



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:40 am GMT

PDB ID : 1B08  
Title : LUNG SURFACTANT PROTEIN D (SP-D) (FRAGMENT)  
Authors : Hakansson, K.; Lim, N.K.; Hoppe, H.-J.; Reid, K.B.M.  
Deposited on : 1998-11-18  
Resolution : 2.30 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

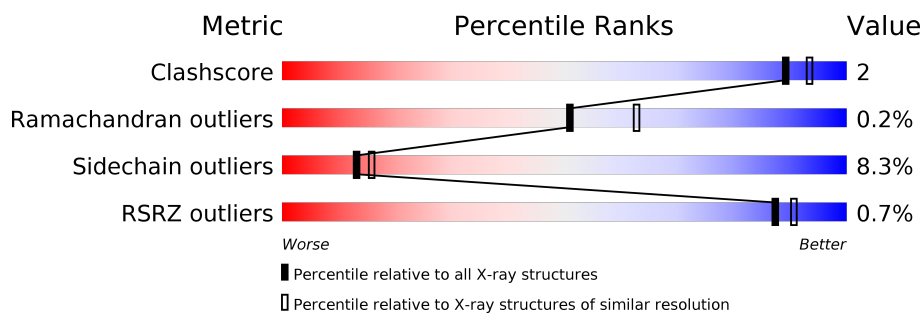
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 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	158	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	158	<div> <div></div> <div>83%</div> <div>10%</div> <div>...</div> </div>
1	C	158	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>. 6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3651 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 PROTEIN (LUNG SURFACTANT PROTEIN D).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1161	728	198	230	5			
1	B	151	Total	C	N	O	S	0	0	0
			1154	723	197	229	5			
1	C	148	Total	C	N	O	S	0	0	0
			1135	711	194	225	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	SER	CONFLICT	UNP P35247
A	200	GLU	GLY	CONFLICT	UNP P35247
A	201	ALA	LEU	CONFLICT	UNP P35247
A	202	GLY	PRO	CONFLICT	UNP P35247
A	203	SER	GLU	CONFLICT	UNP P35247
B	1199	ALA	SER	CONFLICT	UNP P35247
B	1200	GLU	GLY	CONFLICT	UNP P35247
B	1201	ALA	LEU	CONFLICT	UNP P35247
B	1202	GLY	PRO	CONFLICT	UNP P35247
B	1203	SER	GLU	CONFLICT	UNP P35247
C	2199	ALA	SER	CONFLICT	UNP P35247
C	2200	GLU	GLY	CONFLICT	UNP P35247
C	2201	ALA	LEU	CONFLICT	UNP P35247
C	2202	GLY	PRO	CONFLICT	UNP P35247
C	2203	SER	GLU	CONFLICT	UNP P35247

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Ca 3	0	0
2	C	3	Total 3	Ca 3	0	0

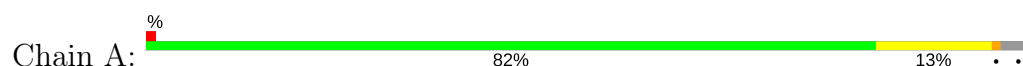
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0
3	B	79	Total 79	O 79	0	0
3	C	47	Total 47	O 47	0	0

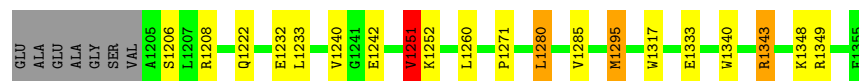
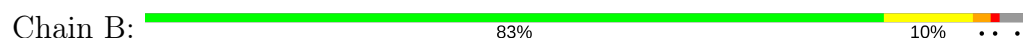
### 3 Residue-property plots [i](#)

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.

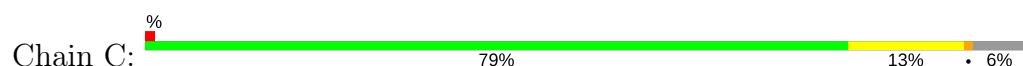
- Molecule 1: PROTEIN (LUNG SURFACTANT PROTEIN D)



- Molecule 1: PROTEIN (LUNG SURFACTANT PROTEIN D)



- Molecule 1: PROTEIN (LUNG SURFACTANT PROTEIN D)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.96Å 109.72Å 56.09Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 18.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.30) 91.8 (18.42-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.30Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.209 , 0.271 0.195 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for l,k,-h 0.047 for h,-k,-l 0.036 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.75	0/1183	1.35	8/1598 (0.5%)
1	B	0.75	0/1176	1.35	12/1588 (0.8%)
1	C	0.71	0/1157	1.29	12/1562 (0.8%)
All	All	0.74	0/3516	1.33	32/4748 (0.7%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2317	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	B	1295	MET	CG-SD-CE	-8.28	86.96	100.20
1	B	1317	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	C	2317	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A	317	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	C	2340	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	B	1340	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	B	1317	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	A	340	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	317	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	A	340	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	C	2340	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	C	2317	TRP	CG-CD2-CE3	6.78	140.00	133.90
1	B	1340	TRP	CE2-CD2-CG	-6.61	102.02	107.30
1	C	2317	TRP	CB-CG-CD1	-6.28	118.84	127.00
1	A	349	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	2306	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	A	208	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	1251	VAL	N-CA-CB	-6.02	98.25	111.50
1	C	2208	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	2343	ARG	NE-CZ-NH2	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2343	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	1349	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	1333	GLU	N-CA-CB	-5.45	100.79	110.60
1	B	1208	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	1343	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	317	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	B	1340	TRP	CB-CG-CD2	-5.10	119.97	126.60
1	C	2219	GLN	CA-CB-CG	-5.10	102.19	113.40
1	A	317	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	C	2340	TRP	CG-CD1-NE1	-5.03	105.08	110.10
1	B	1340	TRP	CG-CD1-NE1	-5.02	105.08	110.10

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	1161	0	1119	6	0
1	B	1154	0	1110	4	0
1	C	1135	0	1089	5	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	66	0	0	1	0
3	B	79	0	0	0	0
3	C	47	0	0	0	0
All	All	3651	0	3318	15	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 2.

All (15) 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:1251:VAL:HG13	1:B:1348:LYS:HB3	1.78	0.64
1:B:1271:PRO:HG3	1:B:1280:LEU:HD12	1.81	0.62
1:A:251:VAL:HG13	1:A:348:LYS:HB3	1.84	0.58
1:C:2324:ASP:HA	1:C:2329:GLU:HB2	1.89	0.54
1:C:2251:VAL:HG13	1:C:2348:LYS:HB3	1.92	0.52
1:C:2238:GLN:HG2	1:C:2283:LEU:HD13	1.93	0.51
1:A:306:TYR:HB2	1:A:308:THR:HG22	1.94	0.49
1:B:1251:VAL:O	1:B:1252:LYS:HG3	2.14	0.48
1:A:227:GLN:O	1:A:231:VAL:HG23	2.14	0.48
1:C:2214:LEU:HA	1:C:2217:GLN:HG2	1.98	0.46
1:A:284:VAL:HG13	1:A:289:GLU:O	2.16	0.44
1:B:1343:ARG:HD2	1:B:1343:ARG:HA	1.84	0.44
1:C:2211:VAL:O	1:C:2214:LEU:HB3	2.19	0.42
1:A:328:SER:HA	3:A:66:HOH:O	2.20	0.41
1:A:251:VAL:HA	1:A:349:ARG:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	150/158 (95%)	145 (97%)	4 (3%)	1 (1%)	25	30
1	B	149/158 (94%)	147 (99%)	2 (1%)	0	100	100
1	C	146/158 (92%)	141 (97%)	5 (3%)	0	100	100
All	All	445/474 (94%)	433 (97%)	11 (2%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ALA

### 5.3.2 Protein sidechains ⓘ

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	122/125 (98%)	113 (93%)	9 (7%)	16	20
1	B	121/125 (97%)	110 (91%)	11 (9%)	11	13
1	C	119/125 (95%)	109 (92%)	10 (8%)	13	15
All	All	362/375 (96%)	332 (92%)	30 (8%)	13	16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	VAL
1	A	212	GLU
1	A	215	GLN
1	A	233	LEU
1	A	259	LEU
1	A	280	LEU
1	A	283	LEU
1	A	295	MET
1	A	308	THR
1	B	1206	SER
1	B	1222	GLN
1	B	1232	GLU
1	B	1233	LEU
1	B	1240	VAL
1	B	1242	GLU
1	B	1251	VAL
1	B	1260	LEU
1	B	1280	LEU
1	B	1285	VAL
1	B	1295	MET
1	C	2215	GLN
1	C	2233	LEU
1	C	2240	VAL
1	C	2251	VAL
1	C	2260	LEU
1	C	2280	LEU

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Mol	Chain	Res	Type
1	C	2283	LEU
1	C	2295	MET
1	C	2303	LYS
1	C	2308	THR

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

Mol	Chain	Res	Type
1	A	222	GLN
1	B	1222	GLN
1	B	1281	GLN
1	C	2220	HIS
1	C	2281	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	152/158 (96%)	-0.54	1 (0%) 87 90	10, 24, 55, 78	0
1	B	151/158 (95%)	-0.62	0 100 100	8, 21, 53, 76	0
1	C	148/158 (93%)	-0.56	2 (1%) 75 80	12, 26, 57, 85	0
All	All	451/474 (95%)	-0.57	3 (0%) 87 90	8, 25, 55, 85	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	ALA	3.1
1	C	2308	THR	2.4
1	C	2209	GLN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	5	1/1	0.98	0.13	1.77	26,26,26,26	0
2	CA	A	3	1/1	0.98	0.11	0.68	31,31,31,31	0
2	CA	B	4	1/1	0.98	0.09	-0.41	21,21,21,21	0
2	CA	C	7	1/1	0.96	0.08	-0.52	27,27,27,27	0
2	CA	A	2	1/1	0.97	0.08	-1.32	26,26,26,26	0
2	CA	A	1	1/1	0.98	0.06	-1.91	27,27,27,27	0
2	CA	C	9	1/1	0.91	0.06	-1.99	45,45,45,45	0
2	CA	C	8	1/1	0.99	0.06	-2.12	31,31,31,31	0
2	CA	B	6	1/1	0.92	0.06	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.