



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:26 pm GMT

PDB ID : 5L80
Title : Structure of Exuperantia EXO-like and SAM-like domains
Authors : Lazzaretti, D.; Veith, K.; Bono, F.
Deposited on : 2016-06-05
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

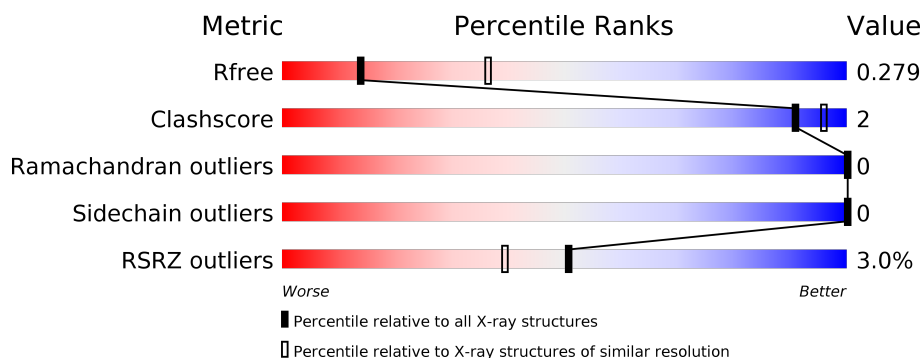
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 $\leq 5\%$. 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	A	353	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 82%, height: 10px; background-color: green;"></div> <div style="width: 1%, height: 10px; background-color: yellow;"></div> <div style="width: 15%, height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;"> % 82% • 15% </div> </div> </div>
1	B	353	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 4%, height: 10px; background-color: red;"></div> <div style="width: 71%, height: 10px; background-color: green;"></div> <div style="width: 5%, height: 10px; background-color: yellow;"></div> <div style="width: 24%, height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;"> 4% 71% 5% 24% </div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8361 atoms, of which 4121 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 Maternal protein exuperantia, Maternal protein exuperantia.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	H	N	O	S	0	0	0
			4616	1496	2305	389	419	7			
1	B	269	Total	C	H	N	O	S	0	0	0
			3734	1227	1816	328	356	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	LEU	-	linker	UNP P28750
A	199	ASP	-	linker	UNP P28750
A	200	ALA	-	linker	UNP P28750
A	201	ASP	-	linker	UNP P28750
A	202	SER	-	linker	UNP P28750
B	198	LEU	-	linker	UNP P28750
B	199	ASP	-	linker	UNP P28750
B	200	ALA	-	linker	UNP P28750
B	201	ASP	-	linker	UNP P28750
B	202	SER	-	linker	UNP P28750

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	3	Total	O	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.54Å 66.59Å 81.33Å 90.00° 113.64° 90.00°	Depositor
Resolution (Å)	47.34 – 2.80 47.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.34-2.80) 99.7 (47.34-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.252 , 0.277 0.253 , 0.279	Depositor DCC
R_{free} test set	969 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8361	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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

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	0.25	0/2348	0.40	0/3180
1	B	0.25	0/1946	0.37	0/2643
All	All	0.25	0/4294	0.38	0/5823

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

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	2311	2305	2269	6	0
1	B	1918	1816	1714	10	0
2	A	8	0	0	0	0
2	B	3	0	0	0	0
All	All	4240	4121	3983	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 2.

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:73:LEU:O	1:A:78:ARG:NH1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASN:OD1	1:B:160:ARG:NH2	2.29	0.66
1:B:337:ALA:O	1:B:341:GLU:N	2.37	0.57
1:A:342:SER:O	1:A:343:TYR:HB3	2.08	0.54
1:B:159:GLU:O	1:B:162:THR:OG1	2.29	0.49
1:B:73:LEU:O	1:B:78:ARG:NH1	2.48	0.46
1:A:39:ASP:OD1	1:A:40:ILE:N	2.45	0.46
1:A:235:GLU:O	1:A:239:ASN:ND2	2.47	0.46
1:B:282:THR:OG1	1:B:283:LEU:N	2.49	0.45
1:B:238:GLU:HA	1:B:241:PHE:CD2	2.53	0.44
1:A:272:ARG:N	1:A:273:PRO:HD2	2.34	0.43
1:B:163:ALA:O	1:B:166:LYS:NZ	2.52	0.42
1:B:336:LYS:O	1:B:340:LEU:N	2.51	0.42
1:B:245:ARG:N	1:B:246:PRO:CD	2.82	0.42
1:B:35:LEU:HG	1:B:241:PHE:CE1	2.55	0.42
1:A:221:GLN:O	1:A:225:SER:N	2.53	0.41

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	291/353 (82%)	285 (98%)	6 (2%)	0	100	100
1	B	257/353 (73%)	252 (98%)	5 (2%)	0	100	100
All	All	548/706 (78%)	537 (98%)	11 (2%)	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	232/306 (76%)	232 (100%)	0	100	100
1	B	164/306 (54%)	164 (100%)	0	100	100
All	All	396/612 (65%)	396 (100%)	0	100	100

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

Some 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 carbohydrates 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 ⓘ

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	A	301/353 (85%)	0.08	2 (0%) 87 83	51, 75, 99, 115	0
1	B	269/353 (76%)	0.30	15 (5%) 25 16	61, 100, 155, 163	0
All	All	570/706 (80%)	0.18	17 (2%) 51 39	51, 84, 136, 163	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	ALA	4.5
1	B	35	LEU	4.3
1	B	300	GLY	3.7
1	B	340	LEU	3.3
1	B	128	PRO	3.2
1	B	341	GLU	2.7
1	B	220	LEU	2.5
1	B	279	PHE	2.4
1	B	136	ILE	2.3
1	B	278	TYR	2.3
1	A	192	LEU	2.2
1	B	135	LEU	2.2
1	B	192	LEU	2.2
1	B	320	ILE	2.1
1	B	218	VAL	2.1
1	B	285	HIS	2.1
1	A	187	TYR	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.