



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 6, 2016 – 07:56 AM EST

PDB ID : 5GRS  
EMDB ID: : EMD-9537  
Title : Complex structure of the fission yeast SREBP-SCAP binding domains  
Authors : Gong, X.; Qian, H.W.; Wu, J.P.; Yan, N.  
Deposited on : 2016-08-12  
Resolution : 5.40 Å(reported)

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

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>  
with specific help available everywhere you see the ⓘ symbol.

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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) : rb-20028442

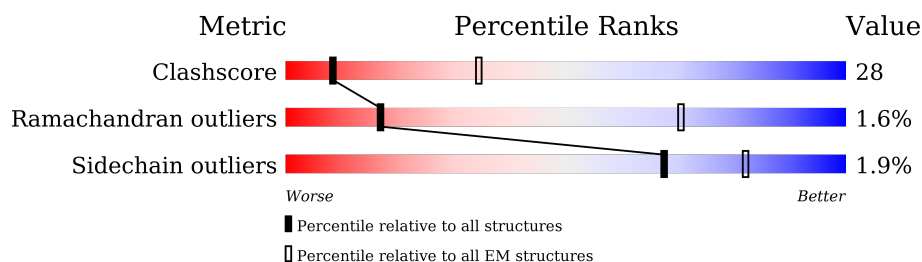
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.40 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
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	396	
1	B	396	
1	C	396	
1	D	396	
2	I	103	
2	J	103	
2	K	103	
2	L	103	
3	E	272	

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Mol	Chain	Length	Quality of chain
3	F	272	<div><div></div><div>44%21%5%30%</div></div>
3	G	272	<div><div></div><div>49%17%•31%</div></div>
3	H	272	<div><div></div><div>43%22%5%•30%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19489 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 Sterol regulatory element-binding protein cleavage-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	1	0
			2986	1908	489	577	12		
1	B	375	Total	C	N	O	S	1	0
			2986	1908	489	577	12		
1	C	375	Total	C	N	O	S	1	0
			2982	1906	488	576	12		
1	D	375	Total	C	N	O	S	1	0
			2986	1908	489	577	12		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	MET	-	expression tag	UNP O43043
A	671	SER	CYS	engineered mutation	UNP O43043
A	873	SER	CYS	engineered mutation	UNP O43043
A	901	SER	CYS	engineered mutation	UNP O43043
A	920	SER	CYS	engineered mutation	UNP O43043
A	941	SER	CYS	engineered mutation	UNP O43043
B	566	MET	-	expression tag	UNP O43043
B	671	SER	CYS	engineered mutation	UNP O43043
B	873	SER	CYS	engineered mutation	UNP O43043
B	901	SER	CYS	engineered mutation	UNP O43043
B	920	SER	CYS	engineered mutation	UNP O43043
B	941	SER	CYS	engineered mutation	UNP O43043
C	566	MET	-	expression tag	UNP O43043
C	671	SER	CYS	engineered mutation	UNP O43043
C	873	SER	CYS	engineered mutation	UNP O43043
C	901	SER	CYS	engineered mutation	UNP O43043
C	920	SER	CYS	engineered mutation	UNP O43043
C	941	SER	CYS	engineered mutation	UNP O43043
D	566	MET	-	expression tag	UNP O43043
D	671	SER	CYS	engineered mutation	UNP O43043
D	873	SER	CYS	engineered mutation	UNP O43043

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Chain	Residue	Modelled	Actual	Comment	Reference
D	901	SER	CYS	engineered mutation	UNP O43043
D	920	SER	CYS	engineered mutation	UNP O43043
D	941	SER	CYS	engineered mutation	UNP O43043

- Molecule 2 is a protein called Sterol regulatory element-binding protein cleavage-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	62	Total	C	N	O	S	0	0
			489	315	80	91	3		
2	J	62	Total	C	N	O	S	0	0
			489	315	80	91	3		
2	K	62	Total	C	N	O	S	0	0
			489	315	80	91	3		
2	L	62	Total	C	N	O	S	0	0
			489	315	80	91	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	983	ALA	-	expression tag	UNP O43043
I	984	HIS	-	expression tag	UNP O43043
I	985	MET	-	expression tag	UNP O43043
I	1010	SER	CYS	engineered mutation	UNP O43043
J	983	ALA	-	expression tag	UNP O43043
J	984	HIS	-	expression tag	UNP O43043
J	985	MET	-	expression tag	UNP O43043
J	1010	SER	CYS	engineered mutation	UNP O43043
K	983	ALA	-	expression tag	UNP O43043
K	984	HIS	-	expression tag	UNP O43043
K	985	MET	-	expression tag	UNP O43043
K	1010	SER	CYS	engineered mutation	UNP O43043
L	983	ALA	-	expression tag	UNP O43043
L	984	HIS	-	expression tag	UNP O43043
L	985	MET	-	expression tag	UNP O43043
L	1010	SER	CYS	engineered mutation	UNP O43043

- Molecule 3 is a protein called Sterol regulatory element-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	189	Total	C	N	O	S	0	0
			1394	890	224	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	191	Total	C	N	O	S	0	0
			1406	901	227	270	8		
3	G	187	Total	C	N	O	S	0	0
			1383	884	222	269	8		
3	H	191	Total	C	N	O	S	0	0
			1410	904	228	270	8		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	625	ALA	-	expression tag	UNP Q9UUD1
E	626	HIS	-	expression tag	UNP Q9UUD1
E	627	MET	-	expression tag	UNP Q9UUD1
E	644	SER	CYS	engineered mutation	UNP Q9UUD1
E	672	SER	CYS	engineered mutation	UNP Q9UUD1
F	625	ALA	-	expression tag	UNP Q9UUD1
F	626	HIS	-	expression tag	UNP Q9UUD1
F	627	MET	-	expression tag	UNP Q9UUD1
F	644	SER	CYS	engineered mutation	UNP Q9UUD1
F	672	SER	CYS	engineered mutation	UNP Q9UUD1
G	625	ALA	-	expression tag	UNP Q9UUD1
G	626	HIS	-	expression tag	UNP Q9UUD1
G	627	MET	-	expression tag	UNP Q9UUD1
G	644	SER	CYS	engineered mutation	UNP Q9UUD1
G	672	SER	CYS	engineered mutation	UNP Q9UUD1
H	625	ALA	-	expression tag	UNP Q9UUD1
H	626	HIS	-	expression tag	UNP Q9UUD1
H	627	MET	-	expression tag	UNP Q9UUD1
H	644	SER	CYS	engineered mutation	UNP Q9UUD1
H	672	SER	CYS	engineered mutation	UNP Q9UUD1

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.

- Chain A:   5%

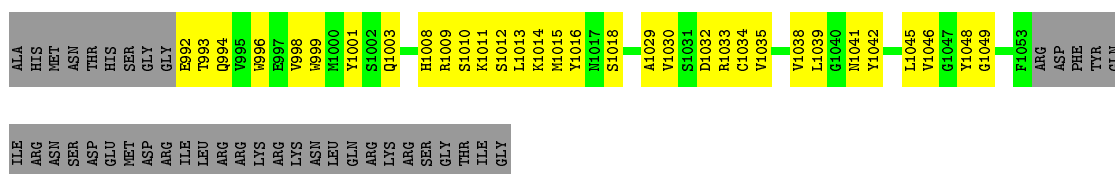
THR	ASP	GLU	LYS	ASN	GLU	ASN	PHE	THR	LEU	ARG	ASN	ARG	LYS	LEU	ARG	THR	ASP	GLU	LYS	ASN	GLU	ASN	PHE	THR	LEU	ARG	THR	ASP	GLU	LYS	ASN	GLU	ASN	PHE	THR	LEU	ARG														
H858	A859	V960	T861	Y866	Y867	Y868	Y869	E872	S873	Y877	I878	I879	L880	N881	K882	V883	D884	Q885	Q886	F887	N888	L889	V890	D896	N897	S898	F904	L907	Q908	E909	E915	S918	V921	M922	S923	S924	D925	G926	I929	M932	R933	R934	S938	G939	I940	S941	D942				
K790	D791	I792	G793	I795	A796	K797	A798	D799	L800	L801	F802	L803	A804	R805	Y809	D810	D813	L814	K815	R816	D817	E818	L819	L820	F823	P826	R827	I828	K829	V830	R831	T832	F833	S834	V837	S838	R841	F842	V843	R844	G845	Q846	V849	S850	S851	L852	S853	F854	C855	F856	T857
Q715	V716	T720	I721	E722	I723	E724	G725	A726	D727	I728	E732	K733	F734	Q735	L736	P739	I740	I741	I744	S745	I746	V747	S748	N752	I753	I754	A755	G756	L757	T758	E759	S760	G761	E762	V763	T764	V765	V766	S767	K768	K769	V772	I773	L778	S779	Q780	I781	K782	L785	V789	
Q650	G651	M652	S655	L656	F657	S658	G659	D660	T661	L662	L665	M666	V667	S668	S669	L672	A673	L674	Q675	H676	S677	V678	H679	C680	A681	M683	S684	M687	F688	M690	M691	T694	A695	K696	D697	D698	E699	K700	K701	N702	F703	E704	L705	V706	V707	V708	E709	S710	E713	T714	
MET	G567	H568	S569	D570	H571	D572	E573	L574	D577	H581	K584	E588	H594	Q595	L596	D597	L598	L599	K600	I601	A602	N606	T609	F610	A611	S612	V613	G614	L615	D616	R617	C618	V621	M622	D623	L624	K630	L631	V632	L633	E636	P639	L642	K643	A644	L647					

- Chain B:

Amino Acid	Count
Met	1
G567	6
G568	6
S569	6
D570	6
H571	6
D572	6
L574	6
D577	6
H581	6
K584	6
E588	6
H594	6
Q595	6
L596	6
D597	6
L598	6
L599	6
A600	6
F601	6
A602	6
M606	6
F610	6
A611	6
S612	6
G613	6
G614	6
L615	6
D616	6
R617	6
C618	6
V621	6
M622	6
D623	6
L624	6
K630	6
L631	6
F632	6
L633	6
E636	6
P639	6
R640	6
T641	6
L642	6
R644	6
L647	6
T720	6
T721	6
T722	6
T723	6
T724	6
G725	6
L656	6
F657	6
T726	6
T727	6
G658	6
L659	6
T728	6
D660	6
T661	6
L662	6
L665	6
N666	6
V667	6
P739	6
T740	6
T741	6
L744	6
S745	6
T746	6
T747	6
S748	6
N752	6
R753	6
T754	6
A755	6
C756	6
T757	6
T758	6
F689	6
S690	6
R691	6
T762	6
F693	6
T763	6
T764	6
R696	6
T766	6
S767	6
K768	6
T769	6
T772	6
T773	6
S774	6
T775	6
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E709	6
S710	6
E713	6
T714	6
T715	6
T716	6

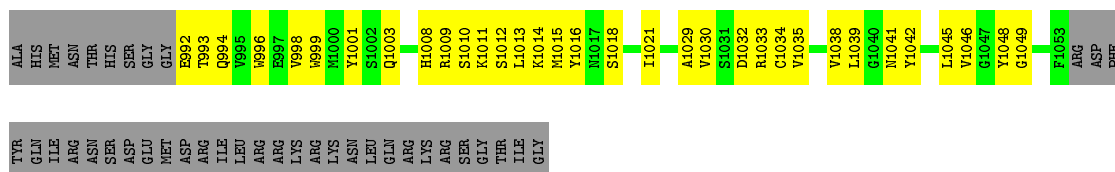






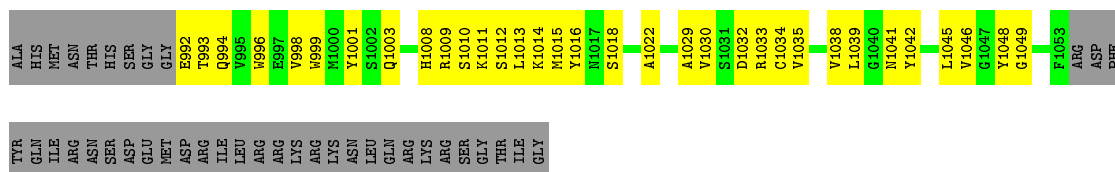
- Molecule 2: Sterol regulatory element-binding protein cleavage-activating protein

Chain J: 28% 32% 40%



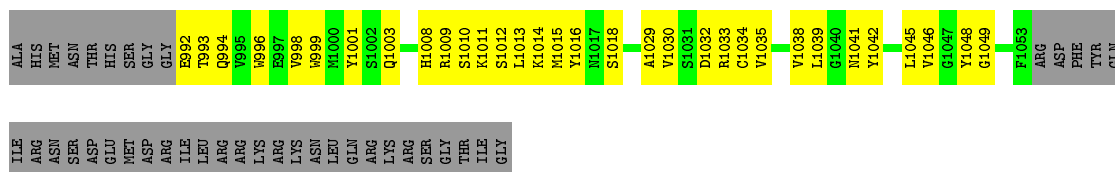
- Molecule 2: Sterol regulatory element-binding protein cleavage-activating protein

Chain K: 28% 32% 40%



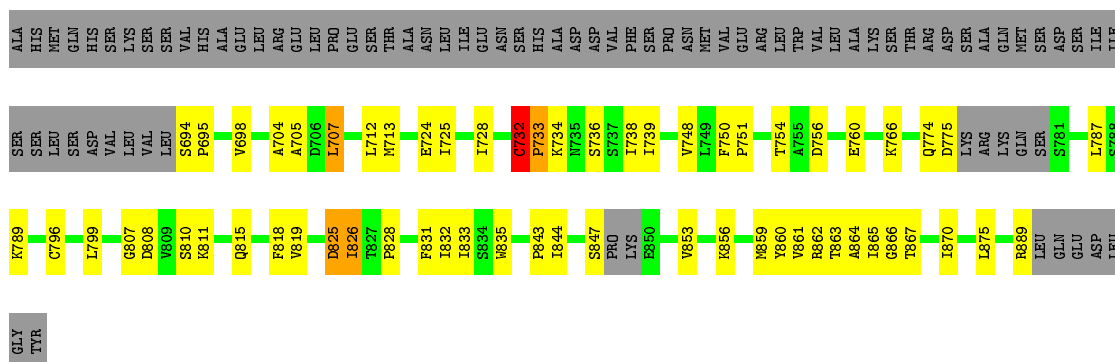
- Molecule 2: Sterol regulatory element-binding protein cleavage-activating protein

Chain L: 29% 31% 40%

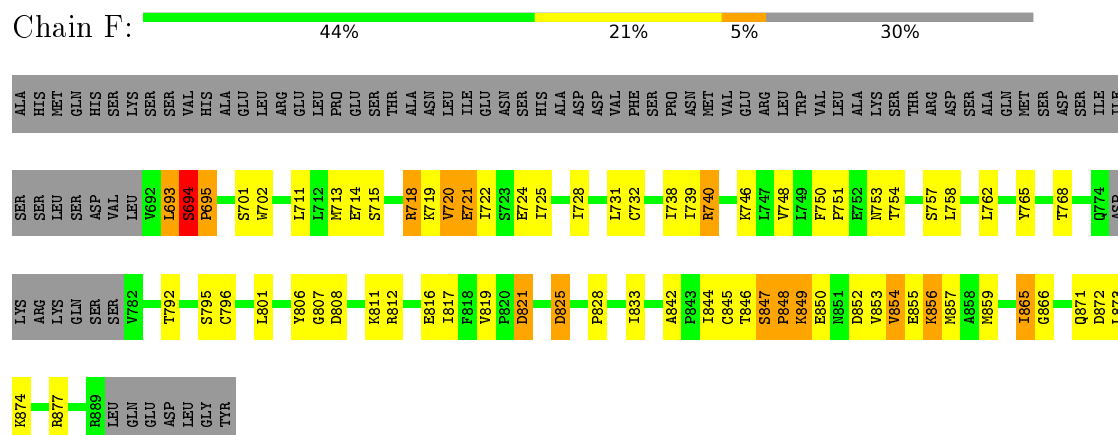


- Molecule 3: Sterol regulatory element-binding protein 1

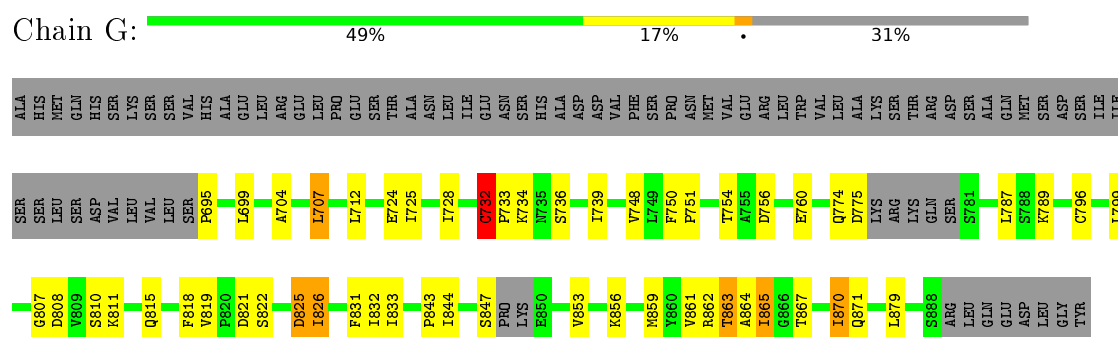
Chain E: 47% 21% 31%



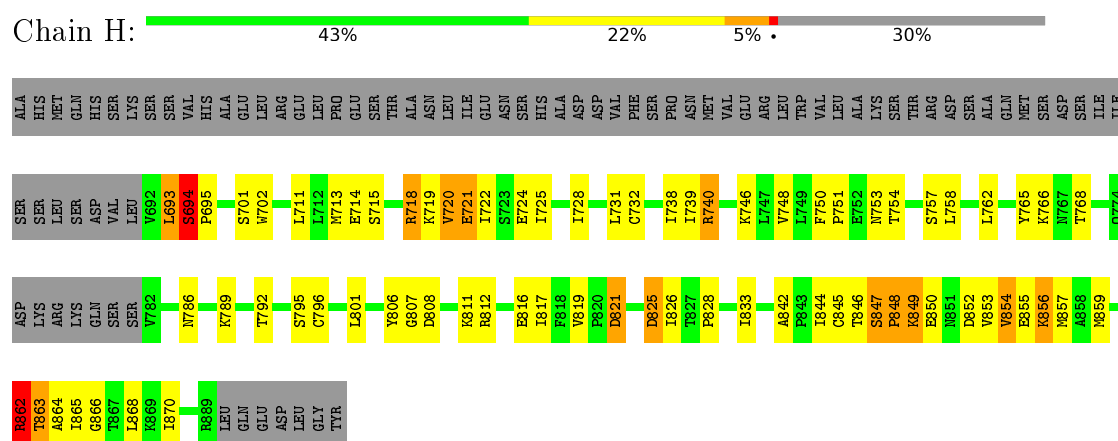
- Molecule 3: Sterol regulatory element-binding protein 1



- Molecule 3: Sterol regulatory element-binding protein 1



- Molecule 3: Sterol regulatory element-binding protein 1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	157243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 2	RMSZ	# Z  > 2
1	A	0.32	0/3054	0.60	0/4147
1	B	0.32	0/3054	0.61	0/4147
1	C	0.32	0/3050	0.61	0/4142
1	D	0.32	0/3054	0.60	0/4147
2	I	0.28	0/500	0.50	0/677
2	J	0.28	0/500	0.50	0/677
2	K	0.28	0/500	0.50	0/677
2	L	0.28	0/500	0.51	0/677
3	E	0.33	1/1413 (0.1%)	0.48	1/1925 (0.1%)
3	F	0.60	6/1427 (0.4%)	0.57	3/1948 (0.2%)
3	G	0.33	0/1402	0.51	1/1909 (0.1%)
3	H	0.60	5/1431 (0.3%)	0.57	3/1952 (0.2%)
All	All	0.37	12/19885 (0.1%)	0.58	8/27025 (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
3	H	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	740	ARG	NE-CZ	-9.46	1.20	1.33
3	H	740	ARG	NE-CZ	-9.43	1.20	1.33
3	F	740	ARG	CZ-NH2	-9.01	1.21	1.33
3	H	740	ARG	CZ-NH2	-8.87	1.21	1.33
3	H	740	ARG	CD-NE	-8.00	1.32	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	694	SER	C-N-CD	6.06	141.13	128.40
3	G	732	CYS	C-N-CD	6.04	141.08	128.40
3	F	694	SER	C-N-CD	6.04	141.07	128.40
3	E	732	CYS	C-N-CD	6.02	141.04	128.40
3	H	847	SER	C-N-CD	5.65	140.26	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	862	ARG	Mainchain

## 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	2986	0	2934	175	0
1	B	2986	0	2934	187	0
1	C	2982	0	2928	183	0
1	D	2986	0	2933	178	0
2	I	489	0	487	36	0
2	J	489	0	487	40	0
2	K	489	0	487	39	0
2	L	489	0	487	36	0
3	E	1394	0	1349	84	0
3	F	1406	0	1364	95	0
3	G	1383	0	1343	49	0
3	H	1410	0	1377	109	0
All	All	19489	0	19110	1086	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 28.

The worst 5 of 1086 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)
3:E:713:MET:CE	3:E:867:THR:HG21	1.08	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:713:MET:CE	3:E:867:THR:CG2	2.04	1.34
3:E:860:TYR:O	3:E:864:ALA:HB3	1.11	1.28
3:E:713:MET:HE3	3:E:867:THR:CG2	1.60	1.27
3:E:860:TYR:O	3:E:864:ALA:CB	1.86	1.23

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	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	17	63
1	B	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	17	63
1	C	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	17	63
1	D	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	17	63
2	I	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
2	J	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
2	K	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
2	L	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
3	E	183/272 (67%)	163 (89%)	16 (9%)	4 (2%)	8	49
3	F	187/272 (69%)	165 (88%)	16 (9%)	6 (3%)	5	41
3	G	181/272 (66%)	160 (88%)	15 (8%)	6 (3%)	5	40
3	H	187/272 (69%)	165 (88%)	14 (8%)	8 (4%)	3	34
All	All	2474/3084 (80%)	2217 (90%)	217 (9%)	40 (2%)	17	56

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	696	LYS

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Mol	Chain	Res	Type
1	B	696	LYS
1	C	696	LYS
1	D	696	LYS
3	E	734	LYS

### 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 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	342/364 (94%)	340 (99%)	2 (1%)	90	95
1	B	342/364 (94%)	340 (99%)	2 (1%)	90	95
1	C	341/364 (94%)	339 (99%)	2 (1%)	90	95
1	D	342/364 (94%)	340 (99%)	2 (1%)	90	95
2	I	54/90 (60%)	54 (100%)	0	100	100
2	J	54/90 (60%)	54 (100%)	0	100	100
2	K	54/90 (60%)	54 (100%)	0	100	100
2	L	54/90 (60%)	54 (100%)	0	100	100
3	E	147/246 (60%)	143 (97%)	4 (3%)	52	79
3	F	147/246 (60%)	134 (91%)	13 (9%)	12	45
3	G	146/246 (59%)	142 (97%)	4 (3%)	52	79
3	H	148/246 (60%)	136 (92%)	12 (8%)	15	50
All	All	2171/2800 (78%)	2130 (98%)	41 (2%)	67	86

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	821	ASP
3	F	856	LYS
3	H	849	LYS
3	F	825	ASP
3	F	849	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	1003	GLN
1	C	844	ASN
1	D	844	ASN
1	B	885	GLN
2	K	1003	GLN

### 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.