



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:53 PM GMT

PDB ID : 1HQZ  
Title : Cofilin homology domain of a yeast actin-binding protein ABP1P  
Authors : Strokopytov, B.V.; Fedorov, A.A.; Mahoney, N.; Drubin, D.G.; Almo, S.C.;  
Burley, S.K.; New York SGX Research Center for Structural Genomics (NYS-GXRC)  
Deposited on : 2000-12-20  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

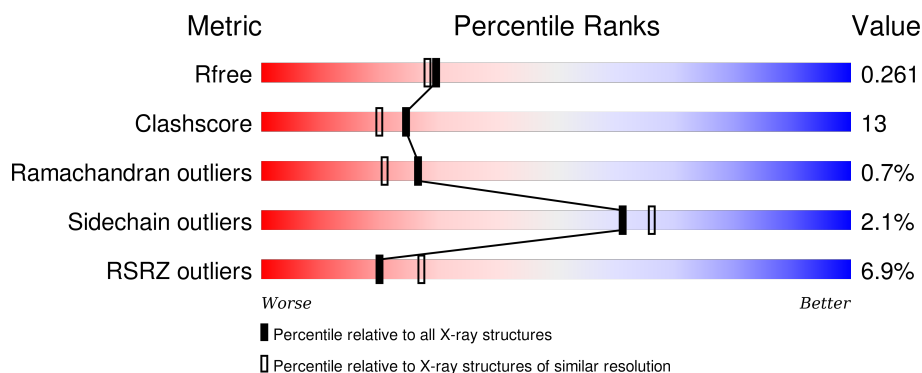
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	141	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
1	2	141	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>..</div> </div> </div>
1	3	141	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>..</div> </div> </div>
1	4	141	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	5	141	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	6	141	<div><div></div><div>5%</div><div>72%</div><div>23%</div><div></div><div></div></div>
1	7	141	<div><div></div><div>12%</div><div>69%</div><div>24%</div><div></div><div>• 5%</div></div>
1	8	141	<div><div></div><div>4%</div><div>71%</div><div>20%</div><div></div><div>• 6%</div></div>
1	9	141	<div><div></div><div>9%</div><div>77%</div><div>18%</div><div></div><div>• •</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10178 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 ACTIN-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	139	Total	C	N	O	S	0	0	0
			1089	689	179	219	2			
1	2	139	Total	C	N	O	S	0	0	0
			1089	689	179	219	2			
1	3	135	Total	C	N	O	S	0	0	0
			1069	678	175	214	2			
1	4	137	Total	C	N	O	S	0	0	0
			1079	684	177	216	2			
1	5	136	Total	C	N	O	S	0	0	0
			1074	681	176	215	2			
1	6	137	Total	C	N	O	S	0	0	0
			1079	684	177	216	2			
1	7	134	Total	C	N	O	S	0	0	0
			1060	674	173	211	2			
1	8	132	Total	C	N	O	S	0	0	0
			1044	663	171	208	2			
1	9	137	Total	C	N	O	S	0	0	0
			1079	684	177	216	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	67	Total	O	0	0
			67	67		
2	2	55	Total	O	0	0
			55	55		
2	3	54	Total	O	0	0
			54	54		
2	4	72	Total	O	0	0
			72	72		
2	5	47	Total	O	0	0
			47	47		

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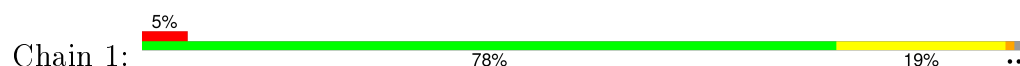
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6	45	Total 45	O 45	0	0
2	7	40	Total 40	O 40	0	0
2	8	75	Total 75	O 75	0	0
2	9	61	Total 61	O 61	0	0

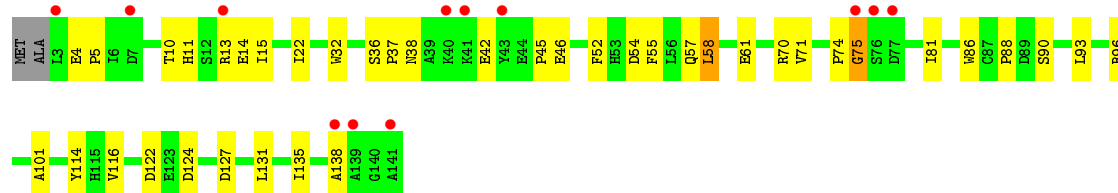
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

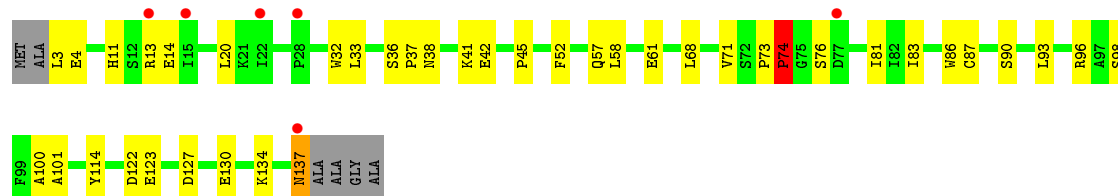
#### • Molecule 1: ACTIN-BINDING PROTEIN



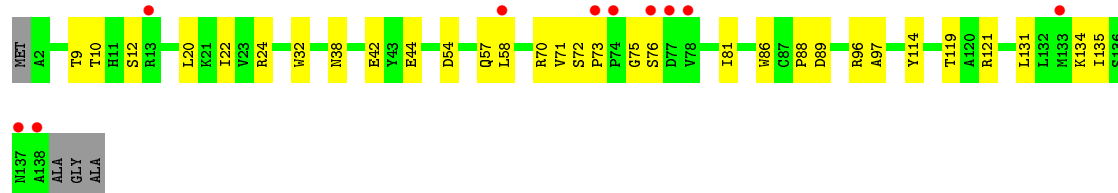
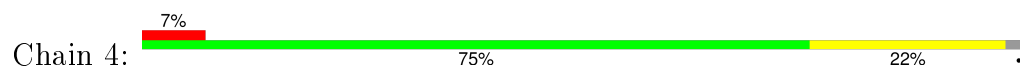
#### • Molecule 1: ACTIN-BINDING PROTEIN



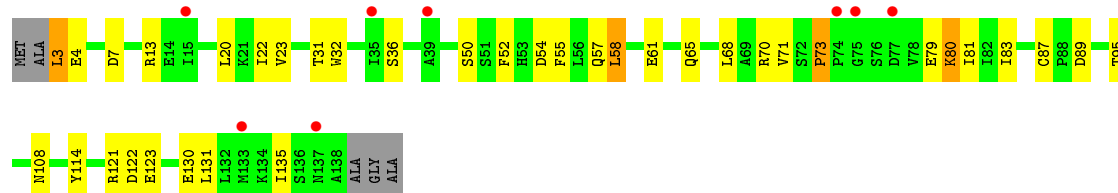
#### • Molecule 1: ACTIN-BINDING PROTEIN



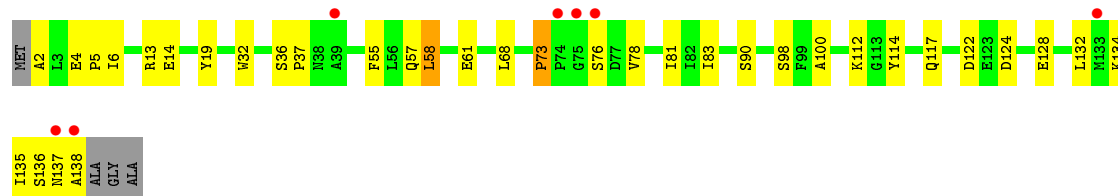
#### • Molecule 1: ACTIN-BINDING PROTEIN



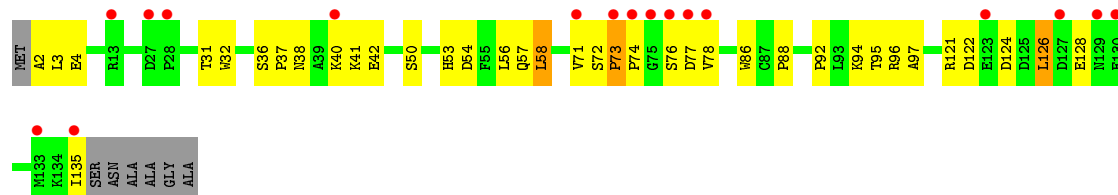
#### • Molecule 1: ACTIN-BINDING PROTEIN



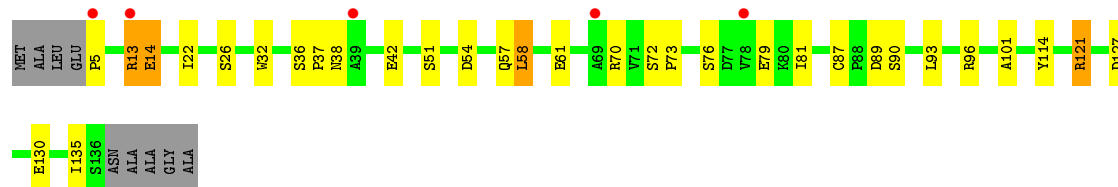
• Molecule 1: ACTIN-BINDING PROTEIN



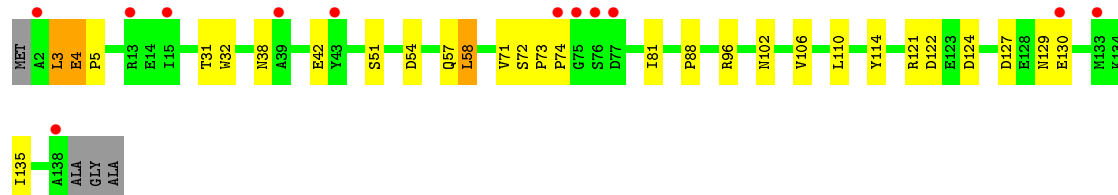
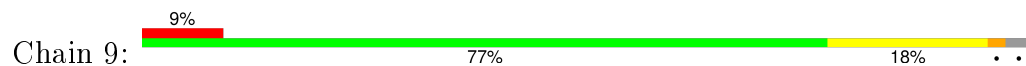
• Molecule 1: ACTIN-BINDING PROTEIN



• Molecule 1: ACTIN-BINDING PROTEIN



• Molecule 1: ACTIN-BINDING PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.48Å 66.68Å 125.10Å 90.00° 108.26° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 14.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (15.00-2.10) 96.1 (14.96-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.213 , 0.259 0.215 , 0.261	Depositor DCC
$R_{free}$ test set	6947 reflections (10.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 68718 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1	0.37	0/1114	0.60	0/1514
1	2	0.35	0/1114	0.58	0/1514
1	3	0.36	0/1094	0.59	0/1488
1	4	0.38	0/1104	0.58	0/1502
1	5	0.36	0/1099	0.58	0/1495
1	6	0.35	0/1104	0.56	0/1502
1	7	0.34	0/1085	0.57	0/1476
1	8	0.37	0/1069	0.59	0/1453
1	9	0.36	0/1104	0.58	0/1502
All	All	0.36	0/9887	0.58	0/13446

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1	1089	0	1048	22	0
1	2	1089	0	1048	40	0
1	3	1069	0	1030	30	0
1	4	1079	0	1040	26	0
1	5	1074	0	1035	36	0
1	6	1079	0	1040	26	0
1	7	1060	0	1024	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	1044	0	1008	26	1
1	9	1079	0	1040	27	0
2	1	67	0	0	2	0
2	2	55	0	0	4	0
2	3	54	0	0	1	0
2	4	72	0	0	1	0
2	5	47	0	0	6	0
2	6	45	0	0	1	0
2	7	40	0	0	1	0
2	8	75	0	0	8	0
2	9	61	0	0	2	0
All	All	10178	0	9313	245	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (245) 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)
1:2:58:LEU:HD13	1:7:3:LEU:HD11	1.29	1.13
1:9:71:VAL:HG11	1:9:135:ILE:HD13	1.47	0.96
1:9:127:ASP:HB3	1:9:130:GLU:HG2	1.49	0.92
1:7:73:PRO:HB3	1:7:135:ILE:HG22	1.54	0.90
1:2:32:TRP:HH2	1:2:58:LEU:HD12	1.39	0.86
1:8:96:ARG:O	2:8:9206:HOH:O	1.94	0.84
1:8:127:ASP:OD2	1:8:130:GLU:HG2	1.81	0.80
1:5:32:TRP:HH2	1:5:58:LEU:HD12	1.47	0.80
2:5:9305:HOH:O	1:6:138:ALA:HA	1.82	0.78
1:4:32:TRP:HH2	1:4:58:LEU:HD12	1.48	0.77
1:4:73:PRO:HG3	1:4:135:ILE:HG22	1.67	0.76
1:9:73:PRO:HG3	1:9:135:ILE:HG22	1.66	0.76
1:4:20:LEU:O	1:4:24:ARG:HB2	1.86	0.76
1:4:32:TRP:CH2	1:4:58:LEU:HD12	2.21	0.75
1:4:76:SER:HA	1:6:76:SER:HB3	1.69	0.75
1:5:3:LEU:HD23	1:5:4:GLU:H	1.51	0.74
1:7:96:ARG:O	2:8:9206:HOH:O	2.05	0.73
1:2:38:ASN:HD21	1:2:42:GLU:HB2	1.51	0.73
1:9:127:ASP:HB3	1:9:130:GLU:CG	2.19	0.73
1:2:116:VAL:HG21	1:2:135:ILE:HA	1.70	0.73
1:5:71:VAL:HG21	1:5:135:ILE:HD13	1.71	0.72
1:2:58:LEU:HD21	1:8:93:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:116:VAL:HG22	1:2:138:ALA:HB3	1.72	0.71
1:3:38:ASN:HD21	1:3:42:GLU:HB2	1.55	0.71
1:2:32:TRP:CH2	1:2:58:LEU:HD12	2.24	0.70
1:9:58:LEU:HD11	2:9:9703:HOH:O	1.90	0.70
1:9:32:TRP:HH2	1:9:58:LEU:HD12	1.55	0.70
1:9:38:ASN:HD21	1:9:42:GLU:HB2	1.57	0.69
1:7:97:ALA:HA	2:8:9206:HOH:O	1.92	0.69
1:1:22:ILE:O	1:1:70:ARG:HD2	1.93	0.68
1:2:38:ASN:ND2	1:2:42:GLU:HB2	2.08	0.67
1:1:76:SER:OG	1:1:78:VAL:HG12	1.95	0.67
1:3:123:GLU:HG3	2:3:9607:HOH:O	1.94	0.66
1:2:122:ASP:OD1	1:2:124:ASP:HB2	1.97	0.65
1:2:138:ALA:HB2	2:2:9480:HOH:O	1.97	0.64
1:3:13:ARG:HH12	1:5:13:ARG:CZ	2.10	0.64
1:2:70:ARG:HD3	2:2:9373:HOH:O	1.97	0.64
1:5:130:GLU:HB2	2:5:9361:HOH:O	1.97	0.63
1:2:57:GLN:C	1:2:58:LEU:HD23	2.19	0.63
1:5:52:PHE:CD1	1:5:71:VAL:HG11	2.33	0.63
1:3:38:ASN:ND2	1:3:42:GLU:HB2	2.13	0.63
1:7:3:LEU:HD23	1:7:94:LYS:HG2	1.81	0.63
1:8:89:ASP:OD2	1:8:121:ARG:NH1	2.31	0.62
1:5:32:TRP:CH2	1:5:58:LEU:HD12	2.34	0.62
1:1:57:GLN:C	1:1:58:LEU:HD23	2.20	0.62
1:6:32:TRP:HH2	1:6:58:LEU:HD12	1.64	0.62
1:2:58:LEU:HD23	1:2:58:LEU:N	2.14	0.61
1:4:57:GLN:C	1:4:58:LEU:HD23	2.20	0.61
1:6:73:PRO:HB3	1:6:136:SER:OG	2.01	0.61
1:5:108:ASN:HB3	2:5:9669:HOH:O	1.99	0.61
1:5:61:GLU:HG3	2:5:9467:HOH:O	2.01	0.61
1:7:126:LEU:HD23	1:7:126:LEU:N	2.15	0.61
1:3:3:LEU:HD21	2:4:9551:HOH:O	1.99	0.60
1:8:32:TRP:HH2	1:8:58:LEU:HD12	1.65	0.60
1:3:73:PRO:HG2	1:3:76:SER:HB3	1.82	0.60
1:1:3:LEU:O	1:1:5:PRO:HD3	2.00	0.60
1:1:13:ARG:HB2	2:1:9412:HOH:O	2.00	0.60
1:4:54:ASP:O	1:4:58:LEU:HG	2.02	0.60
1:2:58:LEU:HD13	1:7:3:LEU:CD1	2.18	0.60
1:9:38:ASN:ND2	1:9:42:GLU:HB2	2.17	0.59
1:5:68:LEU:CD1	1:5:83:ILE:HG22	2.32	0.59
1:2:10:THR:HG21	1:2:42:GLU:OE2	2.01	0.59
1:3:32:TRP:CH2	1:3:58:LEU:HD12	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:13:ARG:HB3	1:8:14:GLU:OE1	2.03	0.58
1:6:73:PRO:HG3	1:6:135:ILE:HG22	1.85	0.58
1:8:58:LEU:HD23	1:8:58:LEU:N	2.18	0.58
1:5:22:ILE:O	1:5:70:ARG:HD2	2.03	0.58
1:5:122:ASP:HB2	2:5:9492:HOH:O	2.03	0.57
1:8:73:PRO:HG2	1:8:76:SER:OG	2.04	0.57
1:5:54:ASP:OD1	1:5:58:LEU:HD21	2.04	0.57
1:9:81:ILE:HB	1:9:114:TYR:HA	1.87	0.57
1:5:3:LEU:CD2	1:5:4:GLU:H	2.17	0.57
1:5:58:LEU:N	1:5:58:LEU:HD23	2.20	0.57
1:5:123:GLU:HG2	2:5:9492:HOH:O	2.05	0.56
1:2:52:PHE:CE1	1:2:71:VAL:HG21	2.40	0.56
1:8:72:SER:HB2	1:8:79:GLU:OE1	2.05	0.56
1:1:13:ARG:HB3	1:1:14:GLU:OE1	2.06	0.56
1:9:71:VAL:CG1	1:9:135:ILE:HD13	2.26	0.56
1:3:4:GLU:OE2	1:3:41:LYS:HD3	2.06	0.56
1:4:76:SER:HA	1:6:76:SER:CB	2.36	0.55
1:3:101:ALA:HB2	1:4:121:ARG:HD3	1.89	0.54
1:4:58:LEU:N	1:4:58:LEU:HD23	2.23	0.54
1:1:32:TRP:HH2	1:1:58:LEU:HD12	1.72	0.54
1:2:127:ASP:O	1:2:131:LEU:HD23	2.08	0.54
1:6:128:GLU:O	1:6:132:LEU:HG	2.08	0.54
1:7:4:GLU:OE1	1:7:95:THR:HG22	2.08	0.54
1:9:32:TRP:CH2	1:9:58:LEU:HD12	2.41	0.54
1:1:58:LEU:HD23	1:1:58:LEU:N	2.23	0.53
1:8:38:ASN:HD21	1:8:42:GLU:HB2	1.73	0.53
1:4:71:VAL:HG12	1:4:72:SER:N	2.23	0.53
1:2:13:ARG:HB3	1:2:14:GLU:OE1	2.07	0.53
1:7:32:TRP:HH2	1:7:58:LEU:HD12	1.72	0.53
1:5:71:VAL:CG2	1:5:135:ILE:HD13	2.38	0.53
1:7:54:ASP:O	1:7:58:LEU:HG	2.10	0.52
1:9:3:LEU:O	1:9:5:PRO:HD3	2.09	0.52
1:5:4:GLU:OE1	1:5:95:THR:HG22	2.09	0.52
1:4:89:ASP:OD2	1:4:121:ARG:NH1	2.43	0.52
1:8:26:SER:HB3	2:8:9713:HOH:O	2.09	0.52
1:2:52:PHE:CD1	1:2:71:VAL:HG21	2.45	0.52
1:8:51:SER:HB3	1:8:54:ASP:OD2	2.10	0.52
1:5:68:LEU:HD13	1:5:83:ILE:HG22	1.92	0.52
1:1:38:ASN:HD21	1:1:42:GLU:HB2	1.73	0.52
1:3:57:GLN:C	1:3:58:LEU:HD23	2.30	0.52
1:3:81:ILE:HB	1:3:114:TYR:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:71:VAL:HG11	1:9:135:ILE:CD1	2.32	0.51
1:4:88:PRO:O	1:4:96:ARG:HD3	2.09	0.51
1:7:36:SER:OG	1:7:37:PRO:HD2	2.11	0.51
1:6:134:LYS:O	1:6:137:ASN:HB3	2.10	0.51
1:3:58:LEU:HD23	1:3:58:LEU:N	2.25	0.51
1:9:102:ASN:O	1:9:106:VAL:HG23	2.10	0.51
1:2:22:ILE:O	1:2:70:ARG:HD2	2.11	0.51
1:7:58:LEU:N	1:7:58:LEU:HD23	2.25	0.51
1:4:73:PRO:HG3	1:4:135:ILE:CG2	2.38	0.50
1:1:14:GLU:OE1	1:1:14:GLU:N	2.45	0.50
1:9:58:LEU:HD23	1:9:58:LEU:N	2.27	0.50
1:3:137:ASN:HD22	1:3:137:ASN:C	2.13	0.50
1:7:31:THR:OG1	1:7:50:SER:HA	2.10	0.50
1:2:46:GLU:HG3	1:7:2:ALA:O	2.11	0.50
1:6:122:ASP:OD1	1:6:124:ASP:HB2	2.12	0.50
1:1:36:SER:OG	1:1:37:PRO:HD2	2.10	0.49
1:3:127:ASP:OD2	1:3:130:GLU:HG2	2.12	0.49
1:6:61:GLU:O	1:6:90:SER:HB2	2.12	0.49
1:8:57:GLN:C	1:8:58:LEU:HD23	2.33	0.49
1:8:38:ASN:ND2	1:8:42:GLU:HB2	2.28	0.49
1:4:81:ILE:HB	1:4:114:TYR:HA	1.94	0.49
1:3:36:SER:OG	1:3:37:PRO:HD2	2.12	0.49
1:3:13:ARG:HB3	1:3:14:GLU:OE1	2.12	0.49
1:8:32:TRP:CH2	1:8:58:LEU:HD12	2.47	0.49
1:2:36:SER:OG	1:2:37:PRO:HD2	2.12	0.49
1:5:57:GLN:C	1:5:58:LEU:HD23	2.33	0.49
1:3:32:TRP:HH2	1:3:58:LEU:HD12	1.76	0.49
1:2:70:ARG:HD3	2:2:9632:HOH:O	2.11	0.49
1:2:15:ILE:HG12	1:2:45:PRO:HD3	1.95	0.48
1:7:86:TRP:HZ3	1:7:126:LEU:HD21	1.78	0.48
1:6:57:GLN:C	1:6:58:LEU:HD23	2.33	0.48
1:9:31:THR:HG21	2:9:9589:HOH:O	2.13	0.48
1:8:81:ILE:HB	1:8:114:TYR:HA	1.95	0.48
1:8:87:CYS:SG	1:8:96:ARG:HG2	2.53	0.48
1:4:10:THR:HG21	1:4:42:GLU:OE2	2.14	0.48
1:7:57:GLN:C	1:7:58:LEU:HD23	2.34	0.47
1:1:38:ASN:ND2	1:1:42:GLU:HB2	2.28	0.47
1:3:134:LYS:HA	1:3:137:ASN:HD21	1.79	0.47
1:9:88:PRO:O	1:9:96:ARG:HD3	2.13	0.47
1:6:2:ALA:O	1:6:5:PRO:HD3	2.15	0.47
1:3:61:GLU:O	1:3:90:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:132:LEU:HA	1:6:135:ILE:HD12	1.97	0.47
1:4:86:TRP:CD1	1:4:88:PRO:HD3	2.49	0.47
1:1:121:ARG:CD	1:2:101:ALA:HA	2.45	0.47
1:4:131:LEU:HD23	1:4:134:LYS:HD2	1.97	0.47
1:2:86:TRP:CD1	1:2:88:PRO:HD3	2.49	0.47
1:3:3:LEU:HD12	1:3:98:SER:OG	2.15	0.47
1:7:38:ASN:HD21	1:7:42:GLU:HB2	1.80	0.46
1:2:81:ILE:HB	1:2:114:TYR:HA	1.97	0.46
1:9:127:ASP:CB	1:9:130:GLU:HG2	2.35	0.46
1:5:52:PHE:O	1:5:55:PHE:HB3	2.15	0.46
1:5:89:ASP:OD1	1:5:121:ARG:HD3	2.14	0.46
1:3:73:PRO:HB2	1:3:74:PRO:HD2	1.98	0.46
1:3:87:CYS:SG	1:3:96:ARG:HG2	2.56	0.46
1:2:46:GLU:HG2	2:2:9303:HOH:O	2.14	0.46
1:9:57:GLN:C	1:9:58:LEU:HD23	2.37	0.46
1:9:122:ASP:OD1	1:9:124:ASP:HB2	2.16	0.46
1:6:36:SER:OG	1:6:37:PRO:HD2	2.16	0.46
1:6:32:TRP:CE3	1:6:55:PHE:HD1	2.34	0.45
1:6:58:LEU:N	1:6:58:LEU:HD23	2.31	0.45
1:6:132:LEU:HD23	1:6:135:ILE:HD12	1.98	0.45
1:1:80:LYS:C	1:1:81:ILE:HD12	2.36	0.45
1:8:5:PRO:HD3	2:8:9523:HOH:O	2.17	0.45
1:2:54:ASP:O	1:2:58:LEU:HG	2.17	0.45
1:7:40:LYS:O	1:7:41:LYS:HB2	2.17	0.44
1:5:68:LEU:HD12	1:5:83:ILE:HG22	1.99	0.44
1:6:13:ARG:HB3	1:6:14:GLU:OE1	2.18	0.44
1:3:68:LEU:CD1	1:3:83:ILE:HG22	2.48	0.44
1:5:73:PRO:HG3	1:5:135:ILE:HG22	1.99	0.44
1:7:71:VAL:HG12	1:7:72:SER:N	2.33	0.44
1:5:31:THR:OG1	1:5:50:SER:HA	2.18	0.44
1:7:86:TRP:CD1	1:7:88:PRO:HD3	2.53	0.44
1:7:122:ASP:OD1	1:7:124:ASP:HB2	2.17	0.44
1:3:20:LEU:HD21	1:5:20:LEU:HD21	1.99	0.44
1:9:71:VAL:HG22	1:9:72:SER:N	2.33	0.44
1:1:81:ILE:HD12	1:1:81:ILE:N	2.33	0.44
1:7:92:PRO:HG2	2:7:9604:HOH:O	2.17	0.44
1:7:53:HIS:HD2	1:7:128:GLU:OE2	2.01	0.44
1:3:100:ALA:HA	1:4:119:THR:HG21	2.00	0.44
1:8:127:ASP:HB3	1:8:130:GLU:HB2	2.00	0.43
1:7:121:ARG:HD2	1:8:101:ALA:HA	1.99	0.43
1:6:81:ILE:HB	1:6:114:TYR:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:51:SER:HB3	1:9:54:ASP:OD2	2.18	0.43
1:9:73:PRO:HA	1:9:74:PRO:HD3	1.93	0.43
1:2:10:THR:HG22	1:2:11:HIS:CE1	2.54	0.43
1:5:71:VAL:HG23	1:5:135:ILE:HG21	2.00	0.43
1:4:22:ILE:O	1:4:70:ARG:HD2	2.18	0.43
1:5:70:ARG:NE	1:5:79:GLU:OE1	2.50	0.43
1:4:70:ARG:HA	1:4:81:ILE:HD13	2.01	0.43
1:7:76:SER:C	1:7:78:VAL:H	2.22	0.43
1:1:128:GLU:O	1:1:132:LEU:HG	2.18	0.43
1:3:86:TRP:CH2	1:3:122:ASP:HA	2.54	0.43
1:9:127:ASP:HB3	1:9:130:GLU:CD	2.38	0.43
1:6:76:SER:OG	1:6:78:VAL:HG22	2.19	0.43
1:5:3:LEU:HD23	1:5:4:GLU:N	2.28	0.43
1:6:6:ILE:HA	2:6:9576:HOH:O	2.19	0.43
1:2:14:GLU:OE1	1:2:14:GLU:N	2.51	0.42
1:8:61:GLU:O	1:8:90:SER:HB2	2.19	0.42
1:8:22:ILE:HA	2:8:9424:HOH:O	2.19	0.42
1:8:70:ARG:HD2	2:8:9424:HOH:O	2.19	0.42
1:3:93:LEU:HD12	1:4:97:ALA:HB1	2.01	0.42
1:6:19:TYR:OH	1:6:112:LYS:O	2.25	0.42
1:3:11:HIS:HE1	1:3:42:GLU:OE1	2.02	0.42
1:7:56:LEU:HD22	1:7:126:LEU:HB2	2.01	0.42
1:8:96:ARG:C	2:8:9206:HOH:O	2.48	0.42
1:1:121:ARG:HD2	1:2:101:ALA:HA	2.00	0.42
1:1:116:VAL:HG21	1:1:135:ILE:HA	2.02	0.42
1:2:15:ILE:CG1	1:2:45:PRO:HD3	2.50	0.42
1:6:2:ALA:HB1	1:6:98:SER:HB3	2.01	0.42
1:5:36:SER:CB	1:5:65:GLN:HE21	2.32	0.42
1:3:52:PHE:CD1	1:3:71:VAL:HG21	2.55	0.42
1:5:3:LEU:CD2	1:5:4:GLU:N	2.82	0.41
1:4:38:ASN:HB3	1:4:44:GLU:OE1	2.20	0.41
1:5:131:LEU:O	1:5:135:ILE:HG13	2.20	0.41
1:6:68:LEU:HD13	1:6:83:ILE:HG22	2.02	0.41
1:1:51:SER:HB3	2:1:9546:HOH:O	2.20	0.41
1:3:33:LEU:HD11	1:3:45:PRO:HB3	2.02	0.41
1:2:10:THR:HG22	1:2:10:THR:O	2.21	0.41
1:4:38:ASN:ND2	1:4:42:GLU:HB2	2.35	0.41
1:2:61:GLU:O	1:2:90:SER:HB2	2.19	0.41
1:7:126:LEU:H	1:7:126:LEU:HD23	1.84	0.41
1:1:97:ALA:CB	1:2:93:LEU:HD12	2.50	0.41
1:1:86:TRP:CD1	1:1:88:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:36:SER:OG	1:8:37:PRO:HD2	2.20	0.41
1:7:4:GLU:OE1	1:7:95:THR:CG2	2.67	0.41
1:9:3:LEU:O	1:9:5:PRO:CD	2.68	0.41
1:4:9:THR:HA	1:4:12:SER:HB3	2.02	0.41
1:2:74:PRO:O	1:2:75:GLY:C	2.58	0.41
1:2:52:PHE:O	1:2:55:PHE:HB3	2.21	0.41
1:5:80:LYS:N	1:5:80:LYS:HD2	2.36	0.41
1:5:23:VAL:HG12	1:5:81:ILE:HD13	2.02	0.41
1:8:135:ILE:O	1:8:135:ILE:HG22	2.21	0.41
1:2:88:PRO:O	1:2:96:ARG:HD3	2.21	0.40
1:1:27:ASP:HA	1:1:28:PRO:HD2	1.90	0.40
1:5:87:CYS:HB3	1:6:100:ALA:CB	2.52	0.40
1:2:4:GLU:HA	1:2:5:PRO:HD3	1.87	0.40
1:7:126:LEU:CD2	1:7:126:LEU:N	2.84	0.40
1:5:83:ILE:HG23	1:5:114:TYR:HB3	2.03	0.40
1:9:4:GLU:HA	1:9:5:PRO:HD2	1.94	0.40
1:6:83:ILE:HD11	1:6:117:GLN:HG3	2.04	0.40
1:4:75:GLY:HA2	1:9:129:ASN:OD1	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:13:ARG:NH2	1:8:13:ARG:NH2[2_655]	2.14	0.06

## 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	1	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
1	2	137/141 (97%)	132 (96%)	4 (3%)	1 (1%)	26	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	133/141 (94%)	125 (94%)	7 (5%)	1 (1%)	24	17
1	4	135/141 (96%)	130 (96%)	5 (4%)	0	100	100
1	5	134/141 (95%)	127 (95%)	6 (4%)	1 (1%)	26	21
1	6	135/141 (96%)	132 (98%)	2 (2%)	1 (1%)	26	21
1	7	132/141 (94%)	125 (95%)	4 (3%)	3 (2%)	8	3
1	8	130/141 (92%)	129 (99%)	1 (1%)	0	100	100
1	9	135/141 (96%)	131 (97%)	3 (2%)	1 (1%)	26	21
All	All	1208/1269 (95%)	1165 (96%)	35 (3%)	8 (1%)	26	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	74	PRO
1	2	75	GLY
1	7	77	ASP
1	5	73	PRO
1	7	73	PRO
1	6	73	PRO
1	9	4	GLU
1	7	74	PRO

### 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	1	118/119 (99%)	115 (98%)	3 (2%)	55	59
1	2	118/119 (99%)	117 (99%)	1 (1%)	86	91
1	3	118/119 (99%)	116 (98%)	2 (2%)	68	74
1	4	118/119 (99%)	118 (100%)	0	100	100
1	5	118/119 (99%)	114 (97%)	4 (3%)	44	45
1	6	118/119 (99%)	116 (98%)	2 (2%)	68	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	116/119 (98%)	114 (98%)	2 (2%)	68	74
1	8	115/119 (97%)	111 (96%)	4 (4%)	43	44
1	9	118/119 (99%)	114 (97%)	4 (3%)	44	45
All	All	1057/1071 (99%)	1035 (98%)	22 (2%)	61	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	3	LEU
1	1	58	LEU
1	1	130	GLU
1	2	58	LEU
1	3	74	PRO
1	3	137	ASN
1	5	3	LEU
1	5	7	ASP
1	5	58	LEU
1	5	80	LYS
1	6	4	GLU
1	6	58	LEU
1	7	58	LEU
1	7	126	LEU
1	8	13	ARG
1	8	14	GLU
1	8	58	LEU
1	8	121	ARG
1	9	3	LEU
1	9	58	LEU
1	9	110	LEU
1	9	121	ARG

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

Mol	Chain	Res	Type
1	1	117	GLN
1	2	117	GLN
1	3	11	HIS
1	3	137	ASN
1	4	53	HIS
1	5	11	HIS

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Mol	Chain	Res	Type
1	5	53	HIS
1	5	129	ASN
1	6	129	ASN
1	7	53	HIS
1	9	53	HIS
1	9	137	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1	139/141 (98%)	0.24	7 (5%) 32 41	27, 41, 62, 71	0
1	2	139/141 (98%)	0.48	12 (8%) 13 18	30, 44, 68, 81	0
1	3	135/141 (95%)	0.30	6 (4%) 38 47	27, 44, 61, 71	0
1	4	137/141 (97%)	0.31	10 (7%) 18 24	25, 38, 74, 86	0
1	5	136/141 (96%)	0.49	8 (5%) 26 34	27, 42, 72, 82	0
1	6	137/141 (97%)	0.35	7 (5%) 32 40	29, 44, 78, 83	0
1	7	134/141 (95%)	0.78	17 (12%) 5 6	28, 51, 80, 92	0
1	8	132/141 (93%)	0.18	5 (3%) 44 53	28, 40, 55, 59	0
1	9	137/141 (97%)	0.50	12 (8%) 12 17	28, 43, 72, 85	0
All	All	1226/1269 (96%)	0.40	84 (6%) 20 27	25, 43, 71, 92	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	7	76	SER	9.3
1	7	75	GLY	8.1
1	9	74	PRO	7.7
1	7	74	PRO	7.6
1	6	74	PRO	6.4
1	2	138	ALA	6.2
1	5	74	PRO	6.0
1	7	77	ASP	5.2
1	7	133	MET	5.0
1	2	3	LEU	5.0
1	1	3	LEU	4.7
1	7	28	PRO	4.6
1	4	74	PRO	4.5
1	7	73	PRO	4.3
1	6	138	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	5	39	ALA	4.3
1	7	13	ARG	4.2
1	4	78	VAL	4.2
1	1	77	ASP	4.0
1	5	77	ASP	4.0
1	4	138	ALA	4.0
1	6	75	GLY	4.0
1	4	76	SER	3.9
1	7	78	VAL	3.9
1	9	138	ALA	3.8
1	9	75	GLY	3.8
1	9	133	MET	3.7
1	6	133	MET	3.7
1	4	133	MET	3.7
1	9	2	ALA	3.7
1	3	28	PRO	3.6
1	8	5	PRO	3.6
1	2	139	ALA	3.4
1	5	137	ASN	3.4
1	3	22	ILE	3.3
1	2	75	GLY	3.3
1	5	15	ILE	3.2
1	4	77	ASP	3.2
1	4	73	PRO	3.2
1	5	133	MET	3.2
1	9	76	SER	3.1
1	8	39	ALA	3.0
1	6	76	SER	3.0
1	7	130	GLU	3.0
1	7	129	ASN	2.8
1	3	137	ASN	2.8
1	7	71	VAL	2.8
1	2	13	ARG	2.7
1	9	39	ALA	2.7
1	1	75	GLY	2.6
1	4	13	ARG	2.6
1	5	35	ILE	2.5
1	6	39	ALA	2.5
1	7	127	ASP	2.5
1	7	27	ASP	2.5
1	3	13	ARG	2.5
1	1	5	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	2	77	ASP	2.5
1	7	135	ILE	2.5
1	1	13	ARG	2.4
1	8	13	ARG	2.4
1	3	15	ILE	2.4
1	9	15	ILE	2.4
1	2	76	SER	2.4
1	8	69	ALA	2.3
1	7	40	LYS	2.3
1	8	78	VAL	2.3
1	3	77	ASP	2.3
1	1	15	ILE	2.2
1	9	77	ASP	2.2
1	6	137	ASN	2.2
1	2	43	TYR	2.2
1	4	137	ASN	2.1
1	9	13	ARG	2.1
1	9	43	TYR	2.1
1	9	130	GLU	2.1
1	7	123	GLU	2.1
1	2	41	LYS	2.1
1	1	40	LYS	2.0
1	5	75	GLY	2.0
1	4	58	LEU	2.0
1	2	7	ASP	2.0
1	2	141	ALA	2.0
1	2	40	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.