



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 10:31 pm BST

PDB ID : 5E4H  
Title : Crystal Structure of Apoenzyme Alpha-kinase Domain of Myosin-II Heavy Chain Kinase A  
Authors : Ye, Q.; Cote, G.P.; Jia, Z.  
Deposited on : 2015-10-06  
Resolution : 2.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

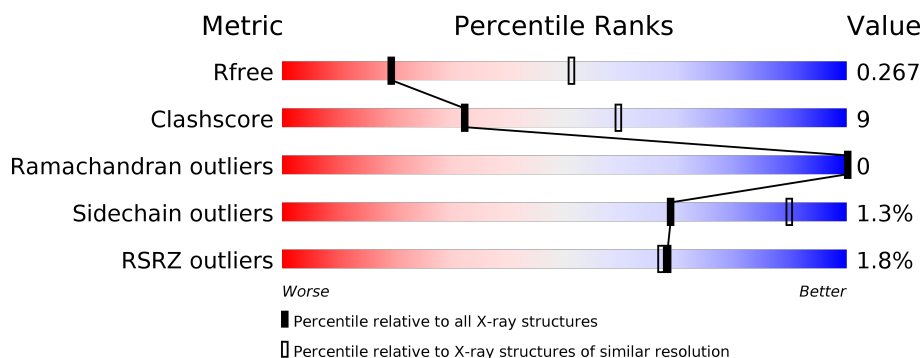
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	307	<div> <div></div> <div>64%18%18%</div> </div>
1	B	307	<div> <div>3%</div> <div>64%16%20%</div> </div>
1	C	307	<div> <div>2%</div> <div>63%17%20%</div> </div>
1	D	307	<div> <div></div> <div>66%17%17%</div> </div>
1	E	307	<div> <div>2%</div> <div>63%19%19%</div> </div>
1	F	307	<div> <div></div> <div>67%14%18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	307	<div><div>%</div><div><div></div><div>67%</div><div>16%</div><div>17%</div></div></div>
1	H	307	<div><div>2%</div><div><div></div><div>64%</div><div>16%</div><div>19%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16069 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 Myosin-II heavy chain kinase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	P	S	0	0	0
			2004	1280	334	376	2	12			
1	B	247	Total	C	N	O	P	S	0	0	0
			1972	1260	328	370	2	12			
1	C	245	Total	C	N	O	P	S	0	0	0
			1957	1252	326	365	2	12			
1	D	256	Total	C	N	O	P	S	0	0	0
			2039	1301	340	384	2	12			
1	E	250	Total	C	N	O	P	S	0	0	0
			1990	1271	332	373	2	12			
1	F	253	Total	C	N	O	P	S	0	0	0
			2012	1286	335	377	2	12			
1	G	256	Total	C	N	O	P	S	0	0	0
			2039	1301	340	384	2	12			
1	H	249	Total	C	N	O	P	S	0	0	0
			1984	1268	331	371	2	12			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	MET	-	expression tag	UNP P42527
A	536	GLY	-	expression tag	UNP P42527
A	537	GLY	-	expression tag	UNP P42527
A	538	HIS	-	expression tag	UNP P42527
A	539	HIS	-	expression tag	UNP P42527
A	540	HIS	-	expression tag	UNP P42527
A	541	HIS	-	expression tag	UNP P42527
A	542	HIS	-	expression tag	UNP P42527
A	543	HIS	-	expression tag	UNP P42527
A	544	GLY	-	expression tag	UNP P42527
A	545	GLU	-	expression tag	UNP P42527
A	546	ASN	-	expression tag	UNP P42527
A	547	LEU	-	expression tag	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
A	548	TYR	-	expression tag	UNP P42527
A	549	PHE	-	expression tag	UNP P42527
A	550	GLN	-	expression tag	UNP P42527
A	551	GLY	-	expression tag	UNP P42527
B	535	MET	-	expression tag	UNP P42527
B	536	GLY	-	expression tag	UNP P42527
B	537	GLY	-	expression tag	UNP P42527
B	538	HIS	-	expression tag	UNP P42527
B	539	HIS	-	expression tag	UNP P42527
B	540	HIS	-	expression tag	UNP P42527
B	541	HIS	-	expression tag	UNP P42527
B	542	HIS	-	expression tag	UNP P42527
B	543	HIS	-	expression tag	UNP P42527
B	544	GLY	-	expression tag	UNP P42527
B	545	GLU	-	expression tag	UNP P42527
B	546	ASN	-	expression tag	UNP P42527
B	547	LEU	-	expression tag	UNP P42527
B	548	TYR	-	expression tag	UNP P42527
B	549	PHE	-	expression tag	UNP P42527
B	550	GLN	-	expression tag	UNP P42527
B	551	GLY	-	expression tag	UNP P42527
C	535	MET	-	expression tag	UNP P42527
C	536	GLY	-	expression tag	UNP P42527
C	537	GLY	-	expression tag	UNP P42527
C	538	HIS	-	expression tag	UNP P42527
C	539	HIS	-	expression tag	UNP P42527
C	540	HIS	-	expression tag	UNP P42527
C	541	HIS	-	expression tag	UNP P42527
C	542	HIS	-	expression tag	UNP P42527
C	543	HIS	-	expression tag	UNP P42527
C	544	GLY	-	expression tag	UNP P42527
C	545	GLU	-	expression tag	UNP P42527
C	546	ASN	-	expression tag	UNP P42527
C	547	LEU	-	expression tag	UNP P42527
C	548	TYR	-	expression tag	UNP P42527
C	549	PHE	-	expression tag	UNP P42527
C	550	GLN	-	expression tag	UNP P42527
C	551	GLY	-	expression tag	UNP P42527
D	535	MET	-	expression tag	UNP P42527
D	536	GLY	-	expression tag	UNP P42527
D	537	GLY	-	expression tag	UNP P42527
D	538	HIS	-	expression tag	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
D	539	HIS	-	expression tag	UNP P42527
D	540	HIS	-	expression tag	UNP P42527
D	541	HIS	-	expression tag	UNP P42527
D	542	HIS	-	expression tag	UNP P42527
D	543	HIS	-	expression tag	UNP P42527
D	544	GLY	-	expression tag	UNP P42527
D	545	GLU	-	expression tag	UNP P42527
D	546	ASN	-	expression tag	UNP P42527
D	547	LEU	-	expression tag	UNP P42527
D	548	TYR	-	expression tag	UNP P42527
D	549	PHE	-	expression tag	UNP P42527
D	550	GLN	-	expression tag	UNP P42527
D	551	GLY	-	expression tag	UNP P42527
E	535	MET	-	expression tag	UNP P42527
E	536	GLY	-	expression tag	UNP P42527
E	537	GLY	-	expression tag	UNP P42527
E	538	HIS	-	expression tag	UNP P42527
E	539	HIS	-	expression tag	UNP P42527
E	540	HIS	-	expression tag	UNP P42527
E	541	HIS	-	expression tag	UNP P42527
E	542	HIS	-	expression tag	UNP P42527
E	543	HIS	-	expression tag	UNP P42527
E	544	GLY	-	expression tag	UNP P42527
E	545	GLU	-	expression tag	UNP P42527
E	546	ASN	-	expression tag	UNP P42527
E	547	LEU	-	expression tag	UNP P42527
E	548	TYR	-	expression tag	UNP P42527
E	549	PHE	-	expression tag	UNP P42527
E	550	GLN	-	expression tag	UNP P42527
E	551	GLY	-	expression tag	UNP P42527
F	535	MET	-	expression tag	UNP P42527
F	536	GLY	-	expression tag	UNP P42527
F	537	GLY	-	expression tag	UNP P42527
F	538	HIS	-	expression tag	UNP P42527
F	539	HIS	-	expression tag	UNP P42527
F	540	HIS	-	expression tag	UNP P42527
F	541	HIS	-	expression tag	UNP P42527
F	542	HIS	-	expression tag	UNP P42527
F	543	HIS	-	expression tag	UNP P42527
F	544	GLY	-	expression tag	UNP P42527
F	545	GLU	-	expression tag	UNP P42527
F	546	ASN	-	expression tag	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
F	547	LEU	-	expression tag	UNP P42527
F	548	TYR	-	expression tag	UNP P42527
F	549	PHE	-	expression tag	UNP P42527
F	550	GLN	-	expression tag	UNP P42527
F	551	GLY	-	expression tag	UNP P42527
G	535	MET	-	expression tag	UNP P42527
G	536	GLY	-	expression tag	UNP P42527
G	537	GLY	-	expression tag	UNP P42527
G	538	HIS	-	expression tag	UNP P42527
G	539	HIS	-	expression tag	UNP P42527
G	540	HIS	-	expression tag	UNP P42527
G	541	HIS	-	expression tag	UNP P42527
G	542	HIS	-	expression tag	UNP P42527
G	543	HIS	-	expression tag	UNP P42527
G	544	GLY	-	expression tag	UNP P42527
G	545	GLU	-	expression tag	UNP P42527
G	546	ASN	-	expression tag	UNP P42527
G	547	LEU	-	expression tag	UNP P42527
G	548	TYR	-	expression tag	UNP P42527
G	549	PHE	-	expression tag	UNP P42527
G	550	GLN	-	expression tag	UNP P42527
G	551	GLY	-	expression tag	UNP P42527
H	535	MET	-	expression tag	UNP P42527
H	536	GLY	-	expression tag	UNP P42527
H	537	GLY	-	expression tag	UNP P42527
H	538	HIS	-	expression tag	UNP P42527
H	539	HIS	-	expression tag	UNP P42527
H	540	HIS	-	expression tag	UNP P42527
H	541	HIS	-	expression tag	UNP P42527
H	542	HIS	-	expression tag	UNP P42527
H	543	HIS	-	expression tag	UNP P42527
H	544	GLY	-	expression tag	UNP P42527
H	545	GLU	-	expression tag	UNP P42527
H	546	ASN	-	expression tag	UNP P42527
H	547	LEU	-	expression tag	UNP P42527
H	548	TYR	-	expression tag	UNP P42527
H	549	PHE	-	expression tag	UNP P42527
H	550	GLN	-	expression tag	UNP P42527
H	551	GLY	-	expression tag	UNP P42527

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is water.

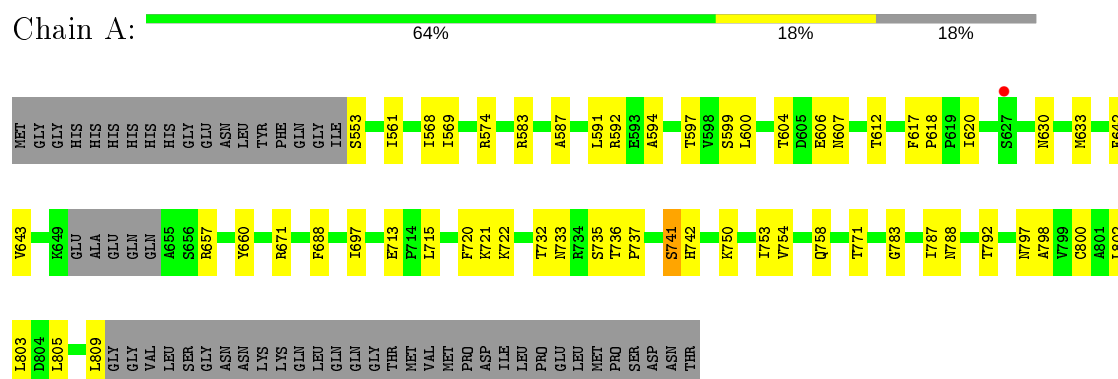
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	13	Total O 13 13	0	0
3	C	5	Total O 5 5	0	0
3	D	9	Total O 9 9	0	0
3	E	7	Total O 7 7	0	0
3	F	7	Total O 7 7	0	0
3	G	11	Total O 11 11	0	0
3	H	3	Total O 3 3	0	0



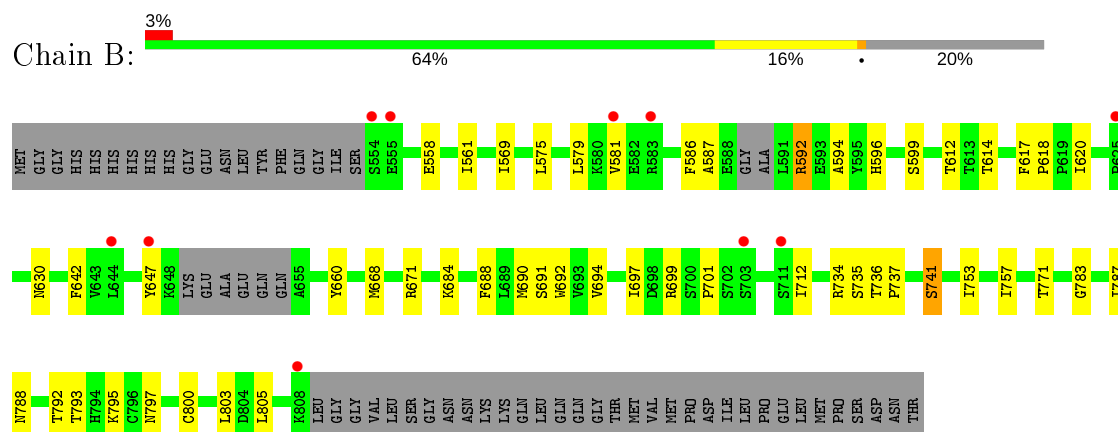
### 3 Residue-property plots [i](#)

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.

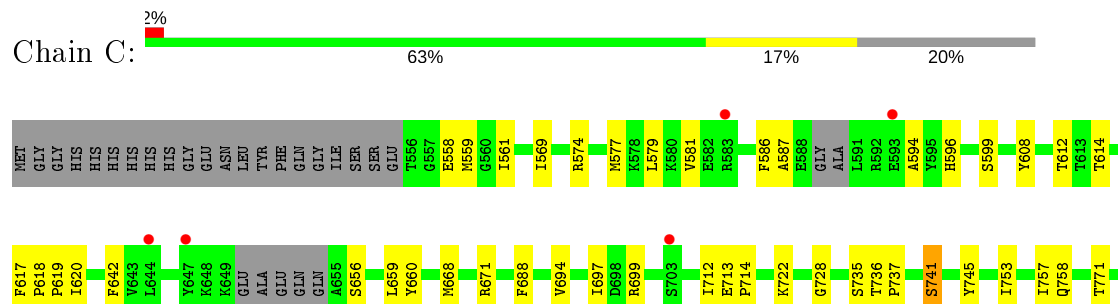
#### • Molecule 1: Myosin-II heavy chain kinase A

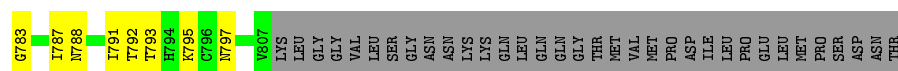


#### • Molecule 1: Myosin-II heavy chain kinase A



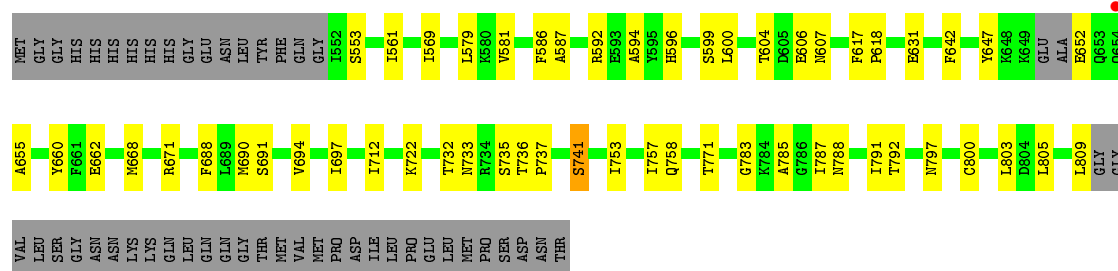
#### • Molecule 1: Myosin-II heavy chain kinase A





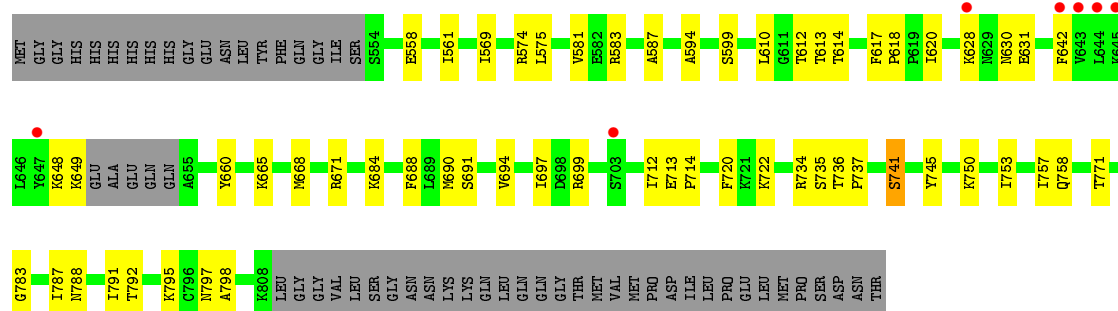
- Molecule 1: Myosin-II heavy chain kinase A

Chain D: 66% 17% 17%



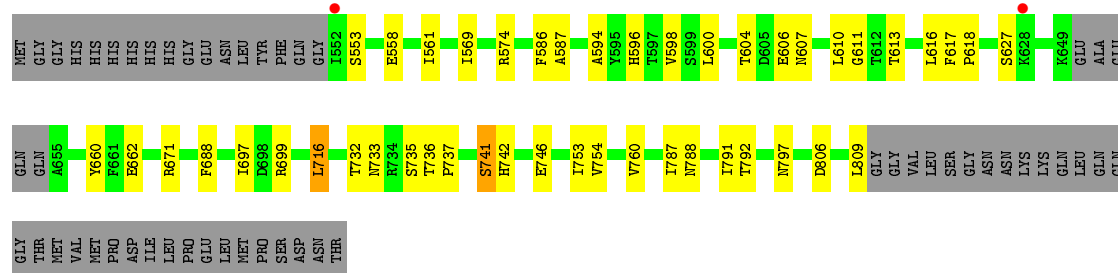
- Molecule 1: Myosin-II heavy chain kinase A

Chain E: 2% 63% 19% 19%



- Molecule 1: Myosin-II heavy chain kinase A

Chain F: 67% 14% 18%



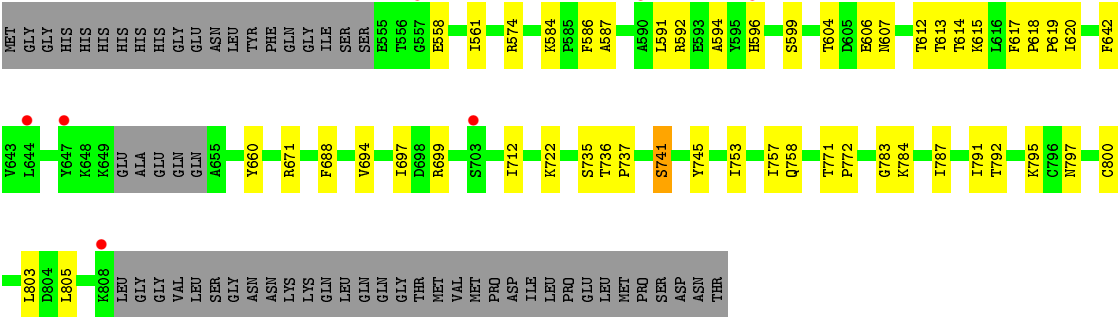
- Molecule 1: Myosin-II heavy chain kinase A

Chain G: 67% 16% 17%





● Molecule 1: Myosin-II heavy chain kinase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.30Å 103.47Å 167.81Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 38.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (40.00-2.90) 97.4 (38.93-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.241 , 0.268 0.241 , 0.267	Depositor DCC
$R_{free}$ test set	3125 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 31.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	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 49.00 % 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 7.9391e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TPO, ZN, PHD

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	0.53	0/2022	0.81	1/2725 (0.0%)
1	B	0.52	0/1989	0.80	0/2680
1	C	0.51	0/1974	0.78	2/2660 (0.1%)
1	D	0.49	0/2057	0.77	0/2772
1	E	0.53	0/2008	0.81	2/2706 (0.1%)
1	F	0.51	0/2030	0.82	1/2736 (0.0%)
1	G	0.52	0/2057	0.77	0/2772
1	H	0.53	0/2002	0.80	1/2698 (0.0%)
All	All	0.52	0/16139	0.80	7/21749 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	577	MET	CG-SD-CE	6.71	110.94	100.20
1	A	583	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	E	583	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	F	716	LEU	CB-CG-CD1	5.25	119.92	111.00
1	E	610	LEU	N-CA-C	5.21	125.08	111.00

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	2004	0	2017	48	0
1	B	1972	0	1980	37	0
1	C	1957	0	1969	31	0
1	D	2039	0	2050	38	0
1	E	1990	0	2002	45	0
1	F	2012	0	2028	26	0
1	G	2039	0	2050	39	0
1	H	1984	0	1997	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	9	0	0	2	0
3	B	13	0	0	1	0
3	C	5	0	0	0	0
3	D	9	0	0	1	0
3	E	7	0	0	2	0
3	F	7	0	0	0	0
3	G	11	0	0	0	0
3	H	3	0	0	0	0
All	All	16069	0	16093	281	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 9.

The worst 5 of 281 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:C:614:THR:HG21	1:C:619:PRO:HA	1.22	1.17
1:H:614:THR:HG21	1:H:619:PRO:HA	1.39	1.03
1:F:716:LEU:HD21	1:F:760:VAL:HG23	1.54	0.87
1:G:566:ASP:OD2	1:G:569:ILE:HD12	1.76	0.85
1:A:630:ASN:HD21	1:A:633:MET:HG2	1.44	0.81

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	246/307 (80%)	239 (97%)	7 (3%)	0	100	100
1	B	239/307 (78%)	229 (96%)	10 (4%)	0	100	100
1	C	237/307 (77%)	229 (97%)	8 (3%)	0	100	100
1	D	250/307 (81%)	241 (96%)	9 (4%)	0	100	100
1	E	244/307 (80%)	236 (97%)	8 (3%)	0	100	100
1	F	247/307 (80%)	238 (96%)	9 (4%)	0	100	100
1	G	250/307 (81%)	243 (97%)	7 (3%)	0	100	100
1	H	243/307 (79%)	232 (96%)	11 (4%)	0	100	100
All	All	1956/2456 (80%)	1887 (96%)	69 (4%)	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	222/268 (83%)	220 (99%)	2 (1%)	78	93
1	B	219/268 (82%)	215 (98%)	4 (2%)	59	85
1	C	217/268 (81%)	215 (99%)	2 (1%)	78	93
1	D	226/268 (84%)	223 (99%)	3 (1%)	69	90
1	E	220/268 (82%)	218 (99%)	2 (1%)	78	93
1	F	223/268 (83%)	218 (98%)	5 (2%)	52	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	226/268 (84%)	223 (99%)	3 (1%)	69	90
1	H	219/268 (82%)	217 (99%)	2 (1%)	78	93
All	All	1772/2144 (83%)	1749 (99%)	23 (1%)	69	90

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	741	SER
1	E	741	SER
1	H	660	TYR
1	E	660	TYR
1	F	598	VAL

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

Mol	Chain	Res	Type
1	C	596	HIS
1	C	738	GLN
1	F	596	HIS
1	C	570	ASN
1	E	758	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	C	612	1	8,10,11	0.92	0	10,14,16	1.12	0
1	TPO	A	612	1	8,10,11	0.71	0	10,14,16	1.54	2 (20%)
1	TPO	G	612	1	8,10,11	0.71	0	10,14,16	1.56	2 (20%)
1	TPO	B	612	1	8,10,11	1.06	0	10,14,16	1.20	1 (10%)
1	PHD	E	663	1	9,11,12	1.05	1 (11%)	10,15,17	2.28	4 (40%)
1	TPO	F	612	1	8,10,11	0.61	0	10,14,16	1.70	2 (20%)
1	PHD	A	663	1	9,11,12	1.15	1 (11%)	10,15,17	2.27	4 (40%)
1	TPO	E	612	1	8,10,11	0.75	0	10,14,16	1.42	1 (10%)
1	PHD	C	663	1	9,11,12	1.36	1 (11%)	10,15,17	2.17	3 (30%)
1	PHD	B	663	1	9,11,12	1.30	1 (11%)	10,15,17	2.33	4 (40%)
1	TPO	H	612	1	8,10,11	0.81	0	10,14,16	1.33	0
1	PHD	D	663	1	9,11,12	0.98	1 (11%)	10,15,17	2.30	4 (40%)
1	PHD	G	663	1	9,11,12	1.23	1 (11%)	10,15,17	2.33	5 (50%)
1	PHD	F	663	1	9,11,12	1.13	1 (11%)	10,15,17	2.25	4 (40%)
1	PHD	H	663	1	9,11,12	1.38	1 (11%)	10,15,17	2.19	4 (40%)
1	TPO	D	612	1	8,10,11	0.74	0	10,14,16	1.54	2 (20%)

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	C	612	1	-	1/9/11/13	-
1	TPO	A	612	1	-	5/9/11/13	-
1	TPO	G	612	1	-	5/9/11/13	-
1	TPO	B	612	1	-	4/9/11/13	-
1	PHD	E	663	1	-	3/8/11/13	-
1	TPO	F	612	1	-	5/9/11/13	-
1	PHD	A	663	1	-	4/8/11/13	-
1	TPO	E	612	1	-	4/9/11/13	-
1	PHD	C	663	1	-	3/8/11/13	-
1	PHD	B	663	1	-	4/8/11/13	-
1	TPO	H	612	1	-	4/9/11/13	-
1	PHD	D	663	1	-	4/8/11/13	-
1	PHD	G	663	1	-	4/8/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PHD	F	663	1	-	4/8/11/13	-
1	PHD	H	663	1	-	3/8/11/13	-
1	TPO	D	612	1	-	1/9/11/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	663	PHD	P-OD1	3.75	1.65	1.59
1	C	663	PHD	P-OD1	3.64	1.64	1.59
1	G	663	PHD	P-OD1	3.43	1.64	1.59
1	B	663	PHD	P-OD1	3.20	1.64	1.59
1	A	663	PHD	P-OD1	3.10	1.64	1.59

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	663	PHD	OD1-CG-CB	4.25	122.79	111.11
1	H	663	PHD	OD1-CG-CB	4.23	122.75	111.11
1	B	663	PHD	OD1-CG-CB	4.23	122.74	111.11
1	G	663	PHD	OD1-CG-CB	4.14	122.50	111.11
1	E	663	PHD	OD1-CG-CB	4.11	122.42	111.11

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	612	TPO	O-C-CA-CB
1	A	612	TPO	N-CA-CB-CG2
1	A	612	TPO	N-CA-CB-OG1
1	A	612	TPO	C-CA-CB-CG2
1	A	612	TPO	CG2-CB-OG1-P

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	612	TPO	2	0
1	A	612	TPO	1	0
1	G	612	TPO	1	0
1	B	612	TPO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	612	TPO	2	0
1	H	612	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/307 (81%)	0.00	1 (0%) 92 93	50, 72, 118, 139	0
1	B	245/307 (79%)	0.10	10 (4%) 37 32	50, 78, 122, 146	0
1	C	243/307 (79%)	0.14	5 (2%) 63 61	50, 80, 127, 147	0
1	D	254/307 (82%)	-0.02	1 (0%) 92 93	45, 69, 116, 155	0
1	E	248/307 (80%)	0.10	7 (2%) 53 49	51, 77, 125, 143	0
1	F	251/307 (81%)	-0.00	2 (0%) 86 86	47, 68, 114, 159	0
1	G	254/307 (82%)	0.02	2 (0%) 86 86	48, 72, 125, 156	0
1	H	247/307 (80%)	0.16	7 (2%) 53 49	51, 82, 127, 155	0
All	All	1992/2456 (81%)	0.06	35 (1%) 68 67	45, 74, 124, 159	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	703	SER	4.2
1	B	554	SER	3.8
1	H	703	SER	3.7
1	B	808	LYS	3.3
1	B	711	SER	3.2

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PHD	G	663	12/13	0.88	0.19	59,87,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PHD	D	663	12/13	0.89	0.17	59,84,104,110	0
1	PHD	A	663	12/13	0.92	0.16	61,87,102,105	0
1	PHD	F	663	12/13	0.92	0.15	56,84,99,100	0
1	PHD	H	663	12/13	0.92	0.12	69,80,97,100	0
1	PHD	C	663	12/13	0.93	0.15	64,80,95,102	0
1	PHD	B	663	12/13	0.93	0.11	73,82,93,96	0
1	PHD	E	663	12/13	0.93	0.12	71,80,95,98	0
1	TPO	C	612	11/12	0.95	0.14	63,71,79,81	0
1	TPO	H	612	11/12	0.95	0.15	69,75,83,86	0
1	TPO	D	612	11/12	0.96	0.18	51,57,60,64	0
1	TPO	A	612	11/12	0.97	0.12	52,62,68,68	0
1	TPO	F	612	11/12	0.97	0.16	51,61,71,76	0
1	TPO	G	612	11/12	0.97	0.18	49,60,66,68	0
1	TPO	E	612	11/12	0.97	0.15	56,66,77,79	0
1	TPO	B	612	11/12	0.98	0.12	56,63,72,73	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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	ZN	G	901	1/1	0.97	0.17	77,77,77,77	0
2	ZN	D	901	1/1	0.99	0.16	72,72,72,72	0
2	ZN	A	901	1/1	0.99	0.17	76,76,76,76	0
2	ZN	B	901	1/1	0.99	0.09	81,81,81,81	0
2	ZN	E	901	1/1	0.99	0.17	77,77,77,77	0
2	ZN	H	901	1/1	0.99	0.12	69,69,69,69	0
2	ZN	C	901	1/1	1.00	0.17	63,63,63,63	0
2	ZN	F	901	1/1	1.00	0.17	72,72,72,72	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.