Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 06:42 pm BST

PDB ID	:	2XU8
Title	:	Structure of Pa1645
Authors	:	Abdelli, W.B.; Moynie, L.; McMahon, S.A.; Liu, H.; Alphey, M.S.; Naismith, J.H.
Deposited on	:	2010-10-15
Resolution	:	1.98 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 (i)) were used in the production of this report:

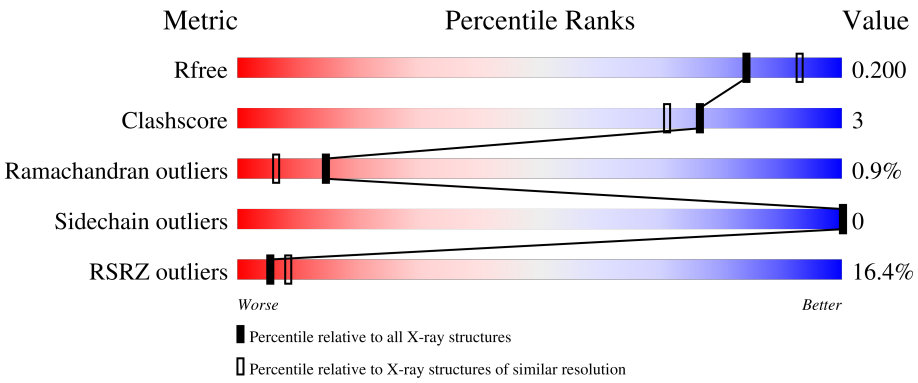
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.98 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}	164625	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	116	16% 94% 6%
1	B	116	14% 96% .
1	C	116	19% 96% .

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	SO4	A	1139	-	-	-	X

2 Entry composition (i)

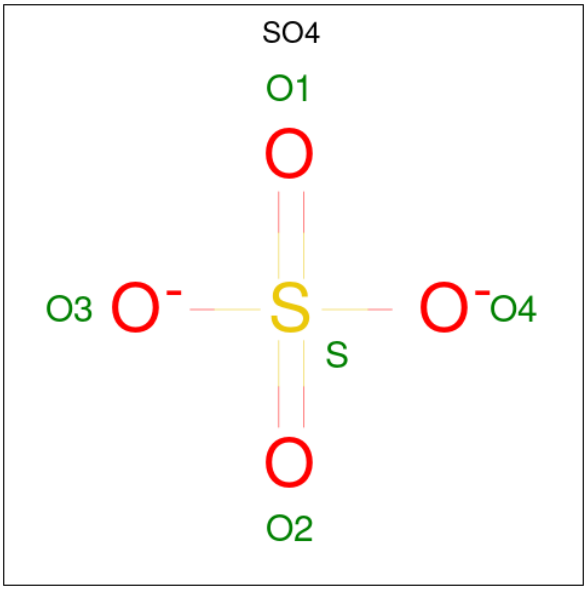
There are 3 unique types of molecules in this entry. The entry contains 3152 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PA1645.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	116	948	601	176	169	2	0	4	0
1	B	116	947	600	178	167	2	0	3	0
1	C	116	956	606	179	169	2	0	4	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0

- Molecule 3 is water.

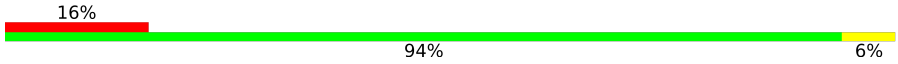
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	95	95	95	0	0
			Total	O		
3	B	86	86	86	0	0
			Total	O		
3	C	65	65	65	0	0

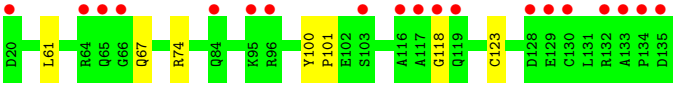
3 Residue-property plots (i)

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: PA1645

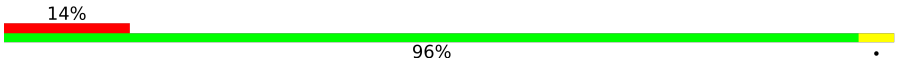
Chain A:

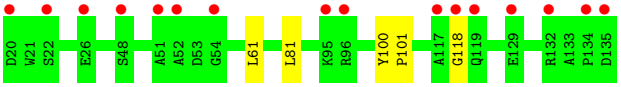




- Molecule 1: PA1645

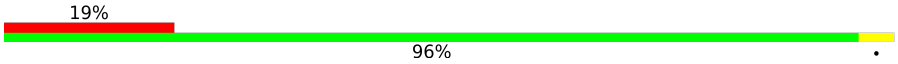
Chain B:

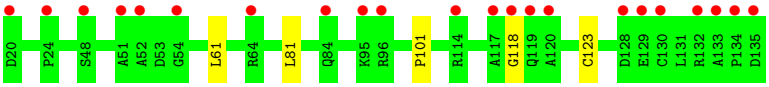




- Molecule 1: PA1645

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	125.97Å 125.97Å 125.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.07 – 1.98 89.07 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.07-1.98) 99.9 (89.07-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.33 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, R_{free}	0.176 , 0.192 0.187 , 0.200	Depositor DCC
R_{free} test set	1772 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.065 for l,-k,h 0.045 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3152	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.46	0/984	0.60	0/1342
1	B	0.42	0/980	0.61	0/1335
1	C	0.42	0/995	0.59	0/1356
All	All	0.43	0/2959	0.60	0/4033

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	A	948	0	928	8	0
1	B	947	0	928	5	0
1	C	956	0	941	5	0
2	A	20	0	0	0	0
2	B	25	0	0	0	0
2	C	10	0	0	0	0
3	A	95	0	0	2	0
3	B	86	0	0	0	0
3	C	65	0	0	0	0
All	All	3152	0	2797	16	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 (16) 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:61[A]:LEU:HD13	1:A:101:PRO:HG2	1.55	0.87
1:A:61[B]:LEU:HD22	1:A:101:PRO:HG2	1.67	0.76
1:C:61[A]:LEU:HD13	1:C:101:PRO:HG2	1.68	0.74
1:B:61[B]:LEU:HD13	1:B:101:PRO:HG2	1.71	0.72
1:C:61[B]:LEU:HD22	1:C:101:PRO:HG2	1.83	0.60
1:A:61[B]:LEU:HD22	1:A:101:PRO:CG	2.31	0.60
1:B:61[A]:LEU:HD22	1:B:101:PRO:HG2	1.83	0.60
1:C:61[B]:LEU:HD22	1:C:101:PRO:CG	2.42	0.49
1:B:61[A]:LEU:HD22	1:B:101:PRO:CG	2.43	0.48
1:A:74:ARG:NH1	3:A:2035:HOH:O	2.47	0.47
1:A:123:CYS:HB3	1:C:81:LEU:HD23	1.97	0.46
1:B:81:LEU:HD23	1:C:123:CYS:HB3	1.99	0.44
1:A:61[A]:LEU:HD13	1:A:101:PRO:CG	2.37	0.43
1:A:67:GLN:HG3	3:A:2044:HOH:O	2.17	0.43
1:A:100:TYR:N	1:A:101:PRO:CD	2.84	0.41
1:B:100:TYR:N	1:B:101:PRO:CD	2.84	0.41

There are no symmetry-related clashes.

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	118/116 (102%)	115 (98%)	2 (2%)	1 (1%)	16 7
1	B	117/116 (101%)	114 (97%)	2 (2%)	1 (1%)	14 6
1	C	119/116 (103%)	116 (98%)	2 (2%)	1 (1%)	16 7
All	All	354/348 (102%)	345 (98%)	6 (2%)	3 (1%)	14 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	B	118	GLY
1	C	118	GLY

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	97/93 (104%)	97 (100%)	0	100	100
1	B	96/93 (103%)	96 (100%)	0	100	100
1	C	98/93 (105%)	98 (100%)	0	100	100
All	All	291/279 (104%)	291 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1139	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	1139	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	C	1137	-	4,4,4	0.23	0	6,6,6	0.26	0
2	SO4	A	1136	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	C	1136	-	4,4,4	0.12	0	6,6,6	0.25	0
2	SO4	B	1136	-	4,4,4	0.22	0	6,6,6	0.40	0
2	SO4	A	1137	-	4,4,4	0.08	0	6,6,6	0.19	0
2	SO4	A	1138	-	4,4,4	0.11	0	6,6,6	0.18	0
2	SO4	B	1140	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	B	1137	-	4,4,4	0.26	0	6,6,6	0.33	0
2	SO4	B	1138	-	4,4,4	0.18	0	6,6,6	0.41	0

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, 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	116/116 (100%)	0.83	19 (16%)	5	8	12, 38, 78, 114	4 (3%)
1	B	116/116 (100%)	0.69	16 (13%)	8	11	12, 37, 69, 84	3 (2%)
1	C	116/116 (100%)	0.93	22 (18%)	4	6	14, 41, 73, 98	4 (3%)
All	All	348/348 (100%)	0.82	57 (16%)	5	8	12, 38, 74, 114	11 (3%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	ASP	5.2
1	A	117	ALA	5.0
1	A	135	ASP	4.0
1	C	117	ALA	4.0
1	A	118	GLY	3.9
1	B	117	ALA	3.9
1	C	128	ASP	3.6
1	B	52	ALA	3.6
1	C	95	LYS	3.6
1	C	120	ALA	3.6
1	A	134	PRO	3.4
1	C	130	CYS	3.4
1	A	96	ARG	3.4
1	C	52	ALA	3.3
1	B	135	ASP	3.3
1	C	133	ALA	3.3
1	C	84	GLN	3.3
1	B	119	GLN	3.2
1	C	118	GLY	3.2
1	A	130	CYS	3.1
1	A	20	ASP	3.1
1	C	119	GLN	3.1
1	A	64	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	22	SER	3.1
1	B	118	GLY	3.0
1	C	129	GLU	3.0
1	C	64	ARG	3.0
1	A	95	LYS	3.0
1	B	95	LYS	3.0
1	B	51	ALA	2.9
1	C	132[A]	ARG	2.8
1	A	133	ALA	2.7
1	A	116	ALA	2.7
1	A	132	ARG	2.7
1	C	96	ARG	2.7
1	C	20	ASP	2.7
1	B	54	GLY	2.6
1	A	129	GLU	2.6
1	C	51	ALA	2.6
1	A	119	GLN	2.5
1	B	134	PRO	2.4
1	B	20	ASP	2.3
1	B	96	ARG	2.3
1	C	54	GLY	2.2
1	B	132[A]	ARG	2.2
1	A	84	GLN	2.2
1	A	66	GLY	2.2
1	C	134	PRO	2.1
1	C	48	SER	2.1
1	B	48	SER	2.1
1	C	24	PRO	2.1
1	A	128	ASP	2.0
1	B	26	GLU	2.0
1	B	129	GLU	2.0
1	A	103[A]	SER	2.0
1	A	65	GLN	2.0
1	C	114	ARG	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)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	SO4	A	1139	5/5	0.79	0.45	204,204,205,206	0
2	SO4	B	1140	5/5	0.84	0.11	62,71,73,73	0
2	SO4	B	1139	5/5	0.93	0.08	62,64,65,65	0
2	SO4	A	1138	5/5	0.94	0.15	58,60,63,67	5
2	SO4	A	1137	5/5	0.96	0.12	35,38,41,41	0
2	SO4	B	1138	5/5	0.97	0.10	35,38,39,43	0
2	SO4	A	1136	5/5	0.98	0.11	33,36,40,40	0
2	SO4	C	1136	5/5	0.98	0.09	31,33,35,35	0
2	SO4	C	1137	5/5	0.98	0.12	35,39,41,42	0
2	SO4	B	1137	5/5	0.99	0.07	27,29,30,31	0
2	SO4	B	1136	5/5	0.99	0.05	27,28,30,32	0

6.5 Other polymers (i)

There are no such residues in this entry.