wwPDB Geometry-Only Validation Summary Report (i)

Jun 16, 2024 – 05:47 AM EDT

PDB ID	:	1SSZ
Title	:	Conformational Mapping of Mini-B: An N-terminal/C-terminal Construct of Surfactant Protein B Using 13C-Enhanced Fourier Transform Infrared (FTIR) Spectroscopy
Authors	:	Waring, A.J.; Walther, F.J.; Gordon, L.M.; Hernandez-Juviel, J.M.; Hong, T.; Sherman, M.A.; Alonso, C.; Alig, T.; Braun, A.; Bacon, D.; Zasadzinski, J.A.
Deposited on	:	2004-03-24
Resolution	:	Not provided

This is a wwPDB Geometry-Only Validation Summary 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 (i) 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 (i)) were used in the production of this report:

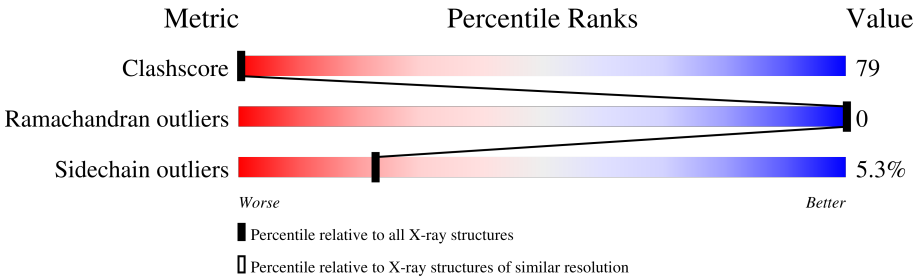
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
INFRARED SPECTROSCOPY

The reported resolution of this entry is unknown.

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))
Clashscore	141614	-
Ramachandran outliers	138981	-
Sidechain outliers	138945	-

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1-A	34	32% 65% .
1	10-A	34	29% 53% 18%
1	2-A	34	50% 38% 9% .
1	3-A	34	29% 59% 12%
1	4-A	34	29% 59% 9% .
1	5-A	34	29% 62% 9%
1	6-A	34	44% 44% 12%
1	7-A	34	15% 76% 9%

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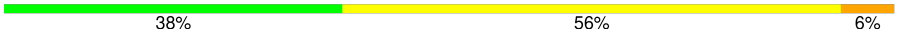
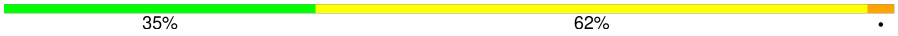
Mol	Chain	Length	Quality of chain
1	8-A	34	
1	9-A	34	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5750 atoms, of which 3050 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 Pulmonary surfactant-associated protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	1-A	34	575	172	305	54	38	6	0	0	0
1	2-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	3-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	4-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	5-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	6-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	7-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	8-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	9-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0
1	10-A	34	Total 575	C 172	H 305	N 54	O 38	S 6	0	0	0

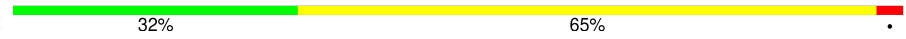
3 Residue-property plots (i)

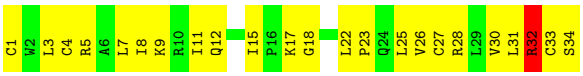
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Pulmonary surfactant-associated protein B

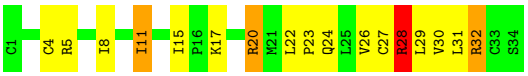
Chain 1-A:





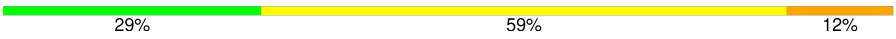
• Molecule 1: Pulmonary surfactant-associated protein B

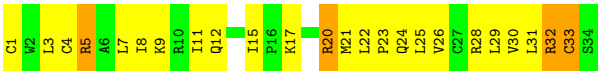
Chain 2-A:



• Molecule 1: Pulmonary surfactant-associated protein B

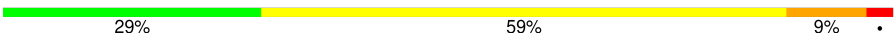
Chain 3-A:

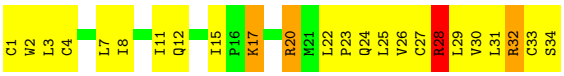




• Molecule 1: Pulmonary surfactant-associated protein B

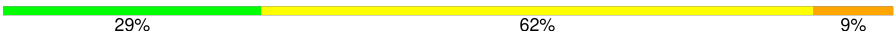
Chain 4-A:





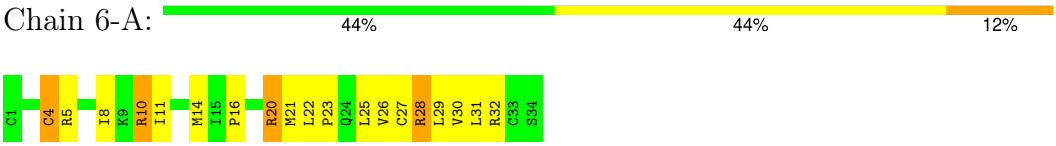
• Molecule 1: Pulmonary surfactant-associated protein B

Chain 5-A:



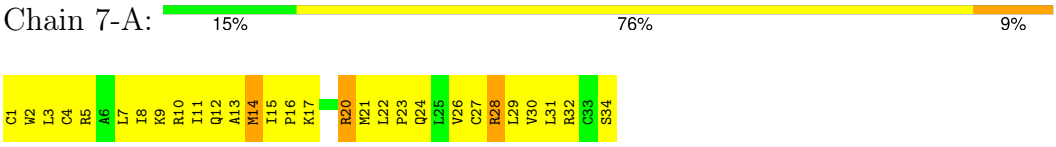
• Molecule 1: Pulmonary surfactant-associated protein B

Chain 6-A:



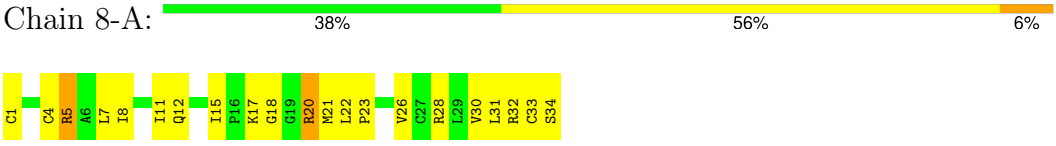
• Molecule 1: Pulmonary surfactant-associated protein B

Chain 7-A:



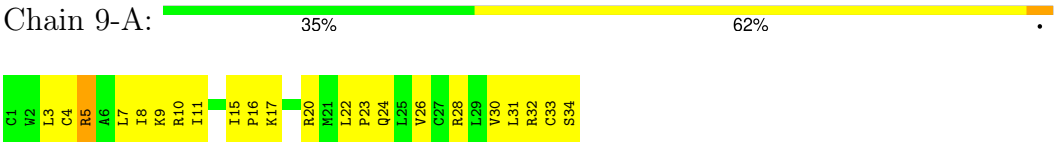
• Molecule 1: Pulmonary surfactant-associated protein B

Chain 8-A:



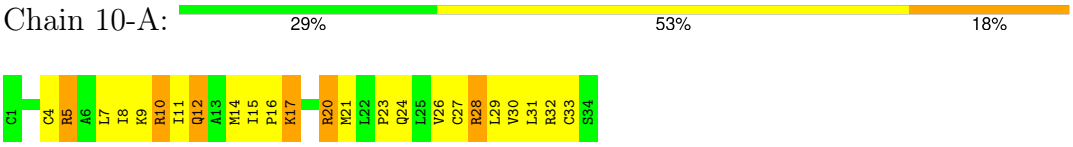
• Molecule 1: Pulmonary surfactant-associated protein B

Chain 9-A:



• Molecule 1: Pulmonary surfactant-associated protein B

Chain 10-A:



4 Model quality

4.1 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	1-A	1.11	0/273	1.29	2/363 (0.6%)
1	2-A	1.08	0/273	1.40	6/363 (1.7%)
1	3-A	1.07	0/273	1.49	8/363 (2.2%)
1	4-A	1.07	0/273	1.37	6/363 (1.7%)
1	5-A	1.07	0/273	1.32	6/363 (1.7%)
1	6-A	1.06	0/273	1.52	8/363 (2.2%)
1	7-A	1.06	0/273	1.44	8/363 (2.2%)
1	8-A	1.10	0/273	1.35	4/363 (1.1%)
1	9-A	1.07	0/273	1.47	8/363 (2.2%)
1	10-A	1.04	0/273	1.54	10/363 (2.8%)
All	All	1.07	0/2730	1.42	66/3630 (1.8%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	10-A	32	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	5-A	5	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	10-A	28	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	10-A	20	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	3-A	5	ARG	NE-CZ-NH1	8.17	124.39	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1-A	270	305	305	48	0
1	2-A	270	305	305	37	0
1	3-A	270	305	305	51	0
1	4-A	270	305	305	46	0
1	5-A	270	305	305	47	0
1	6-A	270	305	305	46	0
1	7-A	270	305	305	65	0
1	8-A	270	305	305	28	0
1	9-A	270	305	305	35	0
1	10-A	270	305	305	51	0
All	All	2700	3050	3050	454	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 79.

The worst 5 of 454 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:A:20:ARG:HG3	1:A:26:VAL:HG11	1.22	1.19
1:A:8:ILE:HD12	1:A:11:ILE:HD11	1.30	1.13
1:A:22:LEU:HB2	1:A:25:LEU:HD23	1.32	1.11
1:A:8:ILE:HG21	1:A:23:PRO:HB3	1.32	1.07
1:A:8:ILE:HD12	1:A:11:ILE:HD11	1.09	1.05

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	1-A	32/34 (94%)	32 (100%)	0	0	100	100
1	2-A	32/34 (94%)	30 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-A	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
1	4-A	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
1	5-A	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
1	6-A	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
1	7-A	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
1	8-A	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
1	9-A	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
1	10-A	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	320/340 (94%)	309 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	1-A	30/30 (100%)	29 (97%)	1 (3%)	38	38
1	2-A	30/30 (100%)	28 (93%)	2 (7%)	16	16
1	3-A	30/30 (100%)	29 (97%)	1 (3%)	38	38
1	4-A	30/30 (100%)	27 (90%)	3 (10%)	7	7
1	5-A	30/30 (100%)	28 (93%)	2 (7%)	16	16
1	6-A	30/30 (100%)	29 (97%)	1 (3%)	38	38
1	7-A	30/30 (100%)	28 (93%)	2 (7%)	16	16
1	8-A	30/30 (100%)	28 (93%)	2 (7%)	16	16
1	9-A	30/30 (100%)	30 (100%)	0	100	100
1	10-A	30/30 (100%)	28 (93%)	2 (7%)	16	16
All	All	300/300 (100%)	284 (95%)	16 (5%)	22	22

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	10-A	12	GLN
1	8-A	20	ARG
1	5-A	20	ARG
1	8-A	5	ARG
1	5-A	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	3-A	12	GLN
1	4-A	24	GLN
1	7-A	24	GLN
1	8-A	12	GLN
1	10-A	12	GLN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.