



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:06 PM UTC

PDB ID : 5EHK / pdb_00005ehk
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

<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

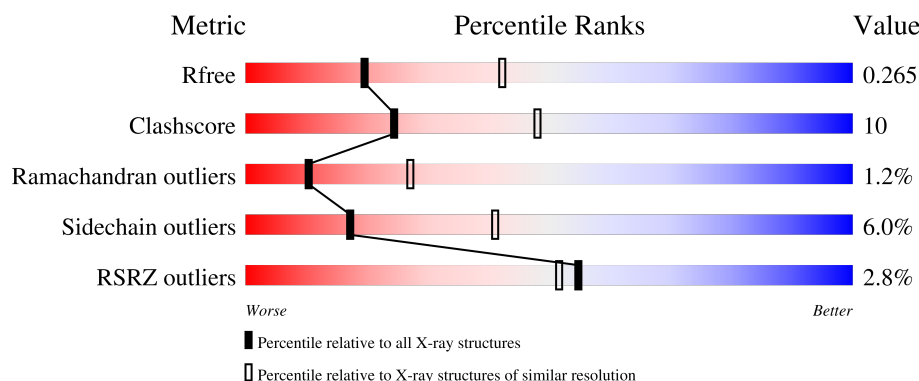
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

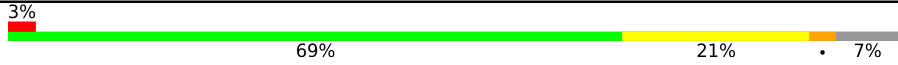
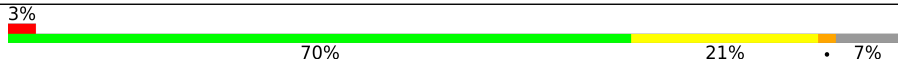
The reported resolution of this entry is 2.71 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	1115	
1	B	1115	

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			

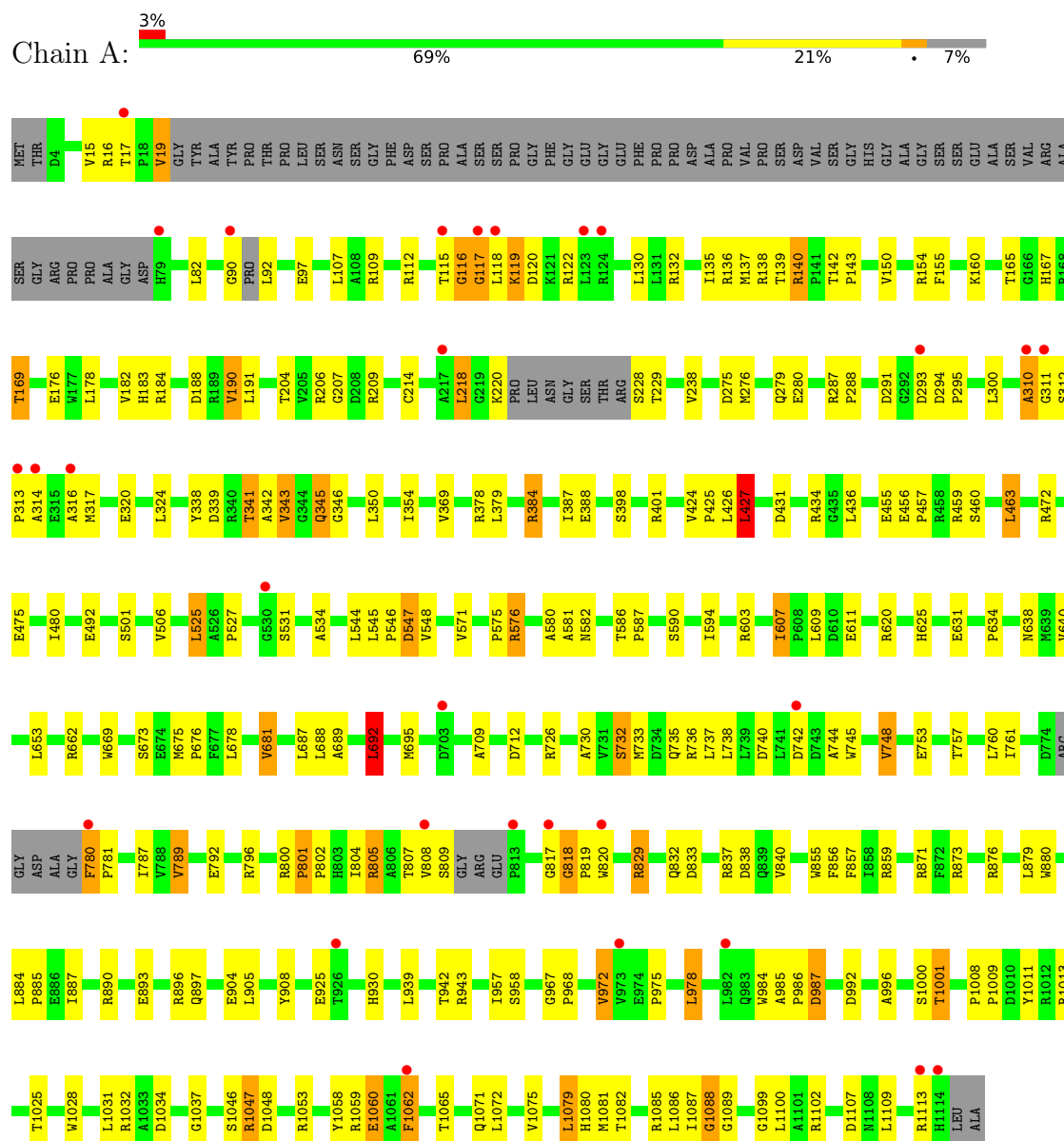
- Molecule 2 is water.

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

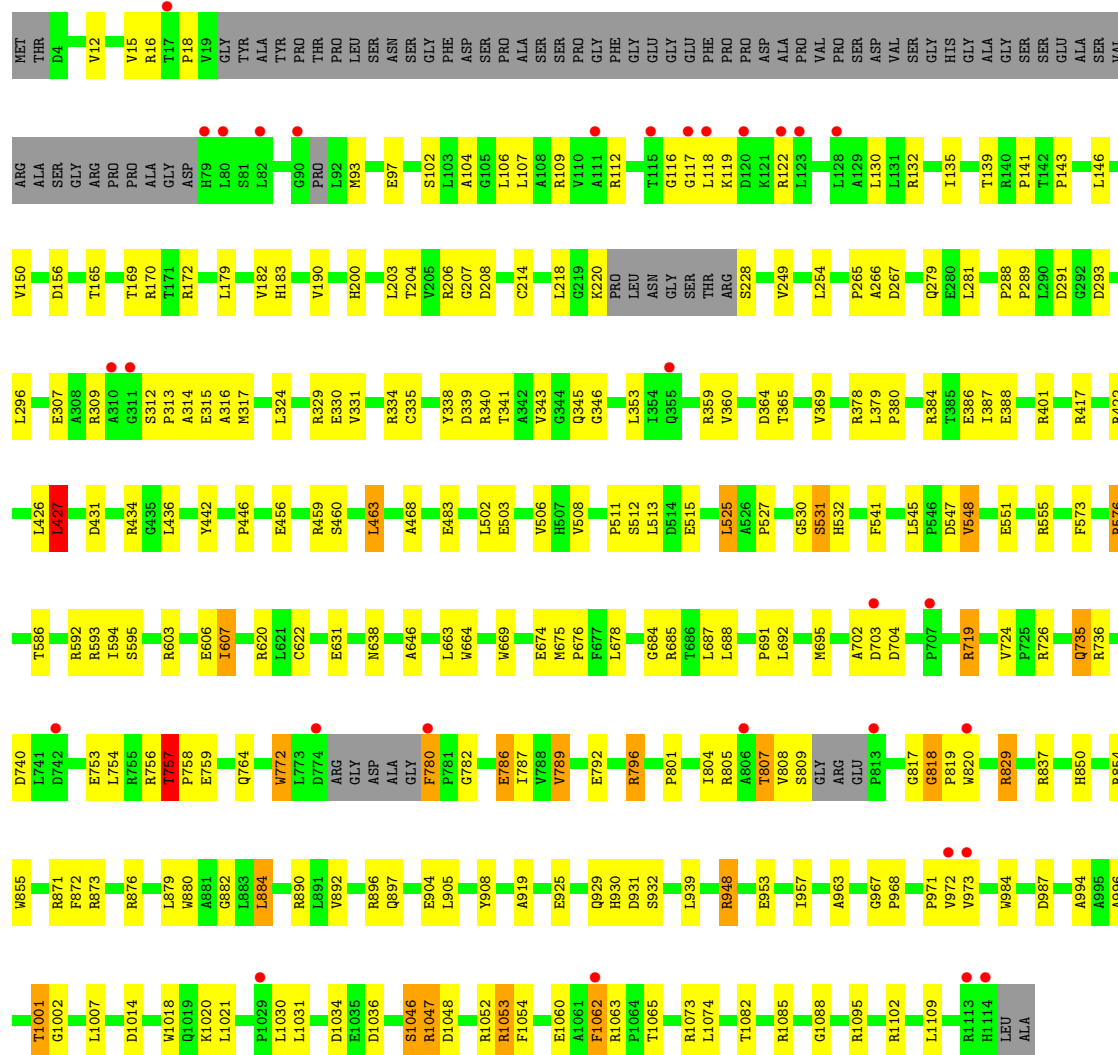
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 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 1.8.2_1309	Depositor
R, R_{free}	0.204 , 0.264 0.207 , 0.265	Depositor DCC
R_{free} test set	3537 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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	0.60	1/8223 (0.0%)	0.98	14/11182 (0.1%)
1	B	0.62	0/8223	0.97	15/11182 (0.1%)
All	All	0.61	1/16446 (0.0%)	0.98	29/22364 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	VAL	CA-C	5.55	1.57	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1089	GLY	N-CA-C	-10.49	99.88	115.72
1	A	757	THR	CA-C-N	7.62	127.66	119.28
1	A	757	THR	C-N-CA	7.62	127.66	119.28
1	A	967	GLY	CA-C-N	7.53	125.16	119.66
1	A	967	GLY	C-N-CA	7.53	125.16	119.66
1	B	884	LEU	CA-C-N	-7.46	112.11	119.64
1	B	884	LEU	C-N-CA	-7.46	112.11	119.64
1	B	309	ARG	N-CA-C	-6.61	105.84	114.04
1	A	801	PRO	O-C-N	6.41	124.16	121.15
1	B	818	GLY	N-CA-C	6.02	124.62	112.34
1	B	967	GLY	CA-C-N	5.98	124.02	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	967	GLY	C-N-CA	5.98	124.02	119.66
1	A	818	GLY	N-CA-C	5.96	124.49	112.34
1	B	218	LEU	N-CA-C	5.84	117.32	111.07
1	B	757	THR	CA-C-N	5.78	126.18	119.47
1	B	757	THR	C-N-CA	5.78	126.18	119.47
1	A	545	LEU	CA-C-N	5.72	125.84	119.32
1	A	545	LEU	C-N-CA	5.72	125.84	119.32
1	B	801	PRO	O-C-N	5.68	123.92	121.31
1	B	364	ASP	N-CA-C	5.59	117.37	111.28
1	A	805	ARG	N-CA-C	-5.47	104.87	112.03
1	A	218	LEU	N-CA-C	5.40	116.85	111.07
1	A	214	CYS	CA-C-N	-5.40	115.02	120.31
1	A	214	CYS	C-N-CA	-5.40	115.02	120.31
1	B	735	GLN	N-CA-C	5.28	118.06	109.24
1	B	968	PRO	O-C-N	5.22	123.71	121.31
1	A	692	LEU	N-CA-C	5.17	116.84	108.26
1	B	1082	THR	N-CA-C	-5.14	105.75	111.36
1	B	592	ARG	N-CA-C	5.01	117.00	109.23

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 [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	8044	0	8012	164	1
1	B	8044	0	8012	162	1
2	A	230	0	0	26	0
2	B	248	0	0	30	0
All	All	16566	0	16024	317	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 (317) 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
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:A:905:LEU:HB2	1:B:905:LEU:HB2	1.69	0.73
1:B:593:ARG:NH1	2:B:1206:HOH:O	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:135:ILE:O	1:B:139:THR:OG1	2.15	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:265:PRO:C	1:B:267:ASP:H	2.09	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
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:1081:MET:HA	1:A:1081:MET:HE2	1.83	0.59
1:A:475:GLU:OE2	2:A:1210:HOH:O	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:116:GLY:C	1:A:118:LEU:H	2.12	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:A:456:GLU:HG2	1:B:456:GLU:HG2	1.86	0.56
1:B:829:ARG:NH1	1:B:1088:GLY:O	2.38	0.56
1:A:207:GLY:HA2	1:B:897:GLN:HB3	1.88	0.55
1:B:12:VAL:HG22	1:B:551:GLU:HG2	1.87	0.55
1:A:1080:HIS:CD2	1:A:1081:MET:HE3	2.41	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: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
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:A:695:MET:HE1	1:A:760:LEU:HD23	1.91	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:A:19:VAL:HG21	1:A:137:MET:HE2	1.92	0.52
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:736:ARG:NH1	2:B:1249:HOH:O	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1002:GLY:HA3	1:B:1102:ARG:CZ	2.38	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:107:LEU:HD11	1:A:130:LEU:HD13	1.92	0.52
1:A:968:PRO:O	1:A:1059:ARG:HD3	2.10	0.52
1:B:183:HIS:NE2	1:B:220:LYS:HE2	2.25	0.52
1:A:675:MET:HE3	1:A:676:PRO:HD2	1.91	0.51
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:OE1	1:A:320:GLU:N	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:A:312:SER:C	1:A:314:ALA:H	2.17	0.49
1:A:675:MET:HE1	1:B:468:ALA:HB2	1.93	0.49
1:B:669:TRP:CD1	1:B:678:LEU:HD13	2.46	0.49
1:B:675:MET:HE3	1:B:676:PRO:HD2	1.94	0.49
1:B:819:PRO:HG2	1:B:820:TRP:CD1	2.47	0.49
1:A:890:ARG:NH1	2:A:1213:HOH:O	2.20	0.49
1:A:984:TRP:HZ3	1:A:996:ALA:O	1.96	0.49
1:A:1075:VAL:O	1:A:1079:LEU:HD22	2.12	0.49
1:A:220:LYS:O	2:A:1214:HOH:O	2.20	0.49
1:B:15:VAL:O	1:B:150:VAL:HA	2.13	0.49
1:B:1020:LYS:HE2	1:B:1030:LEU:HD12	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:B:170:ARG:HH11	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:386:GLU:CD	1:B:685:ARG:HB2	2.39	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:A:434:ARG:NE	2:A:1236:HOH:O	2.37	0.47
1:B:208:ASP:OD1	2:B:1217:HOH:O	2.20	0.47
1:B:312:SER:O	1:B:314:ALA:N	2.39	0.47
1:B:483:GLU:N	1:B:483:GLU:OE1	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:457:PRO:HG2	1:B:459:ARG:NE	2.30	0.46
1:A:1001:THR:CG2	1:A:1102:ARG:HH11	2.28	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:A:1008:PRO:HG3	1:A:1100:LEU:HD12	1.96	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:984:TRP:CZ3	1:B:996:ALA:O	2.69	0.46
1:B:1054:PHE:CZ	1:B:1074:LEU:HD21	2.50	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:434:ARG:NH2	1:B:896:ARG:O	2.50	0.45
1:A:590:SER:O	2:A:1215:HOH:O	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:620:ARG:HH22	1:B:631:GLU:CD	2.25	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: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:931:ASP:OD2	1:B:1085:ARG:HD2	2.17	0.45
1:B:324:LEU:HD11	1:B:360:VAL:HG13	1.99	0.45
1:A:238:VAL:HG22	1:A:276:MET:HE3	1.99	0.44
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:97:GLU:HA	1:B:104:ALA:HB2	2.00	0.44
1:B:296:LEU:HD21	1:B:331:VAL:HG23	1.99	0.44
1:A:838:ASP:CG	1:A:943:ARG:HH22	2.26	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: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:B:265:PRO:C	1:B:267:ASP:N	2.75	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
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:855:TRP:CH2	1:B:932:SER:HB3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1063:ARG:HB2	1:B:1065:THR:HG22	2.00	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:1008:PRO:HD3	1:A:1099:GLY:HA3	2.00	0.43
1:A:1028:TRP:O	1:A:1032:ARG:HG3	2.18	0.43
1:B:170:ARG:HD2	1:B:172:ARG:NE	2.34	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:291:ASP:O	1:A:587:PRO:HA	2.19	0.42
1:A:547:ASP:OD1	1:A:547:ASP:N	2.30	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:275:ASP:O	1:A:279:GLN:HG3	2.19	0.42
1:A:1059:ARG:O	1:A:1062:PHE:HD2	2.02	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: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:837:ARG:HD3	1:B:939:LEU:O	2.19	0.42
1:B:850:HIS:CE1	1:B:882:GLY:C	2.97	0.42
1:B:854:ARG:HA	1:B:929:GLN:OE1	2.19	0.42
1:B:948:ARG:HE	1:B:948:ARG:HB3	1.52	0.42
1:A:1001:THR:HG23	1:A:1102:ARG:HH11	1.85	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:1034:ASP:OD1	1:B:1036:ASP:N	2.52	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: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
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:178:LEU:O	1:A:182:VAL:HG23	2.20	0.41
1:A:184:ARG:CZ	1:A:324:LEU:HD22	2.49	0.41
1:A:294:ASP:HA	1:A:295:PRO:HD2	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ALA:HA	1:A:712:ASP:HB2	2.01	0.41
1:A:857:PHE:CD1	1:A:857:PHE:C	2.98	0.41
1:A:1034:ASP:HB3	1:A:1037:GLY:H	1.85	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:A:140:ARG:HG3	1:A:142:THR:H	1.86	0.41
1:A:580:ALA:HB1	1:A:640:VAL:HG13	2.03	0.41
1:B:279:GLN:HB2	1:B:281:LEU:HD13	2.02	0.41
1:B:315:GLU:C	1:B:317:MET:H	2.29	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:B:512:SER:OG	1:B:515:GLU:HG3	2.21	0.41
1:B:12:VAL:CG2	1:B:551:GLU:HG2	2.50	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:HH11	1:B:434:ARG:HD2	1.72	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:B:702:ALA:C	1:B:704:ASP:H	2.30	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: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:424:VAL:O	1:A:425:PRO:C	2.61	0.40
1:A:544:LEU:C	1:A:546:PRO:HD3	2.46	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

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	1024/1115 (92%)	963 (94%)	50 (5%)	11 (1%)	11	29
1	B	1024/1115 (92%)	963 (94%)	48 (5%)	13 (1%)	9	25
All	All	2048/2230 (92%)	1926 (94%)	98 (5%)	24 (1%)	10	27

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
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%)	756 (93%)	56 (7%)	14	34
1	B	812/868 (94%)	771 (95%)	41 (5%)	22	48
All	All	1624/1736 (94%)	1527 (94%)	97 (6%)	17	41

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	19	VAL
1	A	97	GLU
1	A	120	ASP
1	A	140	ARG
1	A	165	THR
1	A	169	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	343	VAL
1	A	345	GLN
1	A	384	ARG
1	A	427	LEU
1	A	436	LEU
1	A	463	LEU
1	A	472	ARG
1	A	492	GLU
1	A	525	LEU
1	A	531	SER
1	A	547	ASP
1	A	548	VAL
1	A	571	VAL
1	A	576	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	607	ILE
1	A	673	SER
1	A	681	VAL
1	A	687	LEU
1	A	692	LEU
1	A	732	SER
1	A	738	LEU
1	A	748	VAL
1	A	789	VAL
1	A	796	ARG
1	A	829	ARG
1	A	879	LEU
1	A	887	ILE
1	A	904	GLU
1	A	942	THR
1	A	972	VAL
1	A	978	LEU
1	A	987	ASP
1	A	1001	THR
1	A	1047	ARG
1	A	1053	ARG
1	A	1060	GLU
1	A	1062	PHE
1	A	1065	THR
1	A	1072	LEU
1	A	1079	LEU
1	A	1082	THR
1	A	1086	LEU
1	A	1109	LEU
1	B	165	THR
1	B	190	VAL
1	B	204	THR
1	B	343	VAL
1	B	345	GLN
1	B	365	THR
1	B	427	LEU
1	B	436	LEU
1	B	463	LEU
1	B	502	LEU
1	B	513	LEU
1	B	525	LEU
1	B	531	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	547	ASP
1	B	548	VAL
1	B	576	ARG
1	B	607	ILE
1	B	687	LEU
1	B	692	LEU
1	B	719	ARG
1	B	757	THR
1	B	786	GLU
1	B	789	VAL
1	B	796	ARG
1	B	807	THR
1	B	829	ARG
1	B	879	LEU
1	B	892	VAL
1	B	904	GLU
1	B	948	ARG
1	B	987	ASP
1	B	1001	THR
1	B	1007	LEU
1	B	1046	SER
1	B	1047	ARG
1	B	1053	ARG
1	B	1060	GLU
1	B	1062	PHE
1	B	1073	ARG
1	B	1095	ARG
1	B	1109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	645	GLN
1	A	832	GLN
1	B	763	GLN

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 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	1036/1115 (92%)	-0.11	29 (2%) 55 51	6, 32, 68, 108	0
1	B	1036/1115 (92%)	-0.08	30 (2%) 53 50	6, 31, 74, 106	0
All	All	2072/2230 (92%)	-0.10	59 (2%) 55 51	6, 32, 71, 108	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	973	VAL	4.1
1	A	780	PHE	3.9
1	A	310	ALA	3.8
1	B	742	ASP	3.8
1	A	79	HIS	3.7
1	B	118	LEU	3.7
1	B	703	ASP	3.6
1	B	79	HIS	3.6
1	B	82	LEU	3.4
1	B	123	LEU	3.4
1	A	313	PRO	3.3
1	A	820	TRP	3.1
1	B	1114	HIS	3.1
1	A	115	THR	3.1
1	B	1062	PHE	3.0
1	A	1114	HIS	3.0
1	A	742	ASP	3.0
1	B	111	ALA	3.0
1	B	1113	ARG	2.9
1	B	90	GLY	2.9
1	A	17	THR	2.9
1	A	118	LEU	2.9
1	A	123	LEU	2.9
1	B	707	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	17	THR	2.9
1	B	310	ALA	2.8
1	B	80	LEU	2.7
1	A	217	ALA	2.7
1	B	780	PHE	2.7
1	A	90	GLY	2.7
1	A	293	ASP	2.7
1	B	806	ALA	2.6
1	B	128	LEU	2.5
1	B	774	ASP	2.5
1	B	311	GLY	2.5
1	A	973	VAL	2.4
1	A	311	GLY	2.4
1	A	124	ARG	2.4
1	A	817	GLY	2.3
1	A	316	ALA	2.3
1	B	117	GLY	2.3
1	A	813	PRO	2.3
1	B	122	ARG	2.2
1	B	1029	PRO	2.2
1	B	972	VAL	2.2
1	B	115	THR	2.2
1	A	314	ALA	2.2
1	A	982	LEU	2.1
1	A	1113	ARG	2.1
1	B	813	PRO	2.1
1	A	117	GLY	2.1
1	A	530	GLY	2.1
1	A	1062	PHE	2.1
1	A	926	THR	2.1
1	B	355	GLN	2.1
1	A	808	VAL	2.1
1	A	703	ASP	2.0
1	B	120	ASP	2.0
1	B	820	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.