



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 06:59 PM UTC

PDB ID : 8H58 / pdb_00008h58
Title : Crystal structure of YhaJ effector binding domain
Authors : Kim, M.; Ryu, S.E.
Deposited on : 2022-10-12
Resolution : 2.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

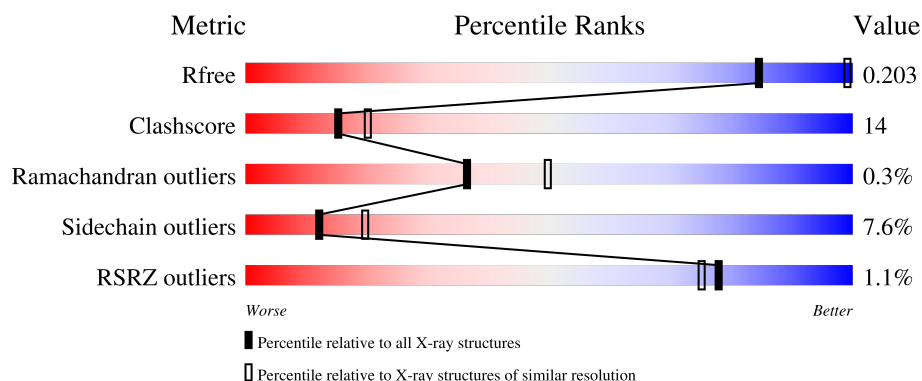
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	207	2% 74% 18% ...
1	B	207	71% 24% ...
1	C	207	68% 25% 5% ...
1	D	207	0% 70% 26% ...
1	E	207	0% 69% 24% ...

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Mol	Chain	Length	Quality of chain
1	F	207	% 72% 24%
1	G	207	% 69% 24% 5%
1	H	207	2% 73% 22%
1	I	207	2% 74% 18%
1	J	207	71% 24%
1	K	207	2% 73% 22%
1	L	207	64% 31%
1	M	207	% 68% 28%
1	N	207	69% 26%
1	O	207	% 76% 18%
1	P	207	69% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25530 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 HTH-type transcriptional regulator YhaJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	B	204	Total	C	N	O	S	0	0	0
			1593	1011	279	295	8			
1	C	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	D	204	Total	C	N	O	S	0	0	0
			1593	1010	278	297	8			
1	E	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	F	205	Total	C	N	O	S	0	0	0
			1606	1019	281	298	8			
1	G	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	H	203	Total	C	N	O	S	0	0	0
			1593	1011	278	296	8			
1	I	201	Total	C	N	O	S	0	0	0
			1575	1000	276	292	7			
1	J	204	Total	C	N	O	S	0	0	0
			1593	1011	279	295	8			
1	K	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	L	203	Total	C	N	O	S	0	0	0
			1592	1010	278	296	8			
1	M	203	Total	C	N	O	S	0	0	0
			1593	1011	279	296	7			
1	N	205	Total	C	N	O	S	0	0	0
			1606	1019	281	298	8			
1	O	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	P	201	Total	C	N	O	S	0	0	0
			1573	1000	273	292	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLY	-	expression tag	UNP P67661
A	93	SER	-	expression tag	UNP P67661
A	94	HIS	-	expression tag	UNP P67661
A	95	MET	-	expression tag	UNP P67661
B	92	GLY	-	expression tag	UNP P67661
B	93	SER	-	expression tag	UNP P67661
B	94	HIS	-	expression tag	UNP P67661
B	95	MET	-	expression tag	UNP P67661
C	92	GLY	-	expression tag	UNP P67661
C	93	SER	-	expression tag	UNP P67661
C	94	HIS	-	expression tag	UNP P67661
C	95	MET	-	expression tag	UNP P67661
D	92	GLY	-	expression tag	UNP P67661
D	93	SER	-	expression tag	UNP P67661
D	94	HIS	-	expression tag	UNP P67661
D	95	MET	-	expression tag	UNP P67661
E	92	GLY	-	expression tag	UNP P67661
E	93	SER	-	expression tag	UNP P67661
E	94	HIS	-	expression tag	UNP P67661
E	95	MET	-	expression tag	UNP P67661
F	92	GLY	-	expression tag	UNP P67661
F	93	SER	-	expression tag	UNP P67661
F	94	HIS	-	expression tag	UNP P67661
F	95	MET	-	expression tag	UNP P67661
G	92	GLY	-	expression tag	UNP P67661
G	93	SER	-	expression tag	UNP P67661
G	94	HIS	-	expression tag	UNP P67661
G	95	MET	-	expression tag	UNP P67661
H	92	GLY	-	expression tag	UNP P67661
H	93	SER	-	expression tag	UNP P67661
H	94	HIS	-	expression tag	UNP P67661
H	95	MET	-	expression tag	UNP P67661
I	92	GLY	-	expression tag	UNP P67661
I	93	SER	-	expression tag	UNP P67661
I	94	HIS	-	expression tag	UNP P67661
I	95	MET	-	expression tag	UNP P67661
J	92	GLY	-	expression tag	UNP P67661
J	93	SER	-	expression tag	UNP P67661
J	94	HIS	-	expression tag	UNP P67661
J	95	MET	-	expression tag	UNP P67661
K	92	GLY	-	expression tag	UNP P67661
K	93	SER	-	expression tag	UNP P67661

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Chain	Residue	Modelled	Actual	Comment	Reference
K	94	HIS	-	expression tag	UNP P67661
K	95	MET	-	expression tag	UNP P67661
L	92	GLY	-	expression tag	UNP P67661
L	93	SER	-	expression tag	UNP P67661
L	94	HIS	-	expression tag	UNP P67661
L	95	MET	-	expression tag	UNP P67661
M	92	GLY	-	expression tag	UNP P67661
M	93	SER	-	expression tag	UNP P67661
M	94	HIS	-	expression tag	UNP P67661
M	95	MET	-	expression tag	UNP P67661
N	92	GLY	-	expression tag	UNP P67661
N	93	SER	-	expression tag	UNP P67661
N	94	HIS	-	expression tag	UNP P67661
N	95	MET	-	expression tag	UNP P67661
O	92	GLY	-	expression tag	UNP P67661
O	93	SER	-	expression tag	UNP P67661
O	94	HIS	-	expression tag	UNP P67661
O	95	MET	-	expression tag	UNP P67661
P	92	GLY	-	expression tag	UNP P67661
P	93	SER	-	expression tag	UNP P67661
P	94	HIS	-	expression tag	UNP P67661
P	95	MET	-	expression tag	UNP P67661

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	2	Total 2	Na 2	0	0
2	M	1	Total 1	Na 1	0	0
2	N	1	Total 1	Na 1	0	0
2	O	1	Total 1	Na 1	0	0
2	P	1	Total 1	Na 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	6	Total 6	O 6	0	0
3	C	4	Total 4	O 4	0	0
3	D	6	Total 6	O 6	0	0
3	E	5	Total 5	O 5	0	0
3	F	4	Total 4	O 4	0	0
3	G	8	Total 8	O 8	0	0
3	H	6	Total 6	O 6	0	0
3	I	7	Total 7	O 7	0	0
3	J	3	Total 3	O 3	0	0
3	K	5	Total 5	O 5	0	0
3	L	8	Total 8	O 8	0	0
3	M	5	Total 5	O 5	0	0
3	N	4	Total 4	O 4	0	0

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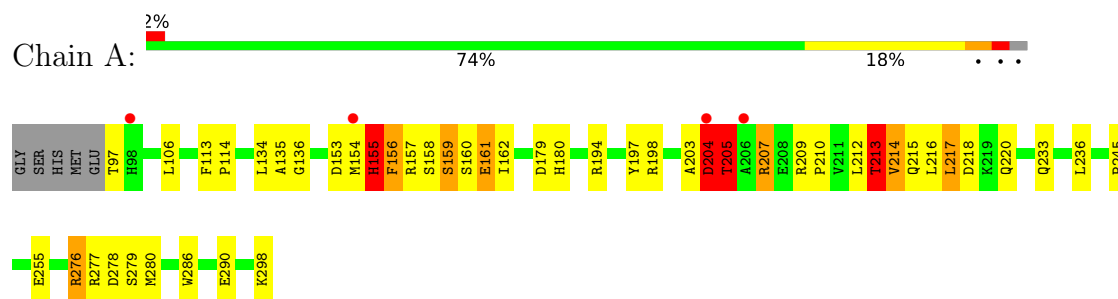
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	8	Total	O	0	0
			8	8		
3	P	5	Total	O	0	0
			5	5		

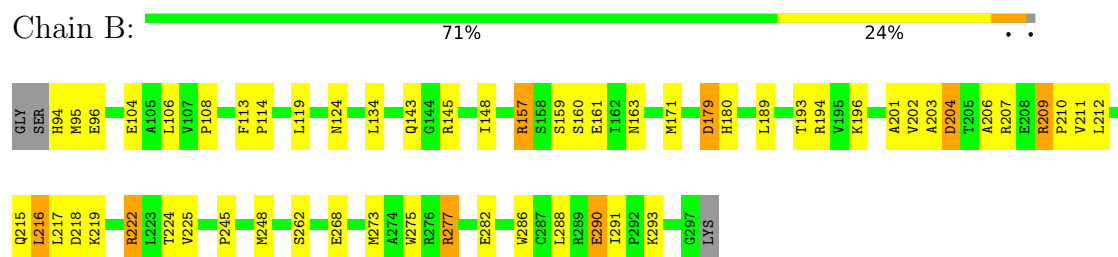
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

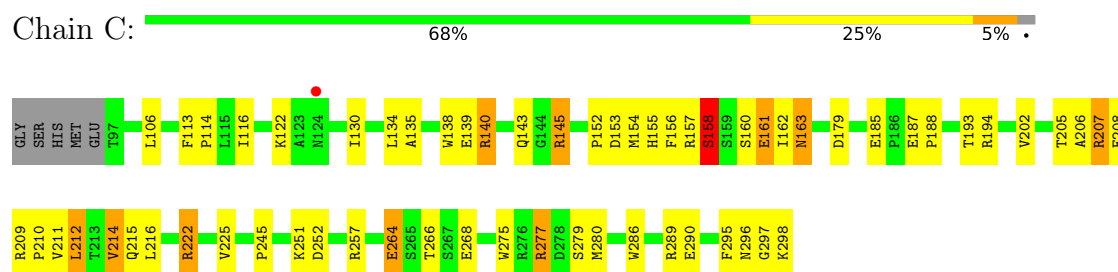
- Molecule 1: HTH-type transcriptional regulator YhaJ



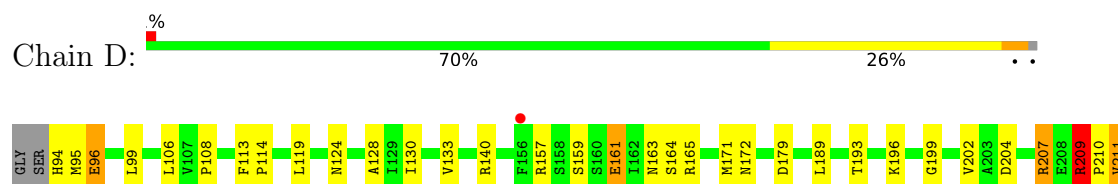
- Molecule 1: HTH-type transcriptional regulator YhaJ



- Molecule 1: HTH-type transcriptional regulator YhaJ



- Molecule 1: HTH-type transcriptional regulator YhaJ

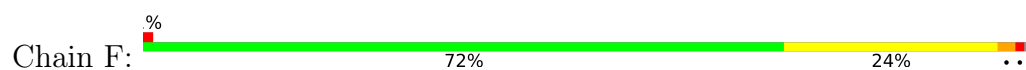




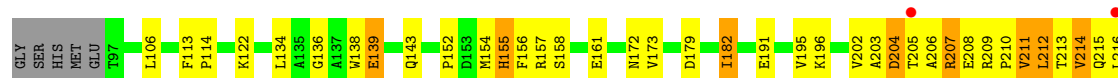
- Molecule 1: HTH-type transcriptional regulator YhaJ



- Molecule 1: HTH-type transcriptional regulator YhaJ



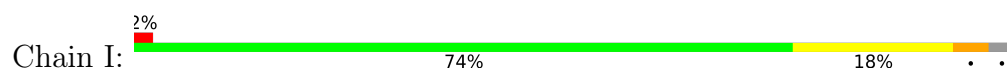
- Molecule 1: HTH-type transcriptional regulator YhaJ

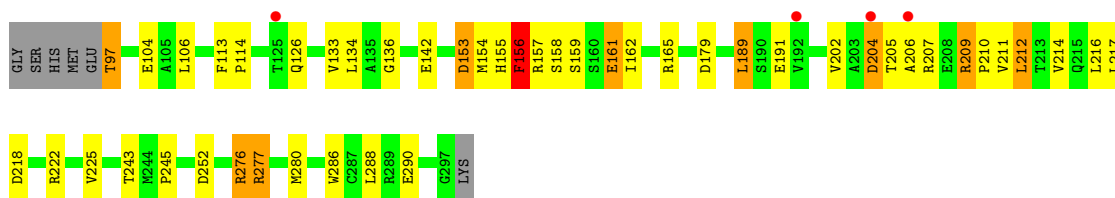


- Molecule 1: HTH-type transcriptional regulator YhaJ



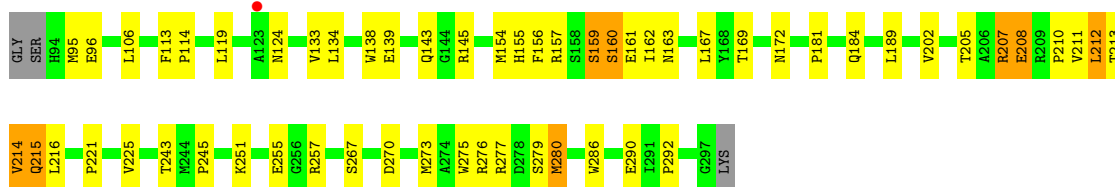
- Molecule 1: HTH-type transcriptional regulator YhaJ





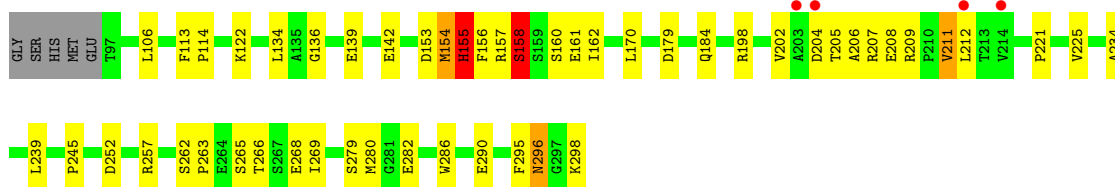
- Molecule 1: HTH-type transcriptional regulator YhaJ

Chain J: 71% 24% . .



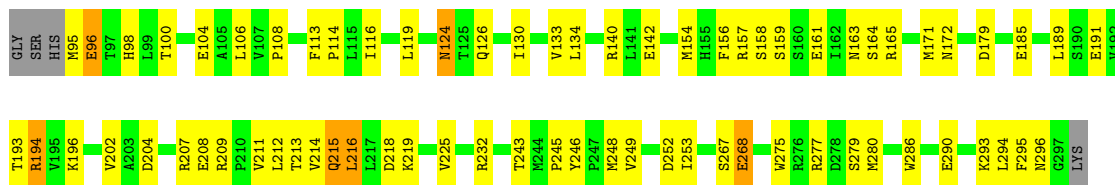
- Molecule 1: HTH-type transcriptional regulator YhaJ

Chain K: 2% 73% 22% . . .



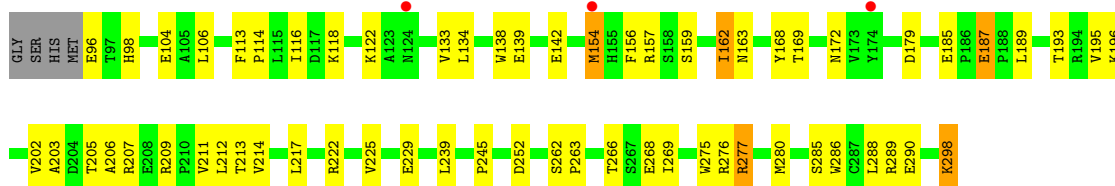
- Molecule 1: HTH-type transcriptional regulator YhaJ

Chain L: 64% 31% . .



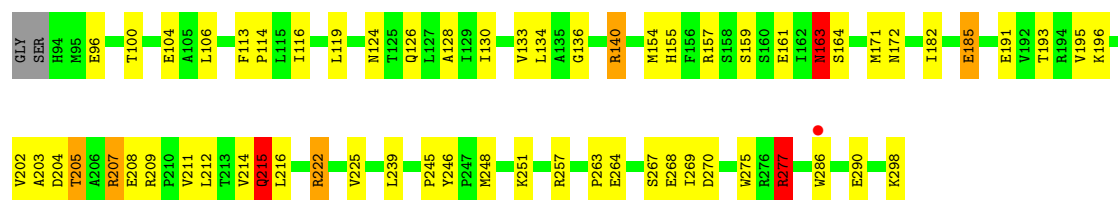
- Molecule 1: HTH-type transcriptional regulator YhaJ

Chain M: 68% 28% . .



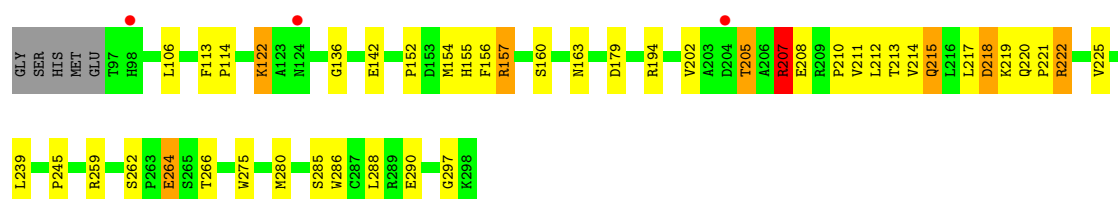
- Molecule 1: HTH-type transcriptional regulator YhaJ

Chain N:  69% 26% ...



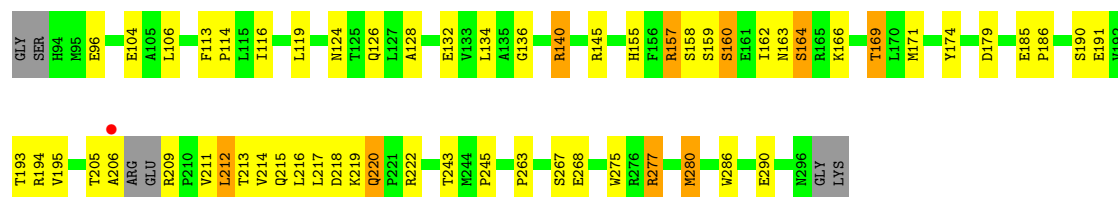
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain O:  % 76% 18% ..



• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain P:  69% 24% ..



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	215.19Å 215.19Å 263.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.91 – 2.64 36.91 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.91-2.64) 99.9 (36.91-2.64)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.236 0.157 , 0.203	Depositor DCC
R_{free} test set	6573 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.220 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.220 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.227 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.227 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.227 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.227 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.256 for h,-h-k,-l	Xtriage

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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.

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Property	Value	Source
Reported twinning fraction	0.139 for H, K, L 0.135 for K, H, -L 0.124 for $-2/3H-1/3K+2/3L$, $-1/3H-2/3K-2/3L$, $2/3H-2/3K+1/3L$ 0.124 for $-1/3H-2/3K-2/3L$, $-2/3H-1/3K+2/3L$, $-2/3H+2/3K-1/3L$ 0.117 for $-1/3H+1/3K-2/3L$, -K, $-4/3H-2/3K+1/3L$ 0.119 for -K, $-1/3H+1/3K-2/3L$, $4/3H+2/3K-1/3L$ 0.120 for $1/3H-1/3K+2/3L$, -H, $-2/3H-4/3K-1/3L$ 0.122 for -H, $1/3H-1/3K+2/3L$, $2/3H+4/3K+1/3L$	Depositor
Outliers	0 of 133605 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25530	wwPDB-VP
Average B, all atoms ($\text{\AA}^2$)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.70	0/1615	1.15	6/2196 (0.3%)
1	B	0.65	1/1624 (0.1%)	1.06	3/2209 (0.1%)
1	C	0.71	0/1615	1.08	7/2196 (0.3%)
1	D	0.69	0/1624	1.05	3/2210 (0.1%)
1	E	0.72	0/1615	1.08	5/2196 (0.2%)
1	F	0.69	0/1637	1.13	10/2225 (0.4%)
1	G	0.70	0/1615	1.07	3/2196 (0.1%)
1	H	0.68	0/1624	1.02	1/2209 (0.0%)
1	I	0.70	1/1606 (0.1%)	1.03	3/2185 (0.1%)
1	J	0.68	0/1624	1.05	3/2209 (0.1%)
1	K	0.72	0/1615	1.10	4/2196 (0.2%)
1	L	0.70	1/1623 (0.1%)	1.08	6/2207 (0.3%)
1	M	0.72	0/1624	1.07	1/2208 (0.0%)
1	N	0.69	0/1637	1.09	8/2225 (0.4%)
1	O	0.69	0/1615	1.13	11/2196 (0.5%)
1	P	0.76	1/1603 (0.1%)	1.12	2/2180 (0.1%)
All	All	0.70	4/25916 (0.0%)	1.08	76/35243 (0.2%)

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	D	0	1
1	F	0	1
1	I	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	155	HIS	CE1-NE2	6.54	1.39	1.32
1	I	153	ASP	CG-OD1	5.67	1.36	1.25
1	L	268	GLU	CD-OE2	5.09	1.35	1.25
1	B	180	HIS	CE1-NE2	5.04	1.37	1.32

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ASP	CA-CB-CG	8.72	121.33	112.60
1	K	179	ASP	CA-CB-CG	8.56	121.16	112.60
1	O	222	ARG	CB-CG-CD	7.96	129.62	111.30
1	O	264	GLU	CB-CA-C	-7.91	97.24	110.68
1	O	157	ARG	CG-CD-NE	7.88	129.34	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	HIS	Peptide
1	D	209	ARG	Mainchain
1	F	132	GLU	Sidechain
1	I	156	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1584	0	1628	50	0
1	B	1593	0	1630	66	0
1	C	1584	0	1630	68	0
1	D	1593	0	1622	40	1
1	E	1584	0	1630	63	1
1	F	1606	0	1647	48	0
1	G	1584	0	1629	48	1
1	H	1593	0	1630	33	1
1	I	1575	0	1617	51	0
1	J	1593	0	1628	50	0
1	K	1584	0	1630	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1592	0	1631	68	3
1	M	1593	0	1636	51	2
1	N	1606	0	1647	54	0
1	O	1584	0	1629	35	2
1	P	1573	0	1610	58	3
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	D	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
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	10	0	0	2	0
3	B	6	0	0	3	0
3	C	4	0	0	1	0
3	D	6	0	0	1	0
3	E	5	0	0	2	0
3	F	4	0	0	0	0
3	G	8	0	0	0	0
3	H	6	0	0	0	0
3	I	7	0	0	4	0
3	J	3	0	0	0	0
3	K	5	0	0	0	0
3	L	8	0	0	5	0
3	M	5	0	0	2	0
3	N	4	0	0	0	0
3	O	8	0	0	0	0
3	P	5	0	0	1	0
All	All	25530	0	26074	699	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 14.

The worst 5 of 699 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:E:98:HIS:HB3	1:F:207:ARG:NH2	1.57	1.20
1:L:296:ASN:OD1	3:L:401:HOH:O	1.61	1.18
1:E:98:HIS:HB3	1:F:207:ARG:CZ	1.76	1.16
1:B:209:ARG:CG	1:B:216:LEU:HD22	1.79	1.13
1:C:185:GLU:OE1	1:C:187:GLU:N	1.85	1.09

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:L:165:ARG:CZ	1:P:160:SER:O[9_544]	1.23	0.97
1:L:165:ARG:NH2	1:P:160:SER:O[9_544]	1.48	0.72
1:L:165:ARG:NE	1:P:160:SER:O[9_544]	1.58	0.62
1:E:209:ARG:NH2	1:G:208:GLU:OE2[3_655]	1.87	0.33
1:M:209:ARG:NH2	1:O:208:GLU:O[2_555]	2.09	0.11

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	200/207 (97%)	188 (94%)	9 (4%)	3 (2%)	8	11
1	B	202/207 (98%)	191 (95%)	11 (5%)	0	100	100
1	C	200/207 (97%)	192 (96%)	8 (4%)	0	100	100
1	D	202/207 (98%)	196 (97%)	6 (3%)	0	100	100
1	E	200/207 (97%)	188 (94%)	12 (6%)	0	100	100
1	F	203/207 (98%)	196 (97%)	7 (3%)	0	100	100
1	G	200/207 (97%)	189 (94%)	10 (5%)	1 (0%)	24	36
1	H	201/207 (97%)	190 (94%)	11 (6%)	0	100	100
1	I	199/207 (96%)	185 (93%)	11 (6%)	3 (2%)	8	11
1	J	202/207 (98%)	192 (95%)	9 (4%)	1 (0%)	24	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	200/207 (97%)	190 (95%)	9 (4%)	1 (0%)	24	36
1	L	201/207 (97%)	196 (98%)	5 (2%)	0	100	100
1	M	201/207 (97%)	191 (95%)	9 (4%)	1 (0%)	24	36
1	N	203/207 (98%)	198 (98%)	5 (2%)	0	100	100
1	O	200/207 (97%)	189 (94%)	11 (6%)	0	100	100
1	P	197/207 (95%)	191 (97%)	6 (3%)	0	100	100
All	All	3211/3312 (97%)	3062 (95%)	139 (4%)	10 (0%)	36	50

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	A	214	VAL
1	I	156	PHE
1	I	161	GLU
1	K	155	HIS

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	173/177 (98%)	163 (94%)	10 (6%)	18	30
1	B	173/177 (98%)	162 (94%)	11 (6%)	16	26
1	C	173/177 (98%)	161 (93%)	12 (7%)	14	23
1	D	173/177 (98%)	155 (90%)	18 (10%)	7	9
1	E	173/177 (98%)	156 (90%)	17 (10%)	7	11
1	F	175/177 (99%)	159 (91%)	16 (9%)	9	13
1	G	173/177 (98%)	157 (91%)	16 (9%)	8	13
1	H	174/177 (98%)	162 (93%)	12 (7%)	14	23
1	I	172/177 (97%)	159 (92%)	13 (8%)	12	20
1	J	173/177 (98%)	160 (92%)	13 (8%)	12	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	173/177 (98%)	166 (96%)	7 (4%)	28	45
1	L	174/177 (98%)	158 (91%)	16 (9%)	8	13
1	M	174/177 (98%)	162 (93%)	12 (7%)	14	23
1	N	175/177 (99%)	161 (92%)	14 (8%)	11	18
1	O	173/177 (98%)	166 (96%)	7 (4%)	28	45
1	P	172/177 (97%)	155 (90%)	17 (10%)	7	10
All	All	2773/2832 (98%)	2562 (92%)	211 (8%)	12	20

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	189	LEU
1	K	265	SER
1	P	166	LYS
1	I	212	LEU
1	J	208	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	143	GLN
1	L	172	ASN
1	O	296	ASN
1	L	163	ASN
1	L	296	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 15 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	202/207 (97%)	-0.04	4 (1%) 65 61	34, 51, 73, 97	0
1	B	204/207 (98%)	-0.03	0 100 100	28, 56, 72, 92	0
1	C	202/207 (97%)	-0.07	1 (0%) 87 85	34, 53, 76, 88	0
1	D	204/207 (98%)	0.08	3 (1%) 72 69	39, 56, 76, 95	0
1	E	202/207 (97%)	-0.06	2 (0%) 79 76	31, 51, 73, 83	0
1	F	205/207 (99%)	-0.10	2 (0%) 79 76	29, 52, 73, 115	0
1	G	202/207 (97%)	-0.06	2 (0%) 79 76	30, 51, 78, 87	0
1	H	203/207 (98%)	-0.01	5 (2%) 58 54	33, 53, 78, 95	0
1	I	201/207 (97%)	-0.03	4 (1%) 65 61	32, 52, 72, 93	0
1	J	204/207 (98%)	0.08	1 (0%) 87 85	26, 57, 73, 85	0
1	K	202/207 (97%)	-0.04	4 (1%) 65 61	37, 53, 70, 84	0
1	L	203/207 (98%)	-0.05	0 100 100	37, 55, 71, 93	0
1	M	203/207 (98%)	-0.07	3 (1%) 72 69	32, 52, 76, 96	0
1	N	205/207 (99%)	-0.12	1 (0%) 87 85	29, 53, 69, 111	0
1	O	202/207 (97%)	-0.11	3 (1%) 72 69	34, 51, 76, 91	0
1	P	201/207 (97%)	-0.08	1 (0%) 87 85	33, 54, 72, 81	0
All	All	3245/3312 (97%)	-0.05	36 (1%) 78 75	26, 53, 74, 115	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ASP	4.7
1	F	286	TRP	3.4
1	A	206	ALA	3.2
1	I	206	ALA	3.1
1	A	98	HIS	3.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	NA	A	302	1/1	0.90	0.09	37,37,37,37	0
2	NA	G	301	1/1	0.91	0.11	40,40,40,40	0
2	NA	F	301	1/1	0.92	0.17	40,40,40,40	0
2	NA	C	301	1/1	0.92	0.10	32,32,32,32	0
2	NA	D	301	1/1	0.93	0.14	49,49,49,49	0
2	NA	J	301	1/1	0.93	0.07	37,37,37,37	0
2	NA	L	302	1/1	0.93	0.14	38,38,38,38	0
2	NA	L	301	1/1	0.96	0.12	46,46,46,46	0
2	NA	H	301	1/1	0.96	0.12	44,44,44,44	0
2	NA	N	301	1/1	0.97	0.29	58,58,58,58	0
2	NA	O	301	1/1	0.97	0.13	32,32,32,32	0
2	NA	I	301	1/1	0.98	0.12	26,26,26,26	0
2	NA	A	301	1/1	0.98	0.11	33,33,33,33	0
2	NA	P	301	1/1	0.98	0.11	43,43,43,43	0
2	NA	M	301	1/1	0.99	0.08	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.