wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 11:08 AM EDT

PDB ID	:	3C4Y
Title	:	Crystal Structure of Apo form of G protein coupled receptor kinase 1 at 7.51A
Authors	:	Singh, P.; Tesmer, J.J.G.
Deposited on	:	2008-01-30
Resolution	:	7.51 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

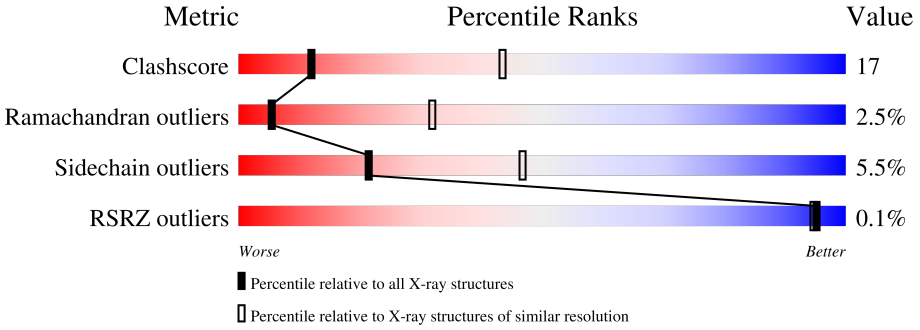
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 7.51 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	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 <=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	543	58% 27% • 12%
1	B	543	57% 27% • 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7629 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 Rhodopsin kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	478	3854	2474	666	695	19	0	0	0
1	B	466	3775	2427	649	680	19	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

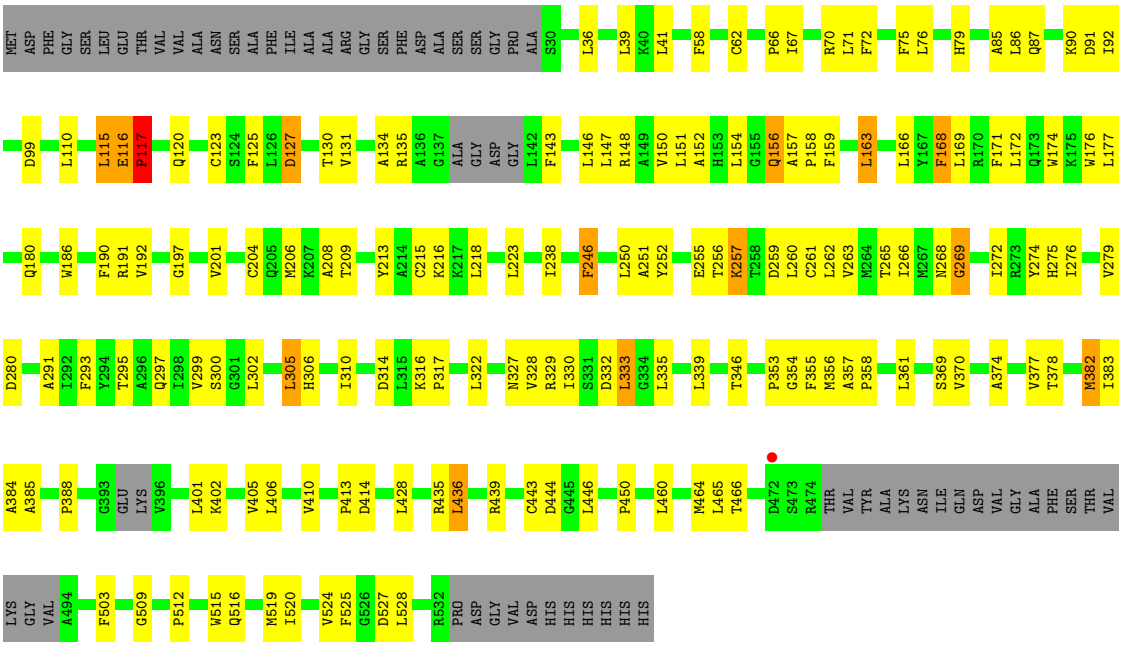
Chain	Residue	Modelled	Actual	Comment	Reference
A	536	VAL	-	expression tag	UNP P28327
A	537	ASP	-	expression tag	UNP P28327
A	538	HIS	-	expression tag	UNP P28327
A	539	HIS	-	expression tag	UNP P28327
A	540	HIS	-	expression tag	UNP P28327
A	541	HIS	-	expression tag	UNP P28327
A	542	HIS	-	expression tag	UNP P28327
A	543	HIS	-	expression tag	UNP P28327
B	536	VAL	-	expression tag	UNP P28327
B	537	ASP	-	expression tag	UNP P28327
B	538	HIS	-	expression tag	UNP P28327
B	539	HIS	-	expression tag	UNP P28327
B	540	HIS	-	expression tag	UNP P28327
B	541	HIS	-	expression tag	UNP P28327
B	542	HIS	-	expression tag	UNP P28327
B	543	HIS	-	expression tag	UNP P28327

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.

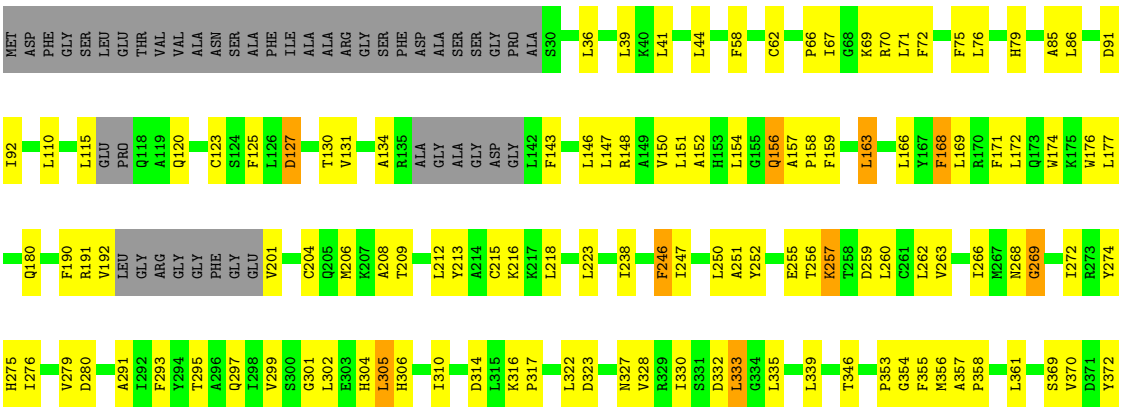
• Molecule 1: Rhodopsin kinase

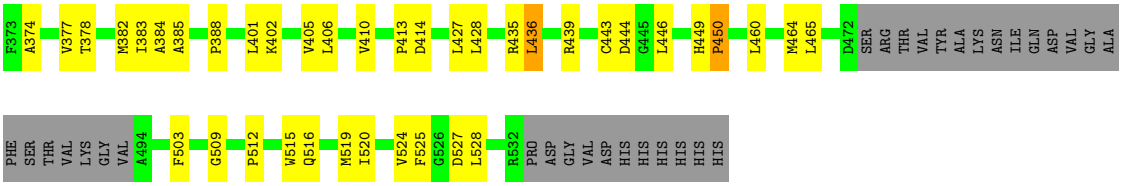
Chain A: 58% 27% • 12%



• Molecule 1: Rhodopsin kinase

Chain B: 57% 27% • 14%




F373
A374
V377
T378
M382
I383
A384
A385
P388
L401
K402
V405
L406
V410
P413
D414
L427
L428
R435
L436
R439
C443
D444
G445
L446
H449
P450
L460
M464
L465
D472
SER
ARG
THR
VAL
TYR
ALA
LYS
ASN
ILE
GLN
ASP
VAL
GLY
ALA
PHE
SER
THR
VAL
LYS
GLY
VAL
A494
F503
G509
P512
W515
Q516
M519
I520
V524
F525
G526
D527
L528
R532
PRO
ASP
GLY
VAL
ASP
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.31Å 123.31Å 192.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 7.51 19.94 – 7.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-7.51) 100.0 (19.94-7.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 7.78Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , (Not available) 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	540.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.14 , 153.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7629	wwPDB-VP
Average B, all atoms (Å^2)	224.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.39	0/3944	0.53	0/5316
1	B	0.38	0/3862	0.53	0/5205
All	All	0.39	0/7806	0.53	0/10521

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	LEU	Peptide
1	A	116	GLU	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	3854	0	3820	133	0
1	B	3775	0	3748	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7629	0	7568	262	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 17.

The worst 5 of 262 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:B:209:THR:HG22	1:B:524:VAL:HG21	1.43	1.00
1:A:209:THR:HG22	1:A:524:VAL:HG21	1.46	0.95
1:B:275:HIS:HA	1:B:279:VAL:HG23	1.51	0.90
1:B:134:ALA:HB2	1:B:146:LEU:HD13	1.52	0.90
1:A:275:HIS:HA	1:A:279:VAL:HG23	1.53	0.88

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	470/543 (87%)	401 (85%)	56 (12%)	13 (3%)	5 30
1	B	456/543 (84%)	394 (86%)	52 (11%)	10 (2%)	6 35
All	All	926/1086 (85%)	795 (86%)	108 (12%)	23 (2%)	5 32

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PRO
1	A	266	ILE
1	A	127	ASP
1	A	257	LYS

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Mol	Chain	Res	Type
1	A	269	GLY

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	401/449 (89%)	378 (94%)	23 (6%)	20	45
1	B	395/449 (88%)	374 (95%)	21 (5%)	22	47
All	All	796/898 (89%)	752 (94%)	44 (6%)	21	47

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	168	PHE
1	B	305	LEU
1	B	191	ARG
1	B	246	PHE
1	B	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	268	ASN
1	B	278	ASN
1	A	278	ASN
1	A	306	HIS
1	B	120	GLN

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 monosaccharides 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)

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	478/543 (88%)	-0.76	1 (0%) 95 93	223, 224, 225, 238	1 (0%)
1	B	466/543 (85%)	-0.74	0 100 100	223, 224, 225, 238	0
All	All	944/1086 (86%)	-0.75	1 (0%) 95 95	223, 224, 225, 238	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	ASP	2.1

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 monosaccharides 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.