



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:21 AM UTC

PDB ID : 8ILT / pdb\_00008ilt  
Title : Crystal structure of Est30  
Authors : Feng, Y.; Luo, Z.  
Deposited on : 2023-03-04  
Resolution : 2.42 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)

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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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

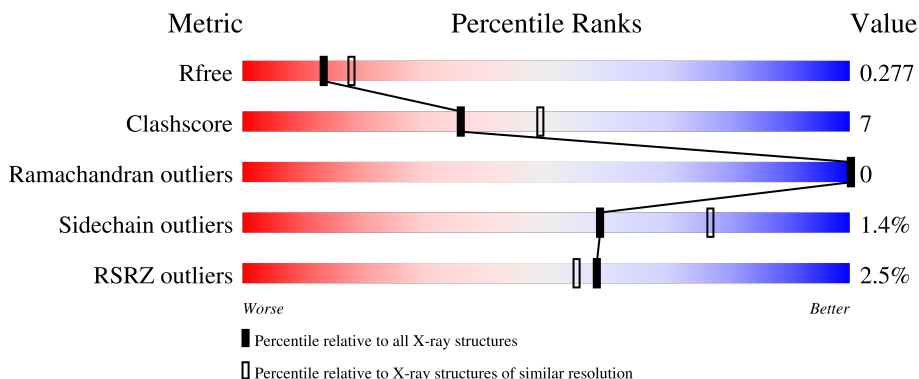
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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.



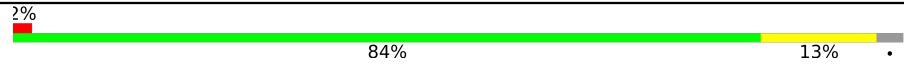

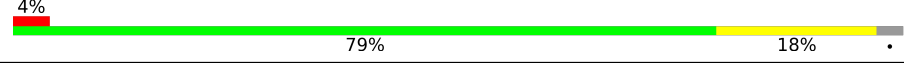
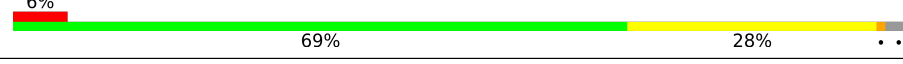
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	255	 90% 8%
1	B	255	 84% 14%
1	C	255	 86% 13%
1	D	255	 84% 13%
1	E	255	 86% 13%

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Mol	Chain	Length	Quality of chain
1	F	255	
1	G	255	
1	H	255	
1	I	255	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18672 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 Carboxylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	Total 2043	C 1315	N 332	O 385	S 11	0	1	0
1	B	250	Total 2040	C 1314	N 329	O 385	S 12	0	3	0
1	C	253	Total 2058	C 1324	N 338	O 385	S 11	0	0	0
1	D	248	Total 2009	C 1295	N 325	O 378	S 11	0	0	0
1	E	254	Total 2076	C 1335	N 341	O 389	S 11	0	2	0
1	F	248	Total 2009	C 1295	N 325	O 378	S 11	0	0	0
1	G	247	Total 2004	C 1291	N 324	O 378	S 11	0	1	0
1	H	248	Total 2009	C 1295	N 325	O 378	S 11	0	0	0
1	I	248	Total 2009	C 1295	N 325	O 378	S 11	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q06174
A	127	SER	MET	engineered mutation	UNP Q06174
A	130	LEU	GLY	engineered mutation	UNP Q06174
A	171	LYS	ILE	engineered mutation	UNP Q06174
A	248	LEU	-	expression tag	UNP Q06174
A	249	GLU	-	expression tag	UNP Q06174
A	250	HIS	-	expression tag	UNP Q06174
A	251	HIS	-	expression tag	UNP Q06174
A	252	HIS	-	expression tag	UNP Q06174
A	253	HIS	-	expression tag	UNP Q06174
A	254	HIS	-	expression tag	UNP Q06174

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Chain	Residue	Modelled	Actual	Comment	Reference
A	255	HIS	-	expression tag	UNP Q06174
B	1	MET	-	initiating methionine	UNP Q06174
B	127	SER	MET	engineered mutation	UNP Q06174
B	130	LEU	GLY	engineered mutation	UNP Q06174
B	171	LYS	ILE	engineered mutation	UNP Q06174
B	248	LEU	-	expression tag	UNP Q06174
B	249	GLU	-	expression tag	UNP Q06174
B	250	HIS	-	expression tag	UNP Q06174
B	251	HIS	-	expression tag	UNP Q06174
B	252	HIS	-	expression tag	UNP Q06174
B	253	HIS	-	expression tag	UNP Q06174
B	254	HIS	-	expression tag	UNP Q06174
B	255	HIS	-	expression tag	UNP Q06174
C	1	MET	-	initiating methionine	UNP Q06174
C	127	SER	MET	engineered mutation	UNP Q06174
C	130	LEU	GLY	engineered mutation	UNP Q06174
C	171	LYS	ILE	engineered mutation	UNP Q06174
C	248	LEU	-	expression tag	UNP Q06174
C	249	GLU	-	expression tag	UNP Q06174
C	250	HIS	-	expression tag	UNP Q06174
C	251	HIS	-	expression tag	UNP Q06174
C	252	HIS	-	expression tag	UNP Q06174
C	253	HIS	-	expression tag	UNP Q06174
C	254	HIS	-	expression tag	UNP Q06174
C	255	HIS	-	expression tag	UNP Q06174
D	1	MET	-	initiating methionine	UNP Q06174
D	127	SER	MET	engineered mutation	UNP Q06174
D	130	LEU	GLY	engineered mutation	UNP Q06174
D	171	LYS	ILE	engineered mutation	UNP Q06174
D	248	LEU	-	expression tag	UNP Q06174
D	249	GLU	-	expression tag	UNP Q06174
D	250	HIS	-	expression tag	UNP Q06174
D	251	HIS	-	expression tag	UNP Q06174
D	252	HIS	-	expression tag	UNP Q06174
D	253	HIS	-	expression tag	UNP Q06174
D	254	HIS	-	expression tag	UNP Q06174
D	255	HIS	-	expression tag	UNP Q06174
E	1	MET	-	initiating methionine	UNP Q06174
E	127	SER	MET	engineered mutation	UNP Q06174
E	130	LEU	GLY	engineered mutation	UNP Q06174
E	171	LYS	ILE	engineered mutation	UNP Q06174
E	248	LEU	-	expression tag	UNP Q06174

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Chain	Residue	Modelled	Actual	Comment	Reference
E	249	GLU	-	expression tag	UNP Q06174
E	250	HIS	-	expression tag	UNP Q06174
E	251	HIS	-	expression tag	UNP Q06174
E	252	HIS	-	expression tag	UNP Q06174
E	253	HIS	-	expression tag	UNP Q06174
E	254	HIS	-	expression tag	UNP Q06174
E	255	HIS	-	expression tag	UNP Q06174
F	1	MET	-	initiating methionine	UNP Q06174
F	127	SER	MET	engineered mutation	UNP Q06174
F	130	LEU	GLY	engineered mutation	UNP Q06174
F	171	LYS	ILE	engineered mutation	UNP Q06174
F	248	LEU	-	expression tag	UNP Q06174
F	249	GLU	-	expression tag	UNP Q06174
F	250	HIS	-	expression tag	UNP Q06174
F	251	HIS	-	expression tag	UNP Q06174
F	252	HIS	-	expression tag	UNP Q06174
F	253	HIS	-	expression tag	UNP Q06174
F	254	HIS	-	expression tag	UNP Q06174
F	255	HIS	-	expression tag	UNP Q06174
G	1	MET	-	initiating methionine	UNP Q06174
G	127	SER	MET	engineered mutation	UNP Q06174
G	130	LEU	GLY	engineered mutation	UNP Q06174
G	171	LYS	ILE	engineered mutation	UNP Q06174
G	248	LEU	-	expression tag	UNP Q06174
G	249	GLU	-	expression tag	UNP Q06174
G	250	HIS	-	expression tag	UNP Q06174
G	251	HIS	-	expression tag	UNP Q06174
G	252	HIS	-	expression tag	UNP Q06174
G	253	HIS	-	expression tag	UNP Q06174
G	254	HIS	-	expression tag	UNP Q06174
G	255	HIS	-	expression tag	UNP Q06174
H	1	MET	-	initiating methionine	UNP Q06174
H	127	SER	MET	engineered mutation	UNP Q06174
H	130	LEU	GLY	engineered mutation	UNP Q06174
H	171	LYS	ILE	engineered mutation	UNP Q06174
H	248	LEU	-	expression tag	UNP Q06174
H	249	GLU	-	expression tag	UNP Q06174
H	250	HIS	-	expression tag	UNP Q06174
H	251	HIS	-	expression tag	UNP Q06174
H	252	HIS	-	expression tag	UNP Q06174
H	253	HIS	-	expression tag	UNP Q06174
H	254	HIS	-	expression tag	UNP Q06174

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Chain	Residue	Modelled	Actual	Comment	Reference
H	255	HIS	-	expression tag	UNP Q06174
I	1	MET	-	initiating methionine	UNP Q06174
I	127	SER	MET	engineered mutation	UNP Q06174
I	130	LEU	GLY	engineered mutation	UNP Q06174
I	171	LYS	ILE	engineered mutation	UNP Q06174
I	248	LEU	-	expression tag	UNP Q06174
I	249	GLU	-	expression tag	UNP Q06174
I	250	HIS	-	expression tag	UNP Q06174
I	251	HIS	-	expression tag	UNP Q06174
I	252	HIS	-	expression tag	UNP Q06174
I	253	HIS	-	expression tag	UNP Q06174
I	254	HIS	-	expression tag	UNP Q06174
I	255	HIS	-	expression tag	UNP Q06174

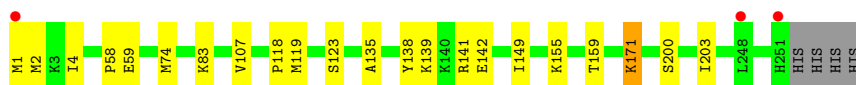
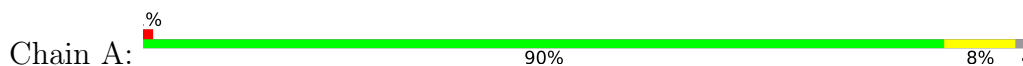
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	75	Total O 75 75	0	0
2	B	61	Total O 61 61	0	0
2	C	73	Total O 73 73	0	0
2	D	55	Total O 55 55	0	0
2	E	50	Total O 50 50	0	0
2	F	34	Total O 34 34	0	0
2	G	23	Total O 23 23	0	0
2	H	30	Total O 30 30	0	0
2	I	14	Total O 14 14	0	0

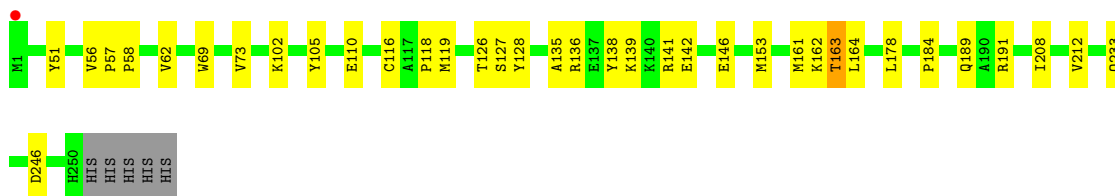
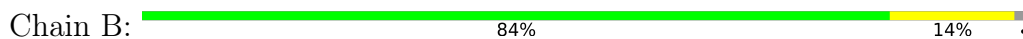
### 3 Residue-property plots [i](#)

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

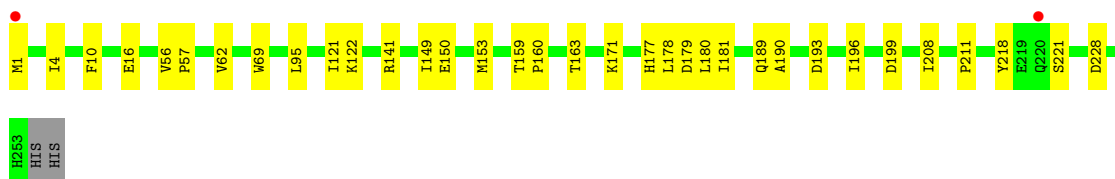
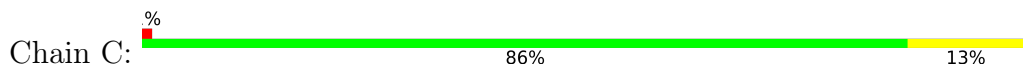
- Molecule 1: Carboxylesterase



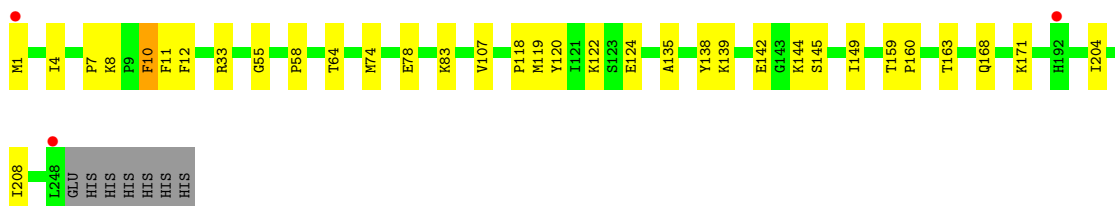
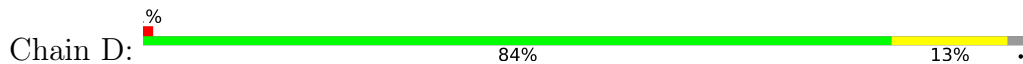
- Molecule 1: Carboxylesterase



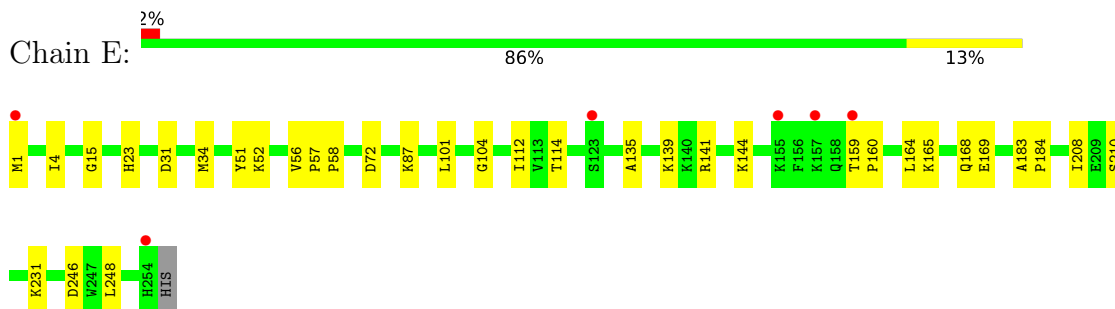
- Molecule 1: Carboxylesterase



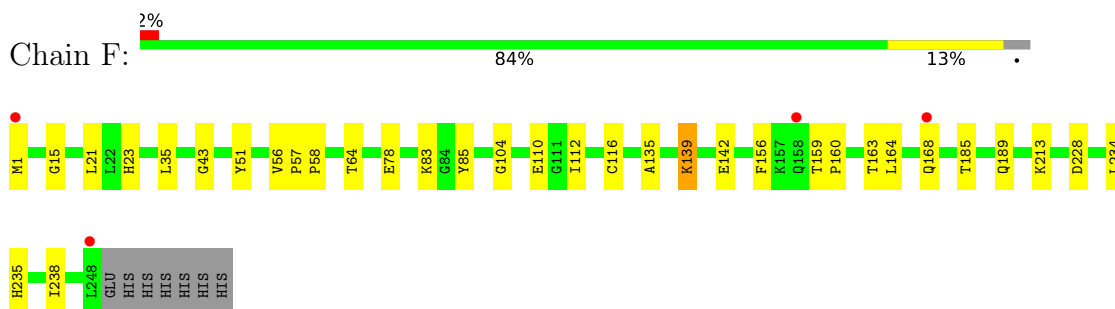
- Molecule 1: Carboxylesterase



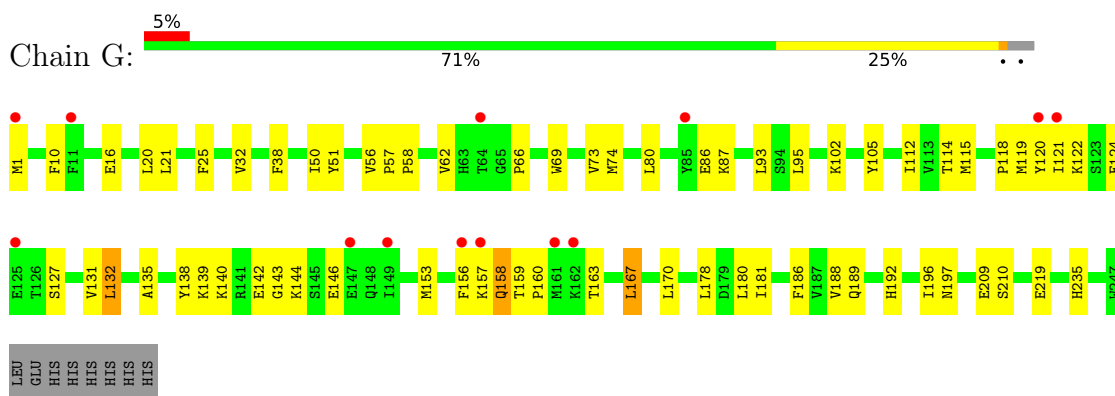
- Molecule 1: Carboxylesterase



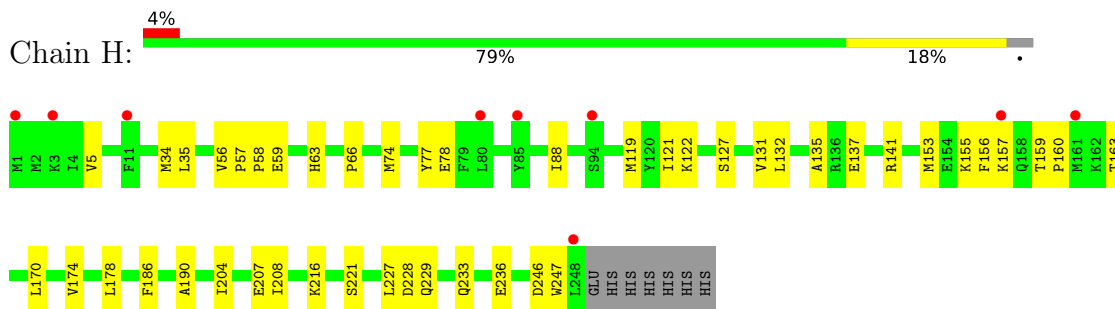
- Molecule 1: Carboxylesterase



- Molecule 1: Carboxylesterase

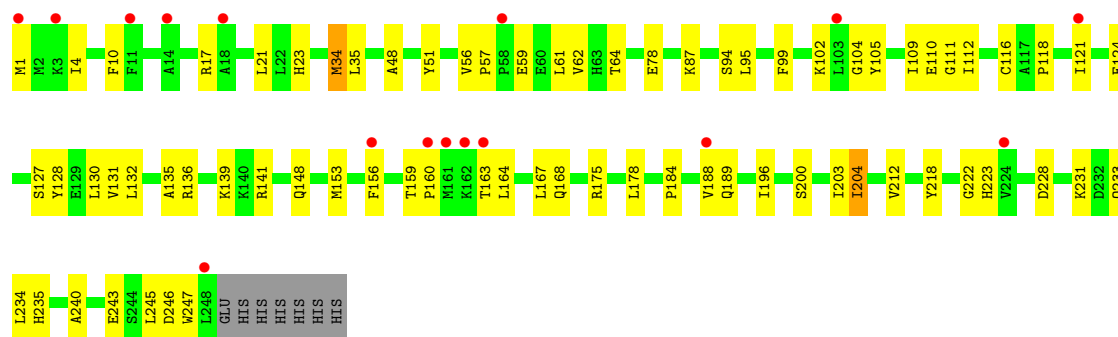


- Molecule 1: Carboxylesterase



- Molecule 1: Carboxylesterase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.96Å 59.99Å 166.04Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	49.54 – 2.42 49.54 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.54-2.42) 99.9 (49.54-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, $R_{free}$	0.214 , 0.273 0.225 , 0.277	Depositor DCC
$R_{free}$ test set	5612 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtrriage
Anisotropy	0.741	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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](#)

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	0.57	0/2100	1.05	0/2839
1	B	0.58	0/2104	0.98	0/2844
1	C	0.59	0/2113	1.03	4/2857 (0.1%)
1	D	0.53	0/2060	1.04	2/2785 (0.1%)
1	E	0.54	0/2140	1.04	1/2894 (0.0%)
1	F	0.55	0/2060	0.99	1/2785 (0.0%)
1	G	0.57	0/2059	1.03	1/2784 (0.0%)
1	H	0.53	0/2060	1.02	1/2785 (0.0%)
1	I	0.53	0/2060	0.98	0/2785
All	All	0.55	0/18756	1.02	10/25358 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63	HIS	N-CA-C	-7.14	102.87	112.94
1	E	31	ASP	CA-CB-CG	6.40	119.00	112.60
1	C	218	TYR	CB-CA-C	5.95	119.82	110.19
1	C	179	ASP	CA-CB-CG	5.94	118.54	112.60
1	D	10	PHE	CA-CB-CG	5.89	119.69	113.80

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	2043	0	1998	15	0
1	B	2040	0	1999	27	0
1	C	2058	0	2010	22	0
1	D	2009	0	1976	26	0
1	E	2076	0	2022	26	0
1	F	2009	0	1976	27	0
1	G	2004	0	1968	42	0
1	H	2009	0	1976	29	0
1	I	2009	0	1976	53	0
2	A	75	0	0	1	0
2	B	61	0	0	1	0
2	C	73	0	0	4	0
2	D	55	0	0	0	0
2	E	50	0	0	1	0
2	F	34	0	0	2	0
2	G	23	0	0	0	0
2	H	30	0	0	4	0
2	I	14	0	0	1	0
All	All	18672	0	17901	262	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 7.

The worst 5 of 262 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:64:THR:O	1:D:163:THR:HG22	1.48	1.11
1:I:188:VAL:HG13	1:I:218:TYR:HE1	1.12	1.10
1:F:64:THR:O	1:F:163:THR:CG2	2.01	1.09
1:F:64:THR:O	1:F:163:THR:HG22	1.56	1.05
1:D:64:THR:O	1:D:163:THR:CG2	2.04	1.05

There are no symmetry-related clashes.

## 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	250/255 (98%)	236 (94%)	14 (6%)	0	100	100
1	B	251/255 (98%)	242 (96%)	9 (4%)	0	100	100
1	C	251/255 (98%)	241 (96%)	10 (4%)	0	100	100
1	D	246/255 (96%)	238 (97%)	8 (3%)	0	100	100
1	E	254/255 (100%)	241 (95%)	13 (5%)	0	100	100
1	F	246/255 (96%)	232 (94%)	14 (6%)	0	100	100
1	G	246/255 (96%)	225 (92%)	21 (8%)	0	100	100
1	H	246/255 (96%)	224 (91%)	22 (9%)	0	100	100
1	I	246/255 (96%)	227 (92%)	19 (8%)	0	100	100
All	All	2236/2295 (97%)	2106 (94%)	130 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	221/224 (99%)	220 (100%)	1 (0%)	81	90
1	B	222/224 (99%)	220 (99%)	2 (1%)	70	84
1	C	222/224 (99%)	221 (100%)	1 (0%)	81	90
1	D	217/224 (97%)	214 (99%)	3 (1%)	59	77
1	E	225/224 (100%)	225 (100%)	0	100	100
1	F	217/224 (97%)	216 (100%)	1 (0%)	81	90
1	G	217/224 (97%)	209 (96%)	8 (4%)	30	49
1	H	217/224 (97%)	213 (98%)	4 (2%)	51	71
1	I	217/224 (97%)	210 (97%)	7 (3%)	34	54
All	All	1975/2016 (98%)	1948 (99%)	27 (1%)	59	77

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	167	LEU
1	H	132	LEU
1	I	167	LEU
1	H	35	LEU
1	H	137	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	158	GLN
1	H	63	HIS
1	G	229	GLN
1	H	75	ASN
1	C	252	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](#)

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

## 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

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	251/255 (98%)	-0.31	3 (1%) 76 74	21, 38, 59, 102	1 (0%)
1	B	250/255 (98%)	-0.20	1 (0%) 88 87	20, 41, 59, 98	3 (1%)
1	C	253/255 (99%)	-0.16	2 (0%) 82 80	27, 40, 67, 92	0
1	D	248/255 (97%)	-0.04	3 (1%) 76 74	30, 44, 69, 96	0
1	E	254/255 (99%)	0.07	6 (2%) 59 56	24, 45, 79, 98	2 (0%)
1	F	248/255 (97%)	0.14	4 (1%) 70 67	35, 50, 70, 104	0
1	G	247/255 (96%)	0.60	13 (5%) 32 28	38, 63, 94, 122	1 (0%)
1	H	248/255 (97%)	0.65	9 (3%) 46 42	41, 65, 97, 113	0
1	I	248/255 (97%)	0.96	16 (6%) 25 21	53, 73, 102, 114	0
All	All	2247/2295 (97%)	0.19	57 (2%) 58 55	20, 50, 88, 122	7 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	248	LEU	5.0
1	F	248	LEU	4.7
1	E	1	MET	4.4
1	H	248	LEU	4.4
1	D	248	LEU	4.2

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.