Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:33 AM GMT

PDB ID : 3KRJ
Title : cFMS tyrosine kinase in complex with 4-Cyano-1H-imidazole-2-carboxylicacid (2-cyclohex-1-enyl-4-piperidin-4-yl-phenyl)-amide
Authors : Schubert, C.
Deposited on : 2009-11-18
Resolution : 2.10 Å(reported)

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 (i)

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		12
Ramachandran outliers		1.3%
Sidechain outliers		6.7%
RSRZ outliers		4.9%

Worse Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
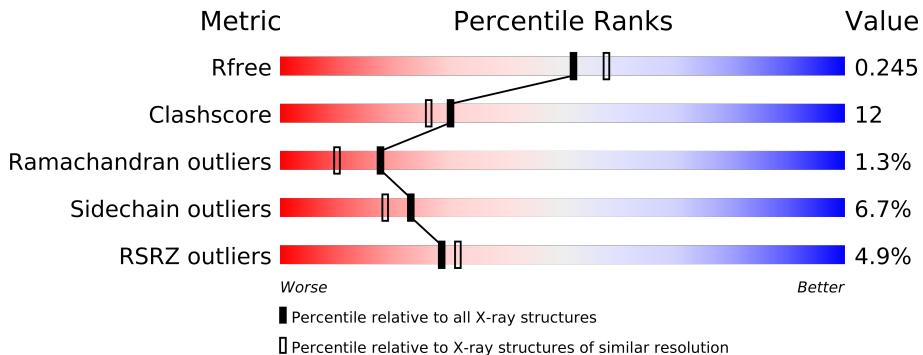
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	335	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4994 atoms, of which 2415 are hydrogens 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 Macrophage colony-stimulating factor 1 receptor, Basic fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total 4795	C 1550	H 2390	N 409	O 431	S 15	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLY	-	EXPRESSION TAG	UNP P07333
A	536	VAL	-	EXPRESSION TAG	UNP P07333
A	537	ASP	-	EXPRESSION TAG	UNP P07333
A	686	SER	CYS	ENGINEERED	UNP P11362

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
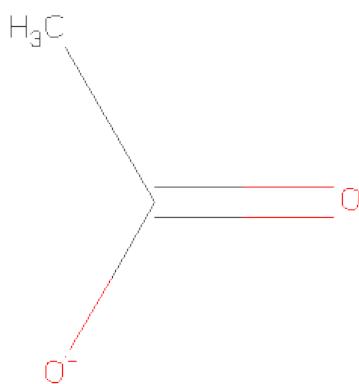
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0

- Molecule 3 is 4-CYANO-N-(2-CYCLOHEX-1-EN-1-YL-4-PIPERIDIN-4-YLPHENYL)-1H-I MIDAZOLE-2-CARBOXAMIDE (three-letter code: KRJ) (formula: $C_{22}H_{25}N_5O$).
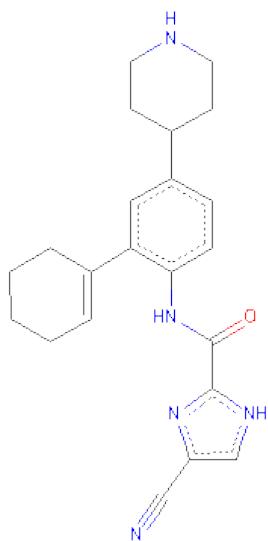
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			53	22	25	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		

3 Residue-property plots ⓘ

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.

• Molecule 1: Macrophage colony-stimulating factor 1 receptor, Basic fibroblast growth factor receptor 1

Chain A:
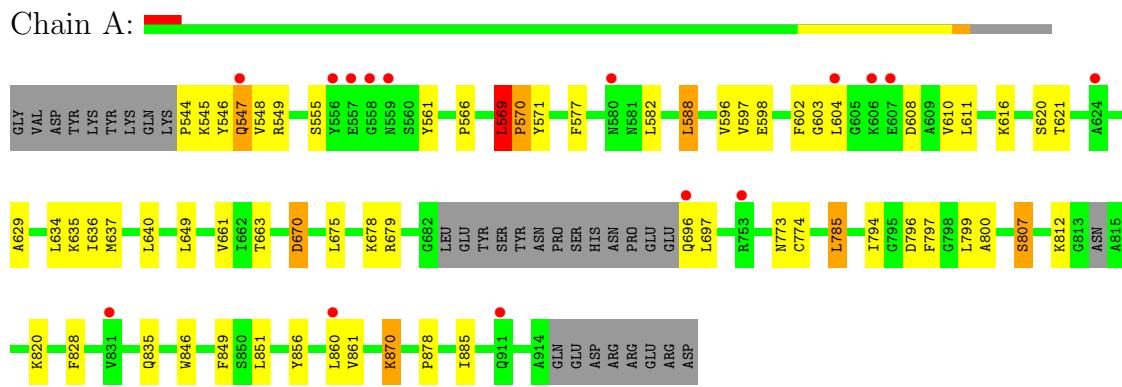
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	82.88Å 82.88Å 144.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.40 – 2.10 16.42 – 2.09	Depositor EDS
% Data completeness (in resolution range)	93.3 (16.40-2.10) 93.4 (16.42-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.09Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.260 0.192 , 0.245	Depositor DCC
R_{free} test set	1924 reflections (9.43%)	DCC
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.52 , 62.7	EDS
Estimated twinning fraction	0.040 for h,-h-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.31$	Xtriage
Outliers	0 of 21108 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4994	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: KRJ, ACT

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	0.23	0/2467	0.46	1/3340 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	544	PRO	N-CA-CB	5.87	110.34	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2   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 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	2405	2390	0	57	0
2	A	4	0	3	0	0
3	A	28	25	0	4	0
4	A	142	0	0	0	0
All	All	2579	2415	3	58	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 12.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:546:TYR:HA	1:A:547:GLN:CB	1.93	0.99
1:A:546:TYR:HA	1:A:547:GLN:HB2	1.52	0.92
1:A:570:PRO:CB	1:A:571:TYR:HA	2.11	0.80
1:A:546:TYR:HA	1:A:547:GLN:HB3	1.76	0.66
1:A:785:LEU:HD13	1:A:797:PHE:CE1	2.31	0.66
1:A:570:PRO:HB3	1:A:571:TYR:HA	1.80	0.62
1:A:546:TYR:CA	1:A:547:GLN:CB	2.76	0.61
1:A:569:LEU:N	1:A:569:LEU:HD13	2.16	0.60
1:A:570:PRO:CB	1:A:571:TYR:CA	2.80	0.59
1:A:569:LEU:HB2	1:A:570:PRO:CD	2.33	0.58
1:A:570:PRO:HB2	1:A:571:TYR:HA	1.87	0.57
1:A:678:LYS:HB2	1:A:697:LEU:HD12	1.87	0.56
1:A:602:PHE:HA	1:A:610:VAL:HG12	1.89	0.54
1:A:820:LYS:NZ	1:A:861:VAL:HG21	2.22	0.54
1:A:596:VAL:CG1	1:A:800:ALA:HB3	2.39	0.53
1:A:569:LEU:HD21	1:A:570:PRO:HD3	1.91	0.52
1:A:566:PRO:O	1:A:570:PRO:HD2	2.10	0.51
1:A:569:LEU:O	1:A:570:PRO:O	2.28	0.51
1:A:570:PRO:HB2	1:A:635:LYS:HG2	1.92	0.51
1:A:820:LYS:HZ3	1:A:861:VAL:HG21	1.75	0.51
1:A:640:LEU:HD22	1:A:774:CYS:HG	1.76	0.50
1:A:637:MET:HE2	1:A:649:LEU:HB2	1.94	0.49
1:A:621:THR:CG2	1:A:621:THR:O	2.59	0.49
1:A:577:PHE:CE1	1:A:604:LEU:HD12	2.48	0.49
1:A:566:PRO:HA	1:A:569:LEU:HD23	1.95	0.49
1:A:548:VAL:HG13	1:A:629:ALA:HB2	1.94	0.48
1:A:846:TRP:CD1	1:A:878:PRO:HG3	2.49	0.48
1:A:545:LYS:O	1:A:547:GLN:HB2	2.15	0.47
1:A:636:ILE:O	1:A:640:LEU:HD13	2.15	0.47
1:A:555:SER:HB3	1:A:773:ASN:ND2	2.29	0.46
1:A:549:ARG:HG3	1:A:796:ASP:OD2	2.15	0.46
1:A:820:LYS:HE3	1:A:856:TYR:HB2	1.97	0.46
1:A:548:VAL:HG21	1:A:548:VAL:O	2.15	0.46
1:A:596:VAL:HG11	1:A:800:ALA:HB3	1.97	0.46
1:A:588:LEU:HD11	1:A:598:GLU:HB2	1.98	0.45
1:A:828:PHE:CE2	1:A:870:LYS:HD3	2.52	0.45
1:A:663:THR:HG1	3:A:923:KRJ:H04	1.82	0.45
3:A:923:KRJ:H12	3:A:923:KRJ:O09	2.17	0.45
1:A:849:PHE:CE2	1:A:885:ILE:HG21	2.51	0.45
1:A:577:PHE:CD1	1:A:604:LEU:HD12	2.52	0.45
1:A:679:ARG:HA	1:A:851:LEU:HD13	2.00	0.44
1:A:555:SER:OG	1:A:561:TYR:HA	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:597:VAL:HG12	1:A:598:GLU:O	2.18	0.44
1:A:588:LEU:HB2	1:A:596:VAL:HG13	1.99	0.43
1:A:577:PHE:CE1	1:A:604:LEU:HA	2.54	0.42
1:A:569:LEU:CB	1:A:570:PRO:CD	2.97	0.42
1:A:569:LEU:HB2	1:A:570:PRO:HD3	2.01	0.42
1:A:588:LEU:HB3	3:A:923:KRJ:H18	2.01	0.42
1:A:670:ASP:HB3	3:A:923:KRJ:H21	2.00	0.42
1:A:678:LYS:HB2	1:A:697:LEU:CD1	2.50	0.42
1:A:546:TYR:CA	1:A:547:GLN:HB2	2.36	0.41
1:A:547:GLN:O	1:A:547:GLN:HG3	2.20	0.41
1:A:569:LEU:HD23	1:A:570:PRO:HD2	2.01	0.41
1:A:616:LYS:HB2	1:A:661:VAL:HB	2.01	0.41
1:A:569:LEU:C	1:A:570:PRO:O	2.60	0.40
1:A:860:LEU:H	1:A:860:LEU:HD21	1.86	0.40
1:A:807:SER:H	1:A:807:SER:HG	1.59	0.40
1:A:569:LEU:CD2	1:A:570:PRO:CD	2.99	0.40

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	299/335 (89%)	287 (96%)	8 (3%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	GLN
1	A	569	LEU
1	A	570	PRO
1	A	603	GLY

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	256/287 (89%)	238 (93%)	18 (7%)	21	17

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

Mol	Chain	Res	Type
1	A	569	LEU
1	A	582	LEU
1	A	588	LEU
1	A	608	ASP
1	A	611	LEU
1	A	620	SER
1	A	634	LEU
1	A	670	ASP
1	A	675	LEU
1	A	696	GLN
1	A	785	LEU
1	A	794	ILE
1	A	799	LEU
1	A	807	SER
1	A	812	LYS
1	A	835[A]	GLN
1	A	835[B]	GLN
1	A	870	LYS

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

Mol	Chain	Res	Type
1	A	645	ASN
1	A	764	GLN
1	A	773	ASN
1	A	805	ASN
1	A	854	ASN
1	A	884	ASN

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 ⓘ

2 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	ACT	A	1	-	1,3,3	1.25	0	0,3,3	0.00	-
3	KRJ	A	923	-	31,31,31	0.99	2 (6%)	41,42,42	1.67	6 (14%)

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	ACT	A	1	-	-	0/0/0/0	0/0/0/0
3	KRJ	A	923	-	-	0/12/34/34	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	923	KRJ	C15-C14	2.23	1.42	1.38
3	A	923	KRJ	C15-C16	2.07	1.43	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	923	KRJ	C27-C28-C23	5.91	116.97	111.06
3	A	923	KRJ	C25-C24-C23	4.10	115.16	111.06
3	A	923	KRJ	C15-C14-C23	3.67	127.52	120.90
3	A	923	KRJ	C13-C14-C23	-3.21	113.94	121.19
3	A	923	KRJ	C24-C23-C28	2.44	114.77	109.31
3	A	923	KRJ	C28-C23-C14	2.35	118.02	112.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	304/335 (90%)	0.18	15 (4%)	28	31	20, 41, 82, 113	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	TYR	6.1
1	A	606	LYS	4.0
1	A	557	GLU	3.7
1	A	580	ASN	3.7
1	A	624	ALA	3.5
1	A	607	GLU	3.2
1	A	696	GLN	3.0
1	A	831	VAL	2.7
1	A	753	ARG	2.6
1	A	547	GLN	2.5
1	A	559	ASN	2.3
1	A	911	GLN	2.1
1	A	604	LEU	2.0
1	A	860	LEU	2.0
1	A	558	GLY	2.0

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(Å^2)	Q<0.9
3	KRJ	A	923	28/28	0.16	1.56	22,41,57,65	0
2	ACT	A	1	4/4	0.12	0.15	35,44,51,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.