



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:13 AM UTC

PDB ID : 5ULM / pdb_00005ulm
Title : Structure of the ASK1 central regulatory region
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Deposited on : 2017-01-24
Resolution : 2.10 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

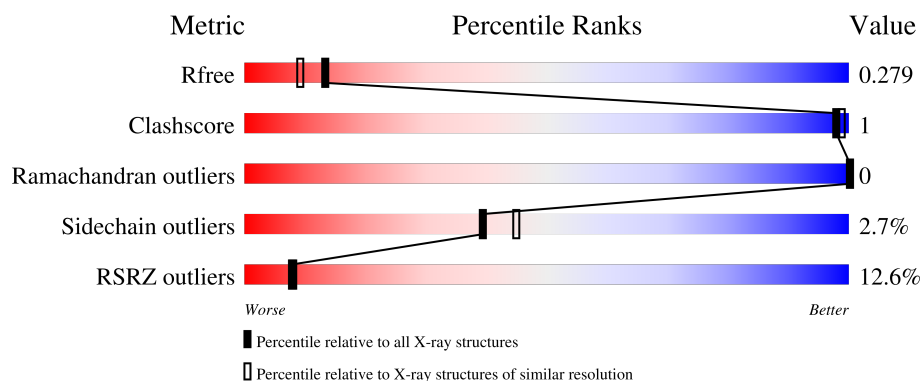
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	393	11% 90% 5% 5%
1	B	393	13% 90% 5% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6450 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.

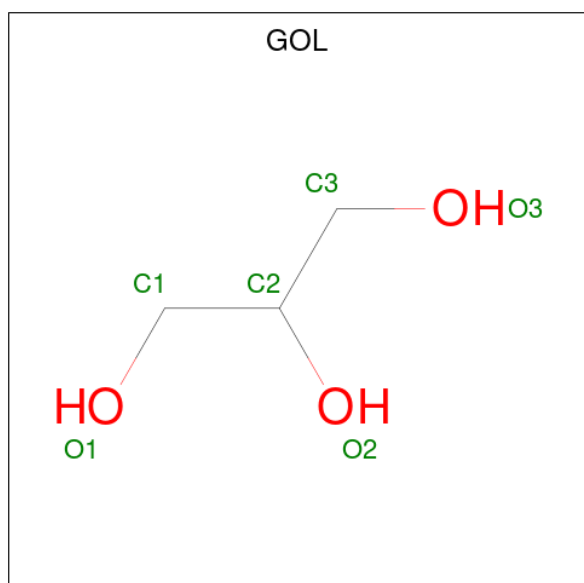
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	1	0
			3034	1965	505	552	12			
1	B	376	Total	C	N	O	S	0	4	0
			3067	1983	512	560	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLY	-	expression tag	UNP Q99683
A	267	PRO	-	expression tag	UNP Q99683
A	268	GLY	-	expression tag	UNP Q99683
B	266	GLY	-	expression tag	UNP Q99683
B	267	PRO	-	expression tag	UNP Q99683
B	268	GLY	-	expression tag	UNP Q99683

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

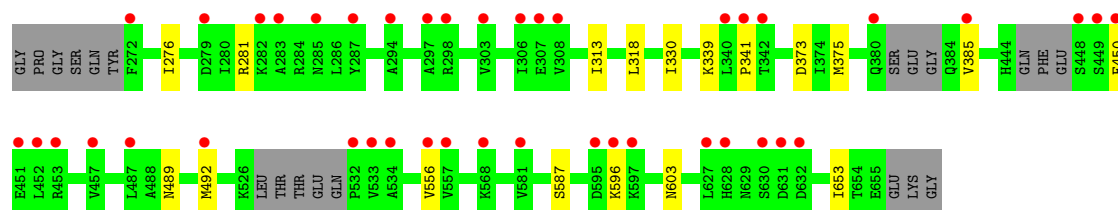
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	173	Total	O	0	0
			173	173		

3 Residue-property plots [i](#)

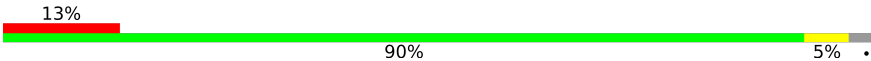
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

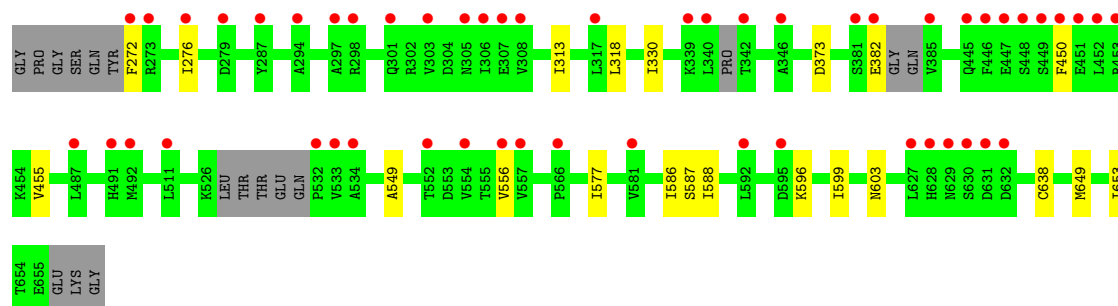
- Molecule 1: Mitogen-activated protein kinase kinase kinase 5

Chain A: 



- Molecule 1: Mitogen-activated protein kinase kinase kinase 5

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.23Å 57.12Å 103.58Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	47.10 – 2.10 47.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.10-2.10) 99.7 (47.10-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.233 , 0.267 0.242 , 0.279	Depositor DCC
R_{free} test set	2430 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6450	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0429e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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

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	0.81	0/3104	0.94	3/4195 (0.1%)
1	B	0.80	0/3142	0.95	3/4244 (0.1%)
All	All	0.80	0/6246	0.95	6/8439 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	GLU	CA-C-O	6.21	131.36	120.80
1	A	341	PRO	CB-CA-C	-5.75	103.23	112.21
1	B	455	VAL	N-CA-C	-5.58	105.08	110.72
1	A	556	VAL	N-CA-C	5.46	116.63	109.21
1	B	556	VAL	N-CA-C	5.35	116.49	109.21
1	A	375	MET	N-CA-C	5.01	116.82	111.36

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	3034	0	3036	3	0
1	B	3067	0	3062	5	0
2	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	170	0	0	1	0
3	B	173	0	0	0	0
All	All	6450	0	6106	8	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 1.

All (8) 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:281:ARG:NH1	3:A:701:HOH:O	2.28	0.56
1:A:587[A]:SER:OG	1:A:603:ASN:ND2	2.39	0.55
1:B:587[A]:SER:OG	1:B:603:ASN:ND2	2.39	0.55
1:B:577:ILE:HG21	1:B:649:MET:HE2	1.89	0.55
1:B:586:ILE:HG22	1:B:588[B]:ILE:HD11	1.92	0.50
1:A:318:LEU:HD22	1:A:330:ILE:HG23	1.99	0.45
1:B:318:LEU:HD22	1:B:330:ILE:HG23	1.99	0.43
1:B:549:ALA:HB2	1:B:638:CYS:HB2	2.03	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	366/393 (93%)	359 (98%)	7 (2%)	0	100	100
1	B	372/393 (95%)	365 (98%)	7 (2%)	0	100	100
All	All	738/786 (94%)	724 (98%)	14 (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	335/353 (95%)	325 (97%)	10 (3%)	36	41
1	B	338/353 (96%)	330 (98%)	8 (2%)	43	49
All	All	673/706 (95%)	655 (97%)	18 (3%)	39	45

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ILE
1	A	313	ILE
1	A	339	LYS
1	A	373	ASP
1	A	385	VAL
1	A	450	PHE
1	A	489	ASN
1	A	492	MET
1	A	596	LYS
1	A	653	ILE
1	B	272	PHE
1	B	276	ILE
1	B	313	ILE
1	B	373	ASP
1	B	450	PHE
1	B	596	LYS
1	B	599	ILE
1	B	653	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	A	489	ASN
1	A	523	HIS
1	A	578	ASN

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Mol	Chain	Res	Type
1	A	600	HIS
1	A	603	ASN
1	A	629	ASN
1	A	651	ASN
1	B	325	GLN
1	B	434	ASN
1	B	523	HIS
1	B	600	HIS
1	B	603	ASN
1	B	629	ASN
1	B	651	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](#)

1 ligand is 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	$\# Z > 2$
2	GOL	B	701	-	5,5,5	0.32	0	5,5,5	0.49	0

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
2	GOL	B	701	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	373/393 (94%)	0.72	42 (11%)	10 10	13, 26, 58, 85	1 (0%)
1	B	376/393 (95%)	0.87	52 (13%)	6 6	11, 26, 60, 96	4 (1%)
All	All	749/786 (95%)	0.79	94 (12%)	8 8	11, 26, 59, 96	5 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	PHE	7.8
1	B	272	PHE	7.1
1	B	557	VAL	6.2
1	B	534	ALA	6.1
1	A	534	ALA	6.0
1	B	450	PHE	5.9
1	B	446	PHE	5.2
1	B	628	HIS	5.2
1	B	449[A]	SER	4.7
1	A	453	ARG	4.6
1	B	340	LEU	4.6
1	A	449	SER	4.5
1	A	557	VAL	4.5
1	A	532	PRO	4.1
1	B	342	THR	4.0
1	B	532	PRO	4.0
1	A	272	PHE	4.0
1	B	306	ILE	3.9
1	B	453	ARG	3.8
1	A	451	GLU	3.8
1	B	533	VAL	3.7
1	B	308	VAL	3.6
1	A	556	VAL	3.5
1	B	382	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	297	ALA	3.4
1	A	452	LEU	3.4
1	B	451	GLU	3.4
1	B	630	SER	3.3
1	B	556	VAL	3.2
1	A	341	PRO	3.2
1	B	297	ALA	3.2
1	A	306	ILE	3.1
1	A	448	SER	3.1
1	A	279	ASP	3.0
1	A	631	ASP	3.0
1	A	308	VAL	3.0
1	B	448	SER	3.0
1	A	595	ASP	2.9
1	B	447	GLU	2.9
1	A	303	VAL	2.8
1	B	303	VAL	2.8
1	A	628	HIS	2.8
1	A	630	SER	2.7
1	B	452	LEU	2.7
1	A	282	LYS	2.7
1	B	339	LYS	2.7
1	B	307	GLU	2.7
1	B	346	ALA	2.6
1	A	307	GLU	2.6
1	B	629	ASN	2.6
1	A	627	LEU	2.6
1	B	385	VAL	2.6
1	B	294	ALA	2.6
1	A	533	VAL	2.6
1	A	294	ALA	2.6
1	A	487	LEU	2.5
1	B	627	LEU	2.5
1	A	385	VAL	2.5
1	B	487	LEU	2.5
1	B	381	SER	2.4
1	B	276	ILE	2.4
1	A	596	LYS	2.4
1	B	632	ASP	2.4
1	B	581	VAL	2.4
1	B	491	HIS	2.4
1	B	511	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	ARG	2.3
1	A	581	VAL	2.3
1	B	279	ASP	2.3
1	A	597	LYS	2.3
1	B	445	GLN	2.3
1	A	340	LEU	2.3
1	B	592	LEU	2.3
1	B	631	ASP	2.3
1	B	492	MET	2.3
1	A	632	ASP	2.2
1	B	317	LEU	2.2
1	A	457	VAL	2.2
1	B	301	GLN	2.2
1	A	283	ALA	2.2
1	B	298	ARG	2.2
1	B	552	THR	2.2
1	B	305	ASN	2.1
1	B	554	VAL	2.1
1	B	287	TYR	2.1
1	A	380	GLN	2.1
1	A	492	MET	2.0
1	A	285	ASN	2.0
1	B	273	ARG	2.0
1	A	342	THR	2.0
1	B	566	PRO	2.0
1	A	287	TYR	2.0
1	B	595	ASP	2.0
1	A	568	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	701	6/6	0.82	0.15	32,41,43,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.