



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 03:32 AM EST

PDB ID : 6DBR
EMDB ID: : EMD-7848
Title : Cryo-EM structure of RAG in complex with one melted RSS and one unmelted RSS
Authors : Wu, H.; Liao, M.; Ru, H.; Mi, W.
Deposited on : 2018-05-03
Resolution : 4.00 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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) : 2.4

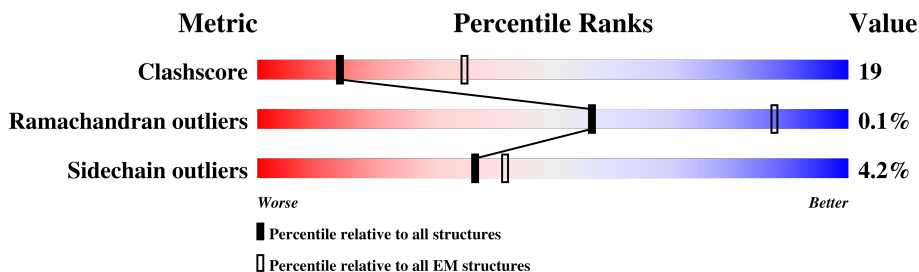
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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

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 ≥ 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	1159	29% 17% . 53%
1	C	1159	29% 17% . 53%
2	B	533	39% 25% . 34%
2	D	533	36% 28% . 34%
3	E	34	44% 56%
4	F	34	35% 65%
5	G	34	44% 56%
6	H	34	41% 59%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17040 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 Recombination activating gene 1 - MBP chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	550	Total	C	N	O	S	0	0
			4437	2784	785	834	34		
1	C	542	Total	C	N	O	S	0	0
			4381	2749	775	823	34		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP P0AEX9
A	-126	GLY	-	expression tag	UNP P0AEX9
A	-125	SER	-	expression tag	UNP P0AEX9
A	-124	SER	-	expression tag	UNP P0AEX9
A	-123	HIS	-	expression tag	UNP P0AEX9
A	-122	HIS	-	expression tag	UNP P0AEX9
A	-121	HIS	-	expression tag	UNP P0AEX9
A	-120	HIS	-	expression tag	UNP P0AEX9
A	-119	HIS	-	expression tag	UNP P0AEX9
A	-118	HIS	-	expression tag	UNP P0AEX9
A	-117	GLY	-	expression tag	UNP P0AEX9
A	-116	THR	-	expression tag	UNP P0AEX9
A	-115	LYS	-	expression tag	UNP P0AEX9
A	-114	THR	-	expression tag	UNP P0AEX9
A	251	GLY	-	linker	UNP P0AEX9
A	252	THR	-	linker	UNP P0AEX9
A	253	ASP	-	linker	UNP P0AEX9
A	254	TYR	-	linker	UNP P0AEX9
A	255	ASP	-	linker	UNP P0AEX9
A	256	ILE	-	linker	UNP P0AEX9
A	257	PRO	-	linker	UNP P0AEX9
A	258	THR	-	linker	UNP P0AEX9
A	259	THR	-	linker	UNP P0AEX9
A	260	LEU	-	linker	UNP P0AEX9
A	261	GLU	-	linker	UNP P0AEX9
A	262	VAL	-	linker	UNP P0AEX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	linker	UNP P0AEX9
A	264	PHE	-	linker	UNP P0AEX9
A	265	GLN	-	linker	UNP P0AEX9
A	266	GLY	-	linker	UNP P0AEX9
A	267	PRO	-	linker	UNP P0AEX9
A	268	LEU	-	linker	UNP P0AEX9
A	269	GLY	-	linker	UNP P0AEX9
A	270	SER	-	linker	UNP P0AEX9
C	-127	MET	-	initiating methionine	UNP P0AEX9
C	-126	GLY	-	expression tag	UNP P0AEX9
C	-125	SER	-	expression tag	UNP P0AEX9
C	-124	SER	-	expression tag	UNP P0AEX9
C	-123	HIS	-	expression tag	UNP P0AEX9
C	-122	HIS	-	expression tag	UNP P0AEX9
C	-121	HIS	-	expression tag	UNP P0AEX9
C	-120	HIS	-	expression tag	UNP P0AEX9
C	-119	HIS	-	expression tag	UNP P0AEX9
C	-118	HIS	-	expression tag	UNP P0AEX9
C	-117	GLY	-	expression tag	UNP P0AEX9
C	-116	THR	-	expression tag	UNP P0AEX9
C	-115	LYS	-	expression tag	UNP P0AEX9
C	-114	THR	-	expression tag	UNP P0AEX9
C	251	GLY	-	linker	UNP P0AEX9
C	252	THR	-	linker	UNP P0AEX9
C	253	ASP	-	linker	UNP P0AEX9
C	254	TYR	-	linker	UNP P0AEX9
C	255	ASP	-	linker	UNP P0AEX9
C	256	ILE	-	linker	UNP P0AEX9
C	257	PRO	-	linker	UNP P0AEX9
C	258	THR	-	linker	UNP P0AEX9
C	259	THR	-	linker	UNP P0AEX9
C	260	LEU	-	linker	UNP P0AEX9
C	261	GLU	-	linker	UNP P0AEX9
C	262	VAL	-	linker	UNP P0AEX9
C	263	LEU	-	linker	UNP P0AEX9
C	264	PHE	-	linker	UNP P0AEX9
C	265	GLN	-	linker	UNP P0AEX9
C	266	GLY	-	linker	UNP P0AEX9
C	267	PRO	-	linker	UNP P0AEX9
C	268	LEU	-	linker	UNP P0AEX9
C	269	GLY	-	linker	UNP P0AEX9
C	270	SER	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Recombination activating gene 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		
2	D	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q1RLW7
B	-1	GLY	-	expression tag	UNP Q1RLW7
B	0	SER	-	expression tag	UNP Q1RLW7
D	-2	GLY	-	expression tag	UNP Q1RLW7
D	-1	GLY	-	expression tag	UNP Q1RLW7
D	0	SER	-	expression tag	UNP Q1RLW7

- Molecule 3 is a DNA chain called Forward strand of unmelted RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	34	Total	C	N	O	P	0	0
			696	331	125	206	34		

- Molecule 4 is a DNA chain called Reverse strand of unmelted RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	34	Total	C	N	O	P	0	0
			698	331	131	202	34		

- Molecule 5 is a DNA chain called Forward strand of melted RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	34	Total	C	N	O	P	0	0
			694	331	122	207	34		

- Molecule 6 is a DNA chain called Reverse strand of melted RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	34	Total	C	N	O	P	0	0
			700	332	133	201	34		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total 1	Zn 1	0
7	C	1	Total 1	Zn 1	0

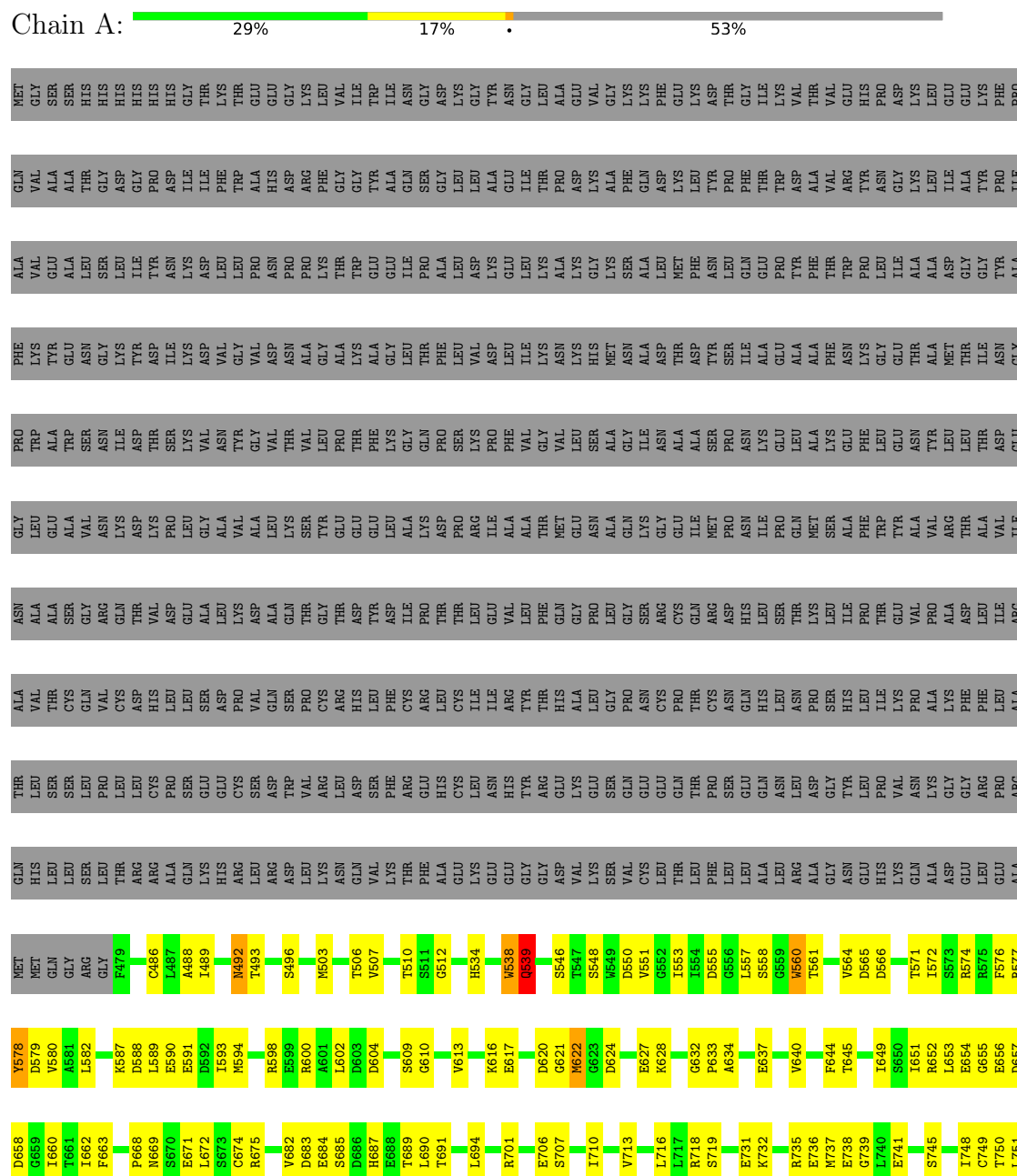
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

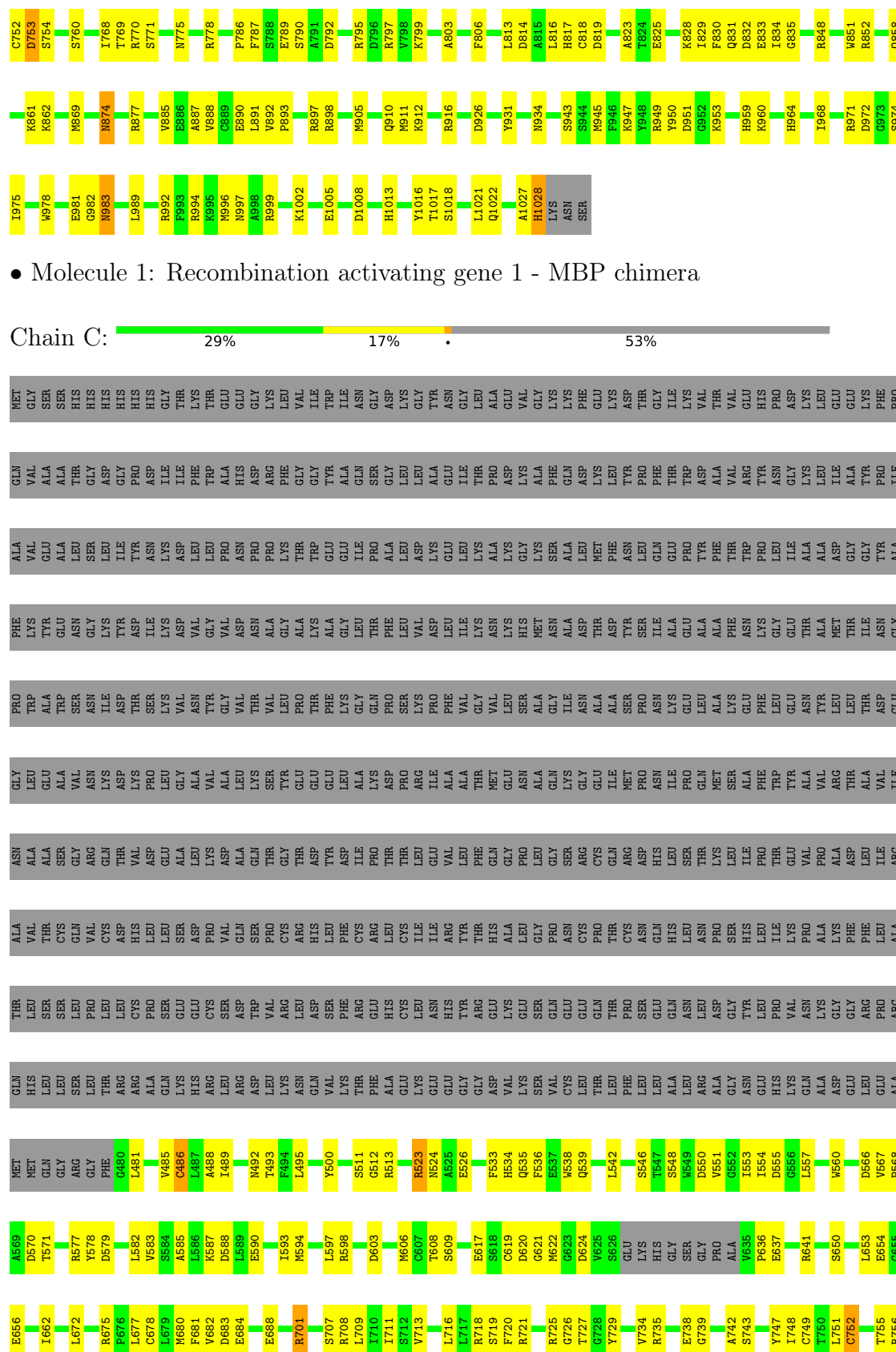
Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total 2	Ca 2	0
8	C	2	Total 2	Ca 2	0

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: Recombination activating gene 1 - MBP chimera





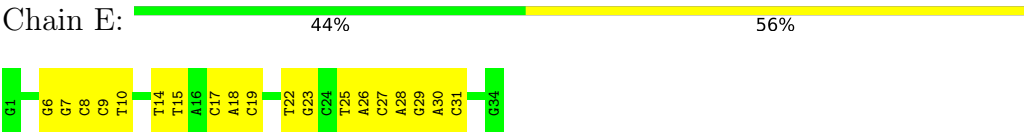


GLU
GLU
ASP
LEU
LEU
LEU
ASP
GLU
SER
GLN
THR
GLY
TYR
TRP
ILE
LYS
CYS
CYS
LEU
SER
CYS
GLN
VAL
ASP
PRO
ASN
ILE
TRP
GLU
PRO
TYR
TYR
SER
THR
LEU
THR
ARG
PRO
ALA
MET
ILE
PHE
CYS
SER
ARG
GLY
GLY
GLY
HIS
TRP
VAL
HIS
ALA
GLN
CYS
MET
LEU
PRO

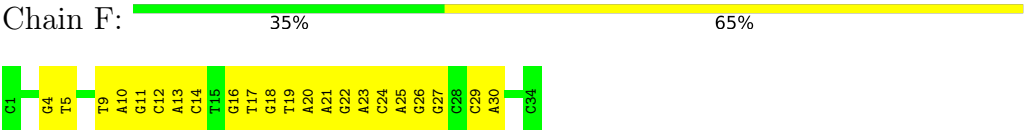
GLU
SER
LEU
LEU
LEU
GLN
SER
GLN
ASP
ASN
SER
LYS
TYR
PHE
CYS
LEU
ASP
HIS
GLY
LEU
PRO
LYS
GLN
GLU
MET
THR
PRO
PRO
LYS
GLN
MET
LEU
PRO
VAL
LYS
ARG
VAL
PRO
MET
LYS
MET
THR
HIS
ARG
LYS
ALA
PRO
VAL
SER
LEU
LYS
MET
THR
PRO
ALA
LYS
THR

PHE
LEU
ARG
ARG
PHE
ASP

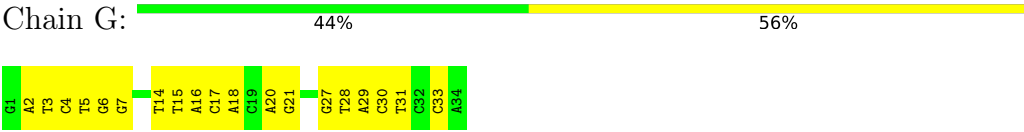
- Molecule 3: Forward strand of unmelted RSS substrate DNA



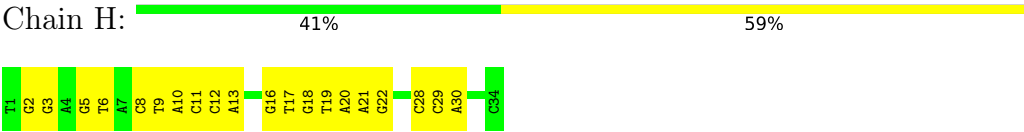
- Molecule 4: Reverse strand of unmelted RSS substrate DNA



- Molecule 5: Forward strand of melted RSS substrate DNA



- Molecule 6: Reverse strand of melted RSS substrate DNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69753	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0/4529	0.61	10/6100 (0.2%)
1	C	0.32	0/4469	0.75	7/6017 (0.1%)
2	B	0.27	0/2784	0.48	1/3784 (0.0%)
2	D	0.32	0/2784	0.52	2/3784 (0.1%)
3	E	0.57	0/779	0.96	0/1200
4	F	0.55	0/783	0.92	0/1206
5	G	0.59	0/776	0.97	0/1195
6	H	0.64	0/786	0.96	0/1211
All	All	0.38	0/17690	0.70	20/24497 (0.1%)

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
1	A	0	3
1	C	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	524	ASN	CB-CG-OD1	27.77	177.13	121.60
1	C	956	ASN	CB-CG-OD1	21.80	165.20	121.60
1	C	956	ASN	CB-CG-ND2	-17.20	75.42	116.70
1	C	524	ASN	CB-CG-ND2	-16.56	76.96	116.70
1	A	1028	HIS	N-CA-CB	-16.16	81.52	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1028	HIS	Sidechain
1	A	539	GLN	Sidechain
1	A	983	ASN	Sidechain
1	C	523	ARG	Peptide
2	D	33	GLN	Sidechain

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	4437	0	4373	168	0
1	C	4381	0	4327	161	0
2	B	2714	0	2665	104	0
2	D	2714	0	2663	132	0
3	E	696	0	384	17	0
4	F	698	0	382	19	0
5	G	694	0	385	29	0
6	H	700	0	382	21	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	2	0	0	0	0
8	C	2	0	0	0	0
All	All	17040	0	15561	615	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 19.

The worst 5 of 615 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:C:774:GLU:OE2	1:C:778:ARG:NH1	1.81	1.14
2:D:338:THR:HG22	2:D:340:PRO:HA	1.41	1.03
1:A:628:LYS:NZ	4:F:17:DT:OP1	1.94	1.00
1:A:539:GLN:OE1	1:A:710:ILE:HG13	1.64	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:283:LYS:NZ	2:D:314:SER:O	1.98	0.97

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	548/1159 (47%)	499 (91%)	47 (9%)	2 (0%)	36	76
1	C	538/1159 (46%)	496 (92%)	42 (8%)	0	100	100
2	B	349/533 (66%)	325 (93%)	24 (7%)	0	100	100
2	D	349/533 (66%)	321 (92%)	28 (8%)	0	100	100
All	All	1784/3384 (53%)	1641 (92%)	141 (8%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	CYS
1	A	512	GLY

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	489/1000 (49%)	469 (96%)	20 (4%)	33	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	484/1000 (48%)	462 (96%)	22 (4%)	30	62
2	B	303/465 (65%)	291 (96%)	12 (4%)	34	64
2	D	303/465 (65%)	290 (96%)	13 (4%)	32	63
All	All	1579/2930 (54%)	1512 (96%)	67 (4%)	37	64

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	336	ASN
1	C	678	CYS
2	D	212	ARG
2	B	341	GLU
1	C	526	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	524	ASN
2	D	33	GLN
1	C	858	GLN
2	B	173	ASN
1	C	822	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.