Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 10:27 AM EST

PDB ID	:	4F1N
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 (i) 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 (1)) were used in the production of this report:

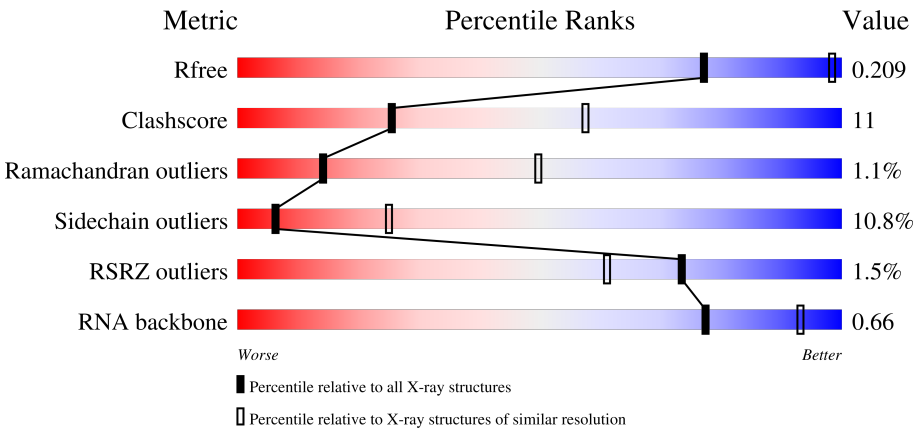
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

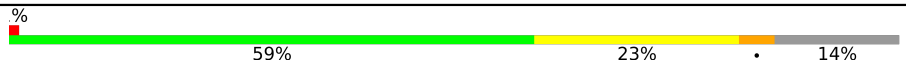
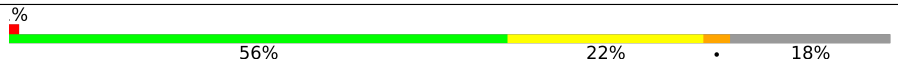
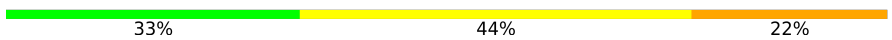
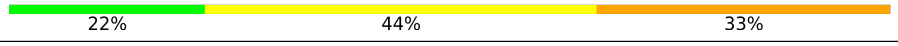
The reported resolution of this entry is 3.19 Å.

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}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)
RNA backbone	3102	1054 (3.50-2.86)

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 <=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	
1	B	1046	
2	E	9	
2	F	9	

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	904	7225	4633	1201	1359	32	0	0	0
1	B	853	6809	4372	1127	1280	30	0	0	0

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*AP*A)-3'.

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

- Molecule 3 is water.

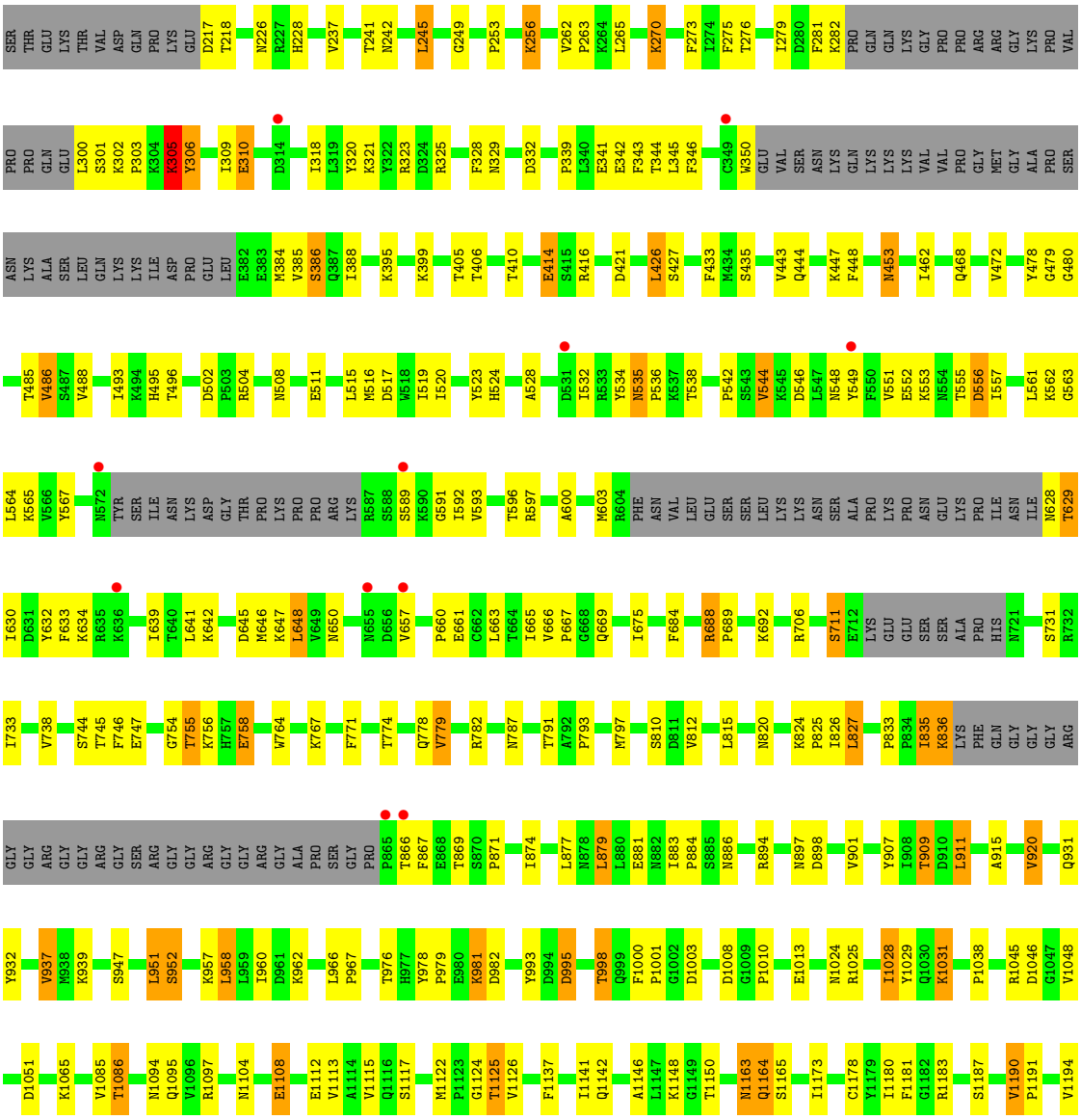
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	20	20	20	0	0
3	E	1	1	1	0	0
3	B	12	12	12	0	0
3	F	1	1	1	0	0

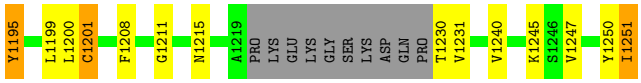
3 Residue-property plots (i)

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: KpAGO

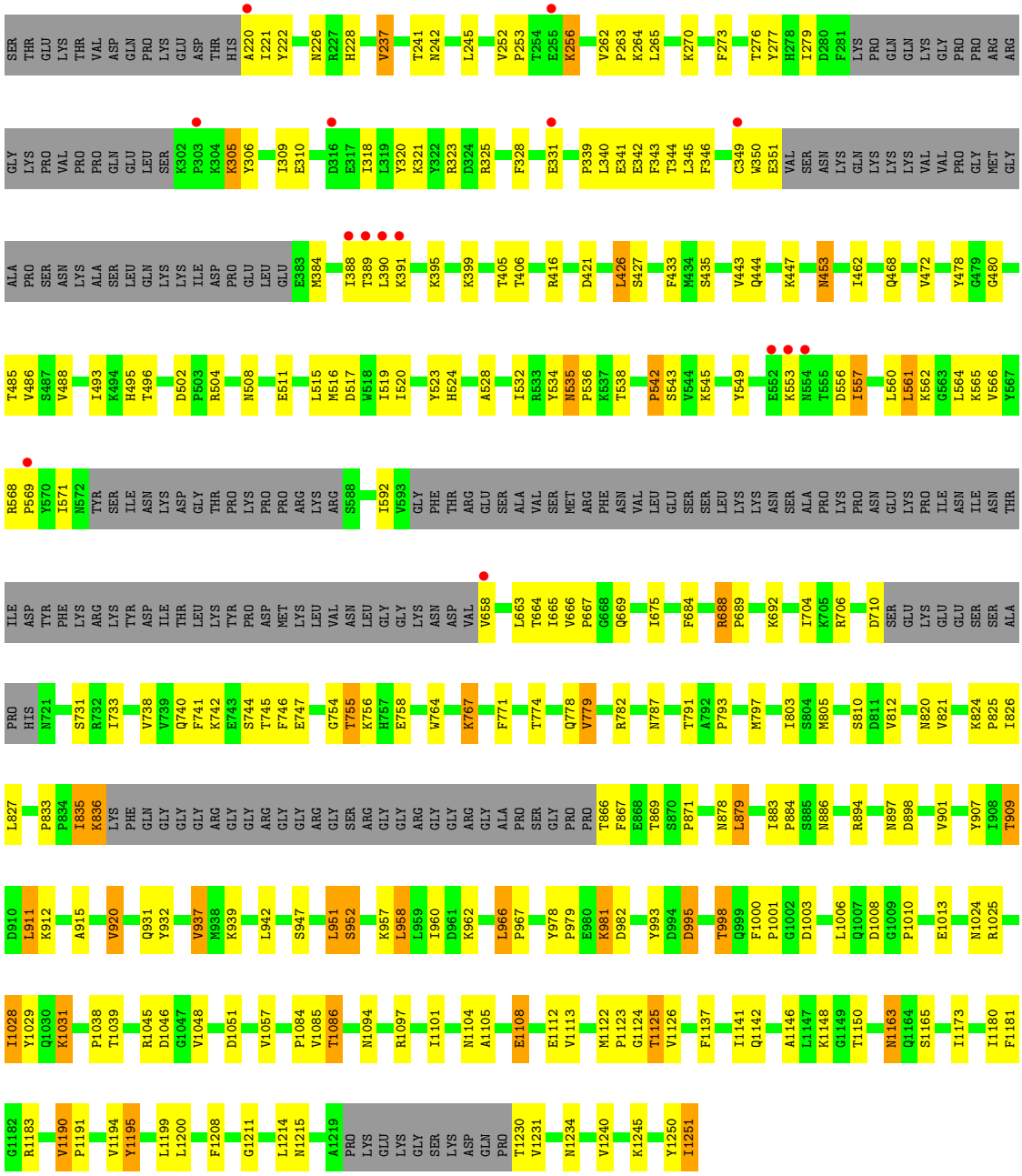
Chain A:





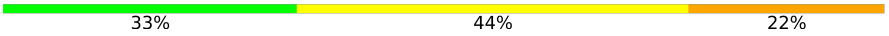
• Molecule 1: KpAGO

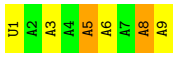
Chain B:



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

Chain E:





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

Chain F: 22% 44% 33%

4 Data and refinement statistics (i)

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 49.52 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.12-3.19) 95.8 (49.52-3.19)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.168 , 0.216 0.161 , 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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.50	0/7382	0.67	2/9981 (0.0%)
1	B	0.51	0/6958	0.68	2/9413 (0.0%)
2	E	1.01	1/201 (0.5%)	1.16	1/310 (0.3%)
2	F	1.08	1/201 (0.5%)	1.22	4/310 (1.3%)
All	All	0.52	2/14742 (0.0%)	0.70	9/20014 (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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	U	OP3-P	-10.60	1.48	1.61
2	E	1	U	OP3-P	-10.32	1.48	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	399	LYS	CD-CE-NZ	8.05	130.21	111.70
2	F	5	A	N1-C6-N6	6.13	122.28	118.60
1	B	305	LYS	CA-CB-CG	6.01	126.63	113.40
2	E	5	A	N1-C6-N6	5.93	122.16	118.60
1	A	329	ASN	C-N-CA	5.32	133.47	122.30
2	F	6	A	N1-C6-N6	5.18	121.71	118.60
1	A	305	LYS	CA-CB-CG	5.06	124.52	113.40
2	F	6	A	C2-N3-C4	-5.06	108.07	110.60
2	F	7	A	N1-C6-N6	5.04	121.62	118.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	220	ALA	Peptide
1	B	542	PRO	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	7225	0	7219	158	0
1	B	6809	0	6799	144	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	303	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 (303) 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:B:755:THR:OG1	1:B:756:LYS:N	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:542:PRO:HA	1:B:543:SER:HB2	1.73	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: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: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: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: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:565:LYS:HA	1:A:591:GLY:HA2	1.88	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:OG	1:A:435:SER:O	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:A:883:ILE:HD12	1:A:884:PRO:HD2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:343:PHE:C	1:A:345:LEU:H	2.13	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: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:435:SER:O	1:B:435:SER:OG	2.23	0.49
1:B:779:VAL:HA	1:B:886:ASN:OD1	2.12	0.49
1:B:1000:PHE:O	1:B:1250:TYR:OH	2.22	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
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:B:343:PHE:C	1:B:345:LEU:H	2.16	0.48
1:A:1195:TYR:O	1:A:1199:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:301:SER:C	1:A:305:LYS:HD2	2.35	0.47
1:A:600:ALA:O	1:A:629:THR:OG1	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:B:939:LYS:NZ	2:F:3:A:OP1	2.47	0.47
1:A:339:PRO:O	1:A:342:GLU:HG2	2.15	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:978:TYR:HE1	1:A:1010:PRO:HB2	1.82	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: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: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:805:MET:HB3	1:B:821:VAL:HG21	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:351:GLU:HG3	1:B:391:LYS:HZ1	1.83	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:778:GLN:CD	1:A:820:ASN:HB2	2.39	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:B:778:GLN:CD	1:B:820:ASN:HB2	2.39	0.43
1:A:516:MET:HA	1:A:519:ILE:HD12	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:384:MET:C	1:A:386:SER:H	2.23	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:384:MET:HE3	1:B:384:MET:HB3	1.89	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 (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	888/1046 (85%)	804 (90%)	74 (8%)	10 (1%)	14	50
1	B	837/1046 (80%)	758 (91%)	70 (8%)	9 (1%)	14	50
All	All	1725/2092 (82%)	1562 (91%)	144 (8%)	19 (1%)	14	50

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	812/929 (87%)	721 (89%)	91 (11%)	6 24
1	B	765/929 (82%)	686 (90%)	79 (10%)	7 27
All	All	1577/1858 (85%)	1407 (89%)	170 (11%)	6 25

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	228	HIS
1	A	237	VAL
1	A	241	THR
1	A	245	LEU
1	A	256	LYS
1	A	265	LEU
1	A	270	LYS
1	A	276	THR
1	A	305	LYS
1	A	306	TYR
1	A	310	GLU
1	A	318	ILE
1	A	386	SER
1	A	414	GLU
1	A	421	ASP
1	A	426	LEU

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Mol	Chain	Res	Type
1	A	427	SER
1	A	453	ASN
1	A	486	VAL
1	A	496	THR
1	A	532	ILE
1	A	546	ASP
1	A	555	THR
1	A	556	ASP
1	A	593	VAL
1	A	603	MET
1	A	629	THR
1	A	632	TYR
1	A	634	LYS
1	A	645	ASP
1	A	648	LEU
1	A	675	ILE
1	A	688	ARG
1	A	692	LYS
1	A	711	SER
1	A	744	SER
1	A	745	THR
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	827	LEU
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

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Mol	Chain	Res	Type
1	A	931	GLN
1	A	937	VAL
1	A	951	LEU
1	A	952	SER
1	A	958	LEU
1	A	966	LEU
1	A	995	ASP
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	1108	GLU
1	A	1113	VAL
1	A	1125	THR
1	A	1137	PHE
1	A	1163	ASN
1	A	1164	GLN
1	A	1165	SER
1	A	1190	VAL
1	A	1195	TYR
1	A	1201	CYS
1	A	1230	THR
1	A	1231	VAL
1	A	1240	VAL
1	A	1245	LYS
1	A	1247	VAL
1	A	1251	ILE
1	B	226	ASN
1	B	228	HIS
1	B	237	VAL
1	B	241	THR
1	B	245	LEU
1	B	256	LYS
1	B	264	LYS
1	B	265	LEU
1	B	270	LYS
1	B	276	THR

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Mol	Chain	Res	Type
1	B	305	LYS
1	B	306	TYR
1	B	310	GLU
1	B	318	ILE
1	B	421	ASP
1	B	426	LEU
1	B	427	SER
1	B	453	ASN
1	B	486	VAL
1	B	496	THR
1	B	532	ILE
1	B	545	LYS
1	B	561	LEU
1	B	571	ILE
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	894	ARG
1	B	897	ASN
1	B	909	THR
1	B	911	LEU
1	B	920	VAL
1	B	931	GLN
1	B	937	VAL

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Mol	Chain	Res	Type
1	B	951	LEU
1	B	952	SER
1	B	958	LEU
1	B	966	LEU
1	B	995	ASP
1	B	998	THR
1	B	1008	ASP
1	B	1028	ILE
1	B	1031	LYS
1	B	1048	VAL
1	B	1051	ASP
1	B	1085	VAL
1	B	1086	THR
1	B	1108	GLU
1	B	1113	VAL
1	B	1125	THR
1	B	1137	PHE
1	B	1163	ASN
1	B	1165	SER
1	B	1190	VAL
1	B	1195	TYR
1	B	1214	LEU
1	B	1230	THR
1	B	1231	VAL
1	B	1240	VAL
1	B	1245	LYS
1	B	1251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	548	ASN
1	A	780	ASN
1	A	820	ASN
1	B	878	ASN
1	B	882	ASN

5.3.3 RNA (i)

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 monosaccharides 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	904/1046 (86%)	-0.34	11 (1%)	79	67	11, 44, 111, 148	0
1	B	853/1046 (81%)	-0.34	15 (1%)	68	55	8, 44, 108, 150	0
2	E	9/9 (100%)	-0.51	0	100	100	30, 35, 67, 175	0
2	F	9/9 (100%)	-0.53	0	100	100	28, 35, 66, 178	0
All	All	1775/2110 (84%)	-0.34	26 (1%)	73	61	8, 44, 110, 178	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	GLU	4.0
1	B	553	LYS	3.7
1	B	552	GLU	3.3
1	B	554	ASN	3.0
1	B	569	PRO	2.9
1	A	572	ASN	2.8
1	B	220	ALA	2.8
1	A	349	CYS	2.8
1	A	655	ASN	2.7
1	A	865	PRO	2.7
1	A	866	THR	2.6
1	B	389	THR	2.5
1	B	658	VAL	2.4
1	B	388	ILE	2.4
1	B	316	ASP	2.4
1	B	255	GLU	2.3
1	A	636	LYS	2.3
1	A	657	VAL	2.2
1	B	349	CYS	2.2
1	A	314	ASP	2.1
1	B	390	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	589	SER	2.1
1	A	531	ASP	2.1
1	B	303	PRO	2.0
1	B	391	LYS	2.0
1	A	549	TYR	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 monosaccharides 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.