wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:58 PM GMT

PDB ID	:	1RJB
Title	:	Crystal Structure of FLT3
Authors	:	Griffith, J.; Black, J.; Faerman, C.; Swenson, L.; Wynn, M.; Lu, F.; Lippke, J.; Saxena, K.
Deposited on	:	2003-11-19
Resolution	:	2.10 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 (i) symbol.

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

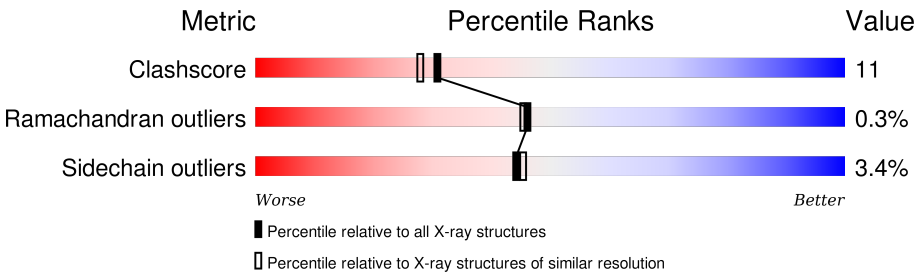
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	344	70% 15% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2716 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 FL cytokine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2406	1563	386	438	19	0	0	0

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	DELETION	UNP P36888
A	?	-	ARG	DELETION	UNP P36888
A	?	-	THR	DELETION	UNP P36888
A	?	-	TRP	DELETION	UNP P36888
A	?	-	THR	DELETION	UNP P36888
A	?	-	GLU	DELETION	UNP P36888
A	?	-	ILE	DELETION	UNP P36888
A	?	-	PHE	DELETION	UNP P36888
A	?	-	LYS	DELETION	UNP P36888
A	?	-	GLU	DELETION	UNP P36888
A	?	-	HIS	DELETION	UNP P36888
A	?	-	ASN	DELETION	UNP P36888
A	?	-	PHE	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	PHE	DELETION	UNP P36888
A	?	-	TYR	DELETION	UNP P36888
A	?	-	PRO	DELETION	UNP P36888
A	?	-	THR	DELETION	UNP P36888
A	?	-	PHE	DELETION	UNP P36888
A	?	-	GLN	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	HIS	DELETION	UNP P36888
A	?	-	PRO	DELETION	UNP P36888
A	?	-	ASN	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	MET	DELETION	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	DELETION	UNP P36888
A	?	-	GLY	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	ARG	DELETION	UNP P36888
A	?	-	GLU	DELETION	UNP P36888
A	?	-	VAL	DELETION	UNP P36888
A	?	-	GLN	DELETION	UNP P36888
A	?	-	ILE	DELETION	UNP P36888
A	?	-	HIS	DELETION	UNP P36888
A	?	-	PRO	DELETION	UNP P36888
A	?	-	ASP	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	ASP	DELETION	UNP P36888
A	?	-	GLN	DELETION	UNP P36888
A	?	-	ILE	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	GLY	DELETION	UNP P36888
A	?	-	LEU	DELETION	UNP P36888
A	?	-	HIS	DELETION	UNP P36888
A	?	-	GLY	DELETION	UNP P36888
A	?	-	ASN	DELETION	UNP P36888
A	?	-	SER	DELETION	UNP P36888
A	?	-	PHE	DELETION	UNP P36888
A	?	-	HIS	DELETION	UNP P36888

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	310	310	310	0	0

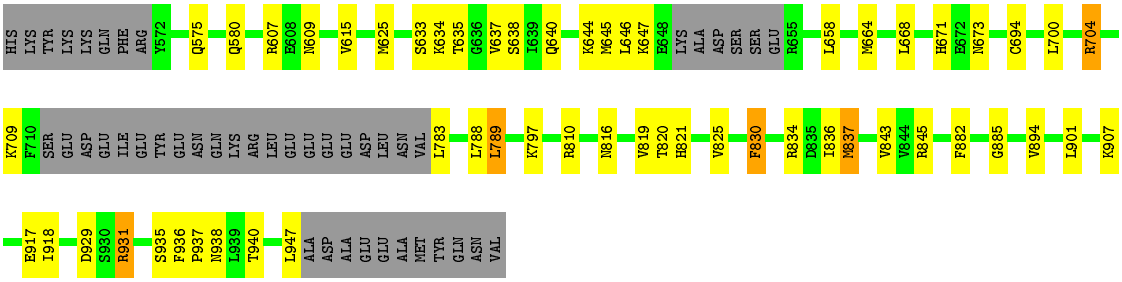
3 Residue-property plots (i)

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 (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.

Note EDS was not executed.

- Molecule 1: FL cytokine receptor

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	80.65Å 80.65Å 150.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.26 – 2.10	Depositor
% Data completeness (in resolution range)	99.1 (29.26-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.210 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2716	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

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	0.52	0/2464	0.72	1/3325 (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	821	HIS	N-CA-C	5.52	125.91	111.00

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	2406	0	2369	52	1
2	A	310	0	0	12	0
All	All	2716	0	2369	52	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 11.

The worst 5 of 52 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:789:LEU:HD12	1:A:947:LEU:HG	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:HIS:HD2	1:A:673:ASN:H	1.15	0.90
1:A:671:HIS:CD2	1:A:673:ASN:H	1.92	0.86
1:A:694:CYS:HA	1:A:820:THR:HG22	1.58	0.83
1:A:694:CYS:HA	1:A:820:THR:CG2	2.18	0.74

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:901:LEU:CD2	1:A:901:LEU:CD2[7_555]	1.96	0.24

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	292/344 (85%)	286 (98%)	5 (2%)	1 (0%)	46 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	634	LYS

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	261/303 (86%)	252 (97%)	9 (3%)	44 45

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	789	LEU
1	A	931	ARG
1	A	837	MET
1	A	704	ARG
1	A	830	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	671	HIS
1	A	816	ASN
1	A	903	GLN
1	A	667	GLN
1	A	847	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 carbohydrates 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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.