Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:11 PM GMT

PDB ID	:	3CCN
Title	:	X-ray structure of c-Met with triazolopyridazine inhibitor.
Authors	:	Abrecht, B.K.; Harmange, J.-C.; Bauer, D.; Dussault, I.; long, A.; Bellon, S.F.
Deposited on	:	2008-02-26
Resolution	:	1.90 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.90 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		0.268
Clashscore		2
Ramachandran outliers		0.4%
Sidechain outliers		0.4%
RSRZ outliers		21.1%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
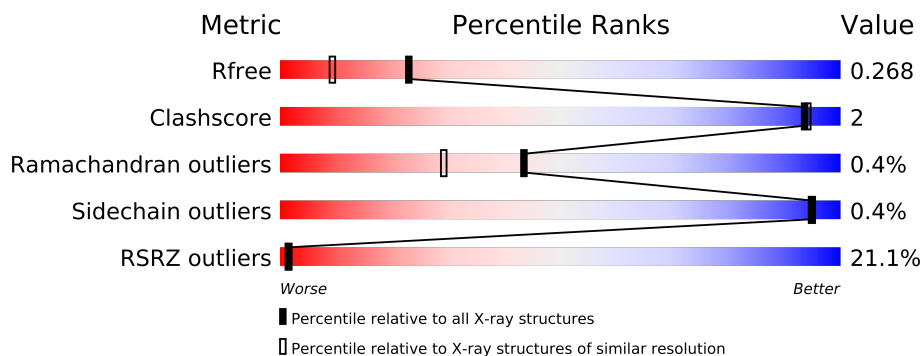
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	310	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2348 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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total 2148	C 1399	N 359	O 375	S 15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	MET	-	INITIATING METHIONINE	UNP P08581
A	1272	LEU	VAL	VARIANT	UNP P08581
A	1351	HIS	-	EXPRESSION TAG	UNP P08581
A	1352	HIS	-	EXPRESSION TAG	UNP P08581
A	1353	HIS	-	EXPRESSION TAG	UNP P08581
A	1354	HIS	-	EXPRESSION TAG	UNP P08581
A	1355	HIS	-	EXPRESSION TAG	UNP P08581
A	1356	HIS	-	EXPRESSION TAG	UNP P08581

- Molecule 2 is 4-[(6-PHENYL[1,2,4]TRIAZOLO[4,3-B]PYRIDAZIN-3-YL)METHYL]PHEN OL (three-letter code: LKG) (formula: $C_{18}H_{14}N_4O$).
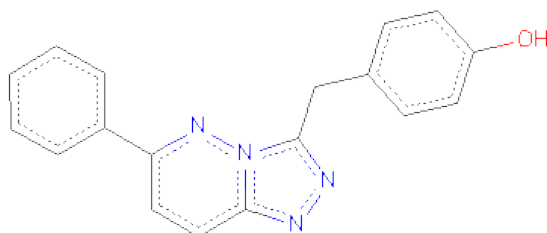
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 23	C 18	N 4	O 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total 177	O 177	0	0

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: Hepatocyte growth factor receptor

Chain A:
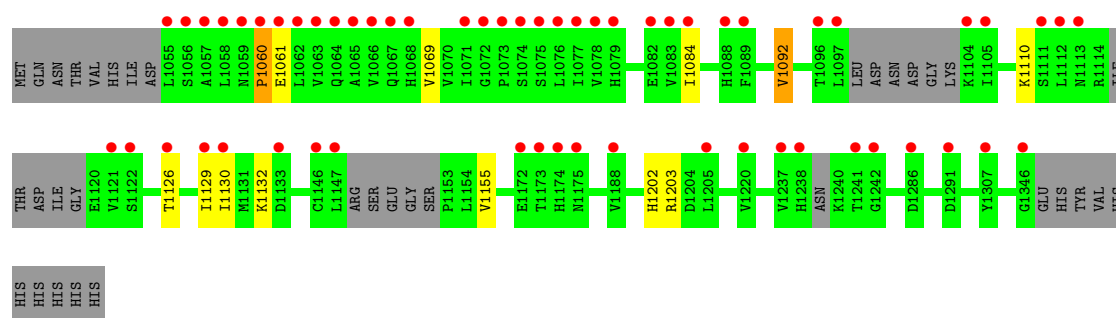
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.06Å 43.44Å 157.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 33.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-1.90) 92.3 (33.50-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.82 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.275 0.233 , 0.268	Depositor DCC
R_{free} test set	1089 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.4	EDS
Estimated twinning fraction	0.039 for k,h,-l	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.31$	Xtriage
Outliers	0 of 21803 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2348	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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: LKG

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	0.43	0/2202	0.52	0/2985

There are no bond length outliers.

There are no bond angle outliers.

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	2148	0	2131	7	0
2	A	23	0	13	0	0
3	A	177	0	0	0	0
All	All	2348	0	2144	7	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 2.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1084:ILE:HG13	1:A:1092:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1069:VAL:HG11	1:A:1129:ILE:HA	1.95	0.48
1:A:1069:VAL:HG12	1:A:1132:LYS:HD3	1.98	0.46
1:A:1202:HIS:O	1:A:1203:ARG:HB2	2.19	0.43
1:A:1126:THR:O	1:A:1130:ILE:HG12	2.20	0.42
1:A:1060:PRO:HB2	1:A:1061:GLU:H	1.58	0.41
1:A:1110:LYS:HB3	1:A:1155:VAL:HB	2.01	0.41

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	265/310 (86%)	258 (97%)	6 (2%)	1 (0%)	43	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1060	PRO

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	232/276 (84%)	231 (100%)	1 (0%)	95	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1092	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1079	HIS
1	A	1167	ASN

5.3.3 RNA (i)

There are no RNA chains 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)

1 ligand is 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	LKG	A	1	-	26,26,26	2.69	3 (11%)	36,36,36	2.30	8 (22%)

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	LKG	A	1	-	-	0/8/8/8	0/2/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	LKG	N2-N1	-9.99	1.24	1.36
2	A	1	LKG	N3-N4	-6.41	1.24	1.37
2	A	1	LKG	C4-C7	-5.31	1.40	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	LKG	C10-N3-N4	7.56	111.43	106.42
2	A	1	LKG	C4-C7-N2	5.74	119.68	115.62
2	A	1	LKG	N3-C10-N1	-5.04	106.90	109.97
2	A	1	LKG	C11-N1-N2	4.91	134.14	125.65
2	A	1	LKG	C11-N4-N3	3.18	110.24	106.48
2	A	1	LKG	C8-C9-C10	-2.94	116.64	119.68
2	A	1	LKG	C11-N1-C10	-2.26	103.38	107.88
2	A	1	LKG	C7-N2-N1	2.21	121.68	117.47

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 (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	275/310 (88%)	1.22	58 (21%)	1	1	13, 27, 54, 56	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1077	ILE	10.9
1	A	1055	LEU	9.5
1	A	1065	ALA	7.8
1	A	1063	VAL	6.6
1	A	1105	ILE	5.9
1	A	1097	LEU	5.8
1	A	1060	PRO	5.7
1	A	1067	GLN	5.4
1	A	1061	GLU	5.0
1	A	1104	LYS	5.0
1	A	1066	VAL	5.0
1	A	1062	LEU	4.9
1	A	1071	ILE	4.7
1	A	1056	SER	4.6
1	A	1082	GLU	4.5
1	A	1147	LEU	4.5
1	A	1057	ALA	4.3
1	A	1174	HIS	4.2
1	A	1075	SER	4.1
1	A	1076	LEU	4.1
1	A	1074	SER	4.1
1	A	1241	THR	4.0
1	A	1346	GLY	3.9
1	A	1172	GLU	3.8
1	A	1237	VAL	3.7
1	A	1078	VAL	3.6
1	A	1072	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1089	PHE	3.5
1	A	1096	THR	3.5
1	A	1059	ASN	3.4
1	A	1130	ILE	3.4
1	A	1175	ASN	3.3
1	A	1083	VAL	3.1
1	A	1112	LEU	3.1
1	A	1073	PRO	2.9
1	A	1121	VAL	2.9
1	A	1064	GLN	2.8
1	A	1220	VAL	2.8
1	A	1079	HIS	2.7
1	A	1088	HIS	2.7
1	A	1111	SER	2.6
1	A	1122	SER	2.6
1	A	1058	LEU	2.6
1	A	1286	ASP	2.6
1	A	1129	ILE	2.5
1	A	1242	GLY	2.5
1	A	1146	CYS	2.5
1	A	1205	LEU	2.4
1	A	1173	THR	2.4
1	A	1113	ASN	2.4
1	A	1238	HIS	2.3
1	A	1084	ILE	2.3
1	A	1307	TYR	2.3
1	A	1068	HIS	2.2
1	A	1126	THR	2.2
1	A	1188	VAL	2.2
1	A	1133	ASP	2.0
1	A	1291	ASP	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 (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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LKG	A	1	23/23	0.10	-1.18	24,26,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.