Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:30 PM GMT

PDB ID	:	1XKJ
Title	:	BACTERIAL LUCIFERASE BETA2 HOMODIMER
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Deposited on	:	1996-10-08
Resolution	:	2.50 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 (i) symbol.

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

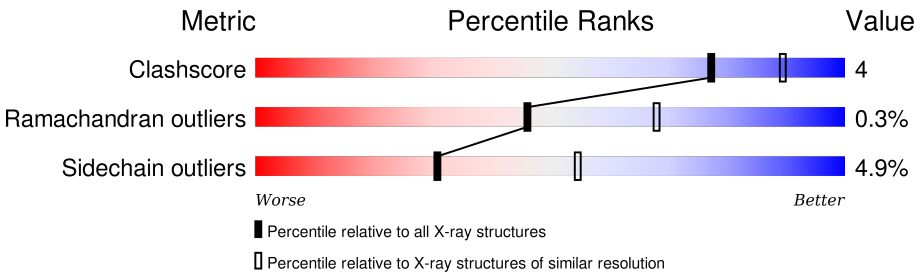
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 <=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	324	86% 13% •
1	B	324	87% 11% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5092 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 BETA2 LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2519	1591	429	484	15	0	0	0
1	B	324	2542	1600	434	493	15	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	14	14	14	0	0
2	B	17	17	17	0	0

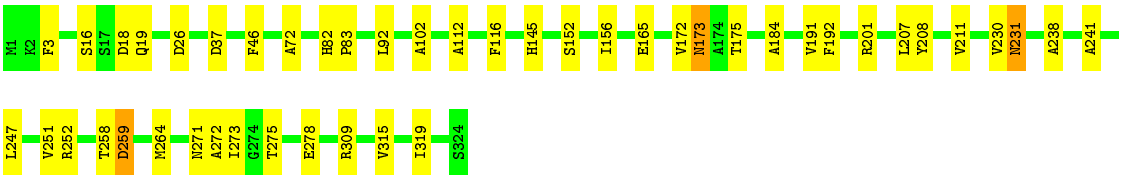
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

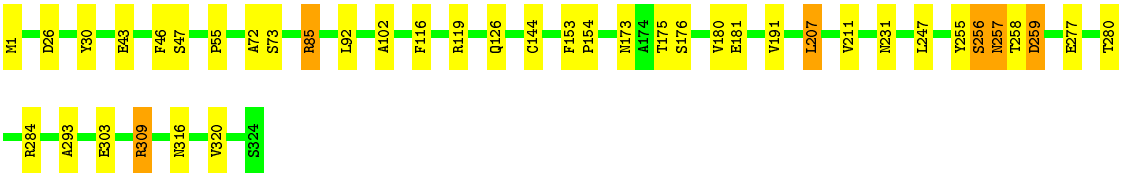
- Molecule 1: BETA2 LUCIFERASE

Chain A:



- Molecule 1: BETA2 LUCIFERASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.40Å 112.40Å 153.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (15.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.191 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5092	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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	0.62	0/2575	0.76	0/3488
1	B	0.64	1/2598 (0.0%)	0.77	3/3518 (0.1%)
All	All	0.63	1/5173 (0.0%)	0.77	3/7006 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	CYS	CB-SG	-5.05	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	258	THR	N-CA-C	-6.90	92.36	111.00
1	B	277	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	B	73	SER	N-CA-C	-5.08	97.30	111.00

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	2519	0	2371	20	0
1	B	2542	0	2401	17	0
2	A	14	0	0	0	0
2	B	17	0	0	0	0
All	All	5092	0	4772	36	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.

All (36) 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:16:SER:H	1:A:19:GLN:NE2	1.67	0.92
1:A:16:SER:H	1:A:19:GLN:HE21	1.36	0.70
1:A:72:ALA:HB2	1:A:102:ALA:HB3	1.80	0.64
1:A:192:PHE:HB3	1:A:201:ARG:HD3	1.85	0.57
1:B:257:ASN:C	1:B:259:ASP:H	2.07	0.57
1:B:207:LEU:O	1:B:211:VAL:HG23	2.09	0.53
1:A:156:ILE:HD13	1:B:116:PHE:CZ	2.45	0.51
1:B:173:ASN:HA	1:B:191:VAL:CG1	2.40	0.51
1:A:275:THR:OG1	1:A:278:GLU:HG3	2.11	0.51
1:B:1:MET:HG3	1:B:293:ALA:O	2.10	0.51
1:B:176:SER:O	1:B:180:VAL:HG23	2.13	0.49
1:A:315:VAL:O	1:A:319:ILE:HG13	2.12	0.48
1:A:251:VAL:HG21	1:A:264:MET:HE1	1.97	0.46
1:A:184:ALA:HA	1:A:208:TYR:CE2	2.51	0.46
1:A:230:VAL:HG22	1:A:272:ALA:HB3	1.98	0.46
1:B:153:PHE:HB2	1:B:154:PRO:HD2	1.98	0.45
1:B:30:TYR:CZ	1:B:309:ARG:HD3	2.52	0.44
1:B:255:TYR:O	1:B:256:SER:C	2.56	0.44
1:A:112:ALA:O	1:A:116:PHE:HB2	2.17	0.44
1:B:119:ARG:HD3	1:B:119:ARG:HA	1.78	0.44
1:A:3:PHE:O	1:A:37:ASP:HB3	2.18	0.43
1:B:181:GLU:HG3	1:B:211:VAL:HG11	2.01	0.43
1:A:271:ASN:O	1:A:273:ILE:N	2.48	0.43
1:A:207:LEU:HD12	1:A:211:VAL:HG23	2.01	0.43
1:B:43:GLU:HB2	1:B:55:PRO:HD3	2.00	0.43
1:B:72:ALA:HB2	1:B:102:ALA:HB3	2.00	0.43
1:B:173:ASN:HB3	1:B:175:THR:HG23	2.01	0.42
1:A:258:THR:O	1:A:259:ASP:CB	2.66	0.42
1:B:316:ASN:O	1:B:320:VAL:HG23	2.20	0.42
1:A:231:ASN:C	1:A:231:ASN:HD22	2.22	0.41
1:A:238:ALA:O	1:A:241:ALA:HB3	2.20	0.41
1:B:280:THR:HG22	1:B:284:ARG:NH1	2.36	0.41
1:B:85:ARG:HG3	1:B:85:ARG:HH11	1.85	0.41
1:A:173:ASN:HB3	1:A:175:THR:HG23	2.03	0.40
1:A:46:PHE:N	1:A:46:PHE:CD1	2.87	0.40
1:A:82:HIS:HA	1:A:83:PRO:HD3	1.97	0.40

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	322/324 (99%)	307 (95%)	14 (4%)	1 (0%)	46	68
1	B	322/324 (99%)	309 (96%)	12 (4%)	1 (0%)	46	68
All	All	644/648 (99%)	616 (96%)	26 (4%)	2 (0%)	46	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ASP
1	B	256	SER

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	263/274 (96%)	250 (95%)	13 (5%)	31	55
1	B	270/274 (98%)	257 (95%)	13 (5%)	31	55
All	All	533/548 (97%)	507 (95%)	26 (5%)	31	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	26	ASP
1	A	92	LEU
1	A	145	HIS

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Mol	Chain	Res	Type
1	A	152	SER
1	A	165	GLU
1	A	172	VAL
1	A	173	ASN
1	A	191	VAL
1	A	231	ASN
1	A	247	LEU
1	A	252	ARG
1	A	309	ARG
1	B	26	ASP
1	B	46	PHE
1	B	47	SER
1	B	85	ARG
1	B	92	LEU
1	B	126	GLN
1	B	207	LEU
1	B	231	ASN
1	B	247	LEU
1	B	257	ASN
1	B	259	ASP
1	B	303	GLU
1	B	309	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	19	GLN
1	A	231	ASN
1	A	232	GLN
1	B	9	ASN
1	B	231	ASN
1	B	232	GLN
1	B	257	ASN

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 (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.