Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 04:52 PM EDT

PDB ID	:	4LSH
Title	:	Ion selectivity of OmpF porin soaked in 0.2M KBr
Authors	:	Balasundaresan, D.; Blachowicz, L.; Roux, B.
Deposited on	:	2013-07-22
Resolution	:	2.20 Å(reported)

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

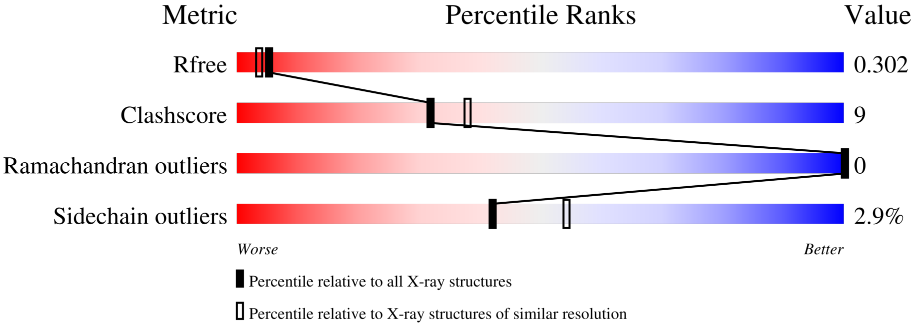
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	402	-	-	X	-
2	BR	A	404	-	-	X	-
2	BR	A	405	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	406	-	-	X	-
2	BR	B	401	-	-	X	-
2	BR	B	404	-	-	X	-
2	BR	B	405	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5491 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 Outer membrane protein F.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	335	Total C N O S 2579 1624 430 522 3	0	0	0
1	B	334	Total C N O S 2574 1621 429 521 3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P02931
B	0	GLY	-	expression tag	UNP P02931

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Br 6 6	0	0
2	B	6	Total Br 6 6	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

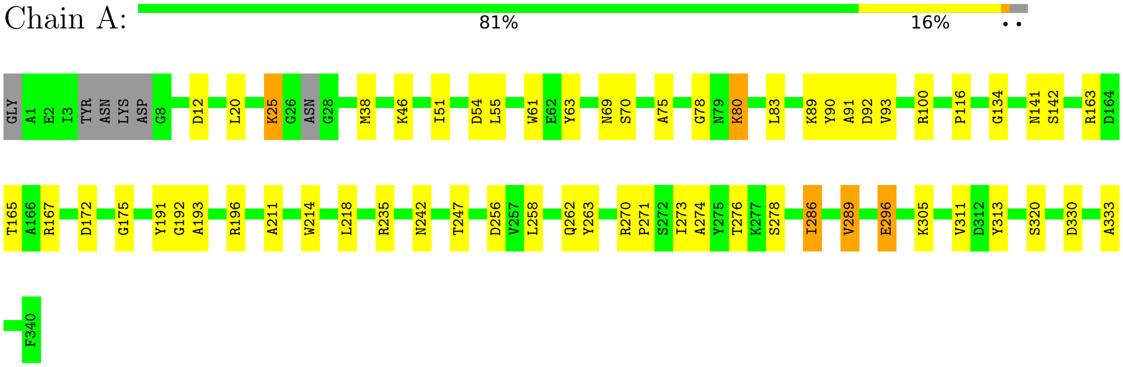
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	159	Total O 159 159	0	0
4	B	166	Total O 166 166	0	0

3 Residue-property plots ⓘ

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.

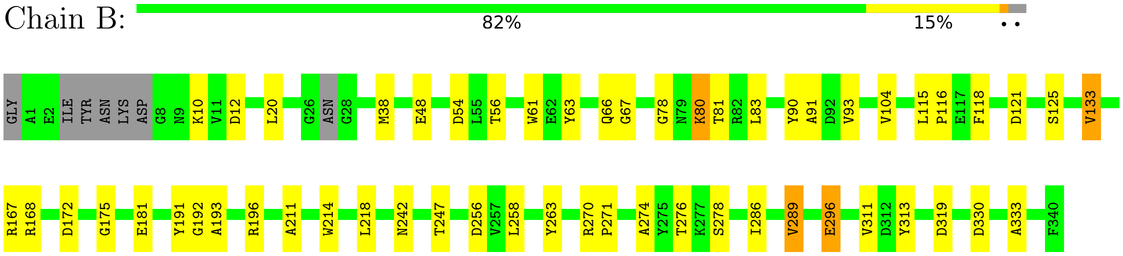
- Molecule 1: Outer membrane protein F

Chain A:



- Molecule 1: Outer membrane protein F

Chain B:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	116.98Å 116.98Å 51.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.89 – 2.20 45.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.89-2.20) 99.7 (45.85-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.245 , 0.293 0.250 , 0.302	Depositor DCC
R_{free} test set	2011 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.378 for -h,-k,l 0.470 for h,-h-k,-l 0.377 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5491	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, BR

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	0.78	0/2632	0.83	3/3556 (0.1%)
1	B	0.79	0/2627	0.87	4/3549 (0.1%)
All	All	0.79	0/5259	0.85	7/7105 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	296	GLU	OE1-CD-OE2	-5.63	116.55	123.30
1	B	133	VAL	CB-CA-C	-5.59	100.77	111.40
1	B	196	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	172	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	196	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	296	GLU	OE1-CD-OE2	-5.04	117.25	123.30

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	2579	0	2395	45	0
1	B	2574	0	2393	38	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	20	1
2	B	6	0	0	14	1
3	A	1	0	0	0	0
4	A	159	0	0	11	2
4	B	166	0	0	5	0
All	All	5491	0	4788	89	3

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 9.

All (89) 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:167:ARG:NH2	2:B:404:BR:BR	2.14	1.36
2:B:402:BR:BR	2:B:404:BR:BR	2.61	1.29
1:B:67:GLY:HA2	2:B:405:BR:BR	1.88	1.28
1:B:270:ARG:HD3	2:B:401:BR:BR	1.92	1.25
1:B:270:ARG:CD	2:B:401:BR:BR	2.51	1.14
1:A:100:ARG:NH1	2:A:402:BR:BR	2.41	1.08
1:B:67:GLY:CA	2:B:405:BR:BR	2.55	1.08
2:B:406:BR:BR	4:B:566:HOH:O	2.27	1.04
1:A:142:SER:N	2:A:406:BR:BR	2.45	1.04
2:A:401:BR:BR	4:A:659:HOH:O	2.32	1.03
1:A:89:LYS:NZ	2:A:406:BR:BR	2.50	0.98
1:B:270:ARG:NE	2:B:401:BR:BR	2.53	0.96
2:A:406:BR:BR	4:A:607:HOH:O	2.44	0.91
1:A:70:SER:O	2:A:405:BR:BR	2.45	0.90
1:A:163:ARG:NH2	2:A:402:BR:BR	2.62	0.88
1:B:67:GLY:C	2:B:405:BR:BR	2.66	0.87
1:A:25:LYS:NZ	4:A:615:HOH:O	1.79	0.85
1:A:134:GLY:HA3	2:A:402:BR:BR	2.34	0.83
1:B:125:SER:HB2	2:B:404:BR:BR	2.34	0.83
1:A:25:LYS:HG2	4:A:600:HOH:O	1.80	0.81
1:A:286:ILE:HD11	1:A:289:VAL:HG22	1.62	0.80
1:A:167:ARG:NH2	2:A:404:BR:BR	2.73	0.76
1:B:66:GLN:O	2:B:405:BR:BR	2.59	0.75
1:B:168:ARG:NH1	2:B:404:BR:BR	2.77	0.73
2:A:406:BR:BR	4:A:610:HOH:O	2.63	0.72
1:B:121:ASP:O	4:B:511:HOH:O	2.14	0.66
1:B:258:LEU:HD13	1:B:276:THR:HG23	1.79	0.65
1:A:134:GLY:CA	2:A:402:BR:BR	3.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:SER:HB2	2:A:406:BR:BR	2.53	0.63
1:A:142:SER:CB	2:A:406:BR:BR	3.02	0.62
1:A:242:ASN:HB3	1:A:247:THR:HB	1.83	0.61
1:A:75:ALA:HA	2:A:405:BR:BR	2.56	0.60
1:A:92:ASP:HB2	4:A:614:HOH:O	2.02	0.59
1:A:116:PRO:HG3	4:A:592:HOH:O	2.03	0.58
1:A:286:ILE:HD11	1:A:289:VAL:CG2	2.35	0.56
1:B:286:ILE:HD11	1:B:289:VAL:HG21	1.88	0.55
2:A:404:BR:BR	4:A:553:HOH:O	2.74	0.54
1:B:48:GLU:OE2	1:B:56:THR:HG21	2.08	0.53
1:A:61:TRP:HA	1:A:83:LEU:O	2.09	0.52
1:B:121:ASP:HB3	4:B:511:HOH:O	2.09	0.52
1:A:69:ASN:HB2	2:A:405:BR:BR	2.64	0.52
1:A:263:TYR:O	1:A:271:PRO:HD2	2.09	0.52
1:B:116:PRO:HG3	4:B:570:HOH:O	2.09	0.52
1:B:181:GLU:HG3	4:B:620:HOH:O	2.09	0.52
1:A:286:ILE:CD1	1:A:289:VAL:HG13	2.40	0.51
1:B:263:TYR:O	1:B:271:PRO:HD2	2.09	0.51
1:A:90:TYR:CD2	1:A:93:VAL:HG21	2.45	0.51
1:B:286:ILE:HD11	1:B:289:VAL:CG2	2.41	0.51
1:A:165:THR:HG23	4:A:539:HOH:O	2.12	0.50
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.46	0.50
1:A:258:LEU:HD23	1:A:276:THR:HG23	1.94	0.50
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.47	0.50
1:B:90:TYR:CD2	1:B:93:VAL:HG21	2.46	0.49
1:B:20:LEU:HG	1:B:38:MET:HB2	1.95	0.49
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.78	0.49
1:A:20:LEU:HG	1:A:38:MET:HB2	1.94	0.48
1:B:125:SER:O	2:B:404:BR:BR	2.86	0.48
1:B:115:LEU:HB2	1:B:118:PHE:O	2.13	0.48
1:B:258:LEU:CD1	1:B:276:THR:HG23	2.44	0.48
1:B:10:LYS:O	1:B:10:LYS:HG3	2.14	0.48
1:A:274:ALA:HB3	1:A:296:GLU:HB3	1.96	0.47
1:B:191:TYR:HD1	1:B:214:TRP:HB3	1.79	0.47
1:B:54:ASP:HB3	1:B:91:ALA:HB2	1.97	0.47
1:B:274:ALA:HB3	1:B:296:GLU:HB3	1.97	0.46
1:A:262:GLN:OE1	1:A:270:ARG:NH1	2.48	0.46
1:B:175:GLY:HA2	1:B:192:GLY:HA2	1.98	0.46
1:A:54:ASP:HB3	1:A:91:ALA:HB2	1.97	0.46
1:B:313:TYR:HE1	1:B:330:ASP:HB3	1.81	0.46
1:B:242:ASN:HB3	1:B:247:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ARG:CG	2:B:401:BR:BR	3.19	0.45
1:A:175:GLY:HA2	1:A:192:GLY:HA2	1.99	0.45
1:A:313:TYR:HE1	1:A:330:ASP:HB3	1.83	0.44
1:B:193:ALA:HA	1:B:211:ALA:O	2.18	0.44
1:A:75:ALA:CA	2:A:405:BR:BR	3.20	0.43
1:A:311:VAL:HA	1:A:333:ALA:O	2.19	0.43
1:A:235:ARG:NH1	4:A:609:HOH:O	2.26	0.42
1:B:311:VAL:HA	1:B:333:ALA:O	2.19	0.42
1:B:61:TRP:HA	1:B:83:LEU:O	2.18	0.42
1:A:256:ASP:OD1	1:A:278:SER:OG	2.29	0.42
1:A:193:ALA:HA	1:A:211:ALA:O	2.19	0.42
1:A:141:ASN:HA	2:A:406:BR:BR	2.75	0.42
1:A:273:ILE:HB	2:A:403:BR:BR	2.74	0.42
1:A:78:GLY:O	1:A:80:LYS:HD3	2.20	0.41
1:B:256:ASP:OD1	1:B:278:SER:OG	2.28	0.41
1:A:46:LYS:HE3	4:A:641:HOH:O	2.21	0.40
1:A:134:GLY:N	2:A:402:BR:BR	3.09	0.40
1:A:51:ILE:HD12	1:A:55:LEU:HG	2.03	0.40
1:A:286:ILE:HD13	1:A:289:VAL:HG13	2.04	0.40
1:B:78:GLY:O	1:B:80:LYS:HD3	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:THR:O	2:B:403:BR:BR[2_655]	2.05	0.15
2:A:402:BR:BR	4:A:572:HOH:O[3_555]	2.15	0.05
4:A:545:HOH:O	4:A:621:HOH:O[3_555]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 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	A	329/341 (96%)	313 (95%)	16 (5%)	0	100	100
1	B	328/341 (96%)	312 (95%)	16 (5%)	0	100	100
All	All	657/682 (96%)	625 (95%)	32 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	257/263 (98%)	249 (97%)	8 (3%)	40	51
1	B	257/263 (98%)	250 (97%)	7 (3%)	44	57
All	All	514/526 (98%)	499 (97%)	15 (3%)	42	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	25	LYS
1	A	80	LYS
1	A	218	LEU
1	A	286	ILE
1	A	289	VAL
1	A	305	LYS
1	A	320	SER
1	B	12	ASP
1	B	80	LYS
1	B	104	VAL
1	B	133	VAL
1	B	218	LEU
1	B	289	VAL
1	B	319	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 13 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 ⓘ

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.