wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 10:06 am BST

PDB ID	:	2OZA
Title	:	Structure of p38alpha complex
Authors	:	White, A.; Pargellis, C.A.; Studts, J.M.; Werneburg, B.G.; Farmer II, B.T.
Deposited on	:	2007-02-25
Resolution	:	2.70 Å(reported)

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

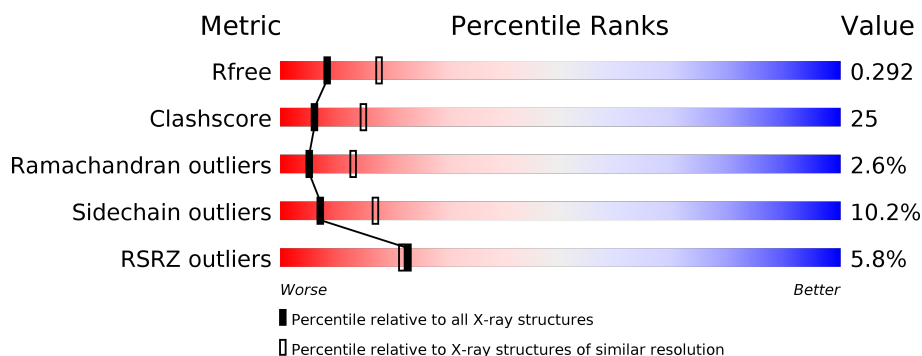|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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		0.292
Clashscore		25
Ramachandran outliers		2.6%
Sidechain outliers		10.2%
RSRZ outliers		5.8%

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	356	6% 48% 40% 5% 7%
2	B	366	5% 49% 38% 5% · 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5500 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total 2703	C 1720	N 468	O 496	S 19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	INSERTION	UNP P49137
A	46	SER	-	INSERTION	UNP P49137

- Molecule 2 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	340	Total 2737	C 1759	N 466	O 500	S 12	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	INSERTION	UNP P47811
B	-4	ALA	-	INSERTION	UNP P47811
B	-3	HIS	-	INSERTION	UNP P47811
B	-2	HIS	-	INSERTION	UNP P47811
B	-1	HIS	-	INSERTION	UNP P47811
B	0	HIS	-	INSERTION	UNP P47811
B	1	HIS	-	INSERTION	UNP P47811

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	28	Total O 28 28		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 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: MAP kinase-activated protein kinase 2
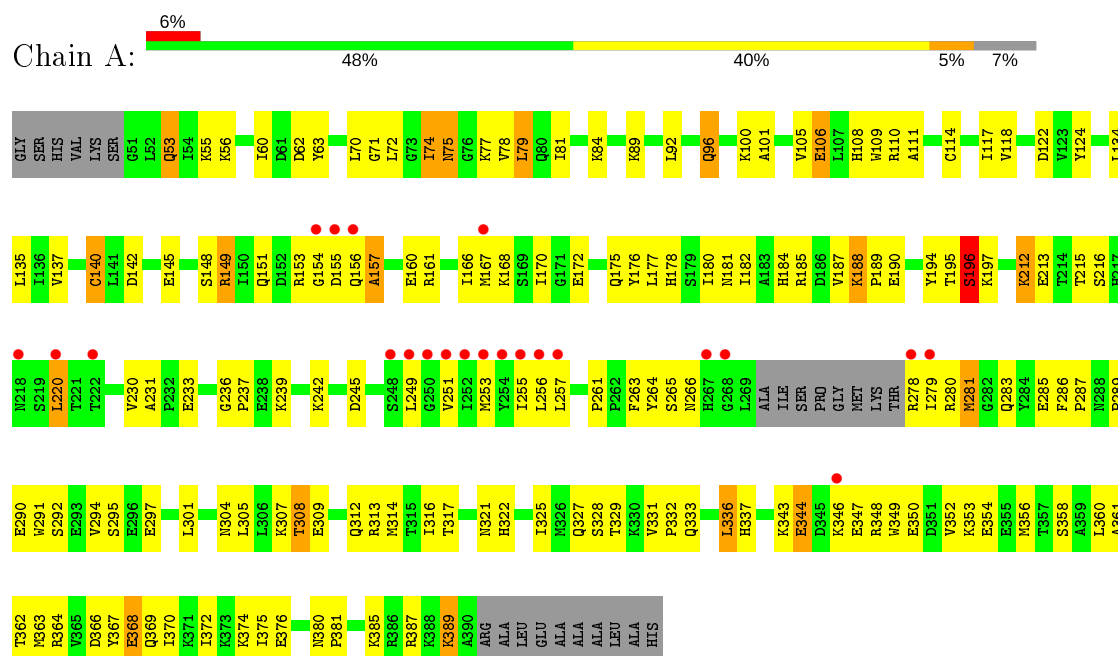
• Molecule 2: Mitogen-activated protein kinase 14
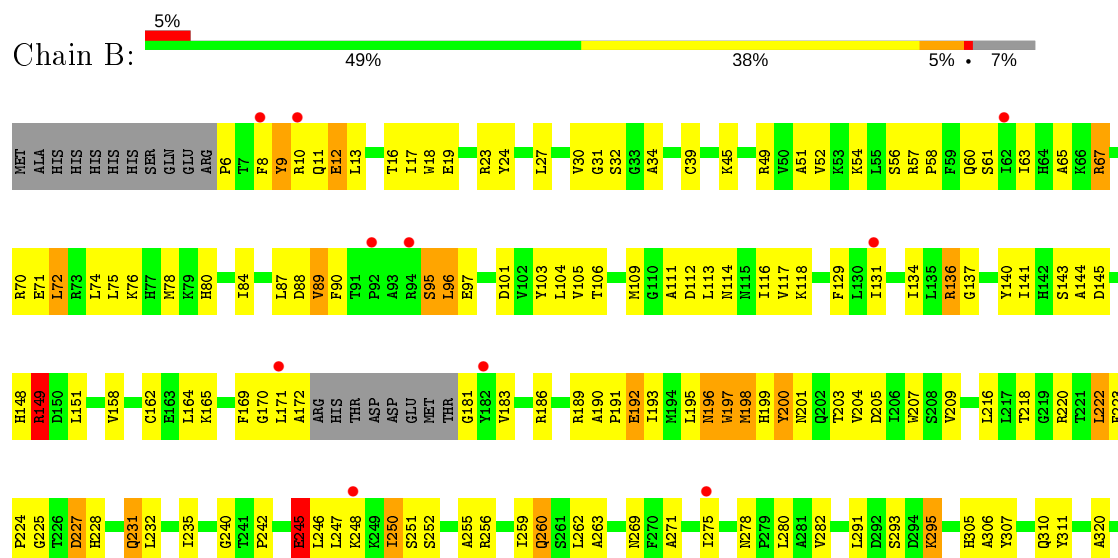
Q325 S326 F327 E328 S329 R330 D331 L332 L333 I334 D335 E336 W337 K338 S339 L340 T341 Y342 D343 E344 V345 I346 V349 L353 ASP GLN GLU GLU MET GLU SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.31Å 83.31Å 231.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.80 – 2.70 26.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (26.80-2.70) 97.9 (26.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$<I/\sigma(I)>$ [1]	2.12 (at 2.72Å)	Xtriage
Refinement program	CNS, CNX	Depositor
R, R_{free}	0.239 , 0.296 0.237 , 0.292	Depositor DCC
R_{free} test set	1110 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å²)	71.2	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 57.4	EDS
L-test for twinning[2]	$<|L|> = 0.52$, $<L^2> = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5500	wwPDB-VP
Average B, all atoms (Å²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.41	0/2759	0.58	0/3722
2	B	0.38	0/2802	0.57	0/3804
All	All	0.39	0/5561	0.57	0/7526

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
2	B	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
2	B	199	HIS	Peptide
2	B	6	PRO	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	2703	0	2741	127	0
2	B	2737	0	2735	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	0	2	0
3	B	28	0	0	1	0
All	All	5500	0	5476	268	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 25.

The worst 5 of 268 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)
2:B:136:ARG:HG2	2:B:136:ARG:HH11	0.97	1.09
2:B:16:THR:HG22	2:B:17:ILE:H	1.24	1.01
2:B:136:ARG:HG2	2:B:136:ARG:NH1	1.75	0.96
2:B:16:THR:HG21	2:B:54:LYS:HE2	1.46	0.94
1:A:154:GLY:N	1:A:155:ASP:HA	1.89	0.87

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	328/356 (92%)	294 (90%)	29 (9%)	5 (2%)	10	26
2	B	336/366 (92%)	291 (87%)	33 (10%)	12 (4%)	3	7
All	All	664/722 (92%)	585 (88%)	62 (9%)	17 (3%)	5	13

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	GLU
2	B	96	LEU

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Mol	Chain	Res	Type
2	B	170	GLY
1	A	74	ILE
1	A	196	SER

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	301/317 (95%)	272 (90%)	29 (10%)	8	19
2	B	299/324 (92%)	267 (89%)	32 (11%)	6	15
All	All	600/641 (94%)	539 (90%)	61 (10%)	7	17

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	LYS
2	B	74	LEU
2	B	291	LEU
1	A	389	LYS
2	B	19	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	ASN
2	B	60	GLN
2	B	228	HIS
1	A	337	HIS
2	B	202	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 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)

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	332/356 (93%)	0.19	22 (6%)	18	16	39, 67, 101, 135	0
2	B	340/366 (92%)	0.18	17 (5%)	28	27	46, 71, 108, 140	0
All	All	672/722 (93%)	0.18	39 (5%)	23	22	39, 69, 107, 140	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	5.8
2	B	326	SER	4.8
1	A	220	LEU	3.7
2	B	62	ILE	3.7
2	B	327	PHE	3.6

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 carbohydrates 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.