



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2QOD / pdb_00002qod
Title : Human EphA3 kinase and juxtamembrane region, Y602F mutant
Authors : Davis, T.; Walker, J.R.; Newman, E.M.; Mackenzie, F.; Butler-Cole, C.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2007-07-20
Resolution : 1.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

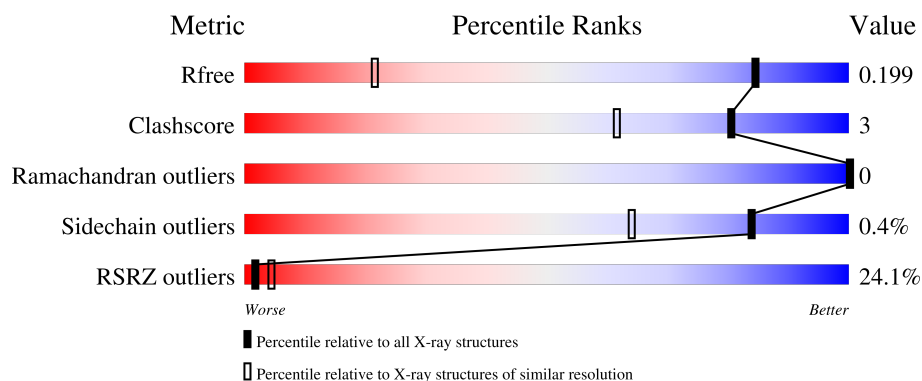
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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}	180053	1380 (1.16-1.12)
Clashscore	190562	1393 (1.16-1.12)
Ramachandran outliers	187476	1369 (1.16-1.12)
Sidechain outliers	187428	1369 (1.16-1.12)
RSRZ outliers	180081	1379 (1.16-1.12)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	373	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2675 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 Ephrin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	19	0
			2305	1477	387	426	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	expression tag	UNP Q6P4R6
A	576	SER	-	expression tag	UNP Q6P4R6
A	602	PHE	TYR	engineered mutation	UNP Q6P4R6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	370	Total	O	0	0
			370	370		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.22Å 38.29Å 76.00Å 90.00° 102.43° 90.00°	Depositor
Resolution (Å)	23.40 – 1.15 23.40 – 1.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (23.40-1.15) 99.3 (23.40-1.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.206 0.200 , 0.199	Depositor DCC
R_{free} test set	5381 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2675	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.48	0/2390	0.62	0/3220

There are no bond length outliers.

There are no bond angle outliers.

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	2305	0	2362	12	0
2	A	370	0	0	3	0
All	All	2675	0	2362	12	0

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 3.

All (12) 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:822[B]:GLU:HG3	2:A:368:HOH:O	1.54	1.05
1:A:627:VAL:HB	1:A:635:VAL:HG23	1.78	0.63
1:A:617:ASP:CG	1:A:619[A]:THR:HG22	2.32	0.55
1:A:862[B]:GLN:NE2	1:A:867:ASN:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASN:ND2	1:A:887:SER:OG	2.43	0.50
1:A:610:HIS:HE1	1:A:615:GLU:OE1	1.97	0.48
1:A:788:ILE:HD12	1:A:788:ILE:H	1.80	0.46
1:A:636:CYS:SG	2:A:299:HOH:O	2.17	0.44
1:A:693:LYS:HA	1:A:694:PRO:C	2.43	0.44
1:A:628:GLY:O	1:A:635:VAL:HG22	2.19	0.43
1:A:814:LEU:HG	1:A:857:MET:HE2	2.02	0.42
1:A:720[A]:VAL:HG23	2:A:26:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	286/373 (77%)	280 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	262/324 (81%)	261 (100%)	1 (0%)	84	64

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

Mol	Chain	Res	Type
1	A	609	VAL

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

Mol	Chain	Res	Type
1	A	610	HIS
1	A	681	ASN
1	A	704	ASN
1	A	855	GLN
1	A	866	ASN
1	A	884	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 oligosaccharides 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

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	274/373 (73%)	1.30	66 (24%) 2 4	5, 14, 27, 34	37 (13%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	627	VAL	7.4
1	A	787	PRO	6.2
1	A	626	VAL	5.8
1	A	628	GLY	5.4
1	A	609	VAL	5.1
1	A	599	PRO	4.9
1	A	788	ILE	4.8
1	A	890	ILE	4.4
1	A	902	LEU	4.4
1	A	892	THR	4.3
1	A	891	ILE	4.1
1	A	623	ILE	4.0
1	A	904	ASP	4.0
1	A	899	SER	4.0
1	A	635	VAL	3.9
1	A	721	ILE	3.9
1	A	630	GLY	3.9
1	A	613	ALA	3.9
1	A	619[A]	THR	3.8
1	A	632	PHE	3.7
1	A	629	ALA	3.7
1	A	597	VAL	3.6
1	A	900	ASN	3.5
1	A	625	LYS	3.5
1	A	624	ASP	3.3
1	A	596	TYR	3.3
1	A	633	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	598	ASP	3.1
1	A	612	PHE	3.1
1	A	829	SER	3.0
1	A	665	ARG	3.0
1	A	660	THR	3.0
1	A	595	THR	2.9
1	A	903	LEU	2.9
1	A	690	THR	2.8
1	A	887	SER	2.8
1	A	886	GLY	2.8
1	A	765	PHE	2.8
1	A	831	GLN	2.7
1	A	883[A]	ARG	2.7
1	A	636	CYS	2.7
1	A	694	PRO	2.6
1	A	901	LEU	2.6
1	A	610	HIS	2.6
1	A	662	LYS	2.6
1	A	797	ALA	2.5
1	A	736	TYR	2.5
1	A	795	ALA	2.5
1	A	611	GLU	2.5
1	A	716	ALA	2.4
1	A	888	LEU	2.4
1	A	659	TYR	2.4
1	A	666	ASP	2.4
1	A	866	ASN	2.3
1	A	841	TYR	2.2
1	A	617	ASP	2.2
1	A	657	VAL	2.2
1	A	826	TRP	2.2
1	A	618	ALA	2.1
1	A	667	PHE	2.1
1	A	677	PHE	2.1
1	A	834	ILE	2.1
1	A	695	VAL	2.1
1	A	621	ILE	2.0
1	A	661	GLU	2.0
1	A	801	PHE	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.