



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2021 – 02:16 PM EDT

PDB ID : 7KYO
Title : PsaBC from *Streptococcus pneumoniae* in complex with Fab
Authors : Maher, M.J.; Sjöhamn, J.
Deposited on : 2020-12-08
Resolution : 2.85 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 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	:	2.23.1
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)	:	2.23.1

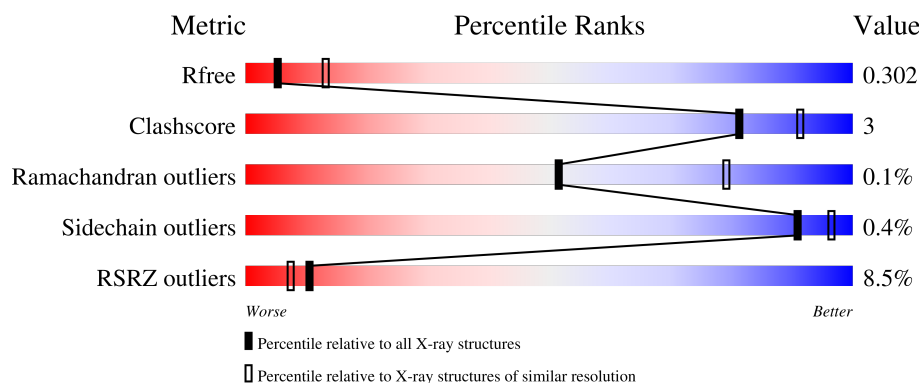
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	B	240	 4% 88% 10% .
2	H	234	 5% 88% . 7%
3	L	218	 11% 93% 6% .
4	C	282	 12% 83% 8% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7045 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 Manganese ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	234	Total	C	N	O	S	0	1	0
			1841	1192	306	338	5			

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	1	0
			1625	1030	266	319	10			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	1	0
			1647	1020	276	344	7			

- Molecule 4 is a protein called Manganese ABC transporter, permease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	258	Total	C	N	O	S	0	0	0
			1899	1273	286	329	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	SER	PHE	conflict	UNP A0A0H2ZPI2

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total	O	0	0
			11	11		

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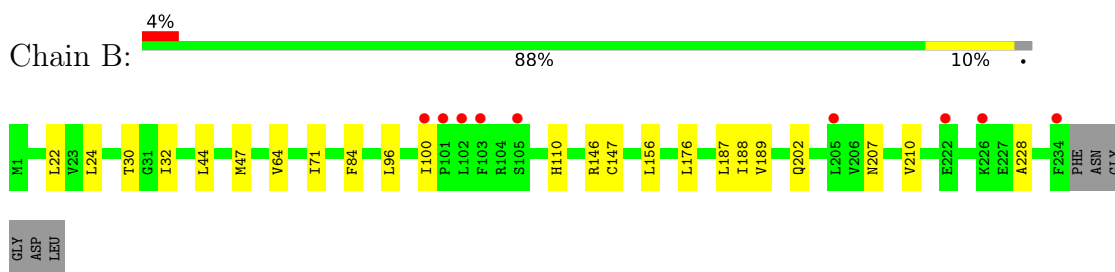
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	6	Total 6	O 6	0	0
5	L	11	Total 11	O 11	0	0
5	C	5	Total 5	O 5	0	0

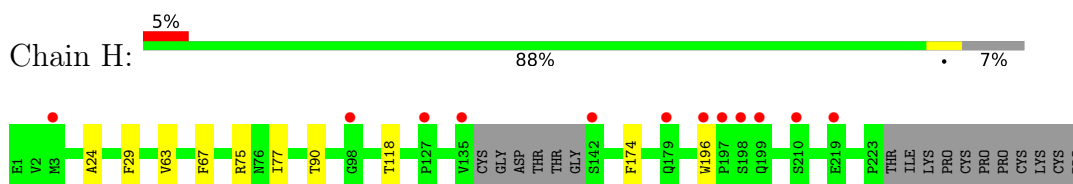
3 Residue-property plots [i](#)

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 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.

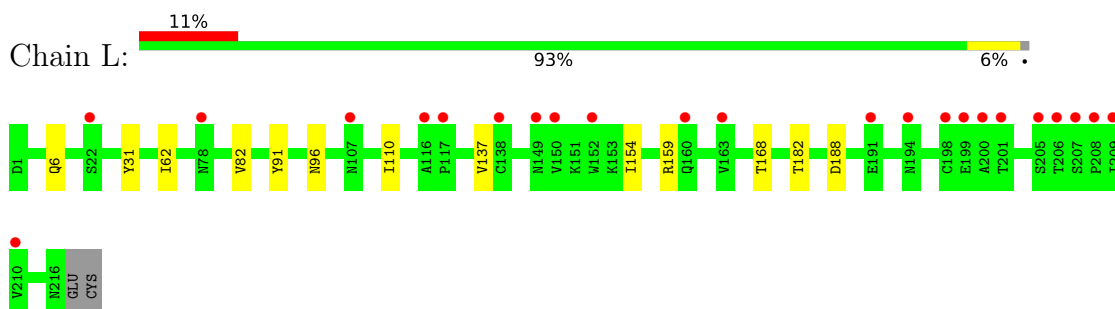
- Molecule 1: Manganese ABC transporter, ATP-binding protein



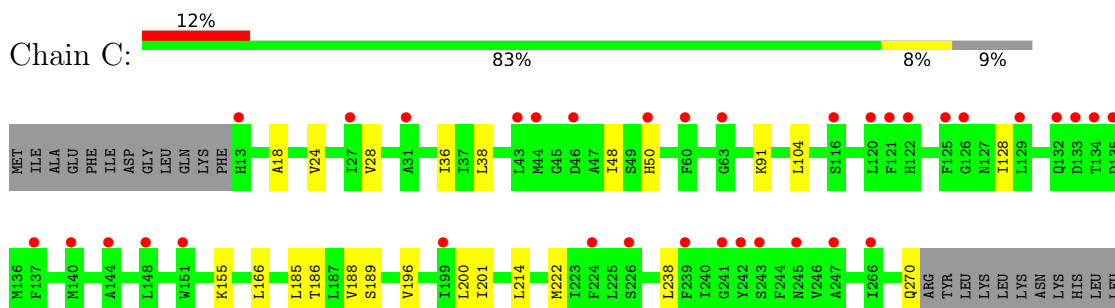
- Molecule 2: Fab heavy chain



- Molecule 3: Fab light chain



- Molecule 4: Manganese ABC transporter, permease protein



LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.66Å 241.70Å 98.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.16 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-2.85) 90.7 (49.16-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.238 , 0.271 0.275 , 0.302	Depositor DCC
R_{free} test set	1689 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7045	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

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	B	0.34	0/1879	0.53	0/2543
2	H	0.34	0/1670	0.54	0/2280
3	L	0.33	0/1690	0.52	0/2306
4	C	0.38	0/1935	0.46	0/2633
All	All	0.35	0/7174	0.51	0/9762

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 [i](#)

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	B	1841	0	1888	13	0
2	H	1625	0	1584	5	0
3	L	1647	0	1522	7	0
4	C	1899	0	2004	16	0
5	B	11	0	0	0	0
5	C	5	0	0	0	0
5	H	6	0	0	0	0
5	L	11	0	0	0	0
All	All	7045	0	6998	37	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 3.

All (37) 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:24:LEU:HD11	1:B:30:THR:HG21	1.76	0.67
4:C:36:ILE:HD11	4:C:185:LEU:HD13	1.77	0.66
4:C:48:ILE:HD11	4:C:186:THR:HG23	1.78	0.65
2:H:24:ALA:HB2	2:H:29:PHE:CZ	2.33	0.64
4:C:28:VAL:HG23	4:C:188:VAL:HG23	1.80	0.62
4:C:189:SER:HA	4:C:201:ILE:HD11	1.82	0.62
1:B:176:LEU:HD13	1:B:188:ILE:HD11	1.85	0.59
4:C:48:ILE:HD11	4:C:186:THR:CG2	2.39	0.53
2:H:75:ARG:HD2	2:H:77:ILE:HD12	1.91	0.52
4:C:214:LEU:HD22	4:C:270:GLN:NE2	2.24	0.52
4:C:50:HIS:CD2	4:C:104:LEU:HD22	2.45	0.52
4:C:128:ILE:HG21	4:C:238:LEU:HD13	1.90	0.52
4:C:38:LEU:HD11	4:C:222:MET:HE2	1.92	0.50
1:B:71:ILE:HD11	1:B:156:LEU:HD13	1.95	0.49
2:H:174:PHE:CD1	3:L:168:THR:HG23	2.51	0.46
1:B:30:THR:HG22	1:B:202:GLN:HB2	1.98	0.46
1:B:146:ARG:CZ	4:C:166:LEU:HD22	2.46	0.46
1:B:96:LEU:HD13	1:B:110:HIS:HB3	1.97	0.45
1:B:32:ILE:HD11	1:B:187:LEU:HD11	1.99	0.45
2:H:63:VAL:HG12	2:H:67:PHE:HB2	1.99	0.45
1:B:84:PHE:CE2	4:C:38:LEU:HD13	2.52	0.44
3:L:154:ILE:HD12	3:L:159:ARG:HD2	1.99	0.44
4:C:196:VAL:HG22	4:C:200:LEU:HB2	1.98	0.44
3:L:82:VAL:CG1	3:L:110:ILE:HD12	2.48	0.44
2:H:90:THR:HG23	2:H:118:THR:HA	1.99	0.44
4:C:18:ALA:HB1	4:C:128:ILE:CG2	2.48	0.44
3:L:62:ILE:N	3:L:62:ILE:HD12	2.34	0.43
4:C:38:LEU:HD11	4:C:222:MET:CE	2.48	0.43
3:L:31:TYR:HB2	3:L:96:ASN:HD21	1.83	0.43
1:B:22:LEU:HD21	1:B:210:VAL:HG21	2.02	0.42
3:L:6:GLN:HE22	3:L:91:TYR:HA	1.84	0.42
1:B:207:ASN:ND2	1:B:228:ALA:O	2.54	0.41
1:B:100:ILE:HD13	4:C:155:LYS:HE3	2.02	0.41
1:B:44:LEU:HD11	1:B:189:VAL:HG23	2.03	0.41
4:C:24:VAL:O	4:C:28:VAL:HG22	2.21	0.41
1:B:47:MET:O	1:B:64:VAL:HG11	2.21	0.40
3:L:137:VAL:HG22	3:L:182:THR:HG22	2.04	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	B	233/240 (97%)	222 (95%)	11 (5%)	0	100	100
2	H	214/234 (92%)	206 (96%)	7 (3%)	1 (0%)	29	57
3	L	215/218 (99%)	204 (95%)	11 (5%)	0	100	100
4	C	256/282 (91%)	250 (98%)	6 (2%)	0	100	100
All	All	918/974 (94%)	882 (96%)	35 (4%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	196	TRP

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	B	201/208 (97%)	200 (100%)	1 (0%)	88	96
2	H	183/200 (92%)	183 (100%)	0	100	100
3	L	183/190 (96%)	182 (100%)	1 (0%)	88	96
4	C	201/227 (88%)	200 (100%)	1 (0%)	88	96
All	All	768/825 (93%)	765 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	147	CYS
3	L	188	ASP
4	C	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	130	GLN
1	B	207	ASN
1	B	231	ASN
2	H	39	GLN
3	L	6	GLN
3	L	42	GLN
3	L	96	ASN
4	C	50	HIS
4	C	194	GLN
4	C	270	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 ⓘ

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	B	234/240 (97%)	0.45	9 (3%) 40 35	26, 32, 42, 54	0
2	H	217/234 (92%)	0.49	12 (5%) 25 20	22, 35, 53, 58	1 (0%)
3	L	216/218 (99%)	0.65	23 (10%) 6 4	24, 33, 44, 47	0
4	C	258/282 (91%)	0.96	35 (13%) 3 2	36, 50, 64, 79	0
All	All	925/974 (94%)	0.65	79 (8%) 10 7	22, 37, 57, 79	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	C	134	THR	5.6
3	L	208	PRO	4.7
3	L	199	GLU	4.4
2	H	197	PRO	4.2
3	L	210	VAL	4.2
1	B	103	PHE	4.2
3	L	198	CYS	4.1
4	C	13	HIS	3.9
2	H	135	VAL	3.7
3	L	116	ALA	3.7
4	C	247	ALA	3.6
4	C	137	PHE	3.6
1	B	105	SER	3.6
3	L	209	ILE	3.6
4	C	63	GLY	3.5
1	B	101	PRO	3.5
4	C	151	TRP	3.4
2	H	179	GLN	3.4
4	C	133	ASP	3.4
3	L	150	VAL	3.4
4	C	140	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	102	LEU	3.2
4	C	116	SER	3.2
4	C	224	PHE	3.1
4	C	44	MET	3.1
4	C	243	SER	3.1
3	L	201	THR	3.1
4	C	121	PHE	3.0
3	L	200	ALA	3.0
4	C	129	LEU	3.0
1	B	100	ILE	2.9
2	H	219	GLU	2.9
4	C	120	LEU	2.9
4	C	242	TYR	2.9
1	B	234	PHE	2.9
3	L	205	SER	2.8
3	L	194	ASN	2.8
4	C	241	GLY	2.7
1	B	226	LYS	2.7
3	L	107	ASN	2.7
2	H	198	SER	2.7
4	C	27	ILE	2.7
2	H	142	SER	2.6
4	C	199	ILE	2.6
3	L	152	TRP	2.6
4	C	122	HIS	2.6
3	L	78	ASN	2.6
2	H	3	MET	2.6
3	L	117	PRO	2.6
2	H	98	GLY	2.5
4	C	126	GLY	2.4
4	C	125	PHE	2.4
4	C	144	ALA	2.4
4	C	31	ALA	2.4
3	L	160	GLN	2.4
4	C	148	LEU	2.4
4	C	239	PHE	2.3
3	L	138	CYS	2.3
4	C	135	ASP	2.3
4	C	266	ILE	2.3
4	C	245	ASN	2.3
4	C	46	ASP	2.2
3	L	22	SER	2.2

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Mol	Chain	Res	Type	RSRZ
4	C	43	LEU	2.2
3	L	191	GLU	2.2
2	H	199	GLN	2.2
2	H	196	TRP	2.2
1	B	222	GLU	2.1
4	C	60	PHE	2.1
3	L	149	ASN	2.1
3	L	207	SER	2.1
4	C	226	SER	2.1
3	L	206	THR	2.1
1	B	205	LEU	2.1
2	H	210	SER	2.1
3	L	163	VAL	2.1
4	C	50	HIS	2.1
2	H	127	PRO	2.0
4	C	132	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 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.