



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 01:15 PM UTC

PDB ID : 3SDM / pdb\_00003sdm  
Title : Structure of oligomeric kinase/RNase Ire1 in complex with an oligonucleotide  
Authors : Korennykh, A.; Korostelev, A.; Egea, P.; Finer-Moore, J.; Zhang, C.; Stroud, R.; Shokat, K.; Walter, P.  
Deposited on : 2011-06-09  
Resolution : 6.60 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.

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

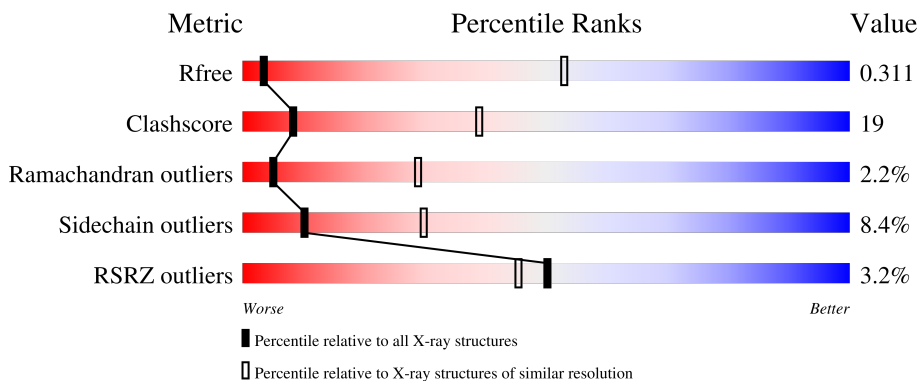
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.60 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.



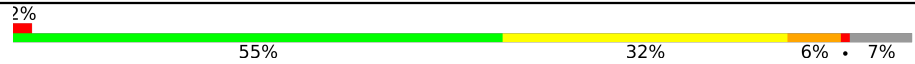

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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  $\geq 3$ , 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	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	448	 2% 55% 32% 6% • 7%
1	G	448	 3% 55% 32% 6% • 7%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 23793 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	418	3399	2162	580	636	3	18	0	0	0
1	B	418	3399	2162	580	636	3	18	0	0	0
1	C	418	3399	2162	580	636	3	18	0	0	0
1	D	418	3399	2162	580	636	3	18	0	0	0
1	E	418	3399	2162	580	636	3	18	0	0	0
1	F	418	3399	2162	580	636	3	18	0	0	0
1	G	418	3399	2162	580	636	3	18	0	0	0

There are 203 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	PRO	-	expression tag	UNP P32361
A	?	-	ASN	deletion	UNP P32361
A	?	-	ASN	deletion	UNP P32361
A	?	-	LEU	deletion	UNP P32361
A	?	-	GLN	deletion	UNP P32361
A	?	-	CYS	deletion	UNP P32361
A	?	-	GLN	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
A	?	-	TYR	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	PRO	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
B	640	PRO	-	expression tag	UNP P32361
B	?	-	ASN	deletion	UNP P32361
B	?	-	ASN	deletion	UNP P32361
B	?	-	LEU	deletion	UNP P32361
B	?	-	GLN	deletion	UNP P32361
B	?	-	CYS	deletion	UNP P32361
B	?	-	GLN	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ARG	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	PHE	deletion	UNP P32361
B	?	-	TYR	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	PRO	deletion	UNP P32361

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	deletion	UNP P32361
C	640	PRO	-	expression tag	UNP P32361
C	?	-	ASN	deletion	UNP P32361
C	?	-	ASN	deletion	UNP P32361
C	?	-	LEU	deletion	UNP P32361
C	?	-	GLN	deletion	UNP P32361
C	?	-	CYS	deletion	UNP P32361
C	?	-	GLN	deletion	UNP P32361
C	?	-	VAL	deletion	UNP P32361
C	?	-	GLU	deletion	UNP P32361
C	?	-	THR	deletion	UNP P32361
C	?	-	GLU	deletion	UNP P32361
C	?	-	HIS	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	ARG	deletion	UNP P32361
C	?	-	HIS	deletion	UNP P32361
C	?	-	THR	deletion	UNP P32361
C	?	-	VAL	deletion	UNP P32361
C	?	-	VAL	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	ASP	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	PHE	deletion	UNP P32361
C	?	-	TYR	deletion	UNP P32361
C	?	-	ASP	deletion	UNP P32361
C	?	-	PRO	deletion	UNP P32361
C	?	-	PHE	deletion	UNP P32361
D	640	PRO	-	expression tag	UNP P32361
D	?	-	ASN	deletion	UNP P32361
D	?	-	ASN	deletion	UNP P32361
D	?	-	LEU	deletion	UNP P32361
D	?	-	GLN	deletion	UNP P32361
D	?	-	CYS	deletion	UNP P32361
D	?	-	GLN	deletion	UNP P32361
D	?	-	VAL	deletion	UNP P32361
D	?	-	GLU	deletion	UNP P32361
D	?	-	THR	deletion	UNP P32361
D	?	-	GLU	deletion	UNP P32361
D	?	-	HIS	deletion	UNP P32361

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	ARG	deletion	UNP P32361
D	?	-	HIS	deletion	UNP P32361
D	?	-	THR	deletion	UNP P32361
D	?	-	VAL	deletion	UNP P32361
D	?	-	VAL	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	ASP	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	PHE	deletion	UNP P32361
D	?	-	TYR	deletion	UNP P32361
D	?	-	ASP	deletion	UNP P32361
D	?	-	PRO	deletion	UNP P32361
D	?	-	PHE	deletion	UNP P32361
E	640	PRO	-	expression tag	UNP P32361
E	?	-	ASN	deletion	UNP P32361
E	?	-	ASN	deletion	UNP P32361
E	?	-	LEU	deletion	UNP P32361
E	?	-	GLN	deletion	UNP P32361
E	?	-	CYS	deletion	UNP P32361
E	?	-	GLN	deletion	UNP P32361
E	?	-	VAL	deletion	UNP P32361
E	?	-	GLU	deletion	UNP P32361
E	?	-	THR	deletion	UNP P32361
E	?	-	GLU	deletion	UNP P32361
E	?	-	HIS	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	ARG	deletion	UNP P32361
E	?	-	HIS	deletion	UNP P32361
E	?	-	THR	deletion	UNP P32361
E	?	-	VAL	deletion	UNP P32361
E	?	-	VAL	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	ASP	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	PHE	deletion	UNP P32361

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	TYR	deletion	UNP P32361
E	?	-	ASP	deletion	UNP P32361
E	?	-	PRO	deletion	UNP P32361
E	?	-	PHE	deletion	UNP P32361
F	640	PRO	-	expression tag	UNP P32361
F	?	-	ASN	deletion	UNP P32361
F	?	-	ASN	deletion	UNP P32361
F	?	-	LEU	deletion	UNP P32361
F	?	-	GLN	deletion	UNP P32361
F	?	-	CYS	deletion	UNP P32361
F	?	-	GLN	deletion	UNP P32361
F	?	-	VAL	deletion	UNP P32361
F	?	-	GLU	deletion	UNP P32361
F	?	-	THR	deletion	UNP P32361
F	?	-	GLU	deletion	UNP P32361
F	?	-	HIS	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	ARG	deletion	UNP P32361
F	?	-	HIS	deletion	UNP P32361
F	?	-	THR	deletion	UNP P32361
F	?	-	VAL	deletion	UNP P32361
F	?	-	VAL	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	ASP	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	PHE	deletion	UNP P32361
F	?	-	TYR	deletion	UNP P32361
F	?	-	ASP	deletion	UNP P32361
F	?	-	PRO	deletion	UNP P32361
F	?	-	PHE	deletion	UNP P32361
G	640	PRO	-	expression tag	UNP P32361
G	?	-	ASN	deletion	UNP P32361
G	?	-	ASN	deletion	UNP P32361
G	?	-	LEU	deletion	UNP P32361
G	?	-	GLN	deletion	UNP P32361
G	?	-	CYS	deletion	UNP P32361
G	?	-	GLN	deletion	UNP P32361
G	?	-	VAL	deletion	UNP P32361
G	?	-	GLU	deletion	UNP P32361

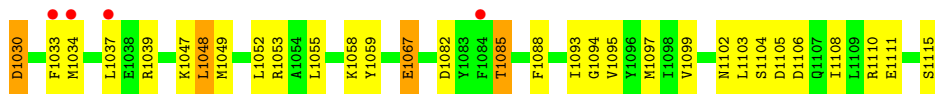
*Continued on next page...*

*Continued from previous page...*

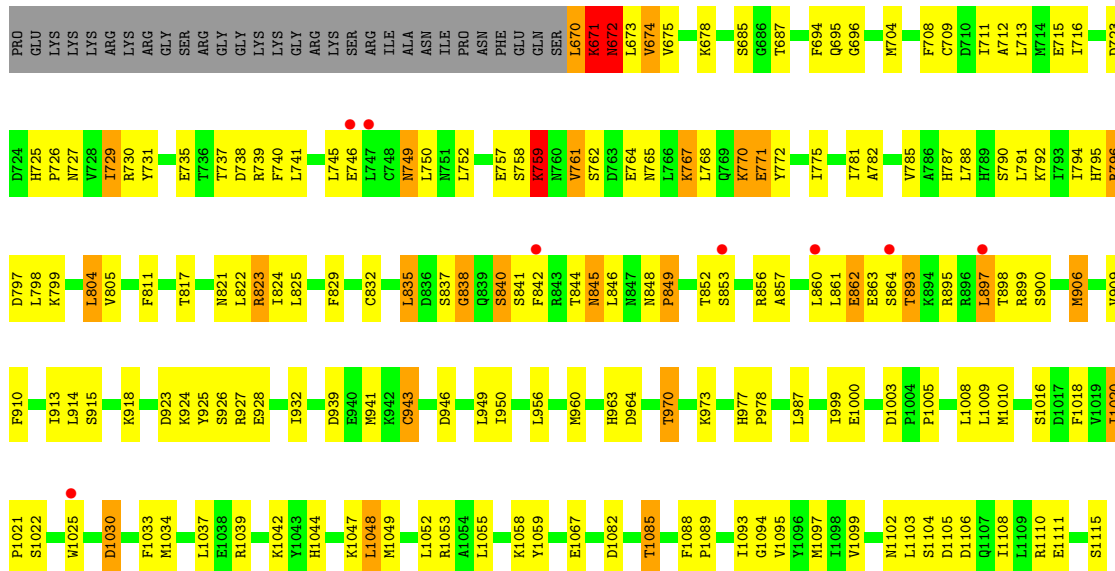
Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	THR	deletion	UNP P32361
G	?	-	GLU	deletion	UNP P32361
G	?	-	HIS	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	ARG	deletion	UNP P32361
G	?	-	HIS	deletion	UNP P32361
G	?	-	THR	deletion	UNP P32361
G	?	-	VAL	deletion	UNP P32361
G	?	-	VAL	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	ASP	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	PHE	deletion	UNP P32361
G	?	-	TYR	deletion	UNP P32361
G	?	-	ASP	deletion	UNP P32361
G	?	-	PRO	deletion	UNP P32361
G	?	-	PHE	deletion	UNP P32361



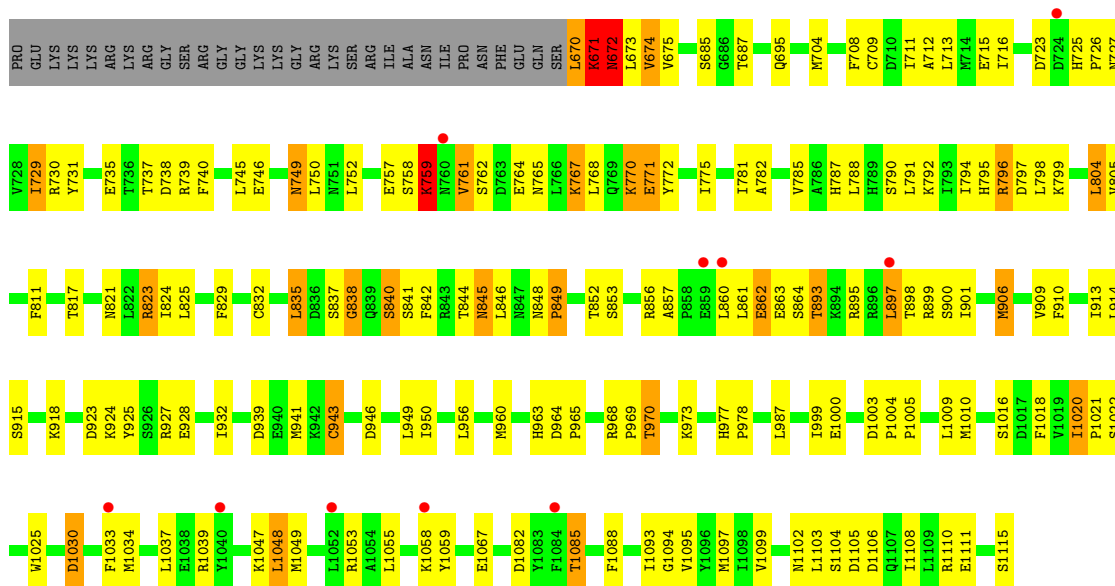




• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

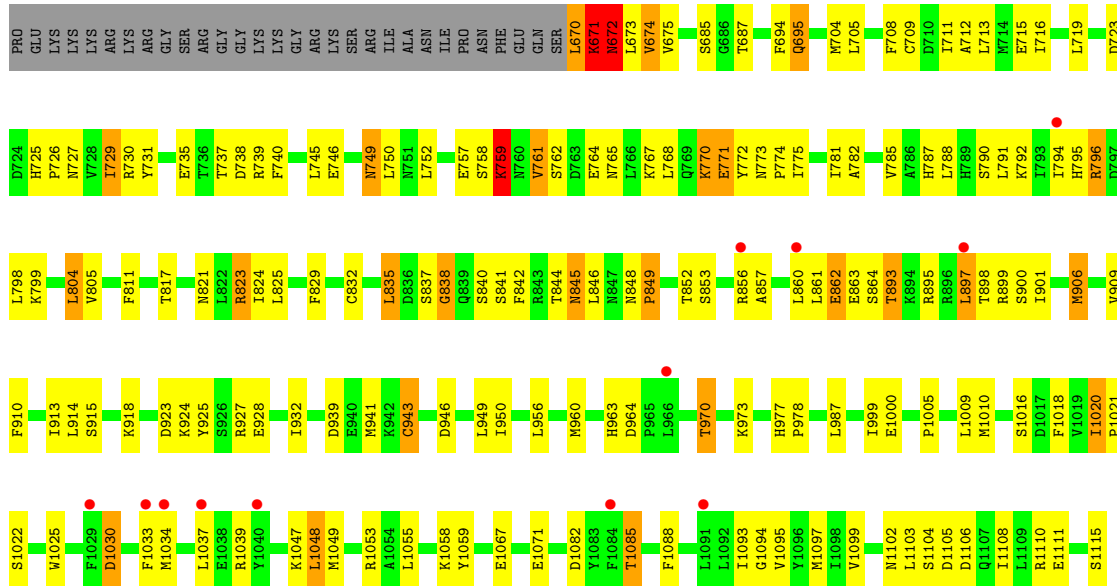


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.65Å 580.67Å 177.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.78 – 6.60 96.78 – 6.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (96.78-6.60) 99.9 (96.78-6.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 6.73Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.286 , 0.317 0.282 , 0.311	Depositor DCC
$R_{free}$ test set	471 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	344.3	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 529.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	23793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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 i

### 5.1 Standard geometry i

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	0.47	0/3437	0.81	3/4629 (0.1%)
1	B	0.46	0/3437	0.81	3/4629 (0.1%)
1	C	0.46	0/3437	0.81	3/4629 (0.1%)
1	D	0.46	0/3437	0.81	3/4629 (0.1%)
1	E	0.46	0/3437	0.81	3/4629 (0.1%)
1	F	0.46	0/3437	0.81	3/4629 (0.1%)
1	G	0.46	0/3437	0.81	3/4629 (0.1%)
All	All	0.46	0/24059	0.81	21/32403 (0.1%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	672	ASN	N-CA-C	-9.98	100.42	112.59
1	F	672	ASN	N-CA-C	-9.97	100.42	112.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	ASN	N-CA-C	-9.97	100.43	112.59
1	G	672	ASN	N-CA-C	-9.97	100.43	112.59
1	E	672	ASN	N-CA-C	-9.96	100.43	112.59

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	671	LYS	Peptide
1	B	671	LYS	Peptide
1	C	671	LYS	Peptide
1	D	671	LYS	Peptide
1	E	671	LYS	Peptide

## 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	3399	0	3409	132	0
1	B	3399	0	3409	132	0
1	C	3399	0	3409	132	1
1	D	3399	0	3409	139	0
1	E	3399	0	3409	137	7
1	F	3399	0	3409	132	0
1	G	3399	0	3409	133	0
All	All	23793	0	23863	913	7

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 19.

The worst 5 of 913 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:D:840:SEP:O2P	1:E:761:VAL:HG11	1.35	1.23
1:A:848:ASN:HB3	1:A:849:PRO:HA	1.42	1.02

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:848:ASN:HB3	1:E:849:PRO:HA	1.42	1.01
1:D:848:ASN:HB3	1:D:849:PRO:HA	1.42	1.01
1:B:848:ASN:HB3	1:B:849:PRO:HA	1.42	1.00

The worst 5 of 7 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)
1:E:1003:ASP:O	1:E:1042:LYS:NZ[4_555]	1.44	0.76
1:E:1003:ASP:O	1:E:1042:LYS:CE[4_555]	1.50	0.70
1:E:1003:ASP:C	1:E:1042:LYS:NZ[4_555]	1.70	0.50
1:E:1003:ASP:OD2	1:E:1044:HIS:NE2[4_555]	1.73	0.47
1:C:761:VAL:CG1	1:E:840:SEP:O2P[2_555]	1.96	0.24

## 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	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	B	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	C	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	D	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	E	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	F	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	G	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
All	All	2891/3136 (92%)	2464 (85%)	364 (13%)	63 (2%)	5	29

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	LYS
1	A	770	LYS
1	A	771	GLU
1	A	862	GLU
1	B	759	LYS

### 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	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	B	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	C	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	D	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	E	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	F	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	G	380/405 (94%)	348 (92%)	32 (8%)	10	30
All	All	2660/2835 (94%)	2436 (92%)	224 (8%)	10	30

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	897	LEU
1	G	1067	GLU
1	E	817	THR
1	G	1048	LEU
1	G	750	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1001	ASN
1	F	1090	ASN
1	G	839	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	C	753	GLN
1	C	725	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

21 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	SEP	F	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	SEP	C	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	D	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	SEP	A	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	TPO	E	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	F	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	TPO	C	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	A	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.42	1 (14%)
1	TPO	G	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	B	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.42	1 (14%)
1	SEP	C	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.74	0
1	SEP	G	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	TPO	D	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.65	2 (20%)
1	SEP	D	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	SEP	G	840	1	8,9,10	1.65	1 (12%)	7,12,14	1.39	1 (14%)
1	SEP	E	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.73	0
1	SEP	E	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.40	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	B	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	TPO	A	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	B	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	F	844	1	8,10,11	3.12	5 (62%)	10,14,16	1.64	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	SEP	F	841	1	-	1/6/8/10	-
1	SEP	C	840	1	-	4/6/8/10	-
1	SEP	D	840	1	-	4/6/8/10	-
1	SEP	A	841	1	-	1/6/8/10	-
1	TPO	E	844	1	-	4/9/11/13	-
1	SEP	F	840	1	-	4/6/8/10	-
1	TPO	C	844	1	-	4/9/11/13	-
1	SEP	A	840	1	-	4/6/8/10	-
1	TPO	G	844	1	-	4/9/11/13	-
1	SEP	B	840	1	-	4/6/8/10	-
1	SEP	C	841	1	-	1/6/8/10	-
1	SEP	G	841	1	-	1/6/8/10	-
1	TPO	D	844	1	-	4/9/11/13	-
1	SEP	D	841	1	-	1/6/8/10	-
1	SEP	G	840	1	-	4/6/8/10	-
1	SEP	E	841	1	-	1/6/8/10	-
1	SEP	E	840	1	-	4/6/8/10	-
1	SEP	B	841	1	-	1/6/8/10	-
1	TPO	A	844	1	-	4/9/11/13	-
1	TPO	B	844	1	-	4/9/11/13	-
1	TPO	F	844	1	-	4/9/11/13	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	844	TPO	O-C	5.56	1.41	1.20
1	D	844	TPO	O-C	5.56	1.41	1.20

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	844	TPO	O-C	5.56	1.41	1.20
1	C	844	TPO	O-C	5.55	1.41	1.20
1	F	844	TPO	O-C	5.55	1.41	1.20

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	844	TPO	O-C-CA	-4.04	114.39	124.77
1	D	844	TPO	O-C-CA	-4.04	114.39	124.77
1	E	844	TPO	O-C-CA	-4.02	114.43	124.77
1	C	844	TPO	O-C-CA	-4.02	114.43	124.77
1	F	844	TPO	O-C-CA	-4.01	114.45	124.77

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	840	SEP	N-CA-CB-OG
1	A	840	SEP	CB-OG-P-O2P
1	A	840	SEP	CB-OG-P-O3P
1	A	844	TPO	N-CA-CB-CG2
1	A	844	TPO	N-CA-CB-OG1

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	840	SEP	1	0
1	D	840	SEP	3	0
1	F	840	SEP	1	0
1	A	840	SEP	1	0
1	B	840	SEP	1	0
1	C	841	SEP	1	0
1	D	841	SEP	2	0
1	E	840	SEP	0	1

## 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 [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, 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	415/448 (92%)	0.15	36 (8%) 16 23	53, 108, 202, 287	0
1	B	415/448 (92%)	-0.04	20 (4%) 35 37	53, 108, 202, 287	0
1	C	415/448 (92%)	-0.41	3 (0%) 84 74	53, 108, 202, 287	0
1	D	415/448 (92%)	-0.31	5 (1%) 76 65	53, 108, 202, 287	0
1	E	415/448 (92%)	-0.24	8 (1%) 66 56	53, 108, 202, 287	0
1	F	415/448 (92%)	-0.16	10 (2%) 59 52	53, 108, 202, 287	0
1	G	415/448 (92%)	-0.15	12 (2%) 53 47	53, 108, 202, 287	0
All	All	2905/3136 (92%)	-0.17	94 (3%) 50 45	53, 108, 203, 287	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1058	LYS	8.9
1	B	860	LEU	7.5
1	A	1033	PHE	6.7
1	B	853	SER	5.9
1	B	856	ARG	5.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	E	841	10/11	0.48	0.18	111,133,156,162	0
1	TPO	A	844	11/12	0.49	0.12	166,194,212,216	0
1	TPO	C	844	11/12	0.52	0.09	166,194,212,216	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	G	844	11/12	0.57	0.07	166,194,212,216	0
1	SEP	C	841	10/11	0.63	0.13	111,133,156,162	0
1	TPO	B	844	11/12	0.65	0.07	166,194,212,216	0
1	TPO	E	844	11/12	0.69	0.06	166,194,212,216	0
1	SEP	G	841	10/11	0.73	0.06	111,133,156,162	0
1	SEP	A	841	10/11	0.76	0.09	111,133,156,162	0
1	TPO	D	844	11/12	0.76	0.07	166,194,212,216	0
1	SEP	E	840	10/11	0.77	0.18	147,153,162,164	0
1	SEP	B	840	10/11	0.81	0.09	147,153,162,164	0
1	SEP	A	840	10/11	0.81	0.08	147,153,162,164	0
1	SEP	D	841	10/11	0.83	0.07	111,133,156,162	0
1	SEP	C	840	10/11	0.84	0.13	147,153,162,164	0
1	SEP	D	840	10/11	0.85	0.06	147,153,162,164	0
1	SEP	F	840	10/11	0.85	0.10	147,153,162,164	0
1	SEP	B	841	10/11	0.86	0.10	111,133,156,162	0
1	SEP	G	840	10/11	0.86	0.11	147,153,162,164	0
1	SEP	F	841	10/11	0.88	0.06	111,133,156,162	0
1	TPO	F	844	11/12	0.89	0.04	166,194,212,216	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.