



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:43 PM UTC

PDB ID : 7NPI / pdb_00007npi
Title : Crystal structure of Mindy2 (C266A) in complex with Lys48-linked penta-ubiquitin (K48-Ub5)
Authors : Lange, S.M.; Armstrong, L.A.; Kulathu, Y.
Deposited on : 2021-02-26
Resolution : 2.81 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

A user guide is available at

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

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

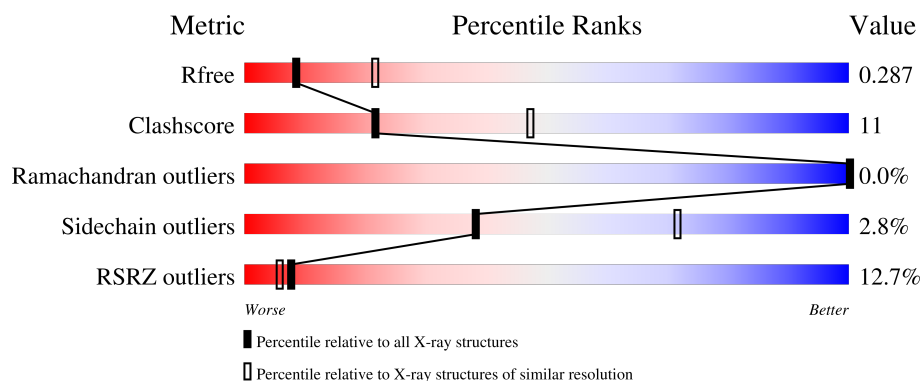
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 of the lower 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 $\leq 5\%$. 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	273	3% 72% 22% • •
1	G	273	5% 68% 27% •
1	M	273	14% 70% 25% • •
1	S	273	6% 65% 30% • •
1	Y	273	4% 67% 28% • •

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Mol	Chain	Length	Quality of chain
1	e	273	
1	k	273	
2	B	76	
2	C	76	
2	D	76	
2	E	76	
2	F	76	
2	H	76	
2	I	76	
2	J	76	
2	K	76	
2	L	76	
2	N	76	
2	O	76	
2	P	76	
2	Q	76	
2	R	76	
2	T	76	
2	U	76	
2	V	76	
2	W	76	
2	X	76	
2	Z	76	
2	a	76	
2	b	76	

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Mol	Chain	Length	Quality of chain
2	c	76	
2	d	76	
2	f	76	
2	g	76	
2	h	76	
2	i	76	
2	j	76	
2	l	76	
2	m	76	
2	n	76	
2	o	76	
2	p	76	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33767 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 Ubiquitin carboxyl-terminal hydrolase MINDY-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2083	1335	337	398	13			
1	G	262	Total	C	N	O	S	0	0	0
			2064	1322	335	394	13			
1	M	263	Total	C	N	O	S	0	0	0
			2055	1316	331	395	13			
1	S	263	Total	C	N	O	S	12	0	0
			2053	1315	328	398	12			
1	Y	263	Total	C	N	O	S	0	0	0
			2072	1327	335	397	13			
1	e	263	Total	C	N	O	S	0	0	0
			2062	1322	335	392	13			
1	k	263	Total	C	N	O	S	0	0	0
			2077	1331	336	397	13			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q8NBR6
A	233	PRO	-	expression tag	UNP Q8NBR6
A	234	LEU	-	expression tag	UNP Q8NBR6
A	235	GLY	-	expression tag	UNP Q8NBR6
A	236	SER	-	expression tag	UNP Q8NBR6
A	237	PRO	-	expression tag	UNP Q8NBR6
A	238	GLU	-	expression tag	UNP Q8NBR6
A	239	PHE	-	expression tag	UNP Q8NBR6
A	240	MET	-	expression tag	UNP Q8NBR6
A	266	ALA	CYS	engineered mutation	UNP Q8NBR6
G	232	GLY	-	expression tag	UNP Q8NBR6
G	233	PRO	-	expression tag	UNP Q8NBR6
G	234	LEU	-	expression tag	UNP Q8NBR6
G	235	GLY	-	expression tag	UNP Q8NBR6
G	236	SER	-	expression tag	UNP Q8NBR6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	237	PRO	-	expression tag	UNP Q8NBR6
G	238	GLU	-	expression tag	UNP Q8NBR6
G	239	PHE	-	expression tag	UNP Q8NBR6
G	240	MET	-	expression tag	UNP Q8NBR6
G	266	ALA	CYS	engineered mutation	UNP Q8NBR6
M	232	GLY	-	expression tag	UNP Q8NBR6
M	233	PRO	-	expression tag	UNP Q8NBR6
M	234	LEU	-	expression tag	UNP Q8NBR6
M	235	GLY	-	expression tag	UNP Q8NBR6
M	236	SER	-	expression tag	UNP Q8NBR6
M	237	PRO	-	expression tag	UNP Q8NBR6
M	238	GLU	-	expression tag	UNP Q8NBR6
M	239	PHE	-	expression tag	UNP Q8NBR6
M	240	MET	-	expression tag	UNP Q8NBR6
M	266	ALA	CYS	engineered mutation	UNP Q8NBR6
S	232	GLY	-	expression tag	UNP Q8NBR6
S	233	PRO	-	expression tag	UNP Q8NBR6
S	234	LEU	-	expression tag	UNP Q8NBR6
S	235	GLY	-	expression tag	UNP Q8NBR6
S	236	SER	-	expression tag	UNP Q8NBR6
S	237	PRO	-	expression tag	UNP Q8NBR6
S	238	GLU	-	expression tag	UNP Q8NBR6
S	239	PHE	-	expression tag	UNP Q8NBR6
S	240	MET	-	expression tag	UNP Q8NBR6
S	266	ALA	CYS	engineered mutation	UNP Q8NBR6
Y	232	GLY	-	expression tag	UNP Q8NBR6
Y	233	PRO	-	expression tag	UNP Q8NBR6
Y	234	LEU	-	expression tag	UNP Q8NBR6
Y	235	GLY	-	expression tag	UNP Q8NBR6
Y	236	SER	-	expression tag	UNP Q8NBR6
Y	237	PRO	-	expression tag	UNP Q8NBR6
Y	238	GLU	-	expression tag	UNP Q8NBR6
Y	239	PHE	-	expression tag	UNP Q8NBR6
Y	240	MET	-	expression tag	UNP Q8NBR6
Y	266	ALA	CYS	engineered mutation	UNP Q8NBR6
e	232	GLY	-	expression tag	UNP Q8NBR6
e	233	PRO	-	expression tag	UNP Q8NBR6
e	234	LEU	-	expression tag	UNP Q8NBR6
e	235	GLY	-	expression tag	UNP Q8NBR6
e	236	SER	-	expression tag	UNP Q8NBR6
e	237	PRO	-	expression tag	UNP Q8NBR6
e	238	GLU	-	expression tag	UNP Q8NBR6

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Chain	Residue	Modelled	Actual	Comment	Reference
e	239	PHE	-	expression tag	UNP Q8NBR6
e	240	MET	-	expression tag	UNP Q8NBR6
e	266	ALA	CYS	engineered mutation	UNP Q8NBR6
k	232	GLY	-	expression tag	UNP Q8NBR6
k	233	PRO	-	expression tag	UNP Q8NBR6
k	234	LEU	-	expression tag	UNP Q8NBR6
k	235	GLY	-	expression tag	UNP Q8NBR6
k	236	SER	-	expression tag	UNP Q8NBR6
k	237	PRO	-	expression tag	UNP Q8NBR6
k	238	GLU	-	expression tag	UNP Q8NBR6
k	239	PHE	-	expression tag	UNP Q8NBR6
k	240	MET	-	expression tag	UNP Q8NBR6
k	266	ALA	CYS	engineered mutation	UNP Q8NBR6

- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
2	C	76	Total	C	N	O	S	0	0	0
			595	375	102	117	1			
2	D	76	Total	C	N	O		207	0	0
			445	273	91	81				
2	E	75	Total	C	N	O	S	0	0	0
			578	364	97	116	1			
2	F	76	Total	C	N	O	S	0	0	0
			589	372	103	113	1			
2	H	73	Total	C	N	O	S	0	0	0
			579	365	99	114	1			
2	I	76	Total	C	N	O	S	0	0	0
			591	372	101	117	1			
2	J	76	Total	C	N	O		5	0	0
			492	303	94	95				
2	K	74	Total	C	N	O	S	0	0	0
			562	355	94	112	1			
2	L	76	Total	C	N	O	S	0	0	0
			593	372	103	117	1			
2	N	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
2	O	76	Total	C	N	O	S	4	0	0
			589	371	101	116	1			
2	P	76	Total	C	N	O		127	0	0
			441	266	90	85				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	71	Total	C	N	O	S	0	0	0
			545	345	92	107	1			
2	R	76	Total	C	N	O	S	0	0	0
			555	349	99	106	1			
2	T	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
2	U	76	Total	C	N	O	S	0	0	0
			595	375	102	117	1			
2	V	76	Total	C	N	O	S	179	0	0
			421	256	85	79	1			
2	W	72	Total	C	N	O		0	0	0
			555	351	91	113				
2	X	76	Total	C	N	O		0	0	0
			565	352	100	113				
2	Z	73	Total	C	N	O	S	0	0	0
			578	365	98	114	1			
2	a	76	Total	C	N	O	S	0	0	0
			593	373	104	115	1			
2	b	76	Total	C	N	O		68	0	0
			464	284	93	87				
2	c	73	Total	C	N	O	S	0	0	0
			566	354	97	114	1			
2	d	76	Total	C	N	O	S	0	0	0
			585	368	103	113	1			
2	f	73	Total	C	N	O	S	0	0	0
			569	359	97	112	1			
2	g	76	Total	C	N	O	S	0	0	0
			599	377	105	116	1			
2	h	76	Total	C	N	O		91	0	0
			439	267	89	83				
2	i	73	Total	C	N	O		0	0	0
			522	329	91	102				
2	j	76	Total	C	N	O		0	0	0
			552	345	100	107				
2	l	73	Total	C	N	O	S	0	0	0
			578	365	98	114	1			
2	m	76	Total	C	N	O	S	0	0	0
			596	375	104	116	1			
2	n	75	Total	C	N	O		56	0	0
			458	274	89	95				
2	o	72	Total	C	N	O		0	0	0
			545	344	91	110				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	p	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	S	1	Total	Na	0	0
			1	1		

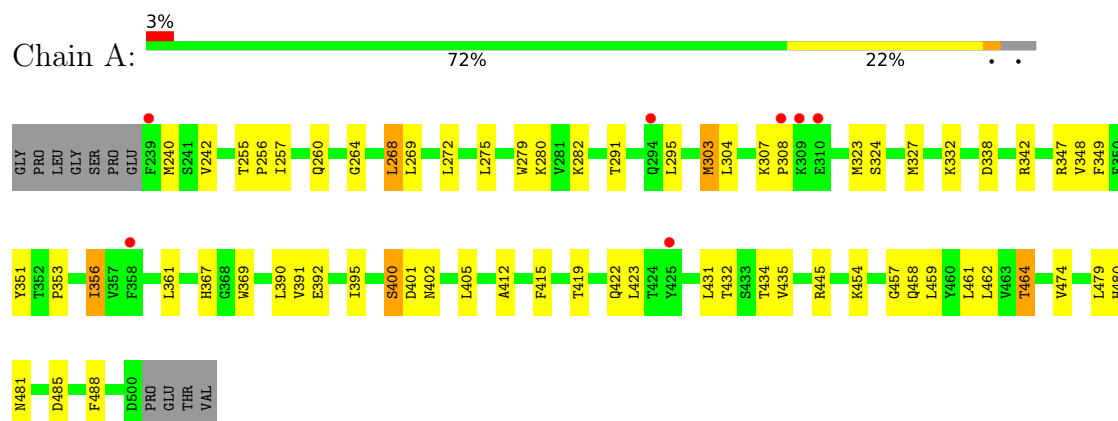
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	E	1	Total	O	0	0
			1	1		
5	G	3	Total	O	0	0
			3	3		
5	M	2	Total	O	0	0
			2	2		
5	T	2	Total	O	0	0
			2	2		
5	Y	1	Total	O	0	0
			1	1		
5	Z	1	Total	O	0	0
			1	1		
5	e	1	Total	O	0	0
			1	1		
5	m	1	Total	O	0	0
			1	1		

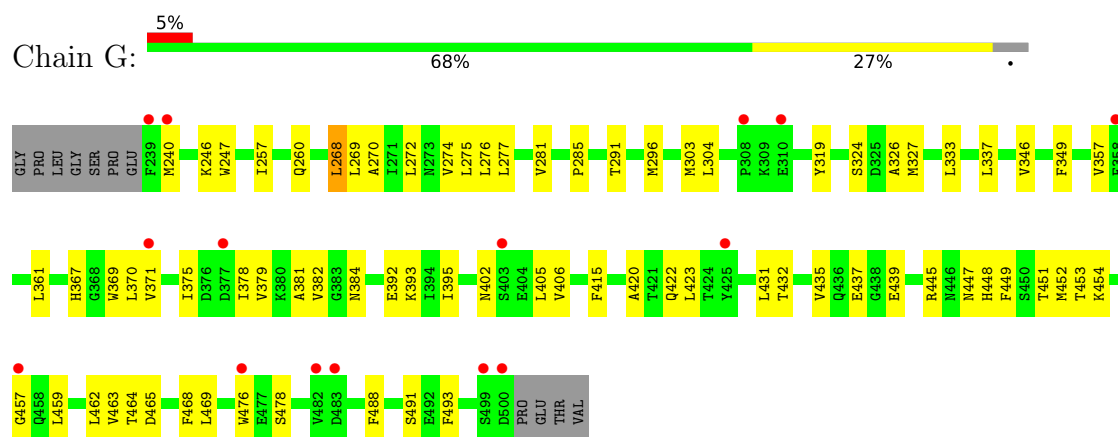
3 Residue-property plots

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 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.

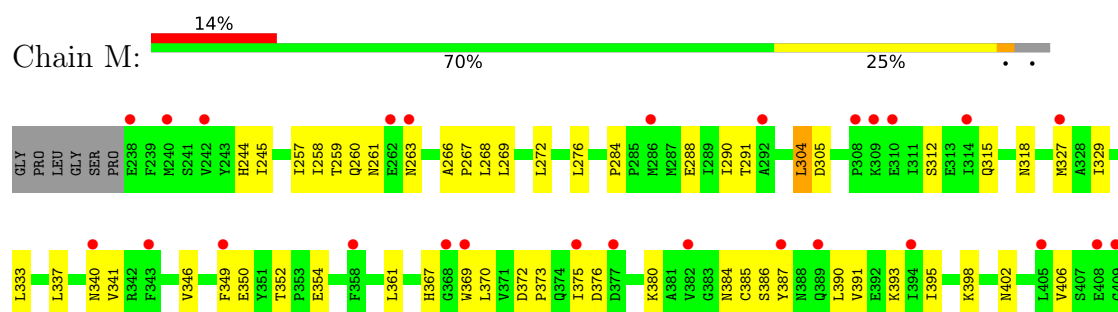
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

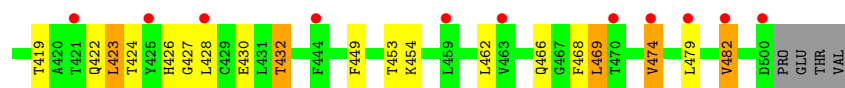


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

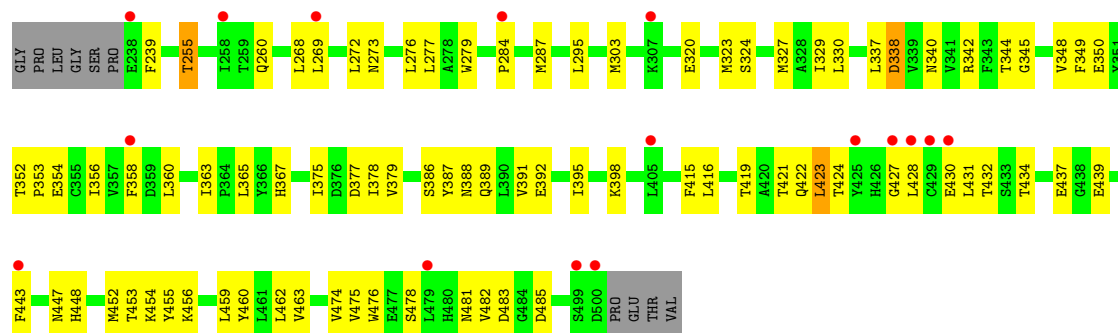


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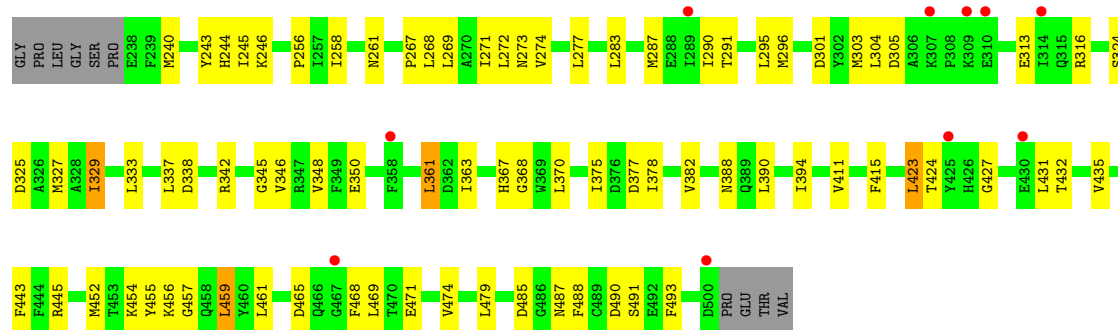




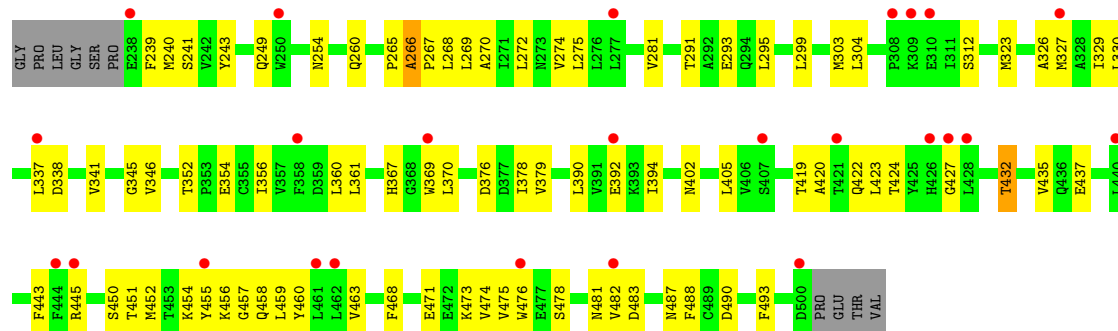
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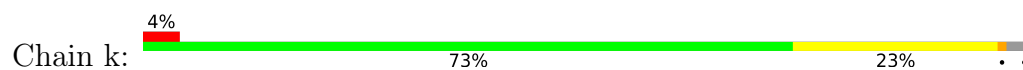
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

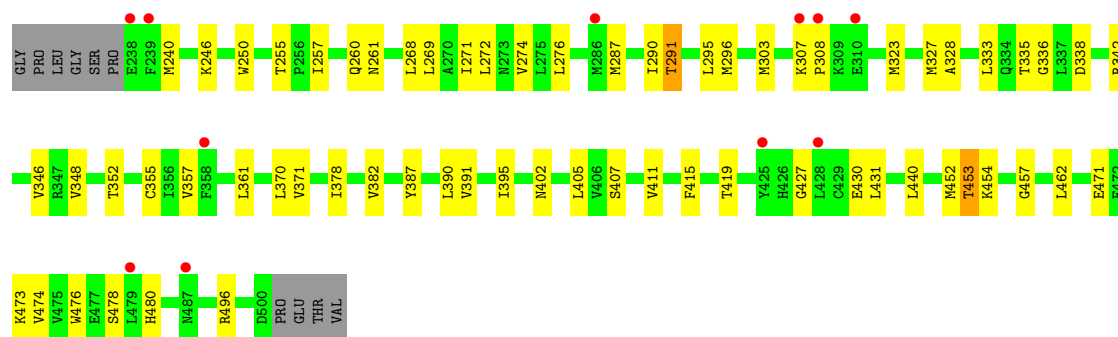


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

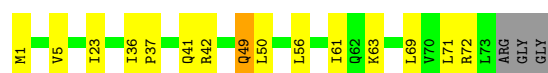
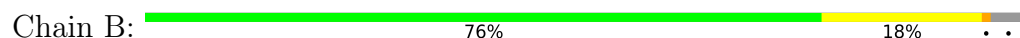


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

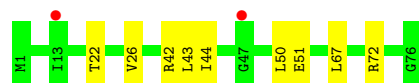
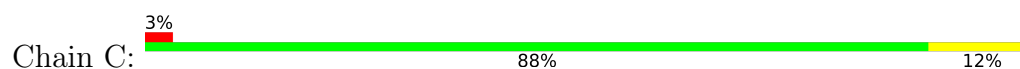




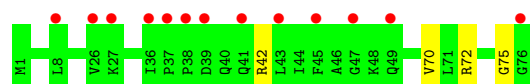
• Molecule 2: Polyubiquitin-C



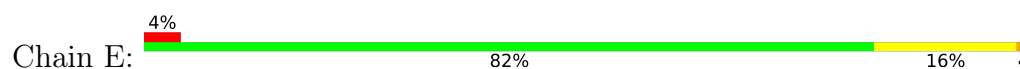
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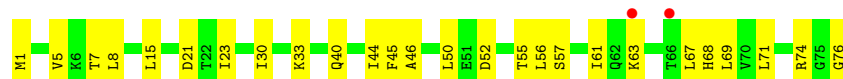
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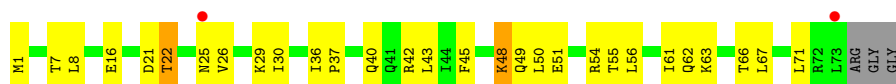


• Molecule 2: Polyubiquitin-C

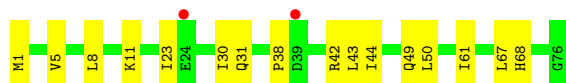
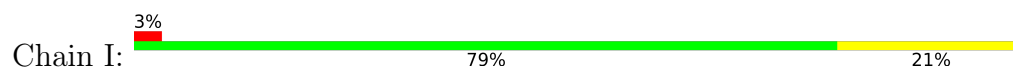


• Molecule 2: Polyubiquitin-C

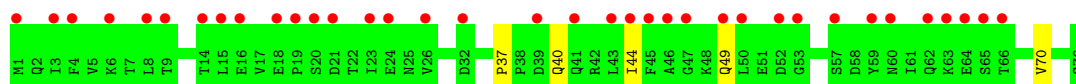
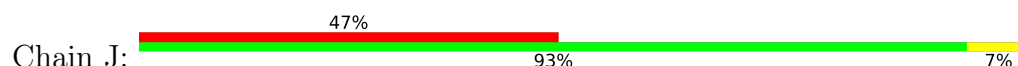




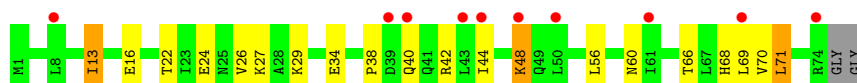
● Molecule 2: Polyubiquitin-C



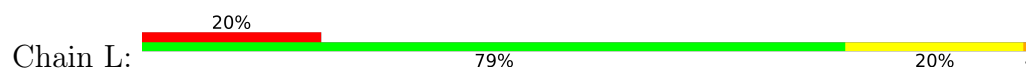
● Molecule 2: Polyubiquitin-C



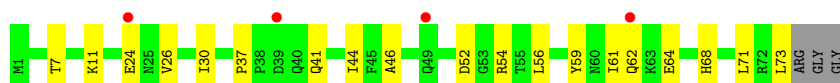
● Molecule 2: Polyubiquitin-C



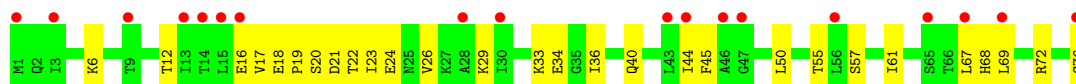
● Molecule 2: Polyubiquitin-C



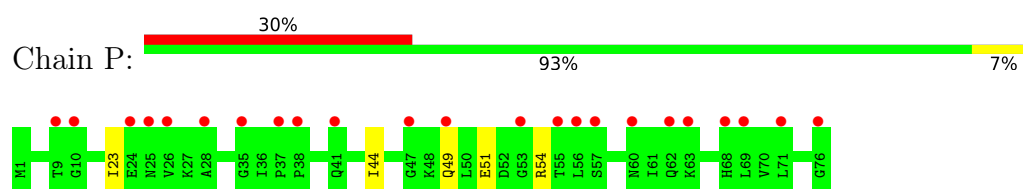
● Molecule 2: Polyubiquitin-C



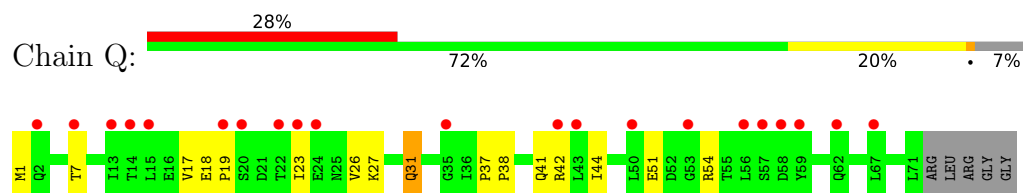
● Molecule 2: Polyubiquitin-C



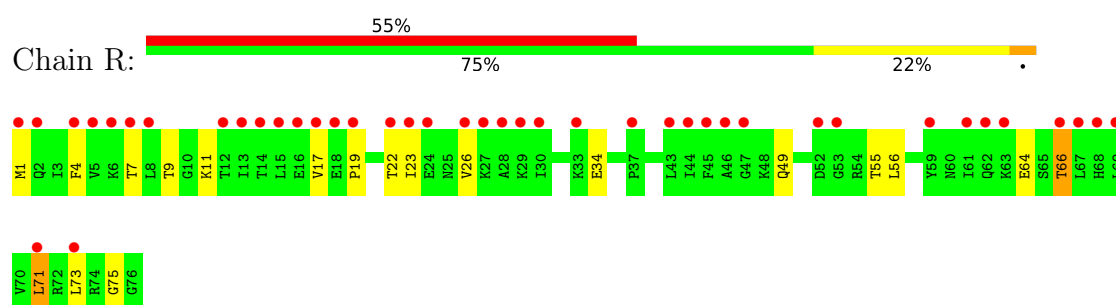
● Molecule 2: Polyubiquitin-C



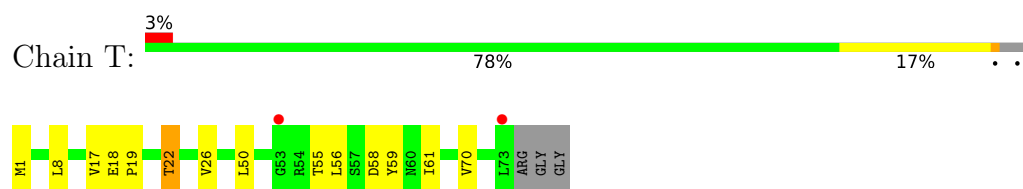
• Molecule 2: Polyubiquitin-C



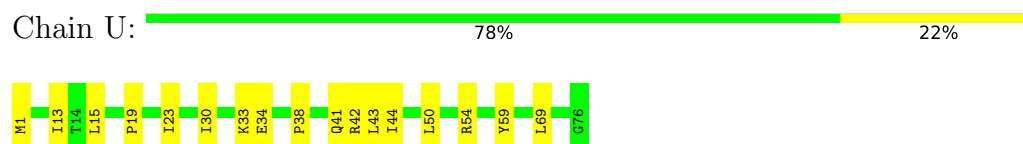
• Molecule 2: Polyubiquitin-C



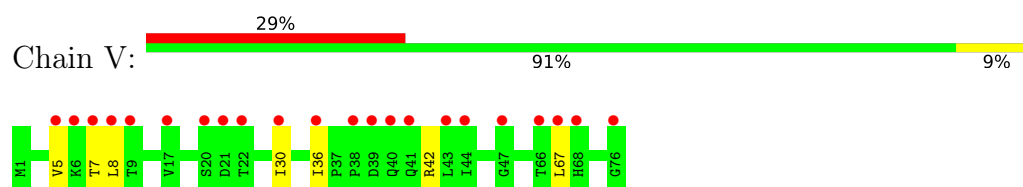
• Molecule 2: Polyubiquitin-C



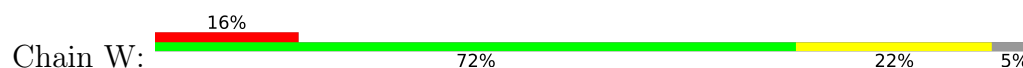
• Molecule 2: Polyubiquitin-C

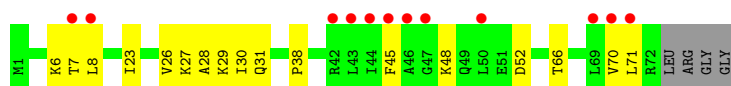


• Molecule 2: Polyubiquitin-C

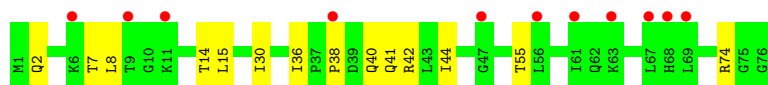
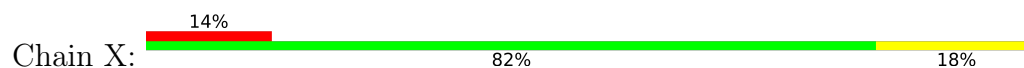


• Molecule 2: Polyubiquitin-C

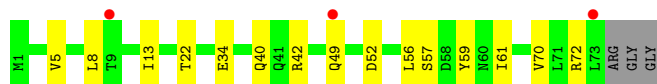
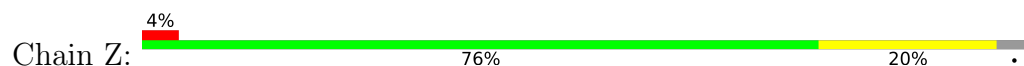




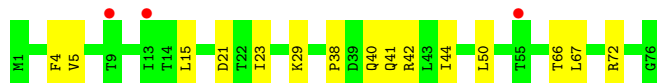
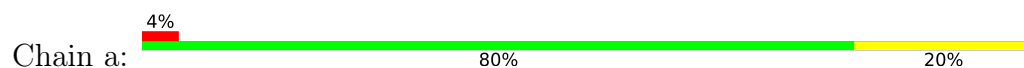
- Molecule 2: Polyubiquitin-C



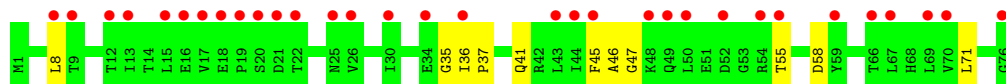
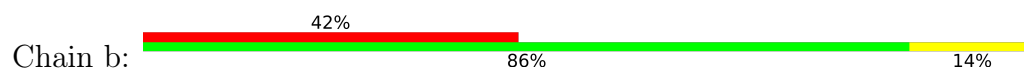
- Molecule 2: Polyubiquitin-C



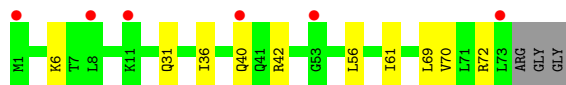
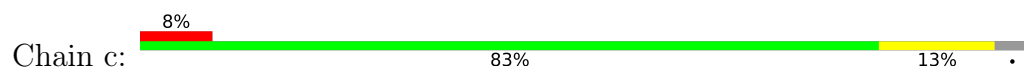
- Molecule 2: Polyubiquitin-C



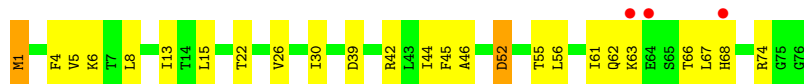
- Molecule 2: Polyubiquitin-C



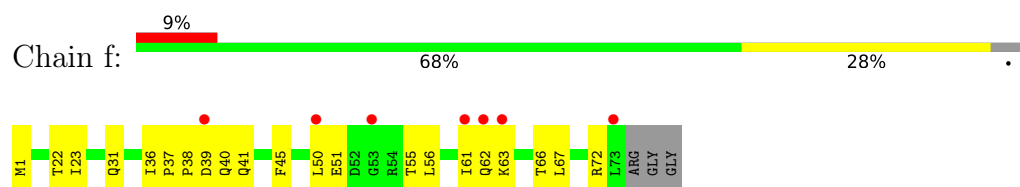
- Molecule 2: Polyubiquitin-C



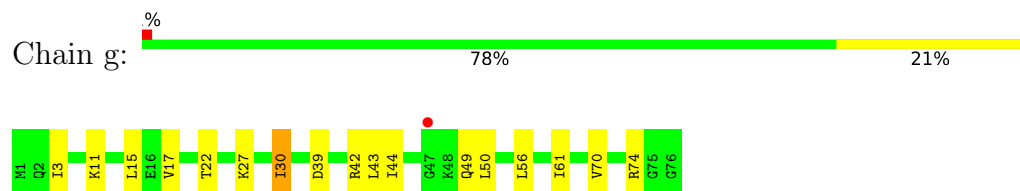
- Molecule 2: Polyubiquitin-C



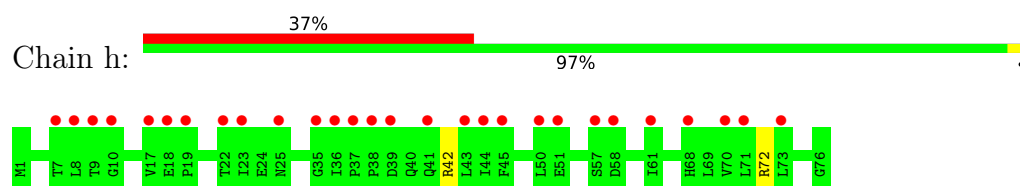
- Molecule 2: Polyubiquitin-C



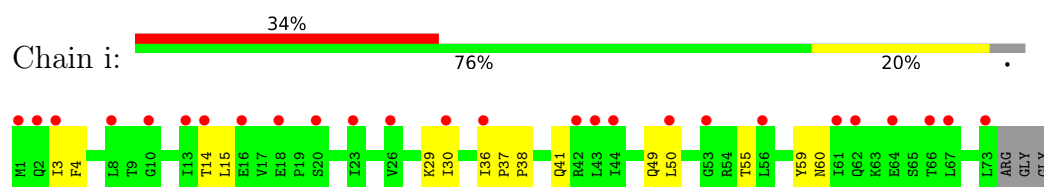
• Molecule 2: Polyubiquitin-C



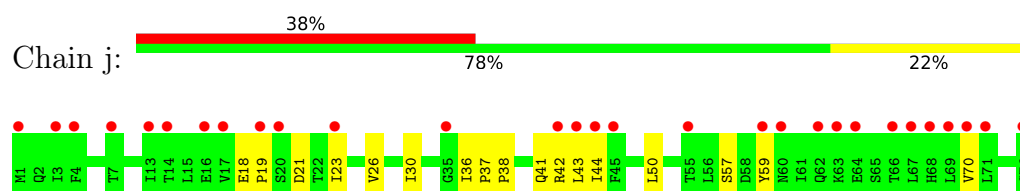
• Molecule 2: Polyubiquitin-C



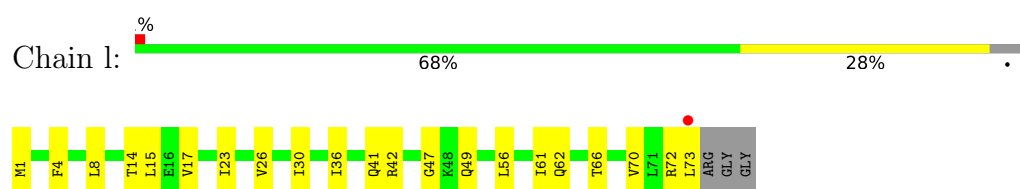
• Molecule 2: Polyubiquitin-C



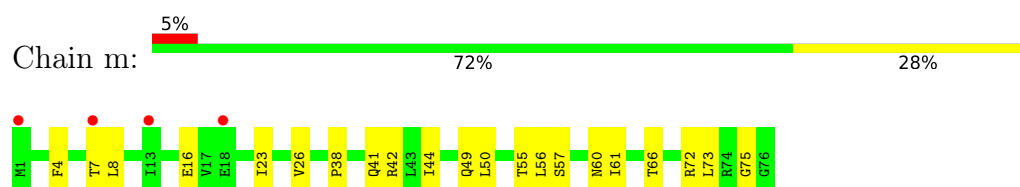
• Molecule 2: Polyubiquitin-C



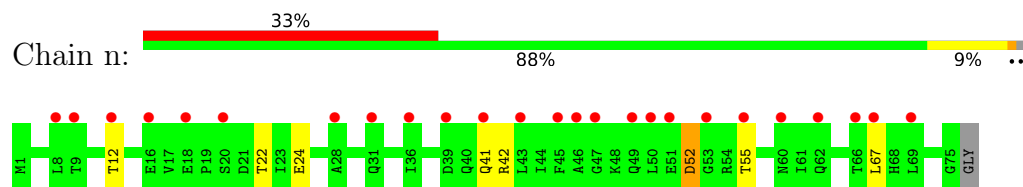
• Molecule 2: Polyubiquitin-C



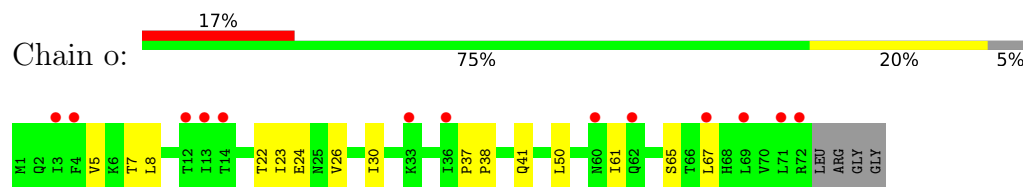
• Molecule 2: Polyubiquitin-C



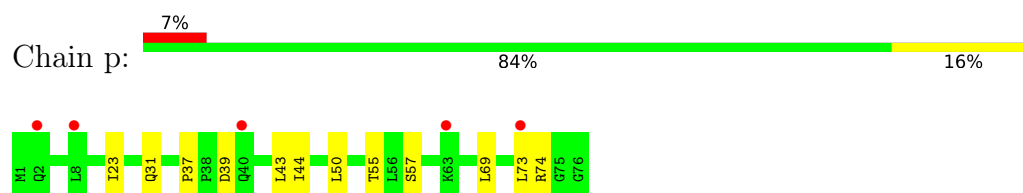
● Molecule 2: Polyubiquitin-C



● Molecule 2: Polyubiquitin-C



● Molecule 2: Polyubiquitin-C



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.06Å 203.07Å 265.04Å 90.00° 107.14° 90.00°	Depositor
Resolution (Å)	126.63 – 2.81 126.63 – 2.81	Depositor EDS
% Data completeness (in resolution range)	44.2 (126.63-2.81) 41.4 (126.63-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.19rc7_4070	Depositor
R, R_{free}	0.228 , 0.288 0.230 , 0.287	Depositor DCC
R_{free} test set	4457 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	33767	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/2131	0.28	0/2903
1	G	0.11	0/2112	0.29	0/2880
1	M	0.13	0/2103	0.32	0/2871
1	S	0.15	0/2101	0.35	0/2871
1	Y	0.17	0/2120	0.34	0/2893
1	e	0.13	0/2109	0.34	0/2877
1	k	0.11	0/2125	0.31	0/2897
2	B	0.11	0/588	0.28	0/792
2	C	0.08	0/601	0.24	0/809
2	D	0.09	0/449	0.25	0/616
2	E	0.09	0/584	0.26	0/789
2	F	0.12	0/595	0.28	0/802
2	H	0.21	0/585	0.31	0/788
2	I	0.11	0/597	0.32	0/805
2	J	0.07	0/497	0.21	0/679
2	K	0.09	0/568	0.29	0/770
2	L	0.13	0/599	0.31	0/808
2	N	0.10	0/588	0.28	0/792
2	O	0.12	0/595	0.33	0/802
2	P	0.07	0/444	0.22	0/611
2	Q	0.13	0/551	0.31	0/745
2	R	0.15	0/561	0.27	0/761
2	T	0.09	0/588	0.26	0/792
2	U	0.08	0/601	0.27	0/809
2	V	0.16	0/423	0.28	0/584
2	W	0.10	0/561	0.29	0/760
2	X	0.10	0/570	0.26	0/773
2	Z	0.12	0/584	0.30	0/788
2	a	0.10	0/599	0.32	0/807
2	b	0.15	0/468	0.34	0/641
2	c	0.08	0/572	0.28	0/773
2	d	0.10	0/591	0.28	0/798

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	f	0.30	0/575	0.46	0/777
2	g	0.10	0/605	0.28	0/813
2	h	0.16	0/443	0.28	0/609
2	i	0.10	0/528	0.27	0/719
2	j	0.12	0/558	0.34	0/757
2	l	0.09	0/584	0.27	0/788
2	m	0.12	0/602	0.32	0/811
2	n	0.07	0/461	0.26	0/636
2	o	0.09	0/551	0.28	0/749
2	p	0.10	0/607	0.27	0/816
All	All	0.13	0/34274	0.30	0/46561

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2083	0	2010	45	0
1	G	2064	0	1968	60	0
1	M	2055	0	1937	63	0
1	S	2053	0	1921	63	0
1	Y	2072	0	1975	62	0
1	e	2062	0	1970	66	0
1	k	2077	0	1985	44	0
2	B	582	0	608	10	0
2	C	595	0	616	5	0
2	D	445	0	315	4	0
2	E	578	0	582	8	0
2	F	589	0	607	20	0
2	H	579	0	598	20	0
2	I	591	0	605	13	0
2	J	492	0	403	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	562	0	559	17	0
2	L	593	0	607	14	0
2	N	582	0	608	14	0
2	O	589	0	602	18	0
2	P	441	0	303	3	0
2	Q	545	0	545	13	0
2	R	555	0	538	13	0
2	T	582	0	607	8	0
2	U	595	0	616	12	0
2	V	421	0	279	4	0
2	W	555	0	557	14	0
2	X	565	0	557	9	0
2	Z	578	0	596	9	0
2	a	593	0	612	11	0
2	b	464	0	350	10	0
2	c	566	0	563	7	0
2	d	585	0	599	16	0
2	f	569	0	576	14	0
2	g	599	0	621	13	0
2	h	439	0	293	3	0
2	i	522	0	481	15	0
2	j	552	0	529	13	0
2	l	578	0	596	13	0
2	m	596	0	615	13	0
2	n	458	0	336	3	0
2	o	545	0	536	8	0
2	p	601	0	629	9	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
4	S	1	0	0	0	0
5	A	4	0	0	1	0
5	E	1	0	0	0	0
5	G	3	0	0	0	0
5	M	2	0	0	0	0
5	T	2	0	0	0	0
5	Y	1	0	0	0	0
5	Z	1	0	0	0	0
5	e	1	0	0	0	0
5	m	1	0	0	0	0
All	All	33767	0	32410	699	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 11.

The worst 5 of 699 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:S:375:ILE:HD11	1:S:378:ILE:CG1	2.04	0.87
1:Y:375:ILE:HD11	1:Y:378:ILE:HD11	1.55	0.87
1:S:375:ILE:HD11	1:S:378:ILE:HG12	1.58	0.85
2:b:36:ILE:HG22	2:b:41:GLN:HE21	1.43	0.83
1:S:329:ILE:HG12	1:S:354:GLU:HG2	1.60	0.82

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 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	260/273 (95%)	251 (96%)	9 (4%)	0	100	100
1	G	260/273 (95%)	240 (92%)	20 (8%)	0	100	100
1	M	261/273 (96%)	245 (94%)	15 (6%)	1 (0%)	30	58
1	S	261/273 (96%)	248 (95%)	13 (5%)	0	100	100
1	Y	261/273 (96%)	246 (94%)	15 (6%)	0	100	100
1	e	261/273 (96%)	248 (95%)	12 (5%)	1 (0%)	30	58
1	k	261/273 (96%)	244 (94%)	17 (6%)	0	100	100
2	B	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
2	C	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	D	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	E	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
2	F	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	H	71/76 (93%)	71 (100%)	0	0	100	100
2	I	74/76 (97%)	72 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	K	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
2	L	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
2	N	71/76 (93%)	71 (100%)	0	0	100	100
2	O	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	P	74/76 (97%)	74 (100%)	0	0	100	100
2	Q	69/76 (91%)	67 (97%)	2 (3%)	0	100	100
2	R	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
2	T	71/76 (93%)	71 (100%)	0	0	100	100
2	U	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	V	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	W	70/76 (92%)	65 (93%)	5 (7%)	0	100	100
2	X	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	Z	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
2	a	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	b	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
2	c	71/76 (93%)	71 (100%)	0	0	100	100
2	d	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	f	71/76 (93%)	64 (90%)	7 (10%)	0	100	100
2	g	74/76 (97%)	74 (100%)	0	0	100	100
2	h	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	i	71/76 (93%)	66 (93%)	5 (7%)	0	100	100
2	j	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	l	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
2	m	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
2	n	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
2	o	70/76 (92%)	69 (99%)	1 (1%)	0	100	100
2	p	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
All	All	4371/4571 (96%)	4194 (96%)	175 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	284	PRO
1	e	266	ALA

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	231/248 (93%)	224 (97%)	7 (3%)	36	69
1	G	225/248 (91%)	220 (98%)	5 (2%)	45	77
1	M	222/248 (90%)	214 (96%)	8 (4%)	31	64
1	S	221/248 (89%)	213 (96%)	8 (4%)	31	64
1	Y	227/248 (92%)	221 (97%)	6 (3%)	40	73
1	e	224/248 (90%)	216 (96%)	8 (4%)	31	64
1	k	227/248 (92%)	222 (98%)	5 (2%)	45	77
2	B	67/68 (98%)	66 (98%)	1 (2%)	57	83
2	C	67/68 (98%)	65 (97%)	2 (3%)	36	69
2	D	20/68 (29%)	20 (100%)	0	100	100
2	E	64/68 (94%)	62 (97%)	2 (3%)	35	69
2	F	64/68 (94%)	63 (98%)	1 (2%)	55	82
2	H	66/68 (97%)	61 (92%)	5 (8%)	12	35
2	I	66/68 (97%)	66 (100%)	0	100	100
2	J	35/68 (52%)	34 (97%)	1 (3%)	37	71
2	K	61/68 (90%)	57 (93%)	4 (7%)	15	41
2	L	66/68 (97%)	65 (98%)	1 (2%)	57	83
2	N	67/68 (98%)	67 (100%)	0	100	100
2	O	65/68 (96%)	63 (97%)	2 (3%)	35	69
2	P	20/68 (29%)	19 (95%)	1 (5%)	22	53
2	Q	59/68 (87%)	57 (97%)	2 (3%)	32	66
2	R	55/68 (81%)	52 (94%)	3 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	67/68 (98%)	65 (97%)	2 (3%)	36	69
2	U	67/68 (98%)	67 (100%)	0	100	100
2	V	15/68 (22%)	14 (93%)	1 (7%)	15	40
2	W	62/68 (91%)	62 (100%)	0	100	100
2	X	59/68 (87%)	57 (97%)	2 (3%)	32	66
2	Z	66/68 (97%)	64 (97%)	2 (3%)	36	69
2	a	66/68 (97%)	66 (100%)	0	100	100
2	b	26/68 (38%)	26 (100%)	0	100	100
2	c	62/68 (91%)	62 (100%)	0	100	100
2	d	64/68 (94%)	60 (94%)	4 (6%)	16	43
2	f	63/68 (93%)	62 (98%)	1 (2%)	55	82
2	g	67/68 (98%)	65 (97%)	2 (3%)	36	69
2	h	18/68 (26%)	18 (100%)	0	100	100
2	i	49/68 (72%)	46 (94%)	3 (6%)	17	44
2	j	54/68 (79%)	53 (98%)	1 (2%)	50	79
2	l	66/68 (97%)	65 (98%)	1 (2%)	57	83
2	m	66/68 (97%)	63 (96%)	3 (4%)	24	57
2	n	29/68 (43%)	26 (90%)	3 (10%)	7	22
2	o	59/68 (87%)	57 (97%)	2 (3%)	32	66
2	p	68/68 (100%)	68 (100%)	0	100	100
All	All	3512/4116 (85%)	3413 (97%)	99 (3%)	38	71

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	55	THR
1	e	338	ASP
1	Y	361	LEU
2	Z	57	SER
1	e	378	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	426	HIS
1	k	466	GLN
2	X	41	GLN
1	k	446	ASN
2	i	60	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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 ²)	Q<0.9
1	A	262/273 (95%)	0.23	7 (2%) 56 46	16, 36, 68, 108	0
1	G	262/273 (95%)	0.63	15 (5%) 29 22	34, 53, 85, 115	0
1	M	263/273 (96%)	1.13	38 (14%) 6 4	54, 80, 113, 134	0
1	S	261/273 (95%)	0.59	16 (6%) 27 20	24, 56, 94, 122	0
1	Y	263/273 (96%)	0.43	10 (3%) 44 35	33, 46, 77, 101	0
1	e	263/273 (96%)	0.81	25 (9%) 14 10	41, 62, 102, 130	0
1	k	263/273 (96%)	0.51	11 (4%) 40 32	32, 54, 93, 124	0
2	B	73/76 (96%)	0.05	0 100 100	12, 26, 42, 62	0
2	C	76/76 (100%)	0.27	2 (2%) 57 47	23, 43, 68, 79	0
2	D	36/76 (47%)	1.80	13 (36%) 1 0	77, 115, 144, 144	0
2	E	75/76 (98%)	0.40	3 (4%) 42 33	23, 57, 87, 117	0
2	F	76/76 (100%)	0.42	2 (2%) 57 47	18, 51, 81, 92	0
2	H	73/76 (96%)	0.62	2 (2%) 56 46	41, 62, 80, 83	0
2	I	76/76 (100%)	0.37	2 (2%) 57 47	38, 60, 82, 109	0
2	J	75/76 (98%)	2.06	36 (48%) 0 0	72, 126, 159, 176	0
2	K	74/76 (97%)	1.01	10 (13%) 7 5	44, 79, 99, 108	0
2	L	76/76 (100%)	1.43	15 (19%) 3 2	50, 97, 126, 150	0
2	N	73/76 (96%)	0.71	4 (5%) 30 23	52, 65, 84, 103	0
2	O	75/76 (98%)	1.28	18 (24%) 2 1	63, 85, 110, 128	0
2	P	52/76 (68%)	1.99	23 (44%) 0 0	80, 129, 149, 163	0
2	Q	71/76 (93%)	1.60	21 (29%) 1 1	69, 106, 127, 133	0
2	R	76/76 (100%)	2.25	42 (55%) 0 0	82, 117, 145, 154	0
2	T	73/76 (96%)	0.11	2 (2%) 56 46	17, 39, 60, 68	0
2	U	76/76 (100%)	0.01	0 100 100	21, 42, 67, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	V	41/76 (53%)	2.48	22 (53%) 0 0	67, 106, 137, 145	0
2	W	72/76 (94%)	1.20	12 (16%) 4 3	77, 95, 110, 116	0
2	X	76/76 (100%)	1.07	11 (14%) 6 4	55, 93, 126, 131	0
2	Z	73/76 (96%)	0.14	3 (4%) 41 32	21, 32, 51, 74	0
2	a	76/76 (100%)	0.48	3 (3%) 43 34	32, 52, 77, 89	0
2	b	63/76 (82%)	2.10	32 (50%) 0 0	78, 119, 146, 152	0
2	c	73/76 (96%)	0.96	6 (8%) 17 12	47, 74, 106, 122	0
2	d	76/76 (100%)	0.47	3 (3%) 43 34	35, 62, 89, 96	0
2	f	73/76 (96%)	0.77	7 (9%) 13 10	43, 63, 97, 112	0
2	g	76/76 (100%)	0.22	1 (1%) 75 66	35, 52, 75, 79	0
2	h	58/76 (76%)	2.13	28 (48%) 0 0	77, 116, 148, 159	0
2	i	73/76 (96%)	1.57	26 (35%) 1 0	69, 94, 120, 139	0
2	j	76/76 (100%)	1.76	29 (38%) 1 0	56, 98, 119, 135	0
2	l	73/76 (96%)	0.21	1 (1%) 73 64	27, 47, 71, 89	0
2	m	76/76 (100%)	0.65	4 (5%) 32 24	34, 61, 88, 97	0
2	n	64/76 (84%)	1.69	25 (39%) 1 0	69, 111, 141, 148	0
2	o	72/76 (94%)	0.94	13 (18%) 3 2	54, 80, 100, 113	0
2	p	76/76 (100%)	0.64	5 (6%) 24 17	46, 73, 111, 122	0
All	All	4310/4571 (94%)	0.82	548 (12%) 8 6	12, 64, 126, 176	0

The worst 5 of 548 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	9	THR	7.6
2	R	5	VAL	7.1
2	b	76	GLY	6.7
2	V	47	GLY	6.4
2	V	39	ASP	6.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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	A	601	1/1	0.88	0.10	49,49,49,49	0
4	NA	A	603	1/1	0.95	0.12	30,30,30,30	0
3	CL	A	602	1/1	0.97	0.09	66,66,66,66	0
4	NA	S	601	1/1	0.99	0.18	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.