Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 06:44 pm BST

PDB ID	:	2WL8
Title	:	X-ray crystal structure of Pex19p
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Deposited on	:	2009-06-22
Resolution	:	2.05 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 (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 (1)) were used in the production of this report:

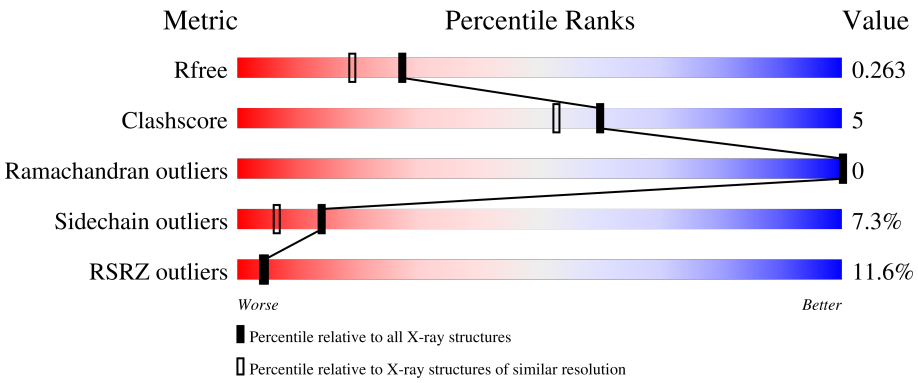
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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% 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	126	6% 71% 16% 13%
1	B	126	2% 69% 12% • 17%
1	C	126	7% 69% 13% • 13%
1	D	126	24% 71% 15% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3715 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 PEROXISOMAL BIOGENESIS FACTOR 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	110	897	570	143	176	8	0	0	0
1	B	104	850	539	136	167	8	0	0	0
1	C	109	889	564	142	175	8	0	0	0
1	D	109	889	564	142	175	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	-	expression tag	UNP P40855
A	159	ALA	-	expression tag	UNP P40855
A	160	MET	-	expression tag	UNP P40855
B	158	GLY	-	expression tag	UNP P40855
B	159	ALA	-	expression tag	UNP P40855
B	160	MET	-	expression tag	UNP P40855
C	158	GLY	-	expression tag	UNP P40855
C	159	ALA	-	expression tag	UNP P40855
C	160	MET	-	expression tag	UNP P40855
D	158	GLY	-	expression tag	UNP P40855
D	159	ALA	-	expression tag	UNP P40855
D	160	MET	-	expression tag	UNP P40855

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	50	50	50	0	0
2	B	75	75	75	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	C	50	50	50	0	0
			Total	O		
2	D	15	15	15	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: PEROXISOMAL BIOGENESIS FACTOR 19

Chain A: 6% 71% 16% 13%

GLY ALA MET GLY MET ASP GLU GLY ASP GLY GLU GLY ASN I171 L174 M175 Q176 S177 I178 M179 L188 L192 K193 E197 K198 Y199 W202 E213 Q221 I228 T236 P237 T238 E241 R247 D260 H263 P264 P265 F278 D279 L280 ASP ALA LEU

• Molecule 1: PEROXISOMAL BIOGENESIS FACTOR 19

Chain B: 2% 69% 12% • 17%

GLY ALA MET GLY MET ASP GLU GLY ASP GLY GLU GLY ASN I171 L172 P173 M179 L192 Y199 P200 E201 R207 P211 P212 E216 Q219 M225 T236 P237 M250 L258 H263 K266 A269 M272 P273 P274 GLY LEU ASN PHE ASP LEU ASP ALA

LEU

• Molecule 1: PEROXISOMAL BIOGENESIS FACTOR 19

Chain C: 7% 69% 13% • 13%

GLY ALA MET GLY MET ASP GLU GLY ASP GLY GLU GLY ASN I171 L174 M175 L192 K193 E194 I195 T196 Y199 P200 E201 W202 L203 Q204 R207 E208 S209 L210 E216 Q219 E235 T236 T242 R247 M250 V251 L252 L258 P265 K266 E267 M272 P273

L276 N277 F278 D279 LEU ASP ALA LEU

• Molecule 1: PEROXISOMAL BIOGENESIS FACTOR 19

Chain D: 24% 71% 15% 13%

GLY ALA MET GLY MET ASP GLU GLY ASP GLY GLU GLY ASN I171 L172 P173 Q176 S177 I178 M179 L183 L192 E197 K198 Y199 P200 E201 W202 L203 Q204 S205 H206 R207 E208 S209 L210 P211 P212 E213 Q214 F215 E216 K217 Y218 K227 T236 E241 D253 D260 H263

P264 P265 K266 E267 L268 A269 G270 E271 M272 D279 LEU ASP ALA LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.15Å 91.12Å 122.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.05 49.44 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.45-2.05) 99.1 (49.44-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.199 , 0.239 0.231 , 0.263	Depositor DCC
R_{free} test set	2400 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3715	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (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	A	0.66	0/918	0.68	0/1242
1	B	0.81	2/870 (0.2%)	0.73	0/1177
1	C	0.72	0/910	0.85	2/1231 (0.2%)
1	D	0.56	0/910	0.62	0/1231
All	All	0.69	2/3608 (0.1%)	0.73	2/4881 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	PRO	N-CD	7.07	1.57	1.47
1	B	199	TYR	CD2-CE2	5.37	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	247	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	C	247	ARG	NE-CZ-NH1	10.37	125.49	120.30

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	A	897	0	878	9	0
1	B	850	0	834	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	889	0	867	13	1
1	D	889	0	867	6	0
2	A	50	0	0	0	0
2	B	75	0	0	1	0
2	C	50	0	0	2	0
2	D	15	0	0	0	0
All	All	3715	0	3446	32	1

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 5.

All (32) 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:266:LYS:HG2	1:C:194:GLU:HB3	1.65	0.76
1:B:269:ALA:HB3	1:C:194:GLU:HG3	1.75	0.69
1:C:192:LEU:O	1:C:196:THR:HG23	1.94	0.68
1:D:263:HIS:HB3	1:D:279:ASP:HA	1.78	0.66
1:C:242:THR:HG22	2:C:2032:HOH:O	2.00	0.62
1:B:263:HIS:HE1	2:C:2041:HOH:O	1.83	0.60
1:A:193:LYS:O	1:A:197:GLU:HG3	2.02	0.60
1:C:272:MET:H	1:C:277:ASN:HD21	1.51	0.58
1:A:179:MET:HG3	1:C:175:MET:HG2	1.88	0.55
1:C:202:TRP:NE1	1:C:267:GLU:HG2	2.21	0.55
1:C:202:TRP:CZ2	1:C:265:PRO:HB3	2.43	0.53
1:C:202:TRP:HE1	1:C:267:GLU:HG2	1.73	0.53
1:A:221:GLN:HE22	1:A:264:PRO:HA	1.74	0.53
1:B:192:LEU:HD12	1:B:225:MET:HE2	1.91	0.52
1:D:171:ILE:HG13	1:D:173:PRO:HD2	1.92	0.51
1:B:216:GLU:HA	1:B:219:GLN:HE21	1.76	0.50
1:B:192:LEU:CD1	1:B:225:MET:HE2	2.42	0.49
1:C:235:GLU:HG3	1:C:247:ARG:HD3	1.93	0.49
1:B:192:LEU:HD12	1:B:225:MET:CE	2.43	0.48
1:C:216:GLU:HA	1:C:219:GLN:HE21	1.80	0.47
1:A:263:HIS:HD2	1:A:264:PRO:O	1.98	0.46
1:D:202:TRP:CZ2	1:D:265:PRO:HB3	2.51	0.45
1:B:201:GLU:HG3	2:B:2019:HOH:O	2.17	0.45
1:A:260:ASP:OD2	1:D:260:ASP:OD2	2.36	0.44
1:C:273:PRO:O	1:C:276:LEU:HB2	2.18	0.44
1:A:199:TYR:OH	1:A:221:GLN:NE2	2.53	0.42
1:A:263:HIS:HA	1:A:278:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PRO:HA	1:B:212:PRO:HD3	1.75	0.42
1:A:202:TRP:CZ2	1:A:265:PRO:HB3	2.56	0.41
1:A:236:THR:HB	1:A:237:PRO:HD2	2.02	0.40
1:D:179:MET:CE	1:D:183:LEU:HD11	2.51	0.40
1:C:171:ILE:O	1:D:227:LYS:HE3	2.20	0.40

All (1) 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:250:MET:CE	1:C:250:MET:CE[3_646]	1.98	0.22

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	108/126 (86%)	107 (99%)	1 (1%)	0	100	100
1	B	102/126 (81%)	102 (100%)	0	0	100	100
1	C	107/126 (85%)	106 (99%)	1 (1%)	0	100	100
1	D	107/126 (85%)	107 (100%)	0	0	100	100
All	All	424/504 (84%)	422 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	104/113 (92%)	97 (93%)	7 (7%)	16 9
1	B	99/113 (88%)	93 (94%)	6 (6%)	18 10
1	C	103/113 (91%)	95 (92%)	8 (8%)	12 5
1	D	103/113 (91%)	94 (91%)	9 (9%)	10 4
All	All	409/452 (90%)	379 (93%)	30 (7%)	14 6

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

Mol	Chain	Res	Type
1	A	174	ILE
1	A	176	GLN
1	A	192	LEU
1	A	213	GLU
1	A	241	GLU
1	A	247	ARG
1	A	280	LEU
1	B	179	MET
1	B	201	GLU
1	B	207	ARG
1	B	236	THR
1	B	250	MET
1	B	258	LEU
1	C	192	LEU
1	C	199	TYR
1	C	236	THR
1	C	242	THR
1	C	252	LEU
1	C	258	LEU
1	C	267	GLU
1	C	276	LEU
1	D	176	GLN
1	D	177	SER
1	D	192	LEU
1	D	197	GLU
1	D	201	GLU
1	D	204	GLN
1	D	213	GLU
1	D	236	THR
1	D	253	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	181	ASN
1	A	204	GLN
1	A	221	GLN
1	A	259	GLN
1	A	263	HIS
1	B	219	GLN
1	B	231	GLN
1	B	263	HIS
1	C	176	GLN
1	C	204	GLN
1	C	219	GLN
1	C	256	GLN
1	C	263	HIS
1	C	277	ASN
1	D	176	GLN
1	D	180	GLN
1	D	221	GLN
1	D	256	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 (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, 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	A	110/126 (87%)	0.96	8 (7%)	15	16	36, 41, 50, 60	0
1	B	104/126 (82%)	0.69	3 (2%)	51	56	33, 41, 50, 63	0
1	C	109/126 (86%)	0.89	9 (8%)	11	11	33, 41, 51, 58	0
1	D	109/126 (86%)	1.57	30 (27%)	0	0	35, 42, 52, 55	0
All	All	432/504 (85%)	1.03	50 (11%)	4	4	33, 42, 51, 63	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	210	LEU	6.8
1	D	209	SER	5.8
1	D	213	GLU	5.7
1	D	208	GLU	5.5
1	D	205	SER	5.4
1	D	267	GLU	5.4
1	D	203	LEU	5.0
1	D	202	TRP	4.7
1	D	207	ARG	4.6
1	D	266	LYS	4.4
1	D	270	GLY	4.4
1	D	212	PRO	4.2
1	D	204	GLN	4.0
1	C	208	GLU	3.9
1	D	206	HIS	3.9
1	C	204	GLN	3.9
1	D	265	PRO	3.8
1	D	201	GLU	3.8
1	C	171	ILE	3.5
1	D	214	GLN	3.4
1	D	198	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	201	GLU	3.2
1	D	216	GLU	3.2
1	D	215	PHE	3.0
1	A	238	THR	2.9
1	D	271	GLU	2.9
1	D	211	PRO	2.9
1	D	268	LEU	2.8
1	D	199	TYR	2.8
1	C	207	ARG	2.6
1	A	237	PRO	2.5
1	C	209	SER	2.4
1	B	272	MET	2.4
1	A	228	ILE	2.4
1	D	241	GLU	2.3
1	B	237	PRO	2.3
1	D	269	ALA	2.3
1	A	178	ILE	2.3
1	D	263	HIS	2.3
1	B	173	PRO	2.2
1	D	272	MET	2.2
1	A	188	LEU	2.2
1	D	218	TYR	2.2
1	A	171	ILE	2.1
1	C	210	LEU	2.1
1	C	174	ILE	2.1
1	C	200	PRO	2.0
1	D	217	LYS	2.0
1	A	213	GLU	2.0
1	A	174	ILE	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.