



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:44 PM EDT

PDB ID : 4F1N / pdb_00004f1n
Title : Crystal structure of Kluyveromyces polysporus Argonaute with a guide RNA
Authors : Nakanishi, K.; Weinberg, D.E.; Bartel, D.P.; Patel, D.J.
Deposited on : 2012-05-07
Resolution : 3.19 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

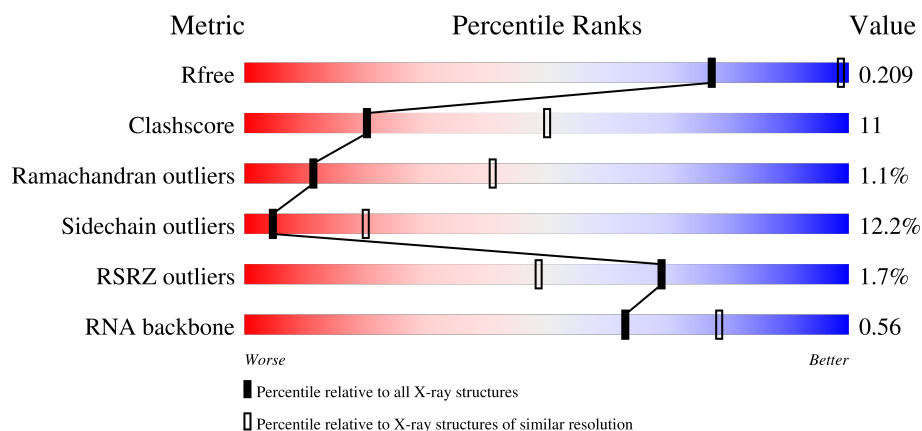
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)
RNA backbone	3983	1138 (3.46-2.90)

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	1046	2% 57% 24% 5% 14%
1	B	1046	% 54% 23% • 18%
2	E	9	44% 44% 11%
2	F	9	44% 44% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14426 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 KpAGO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	904	Total	C	N	O	S	0	0	0
			7225	4633	1201	1359	32			
1	B	853	Total	C	N	O	S	0	0	0
			6809	4372	1127	1280	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	SER	-	expression tag	UNP A7TMA9
B	206	SER	-	expression tag	UNP A7TMA9

- Molecule 2 is a RNA chain called RNA 5'-R(P*UP*AP*AP*AP*AP*AP*AP*A)-3'.

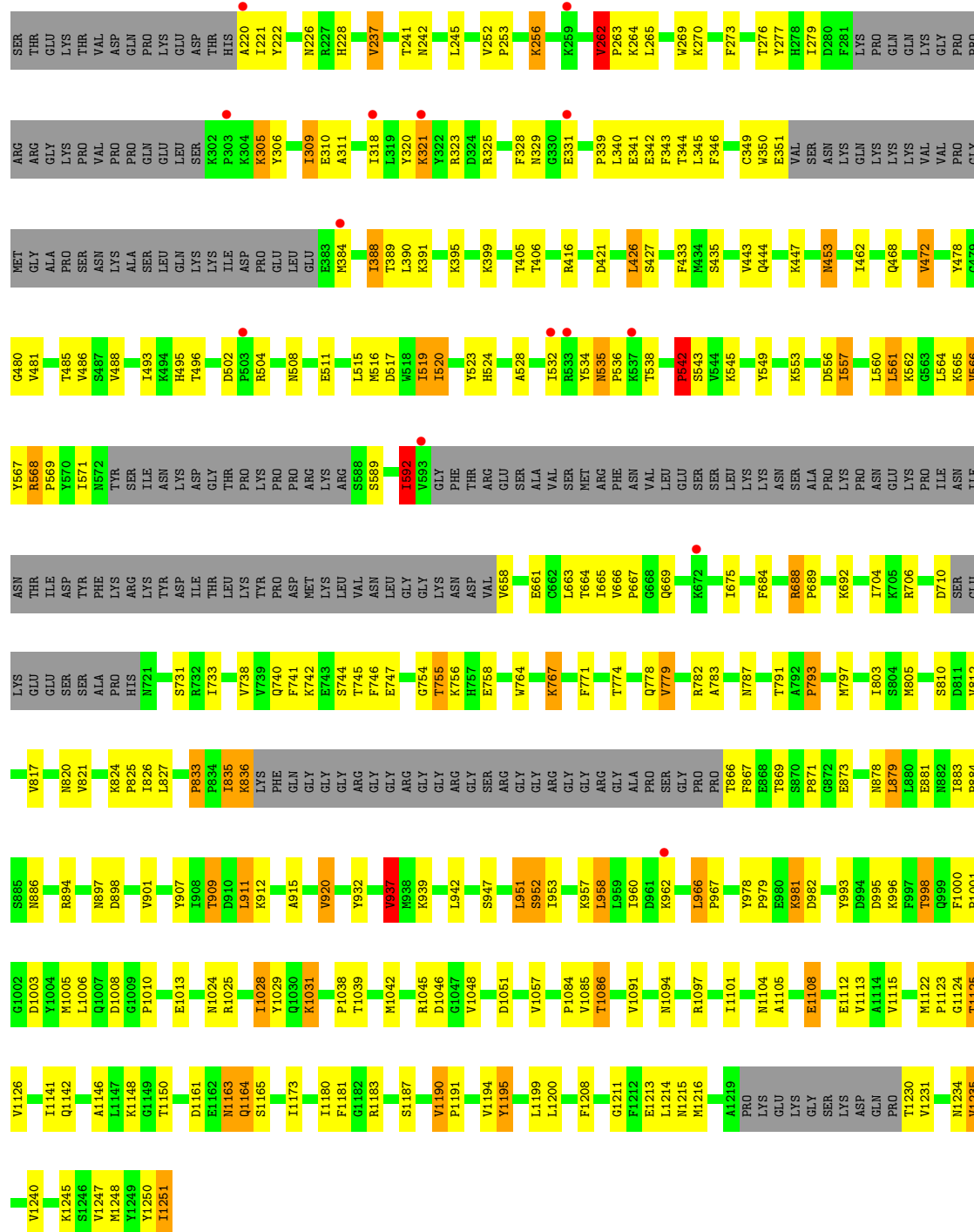
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	P	0	0	0
			179	79	37	54	9			
2	F	9	Total	C	N	O	P	0	0	0
			179	79	37	54	9			

- Molecule 3 is water.

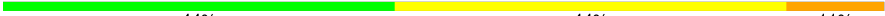
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	E	1	Total	O	0	0
			1	1		
3	B	12	Total	O	0	0
			12	12		
3	F	1	Total	O	0	0
			1	1		



• Molecule 1: KpAGO



• Molecule 2: RNA 5'-R(P*UP*AP*AP*AP*AP*AP*AP*A)-3'

Chain E:  44% 44% 11%



● Molecule 2: RNA 5'-R(P*UP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain F:  44% 44% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	171.55Å 171.55Å 83.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.12 – 3.19 38.12 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.12-3.19) 95.8 (38.12-3.19)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.168 , 0.216 0.163 , 0.209	Depositor DCC
R_{free} test set	1999 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.029 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14426	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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	0.61	0/7382	0.99	22/9981 (0.2%)
1	B	0.60	1/6958 (0.0%)	0.99	25/9413 (0.3%)
2	E	0.42	0/201	0.41	0/310
2	F	0.44	0/201	0.41	0/310
All	All	0.60	1/14742 (0.0%)	0.98	47/20014 (0.2%)

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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	HIS	CE1-NE2	-5.26	1.27	1.32

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	VAL	N-CA-C	8.26	120.00	107.77
1	B	567	TYR	N-CA-C	7.72	120.14	109.18
1	A	329	ASN	N-CA-C	7.44	121.60	112.23
1	B	873	GLU	N-CA-C	-7.37	103.33	111.36
1	A	1235	VAL	N-CA-C	-7.04	106.63	113.53
1	B	1235	VAL	N-CA-C	-7.01	106.66	113.53
1	A	833	PRO	O-C-N	6.92	124.40	121.15
1	A	221	ILE	N-CA-C	6.89	117.67	106.72
1	A	220	ALA	CA-C-N	-6.72	113.95	123.10
1	A	220	ALA	C-N-CA	-6.72	113.95	123.10
1	B	833	PRO	O-C-N	6.65	124.28	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	873	GLU	N-CA-C	-6.64	104.12	111.36
1	A	329	ASN	CA-C-N	6.54	133.47	121.70
1	A	329	ASN	C-N-CA	6.54	133.47	121.70
1	A	481	VAL	N-CA-C	6.49	117.38	107.77
1	A	406	THR	N-CA-C	-6.28	106.58	114.56
1	B	305	LYS	CA-CB-CG	6.26	126.63	114.10
1	B	592	ILE	N-CA-C	6.22	117.79	108.96
1	B	305	LYS	CB-CA-C	-6.07	101.27	110.92
1	A	520	ILE	CB-CA-C	-5.90	104.42	111.97
1	B	399	LYS	CD-CE-NZ	5.72	130.21	111.90
1	A	937	VAL	CB-CA-C	-5.66	103.39	112.16
1	B	937	VAL	CB-CA-C	-5.63	103.43	112.16
1	B	542	PRO	CA-C-O	-5.61	115.38	121.27
1	B	329	ASN	CA-C-N	5.55	132.28	121.41
1	B	329	ASN	C-N-CA	5.55	132.28	121.41
1	B	793	PRO	CA-C-N	5.54	125.54	119.89
1	B	793	PRO	C-N-CA	5.54	125.54	119.89
1	B	388	ILE	N-CA-C	5.40	116.36	108.53
1	A	1164	GLN	CB-CG-CD	5.36	121.70	112.60
1	B	520	ILE	CB-CA-C	-5.34	105.13	111.97
1	B	1161	ASP	N-CA-C	5.33	116.13	107.23
1	B	1164	GLN	CB-CG-CD	5.30	121.61	112.60
1	A	1161	ASP	N-CA-C	5.29	116.07	107.23
1	B	1187	SER	N-CA-C	-5.29	101.85	110.20
1	A	305	LYS	N-CA-CB	5.27	117.66	110.01
1	B	262	VAL	CA-C-N	5.27	126.09	119.98
1	B	262	VAL	C-N-CA	5.27	126.09	119.98
1	A	305	LYS	CA-CB-CG	5.21	124.52	114.10
1	B	817	VAL	N-CA-C	5.14	114.98	107.37
1	A	262	VAL	CA-C-N	5.14	125.94	119.98
1	A	262	VAL	C-N-CA	5.14	125.94	119.98
1	A	871	PRO	N-CA-C	-5.14	103.76	111.57
1	B	568	ARG	CA-C-N	5.10	126.92	121.00
1	B	568	ARG	C-N-CA	5.10	126.92	121.00
1	A	1133	SER	N-CA-C	5.07	116.87	110.33
1	A	533	ARG	N-CA-C	-5.04	105.79	112.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	220	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	B	542	PRO	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	7225	0	7219	169	0
1	B	6809	0	6799	152	0
2	E	179	0	87	5	0
2	F	179	0	87	5	0
3	A	20	0	0	0	0
3	B	12	0	0	1	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	14426	0	14192	322	0

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 11.

All (322) 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:1104:ASN:HB3	1:B:1112:GLU:HG3	1.60	0.84
1:A:447:LYS:HD3	1:A:488:VAL:HG11	1.61	0.82
1:A:1104:ASN:HB3	1:A:1112:GLU:HG3	1.64	0.80
1:A:1126:VAL:HG22	1:A:1141:ILE:HG12	1.64	0.79
1:B:447:LYS:HD3	1:B:488:VAL:HG11	1.64	0.77
1:A:874:ILE:HD12	1:B:871:PRO:HB3	1.68	0.75
1:A:301:SER:HB3	1:A:303:PRO:HG2	1.66	0.74
1:A:1195:TYR:OH	2:E:5:A:OP2	2.05	0.74
1:A:755:THR:OG1	1:A:756:LYS:N	2.20	0.74
1:B:738:VAL:HB	1:B:952:SER:HB3	1.70	0.74
1:A:552:GLU:OE1	1:A:647:LYS:NZ	2.22	0.73
1:B:1126:VAL:HG22	1:B:1141:ILE:HG12	1.71	0.72
1:A:320:TYR:CZ	1:A:323:ARG:NH1	2.57	0.72
1:B:472:VAL:HG12	1:B:485:THR:HG22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:PRO:HA	1:B:543:SER:HB2	1.73	0.71
1:B:755:THR:OG1	1:B:756:LYS:N	2.18	0.71
1:A:472:VAL:HG12	1:A:485:THR:HG22	1.73	0.70
1:B:1195:TYR:OH	2:F:5:A:OP2	2.10	0.70
1:A:217:ASP:OD1	1:A:218:THR:N	2.19	0.70
1:B:320:TYR:CZ	1:B:323:ARG:NH1	2.60	0.70
1:A:824:LYS:HD2	1:A:825:PRO:HD2	1.75	0.68
1:A:958:LEU:HD13	1:A:1173:ILE:HG22	1.75	0.68
1:B:824:LYS:HD2	1:B:825:PRO:HD2	1.76	0.68
1:A:738:VAL:HB	1:A:952:SER:HB3	1.76	0.68
1:B:993:TYR:CD2	1:B:1028:ILE:HD11	2.28	0.68
1:B:958:LEU:HD13	1:B:1173:ILE:HG22	1.76	0.67
1:A:346:PHE:O	1:A:350:TRP:NE1	2.28	0.67
1:A:1003:ASP:OD2	1:A:1025:ARG:NH2	2.21	0.66
1:A:688:ARG:NH2	1:A:1146:ALA:O	2.28	0.66
1:A:689:PRO:HG3	1:A:1150:THR:HG23	1.76	0.66
1:A:993:TYR:CD2	1:A:1028:ILE:HD11	2.30	0.66
1:B:346:PHE:O	1:B:350:TRP:NE1	2.29	0.66
1:B:1211:GLY:O	1:B:1215:ASN:ND2	2.28	0.66
1:A:783:ALA:HB2	1:A:805:MET:HE2	1.77	0.65
1:B:783:ALA:HB2	1:B:805:MET:HE2	1.76	0.65
1:A:1094:ASN:O	1:A:1097:ARG:NH2	2.30	0.65
1:A:1211:GLY:O	1:A:1215:ASN:ND2	2.30	0.65
1:A:826:ILE:HG21	1:A:879:LEU:HD11	1.78	0.64
1:B:1094:ASN:O	1:B:1097:ARG:NH2	2.31	0.64
1:A:1163:ASN:N	1:A:1163:ASN:OD1	2.31	0.62
1:B:453:ASN:OD1	1:B:453:ASN:N	2.25	0.62
1:A:453:ASN:OD1	1:A:453:ASN:N	2.27	0.62
1:A:642:LYS:N	1:A:661:GLU:OE1	2.29	0.62
1:B:1003:ASP:OD2	1:B:1025:ARG:NH2	2.28	0.62
1:B:793:PRO:HG3	1:B:827:LEU:HD11	1.81	0.62
1:B:1183:ARG:HD3	1:B:1251:ILE:HD12	1.81	0.62
1:B:323:ARG:HE	1:B:435:SER:HB2	1.65	0.61
1:B:351:GLU:HG3	1:B:391:LYS:NZ	2.15	0.61
1:A:515:LEU:O	1:A:519:ILE:HG13	2.01	0.61
1:A:1013:GLU:O	1:A:1045:ARG:NH2	2.33	0.60
1:B:515:LEU:O	1:B:519:ILE:HG13	2.02	0.60
1:A:793:PRO:HG3	1:A:827:LEU:HD11	1.82	0.60
1:B:269:TRP:H	1:B:269:TRP:CD1	2.20	0.60
1:A:1190:VAL:HG23	1:A:1191:PRO:HD2	1.84	0.59
1:A:544:VAL:O	1:A:548:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:THR:HG21	1:B:704:ILE:HD11	1.84	0.58
1:B:1124:GLY:HA2	1:B:1142:GLN:O	2.02	0.58
1:B:351:GLU:HG3	1:B:391:LYS:HZ3	1.69	0.58
1:B:658:VAL:N	3:B:1303:HOH:O	2.36	0.57
1:B:1013:GLU:O	1:B:1045:ARG:NH2	2.37	0.57
1:B:557:ILE:HA	1:B:560:LEU:HD23	1.86	0.57
1:A:301:SER:O	1:A:305:LYS:HD2	2.05	0.57
1:A:1124:GLY:HA2	1:A:1142:GLN:O	2.05	0.57
1:B:1086:THR:HG22	1:B:1163:ASN:OD1	2.04	0.57
1:B:341:GLU:HG3	1:B:350:TRP:CH2	2.39	0.57
1:A:1122:MET:O	1:A:1125:THR:OG1	2.22	0.56
1:B:1163:ASN:OD1	1:B:1163:ASN:N	2.38	0.56
1:A:302:LYS:HA	1:A:305:LYS:HG2	1.86	0.56
1:B:1000:PHE:O	1:B:1250:TYR:OH	2.22	0.56
1:A:1148:LYS:HD3	2:E:6:A:C2	2.40	0.56
1:B:1122:MET:O	1:B:1125:THR:OG1	2.23	0.56
1:B:898:ASP:HB3	1:B:901:VAL:HB	1.87	0.56
1:B:957:LYS:O	1:B:962:LYS:NZ	2.34	0.56
1:B:1190:VAL:HG23	1:B:1191:PRO:HD2	1.88	0.56
1:A:343:PHE:C	1:A:345:LEU:H	2.13	0.55
1:A:565:LYS:HA	1:A:591:GLY:HA2	1.88	0.55
1:A:600:ALA:O	1:A:629:THR:OG1	2.23	0.55
1:B:349:CYS:O	1:B:390:LEU:N	2.34	0.55
1:B:993:TYR:HD2	1:B:1028:ILE:HD11	1.69	0.55
1:B:253:PRO:O	1:B:256:LYS:HB2	2.06	0.55
1:B:1148:LYS:HD3	2:F:6:A:C2	2.42	0.55
1:B:515:LEU:HB2	1:B:663:LEU:O	2.06	0.55
1:A:435:SER:O	1:A:435:SER:OG	2.23	0.55
1:B:733:ILE:HD13	1:B:1122:MET:HB3	1.88	0.55
1:A:495:HIS:CE1	1:A:667:PRO:HB3	2.42	0.55
1:B:826:ILE:HG21	1:B:879:LEU:HD11	1.88	0.55
1:A:341:GLU:HG3	1:A:350:TRP:CH2	2.41	0.55
1:B:273:PHE:HB3	1:B:395:LYS:HE2	1.89	0.54
1:A:957:LYS:O	1:A:962:LYS:NZ	2.37	0.54
1:B:528:ALA:HA	1:B:534:TYR:HB3	1.90	0.54
2:E:8:A:O2'	2:E:9:A:OP1	2.22	0.54
1:A:993:TYR:HD2	1:A:1028:ILE:HD11	1.71	0.53
1:A:565:LYS:O	1:A:666:VAL:HG12	2.09	0.53
1:A:898:ASP:HB3	1:A:901:VAL:HB	1.91	0.53
1:B:343:PHE:C	1:B:345:LEU:H	2.16	0.53
1:A:883:ILE:HD12	1:A:884:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TRP:H	1:A:269:TRP:CD1	2.25	0.53
1:A:1086:THR:HG22	1:A:1163:ASN:OD1	2.09	0.53
1:A:528:ALA:HA	1:A:534:TYR:HB3	1.90	0.52
1:A:787:ASN:ND2	1:A:793:PRO:HD3	2.25	0.52
1:B:981:LYS:HG3	1:B:982:ASP:H	1.74	0.52
1:A:281:PHE:O	1:A:282:LYS:HB2	2.09	0.52
1:A:596:THR:OG1	1:A:648:LEU:HD12	2.09	0.52
1:A:939:LYS:NZ	2:E:3:A:OP1	2.42	0.52
1:A:301:SER:C	1:A:305:LYS:HD2	2.35	0.52
1:B:909:THR:HG22	1:B:915:ALA:HB3	1.92	0.52
1:B:833:PRO:O	1:B:835:ILE:HG22	2.10	0.52
1:B:495:HIS:CE1	1:B:667:PRO:HB3	2.45	0.52
1:B:566:VAL:HG23	1:B:664:THR:O	2.10	0.52
1:A:733:ILE:HD13	1:A:1122:MET:HB3	1.92	0.51
1:A:630:ILE:HG12	1:A:641:LEU:HD12	1.91	0.51
1:B:1024:ASN:O	1:B:1028:ILE:HG23	2.10	0.51
1:B:812:VAL:HB	1:B:937:VAL:HG11	1.92	0.51
1:A:508:ASN:HB3	1:A:511:GLU:HB2	1.93	0.51
1:B:565:LYS:O	1:B:666:VAL:HG12	2.11	0.51
1:A:1000:PHE:O	1:A:1250:TYR:OH	2.21	0.51
1:B:1029:TYR:CD2	1:B:1038:PRO:HD3	2.46	0.51
1:A:1183:ARG:HD3	1:A:1251:ILE:HD12	1.93	0.51
1:B:339:PRO:O	1:B:342:GLU:HG2	2.11	0.51
1:A:779:VAL:HA	1:A:886:ASN:OD1	2.11	0.50
1:B:731:SER:HB2	1:B:1125:THR:HG22	1.94	0.50
1:A:731:SER:HB2	1:A:1125:THR:HG22	1.94	0.50
1:A:981:LYS:HG3	1:A:982:ASP:H	1.75	0.50
1:A:502:ASP:OD1	1:A:504:ARG:HD3	2.12	0.50
1:A:279:ILE:HG22	1:A:332:ASP:O	2.11	0.50
1:A:628:ASN:OD1	1:A:629:THR:N	2.44	0.50
1:B:508:ASN:HB3	1:B:511:GLU:HB2	1.93	0.50
1:A:812:VAL:HB	1:A:937:VAL:HG11	1.94	0.50
1:A:833:PRO:O	1:A:835:ILE:HG22	2.12	0.49
1:B:311:ALA:CB	1:B:384:MET:HE1	2.42	0.49
1:B:502:ASP:OD1	1:B:504:ARG:HD3	2.12	0.49
1:B:1200:LEU:HD13	1:B:1250:TYR:CD2	2.48	0.49
1:B:1046:ASP:HB2	1:B:1194:VAL:HG13	1.95	0.49
1:B:321:LYS:O	1:B:325:ARG:NH1	2.45	0.49
1:B:779:VAL:HA	1:B:886:ASN:OD1	2.12	0.49
1:A:535:ASN:ND2	1:A:538:THR:HG23	2.28	0.48
1:A:515:LEU:HB2	1:A:663:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:TYR:HE1	1:A:589:SER:HB3	1.78	0.48
1:B:222:TYR:HB3	1:B:1057:VAL:HG12	1.94	0.48
1:A:836:LYS:HA	1:A:866:THR:O	2.12	0.48
1:A:1195:TYR:O	1:A:1199:LEU:HG	2.13	0.48
1:A:1200:LEU:HD13	1:A:1250:TYR:CD2	2.49	0.48
1:B:535:ASN:ND2	1:B:538:THR:HG23	2.29	0.48
1:B:787:ASN:ND2	1:B:793:PRO:HD3	2.28	0.48
1:A:597:ARG:HA	1:A:647:LYS:HE2	1.96	0.48
1:B:568:ARG:HA	1:B:569:PRO:HD3	1.56	0.48
1:B:516:MET:HA	1:B:519:ILE:HD12	1.95	0.48
1:B:1108:GLU:H	1:B:1108:GLU:HG3	1.43	0.48
1:A:778:GLN:CD	1:A:820:ASN:HB2	2.39	0.48
1:A:253:PRO:O	1:A:256:LYS:HB2	2.13	0.47
1:A:1029:TYR:CD2	1:A:1038:PRO:HD3	2.49	0.47
1:B:778:GLN:CD	1:B:820:ASN:HB2	2.39	0.47
1:B:883:ILE:HD12	1:B:884:PRO:HD2	1.95	0.47
1:B:1001:PRO:HG3	1:B:1028:ILE:CD1	2.45	0.47
1:A:909:THR:HG22	1:A:915:ALA:HB3	1.95	0.47
1:A:321:LYS:O	1:A:325:ARG:NH1	2.47	0.47
1:A:871:PRO:HG3	1:B:878:ASN:HD22	1.78	0.47
1:B:565:LYS:O	1:B:669:GLN:NE2	2.44	0.47
2:F:8:A:O2'	2:F:9:A:OP1	2.22	0.47
1:A:384:MET:C	1:A:386:SER:H	2.23	0.47
1:A:1024:ASN:O	1:A:1028:ILE:HG23	2.15	0.47
1:B:493:ILE:HD13	1:B:665:ILE:HG21	1.97	0.47
1:A:339:PRO:O	1:A:342:GLU:HG2	2.15	0.47
1:B:939:LYS:NZ	2:F:3:A:OP1	2.47	0.47
1:B:435:SER:O	1:B:435:SER:OG	2.23	0.47
1:A:1046:ASP:HB2	1:A:1194:VAL:HG13	1.96	0.46
1:A:1108:GLU:H	1:A:1108:GLU:HG3	1.43	0.46
1:A:549:TYR:CE1	1:A:553:LYS:HB2	2.51	0.46
1:B:561:LEU:HA	1:B:564:LEU:HB2	1.97	0.46
1:A:426:LEU:HD12	1:A:426:LEU:HA	1.78	0.46
1:B:1042:MET:HE2	1:B:1042:MET:HB3	1.62	0.46
1:B:237:VAL:HG13	1:B:1105:ALA:HB2	1.98	0.46
1:B:966:LEU:HD12	1:B:966:LEU:HA	1.84	0.46
1:B:907:TYR:O	1:B:911:LEU:HB3	2.15	0.46
1:B:561:LEU:HB2	1:B:592:ILE:HD11	1.97	0.46
1:A:310:GLU:H	1:A:310:GLU:HG2	1.56	0.46
1:B:406:THR:HG23	1:B:478:TYR:OH	2.16	0.45
1:B:562:LYS:HD2	1:B:562:LYS:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:TYR:CE1	1:B:553:LYS:HB2	2.51	0.45
1:A:947:SER:OG	1:A:998:THR:HG21	2.16	0.45
1:A:320:TYR:CE2	1:A:323:ARG:NH1	2.84	0.45
1:A:561:LEU:O	1:A:563:GLY:N	2.50	0.45
1:A:633:PHE:HB3	1:A:639:ILE:HG13	1.98	0.45
1:B:658:VAL:HG11	1:B:663:LEU:HD13	1.98	0.45
1:B:960:ILE:HD11	1:B:995:ASP:HB2	1.98	0.45
1:A:951:LEU:HD13	1:A:1180:ILE:HG23	1.98	0.45
1:B:564:LEU:O	1:B:592:ILE:HG23	2.17	0.45
1:B:1005:MET:HE2	1:B:1005:MET:HB3	1.82	0.45
1:A:978:TYR:HE1	1:A:1010:PRO:HB2	1.82	0.45
1:A:1042:MET:HB3	1:A:1042:MET:HE2	1.56	0.45
1:A:468:GLN:HG2	1:A:684:PHE:CZ	2.52	0.45
1:A:951:LEU:HA	1:A:951:LEU:HD12	1.55	0.45
1:B:836:LYS:HA	1:B:866:THR:O	2.16	0.45
1:A:309:ILE:HD12	1:A:328:PHE:CG	2.52	0.45
1:A:517:ASP:HA	1:A:520:ILE:HD12	1.99	0.45
1:B:433:PHE:O	1:B:706:ARG:NH1	2.50	0.45
1:A:405:THR:HG22	1:A:416:ARG:HH22	1.82	0.45
1:A:273:PHE:HZ	1:A:399:LYS:HZ1	1.62	0.45
1:A:557:ILE:HG12	1:A:561:LEU:HD11	1.98	0.45
1:B:311:ALA:HB1	1:B:384:MET:HE1	1.99	0.45
1:B:405:THR:HG22	1:B:416:ARG:HH22	1.82	0.45
1:A:960:ILE:HA	1:A:967:PRO:HA	1.99	0.44
1:A:1031:LYS:HB2	1:A:1031:LYS:HE2	1.50	0.44
1:B:688:ARG:NH2	1:B:1146:ALA:O	2.50	0.44
1:A:300:LEU:HA	1:A:305:LYS:NZ	2.32	0.44
1:A:598:GLU:CD	1:A:603:MET:HG2	2.42	0.44
1:B:1216:MET:HE2	1:B:1216:MET:HA	1.98	0.44
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.91	0.44
1:A:523:TYR:CE2	1:A:542:PRO:HG3	2.52	0.44
1:B:566:VAL:CG2	1:B:663:LEU:HG	2.47	0.44
1:B:746:PHE:CD2	1:B:764:TRP:HB3	2.52	0.44
1:B:309:ILE:HD12	1:B:328:PHE:CG	2.52	0.44
1:B:951:LEU:HD13	1:B:1180:ILE:HG23	1.98	0.44
1:A:746:PHE:CD2	1:A:764:TRP:HB3	2.51	0.44
1:A:758:GLU:HB2	1:A:1117:SER:HB2	1.99	0.44
1:B:947:SER:OG	1:B:998:THR:HG21	2.17	0.44
1:B:1115:VAL:C	1:B:1122:MET:HB2	2.43	0.44
1:A:550:PHE:C	1:A:552:GLU:H	2.26	0.44
1:B:805:MET:HB3	1:B:821:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:ASN:C	1:A:1164:GLN:HG2	2.42	0.44
1:A:516:MET:HG2	1:A:660:PRO:HB2	1.99	0.44
1:B:349:CYS:O	1:B:389:THR:HA	2.18	0.44
1:B:1181:PHE:CE2	1:B:1183:ARG:HG2	2.53	0.44
1:A:406:THR:HG23	1:A:478:TYR:OH	2.18	0.43
1:A:433:PHE:HD2	1:A:448:PHE:CE2	2.36	0.43
1:A:262:VAL:HA	1:A:263:PRO:HD3	1.75	0.43
1:A:405:THR:HB	1:A:479:GLY:HA2	2.00	0.43
1:B:262:VAL:HA	1:B:263:PRO:HD3	1.73	0.43
2:F:5:A:C6	2:F:6:A:N6	2.86	0.43
1:B:826:ILE:HD13	1:B:879:LEU:HD11	2.00	0.43
1:B:1101:ILE:HD13	1:B:1101:ILE:HG21	1.77	0.43
1:A:302:LYS:N	1:A:303:PRO:HD2	2.34	0.43
1:A:410:THR:O	1:A:414:GLU:HG3	2.19	0.43
1:A:249:GLY:HA3	1:A:405:THR:OG1	2.19	0.43
1:A:270:LYS:O	1:A:399:LYS:HB3	2.18	0.43
1:A:771:PHE:CZ	1:A:815:LEU:HD13	2.54	0.43
1:B:523:TYR:CE2	1:B:542:PRO:HG3	2.54	0.43
1:B:803:ILE:HD13	1:B:803:ILE:HA	1.91	0.43
1:A:1028:ILE:HD13	1:A:1028:ILE:HG21	1.75	0.43
1:B:320:TYR:CE2	1:B:323:ARG:NH1	2.87	0.43
1:B:978:TYR:HE1	1:B:1010:PRO:HB2	1.83	0.43
1:A:516:MET:HA	1:A:519:ILE:HD12	2.00	0.43
1:B:1248:MET:HE2	1:B:1251:ILE:HG12	2.00	0.43
1:A:273:PHE:HB3	1:A:395:LYS:HE2	2.01	0.42
1:A:564:LEU:O	1:A:592:ILE:HG23	2.19	0.42
1:B:277:TYR:CE2	1:B:340:LEU:HG	2.54	0.42
1:B:493:ILE:CG1	1:B:669:GLN:HB2	2.49	0.42
1:B:979:PRO:HB2	1:B:1208:PHE:CD1	2.54	0.42
1:A:907:TYR:O	1:A:911:LEU:HB3	2.19	0.42
1:B:516:MET:O	1:B:520:ILE:HG13	2.19	0.42
1:A:1001:PRO:HG3	1:A:1028:ILE:CD1	2.50	0.42
1:A:493:ILE:CG1	1:A:669:GLN:HB2	2.49	0.42
1:A:960:ILE:HD11	1:A:995:ASP:HB2	2.01	0.42
1:B:279:ILE:HD11	1:B:388:ILE:HG22	2.01	0.42
1:B:1251:ILE:HD13	1:B:1251:ILE:HA	1.74	0.42
1:A:385:VAL:O	1:A:388:ILE:HG13	2.20	0.42
1:A:1115:VAL:C	1:A:1122:MET:HB2	2.45	0.42
1:A:1163:ASN:O	1:A:1164:GLN:C	2.62	0.42
1:B:493:ILE:HG12	1:B:669:GLN:HB2	2.02	0.42
1:B:920:VAL:HG22	1:B:932:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1195:TYR:O	1:B:1199:LEU:HG	2.18	0.42
1:A:433:PHE:O	1:A:706:ARG:NH1	2.53	0.42
1:A:648:LEU:HD13	1:A:657:VAL:CG1	2.50	0.42
1:B:426:LEU:HD12	1:B:426:LEU:HA	1.77	0.42
1:B:912:LYS:HA	1:B:912:LYS:HD3	1.78	0.42
1:B:689:PRO:HG3	1:B:1150:THR:HG23	2.01	0.42
1:B:960:ILE:HA	1:B:967:PRO:HA	2.01	0.42
1:A:564:LEU:HD21	1:A:665:ILE:HG23	2.01	0.42
1:B:742:LYS:HB2	1:B:771:PHE:O	2.20	0.42
1:A:242:ASN:ND2	1:A:485:THR:O	2.41	0.42
1:A:275:PHE:CZ	1:A:339:PRO:HG3	2.54	0.42
1:A:650:ASN:HB3	1:A:657:VAL:HG22	2.02	0.42
1:B:824:LYS:HA	1:B:825:PRO:HD2	1.91	0.42
1:A:1178:CYS:O	1:A:1187:SER:HA	2.19	0.41
1:B:468:GLN:HG2	1:B:684:PHE:CZ	2.54	0.41
1:B:1039:THR:O	1:B:1084:PRO:HD2	2.20	0.41
1:A:486:VAL:HG11	1:A:1095:GLN:HB3	2.02	0.41
1:A:1181:PHE:CE2	1:A:1183:ARG:HG2	2.55	0.41
1:A:519:ILE:HG13	1:A:519:ILE:H	1.60	0.41
1:A:835:ILE:HG21	1:A:835:ILE:HD13	1.71	0.41
1:B:517:ASP:HA	1:B:520:ILE:HD12	2.01	0.41
1:A:733:ILE:HD12	1:A:1115:VAL:HG12	2.02	0.41
1:A:871:PRO:HG3	1:B:878:ASN:ND2	2.35	0.41
1:B:252:VAL:HA	1:B:253:PRO:HD3	1.90	0.41
1:A:462:ILE:HD12	1:A:556:ASP:HB3	2.02	0.41
1:A:493:ILE:HG12	1:A:669:GLN:HB2	2.03	0.41
1:A:544:VAL:HG13	1:A:646:MET:HG2	2.02	0.41
1:A:877:LEU:O	1:A:881:GLU:HG2	2.21	0.41
1:A:1216:MET:HE2	1:A:1216:MET:HA	2.01	0.41
2:E:5:A:C6	2:E:6:A:N6	2.88	0.41
1:B:242:ASN:ND2	1:B:485:THR:O	2.46	0.41
1:B:256:LYS:HD2	1:B:256:LYS:HA	1.83	0.41
1:B:443:VAL:HG12	1:B:444:GLN:HG3	2.03	0.41
1:B:493:ILE:HD12	1:B:493:ILE:O	2.21	0.41
1:A:641:LEU:HA	1:A:661:GLU:OE1	2.21	0.41
1:B:524:HIS:HD2	1:B:536:PRO:HB3	1.85	0.41
1:A:306:TYR:O	1:A:310:GLU:HG2	2.21	0.41
1:A:343:PHE:C	1:A:345:LEU:N	2.78	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD12	1.84	0.41
1:A:443:VAL:HG12	1:A:444:GLN:HG3	2.02	0.41
1:A:493:ILE:HD12	1:A:493:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LYS:HE3	1:A:589:SER:OG	2.20	0.41
1:A:567:TYR:CE1	1:A:589:SER:HB3	2.55	0.41
1:A:727:MET:HE2	1:A:727:MET:HB3	1.90	0.41
1:A:746:PHE:CE2	1:A:764:TRP:HB3	2.56	0.41
1:A:1251:ILE:HD13	1:A:1251:ILE:HA	1.84	0.41
1:B:767:LYS:HE3	1:B:767:LYS:HB2	1.58	0.41
1:B:835:ILE:HD13	1:B:835:ILE:HG21	1.74	0.41
1:A:384:MET:H	1:A:384:MET:HG2	1.64	0.41
1:B:524:HIS:CD2	1:B:536:PRO:HB3	2.56	0.41
1:B:1006:LEU:HD12	1:B:1006:LEU:HA	1.91	0.41
1:A:524:HIS:CD2	1:A:536:PRO:HB3	2.56	0.40
1:A:979:PRO:HB2	1:A:1208:PHE:CD1	2.56	0.40
1:B:1031:LYS:HE2	1:B:1031:LYS:HB2	1.49	0.40
1:A:256:LYS:HD2	1:A:256:LYS:HA	1.80	0.40
1:B:740:GLN:HG3	1:B:741:PHE:O	2.21	0.40
1:B:462:ILE:HD12	1:B:556:ASP:HB2	2.03	0.40
1:B:942:LEU:HD23	1:B:942:LEU:HA	1.88	0.40
1:B:1123:PRO:HA	1:B:1124:GLY:HA2	1.77	0.40
1:A:920:VAL:HG22	1:A:932:TYR:OH	2.21	0.40
1:A:976:THR:HG23	1:A:1201:CYS:HB3	2.04	0.40
1:B:519:ILE:HG13	1:B:519:ILE:H	1.68	0.40

There are no symmetry-related clashes.

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	888/1046 (85%)	804 (90%)	74 (8%)	10 (1%)	11	41
1	B	837/1046 (80%)	758 (91%)	70 (8%)	9 (1%)	11	41
All	All	1725/2092 (82%)	1562 (91%)	144 (8%)	19 (1%)	11	41

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	VAL
1	A	711	SER
1	B	221	ILE
1	B	981	LYS
1	A	480	GLY
1	A	562	LYS
1	A	981	LYS
1	B	480	GLY
1	B	557	ILE
1	A	551	VAL
1	A	754	GLY
1	A	1164	GLN
1	B	754	GLY
1	A	344	THR
1	B	331	GLU
1	B	344	THR
1	B	1234	ASN
1	A	535	ASN
1	B	535	ASN

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	812/929 (87%)	711 (88%)	101 (12%)	4	19
1	B	765/929 (82%)	673 (88%)	92 (12%)	5	20
All	All	1577/1858 (85%)	1384 (88%)	193 (12%)	5	20

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	227	ARG
1	A	237	VAL
1	A	241	THR

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Mol	Chain	Res	Type
1	A	245	LEU
1	A	256	LYS
1	A	262	VAL
1	A	264	LYS
1	A	265	LEU
1	A	270	LYS
1	A	276	THR
1	A	305	LYS
1	A	306	TYR
1	A	309	ILE
1	A	310	GLU
1	A	318	ILE
1	A	321	LYS
1	A	325	ARG
1	A	384	MET
1	A	386	SER
1	A	388	ILE
1	A	414	GLU
1	A	416	ARG
1	A	421	ASP
1	A	426	LEU
1	A	427	SER
1	A	453	ASN
1	A	472	VAL
1	A	486	VAL
1	A	496	THR
1	A	532	ILE
1	A	546	ASP
1	A	555	THR
1	A	592	ILE
1	A	593	VAL
1	A	629	THR
1	A	634	LYS
1	A	645	ASP
1	A	648	LEU
1	A	661	GLU
1	A	675	ILE
1	A	688	ARG
1	A	692	LYS
1	A	711	SER
1	A	744	SER
1	A	745	THR

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Mol	Chain	Res	Type
1	A	747	GLU
1	A	755	THR
1	A	758	GLU
1	A	767	LYS
1	A	774	THR
1	A	779	VAL
1	A	782	ARG
1	A	791	THR
1	A	797	MET
1	A	810	SER
1	A	835	ILE
1	A	836	LYS
1	A	867	PHE
1	A	869	THR
1	A	879	LEU
1	A	894	ARG
1	A	897	ASN
1	A	909	THR
1	A	911	LEU
1	A	920	VAL
1	A	937	VAL
1	A	951	LEU
1	A	952	SER
1	A	953	ILE
1	A	958	LEU
1	A	966	LEU
1	A	996	LYS
1	A	998	THR
1	A	1008	ASP
1	A	1028	ILE
1	A	1031	LYS
1	A	1048	VAL
1	A	1051	ASP
1	A	1065	LYS
1	A	1085	VAL
1	A	1086	THR
1	A	1091	VAL
1	A	1108	GLU
1	A	1113	VAL
1	A	1125	THR
1	A	1143	SER
1	A	1163	ASN

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Mol	Chain	Res	Type
1	A	1164	GLN
1	A	1165	SER
1	A	1190	VAL
1	A	1195	TYR
1	A	1201	CYS
1	A	1213	GLU
1	A	1230	THR
1	A	1231	VAL
1	A	1235	VAL
1	A	1240	VAL
1	A	1245	LYS
1	A	1247	VAL
1	A	1251	ILE
1	B	226	ASN
1	B	237	VAL
1	B	241	THR
1	B	245	LEU
1	B	256	LYS
1	B	262	VAL
1	B	264	LYS
1	B	265	LEU
1	B	270	LYS
1	B	276	THR
1	B	305	LYS
1	B	306	TYR
1	B	309	ILE
1	B	310	GLU
1	B	318	ILE
1	B	321	LYS
1	B	421	ASP
1	B	426	LEU
1	B	427	SER
1	B	453	ASN
1	B	472	VAL
1	B	486	VAL
1	B	496	THR
1	B	519	ILE
1	B	532	ILE
1	B	545	LYS
1	B	561	LEU
1	B	566	VAL
1	B	571	ILE

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Mol	Chain	Res	Type
1	B	589	SER
1	B	592	ILE
1	B	661	GLU
1	B	675	ILE
1	B	688	ARG
1	B	692	LYS
1	B	710	ASP
1	B	744	SER
1	B	745	THR
1	B	747	GLU
1	B	755	THR
1	B	758	GLU
1	B	767	LYS
1	B	774	THR
1	B	779	VAL
1	B	782	ARG
1	B	791	THR
1	B	797	MET
1	B	810	SER
1	B	835	ILE
1	B	836	LYS
1	B	867	PHE
1	B	869	THR
1	B	879	LEU
1	B	881	GLU
1	B	894	ARG
1	B	897	ASN
1	B	909	THR
1	B	911	LEU
1	B	920	VAL
1	B	937	VAL
1	B	951	LEU
1	B	952	SER
1	B	953	ILE
1	B	958	LEU
1	B	966	LEU
1	B	996	LYS
1	B	998	THR
1	B	1008	ASP
1	B	1028	ILE
1	B	1031	LYS
1	B	1048	VAL

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Mol	Chain	Res	Type
1	B	1051	ASP
1	B	1085	VAL
1	B	1086	THR
1	B	1091	VAL
1	B	1108	GLU
1	B	1113	VAL
1	B	1125	THR
1	B	1163	ASN
1	B	1164	GLN
1	B	1165	SER
1	B	1190	VAL
1	B	1195	TYR
1	B	1213	GLU
1	B	1214	LEU
1	B	1230	THR
1	B	1231	VAL
1	B	1235	VAL
1	B	1240	VAL
1	B	1245	LYS
1	B	1247	VAL
1	B	1251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	814	GLN
1	A	820	ASN
1	A	897	ASN
1	A	1030	GLN
1	A	1079	ASN
1	B	548	ASN
1	B	780	ASN
1	B	820	ASN
1	B	897	ASN
1	B	1030	GLN
1	B	1079	ASN
1	B	1136	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	7/9 (77%)	1 (14%)	1 (14%)
2	F	7/9 (77%)	1 (14%)	1 (14%)
All	All	14/18 (77%)	2 (14%)	2 (14%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	8	A
2	F	8	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	8	A
2	F	8	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	904/1046 (86%)	-0.28	16 (1%) 67 47	11, 44, 111, 148	0
1	B	853/1046 (81%)	-0.28	14 (1%) 70 50	8, 44, 108, 150	0
2	E	9/9 (100%)	-0.87	0 100 100	30, 35, 67, 175	0
2	F	9/9 (100%)	-0.80	0 100 100	28, 35, 66, 178	0
All	All	1775/2110 (84%)	-0.29	30 (1%) 69 49	8, 44, 110, 178	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	GLU	3.7
1	B	532	ILE	3.4
1	B	533	ARG	3.1
1	A	672	LYS	2.9
1	B	503	PRO	2.8
1	A	604	ARG	2.8
1	A	532	ILE	2.7
1	A	533	ARG	2.6
1	A	318	ILE	2.5
1	A	411	GLU	2.5
1	B	537	LYS	2.4
1	A	384	MET	2.4
1	B	303	PRO	2.4
1	A	321	LYS	2.3
1	A	256	LYS	2.3
1	A	300	LEU	2.3
1	B	672	LYS	2.3
1	B	321	LYS	2.3
1	A	1078	GLY	2.2
1	A	264	LYS	2.2
1	B	962	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	217	ASP	2.2
1	A	722	SER	2.2
1	B	259	LYS	2.2
1	B	220	ALA	2.1
1	A	453	ASN	2.1
1	B	318	ILE	2.1
1	B	384	MET	2.1
1	B	593	VAL	2.0
1	A	1219	ALA	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.