wwPDB X-ray Structure Validation Summary Report (i)

Feb 26, 2024 – 06:10 PM JST

PDB ID	:	8ILT
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

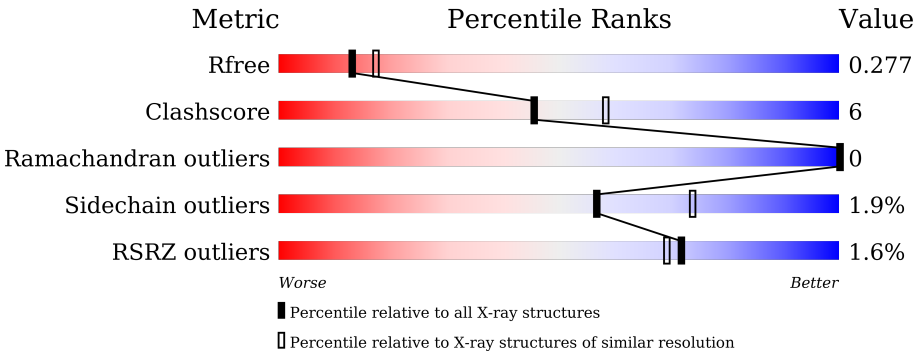
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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 >=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 <=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	91% 7% .
1	B	255	85% 12% .
1	C	255	87% 12% .
1	D	255	% 85% 12% .
1	E	255	87% 12%
1	F	255	% 84% 14% .

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

2 Entry composition (i)

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

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.

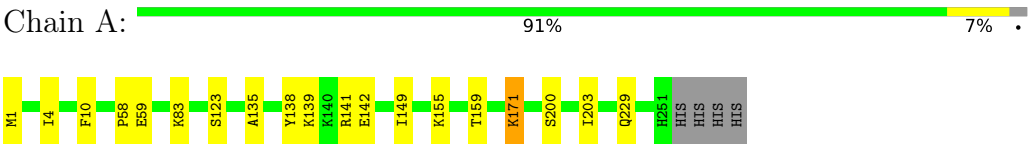
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	75	Total O 75 75	0	0
2	B	61	Total O 61 61	0	0
2	C	73	Total O 73 73	0	0
2	D	55	Total O 55 55	0	0
2	E	50	Total O 50 50	0	0
2	F	34	Total O 34 34	0	0
2	G	23	Total O 23 23	0	0
2	H	30	Total O 30 30	0	0
2	I	14	Total O 14 14	0	0

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.

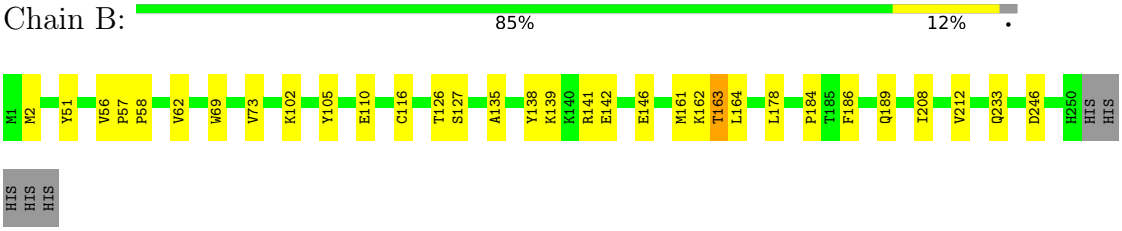
• Molecule 1: Carboxylesterase

Chain A:



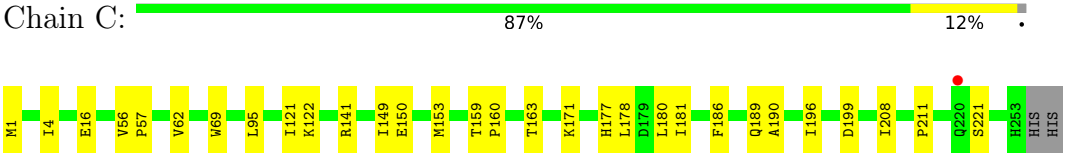
• Molecule 1: Carboxylesterase

Chain B:



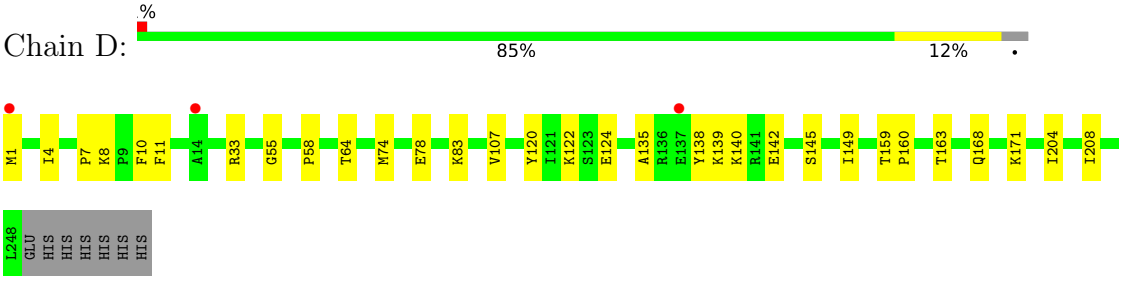
• Molecule 1: Carboxylesterase

Chain C:



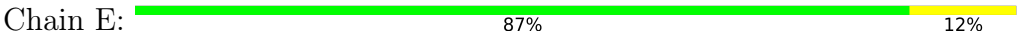
• Molecule 1: Carboxylesterase

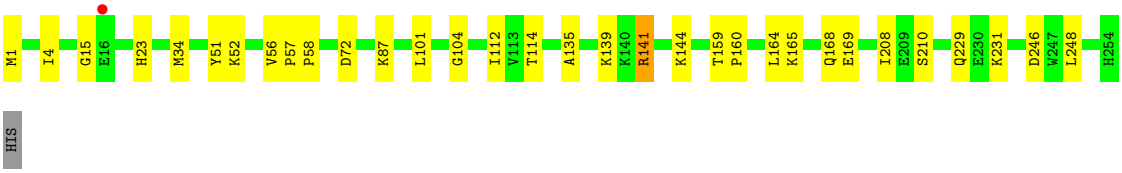
Chain D:



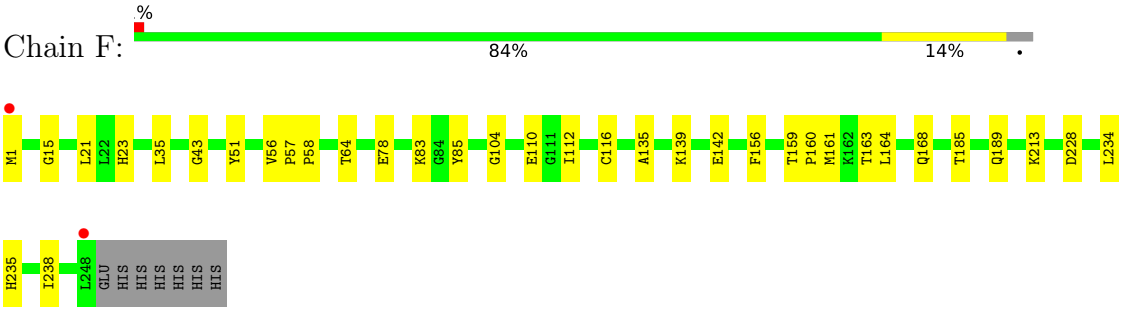
• Molecule 1: Carboxylesterase

Chain E:

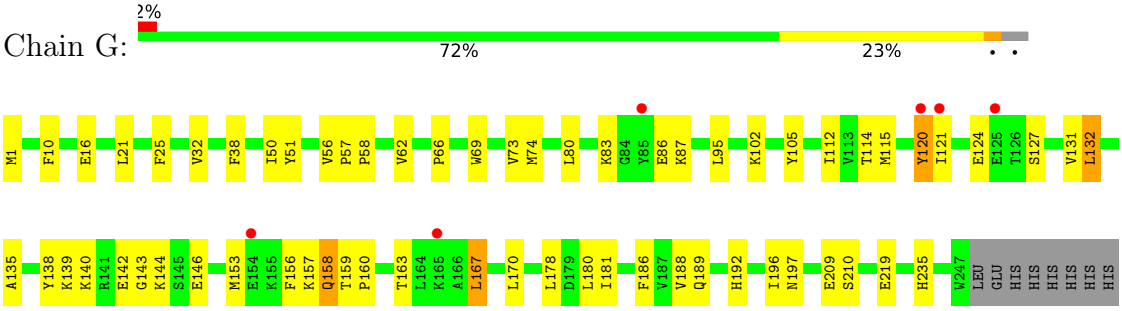




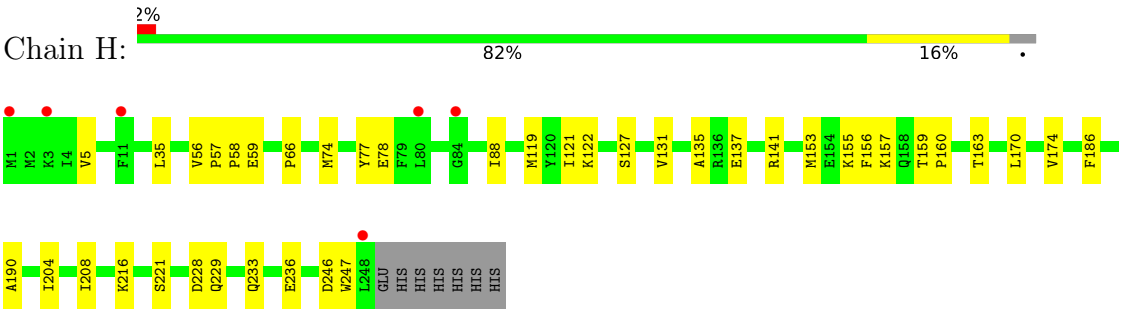
• Molecule 1: Carboxylesterase



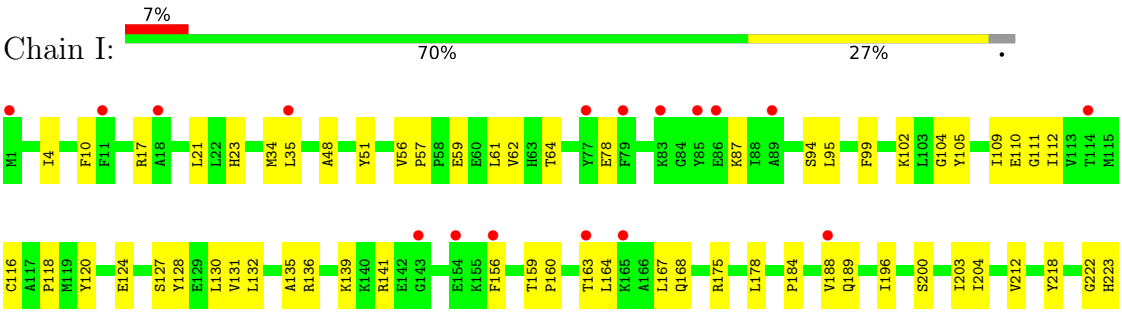
• Molecule 1: Carboxylesterase



• Molecule 1: Carboxylesterase



• Molecule 1: Carboxylesterase



D228
K231
L234
H235
A240
E243
S244
L245
D246
W247
L248
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	149.96Å 59.99Å 166.04Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	49.54 – 2.42 49.49 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.54-2.42) 99.9 (49.49-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.214 , 0.273 0.224 , 0.277	Depositor DCC
R_{free} test set	5611 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18672	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.38	0/2100	0.71	0/2839
1	B	0.38	0/2104	0.65	0/2844
1	C	0.39	0/2113	0.69	0/2857
1	D	0.35	0/2060	0.70	0/2785
1	E	0.35	0/2140	0.70	0/2894
1	F	0.35	0/2060	0.67	0/2785
1	G	0.36	0/2059	0.64	0/2784
1	H	0.35	0/2060	0.66	0/2785
1	I	0.32	0/2060	0.61	0/2785
All	All	0.36	0/18756	0.67	0/25358

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2043	0	1998	12	0
1	B	2040	0	1999	20	0
1	C	2058	0	2010	21	0
1	D	2009	0	1976	22	0
1	E	2076	0	2022	25	0
1	F	2009	0	1976	27	0
1	G	2004	0	1968	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2009	0	1976	24	0
1	I	2009	0	1976	47	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	3	0
2	I	14	0	0	1	0
All	All	18672	0	17901	232	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 6.

The worst 5 of 232 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	218 (99%)	3 (1%)	67	81
1	B	222/224 (99%)	218 (98%)	4 (2%)	59	75
1	C	222/224 (99%)	220 (99%)	2 (1%)	78	89
1	D	217/224 (97%)	213 (98%)	4 (2%)	59	75
1	E	225/224 (100%)	223 (99%)	2 (1%)	78	89
1	F	217/224 (97%)	215 (99%)	2 (1%)	78	89
1	G	217/224 (97%)	207 (95%)	10 (5%)	27	42
1	H	217/224 (97%)	213 (98%)	4 (2%)	59	75
1	I	217/224 (97%)	211 (97%)	6 (3%)	43	62
All	All	1975/2016 (98%)	1938 (98%)	37 (2%)	57	74

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	137	GLU
1	I	167	LEU
1	H	186	PHE
1	I	78	GLU
1	D	140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	63	HIS
1	H	75	ASN
1	I	47	HIS
1	F	235	HIS
1	G	82	ASN

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 monosaccharides 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

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^{th} 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	251/255 (98%)	-0.06	0	100	100	26, 38, 59, 102	0
1	B	250/255 (98%)	-0.10	0	100	100	28, 41, 59, 98	0
1	C	253/255 (99%)	-0.01	1 (0%)	92	91	27, 40, 67, 92	0
1	D	248/255 (97%)	-0.04	3 (1%)	79	76	30, 44, 69, 96	0
1	E	254/255 (99%)	0.02	1 (0%)	92	91	31, 45, 79, 98	0
1	F	248/255 (97%)	0.01	2 (0%)	86	84	35, 50, 70, 104	0
1	G	247/255 (96%)	0.31	6 (2%)	59	56	38, 63, 94, 122	0
1	H	248/255 (97%)	0.27	6 (2%)	59	56	41, 65, 97, 113	0
1	I	248/255 (97%)	0.54	18 (7%)	15	13	53, 73, 102, 114	0
All	All	2247/2295 (97%)	0.10	37 (1%)	72	69	26, 50, 88, 122	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	120	TYR	4.3
1	F	1	MET	4.0
1	I	248	LEU	3.7
1	I	163	THR	3.5
1	I	1	MET	3.4

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 monosaccharides 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.