



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:24 AM GMT

PDB ID : 2QLU
Title : Crystal structure of Activin receptor type II kinase domain from human
Authors : Han, S.
Deposited on : 2007-07-13
Resolution : 2.00 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

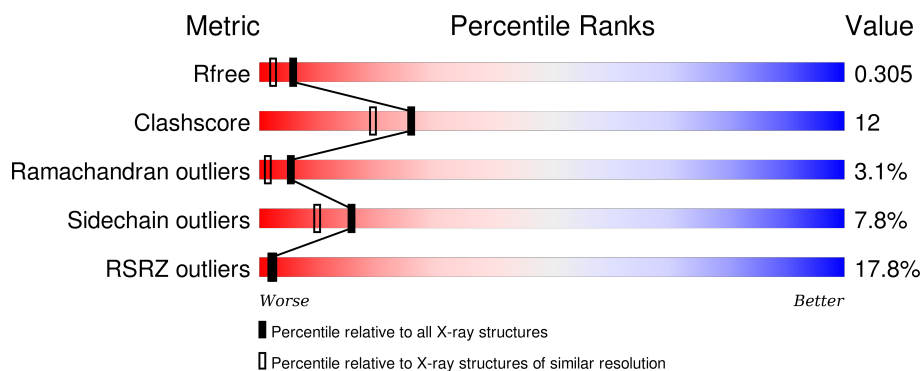
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 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	314	<div> <div>17%</div> <div>67%</div> <div>21%</div> <div>6% • 5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2539 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 Activin receptor type IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2378	1512	419	432	15			

There are 16 discrepancies between the modelled and reference sequences:

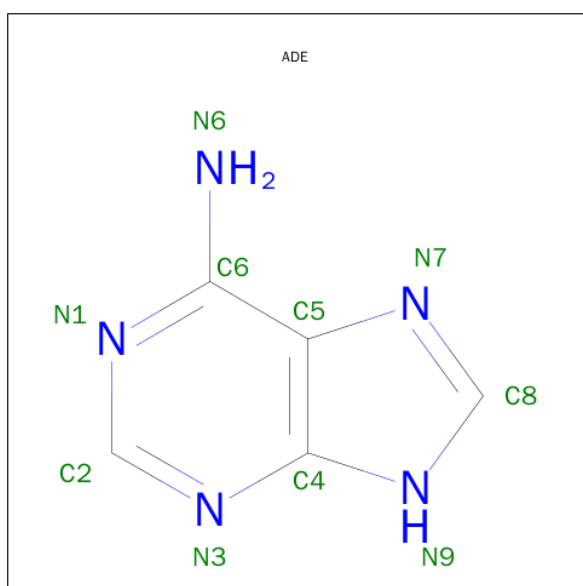
Chain	Residue	Modelled	Actual	Comment	Reference
A	174	MET	-	INITIATING METHIONINE	UNP Q13705
A	175	HIS	-	EXPRESSION TAG	UNP Q13705
A	176	HIS	-	EXPRESSION TAG	UNP Q13705
A	177	HIS	-	EXPRESSION TAG	UNP Q13705
A	178	HIS	-	EXPRESSION TAG	UNP Q13705
A	179	HIS	-	EXPRESSION TAG	UNP Q13705
A	180	HIS	-	EXPRESSION TAG	UNP Q13705
A	181	SER	-	EXPRESSION TAG	UNP Q13705
A	182	SER	-	EXPRESSION TAG	UNP Q13705
A	183	GLY	-	EXPRESSION TAG	UNP Q13705
A	184	LEU	-	EXPRESSION TAG	UNP Q13705
A	185	VAL	-	EXPRESSION TAG	UNP Q13705
A	186	PRO	-	EXPRESSION TAG	UNP Q13705
A	187	ARG	-	EXPRESSION TAG	UNP Q13705
A	188	GLY	-	EXPRESSION TAG	UNP Q13705
A	189	SER	-	EXPRESSION TAG	UNP Q13705

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	5	5		

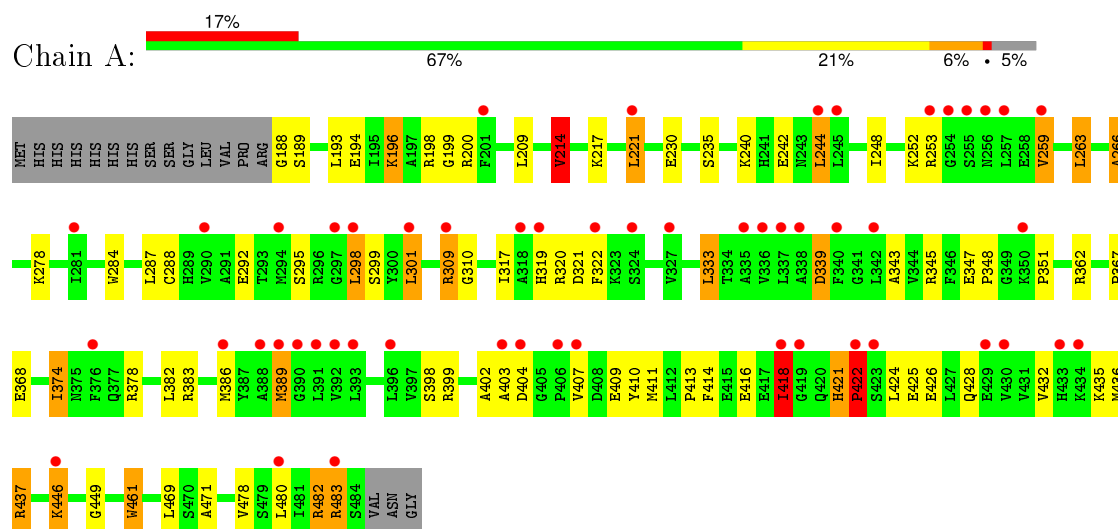
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	A	140	Total 140	O 140	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 ($\text{RSRZ} > 2$). 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: Activin receptor type IIB



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.22Å 98.22Å 71.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.00) 99.4 (29.76-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.283 0.251 , 0.305	Depositor DCC
R_{free} test set	1226 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24012 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2539	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADE, SO4

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	1.30	10/2435 (0.4%)	1.21	16/3291 (0.5%)

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	A	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	GLU	CB-CG	-8.13	1.36	1.52
1	A	244	LEU	CG-CD2	6.41	1.75	1.51
1	A	278	LYS	CD-CE	6.18	1.66	1.51
1	A	389	MET	CG-SD	-5.87	1.65	1.81
1	A	244	LEU	C-O	5.57	1.33	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	A	368	GLU	CB-CA-C	-7.16	96.08	110.40
1	A	214	VAL	CG1-CB-CG2	7.14	122.32	110.90
1	A	437	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	189	SER	N-CA-CB	6.73	120.60	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	PRO	Peptide

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	2378	0	2353	59	1
2	A	10	0	0	0	0
3	A	10	0	4	1	0
4	A	141	0	0	16	0
All	All	2539	0	2357	59	1

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 12.

The worst 5 of 59 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:244:LEU:CD2	1:A:244:LEU:CG	1.75	1.57
1:A:422:PRO:HB3	1:A:426:GLU:OE1	1.60	1.00
1:A:421:HIS:O	1:A:422:PRO:O	1.82	0.98
1:A:244:LEU:CD2	1:A:244:LEU:CD1	2.47	0.92
1:A:399:ARG:HD2	1:A:410:TYR:HB2	1.56	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:OE1	1:A:409:GLU:OE1[7_556]	2.11	0.09

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	295/314 (94%)	268 (91%)	18 (6%)	9 (3%)	5 1

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	ALA
1	A	422	PRO
1	A	253	ARG
1	A	259	VAL
1	A	418	ILE

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	255/270 (94%)	235 (92%)	20 (8%)	16 10

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	ASP
1	A	374	ILE
1	A	446	LYS
1	A	309	ARG
1	A	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	GLN

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](#)

3 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	$\# Z > 2$
2	SO4	A	1	-	4,4,4	1.52	1 (25%)	6,6,6	1.00	1 (16%)
2	SO4	A	2	-	4,4,4	0.10	0	6,6,6	0.82	0
3	ADE	A	488	-	8,11,11	2.42	4 (50%)	4,15,15	2.03	2 (50%)

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
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0
3	ADE	A	488	-	-	0/0/0/0	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	488	ADE	C4-N3	-3.05	1.32	1.37
2	A	1	SO4	O2-S	-2.68	1.38	1.47
3	A	488	ADE	C5-C4	-2.63	1.34	1.40
3	A	488	ADE	C2-N3	2.18	1.36	1.32
3	A	488	ADE	C4-N9	4.87	1.44	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	488	ADE	N3-C2-N1	-3.13	126.50	128.89
3	A	488	ADE	C2-N1-C6	-2.03	115.14	118.77
2	A	1	SO4	O4-S-O3	-2.01	100.82	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	488	ADE	1	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	297/314 (94%)	1.07	53 (17%) 2 2	9, 20, 39, 49	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ALA	8.5
1	A	255	SER	6.9
1	A	254	GLY	5.7
1	A	256	ASN	5.2
1	A	404	ASP	4.7

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(Å ²)	Q<0.9
3	ADE	A	488	10/10	0.94	0.11	-1.35	10,13,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1	5/5	0.99	0.07	-3.82	2,9,14,14	0
2	SO4	A	2	5/5	0.96	0.10	-	55,56,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.