



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:24 PM GMT

PDB ID : 1OU0  
Title : precorrin-8X methylmutase related protein  
Authors : Cuff, M.E.; Joachimiak, A.; Korolev, S.; Savchenko, A.; Edwards, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2003-03-24  
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

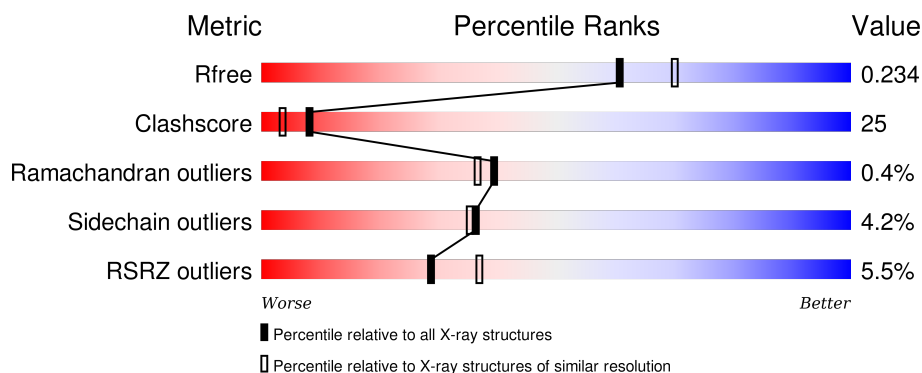
# 1 Overall quality at a glance

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	A	207	<div> <div>3%</div> <div>69%</div> <div>22%</div> <div>8%</div> </div>
1	B	207	<div> <div>6%</div> <div>57%</div> <div>32%</div> <div>7%</div> </div>
1	C	207	<div> <div>3%</div> <div>61%</div> <div>29%</div> <div>8%</div> </div>
1	D	207	<div> <div>7%</div> <div>57%</div> <div>32%</div> <div>8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6434 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 precorrin-8X methylmutase related protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	Se	0	0	0
			1439	909	256	263	3	8			
1	B	193	Total	C	N	O	S	Se	0	0	0
			1468	925	262	270	3	8			
1	C	191	Total	C	N	O	S	Se	0	0	0
			1450	915	260	264	3	8			
1	D	191	Total	C	N	O	S	Se	0	0	0
			1450	915	260	264	3	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	24	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	33	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	63	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	79	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	107	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	124	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	145	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
A	147	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	24	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	33	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	79	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	107	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	124	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	145	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
B	147	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	24	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	33	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	79	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	107	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	124	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	145	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
C	147	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	24	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	33	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	63	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	79	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	107	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	124	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	145	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7
D	147	MSE	MET	MODIFIED RESIDUE	UNP Q9HKE7

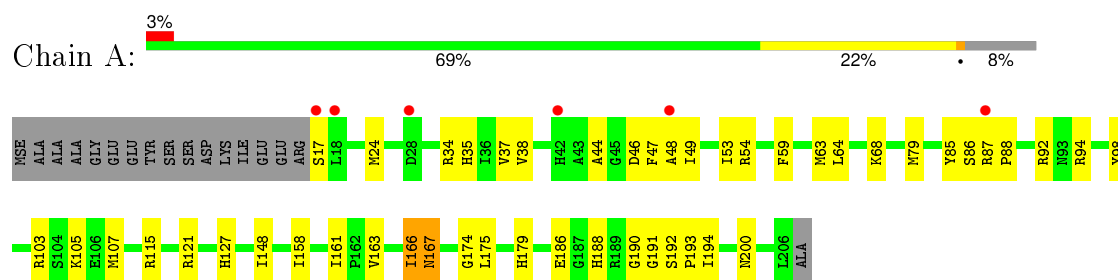
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	194	Total O 194 194	0	0
2	B	120	Total O 120 120	0	0
2	C	156	Total O 156 156	0	0
2	D	157	Total O 157 157	0	0

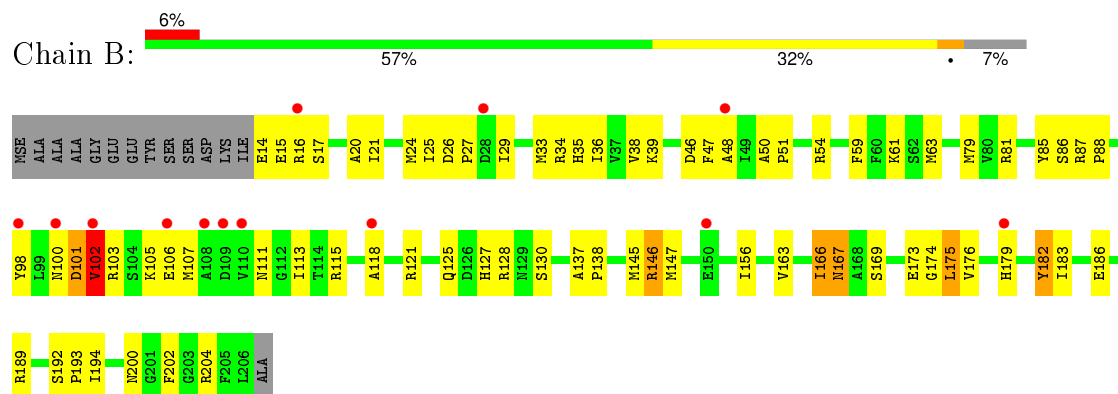
### 3 Residue-property plots [i](#)

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.

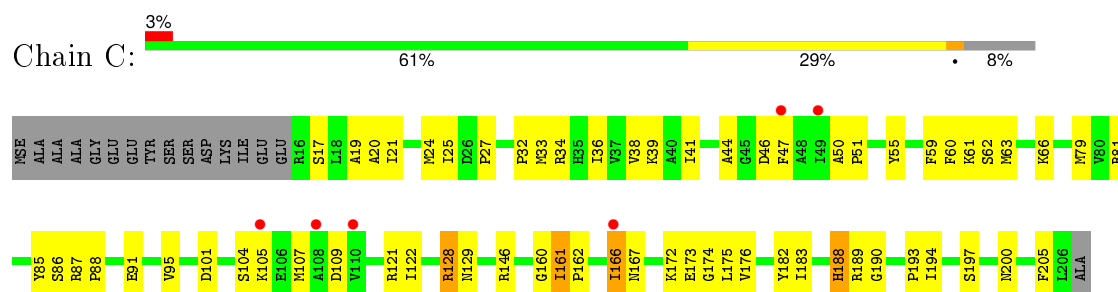
- Molecule 1: precorrin-8X methylmutase related protein



- Molecule 1: precorrin-8X methylmutase related protein

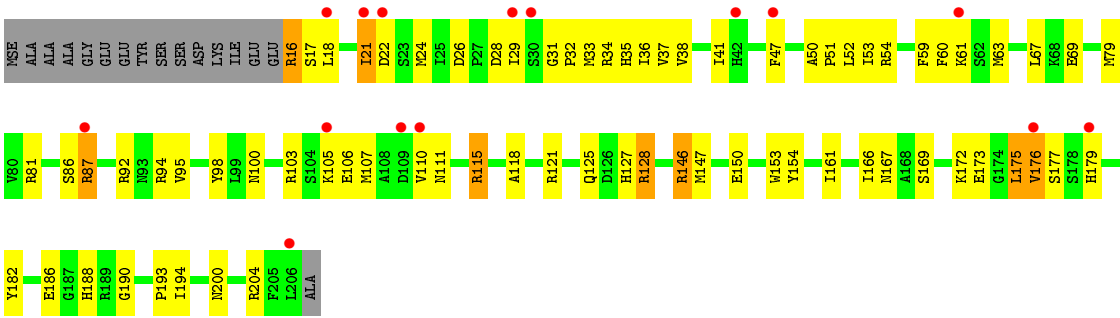


- Molecule 1: precorrin-8X methylmutase related protein



- Molecule 1: precorrin-8X methylmutase related protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.45Å 86.82Å 120.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.24 – 2.10 37.24 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (37.24-2.10) 94.9 (37.24-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.235 0.202 , 0.234	Depositor DCC
$R_{free}$ test set	4399 reflections (10.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 52337 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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	A	0.33	0/1456	0.60	0/1953
1	B	0.31	0/1485	0.59	0/1991
1	C	0.32	0/1467	0.59	0/1967
1	D	0.30	0/1467	0.59	0/1967
All	All	0.32	0/5875	0.60	0/7878

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	182	TYR	Sidechain

### 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	1439	0	1463	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1468	0	1488	75	0
1	C	1450	0	1476	72	0
1	D	1450	0	1476	100	0
2	A	194	0	0	12	0
2	B	120	0	0	9	0
2	C	156	0	0	8	0
2	D	157	0	0	16	0
All	All	6434	0	5903	287	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 25.

All (287) 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:100:ASN:ND2	2:B:314:HOH:O	1.73	1.18
1:D:115:ARG:HH11	1:D:115:ARG:HB2	1.16	1.07
1:C:33:MSE:HE3	1:C:60:PHE:HD1	1.15	1.04
1:C:166:ILE:HG12	1:C:167:ASN:H	1.19	1.03
1:C:166:ILE:H	1:C:166:ILE:HD13	1.21	1.02
1:B:15:GLU:HG3	1:B:16:ARG:H	1.25	1.02
1:D:33:MSE:HE3	1:D:60:PHE:HD1	1.27	1.00
1:D:54:ARG:HE	1:D:186:GLU:HG3	1.36	0.90
1:D:33:MSE:HE3	1:D:60:PHE:CD1	2.08	0.87
1:D:50:ALA:HB3	1:D:51:PRO:HD3	1.55	0.87
1:B:146:ARG:HH12	1:B:147:MSE:HE2	1.37	0.87
1:C:87:ARG:HB3	1:C:87:ARG:NH1	1.90	0.86
1:C:33:MSE:HE3	1:C:60:PHE:CD1	2.08	0.84
1:C:87:ARG:HB3	1:C:87:ARG:HH11	1.42	0.83
1:C:166:ILE:H	1:C:166:ILE:CD1	1.90	0.83
1:A:79:MSE:HE3	1:D:79:MSE:HE3	1.59	0.82
1:C:59:PHE:CE1	1:C:63:MSE:HE3	2.15	0.81
1:C:166:ILE:HG12	1:C:167:ASN:N	1.95	0.81
1:A:54:ARG:HG3	1:A:54:ARG:HH11	1.49	0.78
1:D:61:LYS:HE2	1:D:61:LYS:HA	1.66	0.78
1:B:107:MSE:HE2	1:B:118:ALA:HA	1.64	0.78
1:D:63:MSE:HG3	2:D:275:HOH:O	1.84	0.76
1:C:107:MSE:SE	1:C:121:ARG:HD2	2.39	0.72
1:C:166:ILE:CG1	1:C:167:ASN:H	2.00	0.72
1:D:54:ARG:NE	1:D:186:GLU:HG3	2.05	0.71
1:D:92:ARG:NH1	1:D:92:ARG:HB3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:HH11	1:D:115:ARG:CB	1.97	0.71
1:B:121:ARG:O	1:B:125:GLN:HG3	1.90	0.71
1:D:92:ARG:HH11	1:D:92:ARG:HB3	1.55	0.70
1:C:166:ILE:HD13	1:C:166:ILE:N	2.01	0.70
1:A:92:ARG:HH11	1:A:92:ARG:HG2	1.55	0.70
1:D:18:LEU:HA	1:D:21:ILE:HG12	1.72	0.70
1:A:79:MSE:HE2	1:A:192:SER:HB2	1.74	0.69
1:C:24:MSE:HA	1:C:24:MSE:HE2	1.74	0.69
1:A:193:PRO:HG3	1:D:79:MSE:HE1	1.74	0.69
1:D:147:MSE:HE2	1:D:147:MSE:HA	1.74	0.69
1:A:79:MSE:CE	1:D:79:MSE:HE3	2.23	0.68
1:D:103:ARG:HH11	1:D:103:ARG:HG3	1.56	0.68
1:B:107:MSE:HE1	1:B:121:ARG:HB3	1.76	0.67
1:B:101:ASP:CG	1:B:101:ASP:O	2.33	0.67
1:D:18:LEU:HA	1:D:21:ILE:CG1	2.24	0.67
1:B:15:GLU:HG3	1:B:16:ARG:N	2.04	0.67
1:B:146:ARG:NH1	1:B:147:MSE:HE2	2.09	0.67
1:C:33:MSE:CE	1:C:36:ILE:HG13	2.24	0.67
1:D:105:LYS:HB2	1:D:115:ARG:NH2	2.10	0.66
1:C:33:MSE:HE2	1:C:36:ILE:HG13	1.77	0.66
1:A:79:MSE:HE1	1:D:193:PRO:HG3	1.77	0.65
1:D:21:ILE:HD12	1:D:47:PHE:CE2	2.32	0.65
1:D:59:PHE:CE1	1:D:63:MSE:HE3	2.32	0.65
1:D:115:ARG:HB2	1:D:115:ARG:NH1	2.00	0.65
1:A:79:MSE:HE3	1:D:79:MSE:CE	2.28	0.64
1:D:146:ARG:HG2	1:D:150:GLU:OE2	1.96	0.64
1:B:87:ARG:HB2	1:B:88:PRO:HD3	1.81	0.63
1:D:146:ARG:HH22	1:D:147:MSE:HE3	1.64	0.63
1:D:35:HIS:CE1	1:D:204:ARG:HD3	2.33	0.63
1:A:167:ASN:HB3	2:A:310:HOH:O	1.99	0.63
1:A:54:ARG:NH1	1:A:54:ARG:HG3	2.14	0.62
1:D:107:MSE:HE3	1:D:118:ALA:HA	1.81	0.62
1:D:110:VAL:HG12	1:D:111:ASN:HD22	1.65	0.61
1:D:41:ILE:HD11	1:D:50:ALA:HB2	1.82	0.61
1:D:21:ILE:HG21	1:D:41:ILE:HG21	1.83	0.61
1:C:129:ASN:HB2	2:C:293:HOH:O	2.01	0.60
1:A:98:TYR:OH	1:A:127:HIS:HE1	1.84	0.60
1:A:103:ARG:HD2	2:A:297:HOH:O	2.02	0.60
1:C:34:ARG:O	1:C:38:VAL:HG23	2.01	0.60
1:D:161:ILE:HG22	1:D:190:GLY:HA2	1.82	0.60
1:C:173:GLU:O	1:C:176:VAL:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:MSE:HE1	1:D:121:ARG:HB3	1.84	0.60
1:D:107:MSE:SE	1:D:121:ARG:HD2	2.52	0.59
1:C:61:LYS:HG3	2:C:230:HOH:O	2.02	0.59
1:D:26:ASP:HB3	1:D:29:ILE:HG13	1.84	0.59
1:B:204:ARG:HH11	1:B:204:ARG:HG3	1.65	0.59
1:D:52:LEU:HG	2:D:274:HOH:O	2.01	0.59
1:A:166:ILE:HD13	1:A:166:ILE:C	2.23	0.59
1:B:59:PHE:CZ	1:B:63:MSE:HG3	2.38	0.59
1:B:107:MSE:CE	1:B:118:ALA:HA	2.32	0.58
1:B:128:ARG:HB2	2:B:229:HOH:O	2.02	0.58
1:D:154:TYR:CE2	1:D:179:HIS:HB3	2.38	0.58
1:D:204:ARG:HH11	1:D:204:ARG:HB2	1.67	0.58
1:D:16:ARG:NH1	1:D:16:ARG:HB2	2.19	0.58
1:B:146:ARG:HH22	1:B:147:MSE:CE	2.17	0.58
1:B:101:ASP:O	1:B:101:ASP:OD2	2.22	0.58
1:B:166:ILE:HD13	1:B:166:ILE:O	2.03	0.58
1:B:54:ARG:HD2	1:B:186:GLU:OE2	2.03	0.57
1:D:33:MSE:CE	1:D:36:ILE:HG13	2.34	0.57
1:D:33:MSE:HE2	1:D:33:MSE:HA	1.86	0.57
1:B:146:ARG:HH12	1:B:147:MSE:CE	2.13	0.57
1:A:34:ARG:O	1:A:38:VAL:HG13	2.04	0.57
1:B:102:VAL:HG13	1:B:102:VAL:O	2.05	0.57
1:A:35:HIS:O	1:A:38:VAL:HG22	2.05	0.56
1:A:85:TYR:H	1:A:200:ASN:HD21	1.51	0.56
1:B:105:LYS:HG3	1:B:106:GLU:N	2.19	0.56
1:D:21:ILE:HG23	1:D:47:PHE:CD2	2.41	0.56
1:D:204:ARG:HH11	1:D:204:ARG:CB	2.18	0.56
1:B:81:ARG:HG3	1:B:81:ARG:HH11	1.71	0.56
1:C:85:TYR:H	1:C:200:ASN:HD21	1.53	0.56
1:D:87:ARG:HB3	1:D:87:ARG:NH1	2.21	0.56
1:D:21:ILE:HG23	1:D:47:PHE:CE2	2.41	0.56
1:D:146:ARG:HH12	1:D:147:MSE:HE3	1.71	0.56
1:D:146:ARG:NH2	1:D:147:MSE:HE3	2.20	0.56
1:D:167:ASN:HB2	2:D:267:HOH:O	2.04	0.56
1:D:81:ARG:HD2	2:D:354:HOH:O	2.05	0.56
1:D:121:ARG:O	1:D:125:GLN:HG3	2.07	0.55
1:D:67:LEU:HD12	2:D:275:HOH:O	2.06	0.55
1:B:186:GLU:HG2	2:B:254:HOH:O	2.07	0.55
1:A:17:SER:HB3	2:A:368:HOH:O	2.06	0.55
1:A:59:PHE:CZ	1:A:63:MSE:HG3	2.42	0.55
1:D:51:PRO:HB2	2:D:274:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:O	1:B:38:VAL:HG23	2.06	0.55
1:C:21:ILE:HA	1:C:47:PHE:HE2	1.71	0.55
1:D:110:VAL:HG12	1:D:111:ASN:ND2	2.21	0.54
1:D:16:ARG:HB2	1:D:16:ARG:HH11	1.72	0.54
1:B:50:ALA:HB3	1:B:51:PRO:HD3	1.88	0.54
1:C:160:GLY:C	1:C:162:PRO:HD3	2.28	0.54
1:C:24:MSE:HG3	1:C:47:PHE:CD2	2.42	0.54
1:D:81:ARG:HG3	1:D:95:VAL:HG12	1.89	0.54
1:C:27:PRO:HD3	1:D:166:ILE:HD13	1.88	0.54
1:B:16:ARG:HB2	2:D:355:HOH:O	2.06	0.54
1:C:161:ILE:HG22	1:C:190:GLY:HA2	1.89	0.54
1:A:24:MSE:HE1	1:C:20:ALA:HB1	1.90	0.53
1:A:46:ASP:OD2	1:A:48:ALA:HB3	2.09	0.53
1:C:188:HIS:CD2	1:C:189:ARG:N	2.77	0.53
1:B:194:ILE:HG13	2:B:283:HOH:O	2.08	0.53
1:C:33:MSE:CE	1:C:60:PHE:HD1	2.05	0.53
1:D:103:ARG:NH1	1:D:103:ARG:HG3	2.24	0.53
1:D:87:ARG:HB3	1:D:87:ARG:CZ	2.38	0.52
1:B:61:LYS:HE2	2:B:241:HOH:O	2.08	0.52
1:C:104:SER:HA	1:C:122:ILE:CD1	2.38	0.52
1:B:39:LYS:NZ	1:B:39:LYS:HB3	2.25	0.52
1:D:54:ARG:CZ	2:D:335:HOH:O	2.58	0.51
1:D:33:MSE:HE1	1:D:36:ILE:HG13	1.91	0.51
1:C:188:HIS:HD2	1:C:189:ARG:N	2.08	0.51
1:B:111:ASN:N	1:B:111:ASN:HD22	2.08	0.51
1:C:162:PRO:HD2	1:C:172:LYS:HD3	1.93	0.51
2:A:377:HOH:O	1:D:188:HIS:HB2	2.10	0.51
1:B:107:MSE:HE2	1:B:113:ILE:HD11	1.91	0.51
1:A:86:SER:H	1:A:200:ASN:ND2	2.10	0.50
1:B:204:ARG:NH1	1:B:204:ARG:HG3	2.26	0.50
1:B:182:TYR:C	1:B:182:TYR:CD1	2.84	0.50
1:C:17:SER:O	1:C:21:ILE:HG13	2.11	0.50
1:D:146:ARG:NH1	1:D:147:MSE:HE3	2.26	0.50
1:B:85:TYR:H	1:B:200:ASN:HD21	1.60	0.50
1:D:128:ARG:NH2	1:D:153:TRP:CD1	2.80	0.50
1:B:166:ILE:HG23	1:B:167:ASN:N	2.27	0.50
1:D:146:ARG:HH22	1:D:147:MSE:CE	2.25	0.49
1:D:204:ARG:NH1	1:D:204:ARG:CB	2.74	0.49
1:D:169:SER:O	1:D:173:GLU:HG3	2.12	0.49
1:D:92:ARG:HH11	1:D:92:ARG:CB	2.24	0.49
1:B:101:ASP:OD2	1:B:103:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:PHE:HD2	1:D:61:LYS:HE3	1.77	0.49
1:A:163:VAL:HG22	1:A:191:GLY:N	2.27	0.49
1:B:107:MSE:CE	1:B:121:ARG:HD2	2.42	0.49
1:C:59:PHE:HE1	1:C:63:MSE:HE3	1.71	0.49
1:C:105:LYS:HE3	2:C:242:HOH:O	2.12	0.49
1:B:86:SER:H	1:B:200:ASN:ND2	2.11	0.49
1:C:39:LYS:HD3	1:C:197:SER:O	2.12	0.49
1:C:25:ILE:HD11	1:C:41:ILE:HD12	1.94	0.49
1:A:24:MSE:HE3	1:A:47:PHE:CD1	2.47	0.48
1:B:47:PHE:HZ	1:D:24:MSE:HE2	1.77	0.48
1:C:33:MSE:HE1	1:C:36:ILE:HG13	1.96	0.48
1:A:166:ILE:HD13	1:A:166:ILE:O	2.13	0.48
1:B:21:ILE:HG12	1:B:47:PHE:HE2	1.78	0.48
1:B:79:MSE:CE	1:C:79:MSE:HE2	2.43	0.48
1:B:14:GLU:HB3	2:B:310:HOH:O	2.13	0.48
1:A:166:ILE:HG23	1:A:167:ASN:N	2.28	0.48
1:C:19:ALA:HA	2:C:358:HOH:O	2.14	0.48
1:B:146:ARG:HH22	1:B:147:MSE:HE2	1.77	0.48
1:D:16:ARG:HH11	1:D:17:SER:H	1.60	0.48
2:A:363:HOH:O	1:B:173:GLU:HG2	2.13	0.48
1:B:35:HIS:CE1	1:B:39:LYS:HD2	2.49	0.48
1:B:111:ASN:N	1:B:111:ASN:ND2	2.61	0.48
1:C:109:ASP:HA	2:C:306:HOH:O	2.14	0.48
1:C:24:MSE:HG3	1:C:47:PHE:HD2	1.77	0.47
1:A:161:ILE:HG22	1:A:190:GLY:CA	2.44	0.47
1:C:193:PRO:HD2	2:C:335:HOH:O	2.14	0.47
1:C:87:ARG:HB2	1:C:88:PRO:HD3	1.97	0.47
1:D:34:ARG:O	1:D:38:VAL:HG23	2.14	0.47
1:A:194:ILE:HG13	2:A:215:HOH:O	2.13	0.47
1:A:193:PRO:CG	1:D:79:MSE:HE1	2.43	0.47
1:D:61:LYS:HG2	2:D:230:HOH:O	2.14	0.47
1:D:51:PRO:HD2	2:D:274:HOH:O	2.14	0.47
1:B:128:ARG:HG2	1:B:128:ARG:NH1	2.30	0.47
1:A:79:MSE:HE2	1:A:192:SER:CB	2.44	0.47
1:B:128:ARG:HG2	1:B:128:ARG:HH11	1.80	0.47
1:B:20:ALA:HB2	2:D:349:HOH:O	2.14	0.47
1:C:188:HIS:HD2	1:C:189:ARG:H	1.63	0.47
1:C:55:TYR:HB3	1:C:183:ILE:HG13	1.96	0.47
1:C:59:PHE:CE1	1:C:63:MSE:CE	2.92	0.47
1:A:174:GLY:HA3	2:A:222:HOH:O	2.14	0.47
1:C:161:ILE:N	1:C:162:PRO:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:MSE:SE	1:A:121:ARG:HD2	2.65	0.46
1:B:179:HIS:O	1:B:179:HIS:CD2	2.69	0.46
1:D:175:LEU:C	1:D:177:SER:H	2.19	0.46
1:A:64:LEU:O	1:A:68:LYS:HB2	2.14	0.46
1:C:85:TYR:N	1:C:200:ASN:HD21	2.14	0.46
1:B:46:ASP:OD2	1:B:189:ARG:NH1	2.44	0.46
1:C:50:ALA:HB3	1:C:51:PRO:HD3	1.97	0.46
1:A:49:ILE:O	1:A:53:ILE:HG13	2.16	0.46
1:C:62:SER:O	1:C:66:LYS:HG2	2.16	0.46
1:D:37:VAL:HG13	1:D:53:ILE:HD12	1.98	0.45
1:C:59:PHE:CZ	1:C:63:MSE:HE3	2.50	0.45
1:C:86:SER:H	1:C:200:ASN:ND2	2.14	0.45
1:D:31:GLY:HA3	1:D:32:PRO:HD3	1.82	0.45
1:D:21:ILE:CD1	1:D:47:PHE:CE2	2.99	0.45
1:B:169:SER:O	1:B:173:GLU:HG3	2.16	0.45
1:A:188:HIS:HB2	2:D:338:HOH:O	2.17	0.45
1:C:33:MSE:HA	1:C:33:MSE:HE2	1.99	0.45
1:D:86:SER:H	1:D:200:ASN:ND2	2.13	0.45
1:A:179:HIS:CD2	2:A:210:HOH:O	2.69	0.45
1:B:145:MSE:HE3	1:B:175:LEU:HA	1.99	0.45
1:B:192:SER:N	1:B:193:PRO:CD	2.79	0.45
1:B:26:ASP:OD2	1:B:27:PRO:HD2	2.17	0.45
1:D:204:ARG:HB3	1:D:204:ARG:NH1	2.32	0.44
1:D:154:TYR:HE2	1:D:179:HIS:HB3	1.80	0.44
1:B:166:ILE:CG2	1:B:167:ASN:N	2.79	0.44
1:B:101:ASP:HB2	2:B:322:HOH:O	2.16	0.44
1:A:166:ILE:HB	2:D:279:HOH:O	2.17	0.44
1:A:37:VAL:HG13	1:A:53:ILE:HD12	1.99	0.44
1:A:148:ILE:HD12	1:A:158:ILE:HD11	2.00	0.44
1:A:98:TYR:HE2	1:A:103:ARG:HH22	1.64	0.44
1:C:194:ILE:HG13	2:C:335:HOH:O	2.17	0.44
1:D:33:MSE:HE2	1:D:36:ILE:HG13	1.99	0.44
1:D:60:PHE:CD2	1:D:61:LYS:HE3	2.52	0.44
1:C:87:ARG:HH12	1:C:91:GLU:CD	2.21	0.44
1:B:174:GLY:HA3	2:B:326:HOH:O	2.17	0.44
1:C:32:PRO:HB3	1:C:205:PHE:CZ	2.53	0.44
1:D:18:LEU:CA	1:D:21:ILE:HG12	2.46	0.44
1:A:92:ARG:HH11	1:A:92:ARG:CG	2.25	0.44
1:D:146:ARG:NH2	1:D:147:MSE:CE	2.81	0.44
1:A:127:HIS:HD2	2:A:390:HOH:O	2.00	0.44
1:A:163:VAL:HG22	1:A:190:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:O	1:B:21:ILE:HG13	2.18	0.44
1:D:106:GLU:HG2	2:D:249:HOH:O	2.17	0.44
1:B:33:MSE:HE1	1:B:183:ILE:HD12	1.99	0.44
1:A:87:ARG:NH1	2:A:335:HOH:O	2.51	0.43
1:A:188:HIS:NE2	1:B:51:PRO:HG3	2.33	0.43
1:C:46:ASP:OD2	1:C:189:ARG:NH1	2.51	0.43
1:A:87:ARG:HB3	1:A:88:PRO:HD3	1.99	0.43
1:D:176:VAL:HG12	1:D:182:TYR:OH	2.18	0.43
1:B:24:MSE:SE	1:D:47:PHE:CZ	3.22	0.43
1:C:176:VAL:HA	1:C:182:TYR:CZ	2.53	0.43
1:C:21:ILE:HA	1:C:47:PHE:CE2	2.52	0.43
1:B:36:ILE:HD13	1:B:202:PHE:CE1	2.54	0.43
1:D:194:ILE:HG13	2:D:221:HOH:O	2.18	0.43
1:C:25:ILE:HD11	1:C:41:ILE:CD1	2.48	0.43
1:B:105:LYS:HB3	1:B:115:ARG:CZ	2.49	0.43
1:B:166:ILE:C	1:B:166:ILE:HD13	2.39	0.43
1:C:44:ALA:HB2	1:C:194:ILE:HG12	2.00	0.43
1:B:130:SER:O	1:B:156:ILE:HG23	2.18	0.43
1:B:48:ALA:O	1:B:51:PRO:HD2	2.18	0.42
1:D:41:ILE:CD1	1:D:50:ALA:HB2	2.49	0.42
1:C:174:GLY:HA3	2:C:299:HOH:O	2.18	0.42
1:D:107:MSE:HE3	1:D:118:ALA:CA	2.49	0.42
1:A:161:ILE:HG22	1:A:190:GLY:HA2	2.00	0.42
1:A:44:ALA:HB2	1:A:194:ILE:HD11	2.02	0.42
1:D:69:GLU:O	1:D:92:ARG:NH1	2.52	0.42
1:C:101:ASP:O	1:C:104:SER:HB2	2.19	0.42
1:D:176:VAL:HG12	1:D:182:TYR:CZ	2.54	0.42
1:C:128:ARG:HH11	1:C:128:ARG:HG2	1.83	0.42
1:D:33:MSE:HE2	1:D:36:ILE:CG1	2.49	0.42
1:C:87:ARG:CB	1:C:87:ARG:HH11	2.24	0.42
1:C:33:MSE:HE2	1:C:36:ILE:CG1	2.47	0.42
1:C:50:ALA:HB3	1:C:51:PRO:CD	2.50	0.42
1:A:179:HIS:HD2	2:A:210:HOH:O	2.01	0.42
1:B:163:VAL:HG11	2:B:306:HOH:O	2.19	0.42
1:D:98:TYR:OH	1:D:127:HIS:HE1	2.03	0.42
1:D:41:ILE:HD11	1:D:50:ALA:CB	2.50	0.42
1:C:25:ILE:HB	1:C:34:ARG:NH2	2.35	0.42
1:B:176:VAL:HA	1:B:182:TYR:CZ	2.55	0.42
1:B:98:TYR:OH	1:B:127:HIS:HE1	2.03	0.41
1:D:146:ARG:HB3	1:D:146:ARG:HH11	1.84	0.41
1:C:104:SER:HA	1:C:122:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:OG	1:A:88:PRO:HD2	2.20	0.41
1:B:175:LEU:HD22	1:B:182:TYR:CG	2.55	0.41
1:D:172:LYS:NZ	2:D:223:HOH:O	2.48	0.41
1:B:26:ASP:OD2	1:B:27:PRO:N	2.54	0.41
1:B:137:ALA:HA	1:B:138:PRO:HD3	1.98	0.41
1:A:186:GLU:HG2	2:A:271:HOH:O	2.20	0.41
1:A:105:LYS:HA	1:A:115:ARG:CD	2.51	0.41
1:D:16:ARG:HD3	1:D:18:LEU:N	2.36	0.41
1:A:92:ARG:NH1	1:A:92:ARG:CG	2.83	0.41
1:B:176:VAL:HG12	1:B:182:TYR:CZ	2.56	0.41
1:B:25:ILE:HG23	1:B:29:ILE:HD12	2.02	0.40
1:C:81:ARG:NH1	1:C:95:VAL:O	2.53	0.40
1:C:81:ARG:HG3	1:C:95:VAL:HG12	2.02	0.40
1:C:32:PRO:HB2	1:C:60:PHE:CE1	2.55	0.40
1:D:161:ILE:HG22	1:D:190:GLY:CA	2.51	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	188/207 (91%)	181 (96%)	7 (4%)	0	100	100
1	B	191/207 (92%)	181 (95%)	9 (5%)	1 (0%)	34	30
1	C	189/207 (91%)	180 (95%)	9 (5%)	0	100	100
1	D	189/207 (91%)	175 (93%)	12 (6%)	2 (1%)	17	11
All	All	757/828 (91%)	717 (95%)	37 (5%)	3 (0%)	39	37

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	B	102	VAL
1	D	176	VAL
1	D	22	ASP

### 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	153/156 (98%)	149 (97%)	4 (3%)	54	58
1	B	156/156 (100%)	150 (96%)	6 (4%)	40	40
1	C	154/156 (99%)	148 (96%)	6 (4%)	39	39
1	D	154/156 (99%)	144 (94%)	10 (6%)	21	17
All	All	617/624 (99%)	591 (96%)	26 (4%)	36	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ARG
1	A	166	ILE
1	A	167	ASN
1	A	175	LEU
1	B	101	ASP
1	B	102	VAL
1	B	146	ARG
1	B	166	ILE
1	B	167	ASN
1	B	175	LEU
1	C	128	ARG
1	C	146	ARG
1	C	161	ILE
1	C	166	ILE
1	C	175	LEU
1	C	188	HIS
1	D	16	ARG
1	D	21	ILE
1	D	28	ASP

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Mol	Chain	Res	Type
1	D	87	ARG
1	D	94	ARG
1	D	100	ASN
1	D	115	ARG
1	D	128	ARG
1	D	146	ARG
1	D	175	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	111	ASN
1	A	127	HIS
1	A	151	ASN
1	A	179	HIS
1	A	200	ASN
1	B	111	ASN
1	B	127	HIS
1	B	136	ASN
1	B	179	HIS
1	B	188	HIS
1	B	200	ASN
1	C	127	HIS
1	C	129	ASN
1	C	151	ASN
1	C	188	HIS
1	C	200	ASN
1	D	35	HIS
1	D	111	ASN
1	D	127	HIS
1	D	200	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	A	182/207 (87%)	0.17	6 (3%) 50 59	18, 30, 72, 83	0
1	B	185/207 (89%)	0.57	13 (7%) 19 26	23, 41, 77, 95	0
1	C	183/207 (88%)	0.40	6 (3%) 50 59	20, 35, 59, 83	0
1	D	183/207 (88%)	0.60	15 (8%) 14 20	22, 40, 67, 85	0
All	All	733/828 (88%)	0.44	40 (5%) 29 37	18, 37, 68, 95	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	ILE	6.0
1	B	102	VAL	5.2
1	D	47	PHE	5.0
1	B	110	VAL	5.0
1	A	17	SER	4.8
1	B	179	HIS	3.9
1	C	105	LYS	3.7
1	D	179	HIS	3.6
1	B	109	ASP	3.4
1	D	21	ILE	3.4
1	B	118	ALA	3.3
1	B	106	GLU	3.3
1	B	16	ARG	3.1
1	D	206	LEU	3.1
1	D	61	LYS	3.1
1	D	18	LEU	2.9
1	D	176	VAL	2.9
1	D	29	ILE	2.8
1	A	87	ARG	2.8
1	B	150	GLU	2.8
1	B	108	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	28	ASP	2.6
1	D	87	ARG	2.5
1	D	109	ASP	2.5
1	D	22	ASP	2.4
1	D	105	LYS	2.3
1	A	18	LEU	2.3
1	D	30	SER	2.3
1	A	28	ASP	2.3
1	B	48	ALA	2.3
1	C	47	PHE	2.2
1	D	110	VAL	2.2
1	C	110	VAL	2.2
1	D	42	HIS	2.2
1	C	108	ALA	2.1
1	B	98	TYR	2.1
1	A	42	HIS	2.0
1	B	100	ASN	2.0
1	C	49	ILE	2.0
1	A	48	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 carbohydrates 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.