Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 05:49 PM EDT

PDB ID	:	5V75
Title	:	Structure of Haliangium ochraceum BMC-T HO-5816
Authors	:	Sutter, M.; Aussignargues, C.; Kerfeld, C.A.
Deposited on	:	2017-03-17
Resolution	:	1.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

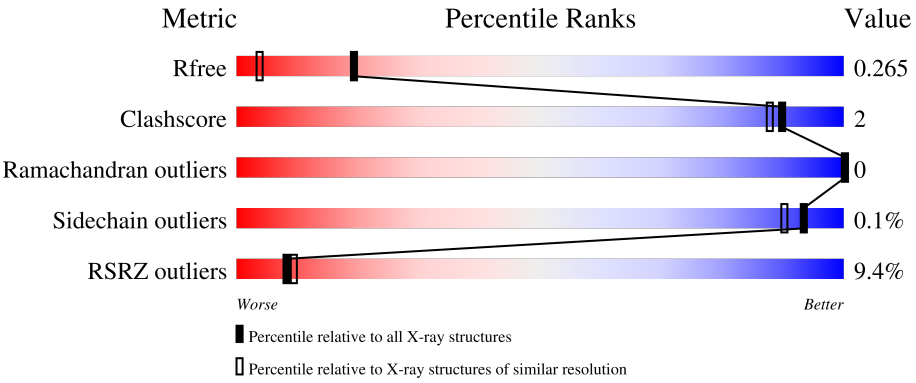
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	212	6% 92% · 7%
1	B	212	8% 92% · 6%
1	C	212	8% 93% · 6%
1	D	212	8% 90% 5% 6%
1	E	212	8% 89% 5% 6%

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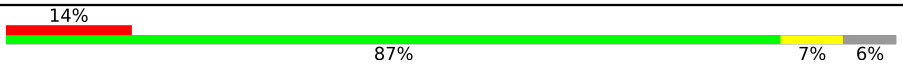
Mol	Chain	Length	Quality of chain
1	F	212	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18923 atoms, of which 9210 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 Microcompartments protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			3018	954	1522	260	279	3			
1	B	199	Total	C	H	N	O	S	0	0	0
			3036	959	1530	262	282	3			
1	C	200	Total	C	H	N	O	S	0	0	0
			3060	967	1543	263	284	3			
1	D	200	Total	C	H	N	O	S	0	0	0
			3051	964	1538	263	283	3			
1	E	200	Total	C	H	N	O	S	0	0	0
			3051	964	1538	263	283	3			
1	F	200	Total	C	H	N	O	S	0	0	0
			3052	964	1539	263	283	3			

- Molecule 2 is water.

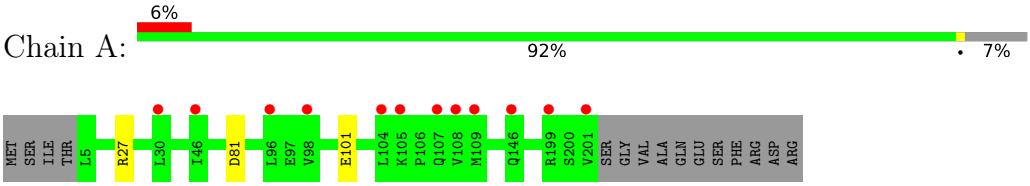
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	106	Total	O	0	0
			106	106		
2	C	116	Total	O	0	0
			116	116		
2	D	108	Total	O	0	0
			108	108		
2	E	109	Total	O	0	0
			109	109		
2	F	101	Total	O	0	0
			101	101		

3 Residue-property plots (i)

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

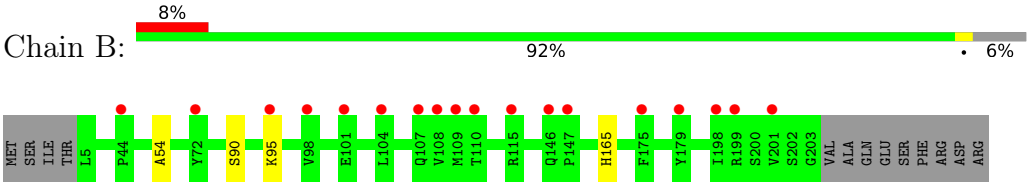
• Molecule 1: Microcompartments protein

Chain A:



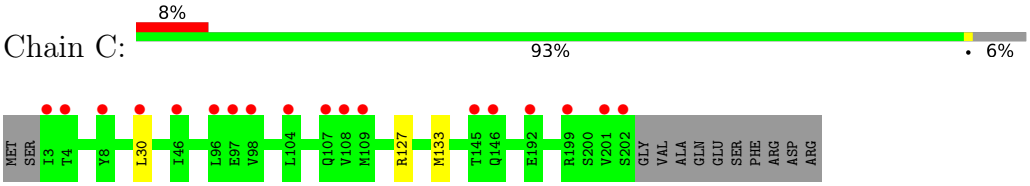
• Molecule 1: Microcompartments protein

Chain B:



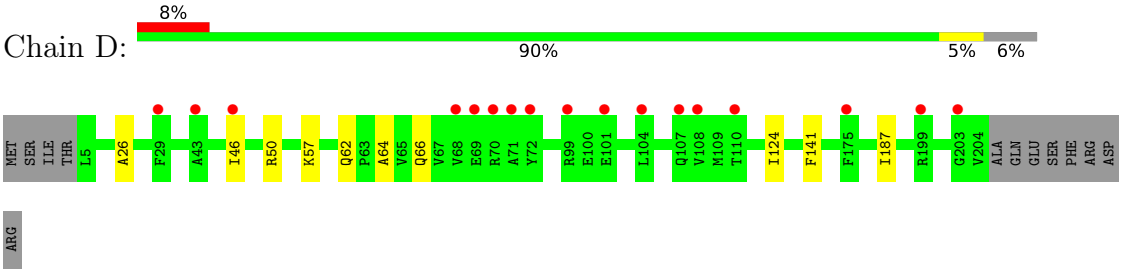
• Molecule 1: Microcompartments protein

Chain C:



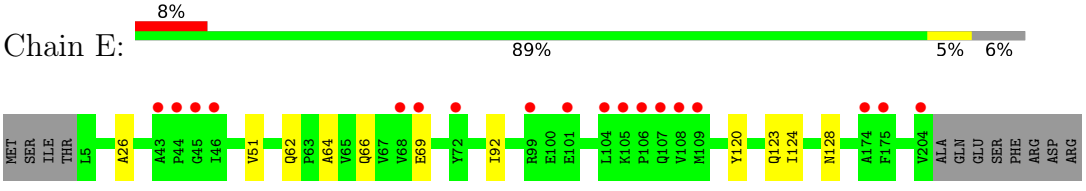
• Molecule 1: Microcompartments protein

Chain D:



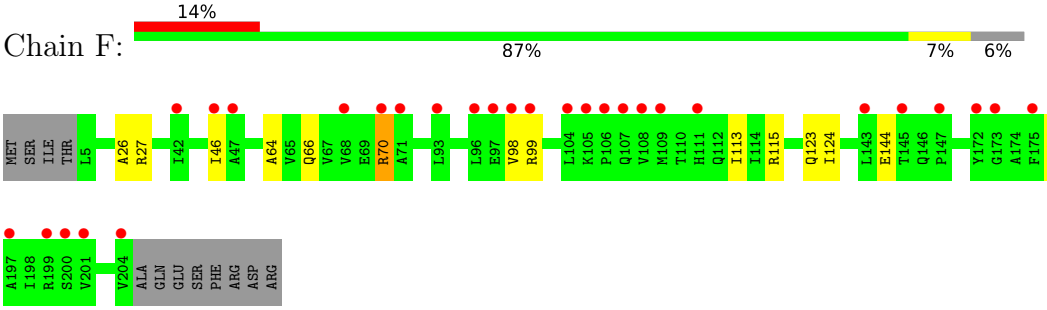
• Molecule 1: Microcompartments protein

Chain E:



• Molecule 1: Microcompartments protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.12Å 126.11Å 139.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.59 – 1.70 38.59 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.59-1.70) 99.2 (38.59-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.70Å)	Xtriage
Refinement program	PHENIX (dev_2650: ???)	Depositor
R, R_{free}	0.226 , 0.266 0.226 , 0.265	Depositor DCC
R_{free} test set	2000 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18923	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6653e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/1522	0.46	0/2071
1	B	0.26	0/1532	0.45	0/2084
1	C	0.27	0/1543	0.47	0/2100
1	D	0.26	0/1539	0.43	0/2094
1	E	0.26	0/1539	0.44	0/2094
1	F	0.26	0/1539	0.44	0/2094
All	All	0.26	0/9214	0.45	0/12537

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	1496	1522	1520	2	1
1	B	1506	1530	1528	2	1
1	C	1517	1543	1543	5	0
1	D	1513	1538	1537	9	0
1	E	1513	1538	1537	8	0
1	F	1513	1539	1537	14	0
2	A	115	0	0	0	1
2	B	106	0	0	2	1
2	C	116	0	0	2	0
2	D	108	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	109	0	0	1	0
2	F	101	0	0	2	0
All	All	9713	9210	9202	32	2

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 2.

All (32) 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:E:69:GLU:OE2	1:F:70:ARG:NH2	2.17	0.77
1:C:133:MET:O	2:C:301:HOH:O	2.09	0.70
1:D:50:ARG:NH2	2:D:304:HOH:O	2.27	0.66
1:D:46:ILE:O	2:D:301:HOH:O	2.15	0.63
1:B:165:HIS:NE2	2:B:302:HOH:O	2.31	0.62
1:D:57:LYS:NZ	2:D:303:HOH:O	2.24	0.60
1:B:54:ALA:HB2	1:B:95:LYS:HD2	1.84	0.59
1:E:120:TYR:O	1:E:123:GLN:HG2	2.02	0.59
1:F:123:GLN:OE1	2:F:301:HOH:O	2.17	0.57
1:C:30:LEU:HD12	1:F:123:GLN:NE2	2.23	0.54
1:D:62:GLN:OE1	2:D:302:HOH:O	2.18	0.52
1:E:62:GLN:OE1	2:E:301:HOH:O	2.19	0.51
1:C:30:LEU:HD12	1:F:123:GLN:HE21	1.76	0.50
1:F:115:ARG:NH1	1:F:184:GLU:HG3	2.25	0.50
1:D:57:LYS:NZ	1:F:115:ARG:O	2.41	0.50
1:D:124:ILE:HG21	1:E:66:GLN:HB3	1.94	0.50
1:F:26:ALA:HB1	1:F:64:ALA:O	2.14	0.47
1:A:101:GLU:OE1	1:A:101:GLU:N	2.43	0.47
1:D:26:ALA:HB1	1:D:64:ALA:O	2.17	0.45
1:C:127:ARG:NH2	2:C:311:HOH:O	2.50	0.44
1:F:144:GLU:HA	1:F:176:GLY:O	2.18	0.43
1:E:26:ALA:HB1	1:E:64:ALA:O	2.19	0.43
1:E:51:VAL:HG13	1:E:92:ILE:HG23	2.01	0.42
1:F:113:ILE:HG21	1:F:115:ARG:NH1	2.34	0.42
1:E:128:ASN:OD1	1:F:27:ARG:NH1	2.50	0.42
1:A:27:ARG:NH1	2:B:307:HOH:O	2.53	0.42
1:D:66:GLN:HB3	1:F:124:ILE:HG21	2.01	0.42
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.91	0.41
1:F:98:VAL:HG12	1:F:99:ARG:O	2.20	0.41
1:E:124:ILE:HG21	1:F:66:GLN:HB3	2.03	0.41
1:D:141:PHE:HB2	1:D:187:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ILE:O	2:F:302:HOH:O	2.21	0.40

All (2) 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)
2:A:358:HOH:O	2:B:320:HOH:O[3_646]	2.05	0.15
1:A:81:ASP:OD2	1:B:90:SER:OG[3_646]	2.19	0.01

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	195/212 (92%)	191 (98%)	4 (2%)	0	100	100
1	B	197/212 (93%)	193 (98%)	4 (2%)	0	100	100
1	C	198/212 (93%)	191 (96%)	7 (4%)	0	100	100
1	D	198/212 (93%)	194 (98%)	4 (2%)	0	100	100
1	E	198/212 (93%)	191 (96%)	7 (4%)	0	100	100
1	F	198/212 (93%)	194 (98%)	4 (2%)	0	100	100
All	All	1184/1272 (93%)	1154 (98%)	30 (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	151/164 (92%)	151 (100%)	0	100	100
1	B	152/164 (93%)	152 (100%)	0	100	100
1	C	154/164 (94%)	154 (100%)	0	100	100
1	D	153/164 (93%)	153 (100%)	0	100	100
1	E	153/164 (93%)	153 (100%)	0	100	100
1	F	153/164 (93%)	152 (99%)	1 (1%)	84	77
All	All	916/984 (93%)	915 (100%)	1 (0%)	93	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	70	ARG

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

Mol	Chain	Res	Type
1	F	123	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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^{th} 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	197/212 (92%)	0.59	12 (6%)	21	23	12, 22, 48, 62	0
1	B	199/212 (93%)	0.50	18 (9%)	9	10	11, 22, 48, 71	0
1	C	200/212 (94%)	0.51	18 (9%)	9	10	11, 21, 47, 62	0
1	D	200/212 (94%)	0.51	17 (8%)	10	12	11, 21, 51, 86	0
1	E	200/212 (94%)	0.48	18 (9%)	9	10	13, 20, 48, 67	0
1	F	200/212 (94%)	0.88	29 (14%)	2	2	11, 26, 51, 68	0
All	All	1196/1272 (94%)	0.58	112 (9%)	8	9	11, 22, 49, 86	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	MET	5.7
1	B	107	GLN	5.4
1	F	68	VAL	5.1
1	D	70	ARG	5.0
1	E	68	VAL	4.8
1	F	147	PRO	4.6
1	F	175	PHE	4.6
1	B	104	LEU	4.5
1	A	201	VAL	4.5
1	D	175	PHE	4.3
1	A	30	LEU	4.2
1	A	98	VAL	4.2
1	F	71	ALA	4.2
1	F	97	GLU	4.0
1	A	104	LEU	3.9
1	E	46	ILE	3.9
1	F	42	ILE	3.9
1	E	204	VAL	3.9
1	F	108	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	146	GLN	3.7
1	A	107	GLN	3.7
1	E	99	ARG	3.6
1	A	109	MET	3.6
1	E	175	PHE	3.5
1	E	69	GLU	3.5
1	D	99	ARG	3.5
1	E	43	ALA	3.5
1	F	172	TYR	3.4
1	C	107	GLN	3.4
1	C	104	LEU	3.4
1	E	72	TYR	3.4
1	E	108	VAL	3.4
1	D	199	ARG	3.4
1	C	30	LEU	3.3
1	B	147	PRO	3.3
1	D	69	GLU	3.2
1	A	96	LEU	3.2
1	A	199	ARG	3.1
1	B	199	ARG	3.1
1	F	47	ALA	3.1
1	F	106	PRO	3.1
1	F	99	ARG	3.1
1	F	107	GLN	3.1
1	D	108	VAL	3.1
1	C	199	ARG	3.0
1	E	101	GLU	3.0
1	B	146	GLN	3.0
1	C	108	VAL	3.0
1	F	197	ALA	3.0
1	A	105	LYS	3.0
1	C	98	VAL	3.0
1	E	106	PRO	2.9
1	D	29	PHE	2.9
1	C	202	SER	2.8
1	F	70	ARG	2.8
1	C	145	THR	2.8
1	A	108	VAL	2.8
1	D	107	GLN	2.8
1	E	45	GLY	2.8
1	D	71	ALA	2.7
1	C	97	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	72	TYR	2.7
1	F	96	LEU	2.7
1	F	200	SER	2.6
1	E	105	LYS	2.6
1	F	201	VAL	2.6
1	E	104	LEU	2.6
1	C	146	GLN	2.6
1	D	46	ILE	2.5
1	B	44	PRO	2.5
1	F	105	LYS	2.5
1	F	199	ARG	2.5
1	B	98	VAL	2.5
1	F	145	THR	2.5
1	D	43	ALA	2.4
1	B	110	THR	2.4
1	C	96	LEU	2.4
1	F	93	LEU	2.4
1	B	72	TYR	2.4
1	B	108	VAL	2.4
1	A	46	ILE	2.4
1	D	110	THR	2.4
1	E	107	GLN	2.4
1	F	204	VAL	2.3
1	D	101	GLU	2.3
1	D	68	VAL	2.3
1	B	95	LYS	2.3
1	B	115	ARG	2.2
1	C	192	GLU	2.2
1	F	173	GLY	2.2
1	C	201	VAL	2.2
1	C	46	ILE	2.2
1	D	203	GLY	2.2
1	B	179	TYR	2.2
1	C	8	TYR	2.2
1	E	44	PRO	2.2
1	F	46	ILE	2.2
1	F	109	MET	2.1
1	F	98	VAL	2.1
1	F	143	LEU	2.1
1	C	4	THR	2.1
1	B	198	ILE	2.1
1	C	109	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	109	MET	2.1
1	D	104	LEU	2.1
1	E	174	ALA	2.1
1	F	111	HIS	2.1
1	B	201	VAL	2.1
1	B	101	GLU	2.1
1	B	175	PHE	2.1
1	C	3	ILE	2.1
1	F	104	LEU	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 monosaccharides 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.