



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 06:17 AM GMT

PDB ID : 1NXK
Title : Crystal structure of staurosporine bound to MAP KAP kinase 2
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Malakian, K.; Telliez, J.B.; Lin, L.L.; Kriz, R.W.; Seehra, J.; Somers, W.S.;
Stahl, M.L.
Deposited on : 2003-02-10
Resolution : 2.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

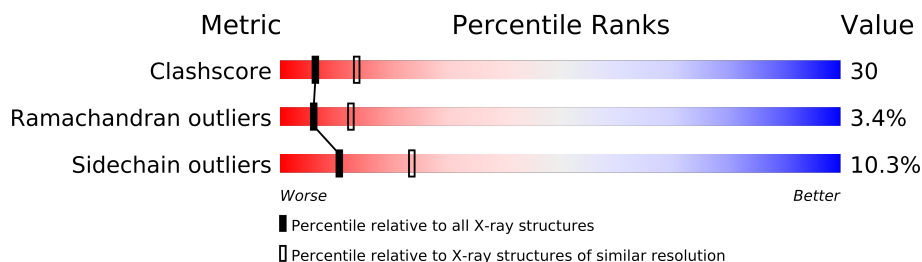
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	400	
1	B	400	
1	C	400	
1	D	400	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9405 atoms, of which 0 are hydrogen and 0 are deuterium.

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	290	Total	C	N	O	S	Se	0	0	0
			2289	1471	388	413	6	11			
1	B	283	Total	C	N	O	S	Se	0	0	0
			2234	1425	382	410	6	11			
1	C	306	Total	C	N	O	S	Se	0	0	0
			2438	1557	421	442	6	12			
1	D	288	Total	C	N	O	S	Se	0	0	0
			2252	1452	373	410	6	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	314	MSE	MET	MODIFIED RESIDUE	UNP P49137

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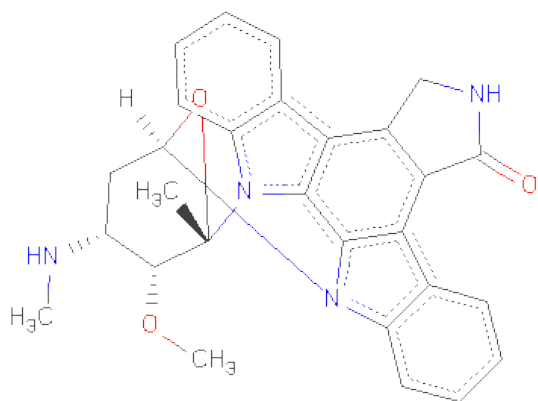
Chain	Residue	Modelled	Actual	Comment	Reference
B	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	356	MSE	MET	MODIFIED RESIDUE	UNP P49137

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	28	4	3		
3	B	1	Total	C	N	O	0	0
			35	28	4	3		

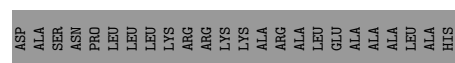
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			35	28	4	3		
3	D	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	16	Total	O	0	0
			16	16		
4	C	9	Total	O	0	0
			9	9		
4	D	7	Total	O	0	0
			7	7		



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	160.20Å 160.20Å 133.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.239 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9405	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: STU, SO4

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	0.76	3/2331 (0.1%)	0.95	3/3140 (0.1%)
1	B	0.79	2/2271 (0.1%)	0.99	3/3057 (0.1%)
1	C	0.75	1/2481 (0.0%)	0.91	2/3337 (0.1%)
1	D	0.66	0/2295	0.86	0/3100
All	All	0.74	6/9378 (0.1%)	0.93	8/12634 (0.1%)

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	3
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	NE1-CE2	8.77	1.49	1.37
1	C	324	TRP	NE1-CE2	8.66	1.48	1.37
1	A	109	TRP	NE1-CE2	8.65	1.48	1.37
1	A	291	TRP	NE1-CE2	8.64	1.48	1.37
1	B	247	TRP	NE1-CE2	8.64	1.48	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	PHE	O-C-N	-7.70	110.39	122.70
1	B	303	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	282	GLY	N-CA-C	-5.54	99.25	113.10
1	B	110	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	183	ALA	N-CA-C	-5.30	96.70	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	103	ARG	Sidechain
1	A	119	ARG	Sidechain
1	B	158	PHE	Mainchain
1	B	176	TYR	Sidechain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2289	0	2258	148	0
1	B	2234	0	2197	137	0
1	C	2438	0	2414	152	0
1	D	2252	0	2194	157	0
2	B	10	0	0	0	0
3	A	35	0	26	3	0
3	B	35	0	26	2	0
3	C	35	0	26	1	0
3	D	35	0	26	7	0
4	A	10	0	0	0	0
4	B	16	0	0	0	0
4	C	9	0	0	0	0
4	D	7	0	0	0	0
All	All	9405	0	9167	561	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 30.

The worst 5 of 561 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:ASN:HD22	1:A:269:LEU:HG	1.30	0.96
1:A:158:PHE:CE1	1:A:162:GLU:HB3	2.00	0.95
1:C:328:SER:O	1:C:331:VAL:HG12	1.66	0.94
1:A:260:TYR:HE2	1:A:290:GLU:HG2	1.30	0.94
1:D:167:MSE:HG3	1:D:253:MSE:HG3	1.47	0.94

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	284/400 (71%)	250 (88%)	25 (9%)	9 (3%)	6	14
1	B	277/400 (69%)	241 (87%)	26 (9%)	10 (4%)	5	11
1	C	302/400 (76%)	261 (86%)	30 (10%)	11 (4%)	5	11
1	D	282/400 (70%)	241 (86%)	32 (11%)	9 (3%)	6	14
All	All	1145/1600 (72%)	993 (87%)	113 (10%)	39 (3%)	6	12

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
1	B	66	THR
1	B	239	LYS
1	C	42	GLN
1	C	237	PRO

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	246/345 (71%)	224 (91%)	22 (9%)	14	31
1	B	241/345 (70%)	213 (88%)	28 (12%)	8	18
1	C	263/345 (76%)	231 (88%)	32 (12%)	7	17
1	D	241/345 (70%)	221 (92%)	20 (8%)	16	35
All	All	991/1380 (72%)	889 (90%)	102 (10%)	10	23

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	331	VAL
1	C	133	CYS
1	D	264	TYR
1	B	334	THR
1	C	45	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	337	HIS
1	C	151	GLN
1	D	266	ASN
1	C	42	GLN
1	C	57	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	STU	A	401	-	40,42,42	2.21	12 (30%)	62,68,68	2.06	18 (29%)
2	SO4	B	401	-	4,4,4	1.54	1 (25%)	6,6,6	0.64	0
2	SO4	B	402	-	4,4,4	1.58	1 (25%)	6,6,6	0.64	0
3	STU	B	403	-	40,42,42	2.22	14 (35%)	62,68,68	1.61	10 (16%)
3	STU	C	401	-	40,42,42	2.12	15 (37%)	62,68,68	2.04	16 (25%)
3	STU	D	401	-	40,42,42	2.25	16 (40%)	62,68,68	1.75	14 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	STU	A	401	-	-	0/4/42/42	0/0/8/8
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	STU	B	403	-	-	0/4/42/42	0/0/8/8
3	STU	C	401	-	-	0/4/42/42	0/0/8/8
3	STU	D	401	-	-	0/4/42/42	0/0/8/8

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	STU	C21-C22	5.10	1.60	1.53
3	B	403	STU	C23-N4	5.03	1.58	1.47
3	D	401	STU	C23-N4	5.02	1.58	1.47
3	A	401	STU	C23-N4	5.01	1.58	1.47
3	D	401	STU	C18-N2	4.63	1.45	1.39

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	STU	C28-N4-C23	-7.50	109.64	113.82
3	A	401	STU	C28-N4-C23	-7.32	109.74	113.82
3	B	403	STU	C24-C25-N3	-5.20	106.50	112.48
3	C	401	STU	C24-C25-N3	-4.94	106.79	112.48
3	C	401	STU	C7-C6-C19	-4.88	114.50	121.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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