



wwPDB EM Model Validation Summary Report ⓘ

Mar 2, 2020 – 03:38 PM EST

PDB ID : 6VQX
EMDB ID : EMD-21360
Title : Type I-F CRISPR-Csy complex with its inhibitor AcrF6
Authors : Zhang, K.; Li, S.; Pintilie, G.; Zhu, Y.; Huang, Z.; Chiu, W.
Deposited on : 2020-02-06
Resolution : 3.15 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

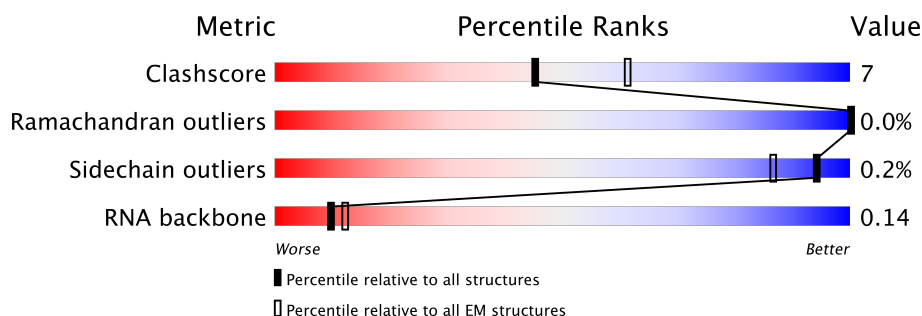
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	100	87% 10% .
2	B	434	74% 23% .
3	C	327	72% 20% . 7%
4	D	360	66% 15% 19%
4	E	360	79% 13% 8%
4	F	360	76% 17% 7%
4	G	360	80% 13% 7%

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Mol	Chain	Length	Quality of chain
4	H	360	<div><div></div><div>74%</div><div>18%</div><div>8%</div></div>
4	I	360	<div><div></div><div>76%</div><div>16%</div><div>8%</div></div>
5	J	187	<div><div></div><div>93%</div><div>7%</div></div>
6	K	60	<div><div></div><div>23%</div><div>55%</div><div>22%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23696 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 AcrF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			737	462	119	154	2		

- Molecule 2 is a protein called CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	422	Total	C	N	O	S	0	0
			3364	2106	634	620	4		

- Molecule 3 is a protein called Type I-F CRISPR-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2395	1517	443	430	5		

- Molecule 4 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2272	1430	409	431	2		
4	E	333	Total	C	N	O	S	0	0
			2579	1617	469	491	2		
4	F	334	Total	C	N	O	S	0	0
			2577	1619	470	486	2		
4	G	335	Total	C	N	O	S	0	0
			2589	1625	471	491	2		
4	H	333	Total	C	N	O	S	0	0
			2573	1615	469	487	2		
4	I	333	Total	C	N	O	S	0	0
			2576	1616	469	489	2		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP A0A444M080
D	2	LYS	-	expression tag	UNP A0A444M080
D	3	SER	-	expression tag	UNP A0A444M080
D	4	SER	-	expression tag	UNP A0A444M080
D	5	HIS	-	expression tag	UNP A0A444M080
D	6	HIS	-	expression tag	UNP A0A444M080
D	7	HIS	-	expression tag	UNP A0A444M080
D	8	HIS	-	expression tag	UNP A0A444M080
D	9	HIS	-	expression tag	UNP A0A444M080
D	10	HIS	-	expression tag	UNP A0A444M080
D	11	GLU	-	expression tag	UNP A0A444M080
D	12	ASN	-	expression tag	UNP A0A444M080
D	13	LEU	-	expression tag	UNP A0A444M080
D	14	TYR	-	expression tag	UNP A0A444M080
D	15	PHE	-	expression tag	UNP A0A444M080
D	16	GLN	-	expression tag	UNP A0A444M080
D	17	SER	-	expression tag	UNP A0A444M080
D	18	ASN	-	expression tag	UNP A0A444M080
D	19	ALA	-	expression tag	UNP A0A444M080
E	1	MET	-	expression tag	UNP A0A444M080
E	2	LYS	-	expression tag	UNP A0A444M080
E	3	SER	-	expression tag	UNP A0A444M080
E	4	SER	-	expression tag	UNP A0A444M080
E	5	HIS	-	expression tag	UNP A0A444M080
E	6	HIS	-	expression tag	UNP A0A444M080
E	7	HIS	-	expression tag	UNP A0A444M080
E	8	HIS	-	expression tag	UNP A0A444M080
E	9	HIS	-	expression tag	UNP A0A444M080
E	10	HIS	-	expression tag	UNP A0A444M080
E	11	GLU	-	expression tag	UNP A0A444M080
E	12	ASN	-	expression tag	UNP A0A444M080
E	13	LEU	-	expression tag	UNP A0A444M080
E	14	TYR	-	expression tag	UNP A0A444M080
E	15	PHE	-	expression tag	UNP A0A444M080
E	16	GLN	-	expression tag	UNP A0A444M080
E	17	SER	-	expression tag	UNP A0A444M080
E	18	ASN	-	expression tag	UNP A0A444M080
E	19	ALA	-	expression tag	UNP A0A444M080
F	1	MET	-	expression tag	UNP A0A444M080
F	2	LYS	-	expression tag	UNP A0A444M080
F	3	SER	-	expression tag	UNP A0A444M080
F	4	SER	-	expression tag	UNP A0A444M080
F	5	HIS	-	expression tag	UNP A0A444M080

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Chain	Residue	Modelled	Actual	Comment	Reference
F	6	HIS	-	expression tag	UNP A0A444M080
F	7	HIS	-	expression tag	UNP A0A444M080
F	8	HIS	-	expression tag	UNP A0A444M080
F	9	HIS	-	expression tag	UNP A0A444M080
F	10	HIS	-	expression tag	UNP A0A444M080
F	11	GLU	-	expression tag	UNP A0A444M080
F	12	ASN	-	expression tag	UNP A0A444M080
F	13	LEU	-	expression tag	UNP A0A444M080
F	14	TYR	-	expression tag	UNP A0A444M080
F	15	PHE	-	expression tag	UNP A0A444M080
F	16	GLN	-	expression tag	UNP A0A444M080
F	17	SER	-	expression tag	UNP A0A444M080
F	18	ASN	-	expression tag	UNP A0A444M080
F	19	ALA	-	expression tag	UNP A0A444M080
G	1	MET	-	expression tag	UNP A0A444M080
G	2	LYS	-	expression tag	UNP A0A444M080
G	3	SER	-	expression tag	UNP A0A444M080
G	4	SER	-	expression tag	UNP A0A444M080
G	5	HIS	-	expression tag	UNP A0A444M080
G	6	HIS	-	expression tag	UNP A0A444M080
G	7	HIS	-	expression tag	UNP A0A444M080
G	8	HIS	-	expression tag	UNP A0A444M080
G	9	HIS	-	expression tag	UNP A0A444M080
G	10	HIS	-	expression tag	UNP A0A444M080
G	11	GLU	-	expression tag	UNP A0A444M080
G	12	ASN	-	expression tag	UNP A0A444M080
G	13	LEU	-	expression tag	UNP A0A444M080
G	14	TYR	-	expression tag	UNP A0A444M080
G	15	PHE	-	expression tag	UNP A0A444M080
G	16	GLN	-	expression tag	UNP A0A444M080
G	17	SER	-	expression tag	UNP A0A444M080
G	18	ASN	-	expression tag	UNP A0A444M080
G	19	ALA	-	expression tag	UNP A0A444M080
H	1	MET	-	expression tag	UNP A0A444M080
H	2	LYS	-	expression tag	UNP A0A444M080
H	3	SER	-	expression tag	UNP A0A444M080
H	4	SER	-	expression tag	UNP A0A444M080
H	5	HIS	-	expression tag	UNP A0A444M080
H	6	HIS	-	expression tag	UNP A0A444M080
H	7	HIS	-	expression tag	UNP A0A444M080
H	8	HIS	-	expression tag	UNP A0A444M080
H	9	HIS	-	expression tag	UNP A0A444M080

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Chain	Residue	Modelled	Actual	Comment	Reference
H	10	HIS	-	expression tag	UNP A0A444M080
H	11	GLU	-	expression tag	UNP A0A444M080
H	12	ASN	-	expression tag	UNP A0A444M080
H	13	LEU	-	expression tag	UNP A0A444M080
H	14	TYR	-	expression tag	UNP A0A444M080
H	15	PHE	-	expression tag	UNP A0A444M080
H	16	GLN	-	expression tag	UNP A0A444M080
H	17	SER	-	expression tag	UNP A0A444M080
H	18	ASN	-	expression tag	UNP A0A444M080
H	19	ALA	-	expression tag	UNP A0A444M080
I	1	MET	-	expression tag	UNP A0A444M080
I	2	LYS	-	expression tag	UNP A0A444M080
I	3	SER	-	expression tag	UNP A0A444M080
I	4	SER	-	expression tag	UNP A0A444M080
I	5	HIS	-	expression tag	UNP A0A444M080
I	6	HIS	-	expression tag	UNP A0A444M080
I	7	HIS	-	expression tag	UNP A0A444M080
I	8	HIS	-	expression tag	UNP A0A444M080
I	9	HIS	-	expression tag	UNP A0A444M080
I	10	HIS	-	expression tag	UNP A0A444M080
I	11	GLU	-	expression tag	UNP A0A444M080
I	12	ASN	-	expression tag	UNP A0A444M080
I	13	LEU	-	expression tag	UNP A0A444M080
I	14	TYR	-	expression tag	UNP A0A444M080
I	15	PHE	-	expression tag	UNP A0A444M080
I	16	GLN	-	expression tag	UNP A0A444M080
I	17	SER	-	expression tag	UNP A0A444M080
I	18	ASN	-	expression tag	UNP A0A444M080
I	19	ALA	-	expression tag	UNP A0A444M080

- Molecule 5 is a protein called CRISPR-associated endonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	187	Total	C	N	O	0	0
			763	385	187	191		


- Molecule 6 is a RNA chain called CrRNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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.

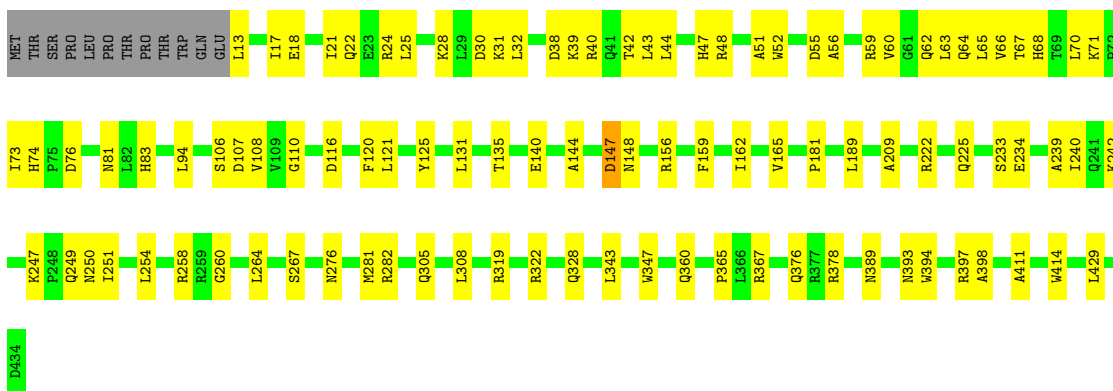
- Molecule 1: AcrF6

Chain A: 



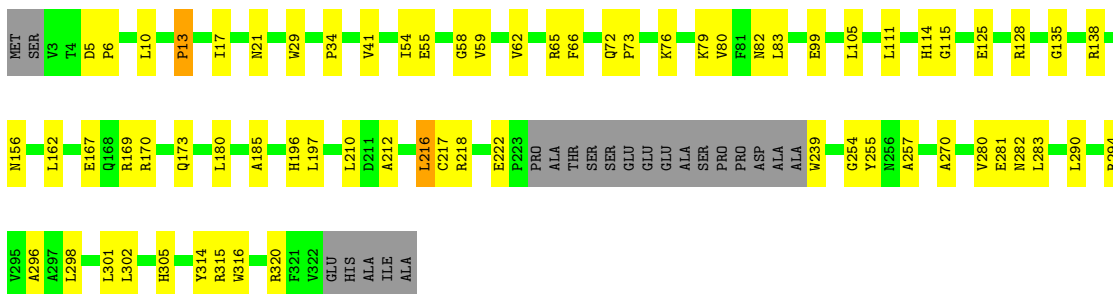
- Molecule 2: CRISPR-associated protein Csy1

Chain B: 



- Molecule 3: Type I-F CRISPR-associated protein Csy2

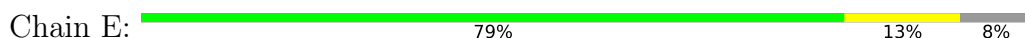
Chain C: 



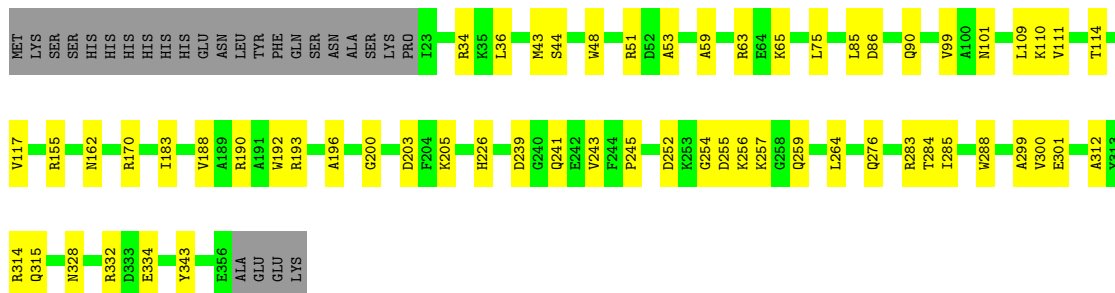
- Molecule 4: CRISPR-associated protein Csy3

Chain D: 

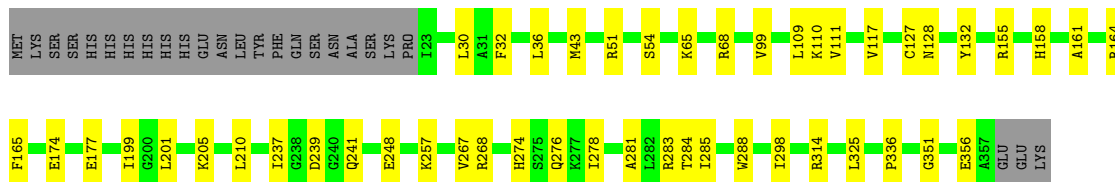
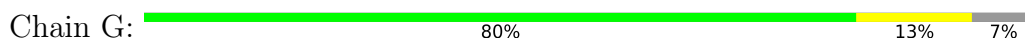
- Molecule 4: CRISPR-associated protein Csy3



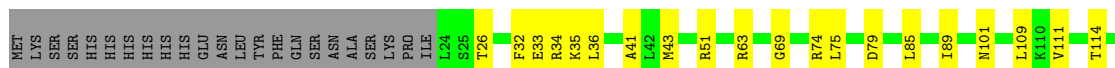
- Molecule 4: CRISPR-associated protein Csy3

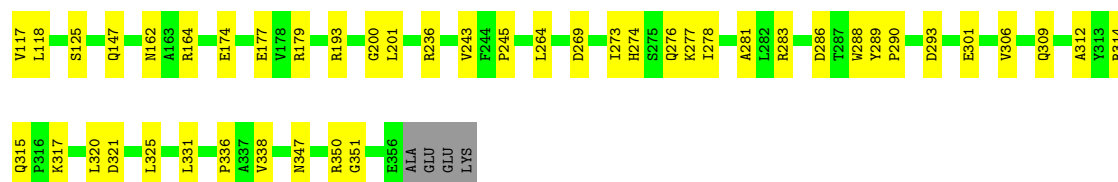


- Molecule 4: CRISPR-associated protein Csy3



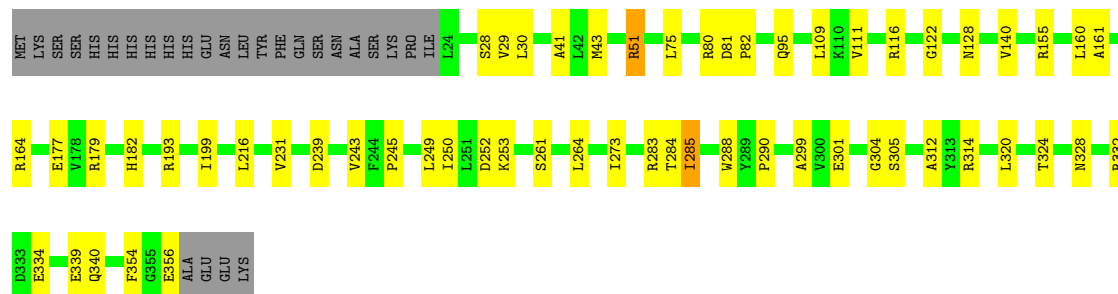
- Molecule 4: CRISPR-associated protein Csy3





• Molecule 4: CRISPR-associated protein Csy3

Chain I: 76% 16% 8%



• Molecule 5: CRISPR-associated endonuclease Cas6/Csy4

Chain J: 93% 7%



• Molecule 6: CrRNA (60-MER)

Chain K: 23% 55% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56455	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	7	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	0.28	0/748	0.53	0/1019
2	B	0.29	0/3445	0.60	4/4675 (0.1%)
3	C	0.31	0/2453	0.55	0/3340
4	D	0.29	0/2315	0.49	0/3143
4	E	0.30	0/2626	0.51	0/3561
4	F	0.31	0/2624	0.50	0/3559
4	G	0.32	0/2636	0.51	0/3575
4	H	0.33	0/2620	0.54	1/3553 (0.0%)
4	I	0.30	0/2623	0.52	1/3557 (0.0%)
5	J	0.25	0/763	0.53	0/956
6	K	0.43	0/1419	0.95	5/2210 (0.2%)
All	All	0.31	0/24272	0.57	11/33148 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1
4	F	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	C	O4'-C1'-N1	11.22	117.18	108.20
6	K	1	C	N1-C2-O2	7.47	123.38	118.90
6	K	1	C	C2-N1-C1'	7.08	126.58	118.80
2	B	189	LEU	CA-CB-CG	6.87	131.10	115.30
2	B	343	LEU	CA-CB-CG	6.77	130.88	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	147	ASP	Peptide
2	B	148	ASN	Peptide
3	C	216	LEU	Peptide
4	F	48	TRP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	737	0	700	6	0
2	B	3364	0	3278	81	0
3	C	2395	0	2390	50	0
4	D	2272	0	2232	35	0
4	E	2579	0	2565	32	0
4	F	2577	0	2568	37	0
4	G	2589	0	2579	30	0
4	H	2573	0	2561	39	0
4	I	2576	0	2563	38	0
5	J	763	0	218	15	0
6	K	1271	0	644	33	0
All	All	23696	0	22298	334	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 334 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)
2:B:65:LEU:HD11	2:B:106:SER:OG	1.35	1.24
5:J:175:CYS:HA	6:K:57:G:OP1	1.38	1.23
5:J:175:CYS:CB	6:K:56:G:H3'	1.82	1.10
2:B:67:THR:HG22	2:B:83:HIS:HA	1.14	1.09
2:B:67:THR:HG22	2:B:83:HIS:CA	1.95	0.95

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 PDB entries followed by that with respect to all EM entries.

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	95/100 (95%)	87 (92%)	8 (8%)	0	100	100
2	B	420/434 (97%)	375 (89%)	45 (11%)	0	100	100
3	C	301/327 (92%)	277 (92%)	23 (8%)	1 (0%)	43	78
4	D	287/360 (80%)	268 (93%)	19 (7%)	0	100	100
4	E	331/360 (92%)	311 (94%)	20 (6%)	0	100	100
4	F	332/360 (92%)	311 (94%)	21 (6%)	0	100	100
4	G	333/360 (92%)	305 (92%)	28 (8%)	0	100	100
4	H	331/360 (92%)	310 (94%)	21 (6%)	0	100	100
4	I	331/360 (92%)	303 (92%)	28 (8%)	0	100	100
5	J	185/187 (99%)	141 (76%)	44 (24%)	0	100	100
All	All	2946/3208 (92%)	2688 (91%)	257 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	13	PRO

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 PDB entries followed by that with respect to all EM entries.

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	74/76 (97%)	74 (100%)	0	100	100
2	B	348/365 (95%)	347 (100%)	1 (0%)	93	97
3	C	252/270 (93%)	252 (100%)	0	100	100
4	D	230/290 (79%)	229 (100%)	1 (0%)	92	97
4	E	265/290 (91%)	265 (100%)	0	100	100
4	F	263/290 (91%)	263 (100%)	0	100	100
4	G	265/290 (91%)	264 (100%)	1 (0%)	92	97
4	H	263/290 (91%)	263 (100%)	0	100	100
4	I	264/290 (91%)	263 (100%)	1 (0%)	92	97
5	J	3/160 (2%)	3 (100%)	0	100	100
All	All	2227/2611 (85%)	2223 (100%)	4 (0%)	94	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	376	GLN
4	D	51	ARG
4	G	68	ARG
4	I	51	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	306	HIS
4	D	101	ASN
4	G	309	GLN
3	C	269	ASN
4	I	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	K	59/60 (98%)	33 (55%)	0

5 of 33 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	K	3	A
6	K	4	A
6	K	9	U
6	K	10	U
6	K	14	G

There are no RNA pucker outliers to report.

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.