



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 07:32 am BST

PDB ID : 5VK0  
Title : Crystal structure of human MDM2 in complex with a 12-mer lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI  
Authors : Tolbert, W.D.; Gohain, N.; Pazgier, M.  
Deposited on : 2017-04-20  
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

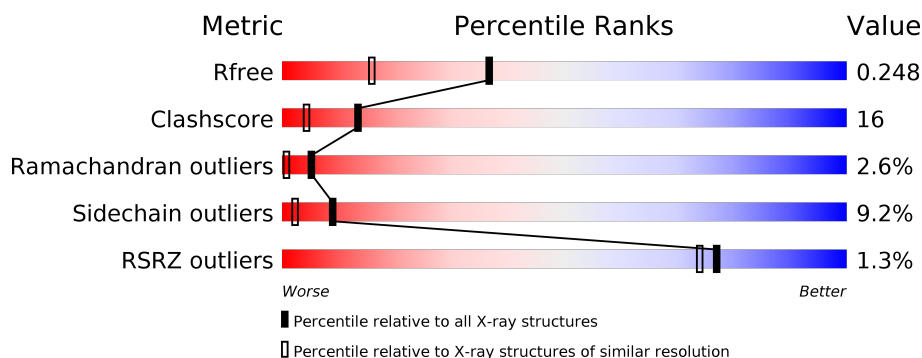
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	85	<div> <div>66%</div> <div>31%</div> <div>..</div> </div>
1	C	85	<div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	E	85	<div> <div>2%</div> <div>66%</div> <div>27%</div> <div>5%</div> <div>.</div> </div>
1	G	85	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	I	85	<div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	K	85	<div> <div>6%</div> <div>45%</div> <div>44%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	85	
1	O	85	
1	Q	85	
1	S	85	
1	U	85	
1	W	85	
2	B	14	
2	D	14	
2	F	14	
2	H	14	
2	J	14	
2	L	14	
2	N	14	
2	P	14	
2	R	14	
2	T	14	
2	V	14	
2	X	14	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10147 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			706	462	116	124	4			
1	C	85	Total	C	N	O	S	0	2	0
			723	473	119	126	5			
1	E	83	Total	C	N	O	S	0	0	0
			689	452	114	119	4			
1	G	85	Total	C	N	O	S	0	0	0
			706	462	116	124	4			
1	I	85	Total	C	N	O	S	0	0	0
			706	462	116	124	4			
1	K	85	Total	C	N	O	S	0	0	0
			706	462	116	124	4			
1	M	85	Total	C	N	O	S	0	0	0
			706	462	116	124	4			
1	O	83	Total	C	N	O	S	0	0	0
			689	452	114	119	4			
1	Q	83	Total	C	N	O	S	0	0	0
			689	452	114	119	4			
1	S	85	Total	C	N	O	S	0	0	0
			706	462	116	124	4			
1	U	84	Total	C	N	O	S	0	0	0
			698	457	115	122	4			
1	W	84	Total	C	N	O	S	0	0	0
			698	457	115	122	4			

- Molecule 2 is a protein called Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			
2	D	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			
2	H	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			
2	J	14	Total	C	N	O	S	0	1	1
			113	74	16	21	2			
2	L	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			
2	N	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			
2	P	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			
2	R	14	Total	C	N	O	S	0	1	1
			113	74	16	21	2			
2	T	14	Total	C	N	O	S	0	1	1
			116	76	16	22	2			
2	V	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			
2	X	14	Total	C	N	O	S	0	0	1
			107	71	15	19	2			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	3	Total	O	0	0
			3	3		
4	C	34	Total	O	0	0
			34	34		
4	D	5	Total	O	0	0
			5	5		
4	E	30	Total	O	0	0
			30	30		

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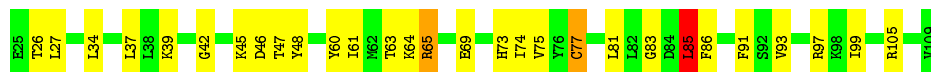
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	5	Total 5	O 5	0	0
4	G	35	Total 35	O 35	0	0
4	H	3	Total 3	O 3	0	0
4	I	31	Total 31	O 31	0	0
4	J	9	Total 9	O 9	0	0
4	K	25	Total 25	O 25	0	0
4	L	2	Total 2	O 2	0	0
4	M	42	Total 42	O 42	0	0
4	N	5	Total 5	O 5	0	0
4	O	27	Total 27	O 27	0	0
4	P	6	Total 6	O 6	0	0
4	Q	24	Total 24	O 24	0	0
4	R	10	Total 10	O 10	0	0
4	S	23	Total 23	O 23	0	0
4	T	4	Total 4	O 4	0	0
4	U	38	Total 38	O 38	0	0
4	V	4	Total 4	O 4	0	0
4	W	22	Total 22	O 22	0	0
4	X	9	Total 9	O 9	0	0

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

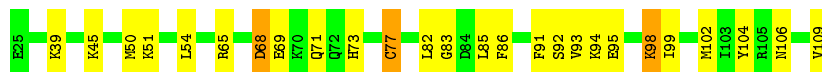
- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 



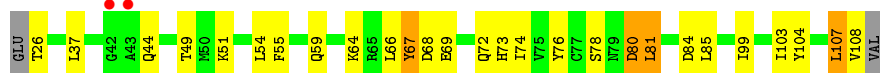
- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain C: 




- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain E: 



- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain G: 

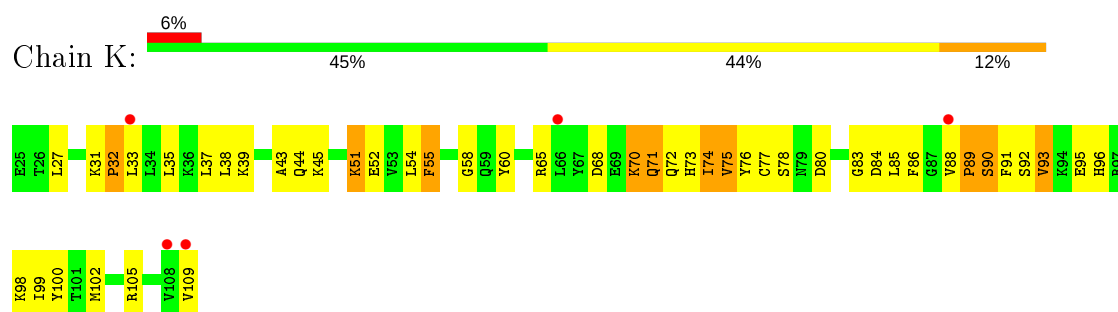


- Molecule 1: E3 ubiquitin-protein ligase Mdm2

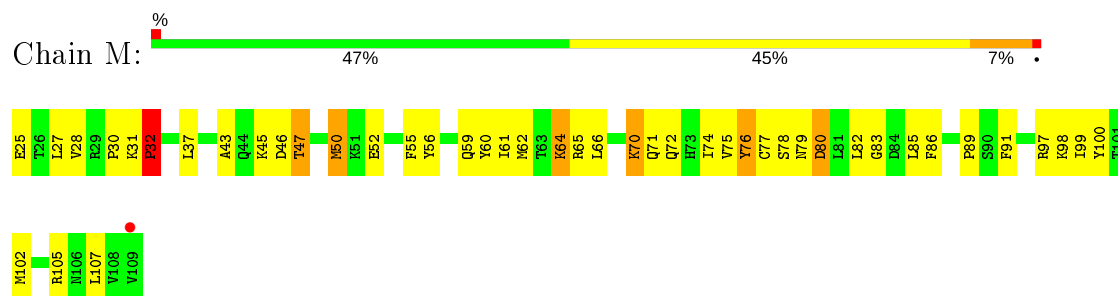
Chain I: 



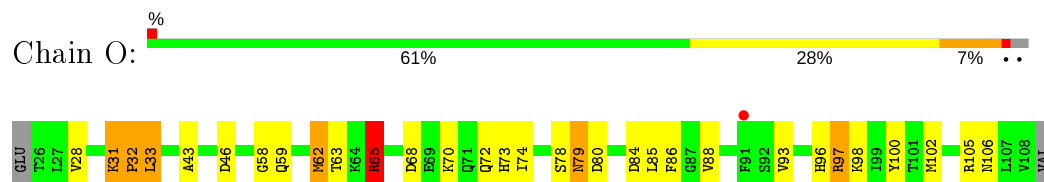
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



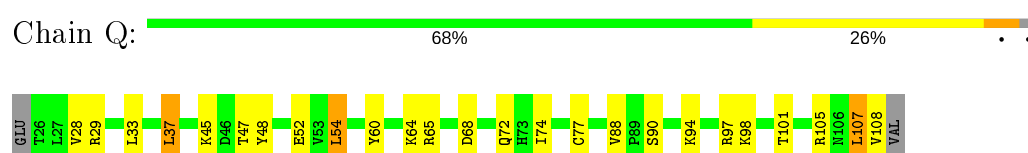
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



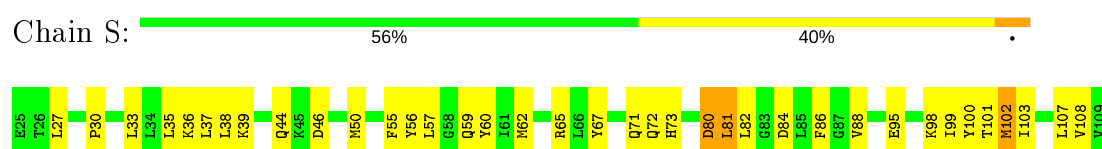
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



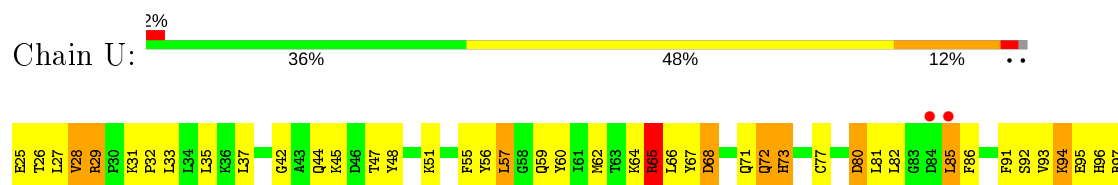
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



- Molecule 1: E3 ubiquitin-protein ligase Mdm2



- Molecule 1: E3 ubiquitin-protein ligase Mdm2







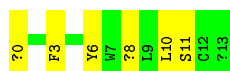
- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain W: 66% 28% 5%



- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI

Chain B: 57% 43%



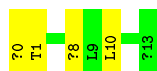
- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI

Chain D: 57% 43%



- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI

Chain F: 71% 29%



- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI

Chain H: 64% 29% 7%



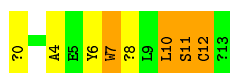
- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI

Chain J: 64% 36%

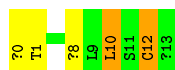


- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI

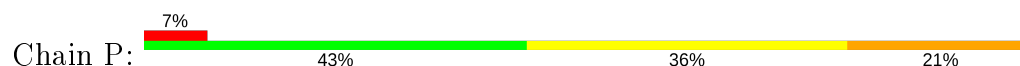
Chain L: 43% 29% 29%



- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI



- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI



- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI



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- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI



- Molecule 2: Lysine-cysteine side chain dithiocarbamate stapled peptide inhibitor PMI



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.84Å 157.47Å 196.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 1.80 41.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (41.70-1.80) 95.2 (41.69-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.198 , 0.247 0.201 , 0.248	Depositor DCC
$R_{free}$ test set	6146 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 25.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.437 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.447 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.338 for H, K, L 0.320 for 1/2H+1/2K, 3/2H-1/2K, -L 0.343 for -1/2H+1/2K, 3/2H+1/2K, -L	Depositor
Outliers	0 of 123343 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACE, 9E7, NH2

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	1.01	0/720	1.30	6/968 (0.6%)
1	C	1.02	1/737 (0.1%)	1.18	2/989 (0.2%)
1	E	1.03	0/703	1.32	4/946 (0.4%)
1	G	0.98	0/720	1.17	4/968 (0.4%)
1	I	1.02	1/720 (0.1%)	1.08	0/968
1	K	0.95	0/720	1.27	7/968 (0.7%)
1	M	1.04	0/720	1.31	5/968 (0.5%)
1	O	1.07	0/703	1.27	3/946 (0.3%)
1	Q	1.00	0/703	1.23	6/946 (0.6%)
1	S	1.04	0/720	1.31	4/968 (0.4%)
1	U	1.02	0/712	1.26	4/958 (0.4%)
1	W	0.98	0/712	1.14	4/958 (0.4%)
2	B	0.87	0/95	1.42	2/128 (1.6%)
2	D	0.97	0/95	2.38	2/128 (1.6%)
2	F	0.88	0/95	2.20	2/128 (1.6%)
2	H	1.03	0/95	1.73	1/128 (0.8%)
2	J	0.87	0/101	1.52	2/136 (1.5%)
2	L	0.92	0/95	1.34	1/128 (0.8%)
2	N	0.97	0/95	2.04	2/128 (1.6%)
2	P	1.00	0/95	1.77	2/128 (1.6%)
2	R	0.77	0/101	1.45	3/136 (2.2%)
2	T	0.83	0/104	2.02	2/140 (1.4%)
2	V	1.06	0/95	2.35	3/128 (2.3%)
2	X	0.86	0/95	1.86	2/128 (1.6%)
All	All	1.00	2/9751 (0.0%)	1.33	73/13115 (0.6%)

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	K	0	1
1	Q	0	1
1	U	0	1
2	B	0	1
2	D	0	3
2	F	0	1
2	H	0	1
2	J	0	1
2	L	0	2
2	N	0	1
2	P	0	2
2	R	0	2
2	T	0	1
2	V	0	1
2	X	0	1
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	77	CYS	CB-SG	-5.91	1.72	1.81
1	I	60	TYR	CB-CG	5.08	1.59	1.51

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	0	ACE	O-C-N	-19.09	92.16	122.70
2	D	0	ACE	C-N-CA	17.53	165.53	121.70
2	T	0	ACE	O-C-N	-17.01	95.48	122.70
2	V	0	ACE	C-N-CA	16.75	163.58	121.70
2	N	0	ACE	O-C-N	-16.37	96.50	122.70

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	9E7	Mainchain
2	D	11	SER	Peptide
2	D	7	TRP	Mainchain
2	D	8	9E7	Mainchain
2	F	8	9E7	Mainchain

## 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	706	0	740	26	0
1	C	723	0	760	18	0
1	E	689	0	725	17	0
1	G	706	0	740	17	0
1	I	706	0	740	9	0
1	K	706	0	740	41	1
1	M	706	0	740	39	0
1	O	689	0	725	28	0
1	Q	689	0	725	22	0
1	S	706	0	740	28	0
1	U	698	0	731	50	1
1	W	698	0	731	23	0
2	B	107	0	85	3	0
2	D	107	0	84	1	0
2	F	107	0	84	1	0
2	H	107	0	85	2	0
2	J	113	0	89	1	0
2	L	107	0	85	12	0
2	N	107	0	84	2	0
2	P	107	0	83	6	0
2	R	113	0	89	2	0
2	T	116	0	89	12	0
2	V	107	0	84	10	0
2	X	107	0	84	1	0
3	C	1	0	0	0	0
3	X	1	0	0	0	0
4	A	22	0	0	1	0
4	B	3	0	0	0	0
4	C	34	0	0	0	0
4	D	5	0	0	0	0
4	E	30	0	0	0	0
4	F	5	0	0	0	0
4	G	35	0	0	3	0
4	H	3	0	0	0	0
4	I	31	0	0	1	0
4	J	9	0	0	0	0
4	K	25	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	2	0	0	0	0
4	M	42	0	0	2	0
4	N	5	0	0	1	0
4	O	27	0	0	1	0
4	P	6	0	0	0	0
4	Q	24	0	0	2	0
4	R	10	0	0	0	0
4	S	23	0	0	3	0
4	T	4	0	0	1	0
4	U	38	0	0	6	0
4	V	4	0	0	1	0
4	W	22	0	0	0	0
4	X	9	0	0	0	0
All	All	10147	0	9862	316	1

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 16.

The worst 5 of 316 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:U:94:LYS:O	1:U:96:HIS:ND1	1.89	1.05
1:U:102:MET:O	1:U:106:ASN:ND2	1.95	0.98
1:U:105:ARG:NH2	4:U:201:HOH:O	1.97	0.98
1:A:75:VAL:HG11	1:A:91:PHE:CZ	2.07	0.89
1:O:33:LEU:HD21	1:O:85:LEU:HG	1.55	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:SER:OG	1:U:96:HIS:ND1[8_545]	2.12	0.08

## 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 X-ray entries followed by that with respect to entries

of similar resolution.

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	83/85 (98%)	75 (90%)	7 (8%)	1 (1%)	13	3
1	C	85/85 (100%)	84 (99%)	1 (1%)	0	100	100
1	E	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
1	G	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
1	I	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
1	K	83/85 (98%)	72 (87%)	8 (10%)	3 (4%)	3	0
1	M	83/85 (98%)	76 (92%)	5 (6%)	2 (2%)	6	1
1	O	81/85 (95%)	70 (86%)	8 (10%)	3 (4%)	3	0
1	Q	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
1	S	83/85 (98%)	73 (88%)	8 (10%)	2 (2%)	6	1
1	U	82/85 (96%)	65 (79%)	12 (15%)	5 (6%)	1	0
1	W	82/85 (96%)	80 (98%)	1 (1%)	1 (1%)	13	3
2	B	11/14 (79%)	8 (73%)	2 (18%)	1 (9%)	1	0
2	D	11/14 (79%)	8 (73%)	2 (18%)	1 (9%)	1	0
2	F	11/14 (79%)	11 (100%)	0	0	100	100
2	H	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
2	J	12/14 (86%)	10 (83%)	1 (8%)	1 (8%)	1	0
2	L	11/14 (79%)	6 (54%)	2 (18%)	3 (27%)	0	0
2	N	11/14 (79%)	8 (73%)	1 (9%)	2 (18%)	0	0
2	P	11/14 (79%)	7 (64%)	1 (9%)	3 (27%)	0	0
2	R	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	T	12/14 (86%)	10 (83%)	2 (17%)	0	100	100
2	V	11/14 (79%)	7 (64%)	3 (27%)	1 (9%)	1	0
2	X	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
All	All	1125/1188 (95%)	1016 (90%)	80 (7%)	29 (3%)	5	1

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	THR
2	D	12	CYS

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Mol	Chain	Res	Type
1	K	89	PRO
2	L	10	LEU
2	L	12	CYS

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	80/80 (100%)	76 (95%)	4 (5%)	24	10
1	C	82/80 (102%)	78 (95%)	4 (5%)	25	11
1	E	78/80 (98%)	71 (91%)	7 (9%)	9	2
1	G	80/80 (100%)	76 (95%)	4 (5%)	24	10
1	I	80/80 (100%)	74 (92%)	6 (8%)	13	4
1	K	80/80 (100%)	68 (85%)	12 (15%)	3	0
1	M	80/80 (100%)	74 (92%)	6 (8%)	13	4
1	O	78/80 (98%)	66 (85%)	12 (15%)	2	0
1	Q	78/80 (98%)	75 (96%)	3 (4%)	33	18
1	S	80/80 (100%)	70 (88%)	10 (12%)	4	1
1	U	79/80 (99%)	62 (78%)	17 (22%)	1	0
1	W	79/80 (99%)	74 (94%)	5 (6%)	18	6
2	B	10/10 (100%)	10 (100%)	0	100	100
2	D	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	9 (90%)	1 (10%)	7	2
2	H	10/10 (100%)	9 (90%)	1 (10%)	7	2
2	J	11/10 (110%)	9 (82%)	2 (18%)	1	0
2	L	10/10 (100%)	10 (100%)	0	100	100
2	N	10/10 (100%)	8 (80%)	2 (20%)	1	0
2	P	10/10 (100%)	10 (100%)	0	100	100
2	R	11/10 (110%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	11/10 (110%)	9 (82%)	2 (18%)	1	0
2	V	10/10 (100%)	9 (90%)	1 (10%)	7	2
2	X	10/10 (100%)	9 (90%)	1 (10%)	7	2
All	All	1077/1080 (100%)	977 (91%)	100 (9%)	9	2

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	70	LYS
1	O	78	SER
1	U	105	ARG
1	M	76	TYR
1	O	31	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	59	GLN
1	K	79	ASN
1	K	96	HIS
1	M	96	HIS
1	U	71	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	9E7	F	8	2	9,10,11	2.14	1 (11%)	4,10,12	2.01	1 (25%)
2	9E7	D	8	2	9,10,11	1.39	1 (11%)	4,10,12	1.71	1 (25%)
2	9E7	X	8	2	9,10,11	1.87	1 (11%)	4,10,12	2.87	1 (25%)
2	9E7	R	8	2	9,10,11	2.20	1 (11%)	4,10,12	2.64	1 (25%)
2	9E7	P	8	2	9,10,11	1.51	1 (11%)	4,10,12	0.87	0
2	9E7	V	8	2	9,10,11	1.99	1 (11%)	4,10,12	1.52	1 (25%)
2	9E7	T	8	2	9,10,11	1.54	1 (11%)	4,10,12	0.62	0
2	9E7	J	8	2	9,10,11	1.17	2 (22%)	4,10,12	1.11	0
2	9E7	H	8	2	9,10,11	1.76	1 (11%)	4,10,12	0.94	0
2	9E7	N	8	2	9,10,11	1.74	1 (11%)	4,10,12	1.60	1 (25%)
2	9E7	L	8	2	9,10,11	1.59	1 (11%)	4,10,12	0.71	0
2	9E7	B	8	2	9,10,11	1.67	1 (11%)	4,10,12	2.01	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9E7	F	8	2	-	2/7/9/11	-
2	9E7	D	8	2	-	2/7/9/11	-
2	9E7	X	8	2	-	2/7/9/11	-
2	9E7	R	8	2	-	3/7/9/11	-
2	9E7	P	8	2	-	6/7/9/11	-
2	9E7	V	8	2	-	4/7/9/11	-
2	9E7	T	8	2	-	2/7/9/11	-
2	9E7	J	8	2	-	2/7/9/11	-
2	9E7	H	8	2	-	3/7/9/11	-
2	9E7	N	8	2	-	2/7/9/11	-
2	9E7	L	8	2	-	2/7/9/11	-
2	9E7	B	8	2	-	2/7/9/11	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	8	9E7	C1-NZ	5.97	1.51	1.44
2	F	8	9E7	C1-NZ	5.48	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	8	9E7	C1-NZ	5.46	1.51	1.44
2	X	8	9E7	C1-NZ	5.15	1.50	1.44
2	H	8	9E7	C1-NZ	4.97	1.50	1.44

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	8	9E7	CE-NZ-C1	5.41	125.52	113.42
2	R	8	9E7	CE-NZ-C1	5.03	124.67	113.42
2	B	8	9E7	CE-NZ-C1	3.83	121.98	113.42
2	F	8	9E7	CE-NZ-C1	3.46	121.17	113.42
2	N	8	9E7	CE-NZ-C1	3.05	120.24	113.42

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	8	9E7	CD-CE-NZ-C1
2	P	8	9E7	C-CA-CB-CG
2	P	8	9E7	N-CA-CB-CG
2	L	8	9E7	CG-CD-CE-NZ
2	V	8	9E7	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	85/85 (100%)	-0.03	0 100 100	18, 24, 32, 40	0
1	C	85/85 (100%)	-0.17	0 100 100	17, 23, 29, 34	0
1	E	83/85 (97%)	0.03	2 (2%) 59 54	22, 28, 34, 39	0
1	G	85/85 (100%)	0.00	1 (1%) 79 76	16, 24, 32, 38	0
1	I	85/85 (100%)	-0.02	0 100 100	15, 24, 32, 38	0
1	K	85/85 (100%)	0.46	5 (5%) 22 17	22, 32, 40, 47	0
1	M	85/85 (100%)	0.26	1 (1%) 79 76	21, 29, 35, 41	0
1	O	83/85 (97%)	0.26	1 (1%) 79 76	25, 30, 35, 40	0
1	Q	83/85 (97%)	-0.07	0 100 100	16, 23, 31, 37	0
1	S	85/85 (100%)	0.15	0 100 100	19, 27, 35, 43	0
1	U	84/85 (98%)	0.36	2 (2%) 59 54	23, 31, 39, 44	0
1	W	84/85 (98%)	0.07	0 100 100	13, 25, 35, 42	0
2	B	11/14 (78%)	0.28	0 100 100	21, 23, 29, 31	0
2	D	11/14 (78%)	0.19	0 100 100	23, 24, 32, 32	0
2	F	11/14 (78%)	0.18	0 100 100	24, 25, 28, 30	0
2	H	11/14 (78%)	-0.09	0 100 100	15, 18, 21, 27	0
2	J	11/14 (78%)	0.30	0 100 100	17, 18, 26, 29	0
2	L	11/14 (78%)	0.27	0 100 100	24, 26, 28, 31	0
2	N	11/14 (78%)	0.30	0 100 100	22, 24, 28, 33	0
2	P	11/14 (78%)	0.43	1 (9%) 9 7	23, 26, 30, 33	0
2	R	11/14 (78%)	0.34	0 100 100	16, 19, 22, 26	0
2	T	11/14 (78%)	0.20	0 100 100	25, 28, 31, 34	0
2	V	11/14 (78%)	0.83	2 (18%) 1 0	23, 26, 29, 32	0
2	X	11/14 (78%)	-0.04	0 100 100	17, 20, 25, 26	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	1144/1188 (96%)	0.13	15 (1%) 77 74	13, 27, 36, 47	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	109	VAL	4.5
1	K	88	VAL	4.0
1	O	91	PHE	3.3
1	K	33	LEU	2.7
1	U	84	ASP	2.6

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	9E7	T	8	11/12	0.77	0.15	24,26,32,33	0
2	9E7	J	8	11/12	0.84	0.16	17,19,26,32	0
2	9E7	L	8	11/12	0.85	0.15	25,27,30,32	0
2	9E7	B	8	11/12	0.86	0.14	20,22,26,33	0
2	9E7	H	8	11/12	0.88	0.16	17,19,28,31	0
2	9E7	R	8	11/12	0.88	0.14	18,20,29,31	0
2	9E7	V	8	11/12	0.88	0.16	25,27,30,33	0
2	9E7	P	8	11/12	0.89	0.13	25,26,34,36	0
2	9E7	N	8	11/12	0.90	0.16	21,22,26,29	0
2	9E7	F	8	11/12	0.91	0.13	25,27,34,37	0
2	9E7	D	8	11/12	0.93	0.12	22,24,27,28	0
2	9E7	X	8	11/12	0.94	0.10	21,26,30,30	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	X	101	1/1	0.98	0.10	35,35,35,35	0
3	CL	C	201	1/1	0.99	0.12	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.