



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:58 PM BST

PDB ID : 4A8A  
EMDB ID: : EMD-1981  
Title : Asymmetric cryo-EM reconstruction of E. coli DegQ 12-mer in complex with lysozyme  
Authors : Malet, H.; Canellas, F.; Sawa, J.; Yan, J.; Thalassinou, K.; Ehrmann, M.; Clausen, T.; Saibil, H.R.  
Deposited on : 2011-11-20  
Resolution : 14.20 Å (reported)  
Based on PDB ID : 3STJ

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

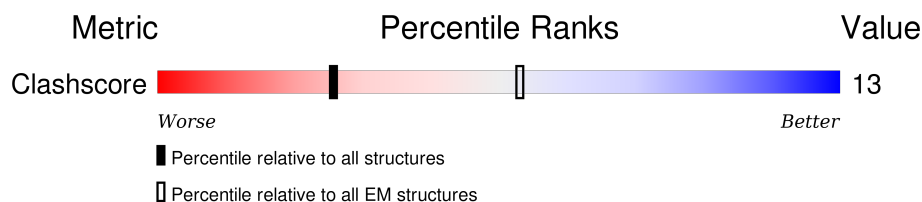
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 14.20 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)	EM structures (#Entries)
Clashscore	114402	924

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	436	 86% • 12%
1	B	436	 87% • 12%
1	C	436	 85% • 12%
1	D	436	 86% • 12%
1	E	436	 86% • 12%
1	F	436	 86% • 12%
1	G	436	 85% • 12%
1	H	436	 86% • 12%
1	I	436	 86% • 12%
1	J	436	 85% • 12%
1	K	436	 87% • 12%

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Mol	Chain	Length	Quality of chain
1	L	436	<div><div></div><div>86%</div><div></div><div>•</div><div>12%</div></div>
2	M	129	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4749 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEGQ.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	385	Total C 385 385	0	385
1	B	385	Total C 385 385	0	385
1	C	385	Total C 385 385	0	385
1	D	385	Total C 385 385	0	385
1	E	385	Total C 385 385	0	385
1	F	385	Total C 385 385	0	385
1	G	385	Total C 385 385	0	385
1	H	385	Total C 385 385	0	385
1	I	385	Total C 385 385	0	385
1	J	385	Total C 385 385	0	385
1	K	385	Total C 385 385	0	385
1	L	385	Total C 385 385	0	385

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
A	429	LEU	-	EXPRESSION TAG	UNP P39099
A	430	GLU	-	EXPRESSION TAG	UNP P39099
A	431	HIS	-	EXPRESSION TAG	UNP P39099
A	432	HIS	-	EXPRESSION TAG	UNP P39099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	433	HIS	-	EXPRESSION TAG	UNP P39099
A	434	HIS	-	EXPRESSION TAG	UNP P39099
A	435	HIS	-	EXPRESSION TAG	UNP P39099
A	436	HIS	-	EXPRESSION TAG	UNP P39099
B	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
B	429	LEU	-	EXPRESSION TAG	UNP P39099
B	430	GLU	-	EXPRESSION TAG	UNP P39099
B	431	HIS	-	EXPRESSION TAG	UNP P39099
B	432	HIS	-	EXPRESSION TAG	UNP P39099
B	433	HIS	-	EXPRESSION TAG	UNP P39099
B	434	HIS	-	EXPRESSION TAG	UNP P39099
B	435	HIS	-	EXPRESSION TAG	UNP P39099
B	436	HIS	-	EXPRESSION TAG	UNP P39099
C	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
C	429	LEU	-	EXPRESSION TAG	UNP P39099
C	430	GLU	-	EXPRESSION TAG	UNP P39099
C	431	HIS	-	EXPRESSION TAG	UNP P39099
C	432	HIS	-	EXPRESSION TAG	UNP P39099
C	433	HIS	-	EXPRESSION TAG	UNP P39099
C	434	HIS	-	EXPRESSION TAG	UNP P39099
C	435	HIS	-	EXPRESSION TAG	UNP P39099
C	436	HIS	-	EXPRESSION TAG	UNP P39099
D	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
D	429	LEU	-	EXPRESSION TAG	UNP P39099
D	430	GLU	-	EXPRESSION TAG	UNP P39099
D	431	HIS	-	EXPRESSION TAG	UNP P39099
D	432	HIS	-	EXPRESSION TAG	UNP P39099
D	433	HIS	-	EXPRESSION TAG	UNP P39099
D	434	HIS	-	EXPRESSION TAG	UNP P39099
D	435	HIS	-	EXPRESSION TAG	UNP P39099
D	436	HIS	-	EXPRESSION TAG	UNP P39099
E	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
E	429	LEU	-	EXPRESSION TAG	UNP P39099
E	430	GLU	-	EXPRESSION TAG	UNP P39099
E	431	HIS	-	EXPRESSION TAG	UNP P39099
E	432	HIS	-	EXPRESSION TAG	UNP P39099
E	433	HIS	-	EXPRESSION TAG	UNP P39099
E	434	HIS	-	EXPRESSION TAG	UNP P39099
E	435	HIS	-	EXPRESSION TAG	UNP P39099
E	436	HIS	-	EXPRESSION TAG	UNP P39099
F	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
F	429	LEU	-	EXPRESSION TAG	UNP P39099

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Chain	Residue	Modelled	Actual	Comment	Reference
F	430	GLU	-	EXPRESSION TAG	UNP P39099
F	431	HIS	-	EXPRESSION TAG	UNP P39099
F	432	HIS	-	EXPRESSION TAG	UNP P39099
F	433	HIS	-	EXPRESSION TAG	UNP P39099
F	434	HIS	-	EXPRESSION TAG	UNP P39099
F	435	HIS	-	EXPRESSION TAG	UNP P39099
F	436	HIS	-	EXPRESSION TAG	UNP P39099
G	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
G	429	LEU	-	EXPRESSION TAG	UNP P39099
G	430	GLU	-	EXPRESSION TAG	UNP P39099
G	431	HIS	-	EXPRESSION TAG	UNP P39099
G	432	HIS	-	EXPRESSION TAG	UNP P39099
G	433	HIS	-	EXPRESSION TAG	UNP P39099
G	434	HIS	-	EXPRESSION TAG	UNP P39099
G	435	HIS	-	EXPRESSION TAG	UNP P39099
G	436	HIS	-	EXPRESSION TAG	UNP P39099
H	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
H	429	LEU	-	EXPRESSION TAG	UNP P39099
H	430	GLU	-	EXPRESSION TAG	UNP P39099
H	431	HIS	-	EXPRESSION TAG	UNP P39099
H	432	HIS	-	EXPRESSION TAG	UNP P39099
H	433	HIS	-	EXPRESSION TAG	UNP P39099
H	434	HIS	-	EXPRESSION TAG	UNP P39099
H	435	HIS	-	EXPRESSION TAG	UNP P39099
H	436	HIS	-	EXPRESSION TAG	UNP P39099
I	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
I	429	LEU	-	EXPRESSION TAG	UNP P39099
I	430	GLU	-	EXPRESSION TAG	UNP P39099
I	431	HIS	-	EXPRESSION TAG	UNP P39099
I	432	HIS	-	EXPRESSION TAG	UNP P39099
I	433	HIS	-	EXPRESSION TAG	UNP P39099
I	434	HIS	-	EXPRESSION TAG	UNP P39099
I	435	HIS	-	EXPRESSION TAG	UNP P39099
I	436	HIS	-	EXPRESSION TAG	UNP P39099
J	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
J	429	LEU	-	EXPRESSION TAG	UNP P39099
J	430	GLU	-	EXPRESSION TAG	UNP P39099
J	431	HIS	-	EXPRESSION TAG	UNP P39099
J	432	HIS	-	EXPRESSION TAG	UNP P39099
J	433	HIS	-	EXPRESSION TAG	UNP P39099
J	434	HIS	-	EXPRESSION TAG	UNP P39099
J	435	HIS	-	EXPRESSION TAG	UNP P39099

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Chain	Residue	Modelled	Actual	Comment	Reference
J	436	HIS	-	EXPRESSION TAG	UNP P39099
K	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
K	429	LEU	-	EXPRESSION TAG	UNP P39099
K	430	GLU	-	EXPRESSION TAG	UNP P39099
K	431	HIS	-	EXPRESSION TAG	UNP P39099
K	432	HIS	-	EXPRESSION TAG	UNP P39099
K	433	HIS	-	EXPRESSION TAG	UNP P39099
K	434	HIS	-	EXPRESSION TAG	UNP P39099
K	435	HIS	-	EXPRESSION TAG	UNP P39099
K	436	HIS	-	EXPRESSION TAG	UNP P39099
L	187	ALA	SER	ENGINEERED MUTATION	UNP P39099
L	429	LEU	-	EXPRESSION TAG	UNP P39099
L	430	GLU	-	EXPRESSION TAG	UNP P39099
L	431	HIS	-	EXPRESSION TAG	UNP P39099
L	432	HIS	-	EXPRESSION TAG	UNP P39099
L	433	HIS	-	EXPRESSION TAG	UNP P39099
L	434	HIS	-	EXPRESSION TAG	UNP P39099
L	435	HIS	-	EXPRESSION TAG	UNP P39099
L	436	HIS	-	EXPRESSION TAG	UNP P39099

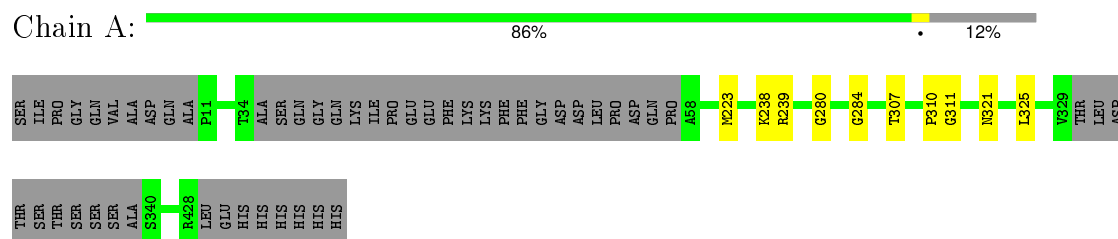
- Molecule 2 is a protein called LYSOZYME C.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	M	129	Total C 129 129	0	129

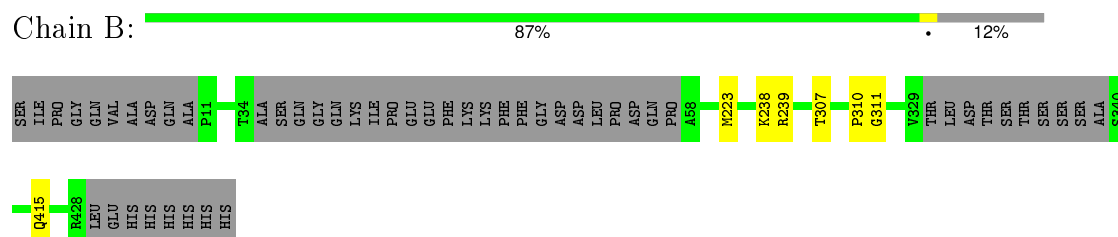
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

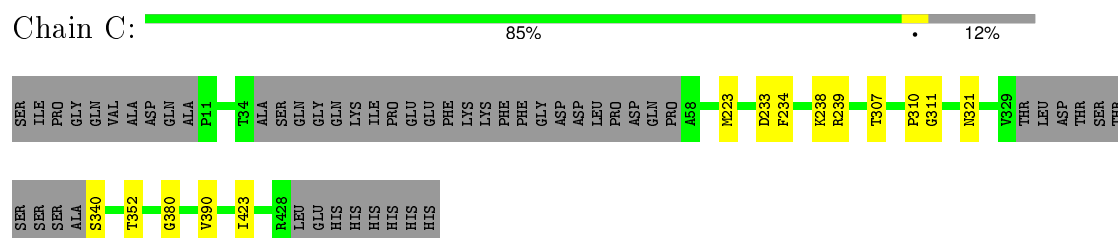
- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEQ



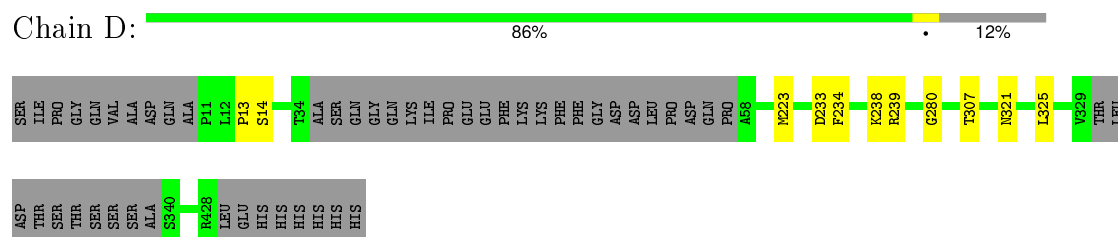
- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEQ



- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEQ




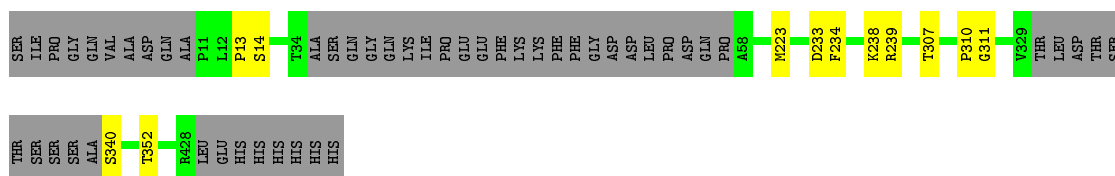
- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEQ




- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEQ

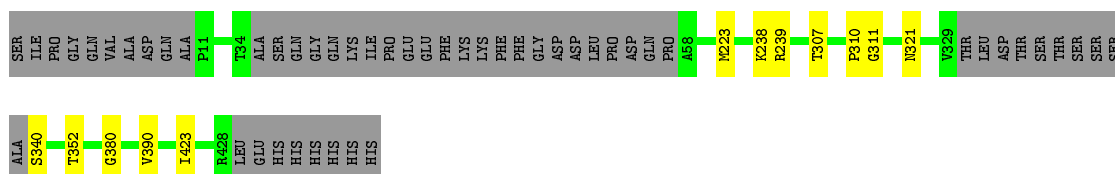


Chain E:  86% 12%




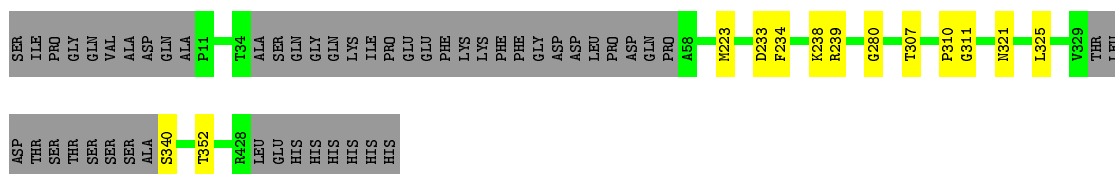
- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEGQ

Chain F:  86% 12%




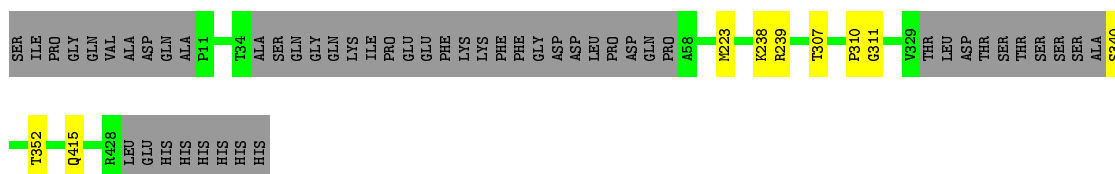
- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEGQ

Chain G:  85% 12%




- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEGQ

Chain H:  86% 12%




- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEGQ

Chain I:  86% 12%



- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEGQ

Chain J:  85% 12%



Q415	SER	ILE	PRO	GLN	GLY	VAL	ALA	ASP	GLN	ALA	P11	T24	ALA	SER	GLN	GLY	GLN	LYS	ILE	PRO	GLU	GLU	PHE	LYS	PHE	PHE	GLY	ASP	ASP	PRO	ASP	GLN	PRO	ASP	M223	K238	R239	T307	P310	G311	V329	THR	LEU	ASP	THR	SER	THR	SER	SER	SER	ALA	E340
------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Molecule 1: PERIPLASMIC PH-DEPENDENT SERINE ENDOPROTEASE DEGO

Sequence logo for the 1000bp upstream region of the human POU3F1 gene. The x-axis represents positions from -980 to +10. The y-axis represents the information content in bits. The background is color-coded by amino acid type: Serine (S), Threonine (T), Aspartate (D), Glutamate (E), Asparagine (N), Glutamine (Q), Valine (V), Alanine (A), Proline (P), Glycine (G), Leucine (L), Isoleucine (I), Methionine (M), Phenylalanine (F), Tyrosine (Y), Histidine (H), Lysine (K), Arginine (R), and Cysteine (C).

Position	Amino Acid	Information Content (bits)
-980	SER	0.00
-979	ILE	0.00
-978	PRO	0.00
-977	GLY	0.00
-976	GLN	0.00
-975	VAL	0.00
-974	ALA	0.00
-973	ASP	0.00
-972	GLN	0.00
-971	ALA	0.00
-970	P11	0.00
-969	T94	0.00
-968	ALA	0.00
-967	SER	0.00
-966	GLN	0.00
-965	GLY	0.00
-964	GLN	0.00
-963	LYS	0.00
-962	ILE	0.00
-961	GLU	0.00
-960	PRO	0.00
-959	GLU	0.00
-958	PHE	0.00
-957	LYS	0.00
-956	PHE	0.00
-955	PHE	0.00
-954	GLY	0.00
-953	ASP	0.00
-952	ASP	0.00
-951	LEU	0.00
-950	PRO	0.00
-949	ASP	0.00
-948	GLN	0.00
-947	PRO	0.00
-946	A58	0.00
-945	M223	0.00
-944	D233	0.00
-943	F234	0.00
-942	K238	0.00
-941	R239	0.00
-940	T307	0.00
-939	V329	0.00
-938	THR	0.00
-937	LEU	0.00
-936	ASP	0.00
-935	THR	0.00
-934	SER	0.00
-933	THR	0.00
-932	SER	0.00
-931	SER	0.00
-930	ALA	0.00
-929	G380	0.00
-928	V390	0.00
-927	I411	0.00
-926	I423	0.00
-925	R428	0.00
-924	LEU	0.00
-923	GLU	0.00
-922	HIS	0.00
-921	HIS	0.00
-920	HIS	0.00
-919	HIS	0.00
-918	HIS	0.00
-917	HIS	0.00

- Molecule 2: LYSOZYME C

Chain M:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [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	385	0	0	7	0
1	B	385	0	0	4	0
1	C	385	0	0	9	0
1	D	385	0	0	7	0
1	E	385	0	0	6	0
1	F	385	0	0	8	0
1	G	385	0	0	8	0
1	H	385	0	0	5	0
1	I	385	0	0	7	0
1	J	385	0	0	8	0
1	K	385	0	0	4	0
1	L	385	0	0	7	0
2	M	129	0	0	0	0
All	All	4749	0	0	64	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 13.

The worst 5 of 64 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:F:238:LYS:CA	1:F:239:ARG:CA	2.66	0.73
1:L:238:LYS:CA	1:L:239:ARG:CA	2.69	0.71
1:G:238:LYS:CA	1:G:239:ARG:CA	2.72	0.67
1:D:13:PRO:CA	1:D:14:SER:CA	2.73	0.66
1:C:238:LYS:CA	1:C:239:ARG:CA	2.74	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 carbohydrates 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.