



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:05 pm BST

PDB ID : 1Z7M  
Title : ATP Phosphoribosyl transferase (HisZG ATP-PRTase) from *Lactococcus lactis*  
Authors : Champagne, K.S.; Sissler, M.; Larrabee, Y.; Doublié, S.; Francklyn, C.S.  
Deposited on : 2005-03-25  
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

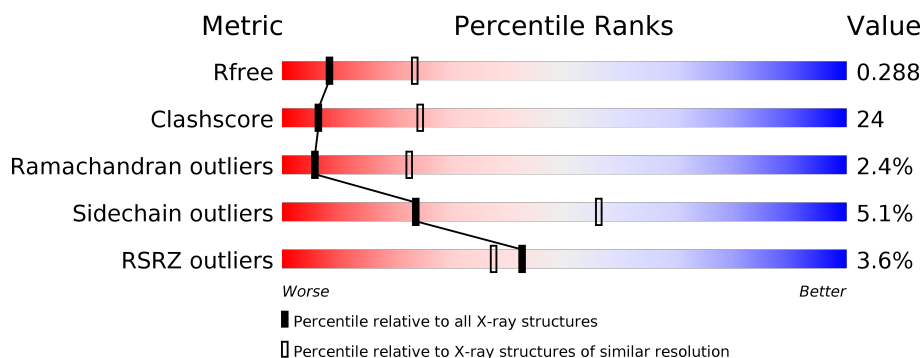
# 1 Overall quality at a glance

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	344	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	344	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>• •</div> <div>8%</div> </div> </div>
1	C	344	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>29%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	344	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>• •</div> <div>9%</div> </div> </div>
2	E	208	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>6%</div> <div>•</div> </div> </div>
2	F	208	<div> <div>9%</div> <div> <div></div> <div>48%</div> <div>45%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	208	
2	H	208	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	WO4	A	329	-	-	-	X
3	WO4	F	210	-	-	-	X
4	PO4	B	329	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16609 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 ATP phosphoribosyltransferase regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	12	0	0
			2526	1624	408	483	11			
1	B	318	Total	C	N	O	S	22	0	0
			2584	1657	424	492	11			
1	C	302	Total	C	N	O	S	11	0	0
			2455	1579	396	469	11			
1	D	314	Total	C	N	O	S	16	0	0
			2557	1642	418	486	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	CLONING ARTIFACT	UNP Q02147
A	-14	ARG	-	CLONING ARTIFACT	UNP Q02147
A	-13	GLY	-	CLONING ARTIFACT	UNP Q02147
A	-12	SER	-	CLONING ARTIFACT	UNP Q02147
A	-11	HIS	-	EXPRESSION TAG	UNP Q02147
A	-10	HIS	-	EXPRESSION TAG	UNP Q02147
A	-9	HIS	-	EXPRESSION TAG	UNP Q02147
A	-8	HIS	-	EXPRESSION TAG	UNP Q02147
A	-7	HIS	-	EXPRESSION TAG	UNP Q02147
A	-6	HIS	-	EXPRESSION TAG	UNP Q02147
A	-5	GLY	-	CLONING ARTIFACT	UNP Q02147
A	-4	SER	-	CLONING ARTIFACT	UNP Q02147
A	-3	ILE	-	CLONING ARTIFACT	UNP Q02147
A	-2	GLU	-	CLONING ARTIFACT	UNP Q02147
A	-1	GLY	-	CLONING ARTIFACT	UNP Q02147
A	0	ARG	-	CLONING ARTIFACT	UNP Q02147
B	-15	MET	-	CLONING ARTIFACT	UNP Q02147
B	-14	ARG	-	CLONING ARTIFACT	UNP Q02147
B	-13	GLY	-	CLONING ARTIFACT	UNP Q02147
B	-12	SER	-	CLONING ARTIFACT	UNP Q02147
B	-11	HIS	-	EXPRESSION TAG	UNP Q02147

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP Q02147
B	-9	HIS	-	EXPRESSION TAG	UNP Q02147
B	-8	HIS	-	EXPRESSION TAG	UNP Q02147
B	-7	HIS	-	EXPRESSION TAG	UNP Q02147
B	-6	HIS	-	EXPRESSION TAG	UNP Q02147
B	-5	GLY	-	CLONING ARTIFACT	UNP Q02147
B	-4	SER	-	CLONING ARTIFACT	UNP Q02147
B	-3	ILE	-	CLONING ARTIFACT	UNP Q02147
B	-2	GLU	-	CLONING ARTIFACT	UNP Q02147
B	-1	GLY	-	CLONING ARTIFACT	UNP Q02147
B	0	ARG	-	CLONING ARTIFACT	UNP Q02147
C	-15	MET	-	CLONING ARTIFACT	UNP Q02147
C	-14	ARG	-	CLONING ARTIFACT	UNP Q02147
C	-13	GLY	-	CLONING ARTIFACT	UNP Q02147
C	-12	SER	-	CLONING ARTIFACT	UNP Q02147
C	-11	HIS	-	EXPRESSION TAG	UNP Q02147
C	-10	HIS	-	EXPRESSION TAG	UNP Q02147
C	-9	HIS	-	EXPRESSION TAG	UNP Q02147
C	-8	HIS	-	EXPRESSION TAG	UNP Q02147
C	-7	HIS	-	EXPRESSION TAG	UNP Q02147
C	-6	HIS	-	EXPRESSION TAG	UNP Q02147
C	-5	GLY	-	CLONING ARTIFACT	UNP Q02147
C	-4	SER	-	CLONING ARTIFACT	UNP Q02147
C	-3	ILE	-	CLONING ARTIFACT	UNP Q02147
C	-2	GLU	-	CLONING ARTIFACT	UNP Q02147
C	-1	GLY	-	CLONING ARTIFACT	UNP Q02147
C	0	ARG	-	CLONING ARTIFACT	UNP Q02147
D	-15	MET	-	CLONING ARTIFACT	UNP Q02147
D	-14	ARG	-	CLONING ARTIFACT	UNP Q02147
D	-13	GLY	-	CLONING ARTIFACT	UNP Q02147
D	-12	SER	-	CLONING ARTIFACT	UNP Q02147
D	-11	HIS	-	EXPRESSION TAG	UNP Q02147
D	-10	HIS	-	EXPRESSION TAG	UNP Q02147
D	-9	HIS	-	EXPRESSION TAG	UNP Q02147
D	-8	HIS	-	EXPRESSION TAG	UNP Q02147
D	-7	HIS	-	EXPRESSION TAG	UNP Q02147
D	-6	HIS	-	EXPRESSION TAG	UNP Q02147
D	-5	GLY	-	CLONING ARTIFACT	UNP Q02147
D	-4	SER	-	CLONING ARTIFACT	UNP Q02147
D	-3	ILE	-	CLONING ARTIFACT	UNP Q02147
D	-2	GLU	-	CLONING ARTIFACT	UNP Q02147
D	-1	GLY	-	CLONING ARTIFACT	UNP Q02147

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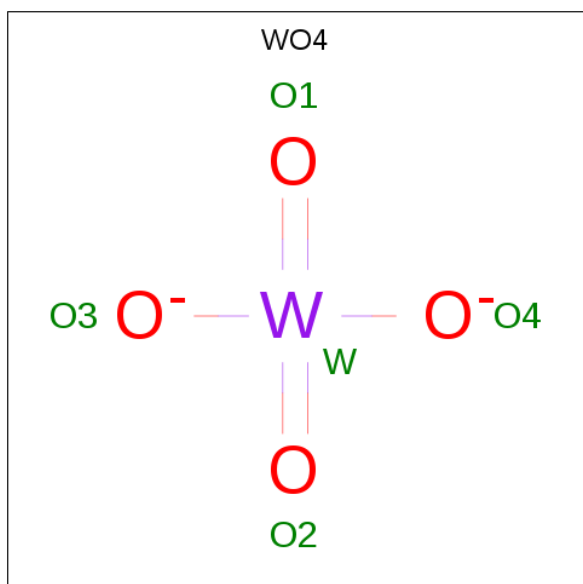
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ARG	-	CLONING ARTIFACT	UNP Q02147

- Molecule 2 is a protein called ATP phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	200	Total	C	N	O	S	5	0	0
			1610	1034	263	309	4			
2	F	201	Total	C	N	O	S	0	0	0
			1611	1035	263	309	4			
2	G	203	Total	C	N	O	S	5	0	0
			1632	1048	267	313	4			
2	H	199	Total	C	N	O	S	4	0	0
			1594	1025	259	306	4			

- Molecule 3 is TUNGSTATE(VI)ION (three-letter code: WO4) (formula: O<sub>4</sub>W).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	W	0	0
			5	4	1		
3	F	1	Total	O	W	0	0
			5	4	1		

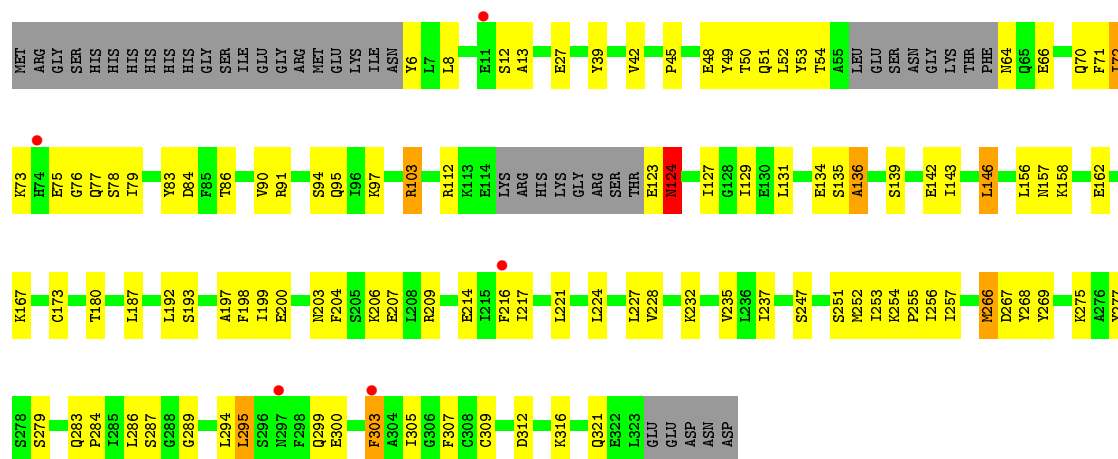
- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



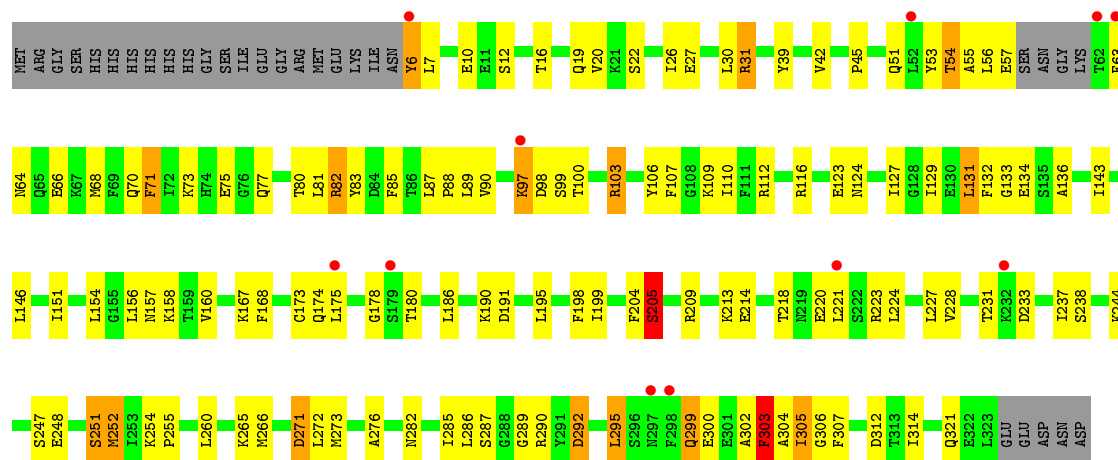
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		



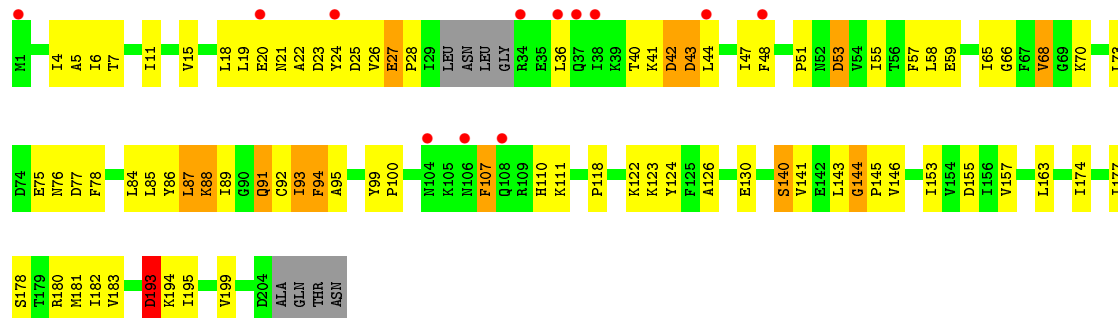




• Molecule 1: ATP phosphoribosyltransferase regulatory subunit

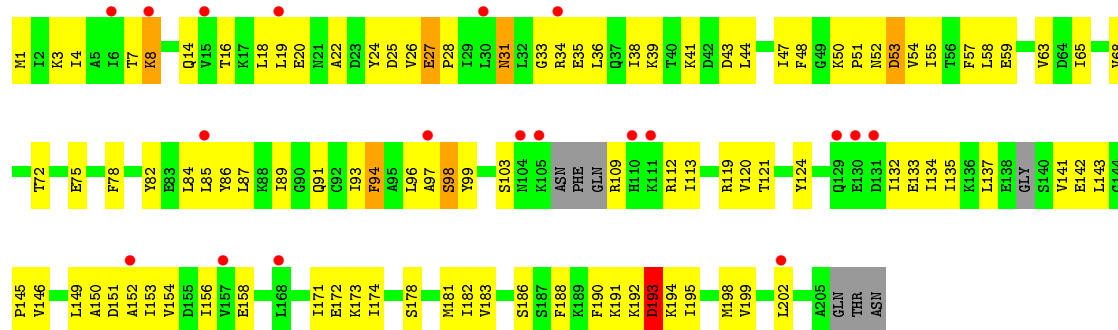


• Molecule 2: ATP phosphoribosyltransferase

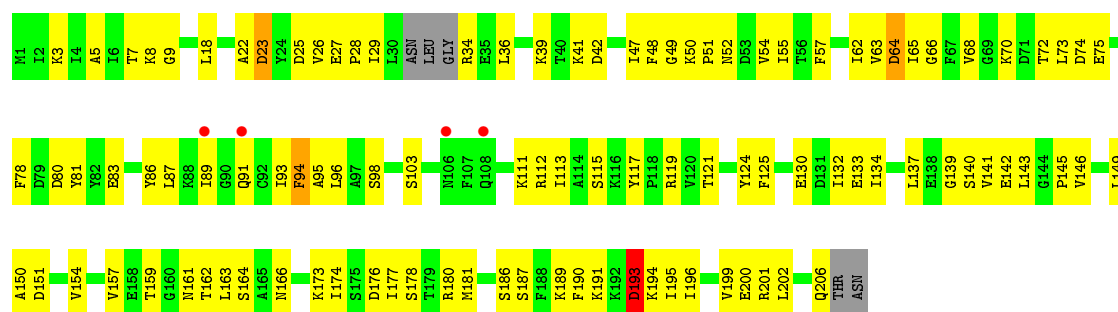


• Molecule 2: ATP phosphoribosyltransferase

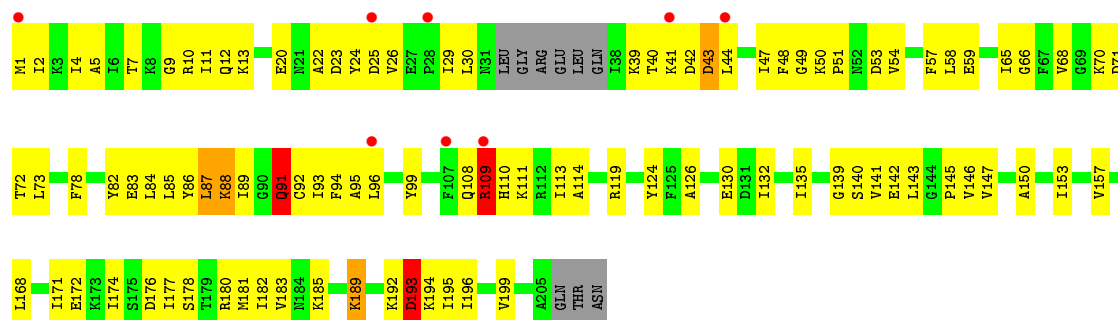




• Molecule 2: ATP phosphoribosyltransferase



• Molecule 2: ATP phosphoribosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.68 Å   222.94 Å   86.38 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 2.90 39.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.90) 88.2 (39.85-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.90 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.245   ,   0.285 0.254   ,   0.288	Depositor DCC
$R_{free}$ test set	2820 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: WO4, PO4

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	0.54	0/2567	0.72	0/3446
1	B	0.50	0/2627	0.67	2/3526 (0.1%)
1	C	0.52	1/2494 (0.0%)	0.68	0/3348
1	D	0.49	2/2599 (0.1%)	0.67	1/3488 (0.0%)
2	E	0.42	0/1632	0.62	0/2193
2	F	0.40	0/1631	0.63	0/2191
2	G	0.43	0/1654	0.66	0/2223
2	H	0.46	1/1616 (0.1%)	0.70	4/2173 (0.2%)
All	All	0.48	4/16820 (0.0%)	0.67	7/22588 (0.0%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	205	SER	C-N	-7.60	1.16	1.34
2	H	110	HIS	C-N	-7.58	1.16	1.34
1	D	303	PHE	C-O	5.35	1.33	1.23
1	C	309	CYS	CB-SG	-5.28	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	109	ARG	CB-CA-C	7.36	125.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	110	HIS	C-N-CA	6.03	136.78	121.70
2	H	110	HIS	CB-CA-C	-5.59	99.21	110.40
1	B	59	ASN	CB-CA-C	-5.42	99.56	110.40
2	H	110	HIS	N-CA-C	5.15	124.91	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	205	SER	Mainchain

## 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	2526	0	2554	115	0
1	B	2584	0	2616	118	0
1	C	2455	0	2480	121	0
1	D	2557	0	2587	117	0
2	E	1610	0	1655	87	0
2	F	1611	0	1664	101	0
2	G	1632	0	1679	98	0
2	H	1594	0	1638	89	0
3	A	5	0	0	0	0
3	F	5	0	0	0	0
4	B	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	1	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
All	All	16609	0	16873	800	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 24.

The worst 5 of 800 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:71:PHE:CE1	1:A:79:ILE:HD11	1.26	1.59
1:C:73:LYS:HE2	1:C:77:GLN:CB	1.39	1.51
1:B:58:SER:HB3	1:B:267:ASP:CB	1.53	1.36
1:C:73:LYS:CE	1:C:77:GLN:HB2	1.52	1.36
1:A:71:PHE:CE1	1:A:79:ILE:CD1	2.14	1.30

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	307/344 (89%)	274 (89%)	29 (9%)	4 (1%)	12	37
1	B	316/344 (92%)	286 (90%)	26 (8%)	4 (1%)	12	37
1	C	296/344 (86%)	274 (93%)	16 (5%)	6 (2%)	7	27
1	D	310/344 (90%)	281 (91%)	21 (7%)	8 (3%)	5	20
2	E	196/208 (94%)	170 (87%)	20 (10%)	6 (3%)	4	16
2	F	195/208 (94%)	162 (83%)	25 (13%)	8 (4%)	3	11
2	G	199/208 (96%)	167 (84%)	25 (13%)	7 (4%)	3	14
2	H	195/208 (94%)	165 (85%)	24 (12%)	6 (3%)	4	16
All	All	2014/2208 (91%)	1779 (88%)	186 (9%)	49 (2%)	6	22

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	TYR
1	A	299	GLN
1	B	61	LYS
1	D	99	SER
1	D	134	GLU

### 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	282/311 (91%)	268 (95%)	14 (5%)	24	57
1	B	288/311 (93%)	270 (94%)	18 (6%)	18	46
1	C	274/311 (88%)	260 (95%)	14 (5%)	24	56
1	D	285/311 (92%)	268 (94%)	17 (6%)	19	49
2	E	180/186 (97%)	166 (92%)	14 (8%)	12	34
2	F	180/186 (97%)	176 (98%)	4 (2%)	52	81
2	G	182/186 (98%)	178 (98%)	4 (2%)	52	81
2	H	178/186 (96%)	169 (95%)	9 (5%)	24	56
All	All	1849/1988 (93%)	1755 (95%)	94 (5%)	24	56

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	266	MET
1	D	97	LYS
2	H	43	ASP
1	C	267	ASP
1	D	31	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	283	GLN
2	E	91	GLN
2	H	31	ASN
1	D	310	HIS
1	D	321	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PO4	F	209	-	4,4,4	1.69	0	6,6,6	0.42	0
3	WO4	F	210	-	2,4,4	1.19	0	-		
3	WO4	A	329	-	2,4,4	1.13	0	-		
4	PO4	B	329	-	4,4,4	6.87	3 (75%)	6,6,6	3.57	4 (66%)
4	PO4	D	329	-	4,4,4	1.62	0	6,6,6	0.44	0
4	PO4	G	209	-	4,4,4	1.63	0	6,6,6	0.43	0
4	PO4	E	209	-	4,4,4	1.66	0	6,6,6	0.43	0
4	PO4	H	209	-	4,4,4	1.60	0	6,6,6	0.43	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	329	PO4	P-O3	9.85	1.84	1.54
4	B	329	PO4	P-O1	-7.99	1.32	1.50
4	B	329	PO4	P-O2	-5.28	1.38	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	329	PO4	O4-P-O3	-5.18	91.35	107.97
4	B	329	PO4	O2-P-O1	4.74	128.24	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	329	PO4	O3-P-O2	-3.54	96.61	107.97
4	B	329	PO4	O3-P-O1	-3.27	98.91	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	209	PO4	1	0
4	B	329	PO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	205:SER	C	206:LYS	N	1.16
1	H	110:HIS	C	111:LYS	N	1.16

## 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	311/344 (90%)	0.21	11 (3%) 44 38	39, 55, 87, 98	3 (0%)
1	B	317/344 (92%)	0.28	4 (1%) 77 77	49, 66, 87, 99	6 (1%)
1	C	302/344 (87%)	0.20	5 (1%) 70 69	43, 66, 88, 93	3 (0%)
1	D	314/344 (91%)	0.39	11 (3%) 44 38	52, 77, 94, 99	4 (1%)
2	E	200/208 (96%)	0.37	12 (6%) 21 18	47, 77, 94, 99	2 (1%)
2	F	201/208 (96%)	0.66	19 (9%) 8 6	69, 80, 93, 100	0
2	G	203/208 (97%)	0.37	4 (1%) 65 63	56, 75, 91, 98	1 (0%)
2	H	199/208 (95%)	0.41	8 (4%) 38 33	61, 75, 92, 97	1 (0%)
All	All	2047/2208 (92%)	0.34	74 (3%) 42 37	39, 72, 92, 100	20 (0%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	ASN	7.3
2	E	108	GLN	5.9
2	G	89	ILE	5.3
2	E	36	LEU	4.6
2	E	106	ASN	4.4

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

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

### 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	Q<0.9
3	WO4	A	329	5/5	0.33	0.56	161,161,161,162	5
3	WO4	F	210	5/5	0.59	0.53	162,162,162,162	5
4	PO4	B	329	5/5	0.82	0.45	103,103,104,127	0
4	PO4	F	209	5/5	0.86	0.13	103,103,104,104	0
4	PO4	D	329	5/5	0.88	0.30	103,104,104,105	0
4	PO4	G	209	5/5	0.91	0.12	102,102,103,103	0
4	PO4	E	209	5/5	0.94	0.10	105,105,106,106	0
4	PO4	H	209	5/5	0.95	0.08	84,86,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.