



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 4CDI / pdb\_00004cdi  
Title : Crystal structure of AcrB-AcrZ complex  
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Deposited on : 2013-10-31  
Resolution : 3.70 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

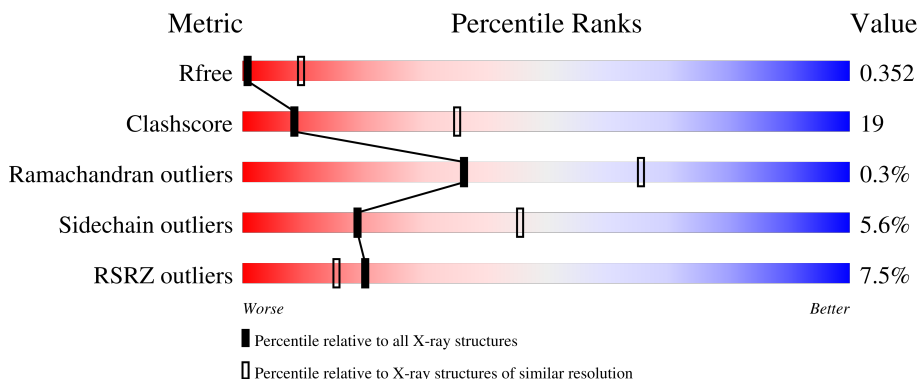
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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  $\geq 3$ , 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	1049	
2	C	49	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8114 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 ACRIFLAVINE RESISTANCE PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1032	7788	5013	1285	1446	44	0	0	0

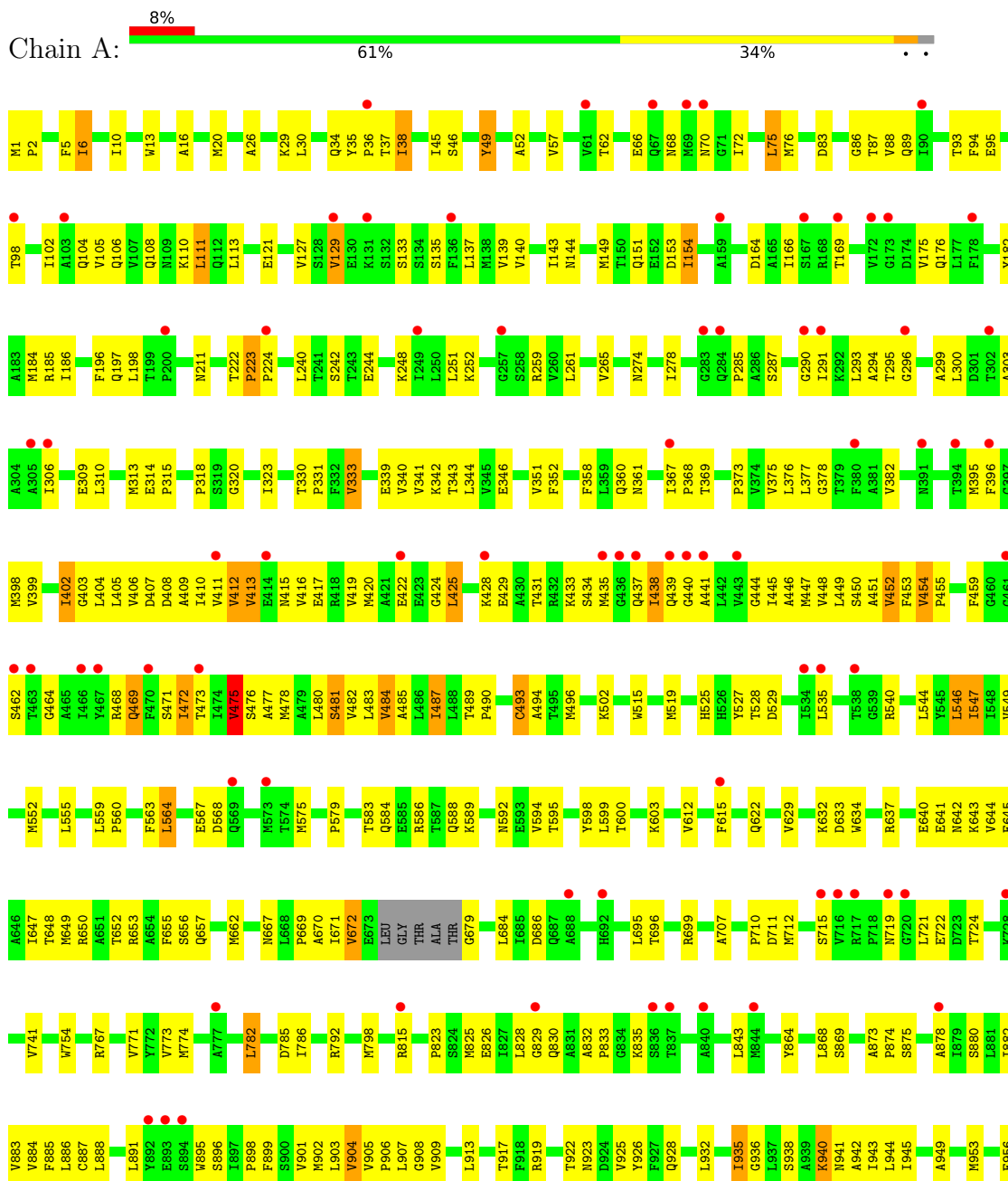
- Molecule 2 is a protein called PREDICTED PROTEIN.

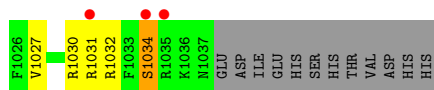
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	46	326	219	48	56	3	0	0	0

### 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.

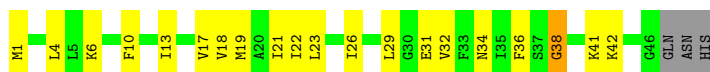
#### • Molecule 1: ACRIFLAVINE RESISTANCE PROTEIN B





- Molecule 2: PREDICTED PROTEIN

Chain C: 53% 39% • 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.21Å 146.21Å 543.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.91 – 3.70 24.91 – 3.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (24.91-3.70) 94.1 (24.91-3.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 3.74Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.339 , 0.361 0.335 , 0.352	Depositor DCC
$R_{free}$ test set	1161 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	142.3	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 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	0.79	0/7936	0.99	11/10780 (0.1%)
2	C	0.81	0/330	1.04	1/448 (0.2%)
All	All	0.79	0/8266	0.99	12/11228 (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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	111	LEU	N-CA-C	-8.12	102.43	111.28
1	A	454	VAL	N-CA-CB	7.78	115.40	110.50
1	A	49	TYR	CA-C-N	5.89	127.48	120.23
1	A	49	TYR	C-N-CA	5.89	127.48	120.23
2	C	38	GLY	N-CA-C	5.64	121.94	112.85
1	A	299	ALA	N-CA-C	5.52	116.98	110.97
1	A	223	PRO	N-CA-C	-5.26	104.28	110.70
1	A	382	VAL	N-CA-C	5.23	116.01	110.72
1	A	782	LEU	CA-C-N	5.23	124.85	119.05
1	A	782	LEU	C-N-CA	5.23	124.85	119.05
1	A	475	VAL	CB-CA-C	-5.20	105.04	112.22
1	A	438	ILE	N-CA-C	5.10	116.40	112.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	THR	Mainchain,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	7788	0	7885	295	0
2	C	326	0	346	24	0
All	All	8114	0	8231	311	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 19.

All (311) 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)
2:C:6:LYS:HG3	2:C:10:PHE:CE2	1.53	1.43
2:C:6:LYS:CG	2:C:10:PHE:HE2	1.52	1.20
1:A:575:MET:HE2	1:A:662:MET:HE2	1.27	1.15
1:A:575:MET:CE	1:A:662:MET:HE2	1.88	1.02
2:C:6:LYS:CG	2:C:10:PHE:CE2	2.35	0.96
1:A:575:MET:CE	1:A:662:MET:CE	2.49	0.89
1:A:884:VAL:HG12	1:A:902:MET:HE1	1.56	0.87
1:A:70:ASN:O	1:A:110:LYS:NZ	2.08	0.86
1:A:555:LEU:HD22	1:A:913:LEU:HB3	1.59	0.85
1:A:960:LEU:HD21	1:A:1030:ARG:HB2	1.58	0.84
2:C:6:LYS:HG3	2:C:10:PHE:HE2	0.69	0.83
2:C:6:LYS:O	2:C:10:PHE:HD2	1.59	0.83
1:A:540:ARG:HD2	2:C:38:GLY:HA3	1.64	0.79
1:A:575:MET:HE1	1:A:662:MET:CE	2.14	0.78
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.66	0.78
2:C:6:LYS:O	2:C:10:PHE:CD2	2.37	0.78
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.73	0.70
1:A:568:ASP:OD1	1:A:634:TRP:NE1	2.24	0.70
1:A:540:ARG:HD2	2:C:38:GLY:CA	2.21	0.70
1:A:684:LEU:HD22	1:A:695:LEU:HD11	1.72	0.70
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:SER:HB3	1:A:1014:ALA:HB1	1.73	0.70
1:A:360:GLN:O	1:A:361:ASN:ND2	2.25	0.69
1:A:632:LYS:O	1:A:637:ARG:NH1	2.25	0.69
1:A:422:GLU:OE1	1:A:422:GLU:N	2.25	0.69
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.75	0.69
1:A:395:MET:HA	1:A:398:MET:HE3	1.73	0.69
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.75	0.68
1:A:454:VAL:HG12	1:A:475:VAL:HG21	1.75	0.68
1:A:137:LEU:HD21	1:A:303:ALA:HB2	1.75	0.67
1:A:633:ASP:OD1	1:A:634:TRP:N	2.27	0.67
1:A:721:LEU:HD13	1:A:815:ARG:HD3	1.75	0.67
1:A:598:TYR:HE2	1:A:629:VAL:HG21	1.61	0.66
1:A:76:MET:HE3	1:A:95:GLU:HA	1.79	0.65
1:A:248:LYS:HA	1:A:261:LEU:HD23	1.79	0.64
1:A:885:PHE:HA	1:A:902:MET:HE3	1.79	0.64
1:A:1030:ARG:O	1:A:1034:SER:OG	2.14	0.64
1:A:898:PRO:O	1:A:901:VAL:HG12	1.98	0.64
1:A:899:PHE:O	1:A:903:LEU:HD12	1.98	0.64
1:A:6:ILE:O	1:A:428:LYS:NZ	2.30	0.63
1:A:451:ALA:HB1	1:A:883:VAL:HG13	1.81	0.63
1:A:546:LEU:O	1:A:549:VAL:HG12	1.99	0.63
1:A:38:ILE:HG22	1:A:462:SER:HB2	1.80	0.63
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.80	0.62
1:A:712:MET:SD	1:A:835:LYS:HE2	2.38	0.62
1:A:402:ILE:O	1:A:406:VAL:HG13	1.99	0.62
1:A:984:LEU:HA	1:A:987:MET:HG2	1.82	0.62
1:A:453:PHE:HB3	1:A:932:LEU:HD22	1.80	0.62
1:A:453:PHE:CE1	1:A:475:VAL:HG22	2.35	0.61
1:A:485:ALA:O	1:A:490:PRO:HD3	2.00	0.61
1:A:358:PHE:CZ	2:C:19:MET:HE1	2.36	0.61
1:A:367:ILE:HG13	1:A:496:MET:HE2	1.83	0.61
1:A:197:GLN:HB3	1:A:798:MET:HE3	1.82	0.61
1:A:110:LYS:HA	1:A:113:LEU:HG	1.83	0.60
1:A:926:TYR:HB3	1:A:1003:VAL:HG23	1.83	0.60
1:A:104:GLN:O	1:A:108:GLN:HG2	2.02	0.60
1:A:37:THR:HG21	1:A:296:GLY:HA2	1.82	0.60
1:A:20:MET:HA	1:A:377:LEU:HD11	1.82	0.60
1:A:903:LEU:O	1:A:906:PRO:HD2	2.02	0.60
1:A:153:ASP:OD1	1:A:182:TYR:OH	2.20	0.59
1:A:404:LEU:HD11	1:A:449:LEU:HD21	1.83	0.59
1:A:375:VAL:CG1	1:A:405:LEU:HD22	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:HE2	1:A:672:VAL:H	1.50	0.59
1:A:898:PRO:O	1:A:902:MET:HG2	2.03	0.59
1:A:679:GLY:HA2	1:A:830:GLN:HB3	1.85	0.58
1:A:884:VAL:HG12	1:A:902:MET:CE	2.30	0.58
1:A:448:VAL:CG2	1:A:884:VAL:HG13	2.34	0.58
1:A:340:VAL:HG12	1:A:395:MET:HE3	1.86	0.58
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.85	0.58
1:A:36:PRO:O	1:A:38:ILE:HG13	2.04	0.57
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.39	0.57
1:A:94:PHE:HB3	1:A:98:THR:HG21	1.86	0.57
1:A:563:PHE:O	1:A:564:LEU:HD23	2.03	0.57
1:A:901:VAL:HG23	1:A:942:ALA:HB3	1.86	0.57
1:A:139:VAL:HG22	1:A:290:GLY:HA2	1.87	0.57
1:A:644:VAL:O	1:A:648:THR:HG23	2.04	0.57
1:A:575:MET:HE2	1:A:662:MET:CE	2.13	0.57
1:A:454:VAL:N	1:A:455:PRO:HD2	2.20	0.56
1:A:544:LEU:HD12	1:A:547:ILE:HG12	1.87	0.56
1:A:110:LYS:HB2	1:A:113:LEU:HD12	1.87	0.56
1:A:712:MET:HG2	1:A:843:LEU:HD22	1.87	0.56
1:A:102:ILE:HA	1:A:105:VAL:HG22	1.87	0.56
2:C:13:ILE:O	2:C:17:VAL:HG23	2.06	0.56
1:A:169:THR:OG1	1:A:309:GLU:OE2	2.23	0.56
1:A:425:LEU:HD12	1:A:429:GLU:HB3	1.87	0.56
1:A:1032:ARG:NH2	2:C:42:LYS:O	2.39	0.56
1:A:653:ARG:O	1:A:656:SER:OG	2.25	0.55
1:A:396:PHE:O	1:A:399:VAL:HG12	2.05	0.55
1:A:568:ASP:OD2	1:A:644:VAL:HG23	2.07	0.55
1:A:560:PRO:HG2	1:A:922:THR:HG22	1.89	0.55
1:A:83:ASP:OD1	1:A:87:THR:OG1	2.24	0.55
1:A:20:MET:HA	1:A:377:LEU:CD1	2.37	0.55
1:A:984:LEU:HD23	1:A:987:MET:HG3	1.90	0.54
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.05	0.54
1:A:196:PHE:O	1:A:252:LYS:NZ	2.27	0.54
1:A:792:ARG:HD3	1:A:798:MET:HE1	1.90	0.54
2:C:6:LYS:CD	2:C:10:PHE:HE2	2.20	0.54
1:A:339:GLU:O	1:A:343:THR:HG23	2.07	0.54
1:A:434:SER:HA	1:A:437:GLN:OE1	2.07	0.54
1:A:2:PRO:O	1:A:6:ILE:HD12	2.07	0.54
1:A:144:ASN:HA	1:A:320:GLY:O	2.08	0.54
1:A:719:ASN:HB2	1:A:828:LEU:HD13	1.89	0.54
1:A:449:LEU:HD13	1:A:936:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:O	1:A:480:LEU:HG	2.08	0.53
1:A:137:LEU:HD13	1:A:293:LEU:HD21	1.90	0.53
1:A:412:VAL:O	1:A:416:VAL:HG23	2.08	0.53
1:A:973:ARG:NH1	1:A:977:MET:SD	2.81	0.53
1:A:721:LEU:HD13	1:A:815:ARG:CD	2.38	0.53
1:A:588:GLN:O	1:A:592:ASN:ND2	2.41	0.53
1:A:974:PRO:O	1:A:978:THR:HG23	2.08	0.53
1:A:358:PHE:CD2	1:A:977:MET:HG2	2.43	0.53
1:A:413:VAL:HA	1:A:493:CYS:SG	2.48	0.53
1:A:415:ASN:ND2	1:A:437:GLN:HE21	2.05	0.53
1:A:464:GLY:O	1:A:468:ARG:HG2	2.09	0.53
1:A:885:PHE:HA	1:A:902:MET:CE	2.39	0.53
1:A:1021:PHE:O	1:A:1024:VAL:HG22	2.09	0.53
1:A:477:ALA:O	1:A:481:SER:HB3	2.08	0.52
1:A:407:ASP:HA	1:A:410:ILE:HG12	1.89	0.52
1:A:971:ARG:NH1	1:A:974:PRO:HB2	2.24	0.52
1:A:398:MET:O	1:A:402:ILE:HG23	2.10	0.52
1:A:932:LEU:O	1:A:935:ILE:HG13	2.09	0.52
1:A:944:LEU:HD12	1:A:971:ARG:HH21	1.74	0.52
1:A:559:LEU:HD23	1:A:923:ASN:HB2	1.91	0.52
1:A:197:GLN:CB	1:A:798:MET:HE3	2.40	0.52
1:A:352:PHE:HD1	1:A:369:THR:HG21	1.73	0.52
1:A:444:GLY:HA3	1:A:891:LEU:HD12	1.91	0.52
1:A:449:LEU:HD23	1:A:478:MET:SD	2.50	0.52
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.91	0.52
1:A:868:LEU:O	1:A:869:SER:OG	2.26	0.52
1:A:1032:ARG:NH1	2:C:41:LYS:CB	2.72	0.52
1:A:10:ILE:O	1:A:13:TRP:N	2.42	0.51
1:A:49:TYR:CD2	1:A:52:ALA:HB2	2.45	0.51
1:A:987:MET:HE2	1:A:1008:MET:HE1	1.92	0.51
1:A:417:GLU:O	1:A:420:MET:HG2	2.10	0.51
1:A:903:LEU:HD22	1:A:1025:PHE:CD1	2.46	0.51
1:A:431:THR:HG21	1:A:494:ALA:HB2	1.93	0.51
1:A:904:VAL:HG11	1:A:1022:VAL:HG22	1.93	0.51
1:A:26:ALA:O	1:A:30:LEU:HB2	2.10	0.51
1:A:880:SER:O	1:A:884:VAL:HG23	2.11	0.51
1:A:997:SER:HA	1:A:1000:GLN:HE22	1.76	0.51
1:A:377:LEU:HD12	1:A:378:GLY:N	2.26	0.51
1:A:527:TYR:OH	1:A:1019:ILE:O	2.29	0.51
2:C:6:LYS:HG3	2:C:10:PHE:CD2	2.30	0.51
1:A:83:ASP:HA	1:A:815:ARG:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:ALA:O	1:A:953:MET:HG2	2.11	0.50
1:A:1013:THR:O	1:A:1017:LEU:HB3	2.11	0.50
1:A:447:MET:O	1:A:450:SER:OG	2.27	0.50
1:A:62:THR:O	1:A:66:GLU:HG3	2.11	0.50
1:A:143:ILE:HD13	1:A:285:PRO:O	2.11	0.50
1:A:449:LEU:CD1	1:A:936:GLY:HA3	2.41	0.50
1:A:35:TYR:OH	1:A:670:ALA:O	2.23	0.50
1:A:143:ILE:HD12	1:A:144:ASN:H	1.75	0.50
1:A:449:LEU:O	1:A:452:VAL:HG22	2.11	0.50
1:A:707:ALA:O	1:A:710:PRO:HD3	2.11	0.50
1:A:919:ARG:HH11	1:A:1005:THR:HG21	1.77	0.50
1:A:410:ILE:HD11	1:A:978:THR:HA	1.93	0.50
1:A:600:THR:O	1:A:603:LYS:NZ	2.42	0.50
1:A:962:GLU:OE1	1:A:962:GLU:N	2.44	0.50
1:A:375:VAL:HG13	1:A:480:LEU:HD12	1.92	0.50
1:A:431:THR:O	1:A:435:MET:HG2	2.12	0.50
1:A:615:PHE:O	1:A:615:PHE:CD1	2.65	0.50
1:A:792:ARG:HB2	1:A:798:MET:HE1	1.94	0.49
1:A:696:THR:HA	1:A:825:MET:HE1	1.95	0.49
1:A:135:SER:OG	1:A:672:VAL:O	2.17	0.49
1:A:198:LEU:HD13	1:A:251:LEU:HD13	1.93	0.49
1:A:453:PHE:HE1	1:A:475:VAL:HG22	1.75	0.49
1:A:989:LEU:HG	1:A:1000:GLN:HB2	1.93	0.49
1:A:102:ILE:O	1:A:106:GLN:HG3	2.13	0.49
1:A:448:VAL:O	1:A:452:VAL:HG13	2.13	0.49
1:A:369:THR:O	1:A:373:PRO:HD2	2.13	0.48
1:A:438:ILE:O	1:A:441:ALA:N	2.41	0.48
1:A:409:ALA:O	1:A:413:VAL:HG13	2.13	0.48
1:A:525:HIS:NE2	1:A:529:ASP:OD2	2.46	0.48
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.48	0.48
1:A:649:MET:O	1:A:652:THR:OG1	2.26	0.48
1:A:913:LEU:O	1:A:917:THR:HG23	2.14	0.48
2:C:18:VAL:HA	2:C:21:ILE:HD12	1.94	0.48
1:A:686:ASP:HB2	1:A:695:LEU:HD22	1.96	0.48
1:A:1:MET:HE3	1:A:487:ILE:HD11	1.96	0.48
1:A:2:PRO:HB2	1:A:435:MET:HG3	1.96	0.48
1:A:440:GLY:O	1:A:891:LEU:HD13	2.14	0.48
1:A:719:ASN:ND2	1:A:826:GLU:OE2	2.47	0.48
2:C:6:LYS:CD	2:C:10:PHE:CE2	2.95	0.48
1:A:437:GLN:HG2	1:A:438:ILE:HG23	1.96	0.48
1:A:940:LYS:HE3	1:A:941:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.96	0.47
1:A:310:LEU:HD21	1:A:323:ILE:HD12	1.95	0.47
1:A:715:SER:O	1:A:829:GLY:HA2	2.14	0.47
1:A:445:ILE:HG22	1:A:943:ILE:HD13	1.97	0.47
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.96	0.47
1:A:415:ASN:O	1:A:419:VAL:HG23	2.15	0.47
1:A:583:THR:HG22	1:A:586:ARG:HD3	1.96	0.47
1:A:641:GLU:O	1:A:650:ARG:NH2	2.41	0.47
1:A:34:GLN:HB3	1:A:333:VAL:CG1	2.45	0.46
1:A:528:THR:HG21	1:A:969:ARG:HD3	1.96	0.46
1:A:314:GLU:N	1:A:314:GLU:OE1	2.48	0.46
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.98	0.46
1:A:586:ARG:O	1:A:589:LYS:HB3	2.14	0.46
1:A:901:VAL:HG23	1:A:942:ALA:CB	2.45	0.46
1:A:151:GLN:HE22	1:A:278:ILE:HG23	1.80	0.46
1:A:433:LYS:O	1:A:437:GLN:OE1	2.34	0.46
1:A:34:GLN:HB3	1:A:333:VAL:HG11	1.97	0.46
1:A:471:SER:O	1:A:475:VAL:HG23	2.16	0.46
1:A:399:VAL:O	1:A:402:ILE:HG13	2.16	0.46
1:A:515:TRP:NE1	1:A:519:MET:SD	2.80	0.46
1:A:137:LEU:CD2	1:A:303:ALA:HB2	2.44	0.46
1:A:873:ALA:N	1:A:874:PRO:HD2	2.30	0.46
1:A:72:ILE:HG22	1:A:106:GLN:HB3	1.99	0.46
1:A:242:SER:OG	1:A:244:GLU:OE1	2.34	0.46
1:A:300:LEU:HD23	1:A:300:LEU:O	2.15	0.46
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.97	0.45
1:A:643:LYS:O	1:A:647:ILE:HG13	2.15	0.45
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.99	0.45
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.98	0.45
1:A:782:LEU:O	1:A:785:ASP:HB2	2.17	0.45
1:A:412:VAL:HB	1:A:438:ILE:HD11	1.97	0.45
1:A:960:LEU:HD21	1:A:1030:ARG:CB	2.37	0.45
1:A:987:MET:HB2	1:A:988:PRO:HD3	1.98	0.45
1:A:438:ILE:O	1:A:439:GLN:C	2.59	0.45
1:A:722:GLU:O	1:A:724:THR:HG23	2.17	0.45
1:A:313:MET:C	1:A:315:PRO:HD2	2.42	0.45
1:A:540:ARG:NH2	2:C:36:PHE:CB	2.80	0.45
1:A:559:LEU:HD12	1:A:560:PRO:HD2	2.00	0.45
1:A:895:TRP:O	1:A:896:SER:OG	2.28	0.45
1:A:1027:VAL:O	1:A:1031:ARG:N	2.45	0.45
1:A:110:LYS:HE2	1:A:110:LYS:HB3	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:N	1:A:290:GLY:O	2.50	0.44
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.51	0.44
1:A:888:LEU:HD13	1:A:901:VAL:HG11	2.00	0.44
1:A:184:MET:HB3	1:A:771:VAL:HG22	1.99	0.44
1:A:352:PHE:CD1	1:A:369:THR:HG21	2.52	0.44
1:A:645:GLU:O	1:A:649:MET:HG2	2.18	0.44
1:A:358:PHE:CG	1:A:977:MET:HG2	2.53	0.44
2:C:23:LEU:HD23	2:C:26:ILE:HD11	1.99	0.44
1:A:16:ALA:O	1:A:20:MET:HG3	2.18	0.44
1:A:72:ILE:HG13	1:A:75:LEU:HD22	2.00	0.44
1:A:402:ILE:HG13	1:A:403:GLY:N	2.33	0.44
1:A:49:TYR:CE1	1:A:121:GLU:HB2	2.53	0.43
1:A:149:MET:HE1	1:A:318:PRO:HG2	1.99	0.43
1:A:407:ASP:OD1	1:A:408:ASP:N	2.51	0.43
1:A:686:ASP:HB3	1:A:823:PRO:HB2	2.00	0.43
1:A:832:ALA:HB1	1:A:833:PRO:HD2	2.00	0.43
1:A:882:ILE:HD13	1:A:882:ILE:HA	1.94	0.43
2:C:31:GLU:O	2:C:34:ASN:HB2	2.18	0.43
1:A:102:ILE:O	1:A:105:VAL:HG22	2.19	0.43
1:A:594:VAL:HG13	1:A:655:PHE:CZ	2.52	0.43
1:A:344:LEU:HD11	1:A:376:LEU:HD22	2.00	0.43
2:C:29:LEU:HA	2:C:32:VAL:HG22	2.00	0.43
1:A:480:LEU:O	1:A:484:VAL:HG13	2.18	0.43
1:A:453:PHE:CD1	1:A:475:VAL:HG22	2.53	0.43
1:A:958:LYS:HE3	1:A:962:GLU:HG2	2.00	0.43
1:A:988:PRO:O	1:A:991:ILE:HG13	2.19	0.43
1:A:973:ARG:O	1:A:974:PRO:C	2.62	0.43
1:A:711:ASP:OD1	1:A:711:ASP:N	2.51	0.43
1:A:992:SER:CB	1:A:1000:GLN:HE21	2.32	0.43
1:A:111:LEU:HD12	1:A:129:VAL:HG23	2.00	0.42
1:A:535:LEU:HD12	1:A:535:LEU:HA	1.87	0.42
1:A:45:ILE:HG12	1:A:129:VAL:HG22	2.01	0.42
1:A:373:PRO:O	1:A:377:LEU:HG	2.18	0.42
1:A:110:LYS:C	1:A:113:LEU:H	2.27	0.42
1:A:403:GLY:O	1:A:406:VAL:HG22	2.19	0.42
1:A:552:MET:SD	1:A:909:VAL:HG21	2.60	0.42
1:A:699:ARG:HD3	1:A:825:MET:HE3	2.01	0.42
1:A:111:LEU:HD11	1:A:127:VAL:HG12	2.01	0.42
1:A:567:GLU:HG2	1:A:998:GLY:HA3	2.01	0.42
1:A:88:VAL:HG12	1:A:89:GLN:N	2.35	0.42
1:A:459:PHE:O	1:A:464:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:O	1:A:472:ILE:HG23	2.19	0.42
1:A:166:ILE:HG22	1:A:175:VAL:HG21	2.01	0.42
1:A:411:VAL:O	1:A:415:ASN:HB2	2.20	0.42
1:A:669:PRO:O	1:A:671:ILE:N	2.53	0.42
1:A:904:VAL:HA	1:A:907:LEU:HG	2.02	0.42
1:A:549:VAL:O	1:A:552:MET:HB3	2.19	0.41
2:C:19:MET:O	2:C:22:ILE:HG13	2.20	0.41
1:A:164:ASP:OD2	1:A:767:ARG:NH2	2.45	0.41
1:A:612:VAL:HG21	1:A:615:PHE:HB3	2.01	0.41
1:A:407:ASP:O	1:A:411:VAL:HG22	2.20	0.41
1:A:944:LEU:HB3	1:A:971:ARG:HE	1.86	0.41
1:A:984:LEU:HA	1:A:987:MET:CG	2.49	0.41
1:A:358:PHE:CE2	2:C:19:MET:HE1	2.55	0.41
1:A:449:LEU:HG	1:A:453:PHE:CE2	2.55	0.41
1:A:669:PRO:C	1:A:671:ILE:N	2.77	0.41
1:A:928:GLN:O	1:A:932:LEU:HD12	2.21	0.41
1:A:166:ILE:HA	1:A:309:GLU:HG2	2.03	0.41
1:A:186:ILE:HB	1:A:773:VAL:HG23	2.03	0.41
1:A:330:THR:O	1:A:333:VAL:N	2.53	0.41
1:A:448:VAL:HG11	1:A:888:LEU:HD21	2.02	0.41
1:A:469:GLN:O	1:A:473:THR:OG1	2.28	0.41
1:A:644:VAL:HG11	1:A:667:ASN:ND2	2.36	0.41
1:A:988:PRO:O	1:A:992:SER:HB2	2.21	0.41
1:A:1008:MET:HE3	1:A:1008:MET:HB2	1.89	0.41
1:A:1024:VAL:HA	1:A:1027:VAL:HG22	2.01	0.41
1:A:886:LEU:HD12	1:A:887:CYS:N	2.36	0.41
1:A:980:LEU:HD21	2:C:19:MET:HB2	2.02	0.41
1:A:294:ALA:O	1:A:295:THR:C	2.64	0.40
2:C:1:MET:O	2:C:4:LEU:HB2	2.21	0.40
1:A:34:GLN:C	1:A:35:TYR:HD1	2.29	0.40
1:A:49:TYR:HE1	1:A:121:GLU:HB2	1.86	0.40
1:A:342:LYS:O	1:A:346:GLU:HG2	2.20	0.40
1:A:399:VAL:HG21	1:A:989:LEU:HD11	2.03	0.40
1:A:185:ARG:HH22	1:A:774:MET:HE2	1.87	0.40
1:A:891:LEU:HD23	1:A:891:LEU:HA	1.96	0.40
1:A:908:GLY:O	1:A:1010:GLY:HA2	2.20	0.40
1:A:396:PHE:HE2	1:A:1003:VAL:HG21	1.87	0.40
1:A:422:GLU:O	1:A:502:LYS:HB2	2.20	0.40
1:A:454:VAL:N	1:A:455:PRO:CD	2.83	0.40
1:A:1012:VAL:HG23	1:A:1013:THR:N	2.36	0.40
1:A:5:PHE:CD2	1:A:487:ILE:HG23	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:SD	1:A:864:TYR:HE2	2.44	0.40
1:A:274:ASN:C	1:A:274:ASN:OD1	2.64	0.40
1:A:875:SER:O	1:A:878:ALA:HB3	2.21	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	1028/1049 (98%)	957 (93%)	68 (7%)	3 (0%)	36	65
2	C	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
All	All	1072/1098 (98%)	999 (93%)	70 (6%)	3 (0%)	36	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	PRO
1	A	224	PRO
1	A	579	PRO

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	823/855 (96%)	775 (94%)	48 (6%)	18	45
2	C	34/41 (83%)	34 (100%)	0	100	100
All	All	857/896 (96%)	809 (94%)	48 (6%)	19	46

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	29	LYS
1	A	38	ILE
1	A	46	SER
1	A	68	ASN
1	A	75	LEU
1	A	93	THR
1	A	129	VAL
1	A	133	SER
1	A	140	VAL
1	A	154	ILE
1	A	259	ARG
1	A	265	VAL
1	A	333	VAL
1	A	341	VAL
1	A	351	VAL
1	A	402	ILE
1	A	412	VAL
1	A	413	VAL
1	A	425	LEU
1	A	452	VAL
1	A	469	GLN
1	A	472	ILE
1	A	475	VAL
1	A	481	SER
1	A	483	LEU
1	A	484	VAL
1	A	487	ILE
1	A	489	THR
1	A	493	CYS
1	A	546	LEU
1	A	547	ILE

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Mol	Chain	Res	Type
1	A	564	LEU
1	A	640	GLU
1	A	657	GLN
1	A	672	VAL
1	A	741	VAL
1	A	904	VAL
1	A	925	VAL
1	A	935	ILE
1	A	940	LYS
1	A	945	ILE
1	A	956	GLU
1	A	986	VAL
1	A	993	THR
1	A	1003	VAL
1	A	1024	VAL
1	A	1034	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	361	ASN
1	A	415	ASN
1	A	517	ASN
1	A	577	GLN
1	A	605	ASN
1	A	701	GLN
1	A	797	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1032/1049 (98%)	0.60	81 (7%) 19   15	104, 120, 120, 120	0
2	C	46/49 (93%)	0.35	0 100   100	120, 120, 120, 120	0
All	All	1078/1098 (98%)	0.59	81 (7%) 20   15	104, 120, 120, 120	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	PHE	5.9
1	A	844	MET	4.4
1	A	1034	SER	4.3
1	A	534	ILE	4.2
1	A	840	ALA	4.1
1	A	136	PHE	4.1
1	A	443	VAL	4.1
1	A	290	GLY	3.8
1	A	715	SER	3.8
1	A	1035	ARG	3.7
1	A	305	ALA	3.7
1	A	535	LEU	3.6
1	A	70	ASN	3.6
1	A	437	GLN	3.6
1	A	436	GLY	3.6
1	A	777	ALA	3.4
1	A	836	SER	3.4
1	A	173	GLY	3.3
1	A	463	THR	3.3
1	A	296	GLY	3.3
1	A	414	GLU	3.1
1	A	717	ARG	3.0
1	A	249	ILE	2.9
1	A	720	GLY	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	90	ILE	2.9
1	A	394	THR	2.9
1	A	440	GLY	2.8
1	A	995	ALA	2.8
1	A	69	MET	2.7
1	A	284	GLN	2.7
1	A	291	ILE	2.7
1	A	67	GLN	2.7
1	A	538	THR	2.7
1	A	200	PRO	2.6
1	A	224	PRO	2.6
1	A	169	THR	2.6
1	A	1031	ARG	2.6
1	A	178	PHE	2.6
1	A	569	GLN	2.6
1	A	615	PHE	2.6
1	A	892	TYR	2.6
1	A	461	GLY	2.5
1	A	131	LYS	2.5
1	A	716	VAL	2.5
1	A	159	ALA	2.5
1	A	439	GLN	2.5
1	A	380	PHE	2.5
1	A	829	GLY	2.5
1	A	172	VAL	2.5
1	A	306	ILE	2.4
1	A	893	GLU	2.4
1	A	573	MET	2.4
1	A	257	GLY	2.4
1	A	367	ILE	2.4
1	A	719	ASN	2.4
1	A	283	GLY	2.3
1	A	466	ILE	2.3
1	A	98	THR	2.3
1	A	411	VAL	2.3
1	A	728	LYS	2.3
1	A	878	ALA	2.2
1	A	435	MET	2.2
1	A	473	THR	2.2
1	A	36	PRO	2.2
1	A	61	VAL	2.2
1	A	428	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	129	VAL	2.2
1	A	692	HIS	2.2
1	A	837	THR	2.1
1	A	441	ALA	2.1
1	A	894	SER	2.1
1	A	467	TYR	2.1
1	A	688	ALA	2.1
1	A	167	SER	2.1
1	A	462	SER	2.1
1	A	396	PHE	2.1
1	A	391	ASN	2.1
1	A	815	ARG	2.0
1	A	302	THR	2.0
1	A	422	GLU	2.0
1	A	103	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.