



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:06 AM UTC

PDB ID : 3B61 / pdb_00003b61
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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

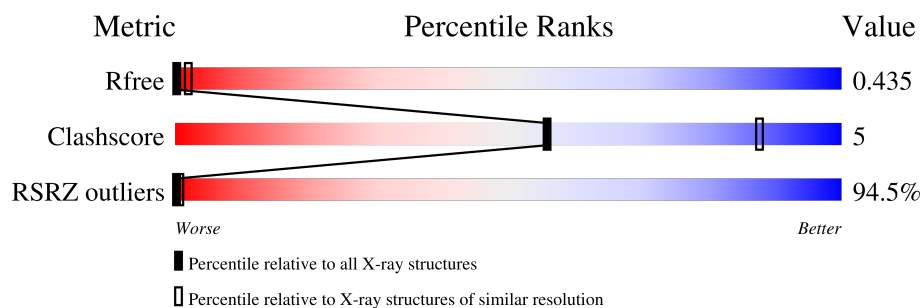
1 Overall quality at a glance

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}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
RSRZ outliers	180081	1122 (5.10-3.90)

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 $\leq 5\%$. 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	90% 97% .
1	B	110	92% 95% ..
1	C	110	95% 97% .
1	D	110	93% 95% ..
1	E	110	94% 97% .
1	F	110	87% 95% ..
1	G	110	95% 97% .

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Mol	Chain	Length	Quality of chain
1	H	110	91% 95% ..

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.

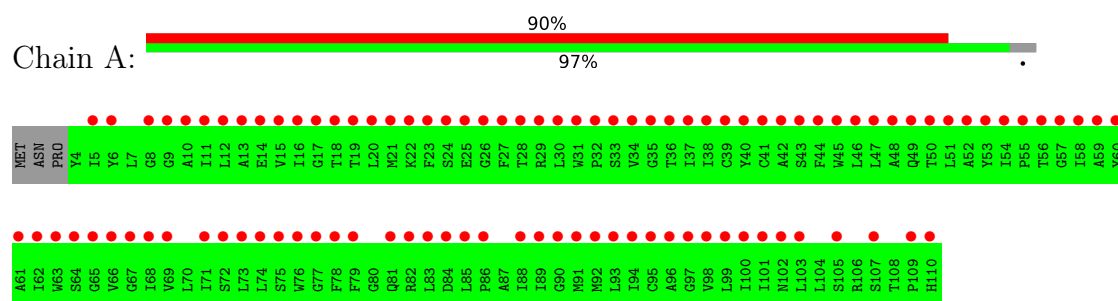
- Molecule 1 is a protein called Multidrug transporter emrE.

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

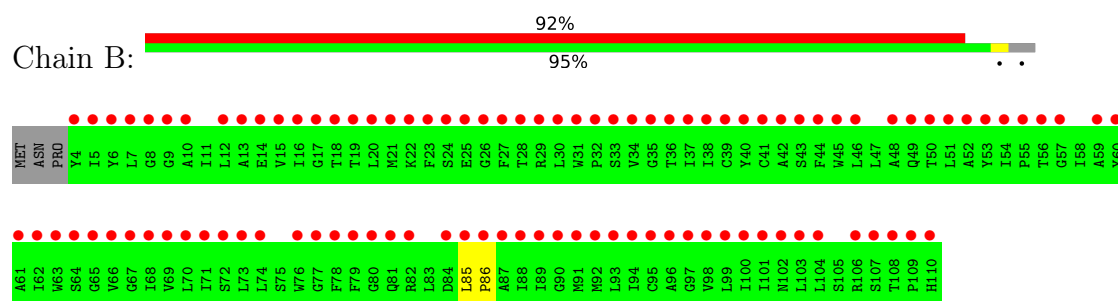
3 Residue-property plots [i](#)

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.

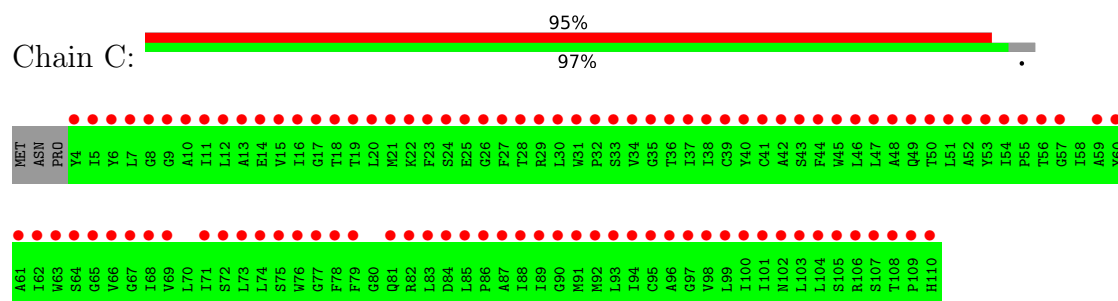
• Molecule 1: Multidrug transporter emrE



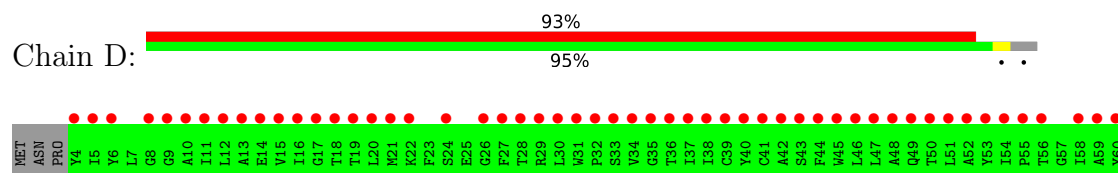
• Molecule 1: Multidrug transporter emrE

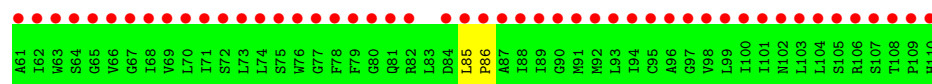


• Molecule 1: Multidrug transporter emrE

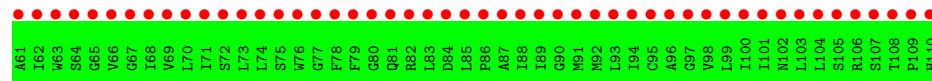
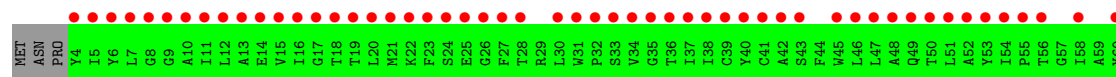


• Molecule 1: Multidrug transporter emrE

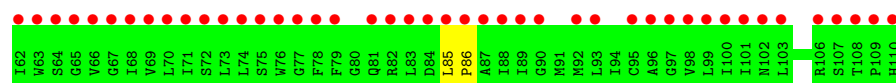
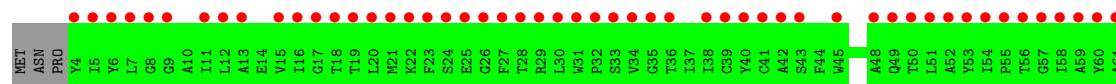
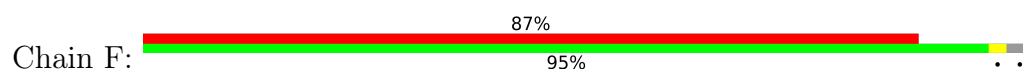




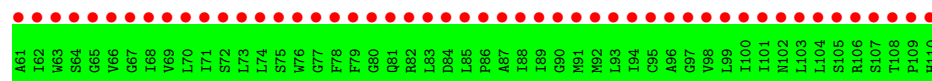
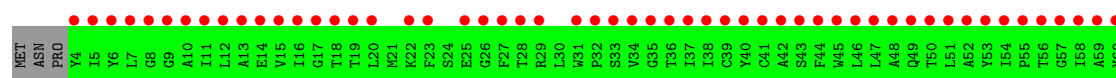
• Molecule 1: Multidrug transporter emrE



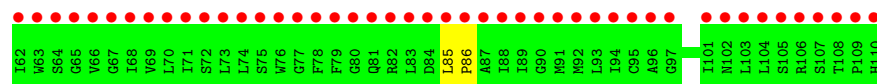
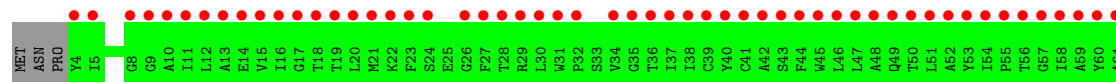
• Molecule 1: Multidrug transporter emrE



• 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	181.00Å 239.20Å 284.20Å 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) 74.8 (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 4.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.318 , 0.362 0.410 , 0.435	Depositor DCC
R_{free} test set	1369 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	187.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	85.45 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.69	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, 0.333 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).

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 oligosaccharides 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%)	9.23	99 (92%) 0 1	82, 228, 336, 336	0
1	B	107/110 (97%)	7.52	101 (94%) 0 1	62, 240, 336, 336	0
1	C	107/110 (97%)	8.39	104 (97%) 0 0	76, 222, 336, 336	0
1	D	107/110 (97%)	8.58	102 (95%) 0 0	61, 209, 336, 336	0
1	E	107/110 (97%)	8.62	103 (96%) 0 0	56, 221, 336, 336	0
1	F	107/110 (97%)	7.30	96 (89%) 0 1	74, 209, 336, 336	0
1	G	107/110 (97%)	7.90	104 (97%) 0 0	48, 229, 336, 336	0
1	H	107/110 (97%)	7.80	100 (93%) 0 1	37, 241, 336, 336	0
All	All	856/880 (97%)	8.17	809 (94%) 0 1	37, 227, 336, 336	0

All (809) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	VAL	46.6
1	A	28	THR	39.4
1	E	84	ASP	35.3
1	A	102	ASN	34.5
1	D	14	GLU	34.3
1	C	31	TRP	32.6
1	E	6	TYR	30.9
1	H	110	HIS	30.6
1	F	83	LEU	30.6
1	A	30	LEU	29.3
1	A	101	ILE	28.7
1	H	105	SER	28.7
1	C	72	SER	28.7
1	A	97	GLY	28.3
1	C	52	ALA	28.1
1	G	35	GLY	27.9

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Mol	Chain	Res	Type	RSRZ
1	A	31	TRP	26.1
1	A	78	PHE	26.0
1	A	99	LEU	24.6
1	F	4	TYR	24.5
1	D	30	LEU	24.5
1	F	5	ILE	24.3
1	G	28	THR	23.7
1	C	75	SER	23.7
1	E	33	SER	23.6
1	H	31	TRP	23.6
1	G	52	ALA	23.6
1	F	19	THR	23.5
1	B	109	PRO	23.5
1	A	79	PHE	23.5
1	E	31	TRP	23.3
1	H	30	LEU	23.1
1	D	32	PRO	22.3
1	C	110	HIS	22.2
1	D	5	ILE	22.2
1	E	78	PHE	22.1
1	B	35	GLY	22.0
1	C	32	PRO	22.0
1	B	110	HIS	21.8
1	H	108	THR	21.6
1	H	51	LEU	21.5
1	D	31	TRP	21.5
1	H	32	PRO	21.5
1	B	80	GLY	21.3
1	G	4	TYR	21.1
1	C	4	TYR	21.1
1	H	79	PHE	21.0
1	A	32	PRO	21.0
1	G	19	THR	20.6
1	E	32	PRO	20.5
1	D	55	PRO	20.3
1	D	9	GLY	20.3
1	D	46	LEU	19.6
1	G	86	PRO	19.6
1	B	30	LEU	19.5
1	C	13	ALA	19.5
1	D	54	ILE	19.1
1	H	101	ILE	19.1

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Mol	Chain	Res	Type	RSRZ
1	D	56	THR	19.0
1	A	100	ILE	18.8
1	E	7	LEU	18.8
1	H	109	PRO	18.5
1	H	56	THR	18.5
1	B	108	THR	18.5
1	E	35	GLY	18.4
1	E	83	LEU	18.3
1	D	109	PRO	18.2
1	D	27	PHE	18.1
1	C	74	LEU	18.0
1	D	49	GLN	17.7
1	D	48	ALA	17.7
1	H	104	LEU	17.6
1	E	87	ALA	17.6
1	D	15	VAL	17.5
1	E	10	ALA	17.5
1	E	90	GLY	17.5
1	G	84	ASP	17.3
1	B	32	PRO	17.2
1	G	16	ILE	17.1
1	D	80	GLY	16.9
1	C	71	ILE	16.6
1	C	86	PRO	16.6
1	F	21	MET	16.6
1	B	31	TRP	16.6
1	F	23	PHE	16.5
1	E	85	LEU	16.4
1	C	76	TRP	16.3
1	E	45	TRP	16.2
1	A	29	ARG	16.2
1	D	13	ALA	16.1
1	D	34	VAL	16.1
1	A	77	GLY	16.0
1	H	16	ILE	15.9
1	H	52	ALA	15.7
1	E	77	GLY	15.6
1	D	16	ILE	15.4
1	E	36	THR	15.2
1	F	24	SER	15.2
1	C	99	LEU	15.2
1	A	96	ALA	15.2

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Mol	Chain	Res	Type	RSRZ
1	F	31	TRP	15.2
1	C	73	LEU	15.2
1	D	11	ILE	15.1
1	C	56	THR	15.1
1	G	53	TYR	14.9
1	G	32	PRO	14.9
1	D	110	HIS	14.8
1	B	79	PHE	14.8
1	B	13	ALA	14.8
1	B	77	GLY	14.8
1	B	16	ILE	14.7
1	F	17	GLY	14.6
1	B	17	GLY	14.6
1	C	77	GLY	14.5
1	E	5	ILE	14.5
1	D	33	SER	14.5
1	A	76	TRP	14.5
1	H	55	PRO	14.4
1	F	16	ILE	14.3
1	A	27	PHE	14.3
1	C	60	TYR	14.3
1	C	68	ILE	14.1
1	F	78	PHE	14.0
1	B	107	SER	14.0
1	C	69	VAL	14.0
1	A	72	SER	14.0
1	H	80	GLY	14.0
1	D	86	PRO	13.9
1	A	33	SER	13.9
1	D	89	ILE	13.9
1	G	85	LEU	13.8
1	F	109	PRO	13.7
1	F	51	LEU	13.7
1	B	78	PHE	13.6
1	E	34	VAL	13.6
1	F	82	ARG	13.6
1	E	93	LEU	13.6
1	C	95	CYS	13.5
1	A	68	ILE	13.5
1	H	24	SER	13.5
1	C	87	ALA	13.5
1	H	48	ALA	13.5

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Mol	Chain	Res	Type	RSRZ
1	G	76	TRP	13.4
1	B	56	THR	13.4
1	D	17	GLY	13.3
1	F	20	LEU	13.3
1	A	56	THR	13.3
1	G	87	ALA	13.2
1	C	90	GLY	13.2
1	E	46	LEU	13.1
1	G	34	VAL	13.1
1	G	37	ILE	13.0
1	G	89	ILE	12.8
1	H	26	GLY	12.6
1	D	79	PHE	12.6
1	B	73	LEU	12.6
1	B	48	ALA	12.6
1	A	103	LEU	12.6
1	F	52	ALA	12.6
1	C	96	ALA	12.5
1	F	8	GLY	12.5
1	G	38	ILE	12.4
1	D	12	LEU	12.4
1	G	83	LEU	12.4
1	E	9	GLY	12.3
1	H	86	PRO	12.3
1	B	34	VAL	12.2
1	G	82	ARG	12.2
1	B	14	GLU	12.1
1	G	109	PRO	12.1
1	D	6	TYR	12.1
1	C	84	ASP	11.9
1	B	20	LEU	11.7
1	H	106	ARG	11.7
1	E	43	SER	11.6
1	B	12	LEU	11.5
1	F	79	PHE	11.5
1	H	15	VAL	11.4
1	E	37	ILE	11.3
1	H	49	GLN	11.2
1	E	25	GLU	11.2
1	G	95	CYS	11.2
1	F	48	ALA	11.1
1	D	85	LEU	11.1

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Mol	Chain	Res	Type	RSRZ
1	G	41	CYS	11.1
1	H	42	ALA	10.9
1	E	88	ILE	10.9
1	A	93	LEU	10.9
1	H	50	THR	10.9
1	D	8	GLY	10.9
1	E	72	SER	10.9
1	G	88	ILE	10.8
1	E	91	MET	10.8
1	B	9	GLY	10.7
1	C	85	LEU	10.7
1	F	36	THR	10.7
1	E	56	THR	10.7
1	F	84	ASP	10.6
1	C	109	PRO	10.6
1	C	91	MET	10.5
1	E	96	ALA	10.5
1	A	69	VAL	10.5
1	C	64	SER	10.4
1	C	89	ILE	10.4
1	C	67	GLY	10.4
1	F	53	TYR	10.3
1	H	12	LEU	10.3
1	C	34	VAL	10.3
1	B	89	ILE	10.2
1	B	86	PRO	10.1
1	F	93	LEU	10.1
1	C	45	TRP	10.0
1	E	82	ARG	10.0
1	G	96	ALA	10.0
1	G	57	GLY	10.0
1	G	20	LEU	10.0
1	C	9	GLY	9.9
1	A	71	ILE	9.9
1	F	33	SER	9.9
1	E	97	GLY	9.9
1	A	43	SER	9.9
1	H	58	ILE	9.9
1	D	39	CYS	9.8
1	E	26	GLY	9.8
1	E	49	GLN	9.8
1	F	73	LEU	9.8

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Mol	Chain	Res	Type	RSRZ
1	B	24	SER	9.7
1	A	41	CYS	9.6
1	G	92	MET	9.6
1	F	45	TRP	9.5
1	G	33	SER	9.4
1	G	110	HIS	9.4
1	E	50	THR	9.4
1	B	57	GLY	9.4
1	C	39	CYS	9.3
1	B	41	CYS	9.3
1	B	49	GLN	9.3
1	G	29	ARG	9.3
1	D	64	SER	9.2
1	E	89	ILE	9.2
1	F	25	GLU	9.2
1	A	81	GLN	9.2
1	H	4	TYR	9.2
1	A	86	PRO	9.1
1	A	38	ILE	9.1
1	H	27	PHE	9.1
1	C	25	GLU	9.1
1	A	89	ILE	9.0
1	E	30	LEU	9.0
1	G	36	THR	9.0
1	E	73	LEU	9.0
1	B	4	TYR	9.0
1	A	92	MET	8.9
1	A	45	TRP	8.9
1	B	39	CYS	8.9
1	D	47	LEU	8.9
1	D	108	THR	8.8
1	H	103	LEU	8.8
1	C	78	PHE	8.8
1	H	13	ALA	8.7
1	G	77	GLY	8.7
1	B	45	TRP	8.7
1	A	64	SER	8.6
1	G	26	GLY	8.6
1	D	95	CYS	8.5
1	A	9	GLY	8.5
1	E	95	CYS	8.5
1	C	92	MET	8.4

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Mol	Chain	Res	Type	RSRZ
1	G	68	ILE	8.4
1	E	52	ALA	8.4
1	C	16	ILE	8.4
1	A	75	SER	8.4
1	H	45	TRP	8.4
1	H	53	TYR	8.3
1	G	64	SER	8.3
1	F	89	ILE	8.3
1	A	65	GLY	8.2
1	D	63	TRP	8.2
1	A	85	LEU	8.2
1	G	91	MET	8.2
1	C	88	ILE	8.2
1	G	100	ILE	8.2
1	F	6	TYR	8.1
1	A	18	THR	8.1
1	A	42	ALA	8.1
1	B	67	GLY	8.1
1	A	73	LEU	8.1
1	F	70	LEU	8.1
1	G	9	GLY	8.0
1	E	67	GLY	8.0
1	B	84	ASP	8.0
1	E	76	TRP	8.0
1	G	27	PHE	8.0
1	A	52	ALA	7.9
1	B	87	ALA	7.9
1	E	39	CYS	7.9
1	B	81	GLN	7.9
1	D	81	GLN	7.9
1	E	11	ILE	7.9
1	E	68	ILE	7.9
1	A	67	GLY	7.9
1	A	37	ILE	7.8
1	B	88	ILE	7.8
1	F	28	THR	7.8
1	G	107	SER	7.8
1	F	97	GLY	7.8
1	B	72	SER	7.8
1	D	28	THR	7.8
1	F	96	ALA	7.8
1	A	39	CYS	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	60	TYR	7.6
1	H	102	ASN	7.6
1	C	83	LEU	7.6
1	B	61	ALA	7.6
1	E	92	MET	7.6
1	H	78	PHE	7.6
1	F	87	ALA	7.6
1	E	51	LEU	7.6
1	F	68	ILE	7.6
1	F	12	LEU	7.5
1	B	64	SER	7.5
1	H	17	GLY	7.5
1	G	13	ALA	7.5
1	F	49	GLN	7.5
1	F	69	VAL	7.5
1	C	65	GLY	7.4
1	G	99	LEU	7.4
1	F	65	GLY	7.4
1	G	45	TRP	7.4
1	F	61	ALA	7.3
1	B	26	GLY	7.3
1	D	73	LEU	7.3
1	B	60	TYR	7.3
1	F	60	TYR	7.3
1	E	48	ALA	7.3
1	D	41	CYS	7.2
1	D	65	GLY	7.2
1	F	72	SER	7.2
1	F	85	LEU	7.2
1	B	42	ALA	7.2
1	A	88	ILE	7.2
1	C	93	LEU	7.2
1	D	70	LEU	7.2
1	F	86	PRO	7.2
1	G	40	TYR	7.2
1	E	102	ASN	7.2
1	E	64	SER	7.1
1	C	57	GLY	7.1
1	F	92	MET	7.1
1	B	46	LEU	7.1
1	A	36	THR	7.1
1	E	17	GLY	7.1

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Mol	Chain	Res	Type	RSRZ
1	H	73	LEU	7.1
1	G	65	GLY	7.0
1	F	58	ILE	7.0
1	H	20	LEU	7.0
1	G	48	ALA	7.0
1	D	84	ASP	7.0
1	E	65	GLY	7.0
1	F	110	HIS	7.0
1	D	96	ALA	6.9
1	A	50	THR	6.9
1	G	39	CYS	6.9
1	H	76	TRP	6.9
1	A	19	THR	6.9
1	G	98	VAL	6.9
1	C	24	SER	6.9
1	C	100	ILE	6.9
1	G	58	ILE	6.9
1	E	86	PRO	6.9
1	A	84	ASP	6.9
1	A	21	MET	6.9
1	G	72	SER	6.8
1	B	19	THR	6.8
1	C	26	GLY	6.8
1	E	22	LYS	6.8
1	H	28	THR	6.8
1	G	102	ASN	6.8
1	H	67	GLY	6.8
1	A	51	LEU	6.8
1	E	75	SER	6.8
1	F	62	ILE	6.8
1	H	36	THR	6.7
1	A	49	GLN	6.7
1	G	106	ARG	6.7
1	G	66	VAL	6.7
1	D	97	GLY	6.7
1	F	29	ARG	6.7
1	F	71	ILE	6.7
1	B	69	VAL	6.7
1	A	83	LEU	6.7
1	F	57	GLY	6.6
1	F	39	CYS	6.6
1	B	68	ILE	6.6

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Mol	Chain	Res	Type	RSRZ
1	F	41	CYS	6.6
1	H	64	SER	6.6
1	C	40	TYR	6.6
1	A	13	ALA	6.6
1	D	67	GLY	6.6
1	D	42	ALA	6.6
1	E	18	THR	6.5
1	G	75	SER	6.5
1	G	93	LEU	6.5
1	D	40	TYR	6.5
1	G	63	TRP	6.5
1	D	107	SER	6.5
1	H	81	GLN	6.5
1	B	53	TYR	6.5
1	F	26	GLY	6.4
1	F	67	GLY	6.4
1	E	19	THR	6.4
1	B	92	MET	6.4
1	A	95	CYS	6.4
1	D	50	THR	6.4
1	H	39	CYS	6.4
1	D	4	TYR	6.4
1	H	82	ARG	6.4
1	A	22	LYS	6.3
1	A	17	GLY	6.3
1	A	25	GLU	6.3
1	C	41	CYS	6.3
1	H	40	TYR	6.3
1	F	56	THR	6.3
1	H	89	ILE	6.3
1	G	10	ALA	6.3
1	D	66	VAL	6.3
1	A	46	LEU	6.3
1	B	40	TYR	6.3
1	G	22	LYS	6.3
1	A	62	ILE	6.3
1	G	49	GLN	6.3
1	C	20	LEU	6.3
1	C	108	THR	6.3
1	E	41	CYS	6.2
1	D	72	SER	6.2
1	H	61	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	88	ILE	6.2
1	H	63	TRP	6.2
1	A	35	GLY	6.2
1	D	94	ILE	6.2
1	B	65	GLY	6.2
1	E	40	TYR	6.2
1	A	48	ALA	6.2
1	H	84	ASP	6.2
1	F	64	SER	6.1
1	B	85	LEU	6.1
1	D	69	VAL	6.1
1	B	27	PHE	6.1
1	C	66	VAL	6.1
1	C	105	SER	6.1
1	C	38	ILE	6.1
1	A	66	VAL	6.1
1	E	20	LEU	6.0
1	G	43	SER	6.0
1	A	82	ARG	6.0
1	C	42	ALA	6.0
1	B	94	ILE	6.0
1	F	66	VAL	6.0
1	B	23	PHE	6.0
1	G	14	GLU	6.0
1	C	10	ALA	6.0
1	D	26	GLY	5.9
1	F	102	ASN	5.9
1	G	6	TYR	5.9
1	F	63	TRP	5.9
1	C	81	GLN	5.9
1	B	21	MET	5.9
1	B	25	GLU	5.9
1	E	74	LEU	5.9
1	G	103	LEU	5.9
1	C	53	TYR	5.9
1	B	90	GLY	5.9
1	B	10	ALA	5.9
1	B	102	ASN	5.9
1	C	97	GLY	5.9
1	E	81	GLN	5.9
1	D	61	ALA	5.8
1	A	24	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	78	PHE	5.8
1	E	58	ILE	5.8
1	A	14	GLU	5.8
1	A	15	VAL	5.8
1	E	99	LEU	5.8
1	A	20	LEU	5.7
1	D	62	ILE	5.7
1	A	110	HIS	5.7
1	H	88	ILE	5.7
1	G	81	GLN	5.7
1	D	92	MET	5.7
1	H	90	GLY	5.7
1	E	38	ILE	5.7
1	A	63	TRP	5.7
1	B	50	THR	5.7
1	G	11	ILE	5.7
1	D	90	GLY	5.6
1	E	62	ILE	5.6
1	D	91	MET	5.6
1	G	105	SER	5.6
1	B	62	ILE	5.6
1	G	108	THR	5.6
1	A	40	TYR	5.6
1	G	60	TYR	5.6
1	A	34	VAL	5.6
1	D	20	LEU	5.6
1	C	63	TRP	5.6
1	F	27	PHE	5.5
1	C	98	VAL	5.5
1	E	69	VAL	5.5
1	A	91	MET	5.5
1	G	90	GLY	5.5
1	G	80	GLY	5.5
1	C	37	ILE	5.5
1	C	102	ASN	5.5
1	G	94	ILE	5.5
1	E	80	GLY	5.5
1	H	70	LEU	5.4
1	D	98	VAL	5.4
1	H	69	VAL	5.4
1	B	103	LEU	5.4
1	D	36	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	36	THR	5.4
1	E	71	ILE	5.4
1	C	82	ARG	5.4
1	C	62	ILE	5.4
1	G	50	THR	5.4
1	G	56	THR	5.4
1	A	61	ALA	5.4
1	B	74	LEU	5.4
1	E	53	TYR	5.4
1	G	42	ALA	5.4
1	B	38	ILE	5.3
1	H	87	ALA	5.3
1	C	79	PHE	5.3
1	D	75	SER	5.3
1	D	103	LEU	5.3
1	G	71	ILE	5.3
1	E	98	VAL	5.3
1	G	73	LEU	5.3
1	E	14	GLU	5.3
1	D	60	TYR	5.3
1	E	4	TYR	5.3
1	D	43	SER	5.3
1	B	66	VAL	5.3
1	F	55	PRO	5.3
1	B	18	THR	5.2
1	B	71	ILE	5.2
1	B	63	TRP	5.2
1	G	18	THR	5.2
1	B	43	SER	5.2
1	A	44	PHE	5.2
1	H	54	ILE	5.2
1	F	99	LEU	5.2
1	B	29	ARG	5.2
1	C	107	SER	5.2
1	C	61	ALA	5.2
1	E	66	VAL	5.2
1	F	76	TRP	5.2
1	E	23	PHE	5.2
1	F	108	THR	5.1
1	G	47	LEU	5.1
1	A	23	PHE	5.1
1	B	51	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	94	ILE	5.1
1	G	78	PHE	5.1
1	B	70	LEU	5.1
1	F	81	GLN	5.1
1	G	97	GLY	5.1
1	D	76	TRP	5.1
1	C	28	THR	5.0
1	F	15	VAL	5.0
1	H	65	GLY	5.0
1	F	38	ILE	5.0
1	C	7	LEU	5.0
1	D	58	ILE	5.0
1	H	85	LEU	5.0
1	C	22	LYS	5.0
1	D	38	ILE	5.0
1	E	104	LEU	5.0
1	D	35	GLY	5.0
1	B	99	LEU	4.9
1	G	79	PHE	4.9
1	B	98	VAL	4.9
1	D	101	ILE	4.9
1	F	54	ILE	4.9
1	C	44	PHE	4.9
1	E	107	SER	4.9
1	D	93	LEU	4.9
1	F	35	GLY	4.9
1	H	91	MET	4.9
1	C	18	THR	4.9
1	C	94	ILE	4.8
1	G	12	LEU	4.8
1	A	57	GLY	4.8
1	A	53	TYR	4.8
1	E	100	ILE	4.8
1	H	62	ILE	4.8
1	D	45	TRP	4.8
1	A	11	ILE	4.7
1	C	49	GLN	4.7
1	A	12	LEU	4.7
1	C	101	ILE	4.7
1	H	93	LEU	4.7
1	H	43	SER	4.7
1	B	82	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	54	ILE	4.7
1	H	72	SER	4.7
1	E	105	SER	4.6
1	H	92	MET	4.6
1	H	60	TYR	4.6
1	F	75	SER	4.6
1	E	109	PRO	4.6
1	A	58	ILE	4.6
1	A	10	ALA	4.6
1	C	48	ALA	4.6
1	E	42	ALA	4.6
1	E	21	MET	4.6
1	H	74	LEU	4.6
1	H	23	PHE	4.5
1	C	17	GLY	4.5
1	A	8	GLY	4.5
1	H	41	CYS	4.5
1	D	82	ARG	4.5
1	E	101	ILE	4.5
1	A	47	LEU	4.5
1	E	103	LEU	4.5
1	A	16	ILE	4.5
1	C	50	THR	4.5
1	D	29	ARG	4.5
1	E	12	LEU	4.4
1	F	11	ILE	4.4
1	B	96	ALA	4.4
1	F	90	GLY	4.4
1	D	100	ILE	4.4
1	E	70	LEU	4.4
1	B	100	ILE	4.4
1	E	16	ILE	4.4
1	H	97	GLY	4.4
1	G	69	VAL	4.4
1	E	15	VAL	4.3
1	E	63	TRP	4.3
1	C	43	SER	4.3
1	C	104	LEU	4.3
1	F	32	PRO	4.3
1	H	21	MET	4.3
1	H	35	GLY	4.3
1	F	103	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	34	VAL	4.2
1	D	77	GLY	4.2
1	D	68	ILE	4.2
1	C	8	GLY	4.2
1	D	104	LEU	4.2
1	H	46	LEU	4.2
1	E	13	ALA	4.2
1	A	90	GLY	4.2
1	A	107	SER	4.2
1	D	74	LEU	4.2
1	D	102	ASN	4.2
1	C	35	GLY	4.2
1	B	37	ILE	4.2
1	H	9	GLY	4.1
1	H	18	THR	4.1
1	D	10	ALA	4.1
1	F	59	ALA	4.1
1	E	60	TYR	4.1
1	H	77	GLY	4.1
1	A	26	GLY	4.1
1	G	17	GLY	4.1
1	E	110	HIS	4.1
1	B	97	GLY	4.1
1	G	46	LEU	4.1
1	H	34	VAL	4.1
1	H	10	ALA	4.1
1	F	40	TYR	4.1
1	G	67	GLY	4.1
1	C	14	GLU	4.0
1	D	37	ILE	4.0
1	C	33	SER	4.0
1	H	8	GLY	4.0
1	H	75	SER	4.0
1	H	29	ARG	4.0
1	E	27	PHE	4.0
1	H	95	CYS	4.0
1	G	74	LEU	3.9
1	H	11	ILE	3.9
1	C	103	LEU	3.9
1	F	22	LYS	3.9
1	G	62	ILE	3.9
1	H	38	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	87	ALA	3.9
1	E	8	GLY	3.8
1	H	57	GLY	3.8
1	D	99	LEU	3.8
1	F	42	ALA	3.8
1	C	47	LEU	3.8
1	C	29	ARG	3.8
1	F	107	SER	3.7
1	B	59	ALA	3.7
1	C	30	LEU	3.7
1	B	93	LEU	3.7
1	E	47	LEU	3.7
1	H	96	ALA	3.7
1	D	59	ALA	3.7
1	D	18	THR	3.7
1	B	55	PRO	3.7
1	E	24	SER	3.7
1	E	54	ILE	3.7
1	E	106	ARG	3.6
1	C	11	ILE	3.6
1	B	44	PHE	3.6
1	G	15	VAL	3.6
1	F	106	ARG	3.6
1	B	8	GLY	3.6
1	C	23	PHE	3.6
1	C	12	LEU	3.6
1	D	105	SER	3.6
1	E	79	PHE	3.6
1	D	44	PHE	3.5
1	C	21	MET	3.5
1	B	22	LYS	3.5
1	G	54	ILE	3.5
1	G	51	LEU	3.5
1	B	36	THR	3.5
1	A	94	ILE	3.5
1	B	101	ILE	3.5
1	F	88	ILE	3.4
1	G	5	ILE	3.4
1	G	8	GLY	3.4
1	C	19	THR	3.4
1	D	21	MET	3.4
1	F	30	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	74	LEU	3.4
1	C	51	LEU	3.4
1	F	100	ILE	3.4
1	D	53	TYR	3.3
1	C	54	ILE	3.3
1	G	61	ALA	3.3
1	G	44	PHE	3.3
1	B	6	TYR	3.3
1	G	104	LEU	3.3
1	E	61	ALA	3.3
1	G	101	ILE	3.3
1	D	19	THR	3.2
1	D	106	ARG	3.2
1	E	94	ILE	3.2
1	G	70	LEU	3.2
1	C	55	PRO	3.2
1	B	5	ILE	3.2
1	D	71	ILE	3.2
1	A	74	LEU	3.2
1	G	23	PHE	3.2
1	B	104	LEU	3.2
1	H	14	GLU	3.1
1	C	6	TYR	3.1
1	A	55	PRO	3.1
1	H	19	THR	3.1
1	B	76	TRP	3.1
1	F	98	VAL	3.0
1	H	71	ILE	3.0
1	F	13	ALA	3.0
1	C	27	PHE	3.0
1	H	83	LEU	3.0
1	B	52	ALA	3.0
1	B	54	ILE	2.9
1	C	5	ILE	2.9
1	H	68	ILE	2.9
1	C	46	LEU	2.9
1	F	77	GLY	2.9
1	F	101	ILE	2.9
1	A	109	PRO	2.8
1	D	52	ALA	2.8
1	F	7	LEU	2.8
1	F	43	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	5	ILE	2.7
1	C	106	ARG	2.7
1	C	59	ALA	2.7
1	D	24	SER	2.6
1	H	22	LYS	2.6
1	F	50	THR	2.6
1	H	47	LEU	2.6
1	G	25	GLU	2.6
1	H	66	VAL	2.5
1	G	59	ALA	2.5
1	G	55	PRO	2.5
1	H	37	ILE	2.5
1	B	95	CYS	2.5
1	F	95	CYS	2.5
1	A	105	SER	2.5
1	B	15	VAL	2.5
1	C	15	VAL	2.5
1	F	9	GLY	2.5
1	A	5	ILE	2.4
1	E	28	THR	2.4
1	B	33	SER	2.4
1	F	18	THR	2.4
1	A	59	ALA	2.4
1	H	59	ALA	2.4
1	D	22	LYS	2.4
1	E	55	PRO	2.3
1	A	6	TYR	2.3
1	H	44	PHE	2.3
1	G	31	TRP	2.2
1	H	107	SER	2.2
1	B	28	THR	2.2
1	B	106	ARG	2.2
1	E	108	THR	2.2
1	B	91	MET	2.2
1	B	7	LEU	2.1
1	D	51	LEU	2.1
1	G	7	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.