



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2017 – 08:57 PM EDT

PDB ID : 5KHS
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

<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-20029077
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-20029077

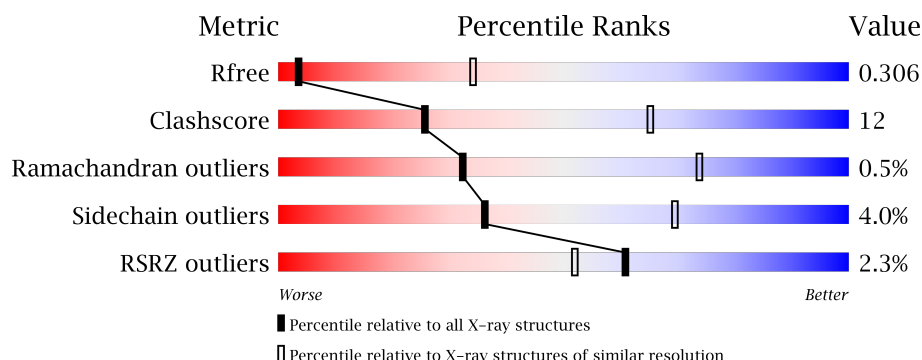
1 Overall quality at a glance

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}	100719	1423 (4.02-3.50)
Clashscore	112137	1087 (4.00-3.52)
Ramachandran outliers	110173	1047 (4.00-3.52)
Sidechain outliers	110143	1041 (4.00-3.52)
RSRZ outliers	101464	1011 (4.00-3.52)

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	<div> <div>2%</div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
1	B	883	<div> <div>2%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>

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			

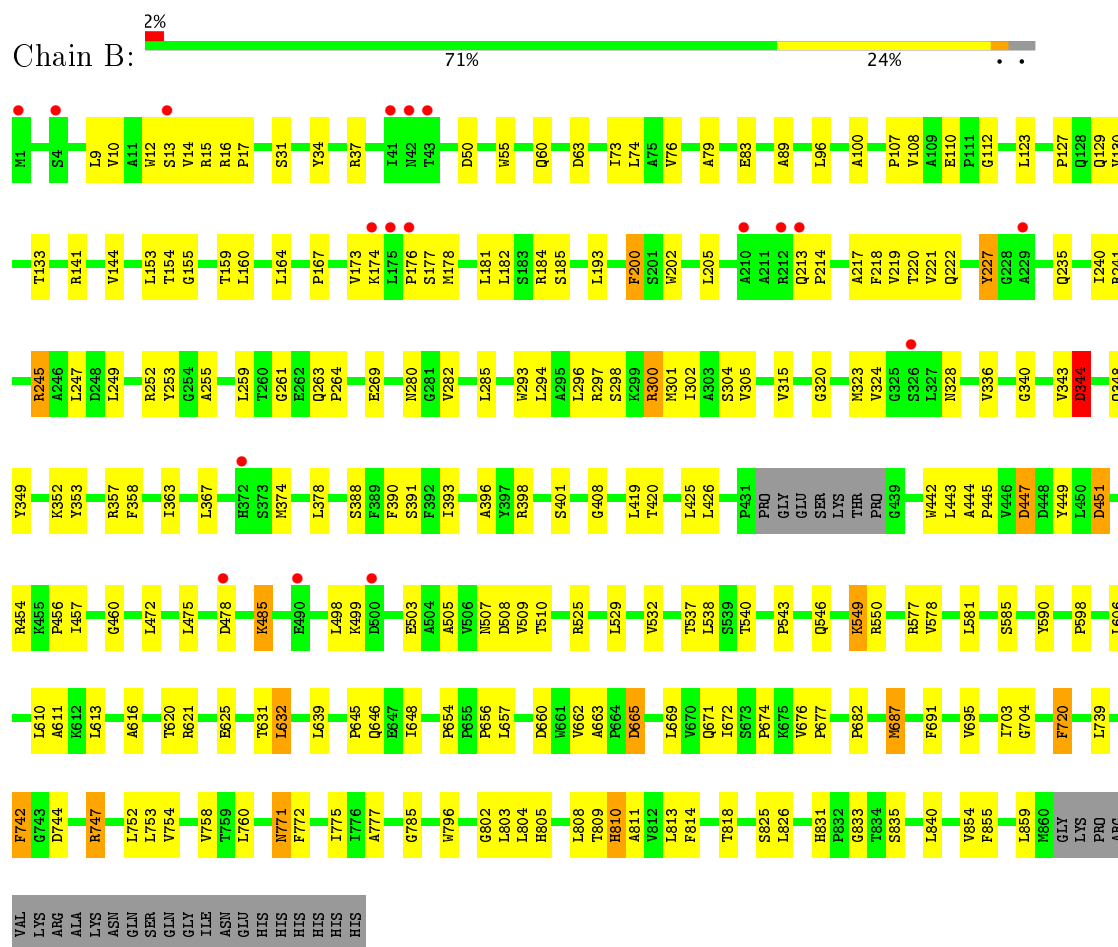
There are 18 discrepancies between the modelled and reference sequences:

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

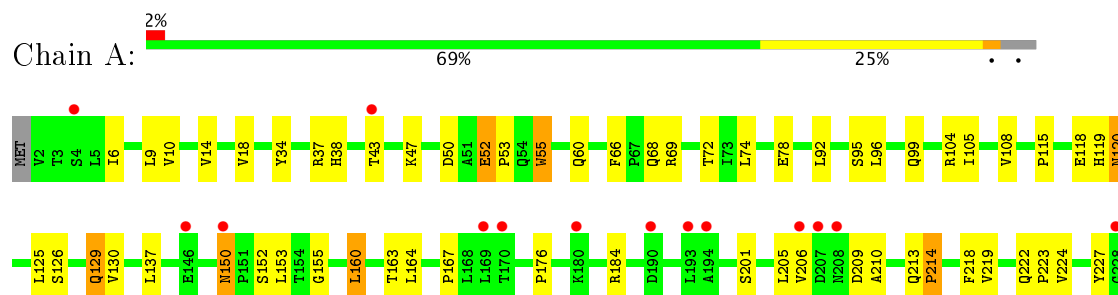
3 Residue-property plots

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: Putative RND superfamily efflux pump membrane protein



- Molecule 1: Putative RND superfamily efflux pump membrane protein



T821	A692	F541	F440	A629
A822	V695	I542	P441	L230
S825	E699	P543	R442	K231
S829	G699	Q546	L443	G233
S830	I703	L560	D447	R241
H831	G704	T565	D448	R245
L840	G705	L581	Y449	A246
Q856	I707	S585	L450	L247
P857	S712	I588	D451	D248
V858	I716	P598	R454	L249
L859	I717	L606	K455	R252
P860	I718	S607	P456	Y253
LYS	A719	L610	I457	G254
PRO	S718	A614	L458	A255
ARG	L720	R626	G460	T383
VAL	L721	L648	T461	F390
LYS	H722	T649	L462	R258
ALA	I728	T652	I466	Q263
ASN	L734	L653	P470	P264
GLN	T738	P654	L471	L265
SER	L739	P655	L472	A266
GLY	F742	P656	L484	D267
ILE	R747	L657	K485	D268
ASN	P751	A663	E490	E269
GLU	H757	P664	S491	G276
HIS	A777	L689	L492	N280
HIS	H805	Q671	V506	T284
HIS	L808	I672	N507	V288
HIS	L808	P677	D508	L292
	A811	V680	V509	V293
	V812	D681	T510	L294
	L813	P682	L516	R300
	F814	L683	L526	N301
	S815	D684	V532	L302
	T818	D685	T537	T308
		N686	L538	G312
				T316
				A322
			N323	
			V324	
			N328	
			S331	
			V336	

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 0.260 , 0.306	Depositor DCC
R_{free} test set	1391 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	1.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , -7.6	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	0.82	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

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	0.25	0/6472	0.45	0/8852
1	B	0.26	1/6477 (0.0%)	0.44	1/8859 (0.0%)
All	All	0.25	1/12949 (0.0%)	0.45	1/17711 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	LYS	CE-NZ	-5.12	1.36	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ASP	CB-CG-OD2	6.05	123.75	118.30

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	6337	0	6566	164	1
1	B	6342	0	6571	151	1
All	All	12679	0	13137	308	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 (308) 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: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:A:363:ILE:HD11	1:A:427:ARG:HG2	1.80	0.63
1:B:74:LEU:HD23	1:B:220:THR:HG23	1.81	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:542:ILE:HD11	1:A:653:LEU:HD11	1.83	0.60
1:B:227:TYR:HE1	1:B:235:GLN:HG3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PRO:HG2	1:A:546:GLN:HG2	1.84	0.59
1:A:440:PHE:CZ	1:A:808:LEU:HD12	2.38	0.58
1:A:300:ARG:HD2	1:A:300:ARG:H	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: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:739:LEU:HD22	1:B:744:ASP:HB3	1.86	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:A:829:SER:O	1:A:831:HIS:N	2.37	0.56
1:B:174:LYS:O	1:B:177:SER:OG	2.24	0.56
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:A:581:LEU:HG	1:A:610:LEU:HD22	1.89	0.55
1:B:808:LEU:HA	1:B:813:LEU:HB2	1.87	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:A:348:GLN:NE2	1:A:811:ALA:O	2.40	0.54
1:B:123:LEU:HD23	1:B:648:ILE:HG22	1.88	0.54
1:A:537:THR:HG22	1:A:538:LEU:H	1.72	0.54
1:A:247:LEU:O	1:A:249:LEU:N	2.34	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:B:654:PRO:HB2	1:B:656:PRO:HD2	1.88	0.54
1:B:129:GLN:N	1:B:129:GLN:OE1	2.37	0.53
1:B:300:ARG:CD	1:B:300:ARG:H	2.20	0.53
1:B:720:PHE:HZ	1:A:470:PRO:HB3	1.73	0.53
1:B:367:LEU:HD11	1:B:426:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PRO:HD2	1:B:648:ILE:HB	1.90	0.53
1:B:753:LEU:HD11	1:A:757:ILE:HD13	1.89	0.53
1:B:34:TYR:HA	1:B:37:ARG:HG2	1.90	0.53
1:A:43:THR:OG1	1:A:266:ALA:O	2.26	0.53
1:B:742:PHE:CD1	1:A:455:LYS:HD2	2.42	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:269:GLU:HB2	1:B:485:LYS:NZ	2.24	0.53
1:A:747:ARG:HG3	1:A:859:LEU:HB3	1.91	0.52
1:B:669:LEU:HD21	1:B:671:GLN:HG3	1.91	0.52
1:A:398:ARG:HA	1:A:401:SER:HB2	1.90	0.52
1:A:50:ASP:HB2	1:A:396:ALA:HB1	1.90	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:240:ILE:HB	1:B:259:LEU:HD21	1.92	0.52
1:B:96:LEU:HB3	1:B:108:VAL:HG21	1.92	0.52
1:A:99:GLN:HB3	1:A:104:ARG:HB2	1.92	0.52
1:B:282:VAL:HA	1:B:285:LEU:HD12	1.90	0.52
1:B:176:PRO:HB3	1:B:598:PRO:HG2	1.91	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:A:247:LEU:C	1:A:249:LEU:H	2.15	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:A:66:PHE:CD1	1:A:663:ALA:HB2	2.46	0.51
1:B:130:VAL:HA	1:B:133:THR:HB	1.93	0.51
1:A:292:LEU:HG	1:A:347:ILE:HD11	1.93	0.50
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:655:PRO:HG2	1:A:656:PRO:HD3	1.94	0.50
1:B:676:VAL:HG13	1:B:687:MET:HE1	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
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

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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:A:324:VAL:HG21	1:A:406:ILE:HD11	1.94	0.49
1:B:110:GLU:HA	1:B:219:VAL:HA	1.94	0.49
1:A:499:LYS:HA	1:A:506:VAL:HG21	1.95	0.49
1:A:284:THR:HG23	1:A:821:THR:HG22	1.94	0.49
1:B:96:LEU:HD13	1:B:221:VAL:HG11	1.93	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:A:703:ILE:HG12	1:A:704:GLY:H	1.76	0.49
1:B:809:THR:HG23	1:B:810:HIS:ND1	2.28	0.49
1:B:390:PHE:CE1	1:B:408:GLY:HA3	2.48	0.49
1:B:73:ILE:HG21	1:B:264:PRO:HG2	1.94	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:585:SER:O	1:A:607:SER:OG	2.28	0.48
1:A:66:PHE:CE2	1:A:669:LEU:HB3	2.46	0.48
1:A:249:LEU:HD22	1:A:253:TYR:HE1	1.78	0.48
1:B:805:HIS:O	1:B:809:THR:HG22	2.14	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:A:328:ASN:ND2	1:A:402:GLU:OE1	2.45	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:B:457:ILE:HG22	1:B:854:VAL:HG13	1.96	0.48
1:A:516:LEU:HD11	1:A:538:LEU:HB3	1.96	0.47
1:B:249:LEU:O	1:B:253:TYR:N	2.25	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:A:355:GLU:HB3	1:A:359:ARG:NH2	2.29	0.47
1:B:200:PHE:CZ	1:B:205:LEU:HD22	2.50	0.47
1:B:153:LEU:HD11	1:B:625:GLU:HB2	1.95	0.47
1:A:751:PRO:HD3	1:A:859:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:VAL:HG23	1:B:621:ARG:NH2	2.30	0.47
1:A:176:PRO:HB3	1:A:598:PRO:HG2	1.96	0.46
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:B:202:TRP:CD1	1:B:631:THR:HG22	2.50	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: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:B:505:ALA:HB1	1:B:508:ASP:CG	2.36	0.46
1:B:60:GLN:NE2	1:B:63:ASP:OD2	2.48	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:352:LYS:HB2	1:B:374:MET:HE1	1.98	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: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:H	1:B:803:LEU:HD23	1.80	0.45
1:B:550:ARG:HD3	1:B:646:GLN:O	2.16	0.45
1:A:390:PHE:CE1	1:A:408:GLY:HA3	2.51	0.45
1:B:581:LEU:HD22	1:B:610:LEU:HD21	1.98	0.45
1:A:747:ARG:HA	1:A:859:LEU:HD23	1.98	0.45
1:A:507:ASN:HD21	1:A:683:ASN:ND2	2.14	0.45
1:A:252:ARG:O	1:A:626:ARG:NH1	2.48	0.45
1:A:78:GLU:O	1:A:255:ALA:HA	2.17	0.45
1:A:455:LYS:HB3	1:A:456:PRO:HD3	1.99	0.45
1:B:509:VAL:HG23	1:B:672:ILE:HD13	1.98	0.45
1:B:202:TRP:CE2	1:B:632:LEU:HG	2.52	0.45
1:A:480:ASN:HD21	1:A:483:HIS:CE1	2.35	0.45
1:B:662:VAL:HG12	1:B:663:ALA:H	1.81	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
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:A:492:MET:HB3	1:A:492:MET:HE3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLN:NE2	1:A:648:ILE:O	2.31	0.44
1:B:320:GLY:O	1:B:324:VAL:HG22	2.17	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:A:747:ARG:HE	1:A:859:LEU:HA	1.83	0.44
1:B:510:THR:OG1	1:B:510:THR:O	2.33	0.44
1:A:393:ILE:HD11	1:A:405:LEU:HB2	1.98	0.44
1:B:294:LEU:HB3	1:B:814:PHE:CE1	2.53	0.44
1:B:744:ASP:HA	1:B:747:ARG:HB2	1.99	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:A:52:GLU:OE2	1:A:55:TRP:HB2	2.17	0.44
1:B:202:TRP:HD1	1:B:631:THR:HG22	1.82	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:83:GLU:CD	1:B:83:GLU:H	2.22	0.43
1:A:440:PHE:HB3	1:A:443:LEU:HD23	2.00	0.43
1:B:654:PRO:HD2	1:B:657:LEU:HD22	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:A:685:ASP:OD1	1:A:685:ASP:N	2.51	0.43
1:B:296:LEU:HD21	1:B:305:VAL:HG21	2.00	0.43
1:B:221:VAL:HG21	1:B:240:ILE:HD11	2.00	0.43
1:A:288:VAL:O	1:A:292:LEU:HB2	2.19	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:B:9:LEU:HD23	1:B:419:LEU:HB3	1.99	0.43
1:A:738:THR:OG1	1:A:739:LEU:HD12	2.19	0.43
1:A:9:LEU:HD22	1:A:419:LEU:HD23	2.01	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:B:425:LEU:HD23	1:B:425:LEU:HA	1.86	0.43
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:A:480:ASN:OD1	1:A:483:HIS:ND1	2.52	0.42
1:B:388:SER:O	1:B:391:SER:OG	2.32	0.42
1:A:74:LEU:HD21	1:A:218:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:TRP:HD1	1:B:302:ILE:HD11	1.83	0.42
1:B:475:LEU:HD21	1:B:760:LEU:HD22	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:52:GLU:HB2	1:A:53:PRO:HD2	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: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:296:LEU:O	1:B:298:SER:N	2.53	0.42
1:B:739:LEU:O	1:B:739:LEU:HD12	2.20	0.42
1:B:213:GLN:HB3	1:B:214:PRO:HD3	2.01	0.42
1:A:717:ILE:HA	1:A:720:PHE:CE1	2.54	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:458:LEU:HD11	1:A:858:VAL:HG22	2.01	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:B:300:ARG:O	1:B:304:SER:OG	2.27	0.41
1:B:153:LEU:HD13	1:B:577:ARG:HD3	2.02	0.41
1:A:105:ILE:HA	1:A:224:VAL:HG22	2.01	0.41
1:A:300:ARG:CD	1:A:300:ARG:H	2.33	0.41
1:B:167:PRO:HB2	1:B:173:VAL:HG12	2.02	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: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: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: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: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:HA	1:A:610:LEU:HD23	1.90	0.41
1:B:444:ALA:HB3	1:B:445:PRO:HD3	2.02	0.41
1:A:247:LEU:C	1:A:249:LEU:N	2.74	0.41
1:A:663:ALA:HB1	1:A:664:PRO:HD2	2.03	0.41
1:A:458:LEU:HD12	1:A:857:PRO:HB2	2.02	0.41
1:B:227:TYR:CE1	1:B:235:GLN:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:83:GLU:CG	1:B:631:THR:HG23	2.50	0.41
1:B:826:LEU:O	1:B:835:SER:HA	2.21	0.41
1:A:68:GLN:O	1:A:72:THR:HG23	2.21	0.41
1:A:308:THR:HG22	1:A:421:LEU:HB3	2.03	0.40
1:B:141:ARG:HA	1:B:144:VAL:HG12	2.02	0.40
1:A:447:ASP:OD2	1:A:805:HIS:ND1	2.55	0.40
1:A:383:THR:HB	1:A:734:LEU:HD11	2.03	0.40
1:B:182:LEU:HA	1:B:606:LEU:HD12	2.02	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:A:120:ASN:N	1:A:120:ASN:OD1	2.55	0.40
1:A:201:SER:O	1:A:205:LEU:HD13	2.21	0.40
1:B:349:TYR:OH	1:B:367:LEU:O	2.39	0.40
1:A:137:LEU:HB3	1:A:560:LEU:HD11	2.02	0.40
1:B:100:ALA:HB2	1:B:108:VAL:HG23	2.03	0.40
1:B:747:ARG:HA	1:B:747:ARG:HD2	1.90	0.40
1:B:443:LEU:CD1	1:B:804:LEU:HB3	2.52	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	38	77
1	B	849/883 (96%)	791 (93%)	52 (6%)	6 (1%)	25	68
All	All	1697/1766 (96%)	1578 (93%)	110 (6%)	9 (0%)	32	74

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 ⓘ

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%)	635 (96%)	27 (4%)	35	69
1	B	662/690 (96%)	636 (96%)	26 (4%)	37	70
All	All	1324/1380 (96%)	1271 (96%)	53 (4%)	36	69

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	TRP
1	B	200	PHE
1	B	227	TYR
1	B	245	ARG
1	B	252	ARG
1	B	280	ASN
1	B	300	ARG

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Mol	Chain	Res	Type
1	B	323	MET
1	B	344	ASP
1	B	442	TRP
1	B	447	ASP
1	B	449	TYR
1	B	451	ASP
1	B	478	ASP
1	B	507	ASN
1	B	525	ARG
1	B	549	LYS
1	B	632	LEU
1	B	639	LEU
1	B	660	ASP
1	B	665	ASP
1	B	687	MET
1	B	720	PHE
1	B	742	PHE
1	B	747	ARG
1	B	810	HIS
1	A	52	GLU
1	A	55	TRP
1	A	60	GLN
1	A	120	ASN
1	A	129	GLN
1	A	150	ASN
1	A	160	LEU
1	A	227	TYR
1	A	245	ARG
1	A	300	ARG
1	A	376	MET
1	A	397	TYR
1	A	415	LEU
1	A	427	ARG
1	A	428	LEU
1	A	442	TRP
1	A	449	TYR
1	A	484	LEU
1	A	490	GLU
1	A	508	ASP
1	A	626	ARG
1	A	639	LEU
1	A	657	LEU

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Mol	Chain	Res	Type
1	A	685	ASP
1	A	722	HIS
1	A	742	PHE
1	A	747	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	GLN
1	A	150	ASN
1	A	480	ASN
1	A	683	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 carbohydrates 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	852/883 (96%)	-0.04	21 (2%)	58 47	6, 46, 81, 112	0
1	B	853/883 (96%)	-0.01	18 (2%)	64 55	6, 44, 82, 112	0
All	All	1705/1766 (96%)	-0.02	39 (2%)	61 52	6, 45, 82, 112	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ASP	5.8
1	A	170	THR	4.8
1	A	190	ASP	4.4
1	B	174	LYS	3.6
1	A	229	ALA	3.5
1	A	206	VAL	3.5
1	B	213	GLN	3.2
1	B	212	ARG	3.1
1	B	175	LEU	3.1
1	A	193	LEU	3.1
1	A	194	ALA	3.0
1	B	1	MET	2.9
1	B	500	ASP	2.9
1	A	4	SER	2.8
1	A	150	ASN	2.8
1	A	43	THR	2.8
1	A	565	THR	2.6
1	A	230	LEU	2.5
1	A	208	ASN	2.5
1	B	490	GLU	2.5
1	B	4	SER	2.4
1	A	268	ASP	2.4
1	A	685	ASP	2.3
1	B	372	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	13	SER	2.3
1	A	480	ASN	2.2
1	B	41	ILE	2.2
1	B	478	ASP	2.2
1	A	169	LEU	2.2
1	B	210	ALA	2.2
1	A	231	LYS	2.1
1	B	43	THR	2.1
1	A	228	GLY	2.1
1	B	326	SER	2.1
1	A	180	LYS	2.1
1	B	229	ALA	2.0
1	B	42	ASN	2.0
1	A	146	GLU	2.0
1	B	176	PRO	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 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.