



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2QOL / pdb_00002qol
Title : Human EphA3 kinase and juxtamembrane region, Y596:Y602:S768G triple mutant
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Deposited on : 2007-07-20
Resolution : 1.07 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

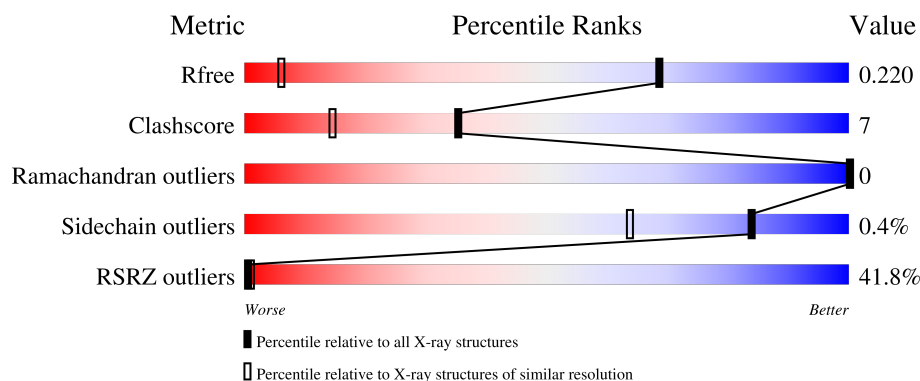
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.07 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	1687 (1.10-1.06)
Clashscore	190562	1727 (1.10-1.06)
Ramachandran outliers	187476	1679 (1.10-1.06)
Sidechain outliers	187428	1676 (1.10-1.06)
RSRZ outliers	180081	1687 (1.10-1.06)

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 2797 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	273	Total	C	N	O	S	0	35	0
			2375	1533	393	434	15			

There are 5 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	596	PHE	TYR	engineered mutation	UNP Q6P4R6
A	602	PHE	TYR	engineered mutation	UNP Q6P4R6
A	768	GLY	SER	engineered mutation	UNP Q6P4R6

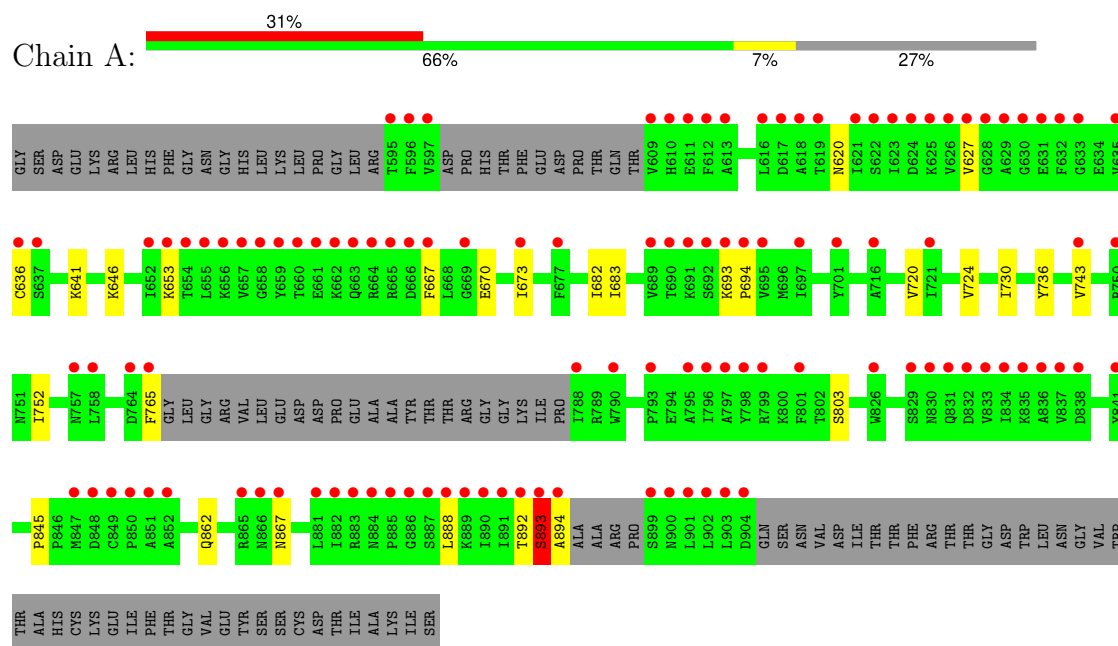
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	422	Total	O	0	0
			422	422		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Ephrin receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.30Å 38.29Å 75.88Å 90.00° 102.15° 90.00°	Depositor
Resolution (Å)	26.55 – 1.07 26.55 – 1.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (26.55-1.07) 92.6 (26.55-1.07)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.211 0.203 , 0.220	Depositor DCC
R_{free} test set	6252 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	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	0.95	EDS
Total number of atoms	2797	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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	0.43	0/2507	0.60	0/3372

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	893	SER	Peptide

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	2375	0	2485	36	0
2	A	422	0	0	13	0
All	All	2797	0	2485	36	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 7.

All (36) 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:743:VAL:HG13	2:A:409:HOH:O	1.83	0.79
1:A:736[B]:TYR:OH	2:A:307:HOH:O	2.03	0.74
1:A:894:ALA:HB3	2:A:337:HOH:O	1.91	0.71
1:A:893:SER:N	1:A:894:ALA:C	2.51	0.68
1:A:803:SER:HA	2:A:409:HOH:O	1.93	0.68
1:A:682[B]:ILE:CD1	1:A:736[B]:TYR:CD2	2.77	0.67
1:A:892:THR:HG22	1:A:893:SER:H	1.60	0.66
1:A:892:THR:HG22	1:A:893:SER:N	2.14	0.63
1:A:670[B]:GLU:HG3	1:A:765[B]:PHE:C	2.24	0.63
1:A:682[B]:ILE:CD1	1:A:736[B]:TYR:HD2	2.12	0.63
1:A:673:ILE:O	2:A:414:HOH:O	2.17	0.60
1:A:683:ILE:O	2:A:408:HOH:O	2.15	0.59
1:A:682[B]:ILE:HD12	1:A:736[B]:TYR:CD2	2.37	0.59
1:A:892:THR:HG22	1:A:894:ALA:C	2.27	0.59
1:A:682[B]:ILE:HD11	1:A:736[B]:TYR:HD2	1.69	0.57
1:A:620[A]:ASN:HD22	1:A:641[A]:LYS:HB3	1.75	0.51
1:A:892:THR:C	1:A:894:ALA:C	2.79	0.51
1:A:845:PRO:HG3	1:A:894:ALA:HB1	1.94	0.50
1:A:636[B]:CYS:SG	2:A:111:HOH:O	2.48	0.50
1:A:894:ALA:CB	2:A:262:HOH:O	2.61	0.49
1:A:888:LEU:HD11	2:A:413:HOH:O	2.13	0.48
1:A:724:VAL:HG11	2:A:413:HOH:O	2.13	0.47
1:A:730:ILE:HD13	1:A:752[B]:ILE:HD13	1.95	0.47
1:A:720[A]:VAL:HG12	1:A:888:LEU:HD13	1.96	0.47
1:A:892:THR:CG2	1:A:893:SER:H	2.24	0.46
1:A:862[B]:GLN:NE2	1:A:867:ASN:O	2.49	0.46
1:A:892:THR:CG2	1:A:893:SER:N	2.79	0.46
1:A:894:ALA:CB	2:A:337:HOH:O	2.57	0.45
1:A:653[A]:LYS:HG2	1:A:667:PHE:CE1	2.53	0.43
1:A:646[B]:LYS:CE	2:A:174:HOH:O	2.66	0.43
1:A:894:ALA:HB2	2:A:262:HOH:O	2.17	0.43
1:A:653[A]:LYS:HG2	1:A:667:PHE:CZ	2.55	0.41
1:A:693:LYS:HA	1:A:694:PRO:C	2.46	0.40
1:A:892:THR:O	1:A:894:ALA:O	2.39	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	301/373 (81%)	296 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	277/323 (86%)	276 (100%)	1 (0%)	84	64

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

Mol	Chain	Res	Type
1	A	893	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	ASN
1	A	757	ASN
1	A	855	GLN
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	273/373 (73%)	2.04	114 (41%) 0 1	5, 11, 21, 27	77 (28%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	632	PHE	10.0
1	A	627	VAL	9.5
1	A	629	ALA	8.8
1	A	894	ALA	8.1
1	A	626	VAL	7.3
1	A	904	ASP	7.2
1	A	635[A]	VAL	6.8
1	A	630	GLY	6.4
1	A	899	SER	6.2
1	A	788	ILE	5.8
1	A	613	ALA	5.8
1	A	891	ILE	5.8
1	A	609	VAL	5.6
1	A	890	ILE	5.5
1	A	625	LYS	5.4
1	A	612	PHE	5.3
1	A	893	SER	5.2
1	A	902	LEU	5.0
1	A	628	GLY	5.0
1	A	883	ARG	4.9
1	A	694	PRO	4.9
1	A	610	HIS	4.8
1	A	596	PHE	4.7
1	A	618	ALA	4.5
1	A	691	LYS	4.5
1	A	657	VAL	4.4
1	A	623	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	837	VAL	4.3
1	A	597	VAL	4.3
1	A	892	THR	4.2
1	A	903	LEU	4.2
1	A	636[A]	CYS	4.1
1	A	900	ASN	4.1
1	A	619[A]	THR	4.1
1	A	826	TRP	4.1
1	A	695	VAL	4.0
1	A	666	ASP	4.0
1	A	659	TYR	4.0
1	A	841	TYR	3.9
1	A	667	PHE	3.8
1	A	658	GLY	3.8
1	A	849	CYS	3.7
1	A	689	VAL	3.7
1	A	901	LEU	3.6
1	A	660	THR	3.6
1	A	882	ILE	3.6
1	A	851	ALA	3.5
1	A	661	GLU	3.5
1	A	665	ARG	3.5
1	A	888	LEU	3.5
1	A	886	GLY	3.5
1	A	631	GLU	3.5
1	A	836	ALA	3.5
1	A	866	ASN	3.4
1	A	765[A]	PHE	3.3
1	A	835	LYS	3.3
1	A	848	ASP	3.3
1	A	847	MET	3.2
1	A	662	LYS	3.2
1	A	690	THR	3.2
1	A	829	SER	3.2
1	A	831	GLN	3.2
1	A	889	LYS	3.1
1	A	673	ILE	3.1
1	A	885	PRO	3.0
1	A	653[A]	LYS	3.0
1	A	797	ALA	3.0
1	A	611	GLU	2.9
1	A	624	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	621	ILE	2.8
1	A	887[A]	SER	2.8
1	A	865[A]	ARG	2.8
1	A	838	ASP	2.8
1	A	881	LEU	2.8
1	A	852	ALA	2.7
1	A	798	TYR	2.7
1	A	834	ILE	2.7
1	A	701	TYR	2.7
1	A	764	ASP	2.7
1	A	801	PHE	2.6
1	A	616	LEU	2.6
1	A	850	PRO	2.6
1	A	669	GLY	2.5
1	A	664	ARG	2.5
1	A	692	SER	2.4
1	A	721[A]	ILE	2.4
1	A	633	GLY	2.4
1	A	663	GLN	2.4
1	A	654	THR	2.4
1	A	799	ARG	2.4
1	A	617	ASP	2.4
1	A	677	PHE	2.4
1	A	758	LEU	2.3
1	A	830	ASN	2.3
1	A	867	ASN	2.3
1	A	790	TRP	2.3
1	A	637	SER	2.3
1	A	833	VAL	2.3
1	A	656	LYS	2.2
1	A	793	PRO	2.2
1	A	757	ASN	2.2
1	A	884	ASN	2.2
1	A	697	ILE	2.2
1	A	796	ILE	2.2
1	A	795	ALA	2.1
1	A	693	LYS	2.1
1	A	743	VAL	2.1
1	A	750[A]	ARG	2.1
1	A	832	ASP	2.1
1	A	595	THR	2.1
1	A	622[A]	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	655	LEU	2.0
1	A	652	ILE	2.0
1	A	716	ALA	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.