



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2016 – 05:45 AM EDT

PDB ID : 5EHK
Title : Crystal structure of tRNA dependent lantibiotic dehydratase MibB from Microbispora sp. 107891
Authors : Hao, Y.; Nair, S.K.
Deposited on : 2015-10-28
Resolution : 2.71 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

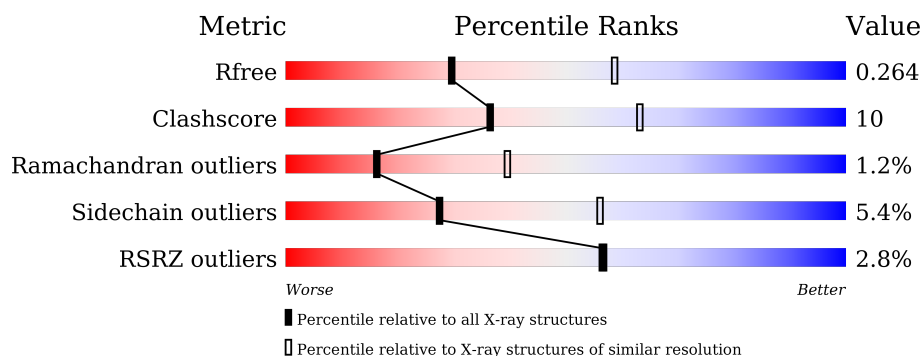
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	1115	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	B	1115	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16566 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 Lantibiotic dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1036	Total	C	N	O	S	0	0	0
			8044	5033	1533	1459	19			
1	B	1036	Total	C	N	O	S	0	0	0
			8044	5033	1533	1459	19			

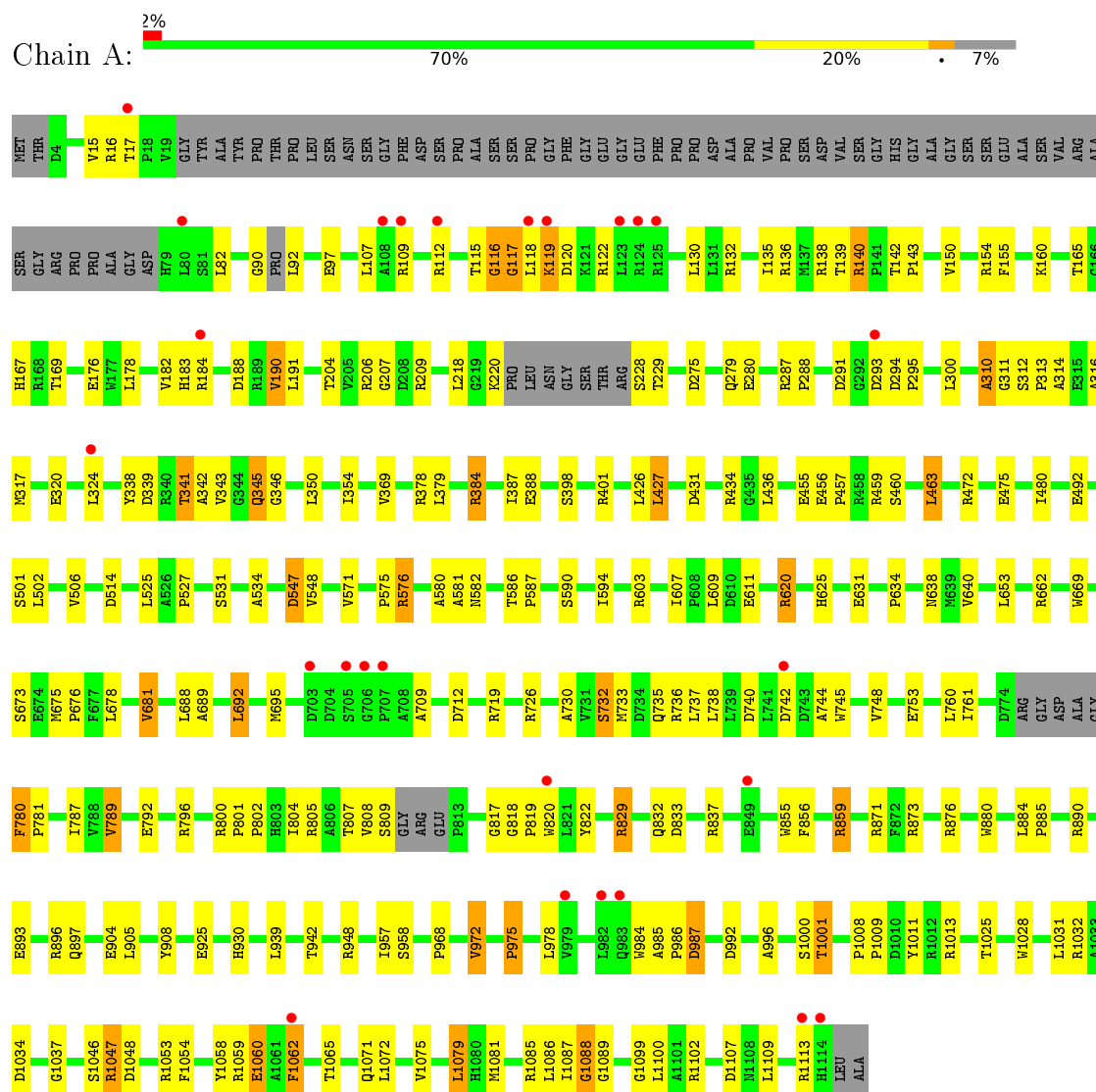
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	0
			230	230		
2	B	248	Total	O	0	0
			248	248		

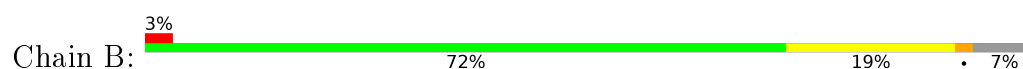
3 Residue-property plots

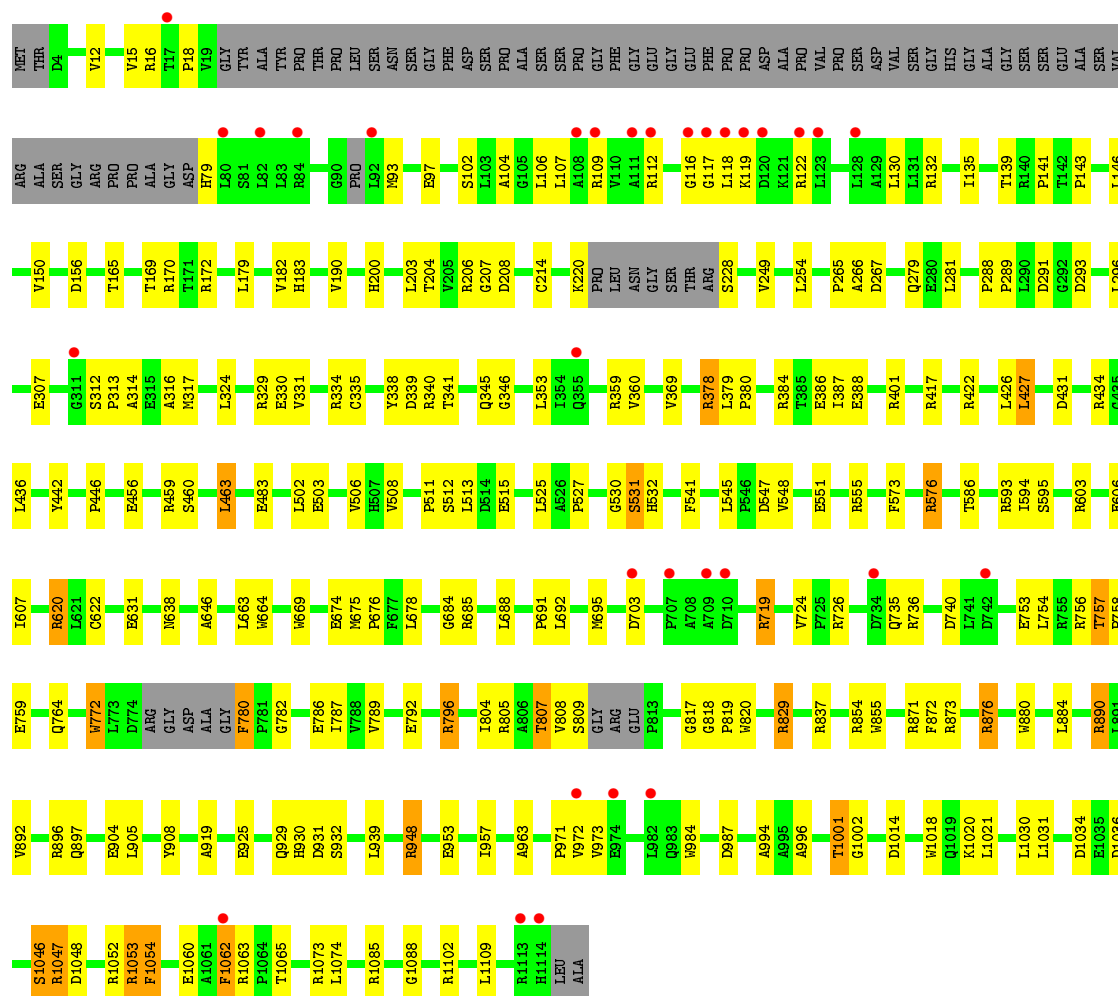
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Lantibiotic dehydratase



• Molecule 1: Lantibiotic dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.14Å 151.11Å 205.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 2.71 45.24 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.1 (45.24-2.71) 96.1 (45.24-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.264 0.202 , 0.264	Depositor DCC
R_{free} test set	3538 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 12.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 70222 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16566	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/8223	0.67	3/11182 (0.0%)
1	B	0.47	0/8223	0.67	0/11182
All	All	0.47	0/16446	0.67	3/22364 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	859	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	859	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	1089	GLY	N-CA-C	-5.29	99.88	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1088	GLY	Peptide
1	A	780	PHE	Peptide
1	B	780	PHE	Peptide

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	8044	0	8012	156	1
1	B	8044	0	8012	158	1
2	A	230	0	0	26	0
2	B	248	0	0	31	0
All	All	16566	0	16024	306	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 (306) 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:541:PHE:O	2:B:1201:HOH:O	1.80	0.98
1:B:808:VAL:O	2:B:1202:HOH:O	1.84	0.93
1:A:688:LEU:O	2:A:1201:HOH:O	1.86	0.93
1:B:220:LYS:O	2:B:1203:HOH:O	1.85	0.93
1:B:786:GLU:OE2	2:B:1204:HOH:O	1.85	0.93
1:A:287:ARG:NH1	2:A:1204:HOH:O	2.01	0.90
1:B:674:GLU:OE2	2:B:1205:HOH:O	1.88	0.90
1:A:809:SER:O	2:A:1202:HOH:O	1.91	0.87
1:A:859:ARG:NE	2:A:1203:HOH:O	2.04	0.85
1:A:119:LYS:HE2	1:A:122:ARG:HB2	1.58	0.84
1:A:832:GLN:OE1	2:A:1203:HOH:O	1.94	0.84
1:A:341:THR:HG22	2:A:1220:HOH:O	1.77	0.83
1:A:426:LEU:O	1:A:427:LEU:HB2	1.78	0.83
1:A:833:ASP:OD1	1:A:859:ARG:NH2	2.12	0.83
1:B:330:GLU:OE1	1:B:359:ARG:NH1	2.14	0.81
1:B:603:ARG:NH1	2:B:1208:HOH:O	2.14	0.80
1:A:132:ARG:NH1	1:A:753:GLU:OE1	2.16	0.79
1:A:807:THR:HG22	1:A:808:VAL:H	1.45	0.79
1:B:807:THR:HG22	1:B:808:VAL:H	1.49	0.76
1:B:156:ASP:OD2	1:B:378:ARG:NH1	2.19	0.76
1:A:582:ASN:OD1	2:A:1206:HOH:O	2.04	0.75
1:A:525:LEU:HD22	1:A:688:LEU:HA	1.69	0.75
1:A:792:GLU:OE2	2:A:1207:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:NH2	2:B:1215:HOH:O	2.20	0.74
1:B:334:ARG:HB2	1:B:353:LEU:HD13	1.69	0.74
1:A:220:LYS:O	2:A:1205:HOH:O	2.03	0.74
1:B:426:LEU:O	1:B:427:LEU:HB2	1.87	0.73
1:B:179:LEU:HA	1:B:182:VAL:HG22	1.71	0.73
1:B:593:ARG:NH1	2:B:1206:HOH:O	2.01	0.73
1:A:905:LEU:HB2	1:B:905:LEU:HB2	1.69	0.73
1:A:341:THR:HG21	1:A:346:GLY:HA3	1.72	0.71
1:A:1047:ARG:NH1	1:A:1048:ASP:OD1	2.25	0.70
1:B:132:ARG:NH1	1:B:753:GLU:OE1	2.23	0.70
1:A:116:GLY:O	1:A:118:LEU:N	2.23	0.69
1:A:871:ARG:NH2	1:A:925:GLU:OE1	2.26	0.69
1:B:379:LEU:HD11	1:B:787:ILE:HD13	1.76	0.68
1:B:329:ARG:NH2	2:B:1223:HOH:O	2.26	0.67
1:B:796:ARG:NH2	2:B:1221:HOH:O	2.26	0.67
1:A:732:SER:OG	1:A:733:MET:N	2.27	0.67
1:A:1001:THR:HG22	1:A:1102:ARG:HD3	1.76	0.67
1:B:1001:THR:O	2:B:1207:HOH:O	2.11	0.67
1:B:818:GLY:HA3	1:B:880:TRP:HE1	1.60	0.66
1:B:527:PRO:O	1:B:736:ARG:NH2	2.27	0.66
1:A:818:GLY:HA3	1:A:880:TRP:HE1	1.60	0.65
1:B:525:LEU:HD22	1:B:688:LEU:HA	1.77	0.65
1:B:719:ARG:HG3	1:B:724:VAL:HB	1.78	0.65
1:B:792:GLU:OE2	2:B:1209:HOH:O	2.14	0.64
1:A:280:GLU:HG2	1:A:287:ARG:HH12	1.63	0.64
1:A:460:SER:HB3	1:A:463:LEU:HB2	1.80	0.64
1:A:732:SER:HB3	1:A:735:GLN:NE2	2.13	0.64
1:B:206:ARG:NH2	1:B:431:ASP:OD1	2.31	0.63
1:A:930:HIS:ND1	1:A:1046:SER:OG	2.32	0.63
1:A:109:ARG:HA	1:A:112:ARG:HG2	1.82	0.62
1:A:228:SER:N	2:A:1226:HOH:O	2.32	0.62
1:A:819:PRO:HG2	1:A:820:TRP:CD1	2.34	0.62
1:B:460:SER:HB3	1:B:463:LEU:HB2	1.80	0.62
1:A:401:ARG:NH1	2:A:1229:HOH:O	2.33	0.61
1:B:214:CYS:HB3	1:B:576:ARG:HH21	1.64	0.61
1:B:819:PRO:HD2	2:B:1278:HOH:O	2.01	0.61
1:B:503:GLU:HB2	1:B:531:SER:HB3	1.81	0.61
1:A:379:LEU:HD11	1:A:787:ILE:HD13	1.82	0.60
1:A:859:ARG:NH1	1:A:1085:ARG:O	2.35	0.60
1:A:586:THR:HG21	1:A:638:ASN:HB3	1.84	0.60
1:A:167:HIS:HB2	1:A:343:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:GLU:OE2	1:A:459:ARG:NH2	2.26	0.59
1:A:896:ARG:O	1:B:434:ARG:NH2	2.35	0.59
1:A:506:VAL:HG12	1:A:525:LEU:HA	1.83	0.59
1:A:856:PHE:HE1	1:A:871:ARG:HE	1.49	0.59
1:A:475:GLU:OE2	2:A:1210:HOH:O	2.17	0.59
1:A:675:MET:HE3	1:A:676:PRO:HD2	1.84	0.59
1:B:135:ILE:O	1:B:139:THR:OG1	2.15	0.59
1:A:90:GLY:O	1:A:92:LEU:N	2.36	0.59
1:A:312:SER:O	1:A:314:ALA:N	2.29	0.58
1:A:893:GLU:HB3	2:A:1373:HOH:O	2.03	0.58
1:B:805:ARG:O	1:B:807:THR:OG1	2.22	0.58
1:B:228:SER:O	2:B:1211:HOH:O	2.18	0.57
1:A:726:ARG:HD2	1:A:742:ASP:HB2	1.85	0.57
1:A:829:ARG:NH1	1:A:1088:GLY:O	2.36	0.57
1:B:586:THR:HG21	1:B:638:ASN:HB3	1.85	0.57
1:B:871:ARG:NH2	1:B:925:GLU:OE1	2.38	0.57
1:B:511:PRO:HD3	1:B:772:TRP:CE2	2.39	0.57
1:B:109:ARG:HA	1:B:112:ARG:HG2	1.87	0.57
1:A:138:ARG:NH1	2:A:1237:HOH:O	2.38	0.57
1:A:527:PRO:O	1:A:736:ARG:NH2	2.34	0.57
1:A:16:ARG:HD3	1:A:143:PRO:HD3	1.87	0.56
1:B:735:GLN:HE22	1:B:757:THR:HG21	1.69	0.56
1:B:957:ILE:HD13	1:B:1031:LEU:HD11	1.88	0.56
1:B:829:ARG:NH1	1:B:1088:GLY:O	2.38	0.56
1:A:456:GLU:HG2	1:B:456:GLU:HG2	1.86	0.56
1:A:207:GLY:HA2	1:B:897:GLN:HB3	1.88	0.55
1:B:265:PRO:C	1:B:267:ASP:H	2.09	0.55
1:B:12:VAL:HG22	1:B:551:GLU:HG2	1.87	0.55
1:B:1047:ARG:NH1	1:B:1048:ASP:OD1	2.40	0.55
1:A:455:GLU:OE2	2:A:1211:HOH:O	2.18	0.54
1:A:695:MET:HE1	1:A:760:LEU:HD23	1.89	0.54
1:A:855:TRP:HA	1:A:871:ARG:O	2.06	0.54
1:B:203:LEU:O	2:B:1212:HOH:O	2.18	0.54
1:B:594:ILE:HG12	1:B:607:ILE:HG23	1.89	0.54
1:B:530:GLY:HA3	1:B:664:TRP:CZ2	2.43	0.54
1:A:978:LEU:HD21	1:A:1000:SER:HA	1.88	0.54
1:A:594:ILE:HG12	1:A:607:ILE:HG23	1.90	0.54
1:A:818:GLY:O	1:A:876:ARG:HG2	2.07	0.54
1:B:1021:LEU:O	2:B:1213:HOH:O	2.19	0.54
1:B:102:SER:CB	2:B:1230:HOH:O	2.55	0.53
1:B:1052:ARG:NH2	2:B:1242:HOH:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HG22	1:A:317:MET:H	1.73	0.53
1:A:829:ARG:NH2	2:A:1240:HOH:O	2.40	0.53
1:B:757:THR:O	1:B:757:THR:OG1	2.22	0.53
1:B:971:PRO:HG2	1:B:1062:PHE:CZ	2.43	0.53
1:B:417:ARG:NH1	2:B:1237:HOH:O	2.36	0.53
1:B:293:ASP:HB3	2:B:1348:HOH:O	2.09	0.53
1:A:434:ARG:NH2	2:A:1236:HOH:O	2.39	0.53
1:A:818:GLY:HA3	1:A:880:TRP:NE1	2.23	0.53
1:B:116:GLY:O	1:B:118:LEU:N	2.38	0.52
1:A:692:LEU:HD21	1:A:761:ILE:HD12	1.92	0.52
1:B:1002:GLY:HA3	1:B:1102:ARG:CZ	2.38	0.52
1:B:736:ARG:NH1	2:B:1249:HOH:O	2.43	0.52
1:A:136:ARG:HG2	1:A:140:ARG:HB3	1.90	0.52
1:B:169:THR:HG22	1:B:339:ASP:OD1	2.09	0.52
1:B:726:ARG:NH1	1:B:740:ASP:OD2	2.43	0.52
1:A:115:THR:O	1:A:117:GLY:N	2.42	0.52
1:A:968:PRO:O	1:A:1059:ARG:HD3	2.10	0.52
1:A:107:LEU:HD11	1:A:130:LEU:HD13	1.92	0.52
1:B:183:HIS:NE2	1:B:220:LYS:HE2	2.25	0.52
1:B:818:GLY:HA3	1:B:880:TRP:NE1	2.26	0.51
1:A:169:THR:HG22	1:A:339:ASP:OD1	2.10	0.51
1:A:837:ARG:HD3	1:A:939:LEU:O	2.11	0.51
1:A:620:ARG:NH2	1:A:631:GLU:OE2	2.43	0.51
1:B:307:GLU:OE2	2:B:1214:HOH:O	2.19	0.51
1:A:908:TYR:OH	2:A:1209:HOH:O	2.15	0.51
1:B:756:ARG:HG2	1:B:757:THR:HG22	1.93	0.51
1:A:342:ALA:HB3	1:A:345:GLN:HG3	1.93	0.51
1:A:1011:TYR:OH	1:A:1107:ASP:OD2	2.27	0.51
1:A:480:ILE:O	2:A:1212:HOH:O	2.19	0.50
1:A:1032:ARG:NH2	2:A:1238:HOH:O	2.39	0.50
1:B:527:PRO:HA	2:B:1271:HOH:O	2.10	0.50
1:B:620:ARG:NH2	1:B:631:GLU:OE2	2.44	0.50
1:B:179:LEU:HD23	1:B:182:VAL:HG21	1.94	0.50
1:A:972:VAL:HB	1:A:986:PRO:HG2	1.94	0.50
1:A:320:GLU:N	1:A:320:GLU:OE1	2.38	0.49
1:A:871:ARG:HH12	1:A:873:ARG:HB2	1.77	0.49
1:A:975:PRO:HB3	1:A:985:ALA:HB2	1.93	0.49
1:B:669:TRP:CD1	1:B:678:LEU:HD13	2.46	0.49
1:B:819:PRO:HG2	1:B:820:TRP:CD1	2.47	0.49
1:A:1075:VAL:O	1:A:1079:LEU:HD22	2.12	0.49
1:A:890:ARG:NH1	2:A:1213:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:TRP:HZ3	1:A:996:ALA:O	1.96	0.49
1:A:220:LYS:O	2:A:1214:HOH:O	2.20	0.49
1:B:1020:LYS:HE2	1:B:1030:LEU:HD12	1.94	0.49
1:B:15:VAL:O	1:B:150:VAL:HA	2.13	0.49
1:A:1009:PRO:O	1:A:1013:ARG:HG2	2.12	0.49
1:A:387:ILE:HD13	1:A:789:VAL:HG11	1.95	0.49
1:B:532:HIS:CE1	1:B:663:LEU:HB3	2.48	0.49
1:B:753:GLU:OE2	1:B:756:ARG:NH1	2.46	0.49
1:A:527:PRO:HG2	1:A:736:ARG:HE	1.77	0.48
1:B:172:ARG:NH1	2:B:1235:HOH:O	2.35	0.48
1:A:160:LYS:HB3	1:A:378:ARG:HB2	1.94	0.48
1:A:730:ALA:HB3	1:A:737:LEU:HB3	1.96	0.48
1:B:401:ARG:NH1	2:B:1252:HOH:O	2.45	0.48
1:A:992:ASP:OD1	1:A:1025:THR:OG1	2.25	0.48
1:B:1001:THR:CG2	1:B:1102:ARG:HE	2.26	0.48
1:A:958:SER:O	1:A:1047:ARG:NH2	2.47	0.48
1:A:293:ASP:HB2	1:A:603:ARG:NH2	2.29	0.47
1:B:170:ARG:HH11	1:B:170:ARG:HG2	1.78	0.47
1:B:508:VAL:O	1:B:782:GLY:HA3	2.14	0.47
1:A:82:LEU:HD22	1:A:745:TRP:CE2	2.49	0.47
1:B:214:CYS:HB3	1:B:576:ARG:NH2	2.28	0.47
1:B:736:ARG:HD3	2:B:1297:HOH:O	2.14	0.47
1:A:987:ASP:OD1	1:A:987:ASP:N	2.45	0.47
1:B:208:ASP:OD1	2:B:1217:HOH:O	2.20	0.47
1:A:434:ARG:NE	2:A:1236:HOH:O	2.37	0.47
1:B:312:SER:O	1:B:314:ALA:N	2.39	0.47
1:B:483:GLU:OE1	1:B:483:GLU:N	2.48	0.47
1:B:919:ALA:O	2:B:1216:HOH:O	2.20	0.47
1:A:800:ARG:HA	1:A:801:PRO:HD3	1.81	0.47
1:A:802:PRO:HB2	1:A:804:ILE:HG12	1.96	0.47
1:A:1001:THR:CG2	1:A:1102:ARG:HH11	2.28	0.46
1:A:457:PRO:HG2	1:B:459:ARG:NE	2.30	0.46
1:A:1008:PRO:HG3	1:A:1100:LEU:HD12	1.96	0.46
1:A:426:LEU:HD22	1:A:609:LEU:HD11	1.96	0.46
1:A:804:ILE:O	1:A:805:ARG:HG3	2.15	0.46
1:B:576:ARG:HA	1:B:576:ARG:HD3	1.67	0.46
1:A:287:ARG:HA	1:A:288:PRO:HD3	1.77	0.46
1:B:426:LEU:O	1:B:427:LEU:CB	2.62	0.46
1:B:818:GLY:HA2	2:B:1278:HOH:O	2.15	0.46
1:A:188:ASP:OD2	1:A:191:LEU:N	2.38	0.46
1:B:1054:PHE:CZ	1:B:1074:LEU:HD21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:TRP:CZ3	1:B:996:ALA:O	2.69	0.46
1:B:573:PHE:CZ	1:B:646:ALA:HB2	2.51	0.46
1:A:384:ARG:O	1:A:388:GLU:HG3	2.16	0.46
1:B:759:GLU:OE1	1:B:759:GLU:N	2.37	0.46
1:A:590:SER:O	2:A:1215:HOH:O	2.20	0.45
1:A:434:ARG:NH2	1:B:896:ARG:O	2.50	0.45
1:B:757:THR:HA	1:B:758:PRO:HD2	1.84	0.45
1:B:890:ARG:HA	1:B:890:ARG:HD2	1.78	0.45
1:A:154:ARG:HG2	1:A:155:PHE:O	2.17	0.45
1:B:512:SER:HA	1:B:780:PHE:CD2	2.51	0.45
1:A:780:PHE:HB2	2:A:1334:HOH:O	2.17	0.45
1:A:206:ARG:NH2	1:A:431:ASP:OD1	2.50	0.45
1:A:611:GLU:OE1	1:A:625:HIS:NE2	2.39	0.45
1:A:800:ARG:NH1	2:A:1244:HOH:O	2.42	0.45
1:A:807:THR:CG2	1:A:808:VAL:H	2.22	0.45
1:B:931:ASP:OD2	1:B:1085:ARG:HD2	2.17	0.45
1:B:146:LEU:HD11	1:B:338:TYR:OH	2.17	0.45
1:B:880:TRP:CE3	1:B:884:LEU:HD22	2.52	0.45
1:B:930:HIS:ND1	1:B:1046:SER:OG	2.49	0.45
1:B:324:LEU:HD11	1:B:360:VAL:HG13	1.99	0.45
1:A:398:SER:O	1:A:662:ARG:NH2	2.42	0.44
1:A:576:ARG:HA	1:A:576:ARG:HD3	1.79	0.44
1:A:634:PRO:HG2	1:A:653:LEU:O	2.18	0.44
1:A:669:TRP:CD1	1:A:678:LEU:HD13	2.52	0.44
1:A:506:VAL:HG12	1:A:525:LEU:HD12	1.99	0.44
1:A:586:THR:HG21	1:A:638:ASN:CB	2.47	0.44
1:B:530:GLY:HA3	1:B:664:TRP:HZ2	1.80	0.44
1:B:820:TRP:CD2	1:B:908:TYR:HD2	2.35	0.44
1:B:984:TRP:HZ3	1:B:996:ALA:O	2.00	0.44
1:B:296:LEU:HD21	1:B:331:VAL:HG23	1.99	0.44
1:B:97:GLU:HA	1:B:104:ALA:HB2	2.00	0.44
1:A:176:GLU:HG3	1:A:218:LEU:O	2.18	0.44
1:A:459:ARG:HB3	1:B:674:GLU:HG3	2.00	0.44
1:B:16:ARG:HD3	1:B:143:PRO:HD3	1.99	0.44
1:B:291:ASP:HA	2:B:1206:HOH:O	2.18	0.44
1:A:116:GLY:C	1:A:118:LEU:H	2.12	0.43
1:A:183:HIS:CE1	1:A:220:LYS:HE2	2.53	0.43
1:B:691:PRO:HG2	1:B:764:GLN:OE1	2.18	0.43
1:A:735:GLN:HE21	1:A:760:LEU:HD13	1.84	0.43
1:A:169:THR:HG21	1:A:338:TYR:CE2	2.53	0.43
1:B:341:THR:HG21	1:B:346:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:963:ALA:HB1	1:B:994:ALA:HA	2.01	0.43
1:A:1058:TYR:OH	1:A:1071:GLN:HB3	2.18	0.43
1:B:1063:ARG:HB2	1:B:1065:THR:HG22	2.00	0.43
1:B:855:TRP:CH2	1:B:932:SER:HB3	2.53	0.43
1:B:622:CYS:HB2	1:B:631:GLU:OE1	2.19	0.43
1:B:871:ARG:HH12	1:B:873:ARG:HB2	1.83	0.43
1:A:1028:TRP:O	1:A:1032:ARG:HG3	2.18	0.43
1:A:1008:PRO:HD3	1:A:1099:GLY:HA3	2.00	0.43
1:B:170:ARG:HD2	1:B:172:ARG:NE	2.34	0.43
1:B:675:MET:HE3	1:B:676:PRO:HD2	2.01	0.43
1:B:200:HIS:HB3	1:B:203:LEU:HG	2.01	0.43
1:B:818:GLY:O	1:B:876:ARG:HG3	2.18	0.43
1:A:169:THR:HG23	1:A:369:VAL:HG13	2.00	0.43
1:B:249:VAL:HG21	1:B:254:LEU:HD13	2.01	0.42
1:A:547:ASP:OD1	1:A:547:ASP:N	2.30	0.42
1:A:291:ASP:O	1:A:587:PRO:HA	2.19	0.42
1:B:386:GLU:CD	1:B:685:ARG:HB2	2.39	0.42
1:B:871:ARG:HG2	1:B:872:PHE:N	2.35	0.42
1:B:1001:THR:HG22	1:B:1102:ARG:HE	1.85	0.42
1:A:1059:ARG:O	1:A:1062:PHE:HD2	2.02	0.42
1:A:275:ASP:O	1:A:279:GLN:HG3	2.19	0.42
1:B:18:PRO:HD3	1:B:141:PRO:HA	2.01	0.42
1:B:595:SER:OG	1:B:606:GLU:OE1	2.34	0.42
1:A:897:GLN:HB3	1:B:207:GLY:HA2	2.01	0.42
1:A:1081:MET:HE2	1:A:1081:MET:HA	2.02	0.42
1:A:167:HIS:HB2	1:A:343:VAL:CG2	2.48	0.42
1:B:620:ARG:NH2	1:B:631:GLU:OE1	2.52	0.42
1:B:854:ARG:HA	1:B:929:GLN:OE1	2.19	0.42
1:B:837:ARG:HD3	1:B:939:LEU:O	2.19	0.42
1:B:948:ARG:HB3	1:B:948:ARG:HE	1.52	0.42
1:A:1001:THR:HG23	1:A:1102:ARG:HH11	1.85	0.42
1:B:1034:ASP:OD1	1:B:1036:ASP:N	2.52	0.42
1:B:506:VAL:HG12	1:B:525:LEU:HD12	2.01	0.42
1:B:854:ARG:HD3	1:B:929:GLN:OE1	2.20	0.42
1:B:551:GLU:O	1:B:555:ARG:HG2	2.19	0.42
1:A:15:VAL:O	1:A:150:VAL:HA	2.20	0.42
1:A:188:ASP:OD2	1:A:190:VAL:HG13	2.20	0.42
1:A:312:SER:C	1:A:314:ALA:H	2.17	0.42
1:A:350:LEU:O	1:A:354:ILE:HG12	2.20	0.42
1:A:744:ALA:O	1:A:748:VAL:HG13	2.20	0.42
1:A:501:SER:HB2	1:A:534:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:CYS:SG	1:B:353:LEU:HD21	2.60	0.41
1:B:106:LEU:HD12	1:B:122:ARG:NE	2.34	0.41
1:B:953:GLU:HG2	1:B:1018:TRP:HZ3	1.85	0.41
1:A:1034:ASP:HB3	1:A:1037:GLY:H	1.85	0.41
1:A:178:LEU:O	1:A:182:VAL:HG23	2.20	0.41
1:A:294:ASP:HA	1:A:295:PRO:HD2	1.90	0.41
1:A:184:ARG:CZ	1:A:324:LEU:HD22	2.49	0.41
1:A:709:ALA:HA	1:A:712:ASP:HB2	2.01	0.41
1:B:107:LEU:HD11	1:B:130:LEU:HD13	2.02	0.41
1:B:545:LEU:HB3	1:B:548:VAL:HG13	2.01	0.41
1:A:957:ILE:HD13	1:A:1031:LEU:HD11	2.03	0.41
1:B:93:MET:SD	1:B:107:LEU:HD13	2.61	0.41
1:A:884:LEU:HB3	1:A:885:PRO:HD3	2.02	0.41
1:B:317:MET:HE3	2:B:1214:HOH:O	2.19	0.41
1:A:140:ARG:HG3	1:A:142:THR:H	1.86	0.41
1:B:279:GLN:HB2	1:B:281:LEU:HD13	2.02	0.41
1:B:384:ARG:O	1:B:388:GLU:HG3	2.19	0.41
1:B:422:ARG:NH2	1:B:809:SER:HB2	2.36	0.41
1:A:580:ALA:HB1	1:A:640:VAL:HG13	2.03	0.41
1:B:512:SER:OG	1:B:515:GLU:HG3	2.21	0.41
1:B:97:GLU:HG2	1:B:104:ALA:HB1	2.02	0.41
1:B:169:THR:HG23	1:B:369:VAL:HG13	2.03	0.41
1:B:434:ARG:HD2	1:B:434:ARG:HH11	1.72	0.41
1:B:12:VAL:CG2	1:B:551:GLU:HG2	2.50	0.41
1:A:310:ALA:HB3	1:A:316:ALA:HB2	2.02	0.40
1:A:681:VAL:HG13	1:A:689:ALA:HB3	2.03	0.40
1:B:379:LEU:HA	1:B:380:PRO:HD3	1.89	0.40
1:A:135:ILE:O	1:A:139:THR:OG1	2.34	0.40
1:A:575:PRO:HG2	1:A:581:ALA:HA	2.03	0.40
1:B:288:PRO:HA	1:B:289:PRO:HD2	1.89	0.40
1:B:620:ARG:HH22	1:B:631:GLU:CD	2.25	0.40
1:B:695:MET:CE	1:B:754:LEU:HD13	2.52	0.40
1:A:726:ARG:NH1	1:A:740:ASP:OD1	2.54	0.40
1:A:871:ARG:NH1	1:A:873:ARG:HB2	2.37	0.40
1:B:387:ILE:HD13	1:B:789:VAL:HG11	2.03	0.40
1:B:442:TYR:O	1:B:446:PRO:HA	2.21	0.40
1:B:804:ILE:O	1:B:805:ARG:HG3	2.21	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:A:1060:GLU:OE2	1:B:1053:ARG:NH2[4_445]	2.18	0.02

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	1024/1115 (92%)	963 (94%)	50 (5%)	11 (1%)	17	42
1	B	1024/1115 (92%)	963 (94%)	48 (5%)	13 (1%)	15	37
All	All	2048/2230 (92%)	1926 (94%)	98 (5%)	24 (1%)	16	39

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY
1	A	427	LEU
1	A	1113	ARG
1	B	427	LEU
1	B	684	GLY
1	A	117	GLY
1	A	119	LYS
1	B	972	VAL
1	B	973	VAL
1	A	311	GLY
1	A	313	PRO
1	B	266	ALA
1	A	310	ALA
1	B	313	PRO
1	B	772	TRP
1	B	117	GLY
1	B	119	LYS
1	B	316	ALA
1	B	703	ASP
1	B	1014	ASP

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Mol	Chain	Res	Type
1	A	817	GLY
1	A	781	PRO
1	A	1087	ILE
1	B	817	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	812/868 (94%)	760 (94%)	52 (6%)	22	47
1	B	812/868 (94%)	777 (96%)	35 (4%)	35	66
All	All	1624/1736 (94%)	1537 (95%)	87 (5%)	27	56

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	97	GLU
1	A	120	ASP
1	A	140	ARG
1	A	165	THR
1	A	190	VAL
1	A	204	THR
1	A	209	ARG
1	A	229	THR
1	A	300	LEU
1	A	341	THR
1	A	345	GLN
1	A	384	ARG
1	A	436	LEU
1	A	463	LEU
1	A	472	ARG
1	A	492	GLU
1	A	502	LEU
1	A	514	ASP

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Mol	Chain	Res	Type
1	A	531	SER
1	A	547	ASP
1	A	548	VAL
1	A	571	VAL
1	A	576	ARG
1	A	620	ARG
1	A	673	SER
1	A	681	VAL
1	A	692	LEU
1	A	719	ARG
1	A	732	SER
1	A	738	LEU
1	A	789	VAL
1	A	796	ARG
1	A	822	TYR
1	A	829	ARG
1	A	904	GLU
1	A	942	THR
1	A	948	ARG
1	A	972	VAL
1	A	975	PRO
1	A	987	ASP
1	A	1001	THR
1	A	1047	ARG
1	A	1053	ARG
1	A	1054	PHE
1	A	1060	GLU
1	A	1062	PHE
1	A	1065	THR
1	A	1072	LEU
1	A	1079	LEU
1	A	1086	LEU
1	A	1109	LEU
1	B	79	HIS
1	B	165	THR
1	B	190	VAL
1	B	204	THR
1	B	345	GLN
1	B	378	ARG
1	B	436	LEU
1	B	463	LEU
1	B	502	LEU

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Mol	Chain	Res	Type
1	B	513	LEU
1	B	531	SER
1	B	547	ASP
1	B	576	ARG
1	B	620	ARG
1	B	692	LEU
1	B	719	ARG
1	B	757	THR
1	B	796	ARG
1	B	807	THR
1	B	829	ARG
1	B	876	ARG
1	B	890	ARG
1	B	892	VAL
1	B	904	GLU
1	B	948	ARG
1	B	987	ASP
1	B	1001	THR
1	B	1046	SER
1	B	1047	ARG
1	B	1053	ARG
1	B	1054	PHE
1	B	1060	GLU
1	B	1062	PHE
1	B	1073	ARG
1	B	1109	LEU

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

Mol	Chain	Res	Type
1	A	183	HIS
1	A	832	GLN
1	A	1019	GLN
1	A	1080	HIS

5.3.3 RNA ⓘ

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	1036/1115 (92%)	-0.10	26 (2%) 61 61	6, 32, 68, 108	0
1	B	1036/1115 (92%)	-0.11	31 (2%) 54 54	6, 31, 74, 106	0
All	All	2072/2230 (92%)	-0.10	57 (2%) 56 57	6, 32, 71, 108	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1114	HIS	9.0
1	B	118	LEU	7.9
1	A	707	PRO	5.6
1	B	742	ASP	5.5
1	A	1113	ARG	5.0
1	B	703	ASP	4.4
1	B	1114	HIS	4.4
1	A	118	LEU	4.2
1	B	116	GLY	4.0
1	A	124	ARG	4.0
1	A	123	LEU	3.8
1	B	128	LEU	3.7
1	B	311	GLY	3.6
1	A	982	LEU	3.4
1	A	119	LYS	3.3
1	A	112	ARG	3.1
1	B	82	LEU	3.1
1	A	705	SER	3.1
1	B	80	LEU	3.1
1	B	111	ALA	3.0
1	A	706	GLY	3.0
1	B	707	PRO	2.9
1	B	709	ALA	2.9
1	A	703	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	119	LYS	2.9
1	A	742	ASP	2.9
1	B	120	ASP	2.9
1	B	123	LEU	2.8
1	B	117	GLY	2.8
1	B	974	GLU	2.7
1	B	84	ARG	2.7
1	B	355	GLN	2.7
1	B	1113	ARG	2.7
1	B	112	ARG	2.5
1	A	820	TRP	2.5
1	B	710	ASP	2.4
1	B	734	ASP	2.4
1	B	972	VAL	2.4
1	A	293	ASP	2.4
1	A	979	VAL	2.4
1	B	1062	PHE	2.3
1	B	108	ALA	2.2
1	B	17	THR	2.2
1	A	125	ARG	2.2
1	A	108	ALA	2.1
1	A	849	GLU	2.1
1	A	80	LEU	2.1
1	A	1062	PHE	2.1
1	A	324	LEU	2.1
1	A	184	ARG	2.1
1	A	109	ARG	2.1
1	A	983	GLN	2.0
1	A	17	THR	2.0
1	B	982	LEU	2.0
1	B	122	ARG	2.0
1	B	92	LEU	2.0
1	B	109	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.