



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4LOG
Title : The crystal structure of the orphan nuclear receptor PNR ligand binding domain fused with MBP
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Deposited on : 2013-07-12
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

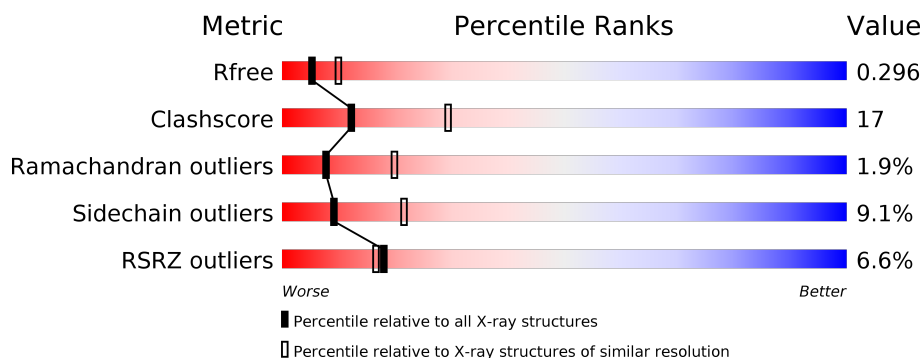
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 $\leq 5\%$. 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	574	
1	B	574	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6234 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 Maltose ABC transporter periplasmic protein and NR2E3 protein chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4334	2799	712	809	14			
1	B	232	Total	C	N	O	S	0	0	0
			1838	1184	314	330	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP K0BGG6
A	369	ASN	-	LINKER	UNP K0BGG6
A	370	ALA	-	LINKER	UNP K0BGG6
A	371	ALA	-	LINKER	UNP K0BGG6
A	372	ALA	-	LINKER	UNP K0BGG6
A	1215	GLU	-	LINKER	UNP K0BGG6
A	1216	PHE	-	LINKER	UNP K0BGG6
A	1405	SER	CYS	ENGINEERED MUTATION	UNP Q8IVZ9
A	1411	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
A	1412	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
A	1413	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
A	1414	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
A	1415	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
A	1416	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
B	1	MET	-	INITIATING METHIONINE	UNP K0BGG6
B	369	ASN	-	LINKER	UNP K0BGG6
B	370	ALA	-	LINKER	UNP K0BGG6
B	371	ALA	-	LINKER	UNP K0BGG6
B	372	ALA	-	LINKER	UNP K0BGG6
B	1215	GLU	-	LINKER	UNP K0BGG6
B	1216	PHE	-	LINKER	UNP K0BGG6
B	1405	SER	CYS	ENGINEERED MUTATION	UNP Q8IVZ9
B	1411	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
B	1412	HIS	-	EXPRESSION TAG	UNP Q8IVZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1413	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
B	1414	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
B	1415	HIS	-	EXPRESSION TAG	UNP Q8IVZ9
B	1416	HIS	-	EXPRESSION TAG	UNP Q8IVZ9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	29	Total O 29 29	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.44Å 184.94Å 85.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.70) 96.4 (29.70-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.285 , 0.307 0.278 , 0.296	Depositor DCC
R_{free} test set	2961 reflections (7.66%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6234	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 [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	0.57	0/4439	0.59	0/6025
1	B	0.62	2/1879 (0.1%)	0.64	0/2548
All	All	0.58	2/6318 (0.0%)	0.61	0/8573

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	TRP	CD2-CE2	5.45	1.47	1.41
1	B	1268	TRP	CD2-CE2	5.04	1.47	1.41

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	4334	0	4340	155	0
1	B	1838	0	1875	69	0
2	A	33	0	0	6	0
2	B	29	0	0	2	0
All	All	6234	0	6215	210	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 17.

The worst 5 of 210 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:1302:VAL:O	1:B:1306:THR:HG22	1.50	1.12
1:A:61:ILE:HD11	1:A:266:ALA:HB1	1.46	0.96
1:B:1400:MET:HE2	1:B:1404:LEU:HG	1.67	0.76
1:A:1275:CYS:HB2	1:A:1276:PRO:HD3	1.68	0.76
1:A:152:ASN:HD21	1:A:155:GLU:HG2	1.53	0.74

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	549/574 (96%)	488 (89%)	53 (10%)	8 (2%)	10	26
1	B	228/574 (40%)	199 (87%)	22 (10%)	7 (3%)	4	9
All	All	777/1148 (68%)	687 (88%)	75 (10%)	15 (2%)	8	20

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1276	PRO
1	B	362	ALA
1	B	1281	PRO
1	A	1275	CYS
1	B	1277	LEU

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	459/472 (97%)	422 (92%)	37 (8%)	11	27
1	B	201/472 (43%)	178 (89%)	23 (11%)	5	13
All	All	660/944 (70%)	600 (91%)	60 (9%)	9	21

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1293	LEU
1	A	1393	LYS
1	B	1384	GLU
1	A	1332	GLU
1	A	1397	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1267	GLN
1	A	1350	GLN
1	B	1290	GLN
1	A	357	GLN
1	B	1341	HIS

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 [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	553/574 (96%)	0.09	23 (4%)	36 35	21, 59, 99, 161	0
1	B	232/574 (40%)	0.42	29 (12%)	3 3	21, 50, 112, 148	7 (3%)
All	All	785/1148 (68%)	0.19	52 (6%)	18 16	21, 57, 104, 161	7 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1281	PRO	12.0
1	A	180	ILE	8.3
1	B	360	ASP	6.8
1	A	1279	ALA	6.3
1	B	337	GLN	6.2

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 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.