



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:13 am BST

PDB ID : 5KWD
Title : Computationally Designed Symmetric Homotetramer
Authors : Fallas, J.A.; Sankaran, B.; Zwart, P.; Baker, D.
Deposited on : 2016-07-17
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

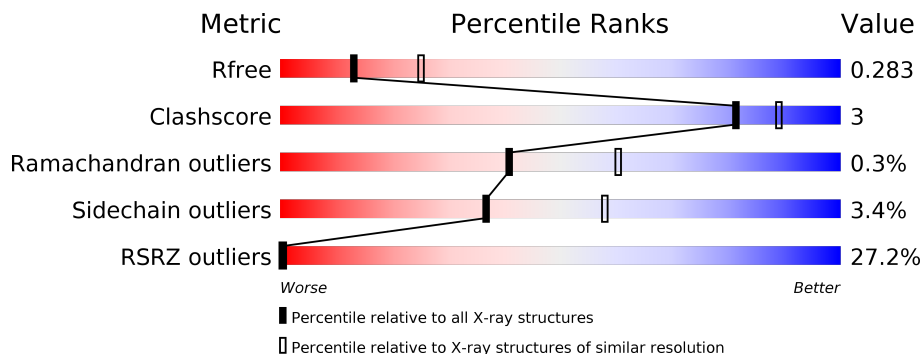
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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	160	<div style="display: flex; align-items: center;"> <div style="width: 19%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">19% 95% 5%</p>
1	B	160	<div style="display: flex; align-items: center;"> <div style="width: 26%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">26% 90% 10%</p>
1	C	160	<div style="display: flex; align-items: center;"> <div style="width: 31%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">31% 90% 8% ..</p>
1	D	160	<div style="display: flex; align-items: center;"> <div style="width: 31%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">31% 93% 6% ..</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9188 atoms, of which 4434 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 Ankyrin repeat-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	160	2329	743	1132	219	233	2	0	0	0
1	B	160	2289	729	1105	216	237	2	0	0	0
1	C	158	2248	720	1088	209	229	2	0	0	0
1	D	159	2286	730	1109	210	235	2	0	0	0

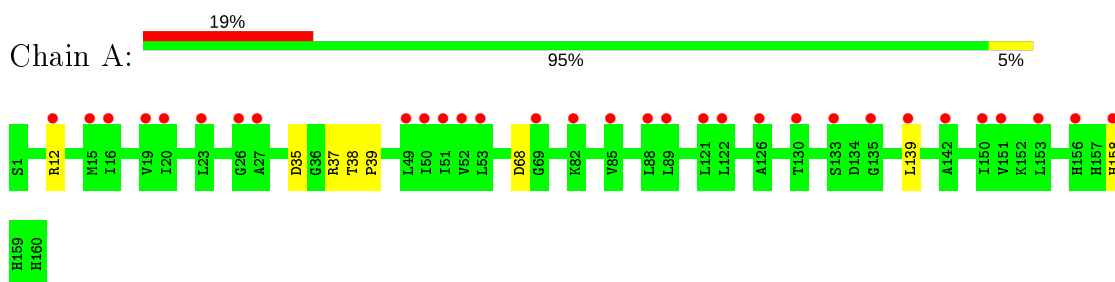
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	12	Total	O	0	0
			12	12		
2	C	4	Total	O	0	0
			4	4		
2	D	11	Total	O	0	0
			11	11		

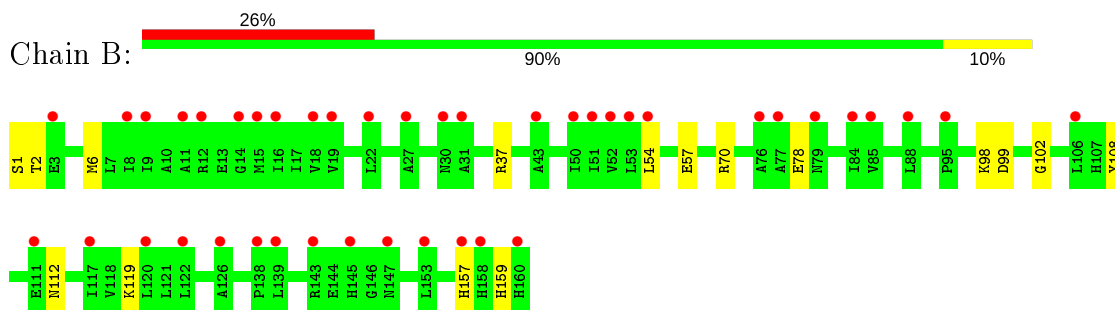
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

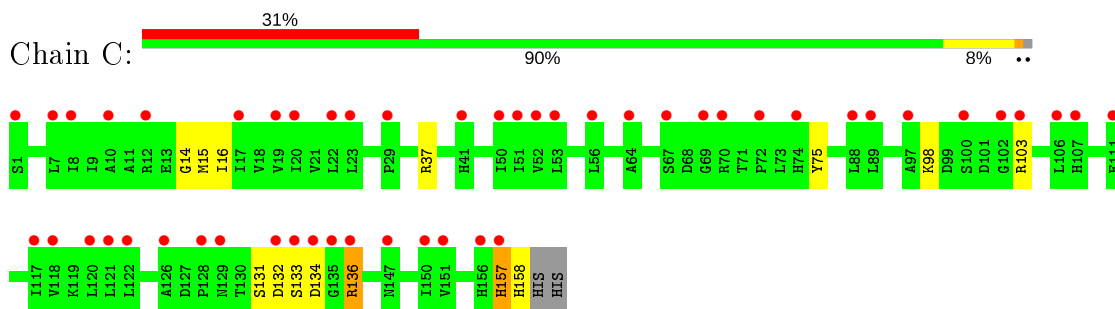
- Molecule 1: Ankyrin repeat-containing protein



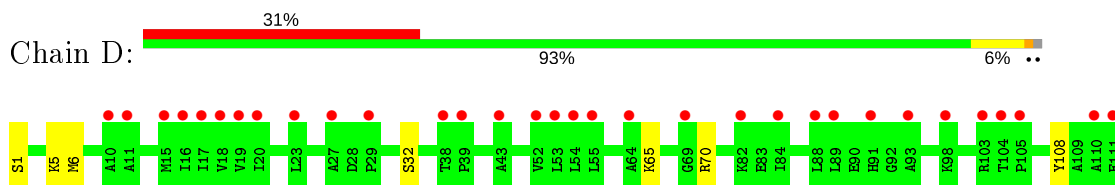
- Molecule 1: Ankyrin repeat-containing protein

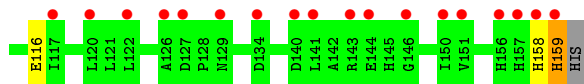


- Molecule 1: Ankyrin repeat-containing protein



- Molecule 1: Ankyrin repeat-containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.77Å 89.47Å 99.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.40 – 2.75 66.40 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.40-2.75) 99.7 (66.40-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.73Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.229 , 0.281 0.230 , 0.283	Depositor DCC
R_{free} test set	1851 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtrriage
Anisotropy	1.001	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9188	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.90% 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

5.1 Standard geometry

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	0.25	0/1219	0.41	0/1654
1	B	0.24	0/1204	0.41	0/1634
1	C	0.24	0/1181	0.41	0/1609
1	D	0.25	0/1198	0.41	0/1628
All	All	0.24	0/4802	0.41	0/6525

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

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	1197	1132	1163	3	0
1	B	1184	1105	1137	8	0
1	C	1160	1088	1099	6	0
1	D	1177	1109	1125	7	0
2	A	9	0	0	1	0
2	B	12	0	0	5	0
2	C	4	0	0	0	0
2	D	11	0	0	2	0
All	All	4754	4434	4524	24	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 3.

All (24) 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:119:LYS:NZ	2:B:201:HOH:O	1.93	0.86
1:D:5:LYS:NZ	2:D:201:HOH:O	2.12	0.82
1:B:99:ASP:OD2	1:B:108:TYR:OH	1.97	0.81
1:D:70:ARG:NH1	1:D:108:TYR:OH	2.13	0.81
1:D:1:SER:N	2:D:202:HOH:O	2.13	0.77
1:B:1:SER:N	2:B:202:HOH:O	2.15	0.75
1:D:158:HIS:HB2	1:D:159:HIS:O	1.88	0.73
1:B:37:ARG:NH2	2:B:203:HOH:O	2.20	0.73
1:A:37:ARG:NH2	1:A:68:ASP:OD2	2.31	0.64
1:D:158:HIS:HB2	1:D:159:HIS:C	2.19	0.62
1:D:158:HIS:N	1:D:159:HIS:HA	2.14	0.62
1:D:116:GLU:OE1	1:D:116:GLU:N	2.33	0.59
1:A:12:ARG:NH1	2:A:203:HOH:O	2.34	0.59
1:C:37:ARG:NH2	1:C:75:TYR:OH	2.39	0.56
1:C:14:GLY:O	1:C:16:ILE:N	2.39	0.56
1:C:157:HIS:O	1:C:158:HIS:HB2	2.08	0.54
1:C:132:ASP:N	1:C:136:ARG:O	2.42	0.52
1:B:78:GLU:O	1:B:112:ASN:ND2	2.43	0.51
1:B:37:ARG:CZ	2:B:203:HOH:O	2.57	0.50
1:B:98:LYS:HE3	1:B:102:GLY:O	2.11	0.50
1:B:70:ARG:NH2	2:B:204:HOH:O	2.23	0.49
1:A:38:THR:HB	1:A:39:PRO:HD2	1.95	0.49
1:C:132:ASP:OD1	1:C:133:SER:N	2.46	0.47
1:C:98:LYS:HA	1:C:103:ARG:O	2.21	0.41

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	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
1	B	158/160 (99%)	150 (95%)	7 (4%)	1 (1%)	25	42
1	C	156/160 (98%)	152 (97%)	3 (2%)	1 (1%)	25	42
1	D	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
All	All	629/640 (98%)	611 (97%)	16 (2%)	2 (0%)	41	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	HIS
1	C	15	MET

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	121/129 (94%)	118 (98%)	3 (2%)	47	67
1	B	121/129 (94%)	116 (96%)	5 (4%)	30	50
1	C	114/129 (88%)	110 (96%)	4 (4%)	36	56
1	D	118/129 (92%)	114 (97%)	4 (3%)	37	58
All	All	474/516 (92%)	458 (97%)	16 (3%)	37	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	139	LEU
1	A	158	HIS
1	B	2	THR
1	B	6	MET
1	B	54	LEU
1	B	57	GLU
1	B	157	HIS
1	C	131	SER

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Mol	Chain	Res	Type
1	C	134	ASP
1	C	136	ARG
1	C	157	HIS
1	D	6	MET
1	D	32	SER
1	D	65	LYS
1	D	159	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	114	HIS

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, 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	160/160 (100%)	1.26	31 (19%) 1 1	31, 42, 62, 76	0
1	B	160/160 (100%)	1.38	42 (26%) 0 0	37, 52, 66, 73	0
1	C	158/160 (98%)	1.65	50 (31%) 0 0	35, 54, 71, 83	0
1	D	159/160 (99%)	1.54	50 (31%) 0 0	33, 49, 67, 81	0
All	All	637/640 (99%)	1.45	173 (27%) 0 0	31, 49, 68, 83	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	GLY	5.6
1	D	158	HIS	4.9
1	C	133	SER	4.8
1	C	156	HIS	4.7
1	C	100	SER	4.6
1	D	146	GLY	4.5
1	B	120	LEU	4.4
1	C	102	GLY	4.4
1	B	160	HIS	4.2
1	D	151	VAL	4.2
1	D	29	PRO	4.1
1	C	20	ILE	4.0
1	C	69	GLY	3.9
1	C	23	LEU	3.8
1	C	107	HIS	3.7
1	D	159	HIS	3.6
1	D	144	GLU	3.6
1	D	117	ILE	3.6
1	D	15	MET	3.6
1	B	122	LEU	3.6
1	D	11	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	145	HIS	3.5
1	B	158	HIS	3.4
1	D	89	LEU	3.4
1	A	150	ILE	3.3
1	A	26	GLY	3.3
1	D	150	ILE	3.3
1	B	11	ALA	3.2
1	A	158	HIS	3.2
1	C	88	LEU	3.2
1	C	8	ILE	3.2
1	D	16	ILE	3.1
1	C	150	ILE	3.1
1	A	151	VAL	3.1
1	C	111	GLU	3.0
1	B	15	MET	3.0
1	B	51	ILE	3.0
1	D	17	ILE	3.0
1	D	110	ALA	3.0
1	B	157	HIS	3.0
1	A	20	ILE	2.9
1	C	157	HIS	2.9
1	A	139	LEU	2.9
1	A	126	ALA	2.9
1	C	126	ALA	2.9
1	C	72	PRO	2.9
1	B	43	ALA	2.9
1	C	50	ILE	2.8
1	A	23	LEU	2.8
1	D	120	LEU	2.8
1	C	134	ASP	2.8
1	B	117	ILE	2.8
1	B	31	ALA	2.8
1	D	93	ALA	2.8
1	D	20	ILE	2.8
1	C	128	PRO	2.8
1	D	126	ALA	2.8
1	B	8	ILE	2.8
1	B	153	LEU	2.8
1	D	43	ALA	2.8
1	B	139	LEU	2.8
1	D	18	VAL	2.7
1	C	147	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	79	ASN	2.7
1	C	7	LEU	2.7
1	C	67	SER	2.7
1	C	132	ASP	2.7
1	B	95	PRO	2.6
1	B	30	ASN	2.6
1	D	19	VAL	2.6
1	D	23	LEU	2.6
1	D	122	LEU	2.6
1	A	16	ILE	2.6
1	A	135	GLY	2.6
1	D	129	ASN	2.6
1	A	49	LEU	2.6
1	B	14	GLY	2.6
1	C	151	VAL	2.6
1	C	1	SER	2.6
1	A	156	HIS	2.6
1	D	143	ARG	2.6
1	B	126	ALA	2.6
1	C	118	VAL	2.5
1	D	88	LEU	2.5
1	C	129	ASN	2.5
1	A	12	ARG	2.5
1	A	153	LEU	2.5
1	D	69	GLY	2.5
1	B	106	LEU	2.5
1	B	12	ARG	2.5
1	C	41	HIS	2.5
1	C	51	ILE	2.5
1	A	89	LEU	2.5
1	C	10	ALA	2.5
1	A	69	GLY	2.4
1	C	52	VAL	2.4
1	D	39	PRO	2.4
1	C	64	ALA	2.4
1	A	82	LYS	2.4
1	D	53	LEU	2.4
1	D	27	ALA	2.4
1	B	22	LEU	2.3
1	D	141	LEU	2.3
1	D	82	LYS	2.3
1	D	84	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	18	VAL	2.3
1	C	19	VAL	2.3
1	C	29	PRO	2.3
1	A	133	SER	2.3
1	C	70	ARG	2.3
1	D	64	ALA	2.3
1	A	19	VAL	2.3
1	B	9	ILE	2.3
1	A	85	VAL	2.3
1	A	122	LEU	2.3
1	D	127	ASP	2.3
1	A	53	LEU	2.2
1	B	3	GLU	2.2
1	D	103	ARG	2.2
1	C	74	HIS	2.2
1	C	122	LEU	2.2
1	D	98	LYS	2.2
1	B	143	ARG	2.2
1	D	52	VAL	2.2
1	A	27	ALA	2.2
1	A	51	ILE	2.2
1	C	17	ILE	2.2
1	D	104	THR	2.2
1	D	111	GLU	2.2
1	C	56	LEU	2.2
1	D	38	THR	2.2
1	A	50	ILE	2.2
1	D	54	LEU	2.2
1	B	27	ALA	2.2
1	C	103	ARG	2.2
1	B	84	ILE	2.1
1	C	120	LEU	2.1
1	C	12	ARG	2.1
1	B	50	ILE	2.1
1	C	89	LEU	2.1
1	C	121	LEU	2.1
1	C	97	ALA	2.1
1	B	19	VAL	2.1
1	B	53	LEU	2.1
1	C	22	LEU	2.1
1	C	117	ILE	2.1
1	B	85	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	53	LEU	2.1
1	D	55	LEU	2.1
1	D	105	PRO	2.1
1	B	52	VAL	2.1
1	D	156	HIS	2.1
1	A	142	ALA	2.1
1	D	140	ASP	2.1
1	B	76	ALA	2.1
1	C	106	LEU	2.1
1	B	138	PRO	2.1
1	A	130	THR	2.1
1	A	121	LEU	2.0
1	A	52	VAL	2.0
1	B	16	ILE	2.0
1	B	147	ASN	2.0
1	D	10	ALA	2.0
1	A	15	MET	2.0
1	B	54	LEU	2.0
1	B	111	GLU	2.0
1	B	77	ALA	2.0
1	D	134	ASP	2.0
1	A	88	LEU	2.0
1	B	88	LEU	2.0
1	C	136	ARG	2.0
1	D	91	HIS	2.0
1	D	157	HIS	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.