



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:00 PM GMT

PDB ID : 1MZN
Title : CRYSTAL STRUCTURE at 1.9 ANGSTROEMS RESOLUTION OF THE HOMODIMER OF HUMAN RXR ALPHA LIGAND BINDING DOMAIN BOUND TO THE SYNTHETIC AGONIST COMPOUND BMS 649 AND A COACTIVATOR PEPTIDE
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Deposited on : 2002-10-09
Resolution : 1.90 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

<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
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

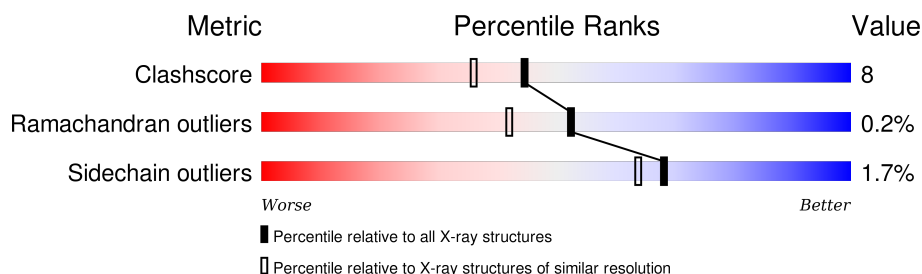
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)


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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	240	
1	C	240	
1	E	240	
1	G	240	
2	B	13	
2	D	13	
2	F	13	

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Mol	Chain	Length	Quality of chain
2	H	13	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment representing 69%, a yellow segment representing 15%, and a grey segment representing 15%. The percentages are labeled below each segment.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8177 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.

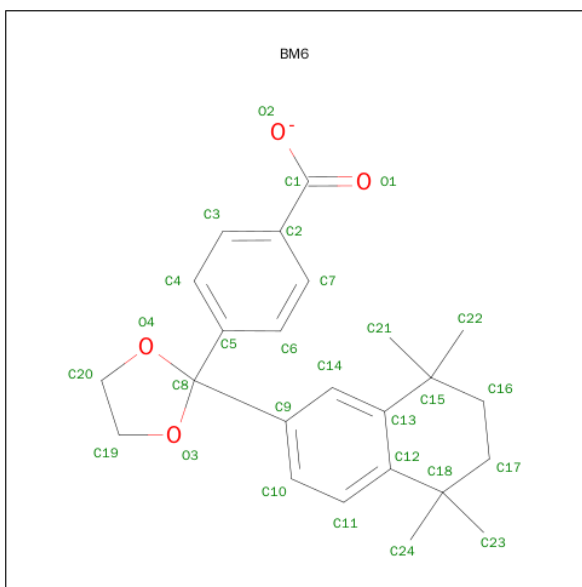
- Molecule 1 is a protein called RXR retinoid X receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1753	1126	299	318	10			
1	C	212	Total	C	N	O	S	0	0	0
			1672	1075	286	301	10			
1	E	224	Total	C	N	O	S	0	0	0
			1753	1126	299	318	10			
1	G	212	Total	C	N	O	S	0	0	0
			1672	1075	286	301	10			

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			98	63	21	14			
2	D	11	Total	C	N	O	0	0	0
			98	63	21	14			
2	F	11	Total	C	N	O	0	0	0
			98	63	21	14			
2	H	11	Total	C	N	O	0	0	0
			98	63	21	14			

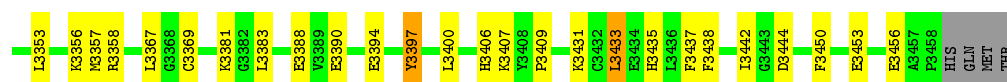
- Molecule 3 is 4-[2-(5,5,8,8-TETRAMETHYL-5,6,7,8-TETRAHYDRO-NAPHTHALEN-2-YL)-[1,3]DIOXOLAN-2-YL]-BENZOIC ACID (three-letter code: BM6) (formula: C₂₄H₂₇O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 24 4	0	0
3	C	1	Total C O 28 24 4	0	0
3	E	1	Total C O 28 24 4	0	0
3	G	1	Total C O 28 24 4	0	0

- Molecule 4 is water.

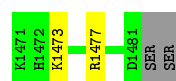
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0
4	B	5	Total O 5 5	0	0
4	C	180	Total O 180 180	0	0
4	E	226	Total O 226 226	0	0
4	F	10	Total O 10 10	0	0
4	G	178	Total O 178 178	0	0
4	H	2	Total O 2 2	0	0



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.12Å 64.69Å 94.78Å 109.97° 92.87° 89.99°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	1.0 (30.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8177	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BM6

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	0.33	0/1788	0.54	0/2421
1	C	0.30	0/1706	0.51	0/2308
1	E	0.33	0/1788	0.53	0/2421
1	G	0.30	0/1706	0.50	0/2308
2	B	0.31	0/99	0.48	0/130
2	D	0.28	0/99	0.42	0/130
2	F	0.29	0/99	0.48	0/130
2	H	0.28	0/99	0.42	0/130
All	All	0.31	0/7384	0.52	0/9978

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	3397	TYR	Sidechain

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	1753	0	1775	26	0
1	C	1672	0	1709	32	0
1	E	1753	0	1775	24	0
1	G	1672	0	1709	33	0
2	B	98	0	108	4	0
2	D	98	0	108	1	0
2	F	98	0	108	5	0
2	H	98	0	108	1	0
3	A	28	0	27	0	0
3	C	28	0	27	0	0
3	E	28	0	27	0	0
3	G	28	0	27	0	0
4	A	222	0	0	5	0
4	B	5	0	0	0	0
4	C	180	0	0	4	0
4	E	226	0	0	3	0
4	F	10	0	0	0	0
4	G	178	0	0	2	0
4	H	2	0	0	0	0
All	All	8177	0	7508	117	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 8.

The worst 5 of 117 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:C:1234:ARG:HH11	1:C:1234:ARG:HG3	1.15	1.05
1:E:2320:VAL:HG21	1:E:2331:HIS:CE1	2.09	0.87
1:G:3453:GLU:O	1:G:3456:GLU:HG2	1.80	0.81
2:F:2477:ARG:O	2:F:2481:ASP:CG	2.18	0.81
1:C:1234:ARG:NH1	1:C:1234:ARG:HG3	1.90	0.77

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	220/240 (92%)	215 (98%)	4 (2%)	1 (0%)	34	21
1	C	208/240 (87%)	206 (99%)	2 (1%)	0	100	100
1	E	220/240 (92%)	214 (97%)	5 (2%)	1 (0%)	34	21
1	G	208/240 (87%)	206 (99%)	2 (1%)	0	100	100
2	B	9/13 (69%)	9 (100%)	0	0	100	100
2	D	9/13 (69%)	6 (67%)	3 (33%)	0	100	100
2	F	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
2	H	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
All	All	892/1012 (88%)	870 (98%)	20 (2%)	2 (0%)	52	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ALA
1	E	2445	THR

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	188/207 (91%)	185 (98%)	3 (2%)	70	66
1	C	182/207 (88%)	178 (98%)	4 (2%)	60	53
1	E	188/207 (91%)	185 (98%)	3 (2%)	70	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	182/207 (88%)	179 (98%)	3 (2%)	70	66
2	B	11/13 (85%)	11 (100%)	0	100	100
2	D	11/13 (85%)	11 (100%)	0	100	100
2	F	11/13 (85%)	11 (100%)	0	100	100
2	H	11/13 (85%)	11 (100%)	0	100	100
All	All	784/880 (89%)	771 (98%)	13 (2%)	68	64

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1383	LEU
1	C	1450	PHE
1	G	3383	LEU
1	C	1294	LEU
1	E	2450	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2435	HIS
2	F	2472	HIS
1	G	3331	HIS
1	C	1435	HIS
1	G	3306	ASN

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

4 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$
3	BM6	A	200	-	28,31,31	1.06	1 (3%)	42,49,49	1.16	3 (7%)
3	BM6	C	1200	-	28,31,31	1.09	1 (3%)	42,49,49	1.43	5 (11%)
3	BM6	E	2200	-	28,31,31	0.96	0	42,49,49	1.13	3 (7%)
3	BM6	G	3200	-	28,31,31	1.02	1 (3%)	42,49,49	1.45	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BM6	A	200	-	-	0/12/44/44	0/4/4/4
3	BM6	C	1200	-	-	0/12/44/44	0/4/4/4
3	BM6	E	2200	-	-	0/12/44/44	0/4/4/4
3	BM6	G	3200	-	-	0/12/44/44	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	200	BM6	C13-C12	2.09	1.44	1.40
3	G	3200	BM6	C11-C12	2.20	1.42	1.39
3	C	1200	BM6	C11-C12	2.27	1.42	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1200	BM6	O4-C8-O3	-5.59	102.21	106.68
3	G	3200	BM6	O4-C8-O3	-4.80	102.84	106.68
3	A	200	BM6	O4-C8-O3	-2.65	104.56	106.68
3	E	2200	BM6	C6-C5-C8	-2.31	116.98	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	200	BM6	C6-C5-C8	-2.06	117.36	120.48

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](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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