



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:24 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 Full wwPDB X-ray Structure Validation 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

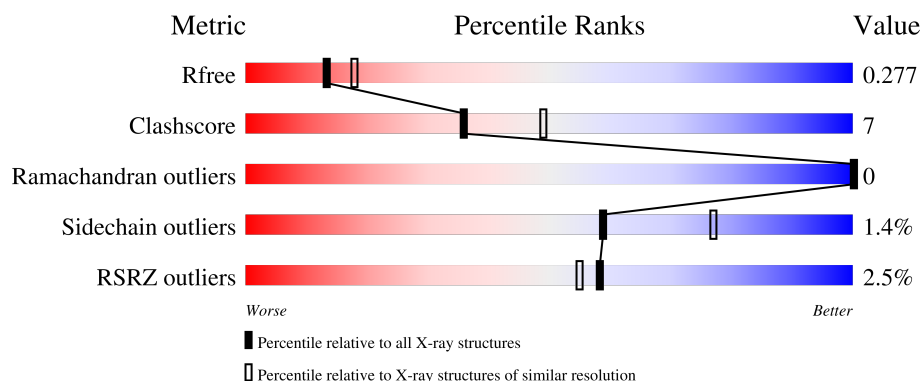
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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 ≥ 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	2% 90% 8% .
1	B	255	84% 14% .
1	C	255	2% 86% 13% .
1	D	255	2% 84% 13% .
1	E	255	2% 86% 13% .

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Mol	Chain	Length	Quality of chain
1	F	255	2% 84% 13%
1	G	255	5% 71% 25%
1	H	255	4% 79% 18%
1	I	255	6% 69% 28%

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
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

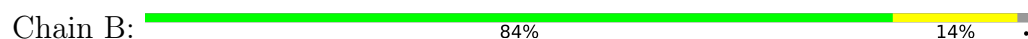
3 Residue-property plots [i](#)

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.

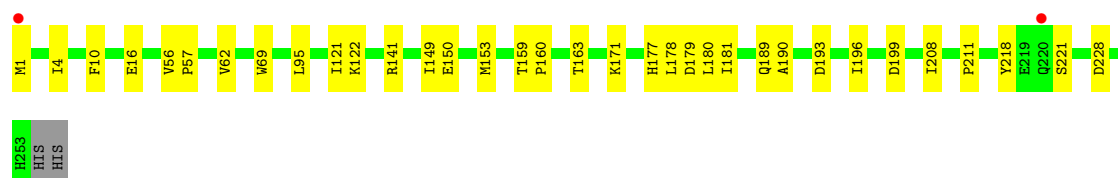
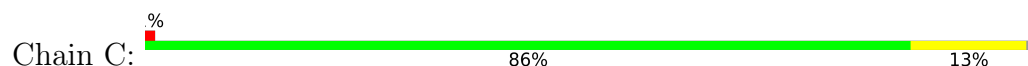
- Molecule 1: Carboxylesterase



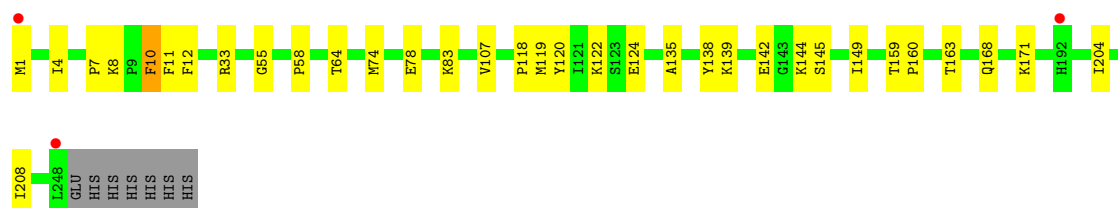
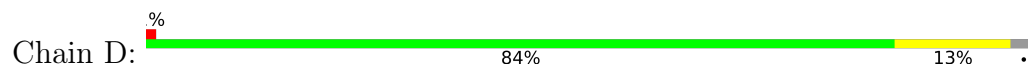
- Molecule 1: Carboxylesterase



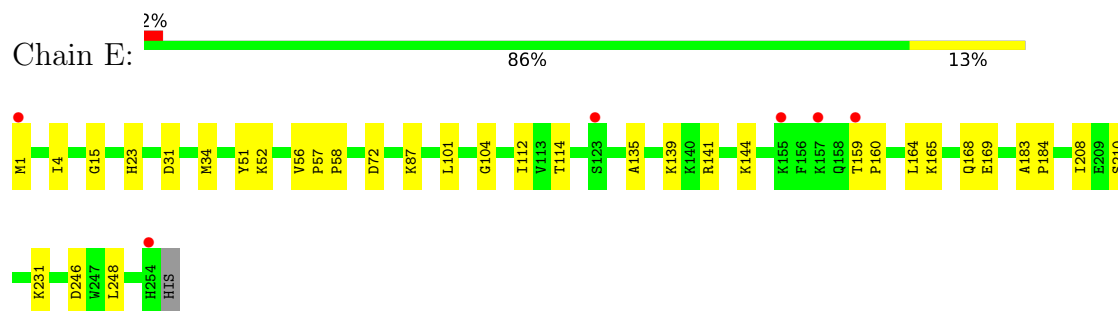
- Molecule 1: Carboxylesterase



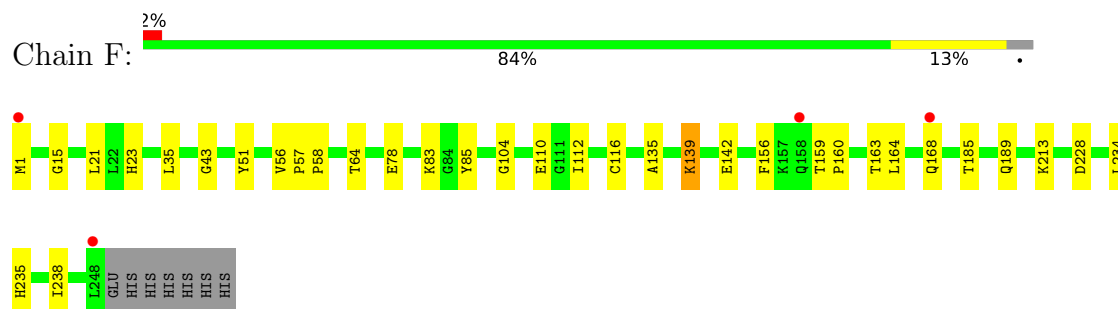
- Molecule 1: Carboxylesterase



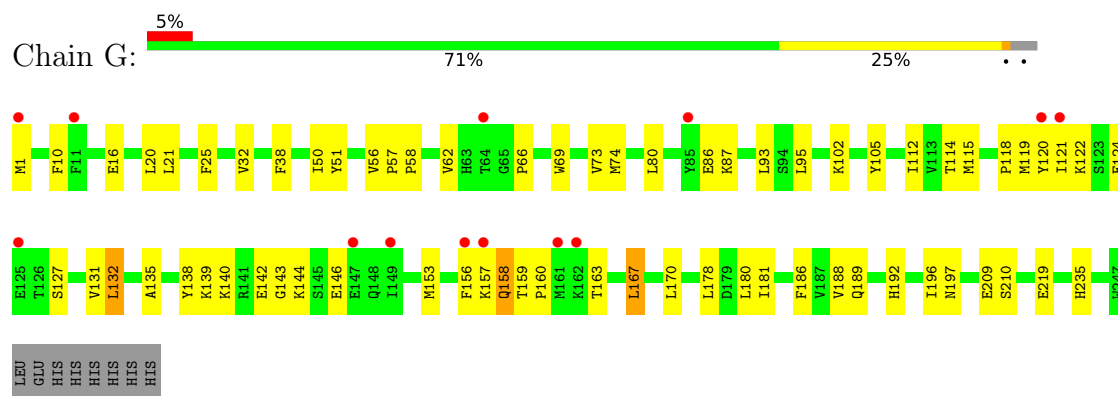
- Molecule 1: Carboxylesterase



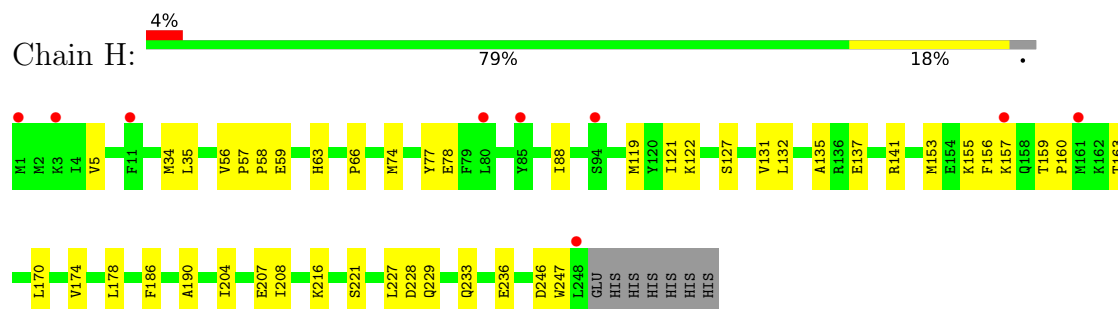
- Molecule 1: Carboxylesterase



- Molecule 1: Carboxylesterase

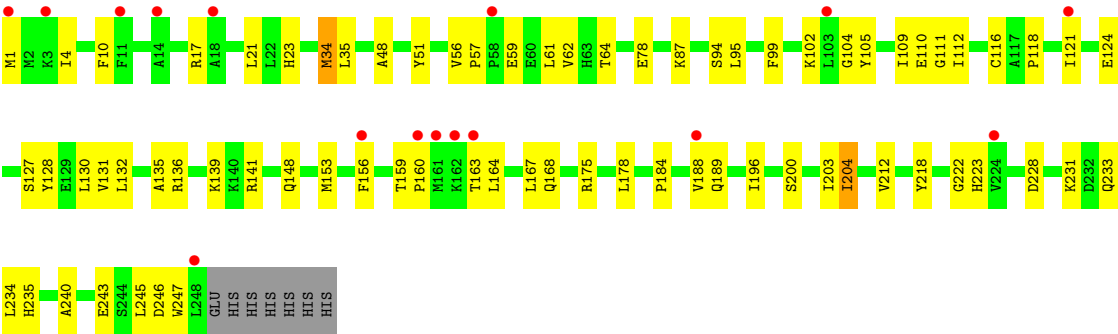


- Molecule 1: Carboxylesterase



- Molecule 1: Carboxylesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.42Å)	Xtriage
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 ²)	41.1	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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.

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	0.57	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.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
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
1	C	228	ASP	CA-CB-CG	5.85	118.45	112.60
1	G	10	PHE	CA-CB-CG	5.23	119.03	113.80
1	F	139	LYS	CB-CA-C	-5.22	101.81	110.68
1	D	12	PHE	CA-CB-CG	5.21	119.01	113.80
1	C	10	PHE	CA-CB-CG	5.15	118.95	113.80

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	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.

All (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
1:I:188:VAL:HG13	1:I:218:TYR:CE1	1.92	1.04
1:E:15:GLY:N	2:E:301:HOH:O	2.01	0.93
1:I:175:ARG:HA	1:I:178:LEU:HD13	1.51	0.92
1:G:115:MET:HG2	1:G:188:VAL:CG2	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:MET:HG2	1:G:188:VAL:HG21	1.56	0.87
1:I:62:VAL:HA	1:I:163:THR:HG21	1.55	0.87
1:F:64:THR:O	1:F:163:THR:HG21	1.74	0.86
1:E:1:MET:SD	1:E:144:LYS:HG2	2.17	0.85
1:H:163:THR:HG22	2:H:317:HOH:O	1.77	0.84
1:F:135:ALA:O	1:F:139:LYS:HG2	1.80	0.81
1:E:101:LEU:HG	1:E:114[A]:THR:HG21	1.61	0.81
1:B:62:VAL:HA	1:B:163:THR:HG21	1.61	0.80
1:E:4:ILE:HG23	1:E:141:ARG:HH11	1.47	0.79
1:F:58:PRO:HG3	1:F:135:ALA:HA	1.67	0.77
1:I:61:LEU:O	1:I:64:THR:HG22	1.85	0.77
1:A:155:LYS:O	1:A:159:THR:HG23	1.85	0.77
1:I:135:ALA:O	1:I:139:LYS:HG2	1.87	0.74
1:D:64:THR:O	1:D:163:THR:HG21	1.89	0.73
1:C:62:VAL:HA	1:C:163:THR:HG21	1.70	0.72
1:D:4:ILE:HD12	1:D:138:TYR:CE1	2.24	0.72
1:I:240:ALA:O	2:I:301:HOH:O	2.07	0.72
1:G:121:ILE:HG13	1:G:124:GLU:CD	2.15	0.70
1:H:127:SER:O	1:H:131:VAL:HG23	1.91	0.70
1:H:156:PHE:O	1:H:160:PRO:HD3	1.92	0.69
1:A:123:SER:OG	1:A:171:LYS:HE3	1.91	0.69
1:E:4:ILE:HD12	1:E:141:ARG:HD3	1.76	0.68
1:I:188:VAL:CG1	1:I:218:TYR:HE1	2.01	0.67
1:D:58:PRO:HG3	1:D:135:ALA:HA	1.77	0.67
1:G:1:MET:SD	1:G:144:LYS:HG3	2.35	0.67
1:E:4:ILE:HG23	1:E:141:ARG:NH1	2.10	0.67
1:D:1:MET:HE3	1:D:144:LYS:HE2	1.78	0.66
1:F:234:LEU:O	1:F:238:ILE:HD12	1.96	0.66
1:E:1:MET:SD	1:E:144:LYS:CG	2.84	0.66
1:C:199:ASP:OD2	1:E:141:ARG:NH1	2.30	0.65
1:H:163:THR:CG2	2:H:317:HOH:O	2.42	0.65
1:I:188:VAL:CG1	1:I:218:TYR:CE1	2.76	0.64
1:B:162:LYS:HE3	1:E:246:ASP:OD2	1.97	0.64
1:G:153:MET:HE2	1:G:153:MET:HA	1.79	0.64
1:H:163:THR:HB	2:H:301:HOH:O	1.97	0.64
1:C:163:THR:HG23	2:C:348:HOH:O	1.98	0.64
1:I:56:VAL:HB	1:I:57:PRO:CD	2.28	0.64
1:B:128:TYR:CE1	1:B:161:MET:HE1	2.32	0.64
1:I:118:PRO:HA	1:I:196:ILE:HG12	1.79	0.63
1:G:135:ALA:HB1	1:G:153:MET:HE1	1.81	0.63
1:G:62:VAL:HA	1:G:163:THR:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:O	1:C:1:MET:HG2	1.99	0.62
1:I:64:THR:O	1:I:163:THR:HG22	1.99	0.62
1:A:4:ILE:HD12	1:A:141:ARG:HG2	1.82	0.62
1:B:138:TYR:O	1:B:142:GLU:HG2	2.00	0.62
1:F:234:LEU:O	1:F:238:ILE:CD1	2.48	0.61
1:D:204:ILE:O	1:D:208:ILE:HG23	2.01	0.61
1:C:4:ILE:CD1	1:C:141:ARG:HG2	2.31	0.60
1:H:119:MET:HE2	1:H:204:ILE:CD1	2.31	0.60
1:B:146:GLU:N	1:B:146:GLU:OE1	2.34	0.60
1:I:56:VAL:HB	1:I:57:PRO:HD2	1.84	0.60
1:I:200:SER:O	1:I:204:ILE:HG13	2.02	0.60
1:E:58:PRO:HG3	1:E:135:ALA:HA	1.84	0.59
1:E:1:MET:SD	1:E:144:LYS:HE3	2.42	0.58
1:B:135:ALA:HB3	1:B:153:MET:HE1	1.85	0.58
1:B:56:VAL:HB	1:B:57:PRO:CD	2.34	0.58
1:G:159:THR:N	1:G:160:PRO:CD	2.66	0.58
1:D:159:THR:N	1:D:160:PRO:CD	2.67	0.58
1:G:1:MET:SD	1:G:144:LYS:CG	2.92	0.57
1:D:124:GLU:HG2	1:D:168:GLN:OE1	2.02	0.57
1:A:138:TYR:O	1:A:142:GLU:HG2	2.04	0.57
1:I:104:GLY:HA3	1:I:112:ILE:HD11	1.86	0.57
1:H:77:TYR:CE1	1:H:88:ILE:HD12	2.40	0.56
1:D:4:ILE:HD12	1:D:138:TYR:CZ	2.40	0.56
1:I:127:SER:O	1:I:131:VAL:HG23	2.05	0.56
1:B:135:ALA:O	1:B:139:LYS:HG2	2.06	0.56
1:F:1:MET:CG	1:F:1:MET:O	2.53	0.56
1:B:136:ARG:HG3	1:B:153:MET:HE2	1.88	0.56
1:B:128:TYR:CD1	1:B:161:MET:HE1	2.40	0.55
1:I:231:LYS:O	1:I:235:HIS:ND1	2.39	0.55
1:C:171:LYS:NZ	2:C:303:HOH:O	2.39	0.55
1:I:124:GLU:HG2	1:I:168:GLN:HE22	1.71	0.55
1:C:4:ILE:HD12	1:C:141:ARG:HG2	1.88	0.55
1:F:15:GLY:HA3	1:F:43:GLY:O	2.07	0.55
1:A:58:PRO:HG3	1:A:135:ALA:HA	1.90	0.54
1:H:153:MET:O	1:H:157:LYS:HG3	2.08	0.54
1:I:95:LEU:HD11	1:I:99:PHE:CE2	2.43	0.54
1:E:208:ILE:HD12	1:E:210:SER:HB2	1.89	0.54
1:F:164:LEU:O	1:F:168:GLN:HG3	2.07	0.54
1:I:102:LYS:HA	1:I:105:TYR:CE2	2.43	0.54
1:D:4:ILE:HD12	1:D:138:TYR:CD1	2.43	0.54
1:D:135:ALA:O	1:D:139:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:THR:N	1:I:160:PRO:CD	2.71	0.53
1:I:23:HIS:CE1	1:I:51:TYR:CD2	2.96	0.53
1:B:233:GLN:NE2	2:B:301:HOH:O	2.32	0.52
1:I:128:TYR:CZ	1:I:132:LEU:HD11	2.44	0.52
1:D:139:LYS:CB	1:D:149:ILE:HD12	2.39	0.52
1:G:192:HIS:CD2	1:G:219:GLU:O	2.63	0.52
1:H:159:THR:N	1:H:160:PRO:CD	2.72	0.52
1:F:21:LEU:HD22	1:F:35:LEU:HD23	1.91	0.52
1:E:159:THR:N	1:E:160:PRO:CD	2.73	0.52
1:E:135:ALA:O	1:E:139:LYS:HG2	2.10	0.52
1:G:192:HIS:NE2	1:G:219:GLU:O	2.43	0.51
1:D:139:LYS:HB2	1:D:149:ILE:HD12	1.91	0.51
1:F:228:ASP:HB3	2:F:315:HOH:O	2.10	0.51
1:D:74:MET:HE1	1:D:107:VAL:HG11	1.92	0.51
1:E:1:MET:SD	1:E:144:LYS:CE	2.98	0.51
1:E:4:ILE:HD12	1:E:141:ARG:CD	2.39	0.51
1:E:101:LEU:CG	1:E:114[A]:THR:HG21	2.38	0.51
1:I:10:PHE:CE2	1:I:48:ALA:HB3	2.46	0.51
1:A:4:ILE:CD1	1:A:141:ARG:HG2	2.41	0.50
1:C:211:PRO:HD2	2:C:331:HOH:O	2.11	0.50
1:E:56:VAL:HB	1:E:57:PRO:CD	2.42	0.50
1:H:121:ILE:HD12	1:H:122:LYS:N	2.27	0.50
1:D:145:SER:O	1:D:149:ILE:HG12	2.12	0.50
1:G:156:PHE:O	1:G:160:PRO:HD3	2.12	0.50
1:A:1:MET:HA	1:A:142:GLU:O	2.12	0.49
1:I:135:ALA:HB1	1:I:153:MET:HE1	1.94	0.49
1:H:56:VAL:HB	1:H:57:PRO:CD	2.42	0.49
1:I:17:ARG:NH1	1:I:243:GLU:OE2	2.45	0.49
1:G:69:TRP:O	1:G:73:VAL:HG23	2.12	0.49
1:C:69:TRP:CE3	1:C:95:LEU:HD21	2.48	0.49
1:H:141:ARG:HH22	1:I:203:ILE:HD13	1.78	0.49
1:I:159:THR:N	1:I:160:PRO:HD3	2.27	0.49
1:G:146:GLU:H	1:G:146:GLU:CD	2.21	0.49
1:B:102:LYS:HA	1:B:105:TYR:CE2	2.48	0.48
1:D:11:PHE:CZ	1:D:83:LYS:HD2	2.47	0.48
1:I:110:GLU:HG3	1:I:245:LEU:HD23	1.94	0.48
1:B:69:TRP:O	1:B:73:VAL:HG23	2.14	0.48
1:G:115:MET:HA	1:G:188:VAL:HG23	1.96	0.48
1:I:34:MET:HE2	1:I:231:LYS:HD2	1.95	0.48
1:F:1:MET:O	1:F:1:MET:HG3	2.14	0.48
1:G:21:LEU:HD23	1:G:32:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:HIS:CE1	1:F:51:TYR:CD2	3.01	0.48
1:F:56:VAL:HB	1:F:57:PRO:HD2	1.94	0.48
1:B:128:TYR:HE1	1:B:161:MET:HE1	1.79	0.47
1:I:87:LYS:HB3	1:I:247:TRP:CZ3	2.49	0.47
1:F:56:VAL:HB	1:F:57:PRO:CD	2.44	0.47
1:G:209:GLU:O	1:G:210:SER:C	2.58	0.47
1:I:116:CYS:HA	1:I:189:GLN:OE1	2.14	0.47
1:B:110:GLU:OE2	1:B:246:ASP:O	2.33	0.47
1:B:161:MET:HE3	1:B:164:LEU:HD12	1.96	0.47
1:D:120:TYR:O	1:D:171:LYS:HE3	2.15	0.47
1:G:25:PHE:HB2	1:G:95:LEU:HD22	1.97	0.47
1:B:58:PRO:CG	1:B:135:ALA:HA	2.45	0.47
1:C:189:GLN:HE22	1:C:196:ILE:HD11	1.79	0.47
1:C:56:VAL:HB	1:C:57:PRO:HD2	1.97	0.47
1:F:83:LYS:HB3	1:F:85:TYR:CE1	2.50	0.47
1:H:155:LYS:O	1:H:159:THR:HG23	2.15	0.47
1:H:170:LEU:O	1:H:174:VAL:HG23	2.15	0.47
1:C:121:ILE:HD12	1:C:122:LYS:N	2.30	0.46
1:G:189:GLN:HE22	1:G:196:ILE:HD11	1.79	0.46
1:H:5:VAL:HB	1:I:203:ILE:HD11	1.97	0.46
1:H:228:ASP:OD1	1:H:229:GLN:N	2.47	0.46
1:E:87:LYS:HE3	1:E:248:LEU:O	2.16	0.46
1:I:109:ILE:HG23	1:I:111:GLY:O	2.15	0.46
1:I:246:ASP:O	1:I:247:TRP:HB2	2.15	0.46
1:G:56:VAL:HB	1:G:57:PRO:CD	2.46	0.46
1:G:120:TYR:HB3	1:G:197:ASN:OD1	2.15	0.46
1:C:189:GLN:NE2	1:C:196:ILE:HD11	2.31	0.45
1:I:34:MET:CE	1:I:231:LYS:HD2	2.47	0.45
1:I:35:LEU:HA	1:I:235:HIS:CD2	2.51	0.45
1:I:222:GLY:O	1:I:223:HIS:C	2.59	0.45
1:A:135:ALA:O	1:A:139:LYS:HG2	2.16	0.45
1:F:159:THR:N	1:F:160:PRO:CD	2.80	0.45
1:C:16:GLU:HG2	2:C:327:HOH:O	2.16	0.45
1:G:139:LYS:HE3	1:G:153:MET:HE3	1.99	0.45
1:G:50:ILE:HG22	1:G:51:TYR:O	2.17	0.45
1:G:127:SER:O	1:G:131:VAL:HG23	2.17	0.45
1:B:127:SER:HB3	1:B:164:LEU:HD22	1.99	0.45
1:C:149:ILE:O	1:C:153:MET:HG2	2.17	0.45
1:I:188:VAL:HG11	1:I:234:LEU:CD1	2.47	0.45
1:A:118:PRO:O	1:A:119:MET:HE2	2.18	0.44
1:G:20:LEU:C	1:G:21:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:HIS:HD2	1:C:180:LEU:HD12	1.81	0.44
1:H:190:ALA:HB1	1:H:221:SER:O	2.17	0.44
1:I:4:ILE:HD11	1:I:141:ARG:HB3	2.00	0.44
1:D:10:PHE:CE2	1:D:33:ARG:HA	2.53	0.44
1:G:21:LEU:HB3	1:G:32:VAL:HG21	1.98	0.44
1:G:178:LEU:HA	1:G:181:ILE:HD12	1.99	0.44
1:I:121:ILE:C	1:I:121:ILE:HD12	2.43	0.44
1:B:184:PRO:HA	1:B:212:VAL:O	2.17	0.44
1:H:66:PRO:HB3	1:H:170:LEU:HD22	2.00	0.44
1:D:118:PRO:O	1:D:119:MET:HE2	2.18	0.44
1:G:118:PRO:O	1:G:119:MET:HE2	2.18	0.44
1:H:204:ILE:O	1:H:208:ILE:HG23	2.18	0.44
1:B:118:PRO:O	1:B:119:MET:HE2	2.17	0.44
1:G:135:ALA:O	1:G:139:LYS:HG2	2.18	0.43
1:I:21:LEU:O	1:I:48:ALA:HA	2.18	0.43
1:A:200:SER:O	1:A:203:ILE:HB	2.18	0.43
1:B:58:PRO:HG3	1:B:135:ALA:HA	2.00	0.43
1:E:104:GLY:HA3	1:E:112:ILE:HD11	2.00	0.43
1:G:102:LYS:HA	1:G:105:TYR:CE2	2.53	0.43
1:A:2:MET:HE1	1:B:191:ARG:HH11	1.84	0.43
1:G:158:GLN:HE21	1:G:158:GLN:HB3	1.59	0.43
1:I:87:LYS:O	1:I:247:TRP:HZ3	1.99	0.43
1:G:122:LYS:HD3	1:G:196:ILE:C	2.43	0.43
1:C:193:ASP:CG	1:C:196:ILE:HG12	2.44	0.43
1:A:59:GLU:OE2	1:A:139:LYS:NZ	2.50	0.43
1:D:1:MET:HA	1:D:142:GLU:O	2.19	0.43
1:A:139:LYS:HB3	1:A:149:ILE:HG12	2.01	0.43
1:F:139:LYS:HA	1:F:142:GLU:OE1	2.19	0.43
1:D:120:TYR:O	1:D:171:LYS:CE	2.67	0.42
1:B:51:TYR:HB3	1:B:69:TRP:CD1	2.55	0.42
1:I:1:MET:HE1	1:I:148:GLN:HE22	1.85	0.42
1:C:177:HIS:CD2	1:C:180:LEU:HD12	2.54	0.42
1:C:159:THR:N	1:C:160:PRO:CD	2.82	0.42
1:D:4:ILE:HD11	1:D:138:TYR:O	2.19	0.42
1:G:66:PRO:HB3	1:G:170:LEU:HD22	2.01	0.42
1:A:74:MET:HE1	1:A:107:VAL:HG11	2.02	0.42
1:B:56:VAL:HB	1:B:57:PRO:HD2	2.02	0.42
1:F:58:PRO:HG3	1:F:135:ALA:CA	2.44	0.42
1:I:156:PHE:O	1:I:160:PRO:HD3	2.20	0.42
1:G:58:PRO:HG3	1:G:135:ALA:HA	2.01	0.42
1:G:140:LYS:O	1:G:143:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:GLN:O	1:H:236:GLU:N	2.53	0.42
1:I:233:GLN:O	1:I:234:LEU:C	2.63	0.42
1:B:178:LEU:O	1:B:208:ILE:HA	2.20	0.42
1:G:112:ILE:HG22	1:G:114[A]:THR:HG23	2.01	0.42
1:C:178:LEU:HA	1:C:181:ILE:HD12	2.01	0.42
1:D:74:MET:HE1	1:D:107:VAL:CG1	2.49	0.42
1:E:23:HIS:CE1	1:E:51:TYR:CD2	3.08	0.42
1:E:165:LYS:O	1:E:169:GLU:HG3	2.20	0.42
1:F:156:PHE:O	1:F:159:THR:OG1	2.36	0.42
1:H:58:PRO:HG3	1:H:135:ALA:HA	2.02	0.42
1:I:128:TYR:HA	1:I:164:LEU:HD11	2.01	0.42
1:C:190:ALA:HB1	1:C:221:SER:O	2.20	0.41
1:F:35:LEU:HA	1:F:235:HIS:CE1	2.54	0.41
1:C:178:LEU:O	1:C:208:ILE:HA	2.20	0.41
1:F:104:GLY:HA3	1:F:112:ILE:HD11	2.01	0.41
1:B:116:CYS:HA	1:B:189:GLN:OE1	2.21	0.41
1:E:183:ALA:O	1:E:184:PRO:C	2.62	0.41
1:H:207:GLU:CD	2:H:303:HOH:O	2.63	0.41
1:H:246:ASP:O	1:H:247:TRP:HB2	2.21	0.41
1:A:83:LYS:NZ	2:A:311:HOH:O	2.53	0.41
1:H:119:MET:HE2	1:H:204:ILE:HD11	2.02	0.41
1:H:119:MET:HE3	1:H:178:LEU:HD11	2.03	0.41
1:I:109:ILE:CG2	1:I:111:GLY:O	2.68	0.41
1:E:34:MET:CE	1:E:231:LYS:HE2	2.51	0.41
1:F:116:CYS:HA	1:F:189:GLN:OE1	2.21	0.41
1:H:58:PRO:HD2	1:H:59:GLU:OE1	2.20	0.41
1:F:110:GLU:OE1	2:F:301:HOH:O	2.21	0.41
1:E:52:LYS:N	1:E:72:ASP:OD2	2.51	0.41
1:E:164:LEU:O	1:E:168:GLN:HG3	2.21	0.41
1:F:15:GLY:N	1:F:43:GLY:O	2.54	0.41
1:G:38:PHE:CE2	1:G:235:HIS:HB3	2.56	0.41
1:I:136:ARG:CG	1:I:136:ARG:HH21	2.34	0.41
1:G:69:TRP:HZ3	1:G:167:LEU:HD12	1.85	0.41
1:H:186:PHE:CD2	1:H:186:PHE:C	2.98	0.41
1:I:184:PRO:HA	1:I:212:VAL:O	2.21	0.41
1:D:7:PRO:CD	1:D:55:GLY:HA3	2.51	0.40
1:D:74:MET:CE	1:D:107:VAL:HG11	2.51	0.40
1:G:138:TYR:O	1:G:142:GLU:HG2	2.21	0.40
1:I:87:LYS:HB3	1:I:247:TRP:CE3	2.56	0.40
1:H:34:MET:HE3	1:H:227:LEU:HD22	2.03	0.40
1:F:185:THR:O	1:F:213:LYS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:GLU:HG3	1:G:87:LYS:HG3	2.03	0.40
1:G:132:LEU:HD11	1:G:157:LYS:HD3	2.02	0.40
1:G:186:PHE:CZ	1:G:188:VAL:CG1	3.04	0.40
1:H:74:MET:O	1:H:78:GLU:HG2	2.21	0.40
1:I:94:SER:HB2	1:I:223:HIS:CE1	2.57	0.40
1:I:34:MET:HE3	1:I:34:MET:HB3	1.86	0.40

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 ⓘ

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

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	B	141	ARG
1	B	163	THR
1	C	150	GLU
1	D	8	LYS
1	D	78	GLU
1	D	122	LYS
1	F	78	GLU
1	G	16	GLU
1	G	74	MET
1	G	80	LEU
1	G	93	LEU
1	G	132	LEU
1	G	158	GLN
1	G	167	LEU
1	G	180	LEU
1	H	35	LEU
1	H	132	LEU

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Mol	Chain	Res	Type
1	H	137	GLU
1	H	216	LYS
1	I	34	MET
1	I	59	GLU
1	I	78	GLU
1	I	130	LEU
1	I	167	LEU
1	I	204	ILE
1	I	228	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	233	GLN
1	B	214	GLN
1	B	250	HIS
1	C	28	ASN
1	C	250	HIS
1	C	252	HIS
1	D	233	GLN
1	E	75	ASN
1	F	158	GLN
1	F	214	GLN
1	F	233	GLN
1	F	235	HIS
1	G	82	ASN
1	G	158	GLN
1	G	168	GLN
1	G	229	GLN
1	H	63	HIS
1	H	75	ASN
1	H	214	GLN
1	I	82	ASN
1	I	148	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	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%)

All (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
1	E	123	SER	4.1
1	D	1	MET	3.9
1	E	254	HIS	3.4
1	B	1	MET	3.3
1	G	120	TYR	3.2
1	I	18	ALA	2.9
1	C	220	GLN	2.9
1	F	1	MET	2.9
1	I	161	MET	2.9
1	I	163	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	251	HIS	2.8
1	G	1	MET	2.7
1	D	192	HIS	2.7
1	G	85	TYR	2.7
1	C	1	MET	2.7
1	G	161	MET	2.7
1	H	1	MET	2.7
1	H	157	LYS	2.6
1	I	224	VAL	2.6
1	I	11	PHE	2.6
1	I	103	LEU	2.6
1	I	156	PHE	2.6
1	I	162	LYS	2.6
1	I	1	MET	2.5
1	H	11	PHE	2.5
1	I	160	PRO	2.5
1	G	156	PHE	2.5
1	H	161	MET	2.4
1	A	248	LEU	2.3
1	H	3	LYS	2.3
1	I	121	ILE	2.3
1	G	11	PHE	2.3
1	H	85	TYR	2.3
1	G	125	GLU	2.3
1	G	121	ILE	2.2
1	G	149	ILE	2.2
1	H	94	SER	2.2
1	I	3	LYS	2.2
1	I	58	PRO	2.2
1	F	168	GLN	2.2
1	E	155	LYS	2.2
1	F	158	GLN	2.2
1	H	80	LEU	2.2
1	G	162	LYS	2.2
1	I	14	ALA	2.2
1	G	157	LYS	2.2
1	A	1	MET	2.1
1	G	147	GLU	2.1
1	I	188	VAL	2.0
1	E	157	LYS	2.0
1	E	159	THR	2.0
1	G	64	THR	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.