Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 05:23 PM JST

PDB ID	:	6LRY
Title	:	Crystal structure of human endothelin ETB receptor in complex with sarafotoxin S6b
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Deposited on	:	2020-01-16
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

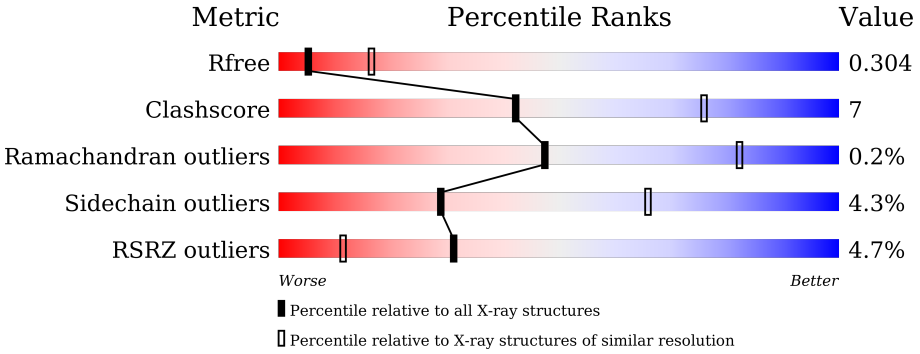
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of 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 <=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	504	5% 76% 15% • 7%
2	B	21	62% 33% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3881 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 Endothelin receptor type B,Endolysin,Endothelin receptor type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3705	2420	618	642	25	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P24530
A	64	GLY	-	expression tag	UNP P24530
A	65	GLY	-	expression tag	UNP P24530
A	124	TYR	ARG	engineered mutation	UNP P24530
A	154	ALA	ASP	engineered mutation	UNP P24530
A	270	ALA	LYS	engineered mutation	UNP P24530
A	1052	THR	CYS	engineered mutation	UNP A0A097J809
A	1095	ALA	CYS	engineered mutation	UNP A0A097J809
A	342	ALA	SER	engineered mutation	UNP P24530
A	381	ALA	ILE	engineered mutation	UNP P24530
A	396	ALA	CYS	engineered mutation	UNP P24530
A	400	ALA	CYS	engineered mutation	UNP P24530
A	405	ALA	CYS	engineered mutation	UNP P24530
A	408	GLU	-	expression tag	UNP P24530
A	409	ASN	-	expression tag	UNP P24530
A	410	LEU	-	expression tag	UNP P24530
A	411	TYR	-	expression tag	UNP P24530
A	412	PHE	-	expression tag	UNP P24530
A	413	GLN	-	expression tag	UNP P24530

- Molecule 2 is a protein called Sarafotoxin-B.

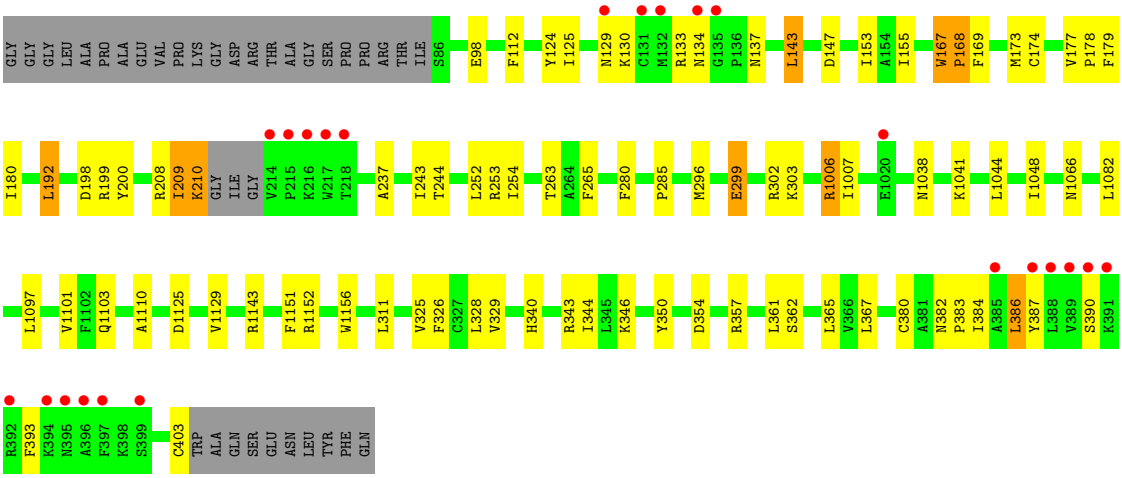
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	21	176	110	27	34	5	0	0	0

3 Residue-property plots (i)

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

• Molecule 1: Endothelin receptor type B,Endolysin,Endothelin receptor type B

Chain A: 5% 76% 15% • 7%



• Molecule 2: Sarafotoxin-B

Chain B: 62% 33% 5%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.12Å 82.28Å 166.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 3.00 49.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.30-3.00) 99.9 (49.30-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.270 , 0.304 0.270 , 0.304	Depositor DCC
R_{free} test set	846 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 70.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3881	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/3787	0.40	0/5145
2	B	0.23	0/180	0.42	0/240
All	All	0.25	0/3967	0.40	0/5385

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 (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	3705	0	3816	51	0
2	B	176	0	157	7	0
All	All	3881	0	3973	54	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 7.

All (54) 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:168:PRO:HA	1:A:253:ARG:HH12	1.47	0.77
1:A:179:PHE:HB2	1:A:237:ALA:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HA	1:A:133:ARG:HD3	1.74	0.70
1:A:354:ASP:O	1:A:357:ARG:NH1	2.29	0.64
1:A:112:PHE:HB2	1:A:155:ILE:HG21	1.83	0.61
1:A:343:ARG:HE	2:B:21:TRP:HD1	1.48	0.61
1:A:263:THR:HG22	1:A:265:PHE:H	1.70	0.56
1:A:1038:ASN:HA	1:A:1041:LYS:HD2	1.88	0.55
2:B:4:LYS:NZ	2:B:5:ASP:OD2	2.40	0.55
1:A:124:TYR:OH	1:A:403:CYS:SG	2.66	0.53
1:A:387:TYR:HD1	1:A:393:PHE:HB3	1.73	0.53
1:A:153:ILE:HD12	1:A:180:ILE:HB	1.91	0.52
1:A:209:ILE:HG13	1:A:210:LYS:HD2	1.92	0.52
1:A:244:THR:HA	1:A:252:LEU:O	2.08	0.51
1:A:200:TYR:HD1	1:A:296:MET:HB2	1.75	0.51
1:A:1156:TRP:HB3	1:A:311:LEU:HD23	1.92	0.51
1:A:387:TYR:HA	1:A:393:PHE:HB3	1.94	0.50
2:B:18:ASP:OD1	2:B:19:VAL:N	2.44	0.50
1:A:280:PHE:O	1:A:285:PRO:HD3	2.12	0.49
1:A:137:ASN:HD22	1:A:137:ASN:H	1.59	0.49
1:A:143:LEU:HG	1:A:192:LEU:HD23	1.95	0.49
1:A:254:ILE:HG12	2:B:16:HIS:HB2	1.93	0.49
1:A:167:TRP:CE3	1:A:169:PHE:HD2	2.30	0.49
1:A:340:HIS:O	1:A:344:ILE:HG12	2.12	0.49
1:A:167:TRP:HZ2	1:A:174:CYS:HB2	1.78	0.48
1:A:299:GLU:OE1	1:A:302:ARG:NH2	2.31	0.48
1:A:1006:ARG:HH21	1:A:1006:ARG:HB3	1.79	0.47
1:A:147:ASP:CG	1:A:382:ASN:HD22	2.17	0.47
1:A:326:PHE:O	1:A:329:VAL:HG22	2.16	0.46
1:A:1006:ARG:NH2	1:A:1007:ILE:HG13	2.31	0.46
1:A:386:LEU:O	1:A:390:SER:OG	2.29	0.46
1:A:350:TYR:CE2	1:A:361:LEU:HD21	2.51	0.46
1:A:325:VAL:O	1:A:329:VAL:HG13	2.15	0.46
1:A:177:VAL:HB	1:A:178:PRO:HD3	1.99	0.45
2:B:14:PHE:O	2:B:18:ASP:N	2.50	0.45
1:A:362:SER:HA	1:A:365:LEU:HD12	2.00	0.44
1:A:169:PHE:HB3	1:A:173:MET:HG3	1.99	0.44
1:A:302:ARG:HE	1:A:1066:ASN:HD21	1.65	0.44
1:A:134:ASN:H	1:A:134:ASN:ND2	2.15	0.44
1:A:125:ILE:O	1:A:129:ASN:HB2	2.18	0.43
1:A:1044:LEU:O	1:A:1048:ILE:HG12	2.19	0.43
1:A:1097:LEU:O	1:A:1101:VAL:HG23	2.19	0.43
1:A:382:ASN:HB2	1:A:383:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:GLN:HB2	1:A:1143:ARG:CZ	2.50	0.42
1:A:167:TRP:O	1:A:253:ARG:NH1	2.53	0.42
1:A:299:GLU:O	1:A:303:LYS:HG2	2.20	0.42
1:A:1082:LEU:HD21	1:A:1110:ALA:HA	2.02	0.42
1:A:384:ILE:HA	1:A:387:TYR:CD2	2.54	0.42
1:A:346:LYS:NZ	2:B:1:CYS:HB2	2.34	0.42
1:A:354:ASP:HB3	1:A:357:ARG:HB3	2.01	0.41
1:A:343:ARG:NH1	2:B:1:CYS:HB3	2.36	0.41
1:A:199:ARG:HA	1:A:199:ARG:HD3	1.71	0.40
1:A:167:TRP:HA	1:A:168:PRO:HD3	1.91	0.40
1:A:1125:ASP:O	1:A:1129:VAL:HG13	2.22	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	464/504 (92%)	448 (97%)	15 (3%)	1 (0%)	47 82
2	B	19/21 (90%)	17 (90%)	2 (10%)	0	100 100
All	All	483/525 (92%)	465 (96%)	17 (4%)	1 (0%)	47 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	PRO

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	401/431 (93%)	384 (96%)	17 (4%)	30	66
2	B	21/21 (100%)	20 (95%)	1 (5%)	25	62
All	All	422/452 (93%)	404 (96%)	18 (4%)	29	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	143	LEU
1	A	167	TRP
1	A	192	LEU
1	A	198	ASP
1	A	208	ARG
1	A	209	ILE
1	A	210	LYS
1	A	243	ILE
1	A	299	GLU
1	A	1006	ARG
1	A	1151	PHE
1	A	1152	ARG
1	A	328	LEU
1	A	367	LEU
1	A	380	CYS
1	A	386	LEU
2	B	1	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	137	ASN
1	A	1120	GLN
1	A	1130	ASN
1	A	373	ASN
1	A	378	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 monosaccharides 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	468/504 (92%)	0.18	23 (4%) 29 11	56, 95, 157, 187	0
2	B	21/21 (100%)	0.07	0 100 100	80, 91, 105, 108	0
All	All	489/525 (93%)	0.18	23 (4%) 31 11	56, 94, 157, 187	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	PRO	7.1
1	A	214	VAL	5.2
1	A	131	CYS	5.2
1	A	397	PHE	5.1
1	A	388	LEU	4.8
1	A	394	LYS	4.1
1	A	132	MET	3.7
1	A	134	ASN	3.7
1	A	391	LYS	3.6
1	A	387	TYR	3.4
1	A	217	TRP	3.4
1	A	395	ASN	3.2
1	A	135	GLY	3.2
1	A	396	ALA	2.9
1	A	216	LYS	2.8
1	A	385	ALA	2.7
1	A	389	VAL	2.6
1	A	129	ASN	2.6
1	A	399	SER	2.6
1	A	1020	GLU	2.4
1	A	218	THR	2.2
1	A	390	SER	2.2
1	A	392	ARG	2.1

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 monosaccharides 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.