Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2021 – 10:06 pm BST

PDB ID	:	7NPI
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 Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

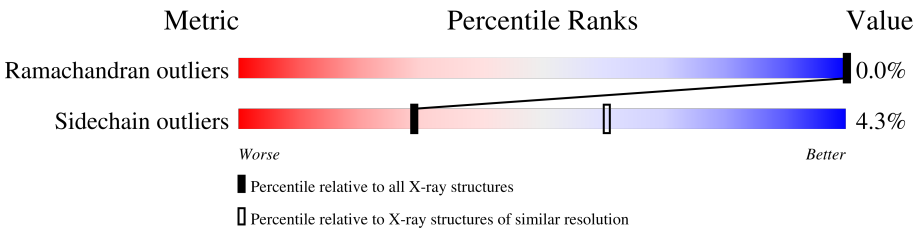
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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))
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	273	93%
1	G	273	91% 5%
1	M	273	94%
1	S	273	94%
1	Y	273	92%
1	e	273	91% 5%
1	k	273	93%
2	B	76	93%
2	C	76	100%

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Mol	Chain	Length	Quality of chain
2	D	76	99%
2	E	76	97%
2	F	76	95% 5%
2	H	76	91% 5%
2	I	76	97%
2	J	76	97%
2	K	76	96%
2	L	76	97%
2	N	76	92%
2	O	76	97%
2	P	76	100%
2	Q	76	91% 7%
2	R	76	95% 5%
2	T	76	93%
2	U	76	100%
2	V	76	100%
2	W	76	88% 7% 5%
2	X	76	95% 5%
2	Z	76	92%
2	a	76	100%
2	b	76	96%
2	c	76	96%
2	d	76	93% 7%
2	f	76	89% 7%
2	g	76	95% 5%

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Mol	Chain	Length	Quality of chain
2	h	76	100%
2	i	76	91% 5%
2	j	76	100%
2	l	76	91% 5%
2	m	76	95% 5%
2	n	76	95%
2	o	76	88% 7% 5%
2	p	76	99%

2 Entry composition (i)

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

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

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

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

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

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

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

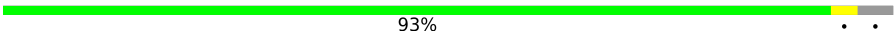
3 Residue-property plots (i)

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.

Note EDS failed to run properly.

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

Chain A:

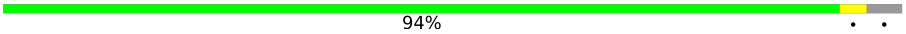


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

Chain G:

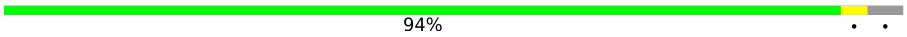
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

Chain M:



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

Chain S:

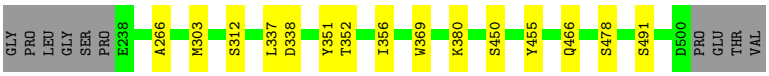


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

Chain Y:

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

Chain e:

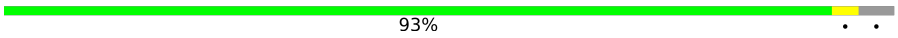


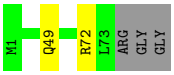
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

Chain k:

• Molecule 2: Polyubiquitin-C

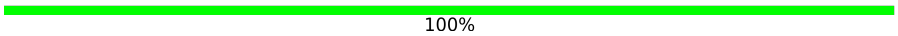
Chain B:





• Molecule 2: Polyubiquitin-C

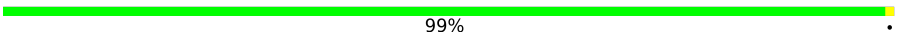
Chain C:



There are no outlier residues recorded for this chain.

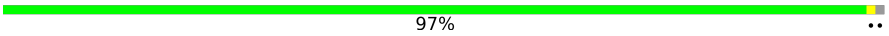
• Molecule 2: Polyubiquitin-C

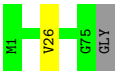
Chain D:



• Molecule 2: Polyubiquitin-C

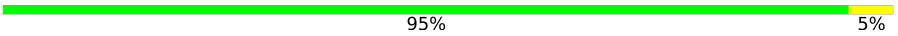
Chain E:





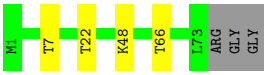
• Molecule 2: Polyubiquitin-C

Chain F:



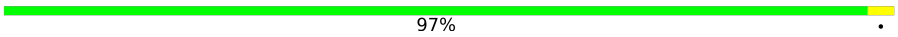
• Molecule 2: Polyubiquitin-C

Chain H:



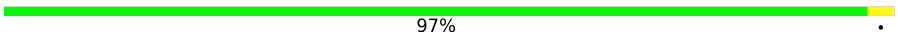
• Molecule 2: Polyubiquitin-C

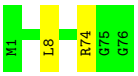
Chain I:



• Molecule 2: Polyubiquitin-C

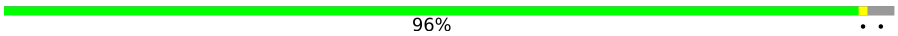
Chain J:

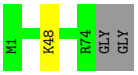




• Molecule 2: Polyubiquitin-C

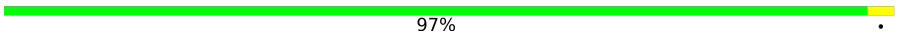
Chain K:





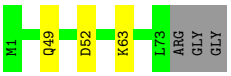
• Molecule 2: Polyubiquitin-C

Chain L:



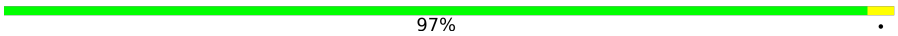
• Molecule 2: Polyubiquitin-C

Chain N:



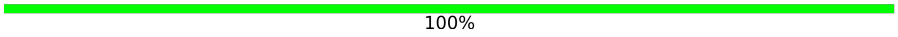
• Molecule 2: Polyubiquitin-C

Chain O:



• Molecule 2: Polyubiquitin-C

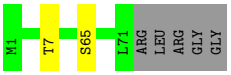
Chain P:



There are no outlier residues recorded for this chain.

• Molecule 2: Polyubiquitin-C

Chain Q: 91% • 7%

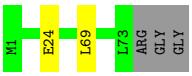


• Molecule 2: Polyubiquitin-C

Chain R: 95% 5%

• Molecule 2: Polyubiquitin-C

Chain T: 93% • •



• Molecule 2: Polyubiquitin-C

Chain U: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: Polyubiquitin-C

Chain V: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: Polyubiquitin-C

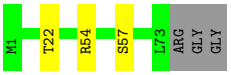
Chain W: 88% 7% 5%

• Molecule 2: Polyubiquitin-C

Chain X: 95% 5%

• Molecule 2: Polyubiquitin-C

Chain Z: 92% • •



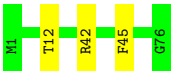
• Molecule 2: Polyubiquitin-C

Chain a: 100%

There are no outlier residues recorded for this chain.

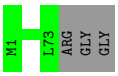
• Molecule 2: Polyubiquitin-C

Chain b: 96%



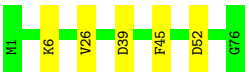
• Molecule 2: Polyubiquitin-C

Chain c: 96%



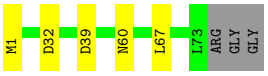
• Molecule 2: Polyubiquitin-C

Chain d: 93% 7%



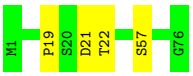
• Molecule 2: Polyubiquitin-C

Chain f: 89% 7%



• Molecule 2: Polyubiquitin-C

Chain g: 95% 5%



• Molecule 2: Polyubiquitin-C

Chain h: 100%

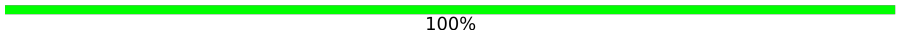
There are no outlier residues recorded for this chain.

• Molecule 2: Polyubiquitin-C

Chain i:

• Molecule 2: Polyubiquitin-C

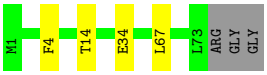
Chain j:



There are no outlier residues recorded for this chain.

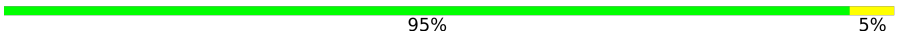
• Molecule 2: Polyubiquitin-C

Chain l:



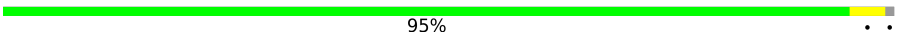
• Molecule 2: Polyubiquitin-C

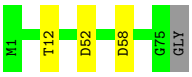
Chain m:



• Molecule 2: Polyubiquitin-C

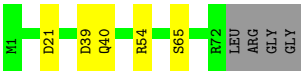
Chain n:





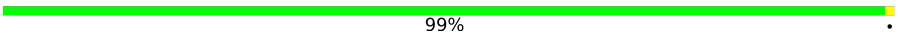
• Molecule 2: Polyubiquitin-C

Chain o:



• Molecule 2: Polyubiquitin-C

Chain p:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	44.2 (126.63-2.81)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.19rc7_4070	Depositor
R, R_{free}	0.228 , 0.288	Depositor
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.249	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.24	0/2131	0.43	0/2903
1	G	0.25	0/2112	0.45	0/2880
1	M	0.25	0/2103	0.47	0/2871
1	S	0.26	0/2101	0.46	0/2871
1	Y	0.26	0/2120	0.47	0/2893
1	e	0.26	0/2109	0.50	0/2877
1	k	0.25	0/2125	0.46	0/2897
2	B	0.25	0/588	0.50	0/792
2	C	0.24	0/601	0.49	0/809
2	D	0.24	0/449	0.49	0/616
2	E	0.24	0/584	0.47	0/789
2	F	0.24	0/595	0.50	0/802
2	H	0.25	0/585	0.49	0/788
2	I	0.25	0/597	0.50	0/805
2	J	0.24	0/497	0.47	0/679
2	K	0.24	0/568	0.51	0/770
2	L	0.24	0/599	0.51	0/808
2	N	0.24	0/588	0.50	0/792
2	O	0.24	0/595	0.51	0/802
2	P	0.22	0/444	0.49	0/611
2	Q	0.24	0/551	0.50	0/745
2	R	0.24	0/561	0.49	0/761
2	T	0.24	0/588	0.49	0/792
2	U	0.24	0/601	0.46	0/809
2	V	0.23	0/423	0.50	0/584
2	W	0.25	0/561	0.50	0/760
2	X	0.24	0/570	0.50	0/773
2	Z	0.24	0/584	0.53	0/788
2	a	0.24	0/599	0.52	0/807
2	b	0.26	0/468	0.56	0/641
2	c	0.24	0/572	0.49	0/773
2	d	0.23	0/591	0.50	0/798

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	f	0.35	0/575	0.59	0/777
2	g	0.24	0/605	0.49	0/813
2	h	0.25	0/443	0.51	0/609
2	i	0.24	0/528	0.48	0/719
2	j	0.24	0/558	0.54	0/757
2	l	0.24	0/584	0.49	0/788
2	m	0.24	0/602	0.53	0/811
2	n	0.23	0/461	0.50	0/636
2	o	0.24	0/551	0.49	0/749
2	p	0.24	0/607	0.51	0/816
All	All	0.25	0/34274	0.49	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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	34	64
1	S	261/273 (96%)	248 (95%)	13 (5%)	0	100	100
1	Y	261/273 (96%)	246 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	261/273 (96%)	248 (95%)	12 (5%)	1 (0%)	34	64
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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%)	41	73
1	G	225/248 (91%)	211 (94%)	14 (6%)	18	45
1	M	222/248 (90%)	216 (97%)	6 (3%)	44	77
1	S	221/248 (89%)	214 (97%)	7 (3%)	39	71
1	Y	227/248 (92%)	216 (95%)	11 (5%)	25	56
1	e	224/248 (90%)	210 (94%)	14 (6%)	18	44
1	k	227/248 (92%)	217 (96%)	10 (4%)	28	60
2	B	67/68 (98%)	65 (97%)	2 (3%)	41	73
2	C	67/68 (98%)	67 (100%)	0	100	100
2	D	20/68 (29%)	19 (95%)	1 (5%)	24	55
2	E	64/68 (94%)	63 (98%)	1 (2%)	62	87
2	F	64/68 (94%)	60 (94%)	4 (6%)	18	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	66/68 (97%)	62 (94%)	4 (6%)	18	46
2	I	66/68 (97%)	64 (97%)	2 (3%)	41	73
2	J	35/68 (52%)	33 (94%)	2 (6%)	20	49
2	K	61/68 (90%)	60 (98%)	1 (2%)	62	87
2	L	66/68 (97%)	64 (97%)	2 (3%)	41	73
2	N	67/68 (98%)	64 (96%)	3 (4%)	27	59
2	O	65/68 (96%)	63 (97%)	2 (3%)	40	72
2	P	20/68 (29%)	20 (100%)	0	100	100
2	Q	59/68 (87%)	57 (97%)	2 (3%)	37	69
2	R	55/68 (81%)	51 (93%)	4 (7%)	14	37
2	T	67/68 (98%)	65 (97%)	2 (3%)	41	73
2	U	67/68 (98%)	67 (100%)	0	100	100
2	V	15/68 (22%)	15 (100%)	0	100	100
2	W	62/68 (91%)	57 (92%)	5 (8%)	11	32
2	X	59/68 (87%)	55 (93%)	4 (7%)	16	40
2	Z	66/68 (97%)	63 (96%)	3 (4%)	27	59
2	a	66/68 (97%)	66 (100%)	0	100	100
2	b	26/68 (38%)	23 (88%)	3 (12%)	5	17
2	c	62/68 (91%)	62 (100%)	0	100	100
2	d	64/68 (94%)	59 (92%)	5 (8%)	12	33
2	f	63/68 (93%)	58 (92%)	5 (8%)	12	33
2	g	67/68 (98%)	63 (94%)	4 (6%)	19	47
2	h	18/68 (26%)	18 (100%)	0	100	100
2	i	49/68 (72%)	45 (92%)	4 (8%)	11	31
2	j	54/68 (79%)	54 (100%)	0	100	100
2	l	66/68 (97%)	62 (94%)	4 (6%)	18	46
2	m	66/68 (97%)	62 (94%)	4 (6%)	18	46
2	n	29/68 (43%)	26 (90%)	3 (10%)	7	21
2	o	59/68 (87%)	54 (92%)	5 (8%)	10	30
2	p	68/68 (100%)	67 (98%)	1 (2%)	65	88
All	All	3512/4116 (85%)	3361 (96%)	151 (4%)	29	60

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LEU
1	A	316	ARG
1	A	332	LYS
1	A	377	ASP
1	A	400	SER
1	A	425	TYR
1	A	464	THR
2	B	49	GLN
2	B	72	ARG
2	D	8	LEU
2	E	26	VAL
2	F	2	GLN
2	F	7	THR
2	F	45	PHE
2	F	52	ASP
1	G	254	ASN
1	G	315	GLN
1	G	324	SER
1	G	351	TYR
1	G	355	CYS
1	G	367	HIS
1	G	384	ASN
1	G	415	PHE
1	G	455	TYR
1	G	478	SER
1	G	479	LEU
1	G	481	ASN
1	G	485	ASP
1	G	491	SER
2	H	7	THR
2	H	22	THR
2	H	48	LYS
2	H	66	THR
2	I	20	SER
2	I	73	LEU
2	J	8	LEU
2	J	74	ARG
2	K	48	LYS
2	L	1	MET
2	L	39	ASP
1	M	251	LYS
1	M	291	THR

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Mol	Chain	Res	Type
1	M	305	ASP
1	M	324	SER
1	M	384	ASN
1	M	432	THR
2	N	49	GLN
2	N	52	ASP
2	N	63	LYS
2	O	1	MET
2	O	63	LYS
2	Q	7	THR
2	Q	65	SER
2	R	17	VAL
2	R	58	ASP
2	R	66	THR
2	R	72	ARG
1	S	255	THR
1	S	320	GLU
1	S	338	ASP
1	S	379	VAL
1	S	410	PHE
1	S	421	THR
1	S	487	ASN
2	T	24	GLU
2	T	69	LEU
2	W	6	LYS
2	W	20	SER
2	W	21	ASP
2	W	45	PHE
2	W	52	ASP
2	X	45	PHE
2	X	55	THR
2	X	60	ASN
2	X	72	ARG
1	Y	295	LEU
1	Y	329	ILE
1	Y	361	LEU
1	Y	377	ASP
1	Y	388	ASN
1	Y	423	LEU
1	Y	440	LEU
1	Y	441	CYS
1	Y	455	TYR

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Mol	Chain	Res	Type
1	Y	459	LEU
1	Y	491	SER
2	Z	22	THR
2	Z	54	ARG
2	Z	57	SER
2	b	12	THR
2	b	42	ARG
2	b	45	PHE
2	d	6	LYS
2	d	26	VAL
2	d	39	ASP
2	d	45	PHE
2	d	52	ASP
1	e	303	MET
1	e	312	SER
1	e	337	LEU
1	e	338	ASP
1	e	351	TYR
1	e	352	THR
1	e	356	ILE
1	e	369	TRP
1	e	380	LYS
1	e	450	SER
1	e	455	TYR
1	e	466	GLN
1	e	478	SER
1	e	491	SER
2	f	1	MET
2	f	32	ASP
2	f	39	ASP
2	f	60	ASN
2	f	67	LEU
2	g	19	PRO
2	g	21	ASP
2	g	22	THR
2	g	57	SER
2	i	4	PHE
2	i	21	ASP
2	i	42	ARG
2	i	55	THR
1	k	261	ASN
1	k	291	THR

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Mol	Chain	Res	Type
1	k	338	ASP
1	k	365	LEU
1	k	371	VAL
1	k	423	LEU
1	k	445	ARG
1	k	453	THR
1	k	478	SER
1	k	479	LEU
2	l	4	PHE
2	l	14	THR
2	l	34	GLU
2	l	67	LEU
2	m	7	THR
2	m	16	GLU
2	m	42	ARG
2	m	63	LYS
2	n	12	THR
2	n	52	ASP
2	n	58	ASP
2	o	21	ASP
2	o	39	ASP
2	o	40	GLN
2	o	54	ARG
2	o	65	SER
2	p	16	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	334	GLN
1	A	402	ASN
1	A	458	GLN
1	A	487	ASN
2	F	40	GLN
1	G	263	ASN
2	J	40	GLN
2	K	60	ASN
2	K	68	HIS
2	L	40	GLN
2	Q	31	GLN
1	S	448	HIS

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Mol	Chain	Res	Type
2	X	41	GLN
2	b	41	GLN
1	e	263	ASN
1	e	315	GLN
2	i	60	ASN
1	k	340	ASN
2	l	62	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.