



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 12:08 am GMT

PDB ID : 5AVL
Title : Crystal structure of LXRalpha in complex with tert-butyl benzoate analog, compound 32b
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Deposited on : 2015-06-17
Resolution : 2.80 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 : 1.7.2 (RC1), CSD as538be (2017)
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

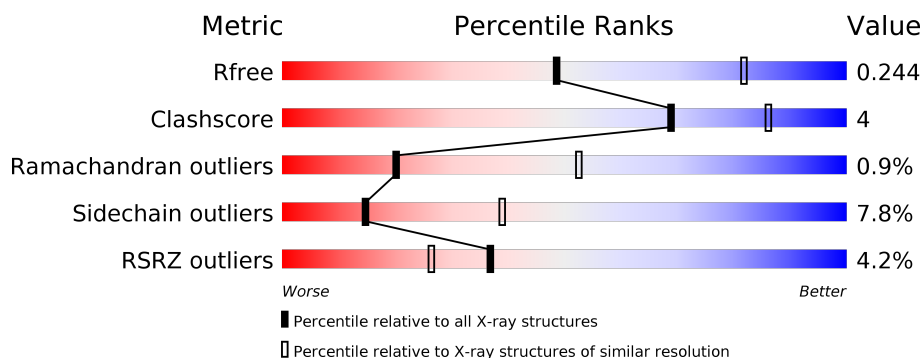
1 Overall quality at a glance

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	283	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>13%</div> <div>•</div> <div>21%</div> </div> </div>
2	B	25	<div> <div>56%</div> <div>•</div> <div>40%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2041 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 Oxysterols receptor LXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1828	1172	316	334	6			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	-	initiating methionine	UNP Q13133
A	166	LYS	-	expression tag	UNP Q13133
A	167	HIS	-	expression tag	UNP Q13133
A	168	GLN	-	expression tag	UNP Q13133
A	169	HIS	-	expression tag	UNP Q13133
A	170	GLN	-	expression tag	UNP Q13133
A	171	HIS	-	expression tag	UNP Q13133
A	172	GLN	-	expression tag	UNP Q13133
A	173	HIS	-	expression tag	UNP Q13133
A	174	GLN	-	expression tag	UNP Q13133
A	175	HIS	-	expression tag	UNP Q13133
A	176	GLN	-	expression tag	UNP Q13133
A	177	HIS	-	expression tag	UNP Q13133
A	178	GLN	-	expression tag	UNP Q13133
A	179	GLN	-	expression tag	UNP Q13133
A	180	PRO	-	expression tag	UNP Q13133
A	181	LEU	-	expression tag	UNP Q13133

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			131	82	27	22			

- Molecule 3 is 2-[4-[4-[[2-[(2-methylpropan-2-yl)oxycarbonyl]-3-oxidanyl-4-(trifluoromethyl)phenyl]methoxy]phenyl]phenyl]ethanoic acid (three-letter code: 4KQ) (formula:

4KQ

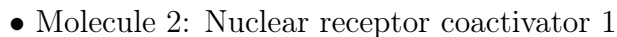
The ORTEP diagram illustrates the chemical structure of 4KQ, a complex molecule featuring a central benzene ring (C14-C19) substituted with a carboxylic acid group (C20-C27) and a trifluoromethyl group (C30-C33). The structure also includes a trifluoromethyl group (C30-C33) and a trifluoromethyl group (C30-C33). The molecule is shown in a perspective view, with atoms labeled with their respective element symbols and coordinates. The structure is a complex molecule with multiple rings and functional groups, including a carboxylic acid and a trifluoromethyl group.

- Molecule 4 is water.



i

- Molecule 1: Oxysterols receptor LXR-alpha



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.91Å 124.91Å 91.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 22.49 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.80) 98.8 (22.49-2.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.192 , 0.243 0.193 , 0.244	Depositor DCC
R_{free} test set	957 reflections (11.70%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2041	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 4KQ

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	0.67	0/1866	0.86	0/2523
2	B	0.60	0/132	0.88	0/175
All	All	0.67	0/1998	0.86	0/2698

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	1828	0	1831	15	0
2	B	131	0	139	1	0
3	A	36	0	24	2	0
4	A	38	0	0	1	0
4	B	8	0	0	1	0
All	All	2041	0	1994	17	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 4.

The worst 5 of 17 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:332:GLN:H	1:A:424:GLN:HE22	1.21	0.86
1:A:207:SER:H	1:A:210:GLN:HE21	1.28	0.82
1:A:323:ARG:HH22	1:A:344:ARG:HH22	1.42	0.67
1:A:326:PHE:HB3	1:A:336:ILE:HD12	1.82	0.61
3:A:501:4KQ:O9	3:A:501:4KQ:O36	2.24	0.54

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	218/283 (77%)	214 (98%)	2 (1%)	2 (1%)	20	52
2	B	13/25 (52%)	12 (92%)	1 (8%)	0	100	100
All	All	231/308 (75%)	226 (98%)	3 (1%)	2 (1%)	20	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	PRO
1	A	317	LYS

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/257 (79%)	185 (92%)	17 (8%)	13	35
2	B	15/24 (62%)	15 (100%)	0	100	100
All	All	217/281 (77%)	200 (92%)	17 (8%)	15	39

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	ARG
1	A	314	THR
1	A	402	LEU
1	A	304	ARG
1	A	438	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	HIS
2	B	695	GLN
1	A	424	GLN
1	A	222	GLN
1	A	431	GLN

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

1 ligand is 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	4KQ	A	501	-	35,38,38	1.10	5 (14%)	53,56,56	1.66	12 (22%)

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	4KQ	A	501	-	-	0/26/28/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	4KQ	C1-C31	-2.57	1.37	1.41
3	A	501	4KQ	C32-C31	-2.32	1.45	1.50
3	A	501	4KQ	O4-C5	-2.28	1.44	1.48
3	A	501	4KQ	C16-C19	-2.07	1.43	1.49
3	A	501	4KQ	O4-C3	2.34	1.39	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	4KQ	C11-C10-C29	-3.74	111.53	119.51
3	A	501	4KQ	C1-C2-C3	-2.76	112.90	117.33
3	A	501	4KQ	F33-C32-C31	-2.69	107.84	112.69
3	A	501	4KQ	C29-C30-C31	-2.33	117.84	121.87
3	A	501	4KQ	C15-C16-C19	-2.30	117.32	121.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	4KQ	2	0

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	224/283 (79%)	-0.42	10 (4%) 34 24	26, 41, 103, 134	0
2	B	15/25 (60%)	-0.63	0 100 100	34, 39, 61, 72	0
All	All	239/308 (77%)	-0.43	10 (4%) 37 26	26, 41, 103, 134	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	6.3
1	A	432	ASP	3.0
1	A	317	LYS	2.7
1	A	447	GLU	2.6
1	A	222	GLN	2.2

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	4KQ	A	501	36/36	0.94	0.18	0.68	34,43,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.