



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID : 3B61
Title : EmrE multidrug transporter, apo crystal form
Authors : Chang, G.; Chen, Y.J.
Deposited on : 2007-10-26
Resolution : 4.50 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 : 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

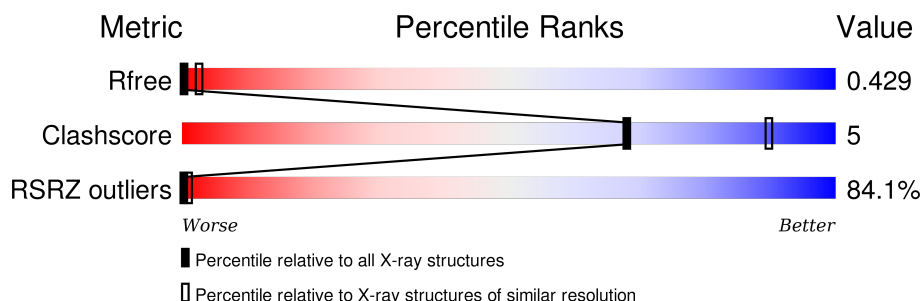
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
RSRZ outliers	91569	1075 (5.40-3.60)

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	110	<div> <div>85%</div> <div>97%</div> </div>
1	B	110	<div> <div>78%</div> <div>95%</div> </div>
1	C	110	<div> <div>83%</div> <div>97%</div> </div>
1	D	110	<div> <div>86%</div> <div>95%</div> </div>
1	E	110	<div> <div>85%</div> <div>97%</div> </div>
1	F	110	<div> <div>79%</div> <div>95%</div> </div>
1	G	110	<div> <div>80%</div> <div>97%</div> </div>
1	H	110	<div> <div>77%</div> <div>95%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 856 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.

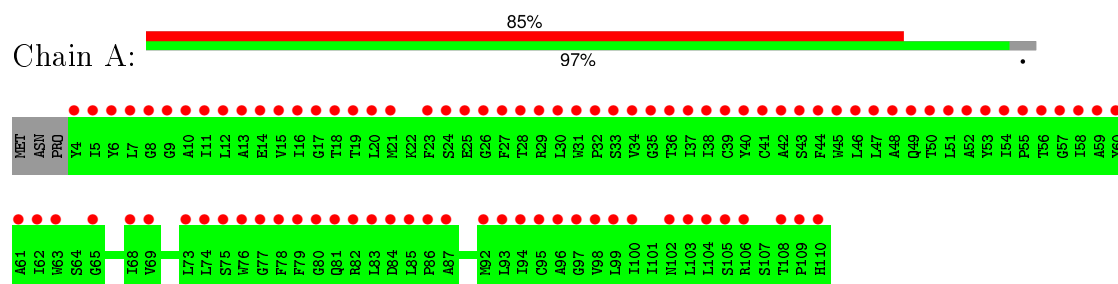
- Molecule 1 is a protein called Multidrug transporter emrE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	107	Total C 107 107	0	0	107
1	B	107	Total C 107 107	0	0	107
1	C	107	Total C 107 107	0	0	107
1	D	107	Total C 107 107	0	0	107
1	E	107	Total C 107 107	0	0	107
1	F	107	Total C 107 107	0	0	107
1	G	107	Total C 107 107	0	0	107
1	H	107	Total C 107 107	0	0	107

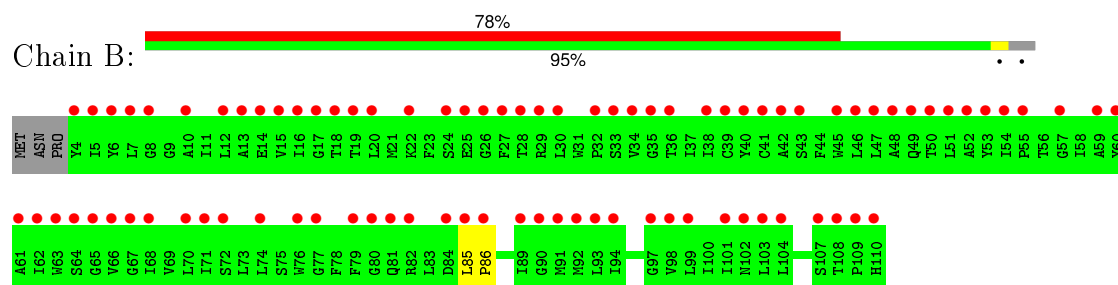
3 Residue-property plots

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.

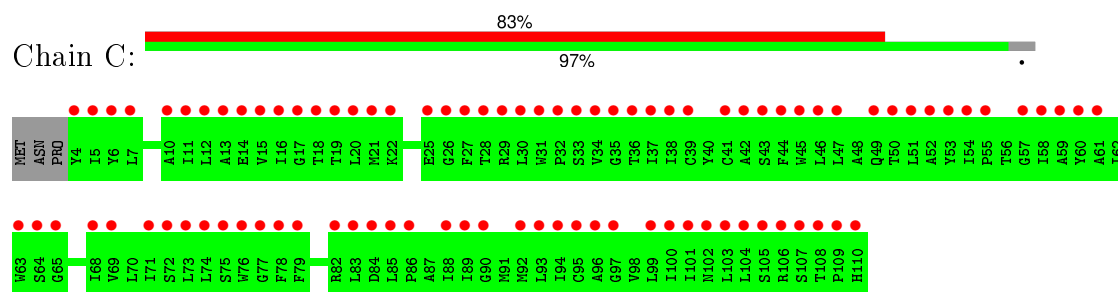
- Molecule 1: Multidrug transporter emrE



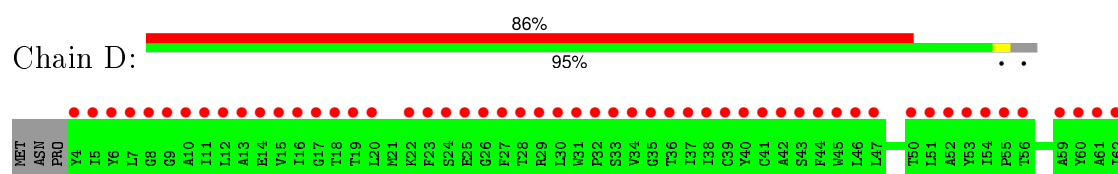
- Molecule 1: Multidrug transporter emrE

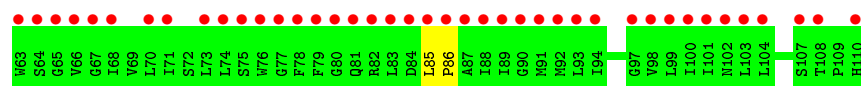


- Molecule 1: Multidrug transporter emrE

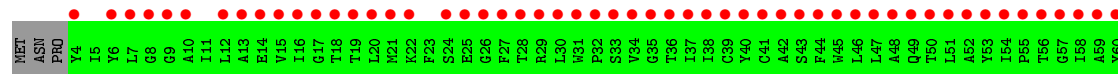
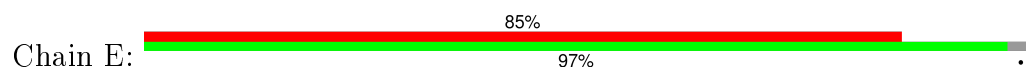


- Molecule 1: Multidrug transporter emrE

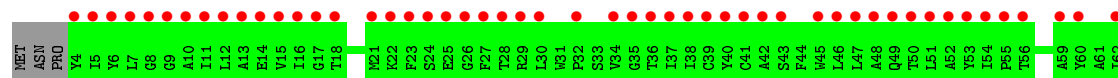
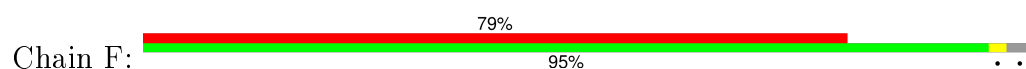




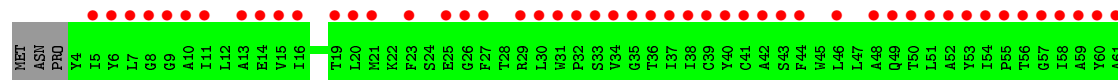
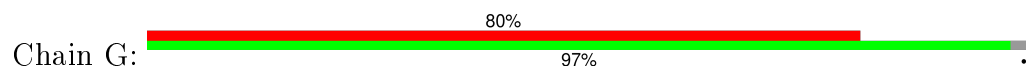
- Molecule 1: Multidrug transporter emrE



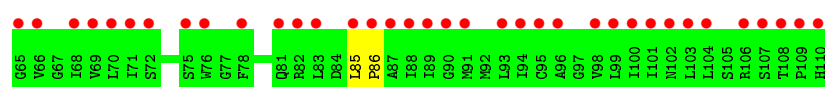
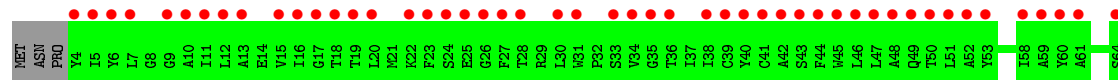
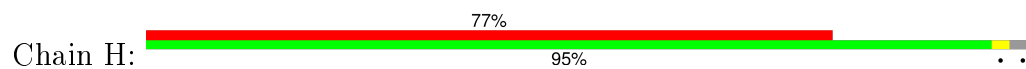
- Molecule 1: Multidrug transporter emrE



- Molecule 1: Multidrug transporter emrE



- Molecule 1: Multidrug transporter emrE



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.00 Å 239.20 Å 284.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 4.50 19.99 – 4.50	Depositor EDS
% Data completeness (in resolution range)	75.8 (19.99-4.50) 75.8 (19.99-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.54 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.318 , 0.362 0.391 , 0.429	Depositor DCC
R_{free} test set	1367 reflections (9.89%)	DCC
Wilson B-factor (Å ²)	187.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 13836 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	856	wwPDB-VP
Average B, all atoms (Å ²)	229.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	107	0	0	0	0
1	B	107	0	0	1	0
1	C	107	0	0	0	0
1	D	107	0	0	1	0
1	E	107	0	0	0	0
1	F	107	0	0	1	0
1	G	107	0	0	0	0
1	H	107	0	0	1	0
All	All	856	0	0	4	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 5.

All (4) 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:H:85:LEU:CA	1:H:86:PRO:CA	2.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:CA	1:D:86:PRO:CA	2.64	0.75
1:F:85:LEU:CA	1:F:86:PRO:CA	2.65	0.75
1:B:85:LEU:CA	1:B:86:PRO:CA	2.66	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

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	107/110 (97%)	8.62	94 (87%) 0 1	82, 228, 336, 336	0
1	B	107/110 (97%)	6.90	86 (80%) 0 1	62, 240, 336, 336	0
1	C	107/110 (97%)	7.55	91 (85%) 0 1	76, 222, 336, 336	0
1	D	107/110 (97%)	7.55	95 (88%) 0 1	61, 209, 336, 336	0
1	E	107/110 (97%)	8.37	94 (87%) 0 1	56, 221, 336, 336	0
1	F	107/110 (97%)	9.46	87 (81%) 0 1	74, 209, 336, 336	0
1	G	107/110 (97%)	7.07	88 (82%) 0 1	48, 229, 336, 336	0
1	H	107/110 (97%)	7.52	85 (79%) 0 1	37, 241, 336, 336	0
All	All	856/880 (97%)	7.88	720 (84%) 0 1	37, 227, 336, 336	0

All (720) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	LEU	46.3
1	E	41	CYS	36.2
1	C	103	LEU	36.0
1	F	81	GLN	35.4
1	F	13	ALA	33.5
1	C	102	ASN	32.3
1	E	87	ALA	31.4
1	A	55	PRO	31.2
1	B	60	TYR	30.2
1	F	35	GLY	29.2
1	F	12	LEU	28.6
1	A	105	SER	28.4
1	C	108	THR	28.3
1	H	59	ALA	28.3
1	H	10	ALA	28.2
1	F	49	GLN	28.0

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Mol	Chain	Res	Type	RSRZ
1	D	8	GLY	27.2
1	E	16	ILE	26.4
1	F	63	TRP	26.2
1	E	47	LEU	25.9
1	B	63	TRP	25.8
1	B	48	ALA	25.6
1	E	26	GLY	24.8
1	A	51	LEU	24.6
1	D	88	ILE	24.6
1	F	45	TRP	24.3
1	E	27	PHE	24.1
1	E	28	THR	22.5
1	H	52	ALA	22.4
1	A	9	GLY	21.9
1	G	103	LEU	21.8
1	B	62	ILE	21.7
1	C	19	THR	21.3
1	E	20	LEU	21.0
1	D	9	GLY	21.0
1	F	94	ILE	20.8
1	E	65	GLY	20.8
1	H	71	ILE	20.8
1	H	46	LEU	20.8
1	D	20	LEU	20.6
1	F	71	ILE	20.6
1	G	60	TYR	20.4
1	F	39	CYS	20.4
1	A	42	ALA	20.3
1	B	49	GLN	20.0
1	F	38	ILE	19.7
1	D	102	ASN	19.6
1	B	61	ALA	19.5
1	D	26	GLY	19.5
1	A	109	PRO	19.4
1	H	19	THR	19.2
1	F	9	GLY	19.1
1	A	38	ILE	19.0
1	D	41	CYS	18.8
1	G	26	GLY	18.8
1	D	19	THR	18.8
1	H	103	LEU	18.7
1	A	12	LEU	18.7

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Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	18.6
1	F	85	LEU	18.3
1	A	35	GLY	18.2
1	A	52	ALA	18.1
1	G	59	ALA	18.0
1	B	91	MET	17.9
1	F	6	TYR	17.8
1	E	45	TRP	17.7
1	G	67	GLY	17.7
1	A	104	LEU	17.5
1	F	46	LEU	17.5
1	A	39	CYS	17.4
1	H	86	PRO	17.3
1	E	86	PRO	17.0
1	F	48	ALA	17.0
1	E	46	LEU	17.0
1	E	21	MET	16.9
1	F	82	ARG	16.8
1	C	105	SER	16.8
1	C	51	LEU	16.6
1	G	13	ALA	16.6
1	F	50	THR	16.4
1	A	110	HIS	16.4
1	A	20	LEU	16.3
1	D	101	ILE	16.3
1	G	42	ALA	16.2
1	B	71	ILE	16.1
1	F	52	ALA	16.0
1	B	39	CYS	16.0
1	G	102	ASN	15.9
1	H	25	GLU	15.9
1	C	6	TYR	15.9
1	C	37	ILE	15.8
1	D	12	LEU	15.8
1	D	31	TRP	15.6
1	E	109	PRO	15.5
1	C	38	ILE	15.5
1	G	31	TRP	15.3
1	B	14	GLU	15.3
1	E	48	ALA	15.2
1	H	45	TRP	15.2
1	G	65	GLY	15.2

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Mol	Chain	Res	Type	RSRZ
1	H	102	ASN	15.1
1	B	29	ARG	15.0
1	F	26	GLY	15.0
1	C	50	THR	15.0
1	A	53	TYR	15.0
1	H	90	GLY	15.0
1	H	88	ILE	14.9
1	H	87	ALA	14.8
1	E	29	ARG	14.8
1	A	27	PHE	14.8
1	H	69	VAL	14.8
1	G	110	HIS	14.7
1	C	12	LEU	14.7
1	F	77	GLY	14.7
1	C	26	GLY	14.6
1	A	61	ALA	14.5
1	A	11	ILE	14.5
1	H	51	LEU	14.4
1	A	19	THR	14.4
1	C	14	GLU	14.4
1	A	10	ALA	14.2
1	D	60	TYR	14.2
1	G	19	THR	14.2
1	A	47	LEU	14.2
1	E	54	ILE	14.1
1	G	6	TYR	14.1
1	E	55	PRO	13.8
1	F	60	TYR	13.8
1	C	109	PRO	13.8
1	C	64	SER	13.7
1	G	79	PHE	13.7
1	F	62	ILE	13.7
1	B	26	GLY	13.6
1	A	6	TYR	13.6
1	D	17	GLY	13.5
1	A	62	ILE	13.5
1	G	66	VAL	13.5
1	F	91	MET	13.4
1	H	16	ILE	13.4
1	H	42	ALA	13.3
1	H	43	SER	13.3
1	F	93	LEU	13.2

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Mol	Chain	Res	Type	RSRZ
1	B	54	ILE	13.2
1	E	7	LEU	13.2
1	A	86	PRO	12.9
1	G	41	CYS	12.9
1	D	71	ILE	12.9
1	H	17	GLY	12.9
1	A	17	GLY	12.8
1	E	15	VAL	12.8
1	G	56	THR	12.8
1	D	62	ILE	12.8
1	E	38	ILE	12.7
1	C	65	GLY	12.7
1	B	35	GLY	12.7
1	F	10	ALA	12.7
1	D	29	ARG	12.6
1	D	51	LEU	12.6
1	G	20	LEU	12.6
1	G	109	PRO	12.5
1	F	99	LEU	12.5
1	G	100	ILE	12.4
1	E	69	VAL	12.3
1	F	4	TYR	12.2
1	H	76	TRP	12.2
1	E	56	THR	12.2
1	F	51	LEU	12.2
1	G	10	ALA	12.0
1	A	4	TYR	12.0
1	F	5	ILE	12.0
1	B	19	THR	11.9
1	D	65	GLY	11.9
1	A	30	LEU	11.9
1	D	61	ALA	11.8
1	E	81	GLN	11.8
1	B	32	PRO	11.8
1	C	25	GLU	11.8
1	H	5	ILE	11.7
1	E	8	GLY	11.6
1	D	59	ALA	11.6
1	G	75	SER	11.5
1	D	82	ARG	11.5
1	A	96	ALA	11.5
1	D	86	PRO	11.5

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Mol	Chain	Res	Type	RSRZ
1	A	31	TRP	11.4
1	B	30	LEU	11.4
1	F	8	GLY	11.4
1	A	78	PHE	11.4
1	A	24	SER	11.4
1	D	52	ALA	11.4
1	F	32	PRO	11.4
1	D	85	LEU	11.3
1	B	13	ALA	11.3
1	F	27	PHE	11.3
1	E	57	GLY	11.3
1	G	37	ILE	11.3
1	C	58	ILE	11.2
1	A	29	ARG	11.2
1	E	30	LEU	11.2
1	H	4	TYR	11.1
1	B	67	GLY	11.1
1	E	18	THR	11.1
1	D	43	SER	11.1
1	H	66	VAL	11.1
1	H	65	GLY	11.1
1	D	91	MET	11.0
1	H	27	PHE	11.0
1	F	104	LEU	11.0
1	F	25	GLU	11.0
1	A	81	GLN	10.9
1	B	102	ASN	10.9
1	G	44	PHE	10.9
1	C	52	ALA	10.9
1	B	4	TYR	10.9
1	D	16	ILE	10.8
1	G	43	SER	10.8
1	F	47	LEU	10.7
1	H	39	CYS	10.7
1	F	87	ALA	10.6
1	H	36	THR	10.6
1	C	71	ILE	10.5
1	C	29	ARG	10.5
1	A	108	THR	10.5
1	G	106	ARG	10.5
1	B	43	SER	10.5
1	F	40	TYR	10.5

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Mol	Chain	Res	Type	RSRZ
1	F	65	GLY	10.4
1	D	38	ILE	10.4
1	A	7	LEU	10.3
1	F	84	ASP	10.3
1	D	39	CYS	10.3
1	C	110	HIS	10.3
1	A	50	THR	10.3
1	H	89	ILE	10.3
1	H	12	LEU	10.3
1	C	7	LEU	10.2
1	H	41	CYS	10.2
1	H	72	SER	10.2
1	F	7	LEU	10.2
1	C	30	LEU	10.2
1	D	25	GLU	10.1
1	E	50	THR	10.1
1	D	32	PRO	10.1
1	D	53	TYR	10.1
1	G	14	GLU	10.1
1	F	86	PRO	10.0
1	E	51	LEU	10.0
1	D	50	THR	10.0
1	E	82	ARG	10.0
1	H	9	GLY	9.9
1	B	17	GLY	9.9
1	H	28	THR	9.9
1	E	52	ALA	9.9
1	C	107	SER	9.9
1	F	22	LYS	9.9
1	F	64	SER	9.8
1	H	99	LEU	9.8
1	B	68	ILE	9.8
1	E	39	CYS	9.8
1	B	40	TYR	9.8
1	A	25	GLU	9.8
1	C	35	GLY	9.7
1	E	110	HIS	9.7
1	E	104	LEU	9.7
1	H	13	ALA	9.7
1	F	53	TYR	9.7
1	B	93	LEU	9.6
1	A	57	GLY	9.6

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Mol	Chain	Res	Type	RSRZ
1	G	25	GLU	9.6
1	D	110	HIS	9.6
1	D	83	LEU	9.5
1	A	95	CYS	9.5
1	F	42	ALA	9.5
1	D	13	ALA	9.5
1	H	75	SER	9.5
1	D	108	THR	9.4
1	F	103	LEU	9.4
1	G	30	LEU	9.3
1	B	70	LEU	9.3
1	A	87	ALA	9.3
1	C	94	ILE	9.3
1	D	107	SER	9.3
1	C	61	ALA	9.3
1	G	29	ARG	9.2
1	F	98	VAL	9.2
1	A	79	PHE	9.2
1	F	36	THR	9.1
1	H	101	ILE	9.1
1	F	72	SER	9.1
1	H	95	CYS	9.1
1	G	49	GLN	9.1
1	G	78	PHE	9.1
1	C	84	ASP	9.0
1	G	50	THR	9.0
1	F	43	SER	9.0
1	H	108	THR	9.0
1	F	29	ARG	9.0
1	C	31	TRP	9.0
1	H	11	ILE	9.0
1	B	103	LEU	9.0
1	A	32	PRO	9.0
1	A	37	ILE	8.9
1	B	5	ILE	8.9
1	E	64	SER	8.8
1	D	4	TYR	8.8
1	A	97	GLY	8.7
1	E	4	TYR	8.7
1	A	68	ILE	8.7
1	F	76	TRP	8.7
1	G	35	GLY	8.7

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Mol	Chain	Res	Type	RSRZ
1	C	68	ILE	8.7
1	H	85	LEU	8.6
1	B	81	GLN	8.6
1	B	92	MET	8.6
1	F	23	PHE	8.6
1	D	35	GLY	8.6
1	E	44	PHE	8.5
1	E	58	ILE	8.5
1	H	110	HIS	8.5
1	G	5	ILE	8.5
1	H	30	LEU	8.5
1	A	65	GLY	8.5
1	B	25	GLU	8.5
1	A	82	ARG	8.4
1	H	50	THR	8.4
1	G	46	LEU	8.4
1	H	6	TYR	8.4
1	H	82	ARG	8.3
1	E	9	GLY	8.3
1	E	98	VAL	8.3
1	D	67	GLY	8.3
1	E	25	GLU	8.2
1	A	14	GLU	8.2
1	B	12	LEU	8.2
1	C	41	CYS	8.2
1	B	7	LEU	8.2
1	E	31	TRP	8.2
1	G	48	ALA	8.2
1	E	32	PRO	8.2
1	C	78	PHE	8.1
1	E	79	PHE	8.1
1	G	38	ILE	8.0
1	B	22	LYS	8.0
1	F	41	CYS	8.0
1	E	10	ALA	8.0
1	H	61	ALA	8.0
1	D	42	ALA	8.0
1	A	48	ALA	7.9
1	B	86	PRO	7.9
1	F	108	THR	7.9
1	C	42	ALA	7.9
1	D	7	LEU	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	85	LEU	7.8
1	B	33	SER	7.8
1	F	18	THR	7.7
1	F	109	PRO	7.7
1	A	69	VAL	7.7
1	B	42	ALA	7.6
1	C	33	SER	7.6
1	E	89	ILE	7.6
1	H	20	LEU	7.6
1	A	16	ILE	7.5
1	D	93	LEU	7.5
1	B	20	LEU	7.5
1	G	81	GLN	7.5
1	C	11	ILE	7.5
1	E	13	ALA	7.5
1	F	21	MET	7.5
1	C	86	PRO	7.5
1	H	109	PRO	7.4
1	D	5	ILE	7.4
1	D	30	LEU	7.4
1	A	21	MET	7.3
1	F	15	VAL	7.3
1	E	36	THR	7.3
1	B	55	PRO	7.3
1	H	107	SER	7.3
1	B	27	PHE	7.3
1	A	98	VAL	7.3
1	C	28	THR	7.2
1	H	33	SER	7.2
1	B	41	CYS	7.2
1	C	97	GLY	7.2
1	F	30	LEU	7.2
1	B	94	ILE	7.2
1	G	7	LEU	7.1
1	A	13	ALA	7.1
1	G	95	CYS	7.1
1	C	16	ILE	7.1
1	G	69	VAL	7.1
1	A	77	GLY	7.1
1	A	40	TYR	7.1
1	G	52	ALA	7.1
1	H	81	GLN	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	106	ARG	7.0
1	F	28	THR	7.0
1	F	17	GLY	7.0
1	A	73	LEU	6.9
1	B	64	SER	6.9
1	F	56	THR	6.9
1	G	86	PRO	6.9
1	B	51	LEU	6.9
1	C	13	ALA	6.9
1	C	75	SER	6.9
1	D	46	LEU	6.9
1	G	61	ALA	6.9
1	D	44	PHE	6.9
1	C	32	PRO	6.9
1	C	59	ALA	6.8
1	C	73	LEU	6.8
1	D	6	TYR	6.8
1	A	60	TYR	6.8
1	C	17	GLY	6.8
1	H	91	MET	6.8
1	E	22	LYS	6.8
1	D	78	PHE	6.7
1	A	100	ILE	6.7
1	B	46	LEU	6.7
1	C	21	MET	6.7
1	G	85	LEU	6.7
1	G	54	ILE	6.6
1	A	5	ILE	6.6
1	E	97	GLY	6.6
1	A	103	LEU	6.6
1	E	19	THR	6.5
1	C	96	ALA	6.5
1	E	78	PHE	6.5
1	E	43	SER	6.5
1	B	110	HIS	6.5
1	F	24	SER	6.4
1	E	59	ALA	6.4
1	E	105	SER	6.4
1	D	18	THR	6.4
1	C	85	LEU	6.4
1	E	99	LEU	6.3
1	H	58	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	G	77	GLY	6.3
1	F	107	SER	6.3
1	G	84	ASP	6.3
1	C	46	LEU	6.3
1	F	92	MET	6.3
1	C	55	PRO	6.3
1	B	6	TYR	6.3
1	G	90	GLY	6.2
1	G	107	SER	6.2
1	A	85	LEU	6.2
1	F	110	HIS	6.2
1	G	11	ILE	6.2
1	G	74	LEU	6.2
1	A	45	TRP	6.2
1	D	24	SER	6.2
1	B	28	THR	6.2
1	G	33	SER	6.2
1	E	106	ARG	6.1
1	D	66	VAL	6.1
1	C	45	TRP	6.1
1	A	94	ILE	6.1
1	F	96	ALA	6.1
1	D	99	LEU	6.1
1	B	50	THR	6.0
1	C	104	LEU	6.0
1	E	42	ALA	6.0
1	F	54	ILE	6.0
1	F	80	GLY	6.0
1	B	84	ASP	6.0
1	F	78	PHE	6.0
1	B	66	VAL	6.0
1	D	36	THR	6.0
1	E	77	GLY	6.0
1	G	71	ILE	6.0
1	H	22	LYS	5.9
1	C	49	GLN	5.9
1	F	102	ASN	5.9
1	F	14	GLU	5.9
1	D	104	LEU	5.9
1	G	34	VAL	5.9
1	G	105	SER	5.8
1	E	80	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	36	THR	5.7
1	C	69	VAL	5.7
1	E	6	TYR	5.7
1	G	39	CYS	5.7
1	G	96	ALA	5.7
1	B	38	ILE	5.7
1	A	8	GLY	5.7
1	H	26	GLY	5.7
1	C	89	ILE	5.6
1	E	71	ILE	5.6
1	D	70	LEU	5.6
1	G	87	ALA	5.6
1	B	101	ILE	5.6
1	D	81	GLN	5.6
1	B	24	SER	5.6
1	G	73	LEU	5.6
1	G	51	LEU	5.5
1	B	107	SER	5.5
1	C	79	PHE	5.5
1	B	108	THR	5.4
1	D	100	ILE	5.4
1	G	58	ILE	5.4
1	H	40	TYR	5.4
1	G	55	PRO	5.4
1	F	70	LEU	5.4
1	D	87	ALA	5.3
1	C	95	CYS	5.3
1	F	55	PRO	5.3
1	E	102	ASN	5.3
1	H	93	LEU	5.3
1	D	11	ILE	5.3
1	E	73	LEU	5.3
1	B	34	VAL	5.3
1	E	40	TYR	5.3
1	C	106	ARG	5.2
1	A	43	SER	5.2
1	C	82	ARG	5.2
1	D	15	VAL	5.2
1	G	64	SER	5.2
1	G	68	ILE	5.2
1	B	74	LEU	5.2
1	H	31	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	68	ILE	5.1
1	H	35	GLY	5.1
1	G	15	VAL	5.1
1	H	78	PHE	5.1
1	G	27	PHE	5.1
1	C	93	LEU	5.1
1	D	74	LEU	5.1
1	D	73	LEU	5.1
1	E	96	ALA	5.0
1	H	68	ILE	5.0
1	A	56	THR	4.9
1	A	58	ILE	4.9
1	C	77	GLY	4.9
1	D	68	ILE	4.9
1	G	23	PHE	4.9
1	C	101	ILE	4.8
1	E	33	SER	4.8
1	C	74	LEU	4.8
1	C	72	SER	4.8
1	E	108	THR	4.8
1	F	59	ALA	4.8
1	E	90	GLY	4.8
1	H	96	ALA	4.7
1	D	54	ILE	4.7
1	A	54	ILE	4.7
1	E	74	LEU	4.7
1	E	66	VAL	4.7
1	F	90	GLY	4.6
1	B	76	TRP	4.6
1	E	88	ILE	4.6
1	G	16	ILE	4.6
1	H	94	ILE	4.5
1	D	77	GLY	4.5
1	A	74	LEU	4.4
1	E	103	LEU	4.4
1	E	68	ILE	4.4
1	B	45	TRP	4.4
1	H	18	THR	4.4
1	D	103	LEU	4.3
1	D	47	LEU	4.3
1	D	27	PHE	4.3
1	G	32	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	17	GLY	4.2
1	G	62	ILE	4.2
1	G	92	MET	4.2
1	H	64	SER	4.2
1	G	80	GLY	4.2
1	G	70	LEU	4.2
1	A	84	ASP	4.2
1	H	104	LEU	4.1
1	C	5	ILE	4.1
1	C	44	PHE	4.1
1	D	10	ALA	4.1
1	H	15	VAL	4.1
1	H	53	TYR	4.1
1	B	47	LEU	4.1
1	A	15	VAL	4.1
1	H	106	ARG	4.1
1	A	18	THR	4.1
1	D	28	THR	4.1
1	B	97	GLY	4.1
1	A	99	LEU	4.0
1	A	26	GLY	4.0
1	H	7	LEU	4.0
1	G	57	GLY	4.0
1	G	40	TYR	3.9
1	A	80	GLY	3.9
1	D	63	TRP	3.9
1	A	33	SER	3.9
1	A	49	GLN	3.9
1	B	104	LEU	3.9
1	H	38	ILE	3.9
1	D	80	GLY	3.9
1	G	8	GLY	3.9
1	B	90	GLY	3.8
1	C	99	LEU	3.8
1	A	36	THR	3.8
1	H	47	LEU	3.8
1	B	80	GLY	3.8
1	G	97	GLY	3.8
1	D	97	GLY	3.8
1	E	85	LEU	3.8
1	D	37	ILE	3.7
1	C	34	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	15	VAL	3.7
1	D	33	SER	3.7
1	B	79	PHE	3.7
1	E	60	TYR	3.7
1	D	23	PHE	3.6
1	D	89	ILE	3.6
1	E	84	ASP	3.6
1	D	55	PRO	3.6
1	C	83	LEU	3.6
1	H	23	PHE	3.6
1	A	93	LEU	3.6
1	C	57	GLY	3.5
1	B	18	THR	3.5
1	F	74	LEU	3.5
1	C	39	CYS	3.5
1	B	99	LEU	3.5
1	B	89	ILE	3.5
1	E	72	SER	3.4
1	G	101	ILE	3.4
1	B	36	THR	3.4
1	B	109	PRO	3.4
1	C	27	PHE	3.4
1	D	56	THR	3.4
1	C	92	MET	3.4
1	E	14	GLU	3.4
1	C	90	GLY	3.3
1	E	101	ILE	3.3
1	C	18	THR	3.3
1	D	79	PHE	3.3
1	C	15	VAL	3.3
1	E	76	TRP	3.3
1	E	34	VAL	3.2
1	C	47	LEU	3.2
1	D	92	MET	3.2
1	F	105	SER	3.2
1	B	53	TYR	3.2
1	F	16	ILE	3.1
1	D	45	TRP	3.1
1	D	98	VAL	3.1
1	G	88	ILE	3.1
1	H	70	LEU	3.1
1	H	83	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	59	ALA	3.0
1	C	53	TYR	3.0
1	F	75	SER	3.0
1	B	10	ALA	3.0
1	D	22	LYS	3.0
1	F	37	ILE	3.0
1	H	60	TYR	3.0
1	D	76	TRP	3.0
1	C	100	ILE	3.0
1	F	34	VAL	3.0
1	A	83	LEU	2.9
1	G	108	THR	2.9
1	A	34	VAL	2.9
1	C	10	ALA	2.9
1	F	95	CYS	2.9
1	E	75	SER	2.9
1	C	88	ILE	2.8
1	C	22	LYS	2.8
1	H	48	ALA	2.8
1	E	53	TYR	2.8
1	A	46	LEU	2.8
1	D	75	SER	2.8
1	G	53	TYR	2.7
1	H	98	VAL	2.7
1	A	75	SER	2.7
1	B	98	VAL	2.7
1	B	52	ALA	2.7
1	D	84	ASP	2.6
1	D	34	VAL	2.6
1	A	23	PHE	2.6
1	E	91	MET	2.6
1	H	44	PHE	2.6
1	G	36	THR	2.5
1	A	102	ASN	2.5
1	G	91	MET	2.5
1	E	95	CYS	2.5
1	D	90	GLY	2.5
1	B	65	GLY	2.5
1	A	76	TRP	2.5
1	E	24	SER	2.4
1	D	64	SER	2.4
1	E	92	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	11	ILE	2.4
1	H	24	SER	2.4
1	D	94	ILE	2.3
1	D	40	TYR	2.3
1	H	49	GLN	2.3
1	H	100	ILE	2.3
1	B	16	ILE	2.2
1	C	43	SER	2.2
1	H	34	VAL	2.2
1	E	49	GLN	2.2
1	G	21	MET	2.2
1	C	63	TRP	2.2
1	A	44	PHE	2.2
1	C	54	ILE	2.2
1	B	82	ARG	2.2
1	C	76	TRP	2.1
1	E	35	GLY	2.1
1	C	60	TYR	2.1
1	A	63	TRP	2.1
1	A	41	CYS	2.1
1	B	57	GLY	2.1
1	G	9	GLY	2.1
1	B	8	GLY	2.1
1	E	37	ILE	2.1
1	C	4	TYR	2.1
1	B	77	GLY	2.1
1	B	72	SER	2.1
1	G	89	ILE	2.1
1	A	28	THR	2.0
1	A	92	MET	2.0
1	E	12	LEU	2.0
1	D	14	GLU	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.