546:GLN:HB3	1:B:549:LYS:HB2	1.77	0.65
1:B:456:PRO:O	1:B:460:GLY:N	2.18	0.64
1:B:181:LEU:O	1:B:185:SER:OG	2.11	0.63
1:B:74:LEU:HD23	1:B:220:THR:HG23	1.81	0.63
1:A:363:ILE:HD11	1:A:427:ARG:HG2	1.80	0.63
1:B:79:ALA:HB2	1:B:255:ALA:HB2	1.81	0.62
1:B:112:GLY:HA2	1:B:503:GLU:HG2	1.81	0.62
1:B:343:VAL:HB	1:B:818:THR:HG21	1.82	0.62
1:B:50:ASP:HB2	1:B:396:ALA:HB1	1.82	0.62
1:A:356:GLU:HG2	1:A:359:ARG:HH21	1.66	0.61
1:A:777:ALA:HB3	1:A:840:LEU:HD12	1.83	0.61
1:B:107:PRO:HG2	1:B:222:GLN:HE21	1.65	0.61
1:A:796:TRP:HZ3	1:A:856:GLN:HG3	1.66	0.60
1:A:786:VAL:HA	1:A:789:LYS:HD2	1.82	0.60
1:A:312:GLY:O	1:A:316:THR:OG1	2.18	0.60
1:A:313:LEU:HD21	1:A:335:MET:HE3	1.83	0.60
1:B:227:TYR:HE1	1:B:235:GLN:HG3	1.67	0.60
1:A:542:ILE:HD11	1:A:653:LEU:HD11	1.83	0.60
1:A:728:ILE:HG23	1:A:782:LEU:HD13	1.84	0.59
1:A:126:SER:H	1:A:129:GLN:NE2	2.00	0.59
1:A:543:PRO:HG2	1:A:546:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CZ	1:A:808:LEU:HD12	2.38	0.58
1:A:300:ARG:H	1:A:300:ARG:HD2	1.69	0.58
1:A:510:THR:HG22	1:A:671:GLN:HG2	1.84	0.58
1:A:581:LEU:HB3	1:A:614:ALA:HB2	1.86	0.57
1:A:796:TRP:CZ3	1:A:856:GLN:HG3	2.39	0.57
1:A:6:ILE:HG23	1:A:419:LEU:HD21	1.86	0.57
1:B:739:LEU:HD22	1:B:744:ASP:HB3	1.86	0.57
1:A:164:LEU:HD13	1:A:588:LEU:HG	1.87	0.57
1:A:440:PHE:CE2	1:A:808:LEU:HD12	2.38	0.57
1:B:73:ILE:HG22	1:B:261:GLY:HA3	1.85	0.57
1:A:265:LEU:HD12	1:A:266:ALA:N	2.20	0.57
1:A:856:GLN:NE2	1:A:859:LEU:O	2.35	0.57
1:B:83:GLU:HG3	1:B:631:THR:HG23	1.87	0.57
1:A:150:ASN:HD22	1:A:152:SER:H	1.53	0.57
1:B:357:ARG:HH21	1:B:358:PHE:HE1	1.53	0.56
1:B:509:VAL:HG21	1:B:695:VAL:HG11	1.86	0.56
1:A:115:PRO:HA	1:A:118:GLU:HB2	1.86	0.56
1:B:720:PHE:CZ	1:A:470:PRO:HB3	2.41	0.56
1:B:174:LYS:O	1:B:177:SER:OG	2.24	0.56
1:A:829:SER:O	1:A:831:HIS:N	2.37	0.56
1:A:247:LEU:C	1:A:249:LEU:H	2.15	0.55
1:A:509:VAL:HG11	1:A:707:ILE:HG13	1.87	0.55
1:A:856:GLN:H	1:A:857:PRO:HD2	1.71	0.55
1:A:456:PRO:O	1:A:460:GLY:N	2.37	0.55
1:B:808:LEU:HA	1:B:813:LEU:HB2	1.87	0.55
1:A:581:LEU:HG	1:A:610:LEU:HD22	1.89	0.55
1:A:348:GLN:OE1	1:A:815:SER:OG	2.13	0.55
1:B:200:PHE:O	1:B:631:THR:HG21	2.06	0.55
1:B:340:GLY:HA2	1:B:818:THR:HG22	1.89	0.55
1:A:34:TYR:HE2	1:A:322:ALA:HB2	1.71	0.55
1:B:123:LEU:HD23	1:B:648:ILE:HG22	1.88	0.54
1:A:348:GLN:NE2	1:A:811:ALA:O	2.40	0.54
1:A:537:THR:HG22	1:A:538:LEU:H	1.72	0.54
1:B:13:SER:OG	1:B:420:THR:O	2.23	0.54
1:B:89:ALA:HB2	1:B:217:ALA:HB1	1.90	0.54
1:A:247:LEU:O	1:A:249:LEU:N	2.34	0.54
1:B:654:PRO:HB2	1:B:656:PRO:HD2	1.88	0.54
1:B:129:GLN:OE1	1:B:129:GLN:N	2.37	0.53
1:B:300:ARG:H	1:B:300:ARG:CD	2.20	0.53
1:B:367:LEU:HD11	1:B:426:LEU:HD12	1.91	0.53
1:B:543:PRO:HD2	1:B:648:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:PHE:HZ	1:A:470:PRO:HB3	1.73	0.53
1:B:34:TYR:HA	1:B:37:ARG:HG2	1.90	0.53
1:B:753:LEU:HD11	1:A:757:ILE:HD13	1.89	0.53
1:B:742:PHE:CD1	1:A:455:LYS:HD2	2.42	0.53
1:A:43:THR:OG1	1:A:266:ALA:O	2.26	0.53
1:B:390:PHE:HA	1:B:393:ILE:HG12	1.89	0.53
1:A:441:PRO:HD2	1:A:442:TRP:CD1	2.43	0.53
1:A:588:LEU:HD13	1:A:606:LEU:HB3	1.91	0.53
1:A:695:VAL:HG13	1:A:707:ILE:HD11	1.89	0.53
1:A:526:LEU:HD22	1:A:695:VAL:HG23	1.90	0.53
1:A:812:VAL:O	1:A:815:SER:HB2	2.09	0.53
1:B:669:LEU:HD21	1:B:671:GLN:HG3	1.91	0.52
1:A:747:ARG:HG3	1:A:859:LEU:HB3	1.91	0.52
1:A:398:ARG:HA	1:A:401:SER:HB2	1.90	0.52
1:A:482:LEU:HD12	1:A:492:MET:HE1	1.91	0.52
1:A:50:ASP:HB2	1:A:396:ALA:HB1	1.90	0.52
1:B:96:LEU:HB3	1:B:108:VAL:HG21	1.92	0.52
1:B:240:ILE:HB	1:B:259:LEU:HD21	1.92	0.52
1:A:209:ASP:OD1	1:A:210:ALA:N	2.43	0.52
1:A:340:GLY:HA3	1:A:822:ALA:HB2	1.91	0.52
1:B:676:VAL:HG22	1:B:687:MET:HE1	1.91	0.52
1:A:99:GLN:HB3	1:A:104:ARG:HB2	1.92	0.52
1:B:176:PRO:HB3	1:B:598:PRO:HG2	1.91	0.52
1:B:282:VAL:HA	1:B:285:LEU:HD12	1.90	0.52
1:A:184:ARG:HD3	1:A:205:LEU:HG	1.92	0.51
1:B:499:LYS:HB2	1:B:682:PRO:HB2	1.92	0.51
1:B:123:LEU:HD13	1:B:645:PRO:CB	2.41	0.51
1:B:336:VAL:HG21	1:B:825:SER:HB3	1.92	0.51
1:B:505:ALA:HB1	1:B:508:ASP:CG	2.36	0.51
1:B:12:TRP:CD1	1:B:16:ARG:HD2	2.45	0.51
1:B:398:ARG:HA	1:B:401:SER:HB2	1.93	0.51
1:B:130:VAL:HA	1:B:133:THR:HB	1.93	0.51
1:A:66:PHE:CD1	1:A:663:ALA:HB2	2.46	0.51
1:B:154:THR:HG22	1:B:577:ARG:HA	1.93	0.50
1:B:796:TRP:NE1	1:B:803:LEU:HB2	2.26	0.50
1:A:292:LEU:HG	1:A:347:ILE:HD11	1.93	0.50
1:A:655:PRO:HG2	1:A:656:PRO:HD3	1.94	0.50
1:B:14:VAL:HG12	1:B:15:ARG:H	1.77	0.50
1:B:178:MET:HB3	1:B:182:LEU:HG	1.94	0.50
1:A:213:GLN:HB2	1:A:214:PRO:HD3	1.92	0.50
1:A:542:ILE:HG13	1:A:648:ILE:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PRO:HG3	1:B:598:PRO:HD2	1.92	0.50
1:B:752:LEU:HD21	1:B:785:GLY:HA3	1.93	0.50
1:B:654:PRO:HG2	1:B:657:LEU:HD13	1.94	0.50
1:A:269:GLU:HG2	1:A:485:LYS:HB3	1.92	0.50
1:B:110:GLU:HA	1:B:219:VAL:HA	1.94	0.49
1:A:324:VAL:HG21	1:A:406:ILE:HD11	1.94	0.49
1:A:499:LYS:HA	1:A:506:VAL:HG21	1.95	0.49
1:B:96:LEU:HD13	1:B:221:VAL:HG11	1.93	0.49
1:A:284:THR:HG23	1:A:821:THR:HG22	1.94	0.49
1:A:263:GLN:N	1:A:264:PRO:HD2	2.26	0.49
1:A:265:LEU:HD12	1:A:266:ALA:H	1.78	0.49
1:A:340:GLY:HA2	1:A:818:THR:HG22	1.94	0.49
1:B:296:LEU:HD13	1:B:301:MET:HB3	1.94	0.49
1:B:677:PRO:HB3	1:A:677:PRO:HB2	1.95	0.49
1:B:809:THR:HG23	1:B:810:HIS:ND1	2.28	0.49
1:A:703:ILE:HG12	1:A:704:GLY:H	1.76	0.49
1:B:73:ILE:HG21	1:B:264:PRO:HG2	1.94	0.49
1:B:390:PHE:CE1	1:B:408:GLY:HA3	2.48	0.49
1:A:10:VAL:O	1:A:14:VAL:HG23	2.13	0.49
1:A:375:GLY:H	1:A:377:PRO:HD2	1.78	0.49
1:A:541:PHE:HD2	1:A:657:LEU:HD21	1.78	0.49
1:A:92:LEU:HD12	1:A:219:VAL:HG11	1.94	0.48
1:A:66:PHE:CE2	1:A:669:LEU:HB3	2.46	0.48
1:A:585:SER:O	1:A:607:SER:OG	2.28	0.48
1:A:249:LEU:HD22	1:A:253:TYR:HE1	1.78	0.48
1:A:776:ILE:HD12	1:A:837:MET:HE2	1.95	0.48
1:B:805:HIS:O	1:B:809:THR:HG22	2.14	0.48
1:B:83:GLU:CD	1:B:83:GLU:H	2.22	0.48
1:A:692:ALA:HB2	1:A:706:PRO:HB2	1.95	0.48
1:A:96:LEU:HB3	1:A:108:VAL:HG21	1.96	0.48
1:B:241:ARG:O	1:B:245:ARG:HB2	2.13	0.48
1:B:247:LEU:O	1:B:249:LEU:N	2.37	0.48
1:A:328:ASN:ND2	1:A:402:GLU:OE1	2.45	0.48
1:B:457:ILE:HG22	1:B:854:VAL:HG13	1.96	0.48
1:B:249:LEU:O	1:B:253:TYR:N	2.25	0.47
1:A:516:LEU:HD11	1:A:538:LEU:HB3	1.96	0.47
1:A:649:THR:N	1:A:652:THR:OG1	2.36	0.47
1:B:585:SER:OG	1:B:611:ALA:HB2	2.15	0.47
1:B:771:ASN:O	1:B:775:ILE:HB	2.15	0.47
1:B:200:PHE:CZ	1:B:205:LEU:HD22	2.50	0.47
1:A:355:GLU:HB3	1:A:359:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HD11	1:B:625:GLU:HB2	1.95	0.47
1:B:578:VAL:HG23	1:B:621:ARG:NH2	2.30	0.47
1:A:751:PRO:HD3	1:A:859:LEU:HD22	1.97	0.47
1:B:184:ARG:HB2	1:B:205:LEU:HD21	1.97	0.46
1:B:357:ARG:NH1	1:B:363:ILE:HG23	2.30	0.46
1:B:754:VAL:O	1:B:758:VAL:HG23	2.15	0.46
1:A:176:PRO:HB3	1:A:598:PRO:HG2	1.96	0.46
1:B:202:TRP:CD1	1:B:631:THR:HG22	2.50	0.46
1:A:442:TRP:CD1	1:A:442:TRP:H	2.33	0.46
1:B:353:TYR:CZ	1:B:426:LEU:HD11	2.50	0.46
1:B:451:ASP:OD2	1:B:802:GLY:N	2.30	0.46
1:B:537:THR:O	1:B:540:THR:OG1	2.25	0.46
1:A:293:TRP:HD1	1:A:302:ILE:HD11	1.79	0.46
1:A:585:SER:HB2	1:A:610:LEU:HB3	1.97	0.46
1:B:60:GLN:NE2	1:B:63:ASP:OD2	2.48	0.46
1:A:352:LYS:HD3	1:A:374:MET:HE1	1.96	0.46
1:A:247:LEU:C	1:A:249:LEU:N	2.74	0.46
1:B:374:MET:HB3	1:B:378:LEU:HD13	1.97	0.46
1:B:10:VAL:O	1:B:14:VAL:HG23	2.16	0.46
1:A:712:SER:O	1:A:716:ILE:HG12	2.16	0.46
1:A:481:PRO:HA	1:A:484:LEU:HD21	1.98	0.45
1:B:31:SER:OG	1:B:315:VAL:HA	2.17	0.45
1:B:703:ILE:HG12	1:B:704:GLY:H	1.82	0.45
1:B:803:LEU:HD23	1:B:803:LEU:H	1.80	0.45
1:A:37:ARG:HG3	1:A:38:HIS:CD2	2.51	0.45
1:A:458:LEU:HD11	1:A:858:VAL:CG2	2.46	0.45
1:B:550:ARG:HD3	1:B:646:GLN:O	2.16	0.45
1:B:581:LEU:HD22	1:B:610:LEU:HD21	1.98	0.45
1:B:768:MET:HE1	1:B:839:LYS:HG2	1.97	0.45
1:A:390:PHE:CE1	1:A:408:GLY:HA3	2.51	0.45
1:A:747:ARG:HA	1:A:859:LEU:HD23	1.98	0.45
1:A:78:GLU:O	1:A:255:ALA:HA	2.17	0.45
1:A:252:ARG:O	1:A:626:ARG:NH1	2.48	0.45
1:A:507:ASN:HD21	1:A:683:ASN:ND2	2.14	0.45
1:B:202:TRP:CE2	1:B:632:LEU:HG	2.52	0.45
1:B:509:VAL:HG23	1:B:672:ILE:HD13	1.98	0.45
1:A:455:LYS:HB3	1:A:456:PRO:HD3	1.99	0.45
1:B:662:VAL:HG12	1:B:663:ALA:H	1.81	0.45
1:A:480:ASN:HD21	1:A:483:HIS:CE1	2.35	0.45
1:B:665:ASP:OD1	1:B:665:ASP:N	2.50	0.45
1:A:18:VAL:HG22	1:A:428:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PHE:HD1	1:A:663:ALA:HB2	1.81	0.45
1:A:69:ARG:NH1	1:A:671:GLN:OE1	2.49	0.45
1:A:808:LEU:CD2	1:A:813:LEU:HD21	2.45	0.45
1:B:320:GLY:O	1:B:324:VAL:HG22	2.17	0.44
1:A:546:GLN:NE2	1:A:648:ILE:O	2.31	0.44
1:B:696:LYS:NZ	1:B:700:PRO:O	2.33	0.44
1:A:119:HIS:ND1	1:A:641:ALA:O	2.51	0.44
1:A:507:ASN:ND2	1:A:682:PRO:O	2.51	0.44
1:B:510:THR:O	1:B:510:THR:OG1	2.33	0.44
1:A:747:ARG:HE	1:A:859:LEU:HA	1.83	0.44
1:B:294:LEU:HB3	1:B:814:PHE:CE1	2.53	0.44
1:B:447:ASP:CG	1:B:804:LEU:HB2	2.42	0.44
1:B:744:ASP:HA	1:B:747:ARG:HB2	1.99	0.44
1:A:393:ILE:HD11	1:A:405:LEU:HB2	1.98	0.44
1:A:160:LEU:HD22	1:A:164:LEU:HD11	2.00	0.44
1:A:222:GLN:HB3	1:A:223:PRO:HD2	2.00	0.44
1:A:480:ASN:HD21	1:A:483:HIS:HE1	1.66	0.44
1:A:230:LEU:HB2	1:A:233:GLY:H	1.82	0.44
1:B:300:ARG:O	1:B:304:SER:OG	2.27	0.44
1:B:202:TRP:HD1	1:B:631:THR:HG22	1.82	0.44
1:A:52:GLU:OE2	1:A:55:TRP:HB2	2.17	0.44
1:A:125:LEU:HB2	1:A:130:VAL:HG23	2.00	0.44
1:A:258:ARG:HB3	1:A:494:THR:HG21	2.00	0.44
1:A:532:VAL:HG13	1:A:672:ILE:HG23	1.99	0.44
1:A:95:SER:OG	1:A:247:LEU:HD11	2.17	0.43
1:B:654:PRO:HD2	1:B:657:LEU:HD22	2.00	0.43
1:A:440:PHE:HB3	1:A:443:LEU:HD23	2.00	0.43
1:B:577:ARG:HD2	1:B:621:ARG:HD2	1.99	0.43
1:B:677:PRO:CB	1:A:677:PRO:HB2	2.47	0.43
1:B:296:LEU:HD21	1:B:305:VAL:HG21	2.00	0.43
1:A:685:ASP:OD1	1:A:685:ASP:N	2.51	0.43
1:B:221:VAL:HG21	1:B:240:ILE:HD11	2.00	0.43
1:B:9:LEU:HD23	1:B:419:LEU:HB3	1.99	0.43
1:B:451:ASP:HA	1:B:454:ARG:NH2	2.34	0.43
1:B:808:LEU:HB2	1:B:813:LEU:HD22	2.01	0.43
1:A:288:VAL:O	1:A:292:LEU:HB2	2.19	0.43
1:A:738:THR:OG1	1:A:739:LEU:HD12	2.19	0.43
1:B:123:LEU:HD13	1:B:645:PRO:HB2	1.99	0.43
1:B:155:GLY:O	1:B:159:THR:HG23	2.19	0.43
1:A:9:LEU:HD22	1:A:419:LEU:HD23	2.01	0.43
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:PRO:HG3	1:B:691:PHE:CE2	2.54	0.42
1:B:772:PHE:O	1:B:775:ILE:HG22	2.18	0.42
1:B:329:MET:HE3	1:B:329:MET:HB2	1.83	0.42
1:A:480:ASN:OD1	1:A:483:HIS:ND1	2.52	0.42
1:B:293:TRP:HD1	1:B:302:ILE:HD11	1.83	0.42
1:A:74:LEU:HD21	1:A:218:PHE:HB3	2.02	0.42
1:B:475:LEU:HD21	1:B:760:LEU:HD22	2.00	0.42
1:B:107:PRO:HG2	1:B:222:GLN:NE2	2.33	0.42
1:B:831:HIS:CD2	1:B:833:GLY:H	2.37	0.42
1:A:52:GLU:HB2	1:A:53:PRO:HD2	2.00	0.42
1:A:363:ILE:HD11	1:A:427:ARG:CG	2.49	0.42
1:A:450:LEU:O	1:A:454:ARG:N	2.52	0.42
1:A:241:ARG:O	1:A:245:ARG:HB2	2.20	0.42
1:A:425:LEU:HD22	1:A:429:PHE:HE2	1.84	0.42
1:B:247:LEU:C	1:B:249:LEU:H	2.25	0.42
1:B:296:LEU:O	1:B:298:SER:N	2.53	0.42
1:B:739:LEU:HD12	1:B:739:LEU:O	2.20	0.42
1:B:213:GLN:HB3	1:B:214:PRO:HD3	2.01	0.42
1:A:71:GLY:C	1:A:223:PRO:HD3	2.45	0.42
1:B:184:ARG:HD2	1:B:205:LEU:HG	2.02	0.42
1:B:529:LEU:HB2	1:B:532:VAL:HG23	2.02	0.42
1:B:537:THR:HG22	1:B:538:LEU:H	1.84	0.42
1:A:717:ILE:HA	1:A:720:PHE:CE1	2.54	0.42
1:B:153:LEU:HD13	1:B:577:ARG:HD3	2.02	0.41
1:B:202:TRP:CZ2	1:B:632:LEU:HG	2.55	0.41
1:B:263:GLN:HB3	1:B:264:PRO:HD3	2.01	0.41
1:A:458:LEU:HD11	1:A:858:VAL:HG22	2.01	0.41
1:B:167:PRO:HB2	1:B:173:VAL:HG12	2.02	0.41
1:A:105:ILE:HA	1:A:224:VAL:HG22	2.01	0.41
1:A:300:ARG:H	1:A:300:ARG:CD	2.33	0.41
1:A:163:THR:HA	1:A:167:PRO:HG2	2.01	0.41
1:A:680:VAL:HG11	1:A:687:MET:HG2	2.01	0.41
1:B:160:LEU:O	1:B:164:LEU:HG	2.20	0.41
1:B:344:ASP:O	1:B:348:GLN:HG2	2.21	0.41
1:A:153:LEU:CD1	1:A:581:LEU:HD11	2.50	0.41
1:A:264:PRO:O	1:A:268:ASP:HB2	2.21	0.41
1:A:336:VAL:HG11	1:A:825:SER:HB3	2.03	0.41
1:B:752:LEU:HD23	1:B:752:LEU:HA	1.86	0.41
1:B:754:VAL:HG11	1:B:855:PHE:CZ	2.56	0.41
1:B:444:ALA:HB3	1:B:445:PRO:HD3	2.02	0.41
1:A:323:MET:HE2	1:A:405:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HD12	1:A:419:LEU:HA	1.94	0.41
1:A:501:SER:HB3	1:A:504:ALA:HB3	2.03	0.41
1:A:610:LEU:HD23	1:A:610:LEU:HA	1.90	0.41
1:A:458:LEU:HD12	1:A:857:PRO:HB2	2.02	0.41
1:A:663:ALA:HB1	1:A:664:PRO:HD2	2.03	0.41
1:B:83:GLU:CG	1:B:631:THR:HG23	2.50	0.41
1:B:227:TYR:CE1	1:B:235:GLN:HG3	2.51	0.41
1:B:826:LEU:O	1:B:835:SER:HA	2.21	0.41
1:A:331:SER:HA	1:A:403:LEU:HD12	2.03	0.41
1:A:462:LEU:O	1:A:466:ILE:HG13	2.21	0.41
1:A:655:PRO:CG	1:A:656:PRO:HD3	2.50	0.41
1:A:68:GLN:O	1:A:72:THR:HG23	2.21	0.41
1:B:141:ARG:HA	1:B:144:VAL:HG12	2.02	0.40
1:A:308:THR:HG22	1:A:421:LEU:HB3	2.03	0.40
1:A:617:ASP:CG	1:A:618:SER:H	2.30	0.40
1:B:182:LEU:HA	1:B:606:LEU:HD12	2.02	0.40
1:A:383:THR:HB	1:A:734:LEU:HD11	2.03	0.40
1:A:447:ASP:OD2	1:A:805:HIS:ND1	2.55	0.40
1:A:294:LEU:HB3	1:A:814:PHE:CE1	2.57	0.40
1:A:422:LEU:HB3	1:A:423:PRO:HD3	2.04	0.40
1:A:481:PRO:O	1:A:485:LYS:HG3	2.22	0.40
1:A:526:LEU:HD21	1:A:699:GLU:HG2	2.03	0.40
1:B:349:TYR:OH	1:B:367:LEU:O	2.39	0.40
1:A:120:ASN:OD1	1:A:120:ASN:N	2.55	0.40
1:A:201:SER:O	1:A:205:LEU:HD13	2.21	0.40
1:A:515:SER:OG	1:A:518:ASP:OD1	2.31	0.40
1:B:100:ALA:HB2	1:B:108:VAL:HG23	2.03	0.40
1:B:443:LEU:CD1	1:B:804:LEU:HB3	2.52	0.40
1:B:747:ARG:HD2	1:B:747:ARG:HA	1.90	0.40
1:A:68:GLN:HG3	1:A:222:GLN:CD	2.46	0.40
1:A:137:LEU:HB3	1:A:560:LEU:HD11	2.02	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]	2.16	0.04

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	848/883 (96%)	787 (93%)	58 (7%)	3 (0%)	30	61
1	B	849/883 (96%)	791 (93%)	52 (6%)	6 (1%)	18	50
All	All	1697/1766 (96%)	1578 (93%)	110 (6%)	9 (0%)	24	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	ARG
1	B	811	ALA
1	B	859	LEU
1	B	771	ASN
1	A	214	PRO
1	B	17	PRO
1	B	328	ASN
1	A	248	ASP
1	A	206	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	662/690 (96%)	662 (100%)	0	100	100
1	B	662/690 (96%)	662 (100%)	0	100	100
All	All	1324/1380 (96%)	1324 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	GLN
1	B	70	ASN
1	B	97	GLN
1	B	222	GLN
1	B	235	GLN
1	A	150	ASN
1	A	480	ASN
1	A	576	GLN
1	A	683	ASN
1	A	690	HIS
1	A	714	ASN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	852/883 (96%)	-1.05	1 (0%) 92 86	6, 46, 81, 112	0
1	B	853/883 (96%)	-1.03	0 100 100	6, 44, 82, 112	0
All	All	1705/1766 (96%)	-1.04	1 (0%) 92 86	6, 45, 82, 112	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ASP	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.