



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:18 AM UTC

PDB ID : 2ONL / pdb_00002onl
Title : Crystal Structure of the p38a-MAPKAP kinase 2 Heterodimer
Authors : Ter Haar, E.
Deposited on : 2007-01-24
Resolution : 4.00 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 ⓘ 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

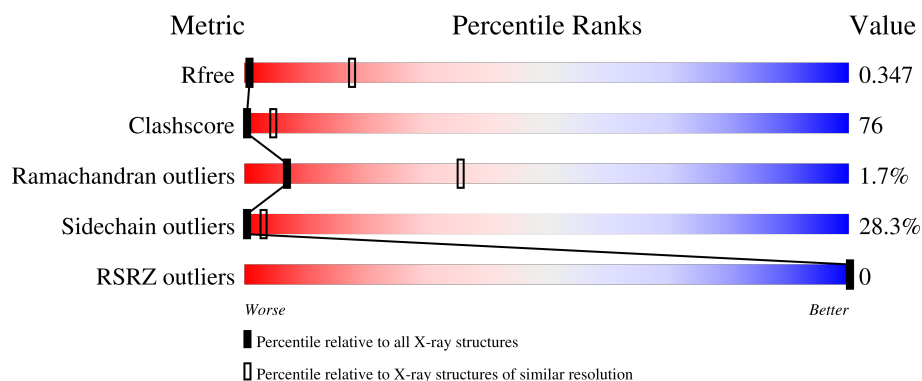
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 $\leq 5\%$. 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	366	
1	B	366	
2	C	406	
2	D	406	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10466 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 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2709	1737	466	494	12			
1	B	339	Total	C	N	O	S	0	0	0
			2714	1740	467	495	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	cloning artifact	UNP Q16539
A	-4	SER	-	cloning artifact	UNP Q16539
A	-3	HIS	-	cloning artifact	UNP Q16539
A	-2	MET	-	cloning artifact	UNP Q16539
A	-1	LEU	-	cloning artifact	UNP Q16539
A	0	GLU	-	cloning artifact	UNP Q16539
A	1	MET	-	cloning artifact	UNP Q16539
B	-5	GLY	-	cloning artifact	UNP Q16539
B	-4	SER	-	cloning artifact	UNP Q16539
B	-3	HIS	-	cloning artifact	UNP Q16539
B	-2	MET	-	cloning artifact	UNP Q16539
B	-1	LEU	-	cloning artifact	UNP Q16539
B	0	GLU	-	cloning artifact	UNP Q16539
B	1	MET	-	cloning artifact	UNP Q16539

- Molecule 2 is a protein called MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	317	Total	C	N	O	S	0	0	0
			2531	1611	440	462	18			
2	D	313	Total	C	N	O	S	0	0	0
			2512	1597	437	460	18			

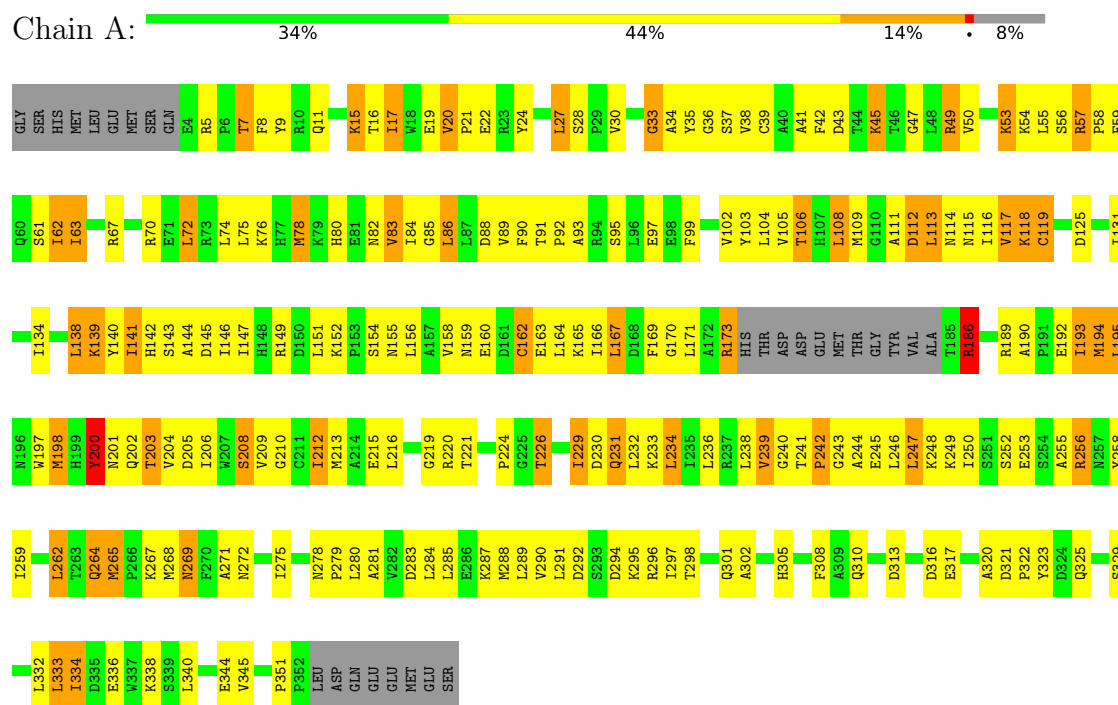
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	cloning artifact	UNP P49137
C	-4	SER	-	cloning artifact	UNP P49137
C	-3	HIS	-	cloning artifact	UNP P49137
C	-2	MET	-	cloning artifact	UNP P49137
C	-1	LEU	-	cloning artifact	UNP P49137
C	0	GLU	-	cloning artifact	UNP P49137
D	-5	GLY	-	cloning artifact	UNP P49137
D	-4	SER	-	cloning artifact	UNP P49137
D	-3	HIS	-	cloning artifact	UNP P49137
D	-2	MET	-	cloning artifact	UNP P49137
D	-1	LEU	-	cloning artifact	UNP P49137
D	0	GLU	-	cloning artifact	UNP P49137

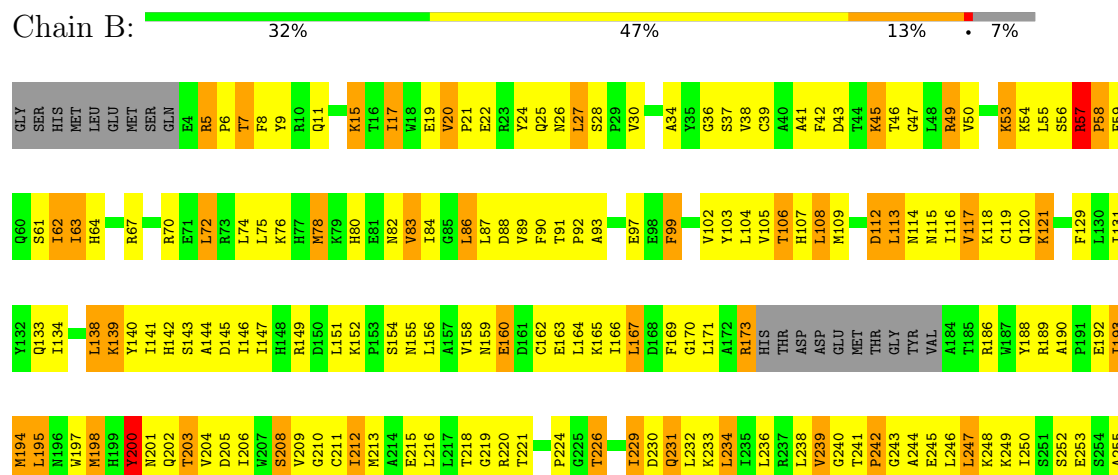
3 Residue-property plots

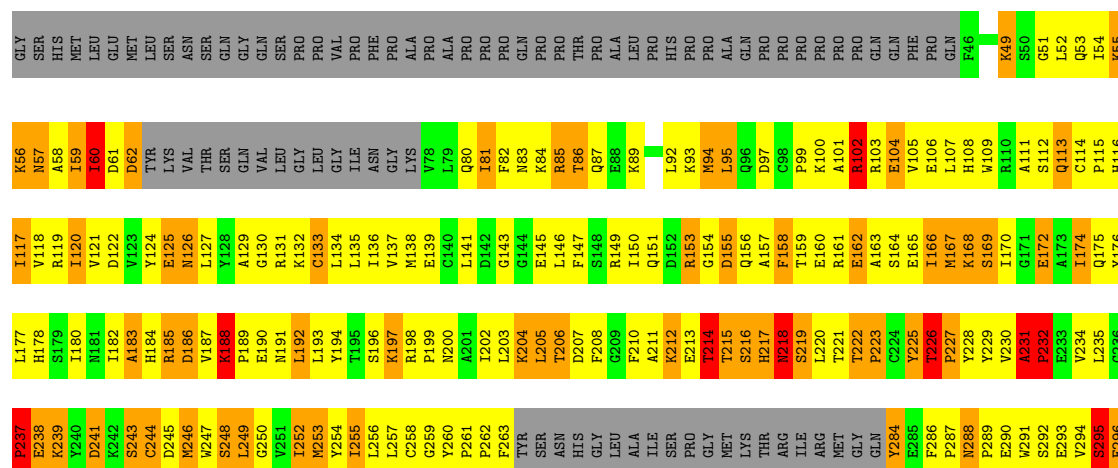
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 14



• Molecule 1: Mitogen-activated protein kinase 14





E297	T357
V298	S358
K299	A359
M300	L360
L301	A361
I302	T362
R303	M363
N304	R364
L305	V365
L306	D366
K307	Y367
T308	E368
E309	Q369
P310	I370
T311	K371
Q312	I372
R313	K373
M314	K374
T315	I375
I316	E376
T317	D377
E318	A378
F319	S379
N320	N380
N321	P381
H322	L382
P323	L383
W324	L384
I325	K385
M326	K386
Q327	K387
S328	K388
T329	K389
K330	A390
V331	R391
P332	A392
Q333	I393
T334	GLU
P335	ALA
L336	ALA
H337	ALA
T338	LEU
S339	ALA
R340	HIS
V341	
L342	
K343	
E344	
D345	
K346	
E347	
R348	
W349	
E350	
D351	
V352	
K353	
E354	
E355	
M356	

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	103.15Å 103.15Å 231.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.34 – 4.00 45.34 – 4.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.34-4.00) 95.9 (45.34-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 4.00Å)	Xtriage
Refinement program	BUSTER-TNT V. 1.1.0	Depositor
R, R_{free}	0.314 , 0.331 0.339 , 0.347	Depositor DCC
R_{free} test set	984 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	106.4	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 336.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.219 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10466	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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	0.33	0/2770	0.84	5/3758 (0.1%)
1	B	0.33	0/2775	0.80	5/3765 (0.1%)
2	C	0.29	0/2583	1.00	18/3480 (0.5%)
2	D	0.32	0/2563	0.89	11/3453 (0.3%)
All	All	0.32	0/10691	0.88	39/14456 (0.3%)

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
1	B	0	1
2	C	0	24
2	D	0	25
All	All	0	52

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	234	VAL	N-CA-C	14.53	128.00	107.37
1	A	265	MET	N-CA-C	9.91	131.71	109.81
1	A	264	GLN	N-CA-C	8.80	120.56	110.97
2	C	297	GLU	N-CA-C	-8.71	101.91	112.54
2	C	258	CYS	N-CA-C	-8.70	102.68	113.38

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Peptide
1	A	33	GLY	Peptide
2	C	153	ARG	Peptide
2	C	154	GLY	Peptide
2	C	89	LYS	Peptide

5.2 Too-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 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	2709	0	2701	305	0
1	B	2714	0	2706	327	0
2	C	2531	0	2509	540	6
2	D	2512	0	2500	506	2
All	All	10466	0	10416	1583	8

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 76.

The worst 5 of 1583 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:159:ASN:C	2:D:370:ILE:HD13	1.35	1.47
2:D:214:THR:HG23	2:D:237:PRO:O	1.24	1.37
2:C:315:THR:CG2	2:C:318:GLU:CB	2.02	1.36
2:D:214:THR:CG2	2:D:238:GLU:HA	1.58	1.33
2:D:99:PRO:O	2:D:103:ARG:HG3	1.22	1.32

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:ALA:CB	2:C:226:THR:OG1[4_574]	1.62	0.58
2:C:58:ALA:CA	2:C:226:THR:OG1[4_574]	1.75	0.45
2:D:58:ALA:CA	2:D:226:THR:O[3_745]	1.87	0.33
2:D:58:ALA:N	2:D:226:THR:O[3_745]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:ALA:N	2:C:226:THR:CG2[4_574]	1.90	0.30

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	334/366 (91%)	307 (92%)	25 (8%)	2 (1%)	21	57
1	B	335/366 (92%)	309 (92%)	23 (7%)	3 (1%)	14	48
2	C	311/406 (77%)	262 (84%)	40 (13%)	9 (3%)	3	26
2	D	307/406 (76%)	247 (80%)	52 (17%)	8 (3%)	4	29
All	All	1287/1544 (83%)	1125 (87%)	140 (11%)	22 (2%)	7	36

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	237	PRO
2	D	232	PRO
2	D	237	PRO
2	C	222	THR
2	C	232	PRO

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	294/325 (90%)	226 (77%)	68 (23%)	1	6
1	B	294/325 (90%)	230 (78%)	64 (22%)	1	6
2	C	272/362 (75%)	179 (66%)	93 (34%)	0	2
2	D	273/362 (75%)	177 (65%)	96 (35%)	0	2
All	All	1133/1374 (82%)	812 (72%)	321 (28%)	0	3

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	81	ILE
2	D	255	ILE
2	D	102	ARG
2	D	174	ILE
2	D	320	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	228	HIS
2	D	96	GLN
1	B	231	GLN
2	D	57	ASN
2	D	113	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 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 [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	338/366 (92%)	-0.90	0 100 100	100, 100, 100, 100	0
1	B	339/366 (92%)	-0.95	0 100 100	100, 100, 100, 100	0
2	C	317/406 (78%)	-0.92	0 100 100	20, 100, 100, 100	0
2	D	313/406 (77%)	-0.92	0 100 100	100, 100, 100, 100	0
All	All	1307/1544 (84%)	-0.92	0 100 100	20, 100, 100, 100	0

There are no RSRZ outliers to report.

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.