



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:15 AM UTC

PDB ID : 7XBR / pdb_00007xbr
Title : Crystal structure of phosphorylated AtMKK5
Authors : Pei, C.J.; Luo, Z.P.; Wu, J.W.; Wang, Z.X.
Deposited on : 2022-03-22
Resolution : 3.20 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

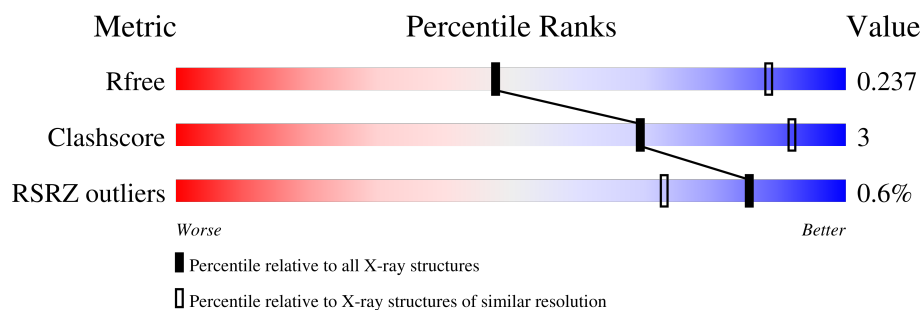
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	295	 80% 8% 11%
1	B	295	 79% 9% 13%
1	C	295	 76% 14% 10%
1	D	295	 72% 15% 13%
1	E	295	 80% 8% 13%
1	G	295	 78% 10% 13%
2	F	295	 73% 14% 13%

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Mol	Chain	Length	Quality of chain
2	H	295	81% 7% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16581 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 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	P	S	0	0	0
			2100	1311	377	394	5	13			
1	B	258	Total	C	N	O	P	S	0	0	0
			2072	1295	369	390	5	13			
1	C	266	Total	C	N	O	P	S	0	0	0
			2121	1322	381	400	5	13			
1	D	256	Total	C	N	O	P	S	0	0	0
			2062	1290	370	385	4	13			
1	E	258	Total	C	N	O	P	S	0	0	0
			2070	1294	369	389	5	13			
1	G	258	Total	C	N	O	P	S	0	0	0
			2029	1271	357	383	5	13			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP Q8RXG3
A	42	GLY	-	expression tag	UNP Q8RXG3
A	43	SER	-	expression tag	UNP Q8RXG3
A	44	SER	-	expression tag	UNP Q8RXG3
A	45	HIS	-	expression tag	UNP Q8RXG3
A	46	HIS	-	expression tag	UNP Q8RXG3
A	47	HIS	-	expression tag	UNP Q8RXG3
A	48	HIS	-	expression tag	UNP Q8RXG3
A	49	HIS	-	expression tag	UNP Q8RXG3
A	50	HIS	-	expression tag	UNP Q8RXG3
A	51	SER	-	expression tag	UNP Q8RXG3
A	52	SER	-	expression tag	UNP Q8RXG3
A	53	GLY	-	expression tag	UNP Q8RXG3
A	54	LEU	-	expression tag	UNP Q8RXG3
A	55	VAL	-	expression tag	UNP Q8RXG3
A	56	PRO	-	expression tag	UNP Q8RXG3
A	57	ARG	-	expression tag	UNP Q8RXG3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLY	-	expression tag	UNP Q8RXG3
A	59	SER	-	expression tag	UNP Q8RXG3
A	60	HIS	-	expression tag	UNP Q8RXG3
A	61	MET	-	expression tag	UNP Q8RXG3
B	41	MET	-	initiating methionine	UNP Q8RXG3
B	42	GLY	-	expression tag	UNP Q8RXG3
B	43	SER	-	expression tag	UNP Q8RXG3
B	44	SER	-	expression tag	UNP Q8RXG3
B	45	HIS	-	expression tag	UNP Q8RXG3
B	46	HIS	-	expression tag	UNP Q8RXG3
B	47	HIS	-	expression tag	UNP Q8RXG3
B	48	HIS	-	expression tag	UNP Q8RXG3
B	49	HIS	-	expression tag	UNP Q8RXG3
B	50	HIS	-	expression tag	UNP Q8RXG3
B	51	SER	-	expression tag	UNP Q8RXG3
B	52	SER	-	expression tag	UNP Q8RXG3
B	53	GLY	-	expression tag	UNP Q8RXG3
B	54	LEU	-	expression tag	UNP Q8RXG3
B	55	VAL	-	expression tag	UNP Q8RXG3
B	56	PRO	-	expression tag	UNP Q8RXG3
B	57	ARG	-	expression tag	UNP Q8RXG3
B	58	GLY	-	expression tag	UNP Q8RXG3
B	59	SER	-	expression tag	UNP Q8RXG3
B	60	HIS	-	expression tag	UNP Q8RXG3
B	61	MET	-	expression tag	UNP Q8RXG3
C	41	MET	-	initiating methionine	UNP Q8RXG3
C	42	GLY	-	expression tag	UNP Q8RXG3
C	43	SER	-	expression tag	UNP Q8RXG3
C	44	SER	-	expression tag	UNP Q8RXG3
C	45	HIS	-	expression tag	UNP Q8RXG3
C	46	HIS	-	expression tag	UNP Q8RXG3
C	47	HIS	-	expression tag	UNP Q8RXG3
C	48	HIS	-	expression tag	UNP Q8RXG3
C	49	HIS	-	expression tag	UNP Q8RXG3
C	50	HIS	-	expression tag	UNP Q8RXG3
C	51	SER	-	expression tag	UNP Q8RXG3
C	52	SER	-	expression tag	UNP Q8RXG3
C	53	GLY	-	expression tag	UNP Q8RXG3
C	54	LEU	-	expression tag	UNP Q8RXG3
C	55	VAL	-	expression tag	UNP Q8RXG3
C	56	PRO	-	expression tag	UNP Q8RXG3
C	57	ARG	-	expression tag	UNP Q8RXG3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	58	GLY	-	expression tag	UNP Q8RXG3
C	59	SER	-	expression tag	UNP Q8RXG3
C	60	HIS	-	expression tag	UNP Q8RXG3
C	61	MET	-	expression tag	UNP Q8RXG3
D	41	MET	-	initiating methionine	UNP Q8RXG3
D	42	GLY	-	expression tag	UNP Q8RXG3
D	43	SER	-	expression tag	UNP Q8RXG3
D	44	SER	-	expression tag	UNP Q8RXG3
D	45	HIS	-	expression tag	UNP Q8RXG3
D	46	HIS	-	expression tag	UNP Q8RXG3
D	47	HIS	-	expression tag	UNP Q8RXG3
D	48	HIS	-	expression tag	UNP Q8RXG3
D	49	HIS	-	expression tag	UNP Q8RXG3
D	50	HIS	-	expression tag	UNP Q8RXG3
D	51	SER	-	expression tag	UNP Q8RXG3
D	52	SER	-	expression tag	UNP Q8RXG3
D	53	GLY	-	expression tag	UNP Q8RXG3
D	54	LEU	-	expression tag	UNP Q8RXG3
D	55	VAL	-	expression tag	UNP Q8RXG3
D	56	PRO	-	expression tag	UNP Q8RXG3
D	57	ARG	-	expression tag	UNP Q8RXG3
D	58	GLY	-	expression tag	UNP Q8RXG3
D	59	SER	-	expression tag	UNP Q8RXG3
D	60	HIS	-	expression tag	UNP Q8RXG3
D	61	MET	-	expression tag	UNP Q8RXG3
E	41	MET	-	initiating methionine	UNP Q8RXG3
E	42	GLY	-	expression tag	UNP Q8RXG3
E	43	SER	-	expression tag	UNP Q8RXG3
E	44	SER	-	expression tag	UNP Q8RXG3
E	45	HIS	-	expression tag	UNP Q8RXG3
E	46	HIS	-	expression tag	UNP Q8RXG3
E	47	HIS	-	expression tag	UNP Q8RXG3
E	48	HIS	-	expression tag	UNP Q8RXG3
E	49	HIS	-	expression tag	UNP Q8RXG3
E	50	HIS	-	expression tag	UNP Q8RXG3
E	51	SER	-	expression tag	UNP Q8RXG3
E	52	SER	-	expression tag	UNP Q8RXG3
E	53	GLY	-	expression tag	UNP Q8RXG3
E	54	LEU	-	expression tag	UNP Q8RXG3
E	55	VAL	-	expression tag	UNP Q8RXG3
E	56	PRO	-	expression tag	UNP Q8RXG3
E	57	ARG	-	expression tag	UNP Q8RXG3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	58	GLY	-	expression tag	UNP Q8RXG3
E	59	SER	-	expression tag	UNP Q8RXG3
E	60	HIS	-	expression tag	UNP Q8RXG3
E	61	MET	-	expression tag	UNP Q8RXG3
G	41	MET	-	initiating methionine	UNP Q8RXG3
G	42	GLY	-	expression tag	UNP Q8RXG3
G	43	SER	-	expression tag	UNP Q8RXG3
G	44	SER	-	expression tag	UNP Q8RXG3
G	45	HIS	-	expression tag	UNP Q8RXG3
G	46	HIS	-	expression tag	UNP Q8RXG3
G	47	HIS	-	expression tag	UNP Q8RXG3
G	48	HIS	-	expression tag	UNP Q8RXG3
G	49	HIS	-	expression tag	UNP Q8RXG3
G	50	HIS	-	expression tag	UNP Q8RXG3
G	51	SER	-	expression tag	UNP Q8RXG3
G	52	SER	-	expression tag	UNP Q8RXG3
G	53	GLY	-	expression tag	UNP Q8RXG3
G	54	LEU	-	expression tag	UNP Q8RXG3
G	55	VAL	-	expression tag	UNP Q8RXG3
G	56	PRO	-	expression tag	UNP Q8RXG3
G	57	ARG	-	expression tag	UNP Q8RXG3
G	58	GLY	-	expression tag	UNP Q8RXG3
G	59	SER	-	expression tag	UNP Q8RXG3
G	60	HIS	-	expression tag	UNP Q8RXG3
G	61	MET	-	expression tag	UNP Q8RXG3

- Molecule 2 is a protein called Mitogen-activated protein kinase kinase 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	257	Total	C	N	O	P	S	0	0	0
			2055	1286	366	386	4	13			
2	H	260	Total	C	N	O	P	S	0	0	0
			2072	1298	370	387	4	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	41	MET	-	initiating methionine	UNP Q8RXG3
F	42	GLY	-	expression tag	UNP Q8RXG3
F	43	SER	-	expression tag	UNP Q8RXG3
F	44	SER	-	expression tag	UNP Q8RXG3
F	45	HIS	-	expression tag	UNP Q8RXG3

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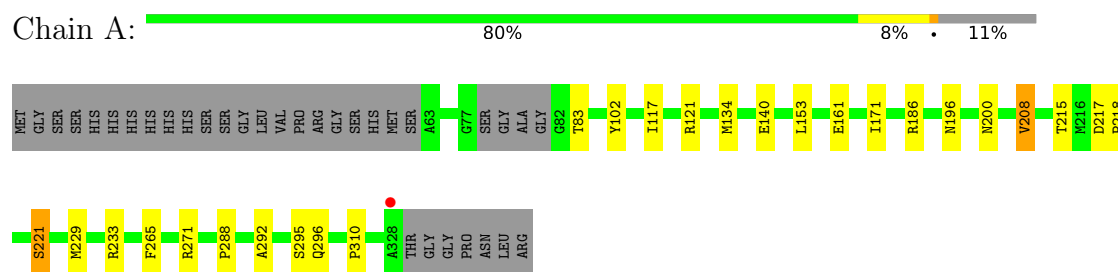
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Chain	Residue	Modelled	Actual	Comment	Reference
F	46	HIS	-	expression tag	UNP Q8RXG3
F	47	HIS	-	expression tag	UNP Q8RXG3
F	48	HIS	-	expression tag	UNP Q8RXG3
F	49	HIS	-	expression tag	UNP Q8RXG3
F	50	HIS	-	expression tag	UNP Q8RXG3
F	51	SER	-	expression tag	UNP Q8RXG3
F	52	SER	-	expression tag	UNP Q8RXG3
F	53	GLY	-	expression tag	UNP Q8RXG3
F	54	LEU	-	expression tag	UNP Q8RXG3
F	55	VAL	-	expression tag	UNP Q8RXG3
F	56	PRO	-	expression tag	UNP Q8RXG3
F	57	ARG	-	expression tag	UNP Q8RXG3
F	58	GLY	-	expression tag	UNP Q8RXG3
F	59	SER	-	expression tag	UNP Q8RXG3
F	60	HIS	-	expression tag	UNP Q8RXG3
F	61	MET	-	expression tag	UNP Q8RXG3
H	41	MET	-	initiating methionine	UNP Q8RXG3
H	42	GLY	-	expression tag	UNP Q8RXG3
H	43	SER	-	expression tag	UNP Q8RXG3
H	44	SER	-	expression tag	UNP Q8RXG3
H	45	HIS	-	expression tag	UNP Q8RXG3
H	46	HIS	-	expression tag	UNP Q8RXG3
H	47	HIS	-	expression tag	UNP Q8RXG3
H	48	HIS	-	expression tag	UNP Q8RXG3
H	49	HIS	-	expression tag	UNP Q8RXG3
H	50	HIS	-	expression tag	UNP Q8RXG3
H	51	SER	-	expression tag	UNP Q8RXG3
H	52	SER	-	expression tag	UNP Q8RXG3
H	53	GLY	-	expression tag	UNP Q8RXG3
H	54	LEU	-	expression tag	UNP Q8RXG3
H	55	VAL	-	expression tag	UNP Q8RXG3
H	56	PRO	-	expression tag	UNP Q8RXG3
H	57	ARG	-	expression tag	UNP Q8RXG3
H	58	GLY	-	expression tag	UNP Q8RXG3
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H	61	MET	-	expression tag	UNP Q8RXG3

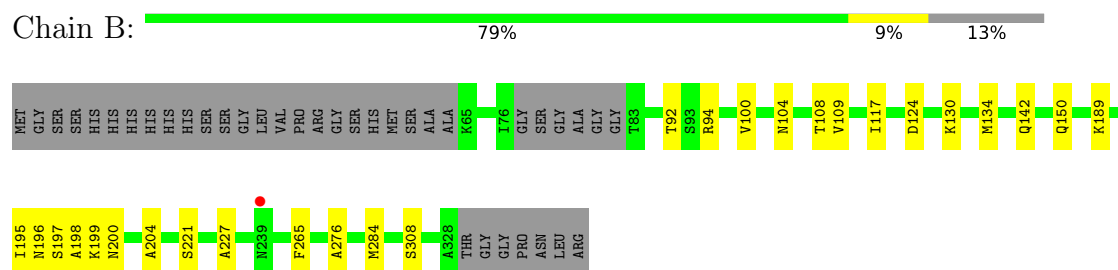
3 Residue-property plots [i](#)

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.

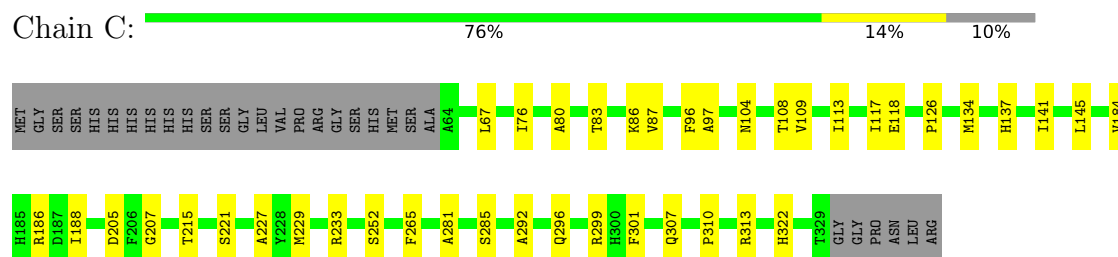
- Molecule 1: Mitogen-activated protein kinase kinase 5



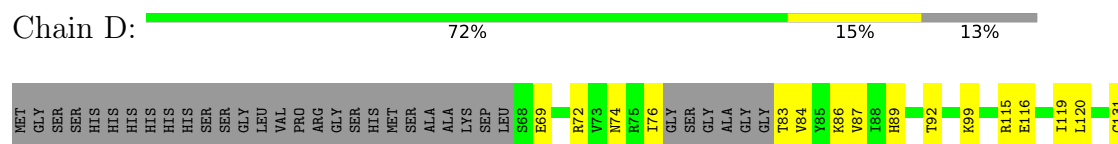
- Molecule 1: Mitogen-activated protein kinase kinase 5

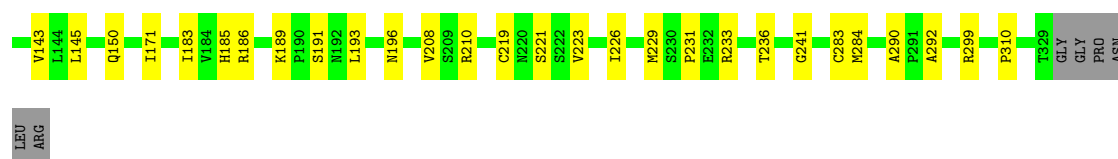


- Molecule 1: Mitogen-activated protein kinase kinase 5

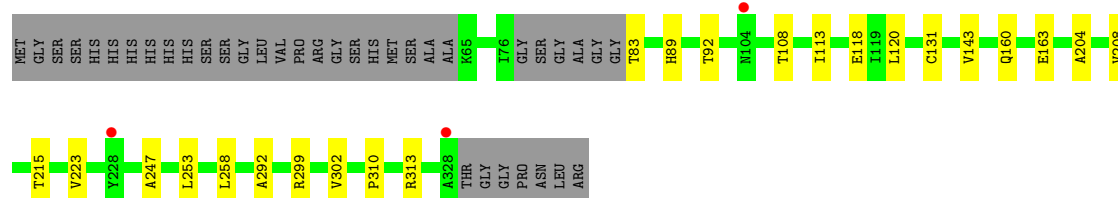
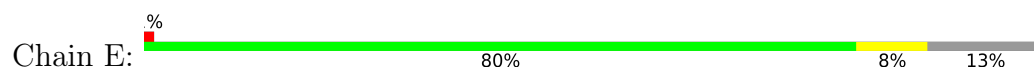


- Molecule 1: Mitogen-activated protein kinase kinase 5

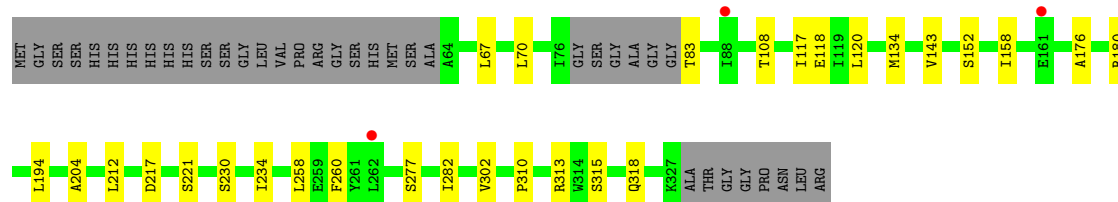
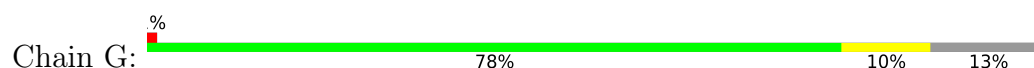




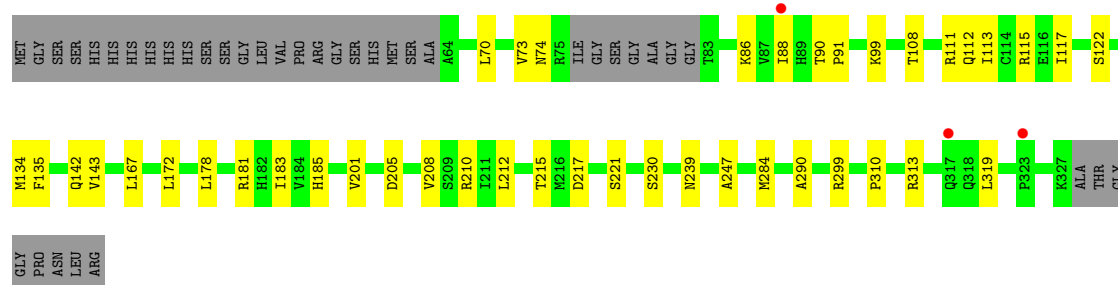
- Molecule 1: Mitogen-activated protein kinase kinase 5



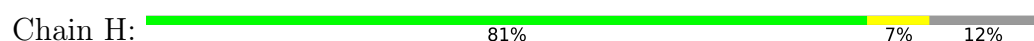
- Molecule 1: Mitogen-activated protein kinase kinase 5



- Molecule 2: Mitogen-activated protein kinase kinase 5



- Molecule 2: Mitogen-activated protein kinase kinase 5



V184	H185	R186	V201	F265	P266	M284	P310	A328	T329	GLY	GLY	PRO	ASN	LEU	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.67Å 198.57Å 202.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 3.20 49.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.13-3.20) 96.7 (49.13-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.246 (Not available) , 0.237	Depositor DCC
R_{free} test set	2647 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	91.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16581	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.08% 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

5.1 Standard geometry

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

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	1.06	0/2090	1.39	8/2821 (0.3%)
1	B	1.04	0/2063	1.39	3/2789 (0.1%)
1	C	1.02	1/2112 (0.0%)	1.40	4/2852 (0.1%)
1	D	1.01	0/2064	1.36	4/2791 (0.1%)
1	E	1.00	0/2060	1.36	5/2784 (0.2%)
1	G	1.01	0/2019	1.35	5/2734 (0.2%)
2	F	1.00	0/2056	1.37	4/2780 (0.1%)
2	H	1.01	0/2074	1.34	2/2805 (0.1%)
All	All	1.02	1/16538 (0.0%)	1.37	35/22356 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	126	PRO	C-O	-5.16	1.17	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	PRO	N-CA-C	7.89	120.33	110.70
1	D	310	PRO	N-CA-C	6.92	119.14	110.70
1	B	204	ALA	CA-C-O	-6.84	115.87	119.77
1	C	310	PRO	N-CA-C	6.84	119.05	110.70
1	E	310	PRO	N-CA-C	6.52	118.65	110.70
2	F	310	PRO	N-CA-C	6.36	118.46	110.70
1	A	153	LEU	N-CA-C	-6.14	105.72	112.72
2	F	208	VAL	N-CA-C	-6.12	107.29	113.47
1	D	208	VAL	N-CA-C	-5.96	107.45	113.47
1	G	310	PRO	N-CA-C	5.94	117.94	110.70
1	E	113	ILE	N-CA-C	-5.86	105.03	110.53
1	C	296	GLN	N-CA-C	-5.83	104.89	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	212	LEU	CA-C-N	5.69	127.83	120.44
1	G	212	LEU	C-N-CA	5.69	127.83	120.44
1	C	205	ASP	CA-CB-CG	5.52	118.12	112.60
2	F	113	ILE	N-CA-C	-5.49	104.97	110.30
2	H	310	PRO	N-CA-C	5.48	117.38	110.70
1	G	217	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	189	LYS	N-CA-C	-5.30	103.45	108.22
1	E	253	LEU	CA-C-N	5.25	125.81	119.98
1	E	253	LEU	C-N-CA	5.25	125.81	119.98
1	A	208	VAL	N-CA-C	-5.24	107.61	112.43
1	D	69	GLU	CB-CA-C	5.18	119.36	111.02
2	H	162	GLN	N-CA-C	-5.18	105.81	111.82
1	A	296	GLN	N-CA-C	-5.15	105.56	111.07
1	A	171	ILE	N-CA-C	-5.15	105.37	110.62
1	G	204	ALA	CA-C-O	-5.12	116.85	119.77
1	B	308	SER	N-CA-C	-5.10	105.62	111.07
1	C	113	ILE	N-CA-C	-5.06	105.56	110.42
1	A	288	PRO	CA-C-O	-5.04	115.83	121.23
1	D	185	HIS	O-C-N	5.04	128.12	122.32
1	E	204	ALA	CA-C-O	-5.03	116.90	119.77
2	F	113	ILE	N-CA-CB	5.03	116.10	110.62
1	A	292	ALA	CA-C-N	5.01	127.00	120.28
1	A	292	ALA	C-N-CA	5.01	127.00	120.28

There are no chirality outliers.

There are no planarity outliers.

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	2100	0	2043	10	0
1	B	2072	0	2008	12	0
1	C	2121	0	2062	17	0
1	D	2062	0	2010	22	0
1	E	2070	0	2010	11	0
1	G	2029	0	1938	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2055	0	1990	26	0
2	H	2072	0	2009	11	0
All	All	16581	0	16070	114	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 3.

All (114) 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:150:GLN:HB2	1:B:195:ILE:HG23	1.66	0.76
1:B:284:MET:HE1	1:C:118:GLU:HA	1.71	0.73
1:A:229:MET:HE2	1:A:233:ARG:HB3	1.75	0.66
2:F:90:THR:OG1	2:F:91:PRO:HD3	1.95	0.66
1:D:284:MET:HE1	1:G:118:GLU:HA	1.77	0.65
1:C:307:GLN:HB2	1:C:313:ARG:HG2	1.81	0.62
1:E:258:LEU:HD13	1:E:302:VAL:HG11	1.80	0.62
2:H:67:LEU:HD22	2:H:137:HIS:HB2	1.81	0.61
1:C:229:MET:HE2	1:C:233:ARG:HB3	1.85	0.58
2:H:101:ILE:HB	2:H:141:ILE:HG23	1.86	0.58
1:A:117:ILE:HG23	1:A:134:MET:HE1	1.86	0.57
1:B:117:ILE:HG23	1:B:134:MET:HE1	1.86	0.56
2:F:122:SER:HB3	2:F:181:ARG:HH22	1.70	0.56
1:C:292:ALA:HA	1:C:299:ARG:HD3	1.87	0.56
1:D:186:ARG:HH21	1:D:219:CYS:HB3	1.69	0.56
1:A:102:TYR:HD1	1:A:140:GLU:HB3	1.71	0.56
2:F:117:ILE:HD12	2:F:134:MET:HE1	1.88	0.55
1:G:315:SER:HB3	1:G:318:GLN:HG2	1.89	0.54
1:D:284:MET:HE2	1:G:117:ILE:HG22	1.88	0.54
1:D:72:ARG:HA	1:D:87:VAL:HG12	1.90	0.54
1:D:74:ASN:HB3	1:D:86:LYS:HB3	1.90	0.54
2:F:290:ALA:HB3	2:F:299:ARG:HG2	1.90	0.53
1:E:120:LEU:HD13	1:E:143:VAL:HG21	1.91	0.53
1:D:120:LEU:HD13	1:D:143:VAL:HG21	1.90	0.52
1:D:290:ALA:HB3	1:D:299:ARG:HG2	1.92	0.52
1:E:247:ALA:HB1	1:E:313:ARG:HD2	1.91	0.52
1:A:121:ARG:HD3	2:H:284:MET:HE2	1.92	0.52
1:D:292:ALA:HA	1:D:299:ARG:HD3	1.91	0.52
1:E:292:ALA:HA	1:E:299:ARG:HD3	1.92	0.52
2:F:112:GLN:HA	2:F:115:ARG:CD	2.39	0.52
2:H:265:PHE:HD2	2:H:266:PRO:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:GLN:HA	2:F:115:ARG:HD2	1.93	0.50
1:E:160:GLN:HB3	1:E:163:GLU:HB3	1.93	0.50
1:B:104:ASN:H	1:B:109:VAL:HG11	1.76	0.50
1:D:171:ILE:HD13	1:D:193:LEU:HD13	1.94	0.50
1:B:198:ALA:O	1:B:199:LYS:HB2	2.12	0.49
1:D:76:ILE:HG13	1:D:84:VAL:HG13	1.95	0.49
1:C:97:ALA:HB3	1:C:145:LEU:HB2	1.95	0.49
2:F:230:SER:HB2	2:F:313:ARG:HH22	1.76	0.49
1:D:115:ARG:HH11	1:D:210:ARG:HG3	1.78	0.49
1:G:234:ILE:HD12	1:G:282:ILE:HD11	1.95	0.49
2:F:172:LEU:HD21	2:F:319:LEU:HB3	1.94	0.48
2:F:167:LEU:HG	2:F:201:VAL:HG21	1.96	0.48
1:D:115:ARG:HD2	1:D:210:ARG:HA	1.95	0.48
1:D:131:CYS:HA	1:D:145:LEU:HA	1.95	0.48
2:F:74:ASN:HB3	2:F:86:LYS:HD3	1.96	0.48
1:A:186:ARG:HH22	1:A:221:SEP:HB3	1.79	0.47
1:C:67:LEU:HD12	1:C:137:HIS:HB2	1.96	0.47
1:D:150:GLN:H	1:D:196:ASN:HA	1.80	0.47
2:F:70:LEU:HA	2:F:88:ILE:O	2.15	0.47
1:G:117:ILE:HG23	1:G:134:MET:HE1	1.96	0.47
1:D:231:PRO:HB3	1:D:283:CYS:HA	1.97	0.47
1:G:67:LEU:HD12	1:G:70:LEU:HD21	1.97	0.47
1:A:186:ARG:HD3	1:A:208:VAL:O	2.15	0.46
2:F:73:VAL:HB	2:F:86:LYS:HG3	1.97	0.46
1:A:196:ASN:HD21	1:A:200:ASN:HD21	1.63	0.46
1:C:188:ILE:O	1:C:252:SER:HB3	2.16	0.46
1:C:184:VAL:HG23	1:C:186:ARG:HD2	1.97	0.46
1:C:117:ILE:HG23	1:C:134:MET:HE1	1.97	0.46
1:D:223:VAL:O	1:D:233:ARG:NH2	2.49	0.46
1:B:92:THR:O	1:B:94:ARG:HG3	2.17	0.45
2:F:247:ALA:HB1	2:F:313:ARG:HD3	1.97	0.45
1:E:131:CYS:SG	1:E:143:VAL:HG23	2.57	0.45
1:B:227:ALA:HB1	1:B:265:PHE:CZ	2.52	0.45
2:H:169:ARG:HH11	2:H:328:ALA:HB3	1.81	0.45
1:C:80:ALA:HB1	1:C:207:GLY:HA3	1.98	0.45
1:A:161:GLU:OE2	1:A:295:SER:OG	2.21	0.45
1:E:118:GLU:HG3	2:F:284:MET:HE1	1.98	0.44
1:G:152:SER:HA	1:G:194:LEU:HA	1.99	0.44
2:F:239:ASN:N	2:F:239:ASN:OD1	2.49	0.44
1:G:176:ALA:O	1:G:180:ARG:NE	2.44	0.44
2:H:177:TYR:O	2:H:181:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:SER:HA	2:H:136:ASP:OD2	2.18	0.44
1:A:217:ASP:HA	1:A:218:PRO:HD3	1.90	0.43
1:C:281:ALA:O	1:C:285:SER:OG	2.33	0.43
1:G:258:LEU:HD22	1:G:302:VAL:HG21	2.00	0.43
2:F:99:LYS:HB3	2:F:143:VAL:HG13	2.00	0.43
2:F:115:ARG:HH21	2:F:210:ARG:HG3	1.83	0.43
2:H:184:VAL:HG23	2:H:186:ARG:HD2	2.01	0.43
1:A:265:PHE:HB2	1:A:271:ARG:HH21	1.83	0.43
1:B:276:ALA:HB1	1:C:141:ILE:HD11	2.00	0.43
1:C:76:ILE:HD11	1:C:86:LYS:HB2	2.00	0.43
1:E:89:HIS:CD2	1:E:92:THR:HG22	2.54	0.42
2:F:135:PHE:HB2	2:F:142:GLN:HB2	2.00	0.42
1:D:89:HIS:ND1	1:D:92:THR:HG22	2.34	0.42
1:B:124:ASP:HA	1:B:130:LYS:HE2	2.02	0.42
1:E:208:VAL:HG22	1:E:223:VAL:HB	2.00	0.42
1:G:120:LEU:HD13	1:G:143:VAL:HG21	2.01	0.42
1:D:236:THR:HB	1:D:241:GLY:HA2	2.01	0.42
1:E:258:LEU:HD12	1:E:258:LEU:HA	1.94	0.42
2:F:115:ARG:NH2	2:F:210:ARG:HG3	2.35	0.42
1:G:230:SER:HB2	1:G:313:ARG:HH22	1.85	0.42
2:H:167:LEU:HG	2:H:201:VAL:HG21	2.00	0.42
1:B:100:VAL:HG12	1:B:142:GLN:HG2	2.02	0.42
1:B:197:SER:O	1:B:199:LYS:HD2	2.20	0.42
2:H:99:LYS:HB3	2:H:143:VAL:HG13	2.02	0.42
1:C:87:VAL:HG23	1:C:96:PHE:HB2	2.02	0.42
2:F:284:MET:HA	2:F:284:MET:HE3	2.02	0.41
2:F:112:GLN:NE2	2:F:115:ARG:HD3	2.35	0.41
2:H:120:LEU:HD13	2:H:143:VAL:HG21	2.01	0.41
1:D:226:ILE:HA	1:D:229:MET:HE2	2.02	0.41
1:B:196:ASN:OD1	1:B:200:ASN:N	2.54	0.41
1:E:118:GLU:HA	2:F:284:MET:CE	2.50	0.41
1:C:104:ASN:HB3	1:C:109:VAL:HG11	2.02	0.41
2:F:111:ARG:O	2:F:115:ARG:HD2	2.21	0.41
2:F:185:HIS:NE2	2:F:205:ASP:O	2.54	0.41
2:F:212:LEU:HD22	2:F:217:ASP:HB3	2.02	0.41
1:C:227:ALA:HB1	1:C:265:PHE:CZ	2.56	0.40
1:C:301:PHE:HB2	1:C:322:HIS:CE1	2.57	0.40
1:D:99:LYS:NZ	1:D:116:GLU:OE2	2.39	0.40
1:D:119:ILE:HG23	1:D:183:ILE:HD13	2.03	0.40
1:D:189:LYS:HE3	1:D:191:SER:HB2	2.04	0.40
2:F:178:LEU:HG	2:F:183:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ILE:HG23	1:G:260:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

37 non-standard protein/DNA/RNA residues 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$
1	TPO	G	83	1	8,10,11	0.79	0	10,14,16	0.97	1 (10%)
1	SEP	A	221	1	8,9,10	0.46	0	7,12,14	1.70	2 (28%)
1	TPO	A	108	1	8,10,11	0.64	0	10,14,16	0.97	0
1	SEP	D	221	1	8,9,10	0.66	0	7,12,14	1.53	2 (28%)
2	TPO	F	108	2	8,10,11	0.67	0	10,14,16	1.09	1 (10%)
1	SEP	G	66	1	8,9,10	0.59	0	7,12,14	0.72	0
1	TPO	B	215	1	8,10,11	0.72	0	10,14,16	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	D	83	1	8,10,11	0.51	0	10,14,16	1.59	1 (10%)
1	TPO	E	108	1	8,10,11	0.56	0	10,14,16	1.31	3 (30%)
1	TPO	D	215	1	8,10,11	0.87	0	10,14,16	0.99	0
1	TPO	B	83	1	8,10,11	0.87	0	10,14,16	0.85	0
1	SEP	C	221	1	8,9,10	0.67	0	7,12,14	1.14	1 (14%)
1	SEP	B	221	1	8,9,10	0.47	0	7,12,14	1.74	2 (28%)
1	TPO	D	108	1	8,10,11	0.46	0	10,14,16	1.22	0
1	SEP	B	66	1	8,9,10	0.64	0	7,12,14	0.83	0
2	SEP	H	221	2	8,9,10	0.64	0	7,12,14	0.98	0
1	TPO	E	215	1	8,10,11	1.13	1 (12%)	10,14,16	0.83	0
1	TPO	C	108	1	8,10,11	0.51	0	10,14,16	1.30	1 (10%)
2	SEP	F	66	2	8,9,10	0.66	0	7,12,14	0.71	0
1	TPO	E	83	1	8,10,11	0.63	0	10,14,16	1.27	1 (10%)
1	TPO	G	108	1	8,10,11	0.53	0	10,14,16	1.36	2 (20%)
2	TPO	H	215	2	8,10,11	0.71	0	10,14,16	1.09	0
2	SEP	F	221	2	8,9,10	0.73	0	7,12,14	1.83	1 (14%)
1	SEP	E	221	1	8,9,10	0.56	0	7,12,14	1.14	0
1	TPO	C	83	1	8,10,11	0.58	0	10,14,16	1.67	2 (20%)
2	TPO	H	108	2	8,10,11	0.59	0	10,14,16	1.20	1 (10%)
1	SEP	E	66	1	8,9,10	0.52	0	7,12,14	0.93	0
1	TPO	A	215	1	8,10,11	0.90	1 (12%)	10,14,16	0.95	0
2	TPO	F	215	2	8,10,11	0.61	0	10,14,16	1.42	1 (10%)
1	TPO	C	215	1	8,10,11	1.24	1 (12%)	10,14,16	0.82	1 (10%)
1	TPO	B	108	1	8,10,11	0.82	0	10,14,16	1.15	2 (20%)
1	TPO	A	83	1	8,10,11	0.63	0	10,14,16	1.20	2 (20%)
1	SEP	C	66	1	8,9,10	0.63	0	7,12,14	1.00	0
1	SEP	G	221	1	8,9,10	0.69	0	7,12,14	1.70	1 (14%)
2	SEP	H	66	2	8,9,10	0.60	0	7,12,14	0.84	0
1	TPO	G	215	1	8,10,11	0.83	0	10,14,16	0.79	0
1	SEP	A	66	1	8,9,10	0.63	0	7,12,14	0.83	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
1	TPO	G	83	1	-	1/9/11/13	-
1	SEP	A	221	1	-	2/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	108	1	-	3/9/11/13	-
1	SEP	D	221	1	-	0/6/8/10	-
2	TPO	F	108	2	-	2/9/11/13	-
1	SEP	G	66	1	-	1/6/8/10	-
1	TPO	B	215	1	-	2/9/11/13	-
1	TPO	D	83	1	-	3/9/11/13	-
1	TPO	E	108	1	-	0/9/11/13	-
1	TPO	D	215	1	-	1/9/11/13	-
1	TPO	B	83	1	-	2/9/11/13	-
1	SEP	C	221	1	-	1/6/8/10	-
1	SEP	B	221	1	-	0/6/8/10	-
1	TPO	D	108	1	-	1/9/11/13	-
1	SEP	B	66	1	-	4/6/8/10	-
2	SEP	H	221	2	-	0/6/8/10	-
1	TPO	E	215	1	-	1/9/11/13	-
1	TPO	C	108	1	-	2/9/11/13	-
2	SEP	F	66	2	-	4/6/8/10	-
1	TPO	E	83	1	-	5/9/11/13	-
1	TPO	G	108	1	-	4/9/11/13	-
2	TPO	H	215	2	-	2/9/11/13	-
2	SEP	F	221	2	-	0/6/8/10	-
1	SEP	E	221	1	-	1/6/8/10	-
1	TPO	C	83	1	-	2/9/11/13	-
2	TPO	H	108	2	-	3/9/11/13	-
1	SEP	E	66	1	-	5/6/8/10	-
1	TPO	A	215	1	-	1/9/11/13	-
2	TPO	F	215	2	-	2/9/11/13	-
1	TPO	C	215	1	-	2/9/11/13	-
1	TPO	B	108	1	-	2/9/11/13	-
1	TPO	A	83	1	-	3/9/11/13	-
1	SEP	C	66	1	-	1/6/8/10	-
1	SEP	G	221	1	-	0/6/8/10	-
2	SEP	H	66	2	-	2/6/8/10	-
1	TPO	G	215	1	-	3/9/11/13	-
1	SEP	A	66	1	-	1/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	TPO	P-OG1	3.00	1.64	1.59
1	E	215	TPO	P-OG1	2.69	1.64	1.59
1	A	215	TPO	P-OG1	2.08	1.63	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	221	SEP	OG-CB-CA	4.27	112.30	108.14
1	G	221	SEP	OG-CB-CA	4.17	112.20	108.14
1	D	83	TPO	P-OG1-CB	-4.09	112.20	123.33
1	C	83	TPO	P-OG1-CB	-3.34	114.25	123.33
2	F	215	TPO	P-OG1-CB	-3.13	114.83	123.33
1	C	108	TPO	P-OG1-CB	-3.09	114.93	123.33
1	A	221	SEP	O3P-P-OG	-3.00	98.85	106.67
1	E	83	TPO	P-OG1-CB	-2.97	115.26	123.33
1	G	108	TPO	P-OG1-CB	-2.88	115.51	123.33
1	B	221	SEP	O3P-P-O2P	2.82	118.36	107.80
1	D	221	SEP	O3P-P-O1P	2.64	121.11	110.83
1	B	221	SEP	O3P-P-OG	-2.63	99.82	106.67
1	E	108	TPO	P-OG1-CB	-2.49	116.56	123.33
2	H	108	TPO	P-OG1-CB	-2.43	116.73	123.33
1	B	108	TPO	P-OG1-CB	-2.41	116.77	123.33
1	C	83	TPO	O3P-P-O2P	2.41	116.85	107.80
1	C	221	SEP	O3P-P-O2P	2.25	116.23	107.80
1	G	83	TPO	O-C-CA	-2.20	119.11	124.77
1	C	215	TPO	O-C-CA	-2.20	119.12	124.77
1	G	108	TPO	O-C-CA	-2.20	119.12	124.77
1	D	221	SEP	OG-P-O1P	-2.18	100.55	106.44
2	F	108	TPO	O-C-CA	-2.10	119.38	124.77
1	E	108	TPO	O3P-P-O2P	2.07	115.55	107.80
1	A	83	TPO	P-OG1-CB	-2.05	117.75	123.33
1	E	108	TPO	O-C-CA	-2.05	119.50	124.77
1	A	221	SEP	O3P-P-O2P	2.03	115.40	107.80
1	B	108	TPO	O-C-CA	-2.02	119.56	124.77
1	A	83	TPO	O-C-CA	-2.02	119.58	124.77

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	SEP	N-CA-CB-OG
1	A	215	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	66	SEP	CB-OG-P-O1P
1	B	66	SEP	CB-OG-P-O2P
1	B	66	SEP	CB-OG-P-O3P
1	B	108	TPO	O-C-CA-CB
1	C	83	TPO	O-C-CA-CB
1	C	108	TPO	O-C-CA-CB
1	C	215	TPO	O-C-CA-CB
1	D	108	TPO	O-C-CA-CB
1	E	66	SEP	C-CA-CB-OG
1	E	83	TPO	N-CA-CB-OG1
1	E	83	TPO	C-CA-CB-CG2
1	E	83	TPO	O-C-CA-CB
2	F	66	SEP	C-CA-CB-OG
2	F	108	TPO	O-C-CA-CB
1	G	83	TPO	O-C-CA-CB
1	G	108	TPO	N-CA-CB-OG1
1	G	108	TPO	C-CA-CB-CG2
2	H	66	SEP	N-CA-CB-OG
2	H	66	SEP	C-CA-CB-OG
2	H	215	TPO	O-C-CA-CB
1	A	83	TPO	CB-OG1-P-O1P
1	B	83	TPO	CG2-CB-OG1-P
1	E	66	SEP	CB-OG-P-O1P
1	G	108	TPO	N-CA-CB-CG2
1	E	221	SEP	CA-CB-OG-P
2	F	66	SEP	CA-CB-OG-P
1	A	108	TPO	C-CA-CB-CG2
1	B	215	TPO	C-CA-CB-CG2
1	D	83	TPO	C-CA-CB-CG2
1	G	215	TPO	C-CA-CB-CG2
1	A	108	TPO	CB-OG1-P-O1P
1	B	108	TPO	CB-OG1-P-O1P
1	A	221	SEP	CB-OG-P-O1P
2	F	66	SEP	CB-OG-P-O1P
1	B	66	SEP	N-CA-CB-OG
1	C	66	SEP	N-CA-CB-OG
1	E	66	SEP	N-CA-CB-OG
2	F	66	SEP	N-CA-CB-OG
1	G	66	SEP	N-CA-CB-OG
1	E	83	TPO	CB-OG1-P-O3P
1	C	108	TPO	CB-OG1-P-O1P
1	E	215	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
2	H	108	TPO	CB-OG1-P-O1P
1	E	66	SEP	CB-OG-P-O3P
1	A	221	SEP	CA-CB-OG-P
1	C	221	SEP	CA-CB-OG-P
1	E	66	SEP	CA-CB-OG-P
1	B	83	TPO	CB-OG1-P-O2P
1	C	215	TPO	CB-OG1-P-O3P
1	D	83	TPO	CB-OG1-P-O3P
2	F	215	TPO	CB-OG1-P-O3P
1	G	215	TPO	CB-OG1-P-O3P
2	H	108	TPO	CB-OG1-P-O3P
2	H	215	TPO	CB-OG1-P-O3P
1	A	83	TPO	C-CA-CB-CG2
1	A	83	TPO	O-C-CA-CB
1	C	83	TPO	C-CA-CB-CG2
1	G	108	TPO	O-C-CA-CB
2	H	108	TPO	O-C-CA-CB
2	F	108	TPO	CB-OG1-P-O1P
1	A	108	TPO	N-CA-CB-CG2
1	B	215	TPO	N-CA-CB-CG2
1	D	83	TPO	N-CA-CB-CG2
1	D	215	TPO	N-CA-CB-CG2
1	E	83	TPO	N-CA-CB-CG2
2	F	215	TPO	N-CA-CB-CG2
1	G	215	TPO	N-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	221	SEP	1	0

5.5 Carbohydrates [i](#)

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 ⓘ

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	257/295 (87%)	-0.44	1 (0%) 88 79	40, 75, 134, 167	0
1	B	253/295 (85%)	-0.44	1 (0%) 88 79	45, 77, 152, 201	0
1	C	261/295 (88%)	-0.50	0 100 100	55, 80, 132, 179	0
1	D	252/295 (85%)	-0.22	0 100 100	71, 107, 147, 172	0
1	E	253/295 (85%)	-0.03	3 (1%) 76 58	64, 115, 162, 177	0
1	G	253/295 (85%)	0.03	3 (1%) 76 58	96, 140, 182, 216	0
2	F	253/295 (85%)	0.02	3 (1%) 76 58	84, 128, 175, 209	0
2	H	256/295 (86%)	-0.33	1 (0%) 88 79	58, 94, 183, 199	0
All	All	2038/2360 (86%)	-0.24	12 (0%) 85 73	40, 106, 166, 216	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	328	ALA	3.3
1	B	239	ASN	2.9
1	A	328	ALA	2.7
1	E	228	TYR	2.7
2	F	317	GLN	2.6
1	G	161	GLU	2.6
1	E	104	ASN	2.4
2	H	83	THR	2.2
2	F	323	PRO	2.1
2	F	88	ILE	2.0
1	G	262	LEU	2.0
1	G	88	ILE	2.0

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

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(Å ²)	Q<0.9
1	TPO	B	83	11/12	0.53	0.11	118,184,222,246	0
1	TPO	G	108	11/12	0.62	0.10	150,188,218,218	0
2	TPO	F	215	11/12	0.66	0.09	151,165,190,194	0
1	TPO	E	108	11/12	0.67	0.09	129,160,193,198	0
1	TPO	D	83	11/12	0.70	0.09	127,138,200,206	0
1	TPO	G	83	11/12	0.70	0.09	154,171,189,202	0
1	TPO	E	215	11/12	0.70	0.10	135,168,180,196	0
2	SEP	H	66	10/11	0.71	0.08	138,185,226,234	0
1	TPO	G	215	11/12	0.72	0.08	141,169,194,197	0
1	SEP	B	66	10/11	0.72	0.09	123,163,198,200	0
1	SEP	G	66	10/11	0.73	0.11	123,177,210,212	0
2	TPO	H	215	11/12	0.73	0.09	131,161,224,232	0
1	SEP	E	66	10/11	0.74	0.09	144,166,193,197	0
1	TPO	D	215	11/12	0.74	0.09	105,132,171,181	0
2	TPO	H	108	11/12	0.76	0.07	156,176,215,247	0
1	TPO	C	215	11/12	0.76	0.10	133,162,180,184	0
1	TPO	B	215	11/12	0.80	0.08	113,132,169,185	0
1	TPO	E	83	11/12	0.80	0.10	124,173,210,215	0
1	TPO	D	108	11/12	0.83	0.09	127,138,173,198	0
1	SEP	G	221	10/11	0.85	0.08	94,112,129,149	0
2	TPO	F	108	11/12	0.85	0.11	118,132,156,182	0
1	TPO	A	108	11/12	0.85	0.08	87,132,145,145	0
2	SEP	F	66	10/11	0.85	0.08	169,181,229,231	0
1	TPO	C	108	11/12	0.89	0.07	106,113,166,173	0
1	TPO	A	215	11/12	0.89	0.07	124,151,176,198	0
1	SEP	D	221	10/11	0.90	0.09	71,106,138,142	0
1	SEP	C	66	10/11	0.90	0.08	113,129,165,176	0
1	TPO	B	108	11/12	0.91	0.06	150,156,164,176	0
1	SEP	E	221	10/11	0.92	0.06	80,95,120,135	0
1	SEP	A	66	10/11	0.92	0.06	99,130,153,169	0
1	TPO	C	83	11/12	0.93	0.07	64,81,112,117	0
1	TPO	A	83	11/12	0.94	0.06	109,134,152,157	0
2	SEP	F	221	10/11	0.94	0.08	64,122,132,133	0
1	SEP	C	221	10/11	0.95	0.06	60,89,111,123	0
1	SEP	A	221	10/11	0.95	0.06	74,83,100,102	0
1	SEP	B	221	10/11	0.96	0.05	64,72,89,97	0
2	SEP	H	221	10/11	0.96	0.05	81,102,112,114	0

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.