



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2016 – 05:09 AM EDT

PDB ID : 5KC7
Title : Crystal structure of Cbln1 (Val55-Gly58 deletion mutant)
Authors : Elegheert, J.; Aricescu, A.R.
Deposited on : 2016-06-05
Resolution : 7.04 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

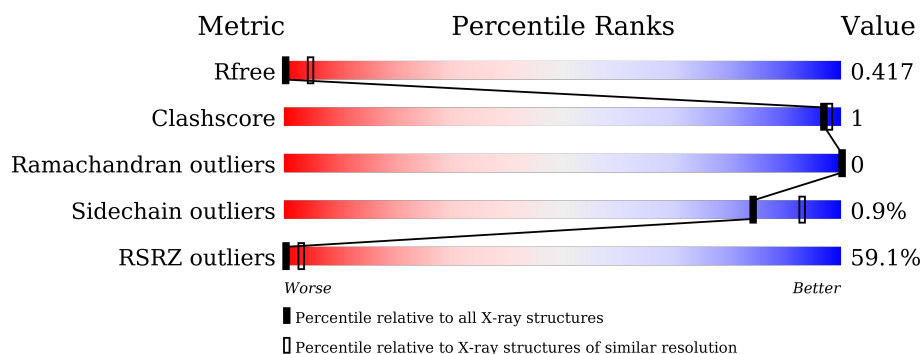
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.04 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	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 ≥ 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	178	<div> <div>61%</div> <div> <div>71%</div> <div>24%</div> </div> </div>
1	B	178	<div> <div>27%</div> <div> <div>72%</div> <div>24%</div> </div> </div>
1	C	178	<div> <div>50%</div> <div> <div>72%</div> <div>24%</div> </div> </div>
1	D	178	<div> <div>42%</div> <div> <div>72%</div> <div>24%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4276 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 Cerebellin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1073	686	186	196	5			
1	B	135	Total	C	N	O	S	0	0	0
			1063	681	183	194	5			
1	C	135	Total	C	N	O	S	0	0	0
			1073	686	186	196	5			
1	D	135	Total	C	N	O	S	0	0	0
			1067	683	183	196	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLU	-	expression tag	UNP P23435
A	26	THR	-	expression tag	UNP P23435
A	27	GLY	-	expression tag	UNP P23435
A	?	-	VAL	deletion	UNP P23435
A	?	-	ARG	deletion	UNP P23435
A	?	-	SER	deletion	UNP P23435
A	?	-	GLY	deletion	UNP P23435
A	194	GLY	-	expression tag	UNP P23435
A	195	THR	-	expression tag	UNP P23435
A	196	LYS	-	expression tag	UNP P23435
A	197	HIS	-	expression tag	UNP P23435
A	198	HIS	-	expression tag	UNP P23435
A	199	HIS	-	expression tag	UNP P23435
A	200	HIS	-	expression tag	UNP P23435
A	201	HIS	-	expression tag	UNP P23435
A	202	HIS	-	expression tag	UNP P23435
B	25	GLU	-	expression tag	UNP P23435
B	26	THR	-	expression tag	UNP P23435
B	27	GLY	-	expression tag	UNP P23435
B	?	-	VAL	deletion	UNP P23435
B	?	-	ARG	deletion	UNP P23435

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P23435
B	?	-	GLY	deletion	UNP P23435
B	194	GLY	-	expression tag	UNP P23435
B	195	THR	-	expression tag	UNP P23435
B	196	LYS	-	expression tag	UNP P23435
B	197	HIS	-	expression tag	UNP P23435
B	198	HIS	-	expression tag	UNP P23435
B	199	HIS	-	expression tag	UNP P23435
B	200	HIS	-	expression tag	UNP P23435
B	201	HIS	-	expression tag	UNP P23435
B	202	HIS	-	expression tag	UNP P23435
C	25	GLU	-	expression tag	UNP P23435
C	26	THR	-	expression tag	UNP P23435
C	27	GLY	-	expression tag	UNP P23435
C	?	-	VAL	deletion	UNP P23435
C	?	-	ARG	deletion	UNP P23435
C	?	-	SER	deletion	UNP P23435
C	?	-	GLY	deletion	UNP P23435
C	194	GLY	-	expression tag	UNP P23435
C	195	THR	-	expression tag	UNP P23435
C	196	LYS	-	expression tag	UNP P23435
C	197	HIS	-	expression tag	UNP P23435
C	198	HIS	-	expression tag	UNP P23435
C	199	HIS	-	expression tag	UNP P23435
C	200	HIS	-	expression tag	UNP P23435
C	201	HIS	-	expression tag	UNP P23435
C	202	HIS	-	expression tag	UNP P23435
D	25	GLU	-	expression tag	UNP P23435
D	26	THR	-	expression tag	UNP P23435
D	27	GLY	-	expression tag	UNP P23435
D	?	-	VAL	deletion	UNP P23435
D	?	-	ARG	deletion	UNP P23435
D	?	-	SER	deletion	UNP P23435
D	?	-	GLY	deletion	UNP P23435
D	194	GLY	-	expression tag	UNP P23435
D	195	THR	-	expression tag	UNP P23435
D	196	LYS	-	expression tag	UNP P23435
D	197	HIS	-	expression tag	UNP P23435
D	198	HIS	-	expression tag	UNP P23435
D	199	HIS	-	expression tag	UNP P23435
D	200	HIS	-	expression tag	UNP P23435
D	201	HIS	-	expression tag	UNP P23435

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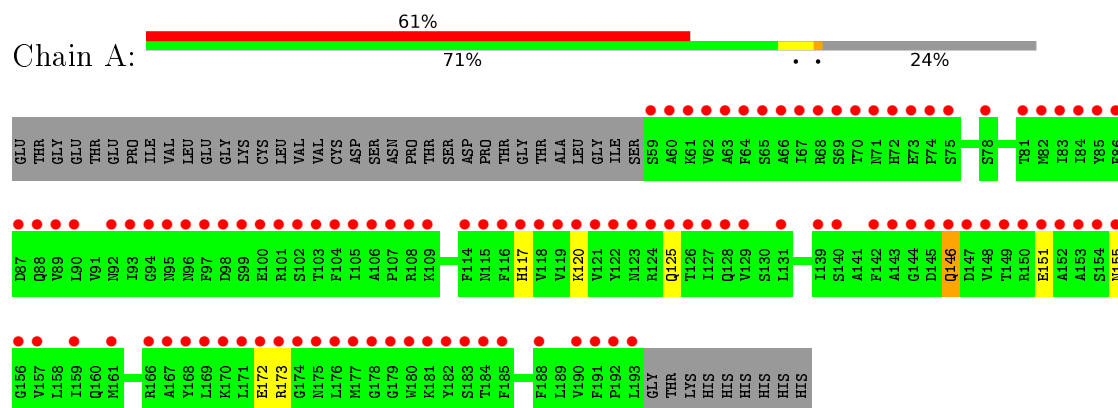
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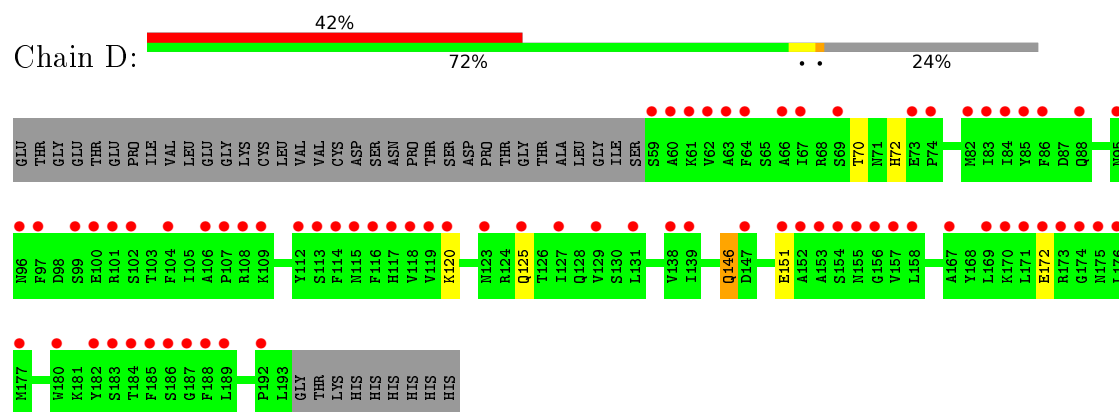
Chain	Residue	Modelled	Actual	Comment	Reference
D	202	HIS	-	expression tag	UNP P23435

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: Cerebellin-1





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	187.45Å 187.45Å 187.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.10 – 7.04 76.53 – 7.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.10-7.04) 100.0 (76.53-7.03)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.96 (at 6.72Å)	Xtriage
Refinement program	PHENIX (dev_2283: ???)	Depositor
R, R_{free}	0.270 , 0.351 0.328 , 0.417	Depositor DCC
R_{free} test set	172 reflections (10.59%)	DCC
Wilson B-factor (Å ²)	402.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 613.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.047 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	4276	wwPDB-VP
Average B, all atoms (Å ²)	469.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.24	0/1097	0.42	0/1481
1	B	0.24	0/1086	0.42	0/1466
1	C	0.24	0/1097	0.42	0/1481
1	D	0.24	0/1091	0.42	0/1474
All	All	0.24	0/4371	0.42	0/5902

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	A	1073	0	1058	4	3
1	B	1063	0	1044	4	1
1	C	1073	0	1058	3	1
1	D	1067	0	1047	3	3
All	All	4276	0	4207	11	4

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 1.

All (11) 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:70:THR:CB	1:D:172:GLU:O	1.95	1.14
1:C:120:LYS:NZ	1:C:125:GLN:O	2.11	0.84
1:D:120:LYS:NZ	1:D:125:GLN:O	2.11	0.84
1:A:120:LYS:NZ	1:A:125:GLN:O	2.11	0.84
1:B:120:LYS:NZ	1:B:125:GLN:O	2.11	0.83
1:B:146:GLN:NE2	1:B:151:GLU:OE2	2.43	0.49
1:A:146:GLN:NE2	1:A:151:GLU:OE2	2.43	0.48
1:D:146:GLN:NE2	1:D:151:GLU:OE2	2.43	0.45
1:A:117:HIS:CE1	1:C:155:ASN:HA	2.56	0.41
1:A:155:ASN:HA	1:B:117:HIS:CE1	2.56	0.41
1:C:146:GLN:NE2	1:C:151:GLU:OE2	2.43	0.40

All (4) 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:B:172:GLU:O	1:C:70:THR:OG1[14_545]	1.45	0.75
1:A:172:GLU:O	1:D:70:THR:OG1[12_455]	1.88	0.32
1:A:173:ARG:N	1:D:72:HIS:CE1[12_455]	2.02	0.18
1:A:173:ARG:CA	1:D:72:HIS:ND1[12_455]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/178 (75%)	130 (98%)	3 (2%)	0	100	100
1	B	133/178 (75%)	130 (98%)	3 (2%)	0	100	100
1	C	133/178 (75%)	130 (98%)	3 (2%)	0	100	100
1	D	133/178 (75%)	130 (98%)	3 (2%)	0	100	100
All	All	532/712 (75%)	520 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	116/153 (76%)	115 (99%)	1 (1%)	84	93
1	B	113/153 (74%)	112 (99%)	1 (1%)	84	93
1	C	116/153 (76%)	115 (99%)	1 (1%)	84	93
1	D	115/153 (75%)	114 (99%)	1 (1%)	84	93
All	All	460/612 (75%)	456 (99%)	4 (1%)	84	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	B	146	GLN
1	C	146	GLN
1	D	146	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	135/178 (75%)	5.58	108 (80%) 0 2	234, 422, 603, 780	0
1	B	135/178 (75%)	1.99	48 (35%) 0 4	333, 421, 654, 762	0
1	C	135/178 (75%)	3.85	89 (65%) 0 3	97, 468, 664, 969	0
1	D	135/178 (75%)	2.55	74 (54%) 0 3	250, 410, 755, 981	0
All	All	540/712 (75%)	3.49	319 (59%) 0 3	97, 439, 676, 981	0

All (319) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	SER	17.4
1	A	144	GLY	16.2
1	C	156	GLY	15.6
1	A	120	LYS	15.6
1	A	151	GLU	14.3
1	A	61	LYS	14.2
1	C	155	ASN	13.8
1	C	59	SER	13.7
1	A	119	VAL	13.2
1	A	150	ARG	13.0
1	A	99	SER	12.9
1	A	85	TYR	12.6
1	C	61	LYS	12.6
1	C	140	SER	12.6
1	C	62	VAL	12.5
1	A	60	ALA	12.4
1	A	62	VAL	12.3
1	A	59	SER	12.0
1	A	86	PHE	11.9
1	A	149	THR	11.8
1	A	101	ARG	11.8

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Mol	Chain	Res	Type	RSRZ
1	A	123	ASN	11.2
1	C	193	LEU	11.0
1	A	103	THR	10.7
1	A	180	TRP	10.7
1	A	97	PHE	10.6
1	C	149	THR	10.5
1	A	179	GLY	10.3
1	B	144	GLY	10.2
1	A	121	VAL	9.9
1	C	144	GLY	9.9
1	B	143	ALA	9.8
1	C	142	PHE	9.8
1	C	139	ILE	9.6
1	C	108	ARG	9.5
1	A	143	ALA	9.5
1	B	151	GLU	9.4
1	C	151	GLU	9.4
1	A	63	ALA	9.3
1	A	145	ASP	9.3
1	A	98	ASP	9.2
1	C	192	PRO	9.1
1	D	156	GLY	9.0
1	A	175	ASN	8.9
1	C	107	PRO	8.8
1	D	155	ASN	8.7
1	C	60	ALA	8.7
1	A	152	ALA	8.6
1	D	107	PRO	8.6
1	A	117	HIS	8.5
1	B	149	THR	8.5
1	D	184	THR	8.4
1	C	143	ALA	8.4
1	A	100	GLU	8.3
1	B	120	LYS	8.0
1	A	107	PRO	7.9
1	A	84	ILE	7.9
1	A	184	THR	7.9
1	A	183	SER	7.8
1	C	141	ALA	7.7
1	C	63	ALA	7.7
1	A	69	SER	7.7
1	A	176	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	74	PRO	7.6
1	C	154	SER	7.6
1	A	104	PHE	7.5
1	A	178	GLY	7.5
1	A	146	GLN	7.5
1	D	62	VAL	7.5
1	A	87	ASP	7.1
1	A	177	MET	7.1
1	A	73	GLU	7.1
1	C	150	ARG	7.0
1	A	108	ARG	7.0
1	A	182	TYR	6.9
1	C	109	LYS	6.8
1	A	68	ARG	6.8
1	B	150	ARG	6.8
1	A	118	VAL	6.7
1	C	157	VAL	6.6
1	A	96	ASN	6.6
1	A	185	PHE	6.6
1	B	193	LEU	6.4
1	D	63	ALA	6.4
1	C	191	PHE	6.3
1	A	93	ILE	6.3
1	A	83	ILE	6.2
1	D	183	SER	6.1
1	A	148	VAL	6.1
1	A	192	PRO	6.1
1	C	175	ASN	6.0
1	B	119	VAL	6.0
1	A	127	ILE	5.9
1	A	167	ALA	5.9
1	D	154	SER	5.8
1	A	181	LYS	5.8
1	C	152	ALA	5.8
1	A	70	THR	5.8
1	C	138	VAL	5.8
1	D	108	ARG	5.8
1	C	169	LEU	5.8
1	A	147	ASP	5.7
1	A	125	GLN	5.7
1	D	117	HIS	5.6
1	C	126	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	84	ILE	5.5
1	C	131	LEU	5.5
1	A	156	GLY	5.4
1	D	153	ALA	5.4
1	D	116	PHE	5.4
1	A	169	LEU	5.4
1	C	127	ILE	5.3
1	C	116	PHE	5.3
1	A	109	LYS	5.3
1	A	171	LEU	5.3
1	A	71	ASN	5.3
1	A	88	GLN	5.2
1	A	66	ALA	5.2
1	D	175	ASN	5.2
1	B	62	VAL	5.2
1	C	102	SER	5.2
1	A	126	THR	5.2
1	A	122	TYR	5.1
1	D	152	ALA	5.1
1	A	67	ILE	5.0
1	C	188	PHE	5.0
1	B	182	TYR	5.0
1	C	129	VAL	5.0
1	A	142	PHE	5.0
1	B	142	PHE	4.9
1	C	93	ILE	4.9
1	D	86	PHE	4.9
1	D	157	VAL	4.8
1	D	59	SER	4.8
1	C	120	LYS	4.8
1	D	114	PHE	4.7
1	B	125	GLN	4.7
1	D	173	ARG	4.7
1	A	128	GLN	4.6
1	A	72	HIS	4.6
1	D	185	PHE	4.6
1	D	66	ALA	4.6
1	B	175	ASN	4.6
1	C	115	ASN	4.5
1	D	118	VAL	4.5
1	A	157	VAL	4.5
1	A	193	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	156	GLY	4.4
1	D	106	ALA	4.4
1	D	115	ASN	4.4
1	C	146	GLN	4.4
1	A	174	GLY	4.4
1	A	64	PHE	4.3
1	C	111	ILE	4.2
1	C	148	VAL	4.2
1	A	188	PHE	4.2
1	D	102	SER	4.2
1	C	74	PRO	4.2
1	D	139	ILE	4.2
1	C	114	PHE	4.1
1	D	100	GLU	4.1
1	B	188	PHE	4.1
1	C	110	GLY	4.1
1	D	104	PHE	4.1
1	B	61	LYS	4.1
1	D	186	SER	4.0
1	B	118	VAL	4.0
1	A	89	VAL	4.0
1	D	174	GLY	4.0
1	B	127	ILE	4.0
1	C	187	GLY	4.0
1	D	187	GLY	4.0
1	A	153	ALA	3.9
1	C	153	ALA	3.9
1	C	160	GLN	3.9
1	A	129	VAL	3.9
1	B	183	SER	3.9
1	C	83	ILE	3.8
1	B	126	THR	3.8
1	A	170	LYS	3.8
1	C	190	VAL	3.8
1	C	125	GLN	3.8
1	D	171	LEU	3.8
1	A	155	ASN	3.7
1	A	94	GLY	3.7
1	C	159	ILE	3.7
1	C	176	LEU	3.7
1	D	127	ILE	3.7
1	C	185	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	154	SER	3.7
1	B	185	PHE	3.6
1	C	133	LEU	3.6
1	B	184	THR	3.6
1	A	115	ASN	3.6
1	B	123	ASN	3.6
1	A	172	GLU	3.6
1	D	74	PRO	3.6
1	C	96	ASN	3.6
1	B	121	VAL	3.6
1	B	84	ILE	3.5
1	D	84	ILE	3.5
1	C	85	TYR	3.5
1	C	174	GLY	3.5
1	C	145	ASP	3.5
1	C	137	PRO	3.4
1	B	152	ALA	3.4
1	B	176	LEU	3.4
1	D	151	GLU	3.4
1	A	95	ASN	3.4
1	C	163	LYS	3.4
1	D	172	GLU	3.4
1	D	169	LEU	3.4
1	D	167	ALA	3.4
1	A	82	MET	3.4
1	A	114	PHE	3.3
1	A	78	SER	3.3
1	A	168	TYR	3.3
1	B	192	PRO	3.3
1	D	101	ARG	3.3
1	D	176	LEU	3.3
1	B	107	PRO	3.2
1	B	86	PHE	3.2
1	B	66	ALA	3.2
1	A	166	ARG	3.2
1	C	118	VAL	3.1
1	A	105	ILE	3.1
1	C	64	PHE	3.1
1	B	63	ALA	3.1
1	D	119	VAL	3.1
1	A	90	LEU	3.1
1	A	124	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	136	TRP	3.0
1	B	145	ASP	3.0
1	A	92	ASN	3.0
1	C	123	ASN	3.0
1	C	128	GLN	3.0
1	C	168	TYR	2.9
1	D	99	SER	2.9
1	A	173	ARG	2.9
1	D	123	ASN	2.9
1	C	130	SER	2.9
1	C	189	LEU	2.9
1	D	192	PRO	2.9
1	C	101	ARG	2.9
1	B	155	ASN	2.9
1	C	75	SER	2.9
1	A	65	SER	2.9
1	A	106	ALA	2.9
1	C	113	SER	2.9
1	B	146	GLN	2.8
1	C	147	ASP	2.8
1	D	170	LYS	2.8
1	D	158	LEU	2.8
1	D	180	TRP	2.8
1	D	120	LYS	2.8
1	D	129	VAL	2.8
1	D	188	PHE	2.8
1	C	124	ARG	2.8
1	D	85	TYR	2.8
1	D	147	ASP	2.7
1	D	109	LYS	2.7
1	B	117	HIS	2.7
1	D	67	ILE	2.7
1	C	158	LEU	2.7
1	A	190	VAL	2.7
1	B	115	ASN	2.7
1	B	59	SER	2.6
1	D	182	TYR	2.6
1	C	135	GLY	2.5
1	B	138	VAL	2.5
1	C	69	SER	2.5
1	B	140	SER	2.5
1	D	73	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	140	SER	2.5
1	B	180	TRP	2.5
1	A	81	THR	2.5
1	C	94	GLY	2.5
1	B	191	PHE	2.5
1	D	113	SER	2.5
1	D	61	LYS	2.5
1	A	131	LEU	2.4
1	B	114	PHE	2.4
1	A	161	MET	2.4
1	C	117	HIS	2.4
1	B	85	TYR	2.4
1	C	167	ALA	2.4
1	D	138	VAL	2.4
1	D	125	GLN	2.4
1	C	132	MET	2.4
1	A	116	PHE	2.3
1	C	112	TYR	2.3
1	B	108	ARG	2.3
1	D	131	LEU	2.3
1	B	157	VAL	2.3
1	D	95	ASN	2.3
1	D	60	ALA	2.3
1	D	69	SER	2.3
1	C	104	PHE	2.3
1	D	88	GLN	2.3
1	C	134	ASN	2.2
1	D	64	PHE	2.2
1	D	82	MET	2.2
1	D	96	ASN	2.2
1	C	119	VAL	2.2
1	D	112	TYR	2.2
1	C	86	PHE	2.2
1	A	75	SER	2.2
1	A	139	ILE	2.1
1	D	189	LEU	2.1
1	D	97	PHE	2.1
1	B	181	LYS	2.1
1	A	191	PHE	2.1
1	C	170	LYS	2.1
1	D	177	MET	2.1
1	D	83	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	ILE	2.0
1	B	139	ILE	2.0
1	C	121	VAL	2.0
1	C	182	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 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.