Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:38 PM GMT

PDB ID	:	1BT9
Title	:	OMPF PORIN MUTANT D74A
Authors	:	Philippsen, A.; Schirmer, T.
Deposited on	:	1998-09-01
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

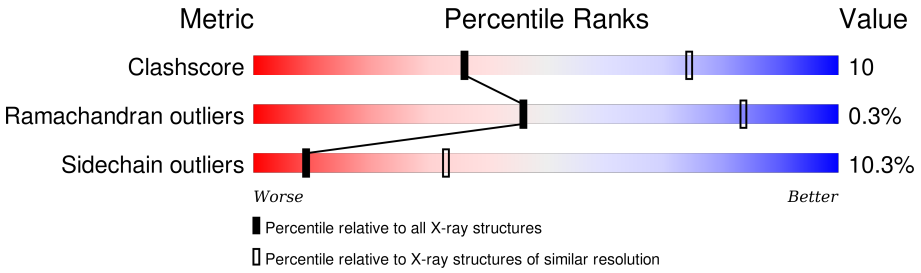
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	340	64% 29% 5% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2640 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 (MATRIX PORIN OUTER MEMBRANE PROTEIN F).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2624	1653	438	530	3	41	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASP	ENGINEERED	UNP P02931

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	16	16	16	0	0

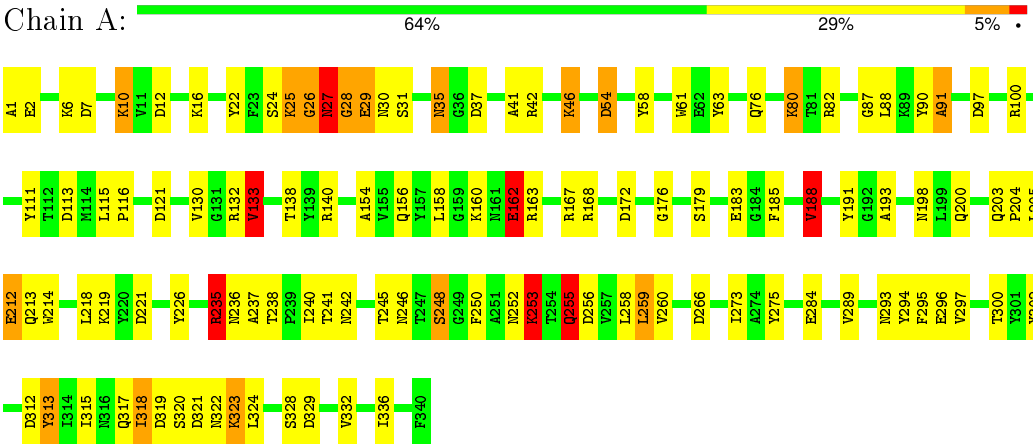
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (MATRIX PORIN OUTER MEMBRANE PROTEIN F)

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.50Å 118.50Å 52.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	91.0 (20.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2640	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.33	8/2680 (0.3%)	1.97	63/3624 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	CA-CB	53.15	2.70	1.53
1	A	28	GLY	CA-C	-19.04	1.21	1.51
1	A	162	GLU	CG-CD	12.67	1.71	1.51
1	A	29	GLU	C-O	11.87	1.46	1.23
1	A	183	GLU	CB-CG	8.89	1.69	1.52
1	A	25	LYS	CA-C	-8.27	1.31	1.52
1	A	28	GLY	C-O	7.78	1.36	1.23
1	A	305	LYS	CB-CG	6.46	1.70	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	ASN	O-C-N	-28.57	74.63	123.20
1	A	28	GLY	O-C-N	-27.68	78.42	122.70
1	A	27	ASN	CA-C-N	22.67	161.54	116.20
1	A	25	LYS	CA-CB-CG	19.46	156.21	113.40
1	A	29	GLU	CB-CA-C	-15.22	79.96	110.40
1	A	100	ARG	NE-CZ-NH2	14.89	127.75	120.30
1	A	25	LYS	CB-CG-CD	14.38	148.99	111.60
1	A	29	GLU	N-CA-CB	-12.45	88.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	A	25	LYS	CB-CA-C	11.39	133.19	110.40
1	A	162	GLU	CG-CD-OE1	11.35	140.99	118.30
1	A	162	GLU	CG-CD-OE2	-11.13	96.03	118.30
1	A	28	GLY	CA-C-O	10.40	139.33	120.60
1	A	26	GLY	CA-C-N	-9.71	95.85	117.20
1	A	82	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	10	LYS	CG-CD-CE	9.30	139.81	111.90
1	A	163	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	221	ASP	CB-CG-OD1	8.66	126.09	118.30
1	A	168	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	100	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	A	37	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	A	82	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	A	140	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	167	ARG	NH1-CZ-NH2	-7.61	111.03	119.40
1	A	29	GLU	CA-C-O	-7.49	104.38	120.10
1	A	183	GLU	CA-CB-CG	-7.36	97.21	113.40
1	A	212	GLU	OE1-CD-OE2	7.28	132.03	123.30
1	A	132	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	A	133	VAL	CB-CA-C	-6.85	98.38	111.40
1	A	29	GLU	O-C-N	6.77	133.53	122.70
1	A	168	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	188	VAL	CB-CA-C	-6.68	98.70	111.40
1	A	256	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	10	LYS	CB-CA-C	6.52	123.45	110.40
1	A	319	ASP	C-N-CA	6.42	137.75	121.70
1	A	235	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	26	GLY	O-C-N	5.99	132.29	122.70
1	A	29	GLU	CA-CB-CG	5.97	126.53	113.40
1	A	2	GLU	OE1-CD-OE2	5.93	130.42	123.30
1	A	113	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	266	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	35	ASN	N-CA-CB	-5.73	100.29	110.60
1	A	12	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	255	GLN	N-CA-CB	5.71	120.87	110.60
1	A	253	LYS	CA-CB-CG	5.63	125.78	113.40
1	A	162	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	260	VAL	CA-CB-CG2	5.58	119.27	110.90
1	A	121	ASP	CB-CG-OD1	5.49	123.25	118.30
1	A	80	LYS	CA-C-O	5.37	131.37	120.10
1	A	58	TYR	CB-CG-CD2	-5.29	117.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	LYS	N-CA-CB	5.26	120.07	110.60
1	A	163	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	313	TYR	CB-CG-CD2	5.21	124.13	121.00
1	A	294	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	7	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	A	22	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	167	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	312	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	132	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	A	295	PHE	N-CA-CB	5.08	119.75	110.60
1	A	226	TYR	CB-CG-CD1	5.05	124.03	121.00
1	A	46	LYS	CA-CB-CG	5.05	124.52	113.40
1	A	76	GLN	CB-CA-C	-5.04	100.32	110.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain
1	A	133	VAL	Mainchain
1	A	162	GLU	Sidechain
1	A	185	PHE	Mainchain
1	A	188	VAL	Mainchain
1	A	236	ASN	Mainchain
1	A	26	GLY	Mainchain
1	A	27	ASN	Mainchain,Peptide
1	A	28	GLY	Mainchain
1	A	29	GLU	Peptide
1	A	307	MET	Mainchain
1	A	54	ASP	Mainchain

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	A	2624	0	2445	48	0
2	A	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2640	0	2445	48	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 10.

All (48) 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:235:ARG:HE	1:A:253:LYS:HD2	1.31	0.93
1:A:205:LEU:HD23	1:A:284:GLU:HG2	1.64	0.78
1:A:31:SER:HA	1:A:329:ASP:HB2	1.72	0.71
1:A:138:THR:OG1	1:A:156:GLN:HG3	1.93	0.68
1:A:259:LEU:HD12	1:A:275:TYR:HD2	1.62	0.64
1:A:115:LEU:HB3	1:A:116:PRO:HD2	1.79	0.62
1:A:24:SER:HB2	1:A:35:ASN:HB2	1.81	0.62
1:A:235:ARG:NE	1:A:253:LYS:HD2	2.09	0.62
1:A:313:TYR:CD1	1:A:332:VAL:HG22	2.36	0.60
1:A:206:GLY:H	1:A:284:GLU:CD	2.09	0.56
1:A:179:SER:CB	1:A:188:VAL:HG13	2.36	0.56
1:A:115:LEU:HD13	1:A:296:GLU:HG3	1.89	0.54
1:A:293:ASN:HB3	1:A:318:ILE:HG12	1.90	0.53
1:A:213:GLN:HE21	1:A:237:ALA:HB1	1.73	0.53
1:A:321:ASP:O	1:A:322:ASN:C	2.47	0.53
1:A:179:SER:HB3	1:A:188:VAL:HG13	1.92	0.52
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.45	0.51
1:A:245:THR:O	1:A:246:ASN:HB2	2.11	0.49
1:A:104:VAL:O	1:A:107:ASP:HB2	2.13	0.48
1:A:87:GLY:HA3	1:A:97:ASP:HB3	1.95	0.47
1:A:205:LEU:HD13	1:A:240:ILE:HD11	1.96	0.47
1:A:111:TYR:CZ	1:A:188:VAL:HG22	2.50	0.47
1:A:241:THR:HG23	1:A:248:SER:OG	2.14	0.46
1:A:255:GLN:HB3	1:A:255:GLN:HE21	1.60	0.46
1:A:30:ASN:ND2	1:A:328:SER:OG	2.47	0.46
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.80	0.46
1:A:193:ALA:HB2	1:A:212:GLU:HG2	1.98	0.46
1:A:179:SER:HB2	1:A:188:VAL:HG13	1.97	0.45
1:A:54:ASP:HB3	1:A:91:ALA:HB2	1.99	0.45
1:A:205:LEU:HD13	1:A:240:ILE:CD1	2.47	0.45
1:A:90:TYR:O	1:A:91:ALA:C	2.54	0.45
1:A:200:GLN:O	1:A:203:GLN:HG2	2.17	0.45
1:A:205:LEU:HD13	1:A:240:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ALA:O	1:A:176:GLY:HA2	2.17	0.44
1:A:203:GLN:HA	1:A:204:PRO:HD3	1.88	0.43
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.83	0.43
1:A:315:ILE:HG22	1:A:317:GLN:NE2	2.32	0.43
1:A:289:VAL:HG21	1:A:324:LEU:HG	2.01	0.42
1:A:242:ASN:O	1:A:246:ASN:N	2.49	0.42
1:A:238:THR:O	1:A:250:PHE:HA	2.20	0.42
1:A:106:TYR:HB2	1:A:130:VAL:O	2.20	0.42
1:A:245:THR:O	1:A:246:ASN:CB	2.68	0.41
1:A:300:THR:HG21	1:A:302:TYR:CZ	2.55	0.41
1:A:273:ILE:HD11	1:A:297:VAL:HG13	2.02	0.41
1:A:321:ASP:O	1:A:323:LYS:NZ	2.40	0.41
1:A:273:ILE:HA	1:A:273:ILE:HD13	1.93	0.41
1:A:158:LEU:O	1:A:172:ASP:HA	2.20	0.41
1:A:16:LYS:O	1:A:41:ALA:HA	2.22	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	338/340 (99%)	316 (94%)	21 (6%)	1 (0%)	46 84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ALA

5.3.2 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	A	262/262 (100%)	235 (90%)	27 (10%)	9 33

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	10	LYS
1	A	25	LYS
1	A	27	ASN
1	A	46	LYS
1	A	80	LYS
1	A	88	LEU
1	A	104	VAL
1	A	133	VAL
1	A	160	LYS
1	A	162	GLU
1	A	188	VAL
1	A	198	ASN
1	A	209	LYS
1	A	218	LEU
1	A	219	LYS
1	A	235	ARG
1	A	248	SER
1	A	252	ASN
1	A	253	LYS
1	A	255	GLN
1	A	258	LEU
1	A	259	LEU
1	A	318	ILE
1	A	320	SER
1	A	323	LYS
1	A	336	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	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

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.