



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 03:28 PM GMT

PDB ID : 2XAE
Title : CRYSTAL STRUCTURE OF HUMAN KINESIN EG5 IN COMPLEX WITH
(R)-2-AMINO-3-((S)-2-METHYL-1,1-DIPHENYLBUTYLTHIO)PROPANO
ICACID
Authors : Kaan, H.Y.K.; Weiss, J.; Menger, D.; Ulaganathan, V.; Tkocz, K.; Laggner,
C.; Popowycz, F.; Joseph, B.; Kozielski, F.
Deposited on : 2010-03-31
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

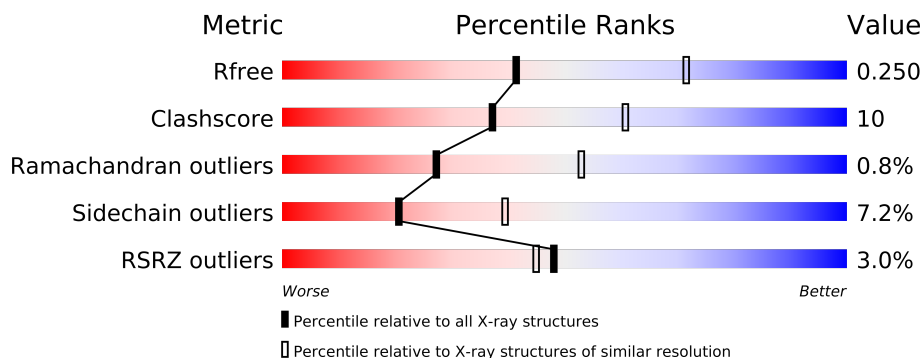
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	
1	C	368	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	2XA	A	1365	-	X

2 Entry composition i

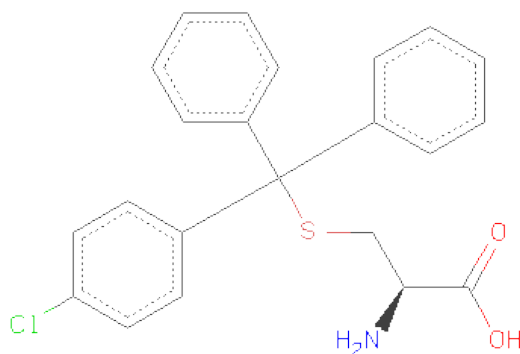
There are 7 unique types of molecules in this entry. The entry contains 8313 atoms, of which 0 are hydrogen and 0 are deuterium.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	6	0
			2584	1626	452	494	12			
1	B	328	Total	C	N	O	S	0	7	0
			2604	1639	453	501	11			
1	C	329	Total	C	N	O	S	0	2	0
			2578	1618	444	506	10			

- Molecule 2 is (2R)-2-AMINO-3-[(4-CHLOROPHENYL)-DIPHENYL-METHYL]SULFANY L-PROPANOICACID (three-letter code: 2XA) (formula: C₂₂H₂₀ClNO₂S).

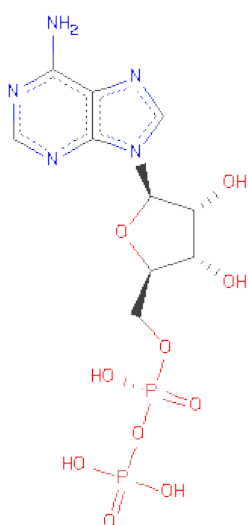


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O S	0	0
			27	22	1	1	2 1		
2	B	1	Total	C	Cl	N	O S	0	0
			27	22	1	1	2 1		
2	C	1	Total	C	Cl	N	O S	0	0
			27	22	1	1	2 1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

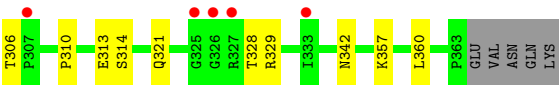
- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	129	Total	O	0	0
			129	129		
7	B	156	Total	O	0	0
			156	156		
7	C	81	Total	O	0	0
			81	81		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.77Å 96.77Å 124.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.23 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.60) 100.0 (29.23-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.257 0.178 , 0.250	Depositor DCC
R_{free} test set	2013 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.5	EDS
Estimated twinning fraction	0.009 for -h,-k,l 0.034 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40185 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8313	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2XA, MG, SO4, ADP, CL

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	1/2640 (0.0%)	0.90	2/3569 (0.1%)
1	B	0.66	0/2665	0.91	6/3603 (0.2%)
1	C	0.59	0/2620	0.84	0/3546
All	All	0.64	1/7925 (0.0%)	0.88	8/10718 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	GLU	CG-CD	6.00	1.60	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	293	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	50	VAL	CB-CA-C	-5.43	101.07	111.40
1	B	177	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	327	ARG	NE-CZ-NH1	5.21	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2584	0	2618	49	0
1	B	2604	0	2635	35	0
1	C	2578	0	2585	69	0
2	A	27	0	19	3	0
2	B	27	0	19	3	0
2	C	27	0	19	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	2	0
4	C	27	0	12	1	0
5	A	1	0	0	1	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
7	A	129	0	0	10	0
7	B	156	0	0	5	0
7	C	81	0	0	5	0
All	All	8313	0	7931	160	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 160 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:ARG:HD2	7:A:2029:HOH:O	1.74	0.86
5:A:1368:CL:CL	7:A:2128:HOH:O	2.34	0.81
1:B:327:ARG:O	1:B:363:PRO:HA	1.83	0.79
1:C:141:HIS:HD2	1:C:142:GLN:HE21	1.31	0.76
1:A:30:LEU:HD13	1:A:31:ALA:N	2.01	0.75

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	328/368 (89%)	316 (96%)	10 (3%)	2 (1%)	33	63
1	B	329/368 (89%)	321 (98%)	7 (2%)	1 (0%)	50	77
1	C	327/368 (89%)	308 (94%)	14 (4%)	5 (2%)	15	30
All	All	984/1104 (89%)	945 (96%)	31 (3%)	8 (1%)	27	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	LYS
1	A	150	ASN
1	A	207	LYS
1	C	123	GLU
1	C	321	GLN

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	289/322 (90%)	272 (94%)	17 (6%)	28	52
1	B	294/322 (91%)	267 (91%)	27 (9%)	13	24
1	C	288/322 (89%)	268 (93%)	20 (7%)	22	42
All	All	871/966 (90%)	807 (93%)	64 (7%)	21	38

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	191	LYS
1	B	304	GLU
1	C	297	ARG
1	B	197	LYS
1	B	240	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	ASN
1	B	262	ASN
1	C	141	HIS
1	B	38	HIS
1	C	183	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	2XA	A	1365	-	29,29,29	1.02	1 (3%)	40,40,40	1.16	2 (5%)
4	ADP	A	1367	3	29,29,29	1.16	1 (3%)	45,45,45	2.15	11 (24%)
2	2XA	B	1365	-	29,29,29	1.30	2 (6%)	40,40,40	1.24	4 (10%)
4	ADP	B	1367	3	29,29,29	1.14	2 (6%)	45,45,45	1.97	8 (17%)
6	SO4	B	1368	-	4,4,4	0.17	0	6,6,6	0.13	0
6	SO4	B	1369	-	4,4,4	0.15	0	6,6,6	0.14	0
2	2XA	C	1364	-	29,29,29	0.87	1 (3%)	40,40,40	1.05	1 (2%)
4	ADP	C	1366	3	29,29,29	1.17	2 (6%)	45,45,45	2.05	11 (24%)
6	SO4	C	1367	-	4,4,4	0.18	0	6,6,6	0.23	0

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	2XA	A	1365	-	-	0/28/28/28	0/3/3/3
4	ADP	A	1367	3	-	0/16/32/32	0/1/3/3
2	2XA	B	1365	-	-	0/28/28/28	0/3/3/3
4	ADP	B	1367	3	-	0/16/32/32	0/1/3/3
6	SO4	B	1368	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1369	-	-	0/0/0/0	0/0/0/0
2	2XA	C	1364	-	-	0/28/28/28	0/3/3/3
4	ADP	C	1366	3	-	0/16/32/32	0/1/3/3
6	SO4	C	1367	-	-	0/0/0/0	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1365	2XA	CB-SG	5.14	1.88	1.81
2	A	1365	2XA	CB-SG	4.47	1.87	1.81
4	C	1366	ADP	C5-C4	3.84	1.49	1.40
4	A	1367	ADP	C5-C4	3.74	1.48	1.40
2	C	1364	2XA	CB-SG	3.47	1.86	1.81

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1366	ADP	N3-C2-N1	-7.62	122.33	128.71
4	A	1367	ADP	N3-C2-N1	-7.30	122.60	128.71
4	B	1367	ADP	N3-C4-N9	6.50	137.17	125.43
4	A	1367	ADP	N3-C4-N9	5.58	135.51	125.43
4	B	1367	ADP	N3-C2-N1	-5.35	124.24	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	328/368 (89%)	-0.32	6 (1%) 65 64	16, 35, 63, 74	0
1	B	328/368 (89%)	-0.26	8 (2%) 56 53	16, 33, 63, 78	0
1	C	329/368 (89%)	-0.04	16 (4%) 28 25	27, 47, 69, 82	0
All	All	985/1104 (89%)	-0.21	30 (3%) 48 45	16, 38, 66, 82	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	LEU	4.8
1	C	325	GLY	3.7
1	B	149	ASP	3.7
1	A	247	GLU	3.2
1	C	271	ASN	3.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	2XA	A	1365	27/27	0.24	2.08	47,58,76,76	0
2	2XA	C	1364	27/27	0.28	1.19	66,70,84,84	0
2	2XA	B	1365	27/27	0.20	0.85	25,42,61,61	0
6	SO4	B	1368	5/5	0.22	0.70	87,88,88,89	0
4	ADP	A	1367	27/27	0.15	0.22	21,47,55,56	0
6	SO4	C	1367	5/5	0.22	0.21	87,87,87,88	0
4	ADP	C	1366	27/27	0.17	-0.11	32,69,73,73	0
3	MG	A	1366	1/1	0.11	-0.41	40,40,40,40	0
6	SO4	B	1369	5/5	0.11	-0.53	91,91,92,92	0
4	ADP	B	1367	27/27	0.11	-0.70	17,37,47,52	0
3	MG	B	1366	1/1	0.11	-1.17	23,23,23,23	0
3	MG	C	1365	1/1	0.10	-2.24	79,79,79,79	0
5	CL	A	1368	1/1	0.10	-6.30	62,62,62,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.