



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:01 AM UTC

PDB ID : 9BBN / pdb_00009bbn
EMDB ID : EMD-44423
Title : Cryo-EM structure of Chikungunya virus asymmetric unit with Fab C9
Authors : Su, G.C.; Galaz-Montoya, J.G.; Pintilie, G.; Jin, J.; Chiu, W.
Deposited on : 2024-04-06
Resolution : 3.30 Å(reported)
Based on initial model : 8FCG

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

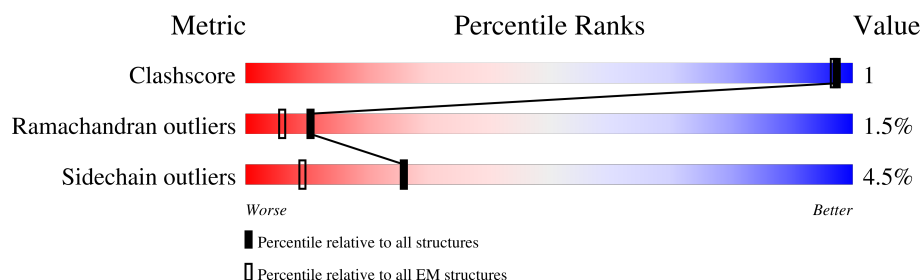
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 of 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	U	60	83% 17%
1	V	60	93% 7%
1	W	60	90% 10%
1	X	60	85% 13% .
2	A	439	95% 5%
2	B	439	93% 6%
2	C	439	93% 6% .
2	D	439	95% 5%
3	E	419	94% 5% .

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Mol	Chain	Length	Quality of chain
3	F	419	 94% 6%
3	G	419	 92% 7% .
3	H	419	 93% 6% .
4	M	234	 87% 10% ..
4	O	234	 88% 9% .
4	Q	234	 88% 9% .
4	S	234	 90% 8% .
5	N	212	 88% 10% .
5	P	212	 86% 12% .
5	R	212	 92% 7% .
5	T	212	 91% 9%
6	I	151	 89% 10% .
6	J	151	 95% . .
6	K	151	 98% ..
6	L	151	 94% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 92155 atoms, of which 45663 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 E3 glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	U	60	Total	C	H	N	O	S	0	0
			950	297	470	84	90	9		
1	W	60	Total	C	H	N	O	S	0	0
			950	297	470	84	90	9		
1	X	60	Total	C	H	N	O	S	0	0
			950	297	470	84	90	9		
1	V	60	Total	C	H	N	O	S	0	0
			950	297	470	84	90	9		

- Molecule 2 is a protein called E1 glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	439	Total	C	H	N	O	S	0	0
			6592	2106	3265	556	638	27		
2	A	439	Total	C	H	N	O	S	0	0
			6591	2106	3264	556	638	27		
2	B	439	Total	C	H	N	O	S	0	0
			6591	2106	3264	556	638	27		
2	D	439	Total	C	H	N	O	S	0	0
			6593	2106	3266	556	638	27		

- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	419	Total	C	H	N	O	S	0	0
			6540	2067	3245	592	608	28		
3	E	419	Total	C	H	N	O	S	0	0
			6544	2067	3249	592	608	28		
3	F	419	Total	C	H	N	O	S	0	0
			6537	2067	3242	592	608	28		
3	H	419	Total	C	H	N	O	S	0	0
			6545	2067	3250	592	608	28		

- Molecule 4 is a protein called Heavy chain of C9.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	M	234	Total	C	H	N	O	S	0	0
			3450	1100	1709	287	347	7		
4	O	234	Total	C	H	N	O	S	0	0
			3450	1100	1709	287	347	7		
4	Q	234	Total	C	H	N	O	S	0	0
			3449	1100	1708	287	347	7		
4	S	234	Total	C	H	N	O	S	0	0
			3450	1100	1709	287	347	7		

- Molecule 5 is a protein called Light chain of C9.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	N	212	Total	C	H	N	O	S	0	0
			3211	1017	1587	276	327	4		
5	P	212	Total	C	H	N	O	S	0	0
			3207	1017	1583	276	327	4		
5	R	212	Total	C	H	N	O	S	0	0
			3213	1017	1589	276	327	4		
5	T	212	Total	C	H	N	O	S	0	0
			3212	1017	1588	276	327	4		


- Molecule 6 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	151	Total	C	H	N	O	S	0	0
			2295	730	1139	204	217	5		
6	K	151	Total	C	H	N	O	S	0	0
			2297	730	1141	204	217	5		
6	I	151	Total	C	H	N	O	S	0	0
			2294	730	1138	204	217	5		
6	L	151	Total	C	H	N	O	S	0	0
			2294	730	1138	204	217	5		

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. 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: E3 glycoprotein

Chain U:  83% 17%




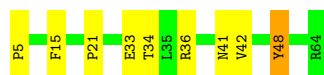
- Molecule 1: E3 glycoprotein

Chain W:  90% 10%



- Molecule 1: E3 glycoprotein

Chain X:  85% 13% .



- Molecule 1: E3 glycoprotein

Chain V:  93% 7%



- Molecule 2: E1 glycoprotein

Chain C:  93% 6% .



- Molecule 2: E1 glycoprotein

Chain A:  95% 5%



- Molecule 2: E1 glycoprotein

Chain B: 93% 6%



- Molecule 2: E1 glycoprotein

Chain D: 95% 5%



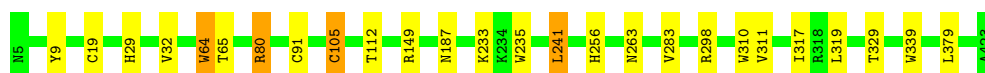
- Molecule 3: E2 glycoprotein

Chain G: 92% 7%



- Molecule 3: E2 glycoprotein

Chain E: 94% 5%



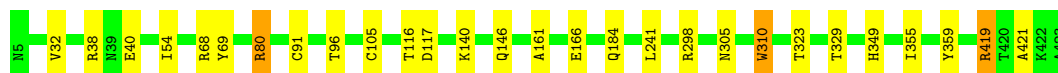
- Molecule 3: E2 glycoprotein

Chain F: 94% 6%




- Molecule 3: E2 glycoprotein

Chain H: 93% 6%




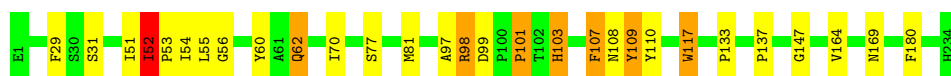
- Molecule 4: Heavy chain of C9

Chain M:  87% 10% ..




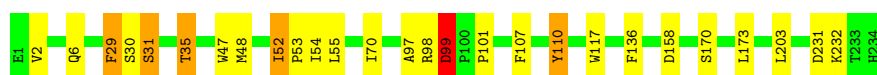
- Molecule 4: Heavy chain of C9

Chain O:  88% 9% .




- Molecule 4: Heavy chain of C9

Chain Q:  88% 9% .




- Molecule 4: Heavy chain of C9

Chain S:  90% 8% .




- Molecule 5: Light chain of C9

Chain N:  88% 10% .



- Molecule 5: Light chain of C9

Chain P:  86% 12% .




- Molecule 5: Light chain of C9

Chain R:  92% 7% .



- Molecule 5: Light chain of C9

Chain T:  91% 9%



- Molecule 6: Capsid protein

Chain J:  95% . .




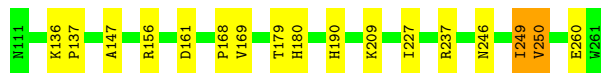
- Molecule 6: Capsid protein

Chain K:  98% ..



- Molecule 6: Capsid protein

Chain I:  89% 10% .



- Molecule 6: Capsid protein

Chain L:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1151475	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	106000	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	U	0.92	0/492	1.58	8/667 (1.2%)
1	V	0.90	0/492	1.50	2/667 (0.3%)
1	W	0.91	0/492	1.48	1/667 (0.1%)
1	X	0.88	0/492	1.49	3/667 (0.4%)
2	A	0.72	0/3409	1.30	7/4651 (0.2%)
2	B	0.71	0/3409	1.28	6/4651 (0.1%)
2	C	0.71	0/3409	1.29	7/4651 (0.2%)
2	D	0.70	0/3409	1.27	4/4651 (0.1%)
3	E	0.80	0/3382	1.39	6/4606 (0.1%)
3	F	0.79	0/3382	1.34	4/4606 (0.1%)
3	G	0.78	0/3382	1.37	6/4606 (0.1%)
3	H	0.79	0/3382	1.36	8/4606 (0.2%)
4	M	0.90	0/1785	1.49	9/2433 (0.4%)
4	O	0.89	0/1785	1.48	10/2433 (0.4%)
4	Q	0.90	0/1785	1.51	10/2433 (0.4%)
4	S	0.92	0/1785	1.49	7/2433 (0.3%)
5	N	0.89	1/1660 (0.1%)	1.47	8/2255 (0.4%)
5	P	0.88	1/1660 (0.1%)	1.44	3/2255 (0.1%)
5	R	0.91	0/1660	1.46	5/2255 (0.2%)
5	T	0.89	0/1660	1.43	4/2255 (0.2%)
6	I	0.87	0/1184	1.45	5/1599 (0.3%)
6	J	0.78	0/1184	1.33	1/1599 (0.1%)
6	K	0.82	0/1184	1.34	2/1599 (0.1%)
6	L	0.80	0/1184	1.33	1/1599 (0.1%)
All	All	0.81	2/47648 (0.0%)	1.38	127/64844 (0.2%)

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	V	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1
2	A	0	4
2	B	0	3
2	C	0	2
3	E	0	2
3	F	0	2
3	G	0	2
3	H	0	2
4	M	0	2
4	O	0	3
4	Q	0	1
4	S	0	1
5	N	0	2
5	T	0	1
6	J	0	1
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	118	PRO	CA-C	5.98	1.55	1.51
5	N	118	PRO	CA-C	5.18	1.55	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	52	ILE	CA-CB-CG1	11.81	130.49	110.40
4	Q	29	PHE	N-CA-C	10.05	125.40	112.34
4	S	35	THR	N-CA-C	9.80	123.74	109.14
3	E	105	CYS	N-CA-C	9.77	117.01	108.22
4	Q	99	ASP	CA-CB-CG	9.54	122.14	112.60
4	Q	35	THR	N-CA-C	9.34	123.08	108.79
4	M	99	ASP	CA-CB-CG	9.26	121.86	112.60
4	S	117	TRP	N-CA-C	8.90	123.66	110.48
4	S	55	LEU	N-CA-C	8.81	125.36	112.94
4	O	31	SER	N-CA-C	8.42	122.11	110.24
4	Q	117	TRP	N-CA-C	8.01	120.56	109.18
4	S	31	SER	N-CA-C	7.78	121.68	110.24
4	O	99	ASP	CA-CB-CG	7.58	120.18	112.60
4	M	60	TYR	N-CA-C	7.41	121.33	110.59
4	O	107	PHE	CA-CB-CG	7.29	121.09	113.80
2	D	134	ARG	NE-CZ-NH2	7.29	125.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	99	ASP	N-CA-C	7.09	125.48	109.81
2	A	134	ARG	NE-CZ-NH2	7.04	125.54	119.20
1	V	5	PRO	CA-N-CD	-6.97	102.25	112.00
2	C	134	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	W	5	PRO	CA-N-CD	-6.76	102.54	112.00
3	F	298	ARG	NE-CZ-NH2	6.74	125.27	119.20
2	C	394	HIS	CA-CB-CG	6.60	120.40	113.80
4	Q	107	PHE	CA-CB-CG	6.55	120.35	113.80
1	X	5	PRO	CA-N-CD	-6.50	102.90	112.00
2	B	134	ARG	NE-CZ-NH2	6.49	125.04	119.20
2	A	398	GLY	CA-C-N	6.49	133.65	121.97
2	A	398	GLY	C-N-CA	6.49	133.65	121.97
5	T	181	SER	N-CA-C	6.35	118.07	110.19
4	O	117	TRP	N-CA-C	6.31	120.33	108.65
4	S	35	THR	CA-CB-CG2	6.30	121.20	110.50
5	R	31	TYR	N-CA-C	6.20	118.55	110.43
4	O	103	HIS	CB-CG-CD2	-6.11	123.26	131.20
3	G	72	ASN	CA-CB-CG	6.07	118.67	112.60
2	A	123	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	V	36	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	U	14	THR	CA-C-N	5.90	128.87	120.49
1	U	14	THR	C-N-CA	5.90	128.87	120.49
5	P	169	ASP	CA-CB-CG	5.90	118.50	112.60
3	H	298	ARG	NE-CZ-NH2	5.88	124.50	119.20
2	C	308	HIS	CB-CG-CD2	-5.83	123.61	131.20
4	Q	31	SER	N-CA-C	5.83	117.94	109.07
4	Q	35	THR	CA-CB-CG2	5.83	120.42	110.50
5	R	60	ARG	NE-CZ-NH2	5.79	124.41	119.20
4	O	98	ARG	NE-CZ-NH2	5.78	124.40	119.20
2	D	123	ARG	NE-CZ-NH2	5.76	124.39	119.20
5	R	97	PHE	CA-CB-CG	5.75	119.56	113.80
3	E	241	LEU	CB-CA-C	5.75	120.73	111.36
3	E	298	ARG	NE-CZ-NH2	5.74	124.36	119.20
4	M	38	ARG	NE-CZ-NH2	5.72	124.35	119.20
5	P	137	ASN	CA-CB-CG	5.69	118.29	112.60
5	N	171	THR	CA-C-N	5.68	132.40	121.54
5	N	171	THR	C-N-CA	5.68	132.40	121.54
5	N	181	SER	N-CA-C	5.66	117.14	110.97
3	G	119	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	U	64	ARG	NE-CZ-NH2	5.62	124.26	119.20
4	O	147	GLY	N-CA-C	5.61	117.28	111.95
4	Q	52	ILE	CA-C-N	5.60	126.84	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	52	ILE	C-N-CA	5.60	126.84	119.84
3	H	117	ASP	CA-CB-CG	5.57	118.17	112.60
6	I	156	ARG	NE-CZ-NH2	5.55	124.19	119.20
4	M	178	HIS	CA-CB-CG	5.54	119.34	113.80
6	I	246	ASN	N-CA-C	5.52	119.32	112.47
4	M	111	TYR	N-CA-C	5.51	117.64	110.53
3	G	298	ARG	NE-CZ-NH2	5.51	124.16	119.20
5	T	96	THR	N-CA-C	5.49	117.84	108.67
1	X	36	ARG	NE-CZ-NH2	5.47	124.13	119.20
3	E	256	HIS	CB-CG-CD2	-5.47	124.08	131.20
4	M	110	TYR	N-CA-C	5.46	117.27	109.14
2	C	398	GLY	CA-C-N	5.43	131.74	121.97
2	C	398	GLY	C-N-CA	5.43	131.74	121.97
2	A	404	VAL	CB-CA-C	-5.39	104.28	111.13
6	K	156	ARG	NE-CZ-NH2	5.38	124.05	119.20
5	N	90	TYR	N-CA-C	5.38	122.26	110.80
6	I	136	LYS	CA-C-N	5.38	126.56	119.84
6	I	136	LYS	C-N-CA	5.38	126.56	119.84
1	U	5	PRO	CA-N-CD	-5.35	104.51	112.00
5	N	118	PRO	N-CA-CB	5.35	106.00	103.22
5	N	30	ASN	CA-CB-CG	5.35	117.95	112.60
4	O	62	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	B	212	ASP	CA-CB-CG	5.31	117.91	112.60
1	U	19	GLN	OE1-CD-NE2	-5.30	117.30	122.60
3	E	149	ARG	NE-CZ-NH2	5.28	123.95	119.20
6	L	156	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	G	117	ASP	CA-CB-CG	5.28	117.88	112.60
5	T	60	ARG	NE-CZ-NH2	5.27	123.95	119.20
2	B	204	GLN	OE1-CD-NE2	-5.27	117.33	122.60
3	F	244	ARG	NE-CZ-NH2	5.25	123.93	119.20
5	R	107	ARG	NE-CZ-NH2	5.25	123.93	119.20
3	G	13	ARG	CB-CA-C	5.23	117.17	109.22
3	E	29	HIS	CB-CG-CD2	-5.22	124.42	131.20
6	K	223	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	G	251	ARG	NE-CZ-NH2	5.22	123.90	119.20
2	C	308	HIS	CA-CB-CG	5.21	119.01	113.80
5	T	197	HIS	CB-CG-CD2	-5.19	124.45	131.20
4	S	100	PRO	N-CA-C	5.19	117.03	110.70
1	U	34	THR	CA-C-N	5.17	127.46	120.38
1	U	34	THR	C-N-CA	5.17	127.46	120.38
4	M	99	ASP	N-CA-C	5.17	121.23	109.81
5	R	89	GLN	OE1-CD-NE2	-5.17	117.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	204	GLN	OE1-CD-NE2	-5.16	117.44	122.60
3	F	408	VAL	N-CA-C	5.14	114.61	108.96
2	A	266	VAL	N-CA-CB	5.13	116.62	110.31
2	B	125	HIS	CB-CG-CD2	-5.12	124.54	131.20
2	C	204	GLN	OE1-CD-NE2	-5.12	117.48	122.60
3	H	68	ARG	N-CA-C	5.12	119.26	112.30
3	H	419	ARG	NE-CZ-NH2	5.11	123.80	119.20
3	F	149	ARG	NE-CZ-NH2	5.11	123.80	119.20
6	I	190	HIS	CB-CG-CD2	-5.10	124.56	131.20
5	P	210	ARG	NE-CZ-NH2	5.10	123.79	119.20
6	J	223	ARG	NE-CZ-NH2	5.10	123.79	119.20
3	H	38	ARG	NE-CZ-NH2	5.09	123.78	119.20
5	N	117	PHE	CA-C-N	5.05	123.30	119.66
5	N	117	PHE	C-N-CA	5.05	123.30	119.66
4	S	138	LEU	N-CA-C	5.05	116.86	111.36
3	H	116	THR	CA-C-N	5.05	128.37	120.75
3	H	116	THR	C-N-CA	5.05	128.37	120.75
4	M	157	LYS	CA-C-N	5.04	129.30	122.19
4	M	157	LYS	C-N-CA	5.04	129.30	122.19
3	H	146	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	U	36	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	X	48	TYR	CB-CA-C	5.03	118.50	110.09
4	Q	98	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	B	303	VAL	CA-C-N	5.00	124.44	119.24
2	B	303	VAL	C-N-CA	5.00	124.44	119.24
2	D	398	GLY	CA-C-N	5.00	130.97	121.97
2	D	398	GLY	C-N-CA	5.00	130.97	121.97

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	206	ARG	Sidechain
2	A	223	ARG	Sidechain
2	A	242	TYR	Sidechain
2	A	247	ARG	Sidechain
2	B	206	ARG	Sidechain
2	B	242	TYR	Sidechain
2	B	247	ARG	Sidechain
2	C	247	ARG	Sidechain
2	C	308	HIS	Sidechain
3	E	80	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	E	9	TYR	Sidechain
3	F	199	TYR	Sidechain
3	F	359	TYR	Sidechain
3	G	244	ARG	Sidechain
3	G	358	TYR	Sidechain
3	H	359	TYR	Sidechain
3	H	80	ARG	Sidechain
6	J	160	TYR	Sidechain
4	M	109	TYR	Sidechain
4	M	110	TYR	Sidechain
5	N	172	TYR	Sidechain
5	N	191	TYR	Sidechain
4	O	109	TYR	Sidechain
4	O	110	TYR	Sidechain
4	O	60	TYR	Sidechain
4	Q	110	TYR	Sidechain
4	S	109	TYR	Sidechain
5	T	90	TYR	Sidechain
1	V	27	TYR	Sidechain
1	V	47	TYR	Sidechain
1	X	48	TYR	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	U	480	470	468	0	0
1	V	480	470	468	0	0
1	W	480	470	468	0	0
1	X	480	470	468	1	0
2	A	3327	3264	3264	0	0
2	B	3327	3264	3264	5	0
2	C	3327	3265	3264	5	0
2	D	3327	3266	3264	4	0
3	E	3295	3249	3245	3	0
3	F	3295	3242	3245	4	0
3	G	3295	3245	3245	8	0
3	H	3295	3250	3245	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	1741	1709	1707	7	0
4	O	1741	1709	1707	5	0
4	Q	1741	1708	1707	5	0
4	S	1741	1709	1707	4	0
5	N	1624	1587	1587	1	0
5	P	1624	1583	1587	5	0
5	R	1624	1589	1587	2	0
5	T	1624	1588	1587	0	0
6	I	1156	1138	1135	1	0
6	J	1156	1139	1135	0	0
6	K	1156	1141	1135	0	0
6	L	1156	1138	1135	0	0
All	All	46492	45663	45624	56	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 1.

All (56) 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)
5:P:93:SER:OG	5:P:94:PRO:HD2	1.96	0.64
4:O:97:ALA:O	4:O:117:TRP:HA	1.97	0.64
3:G:91:CYS:HG	3:G:105:CYS:HG	1.46	0.63
4:Q:47:TRP:CG	4:Q:48:MET:H	2.19	0.60
3:G:64:TRP:CG	4:M:110:TYR:HH	2.19	0.60
4:M:55:LEU:HA	4:M:74:LYS:HB3	1.85	0.58
4:O:52:ILE:HB	4:O:53:PRO:CD	2.34	0.56
4:O:52:ILE:HB	4:O:53:PRO:HD2	1.87	0.56
3:E:64:TRP:CG	4:Q:110:TYR:HH	2.24	0.56
3:H:91:CYS:SG	3:H:105:CYS:HB3	2.48	0.54
4:S:36:TRP:CD1	4:S:51:ILE:HG21	2.44	0.52
5:R:83:ALA:HB3	5:R:85:TYR:CE1	2.45	0.52
2:D:361:ALA:HB3	2:D:404:VAL:CG1	2.40	0.51
3:E:91:CYS:SG	3:E:105:CYS:CB	2.99	0.51
3:E:91:CYS:SG	3:E:105:CYS:HB3	2.51	0.50
5:P:78:ALA:HB3	5:P:79:PRO:HD3	1.93	0.50
6:I:249:ILE:HG22	6:I:250:VAL:H	1.77	0.49
3:G:54:ILE:HD11	3:G:80:ARG:CD	2.43	0.48
2:B:387:ILE:HD11	3:F:278:TYR:CE1	2.49	0.48
4:S:139:ALA:HB3	4:S:140:PRO:HD3	1.97	0.47
2:C:49:CYS:HG	2:C:114:CYS:HG	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:112:GLU:H	2:C:112:GLU:CD	2.24	0.46
3:G:12:ILE:HG22	3:G:235:TRP:HB2	1.98	0.46
3:G:54:ILE:HD11	3:G:80:ARG:HD3	1.97	0.46
4:M:55:LEU:HA	4:M:74:LYS:CB	2.45	0.45
4:M:52:ILE:HB	4:M:53:PRO:CD	2.46	0.45
4:M:157:LYS:HE2	5:N:177:THR:HG21	1.98	0.45
2:C:387:ILE:C	2:C:387:ILE:HD12	2.42	0.45
4:M:99:ASP:HA	4:M:116:VAL:HG13	1.98	0.45
3:F:153:CYS:SG	3:F:266:CYS:HB2	2.58	0.44
4:Q:101:PRO:HB3	5:R:90:TYR:CD1	2.53	0.44
4:S:51:ILE:HG23	4:S:54:ILE:CG2	2.48	0.43
3:F:419:ARG:HG2	3:F:420:THR:H	1.83	0.43
4:Q:47:TRP:CD1	4:Q:48:MET:H	2.37	0.43
3:G:34:LEU:HD23	3:G:34:LEU:H	1.84	0.42
3:H:91:CYS:SG	3:H:105:CYS:CB	3.07	0.42
2:B:259:CYS:HB3	2:B:271:CYS:SG	2.60	0.42
2:D:176:LYS:HE3	2:D:189:TYR:CE1	2.54	0.42
2:C:387:ILE:HD11	3:G:278:TYR:CE1	2.55	0.42
3:H:140:LYS:HE3	3:H:310:TRP:CE2	2.55	0.42
2:C:369:VAL:HG12	2:C:370:CYS:H	1.85	0.42
4:Q:47:TRP:CG	4:Q:48:MET:N	2.87	0.41
2:B:387:ILE:C	2:B:387:ILE:HD12	2.45	0.41
4:O:51:ILE:CD1	4:O:81:MET:HG2	2.51	0.41
5:P:105:ILE:HD13	5:P:105:ILE:H	1.84	0.41
2:D:49:CYS:HB2	2:D:114:CYS:HG	1.85	0.41
4:S:25:PHE:CG	4:S:26:GLY:N	2.88	0.41
5:P:138:PHE:CE2	5:P:172:TYR:HB2	2.55	0.41
3:G:64:TRP:CD1	4:M:110:TYR:HH	2.38	0.41
2:B:187:MET:HE1	2:B:243:TRP:HE1	1.86	0.41
2:B:328:CYS:SG	2:B:370:CYS:HB2	2.61	0.41
3:F:19:CYS:HG	3:F:125:CYS:HG	1.60	0.41
2:D:361:ALA:HB3	2:D:404:VAL:HG11	2.03	0.40
4:O:108:ASN:C	4:O:109:TYR:CD1	3.00	0.40
5:P:174:LEU:C	5:P:174:LEU:HD12	2.46	0.40
1:X:15:PHE:CG	1:X:21:PRO:HD3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	U	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	18
1	V	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
1	W	58/60 (97%)	49 (84%)	6 (10%)	3 (5%)	1	11
1	X	58/60 (97%)	55 (95%)	2 (3%)	1 (2%)	7	30
2	A	437/439 (100%)	413 (94%)	23 (5%)	1 (0%)	43	71
2	B	437/439 (100%)	418 (96%)	18 (4%)	1 (0%)	43	71
2	C	437/439 (100%)	405 (93%)	30 (7%)	2 (0%)	24	55
2	D	437/439 (100%)	409 (94%)	25 (6%)	3 (1%)	18	49
3	E	417/419 (100%)	379 (91%)	38 (9%)	0	100	100
3	F	417/419 (100%)	383 (92%)	31 (7%)	3 (1%)	18	49
3	G	417/419 (100%)	385 (92%)	28 (7%)	4 (1%)	12	40
3	H	417/419 (100%)	387 (93%)	26 (6%)	4 (1%)	12	40
4	M	232/234 (99%)	196 (84%)	30 (13%)	6 (3%)	4	23
4	O	232/234 (99%)	195 (84%)	30 (13%)	7 (3%)	3	20
4	Q	232/234 (99%)	188 (81%)	35 (15%)	9 (4%)	2	16
4	S	232/234 (99%)	197 (85%)	29 (12%)	6 (3%)	4	23
5	N	210/212 (99%)	170 (81%)	30 (14%)	10 (5%)	2	12
5	P	210/212 (99%)	164 (78%)	37 (18%)	9 (4%)	2	14
5	R	210/212 (99%)	174 (83%)	33 (16%)	3 (1%)	9	33
5	T	210/212 (99%)	167 (80%)	37 (18%)	6 (3%)	3	21
6	I	149/151 (99%)	122 (82%)	20 (13%)	7 (5%)	2	12
6	J	149/151 (99%)	133 (89%)	12 (8%)	4 (3%)	4	22
6	K	149/151 (99%)	140 (94%)	8 (5%)	1 (1%)	18	49
6	L	149/151 (99%)	144 (97%)	4 (3%)	1 (1%)	18	49
All	All	6012/6060 (99%)	5376 (89%)	543 (9%)	93 (2%)	11	32

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	60	ASP
4	M	52	ILE
4	M	55	LEU
4	M	136	PHE
4	O	52	ILE
4	O	137	PRO
4	Q	99	ASP
4	Q	136	PHE
6	I	249	ILE
4	S	136	PHE
3	H	69	TYR
3	H	161	ALA
3	G	185	SER
3	G	419	ARG
5	N	172	TYR
2	B	370	CYS
4	O	101	PRO
5	P	79	PRO
5	P	91	GLY
5	P	119	PRO
3	F	185	SER
6	J	247	LYS
4	Q	2	VAL
4	Q	97	ALA
6	I	169	VAL
2	D	370	CYS
4	S	52	ILE
5	T	3	VAL
5	T	184	ASP
1	U	24	PRO
2	C	266	VAL
2	A	399	VAL
5	N	2	ILE
5	N	3	VAL
5	N	80	GLU
4	O	55	LEU
5	P	78	ALA
5	P	166	ASP
6	J	205	THR
4	Q	30	SER
4	Q	53	PRO
5	R	76	ARG

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Mol	Chain	Res	Type
4	S	54	ILE
5	T	141	ARG
6	L	247	LYS
1	W	17	CYS
1	W	32	GLU
3	G	72	ASN
4	M	56	GLY
5	P	167	SER
5	P	181	SER
6	K	247	LYS
4	Q	231	ASP
5	R	157	ASN
3	H	419	ARG
1	U	26	CYS
1	W	11	ALA
1	X	42	VAL
5	N	79	PRO
5	N	119	PRO
5	N	137	ASN
4	O	56	GLY
4	O	77	SER
4	O	133	PRO
5	P	3	VAL
5	P	29	ASN
3	F	72	ASN
3	F	419	ARG
4	Q	158	ASP
5	R	2	ILE
6	I	147	ALA
6	I	161	ASP
6	I	168	PRO
6	I	180	HIS
2	D	152	HIS
2	D	399	VAL
5	T	59	ASP
3	H	421	ALA
2	C	399	VAL
4	M	77	SER
5	N	51	SER
5	N	170	SER
5	N	182	LYS
4	Q	170	SER

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Mol	Chain	Res	Type
4	S	2	VAL
4	S	25	PHE
6	J	131	GLY
5	T	16	GLY
4	M	101	PRO
6	J	123	VAL
6	I	137	PRO
4	S	99	ASP
5	T	2	ILE

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	U	57/57 (100%)	55 (96%)	2 (4%)	32	58
1	V	57/57 (100%)	57 (100%)	0	100	100
1	W	57/57 (100%)	55 (96%)	2 (4%)	32	58
1	X	57/57 (100%)	54 (95%)	3 (5%)	20	49
2	A	369/369 (100%)	354 (96%)	15 (4%)	27	55
2	B	369/369 (100%)	354 (96%)	15 (4%)	27	55
2	C	369/369 (100%)	351 (95%)	18 (5%)	22	51
2	D	369/369 (100%)	361 (98%)	8 (2%)	45	66
3	E	369/369 (100%)	350 (95%)	19 (5%)	21	50
3	F	369/369 (100%)	358 (97%)	11 (3%)	36	61
3	G	369/369 (100%)	351 (95%)	18 (5%)	22	51
3	H	369/369 (100%)	355 (96%)	14 (4%)	29	57
4	M	195/195 (100%)	180 (92%)	15 (8%)	12	37
4	O	195/195 (100%)	183 (94%)	12 (6%)	16	45
4	Q	195/195 (100%)	183 (94%)	12 (6%)	16	45
4	S	195/195 (100%)	184 (94%)	11 (6%)	19	47
5	N	182/182 (100%)	173 (95%)	9 (5%)	22	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	182/182 (100%)	170 (93%)	12 (7%)	15	43
5	R	182/182 (100%)	172 (94%)	10 (6%)	19	48
5	T	182/182 (100%)	174 (96%)	8 (4%)	25	54
6	I	120/120 (100%)	114 (95%)	6 (5%)	22	50
6	J	120/120 (100%)	118 (98%)	2 (2%)	53	71
6	K	120/120 (100%)	119 (99%)	1 (1%)	73	79
6	L	120/120 (100%)	113 (94%)	7 (6%)	18	47
All	All	5168/5168 (100%)	4938 (96%)	230 (4%)	26	53

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	8	CYS
1	U	47	TYR
1	W	52	GLN
1	W	62	GLN
1	X	33	GLU
1	X	34	THR
1	X	41	ASN
2	C	47	ILE
2	C	60	VAL
2	C	108	VAL
2	C	112	GLU
2	C	136	LEU
2	C	163	VAL
2	C	177	ILE
2	C	179	VAL
2	C	184	VAL
2	C	212	ASP
2	C	266	VAL
2	C	267	ARG
2	C	280	ILE
2	C	333	MET
2	C	387	ILE
2	C	402	ILE
2	C	404	VAL
2	C	407	MET
3	G	32	VAL
3	G	57	LYS
3	G	64	TRP

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Mol	Chain	Res	Type
3	G	65	THR
3	G	85	VAL
3	G	110	THR
3	G	193	ASN
3	G	241	LEU
3	G	251	ARG
3	G	263	ASN
3	G	311	VAL
3	G	314	LYS
3	G	323	THR
3	G	329	THR
3	G	334	GLU
3	G	355	ILE
3	G	419	ARG
3	G	422	LYS
2	A	47	ILE
2	A	108	VAL
2	A	177	ILE
2	A	178	VAL
2	A	179	VAL
2	A	184	VAL
2	A	266	VAL
2	A	267	ARG
2	A	280	ILE
2	A	339	ILE
2	A	341	GLU
2	A	387	ILE
2	A	404	VAL
2	A	407	MET
2	A	434	VAL
3	E	19	CYS
3	E	32	VAL
3	E	64	TRP
3	E	65	THR
3	E	80	ARG
3	E	112	THR
3	E	187	ASN
3	E	233	LYS
3	E	235	TRP
3	E	241	LEU
3	E	263	ASN
3	E	283	VAL

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Mol	Chain	Res	Type
3	E	310	TRP
3	E	311	VAL
3	E	317	ILE
3	E	319	LEU
3	E	329	THR
3	E	339	TRP
3	E	379	LEU
4	M	18	VAL
4	M	20	VAL
4	M	29	PHE
4	M	47	TRP
4	M	54	ILE
4	M	57	THR
4	M	70	ILE
4	M	74	LYS
4	M	83	LEU
4	M	87	ARG
4	M	98	ARG
4	M	99	ASP
4	M	119	GLN
4	M	192	LEU
4	M	232	LYS
5	N	14	SER
5	N	47	ILE
5	N	57	ILE
5	N	76	ARG
5	N	77	LEU
5	N	90	TYR
5	N	105	ILE
5	N	119	PRO
5	N	123	GLN
2	B	16	LYS
2	B	47	ILE
2	B	60	VAL
2	B	108	VAL
2	B	177	ILE
2	B	179	VAL
2	B	184	VAL
2	B	266	VAL
2	B	267	ARG
2	B	280	ILE
2	B	299	MET

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Mol	Chain	Res	Type
2	B	341	GLU
2	B	387	ILE
2	B	402	ILE
2	B	407	MET
4	O	29	PHE
4	O	52	ILE
4	O	54	ILE
4	O	62	GLN
4	O	70	ILE
4	O	98	ARG
4	O	101	PRO
4	O	103	HIS
4	O	107	PHE
4	O	164	VAL
4	O	169	ASN
4	O	180	PHE
5	P	2	ILE
5	P	24	ARG
5	P	31	TYR
5	P	72	LEU
5	P	76	ARG
5	P	89	GLN
5	P	90	TYR
5	P	105	ILE
5	P	159	GLN
5	P	171	THR
5	P	174	LEU
5	P	186	GLU
3	F	32	VAL
3	F	54	ILE
3	F	64	TRP
3	F	80	ARG
3	F	85	VAL
3	F	167	ILE
3	F	241	LEU
3	F	257	ILE
3	F	323	THR
3	F	349	HIS
3	F	419	ARG
6	J	213	SER
6	J	223	ARG
6	K	223	ARG

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Mol	Chain	Res	Type
4	Q	6	GLN
4	Q	29	PHE
4	Q	31	SER
4	Q	35	THR
4	Q	52	ILE
4	Q	54	ILE
4	Q	55	LEU
4	Q	70	ILE
4	Q	99	ASP
4	Q	173	LEU
4	Q	203	LEU
4	Q	232	LYS
5	R	27	GLN
5	R	31	TYR
5	R	72	LEU
5	R	76	ARG
5	R	89	GLN
5	R	134	LEU
5	R	145	VAL
5	R	159	GLN
5	R	179	THR
5	R	195	VAL
6	I	179	THR
6	I	209	LYS
6	I	227	ILE
6	I	237	ARG
6	I	250	VAL
6	I	260	GLU
2	D	60	VAL
2	D	67	GLU
2	D	144	VAL
2	D	179	VAL
2	D	266	VAL
2	D	280	ILE
2	D	387	ILE
2	D	407	MET
4	S	31	SER
4	S	35	THR
4	S	52	ILE
4	S	54	ILE
4	S	55	LEU
4	S	60	TYR

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Mol	Chain	Res	Type
4	S	70	ILE
4	S	107	PHE
4	S	111	TYR
4	S	119	GLN
4	S	203	LEU
5	T	24	ARG
5	T	72	LEU
5	T	76	ARG
5	T	82	PHE
5	T	89	GLN
5	T	105	ILE
5	T	131	VAL
5	T	172	TYR
3	H	32	VAL
3	H	40	GLU
3	H	54	ILE
3	H	80	ARG
3	H	96	THR
3	H	166	GLU
3	H	184	GLN
3	H	241	LEU
3	H	305	ASN
3	H	310	TRP
3	H	323	THR
3	H	329	THR
3	H	349	HIS
3	H	355	ILE
6	L	124	THR
6	L	133	LYS
6	L	151	LYS
6	L	159	LYS
6	L	162	LEU
6	L	223	ARG
6	L	245	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	12	ASN
2	C	235	GLN
2	C	351	GLN
2	C	353	GLN

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Mol	Chain	Res	Type
2	C	368	GLN
2	C	373	GLN
3	G	7	ASN
3	G	18	HIS
3	G	49	GLN
3	G	146	GLN
3	G	333	ASN
2	A	235	GLN
3	E	49	GLN
3	E	187	ASN
3	E	218	ASN
3	E	226	HIS
3	E	238	ASN
3	E	299	ASN
5	N	30	ASN
5	N	136	ASN
2	B	138	GLN
2	B	152	HIS
2	B	199	GLN
2	B	235	GLN
2	B	351	GLN
2	B	368	GLN
2	B	373	GLN
4	O	39	GLN
4	O	169	ASN
4	O	185	GLN
4	O	206	GLN
5	P	30	ASN
5	P	37	GLN
5	P	136	ASN
3	F	49	GLN
3	F	142	HIS
3	F	158	GLN
3	F	202	ASN
3	F	207	ASN
3	F	218	ASN
3	F	219	ASN
3	F	238	ASN
3	F	282	GLN
6	K	188	ASN
6	K	233	ASN
4	Q	39	GLN

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Mol	Chain	Res	Type
4	Q	103	HIS
4	Q	185	GLN
4	Q	213	ASN
5	R	37	GLN
5	R	89	GLN
5	R	198	GLN
6	I	246	ASN
2	D	235	GLN
2	D	253	HIS
2	D	351	GLN
2	D	368	GLN
4	S	39	GLN
5	T	30	ASN
5	T	37	GLN
3	H	49	GLN
3	H	353	HIS

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 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 ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44423. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.