



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 3, 2025 – 12:07 PM EDT

PDB ID : 9EHI / pdb_00009ehi
Title : Crystal structure of ENL YEATS in complex with histone H3 methacrylated at K18
Authors : Becht, D.C.; Selvam, K.; Kutateladze, T.G.
Deposited on : 2024-11-22
Resolution : 2.60 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

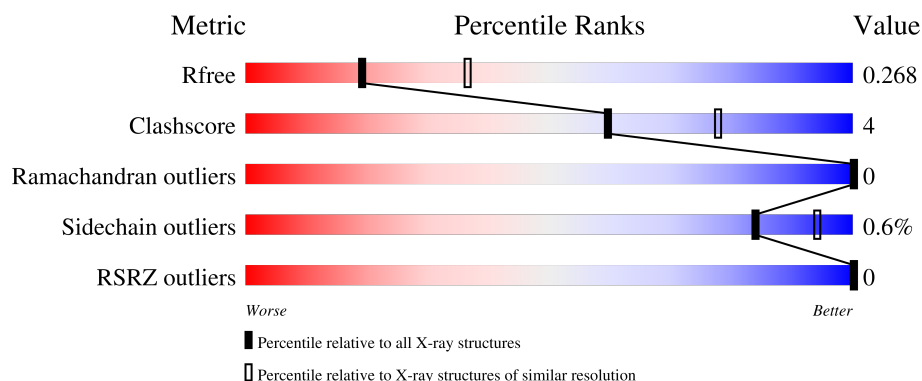
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	145	 90% 6% .
1	B	145	 88% 7% . .
1	C	145	 89% 10% .
1	D	145	 84% 12% . .
1	E	145	 88% 8% .

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Mol	Chain	Length	Quality of chain
1	F	145	 87% 9% .
1	G	145	 92% 5% .
1	H	145	 93% 5% .
1	I	145	 89% 8% .
1	J	145	 91% 6% ..
1	K	145	 86% 10% ..
1	L	145	 91% 7% ..
1	M	145	 89% 8% .
1	N	145	 88% 8% .
1	O	145	 88% 8% ..
1	P	145	 79% 13% .. 5%
2	Q	7	 86% 14%
2	R	7	 86% 14%
2	S	7	 43% 29% 29%
2	T	7	 86% 14%
2	U	7	 86% 14%
2	V	7	 71% 14% 14%
2	W	7	 71% 14% 14%
2	X	7	 29% 14% 29% 29%
2	Y	7	 86% 14%
2	Z	7	 57% 29% 14%
2	a	7	 86% 14%
2	b	7	 71% 29%
2	c	7	 86% 14%
2	d	7	 100%

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Mol	Chain	Length	Quality of chain
2	e	7	<div><div></div><div>86%</div><div>14%</div></div>
2	f	7	<div><div></div><div>57%</div><div>14%</div><div>29%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20056 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 Protein ENL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	1	0
			1159	750	204	197	8			
1	B	139	Total	C	N	O	S	0	3	0
			1165	754	204	197	10			
1	C	143	Total	C	N	O	S	0	1	0
			1192	770	209	204	9			
1	D	140	Total	C	N	O	S	0	1	0
			1167	755	205	198	9			
1	E	139	Total	C	N	O	S	0	3	0
			1166	755	204	197	10			
1	F	139	Total	C	N	O	S	0	1	0
			1161	749	205	198	9			
1	G	141	Total	C	N	O	S	0	0	0
			1170	756	206	199	9			
1	H	142	Total	C	N	O	S	0	1	0
			1182	763	208	201	10			
1	I	140	Total	C	N	O	S	0	0	0
			1164	751	206	199	8			
1	J	142	Total	C	N	O	S	0	0	0
			1180	760	209	202	9			
1	K	140	Total	C	N	O	S	0	1	0
			1167	754	205	199	9			
1	L	143	Total	C	N	O	S	0	2	0
			1202	777	210	206	9			
1	M	141	Total	C	N	O	S	0	1	0
			1161	752	205	196	8			
1	N	140	Total	C	N	O	S	4	0	0
			1163	751	205	198	9			
1	O	140	Total	C	N	O	S	0	3	0
			1180	762	210	199	9			
1	P	138	Total	C	N	O	S	3	0	0
			1142	738	200	196	8			

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	R	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	S	5	Total	C	N	O	4	0	0
			46	29	10	7			
2	T	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	U	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	V	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	W	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	X	5	Total	C	N	O	0	0	0
			46	29	10	7			
2	Y	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	Z	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	a	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	b	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	c	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	d	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	e	7	Total	C	N	O	0	0	0
			59	38	12	9			
2	f	5	Total	C	N	O	0	0	0
			46	29	10	7			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	I	1	Total	C	N	O	S	0	1
			24	12	2	8	2		
3	N	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	P	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	S	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	24	Total	O	0	0
			24	24		
4	C	15	Total	O	0	0
			15	15		
4	D	18	Total	O	0	0
			18	18		
4	E	29	Total	O	0	0
			29	29		
4	F	22	Total	O	0	0
			22	22		
4	G	18	Total	O	0	0
			18	18		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	20	Total 20	O 20	0	0
4	I	16	Total 16	O 16	0	0
4	J	24	Total 24	O 24	0	0
4	K	19	Total 19	O 19	0	0
4	L	23	Total 23	O 23	0	0
4	M	19	Total 19	O 19	0	0
4	N	17	Total 17	O 17	0	0
4	O	14	Total 14	O 14	0	0
4	P	15	Total 15	O 15	0	0
4	Q	7	Total 7	O 7	0	0
4	R	5	Total 5	O 5	0	0
4	S	1	Total 1	O 1	0	0
4	T	4	Total 4	O 4	0	0
4	U	3	Total 3	O 3	0	0
4	V	4	Total 4	O 4	0	0
4	W	3	Total 3	O 3	0	0
4	Y	2	Total 2	O 2	0	0
4	Z	2	Total 2	O 2	0	0
4	a	1	Total 1	O 1	0	0
4	b	2	Total 2	O 2	0	0
4	c	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	d	2	Total	O	0	0
			2	2		
4	e	1	Total	O	0	0
			1	1		
4	f	1	Total	O	0	0
			1	1		

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 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: Protein ENL

Chain A:  90% 6% .




- Molecule 1: Protein ENL

Chain B:  88% 7% . .




- Molecule 1: Protein ENL

Chain C:  89% 10% .




- Molecule 1: Protein ENL

Chain D:  84% 12% . .




- Molecule 1: Protein ENL

Chain E:  88% 8% .



- Molecule 1: Protein ENL

Chain F:  87% 9% .



• Molecule 1: Protein ENL

Chain G: 92% 5% .



• Molecule 1: Protein ENL

Chain H: 93% 5% .



• Molecule 1: Protein ENL

Chain I: 89% 8% .



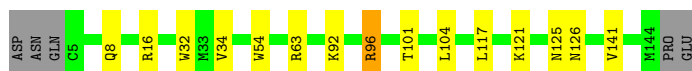
• Molecule 1: Protein ENL

Chain J: 91% 6% ..



• Molecule 1: Protein ENL

Chain K: 86% 10% ..



• Molecule 1: Protein ENL

Chain L: 91% 7% ..



• Molecule 1: Protein ENL

Chain M: 89% 8% .



- Molecule 1: Protein ENL

Chain N: 88% 8% .



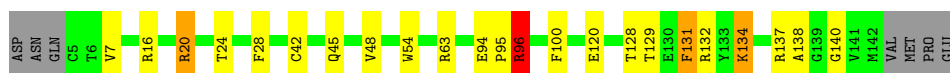
- Molecule 1: Protein ENL

Chain O: 88% 8% . .



- Molecule 1: Protein ENL

Chain P: 79% 13% . . 5%



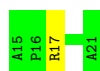
- Molecule 2: Histone H3.1

Chain Q: 86% 14%



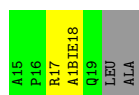
- Molecule 2: Histone H3.1

Chain R: 86% 14%



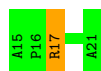
- Molecule 2: Histone H3.1

Chain S: 43% 29% 29%



- Molecule 2: Histone H3.1

Chain T: 86% 14%



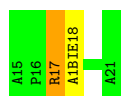
- Molecule 2: Histone H3.1

Chain U: 86% 14%



- Molecule 2: Histone H3.1

Chain V: 71% 14% 14%



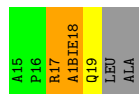
- Molecule 2: Histone H3.1

Chain W: 71% 14% 14%



- Molecule 2: Histone H3.1

Chain X: 29% 14% 29% 29%



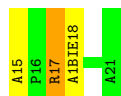
- Molecule 2: Histone H3.1

Chain Y: 86% 14%



- Molecule 2: Histone H3.1

Chain Z: 57% 29% 14%



- Molecule 2: Histone H3.1

Chain a: 86% 14%




- Molecule 2: Histone H3.1

Chain b:  71% 29%



- Molecule 2: Histone H3.1

Chain c:  86% 14%




- Molecule 2: Histone H3.1

Chain d:  100%

There are no outlier residues recorded for this chain.

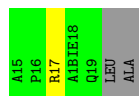
- Molecule 2: Histone H3.1

Chain e:  86% 14%



- Molecule 2: Histone H3.1

Chain f:  57% 14% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.46Å 98.41Å 118.45Å 87.59° 90.00° 90.02°	Depositor
Resolution (Å)	37.18 – 2.60 37.18 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.18-2.60) 97.7 (37.18-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.219 , 0.267 0.225 , 0.268	Depositor DCC
R_{free} test set	3588 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 15.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l 0.037 for -h,k,-l 0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20056	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2621e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1BIE, MES

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	0.40	0/1197	0.76	0/1619
1	B	0.43	0/1209	0.82	0/1635
1	C	0.41	0/1231	0.79	0/1665
1	D	0.41	0/1205	0.76	0/1629
1	E	0.42	0/1210	0.80	0/1636
1	F	0.39	0/1196	0.77	0/1617
1	G	0.41	0/1206	0.77	0/1631
1	H	0.41	0/1221	0.79	0/1651
1	I	0.39	0/1199	0.78	0/1621
1	J	0.43	0/1215	0.77	0/1642
1	K	0.39	0/1205	0.80	0/1629
1	L	0.41	0/1244	0.79	0/1682
1	M	0.38	0/1199	0.76	0/1623
1	N	0.41	0/1198	0.78	0/1619
1	O	0.38	0/1221	0.79	0/1649
1	P	0.47	0/1177	0.92	1/1592 (0.1%)
2	Q	0.44	0/44	1.02	0/57
2	R	0.50	0/44	0.79	0/57
2	S	0.56	0/31	0.89	0/39
2	T	0.40	0/44	1.02	0/57
2	U	0.55	0/44	0.95	0/57
2	V	0.43	0/44	1.16	0/57
2	W	0.44	0/44	1.03	0/57
2	X	0.53	0/31	1.20	0/39
2	Y	0.47	0/44	1.21	0/57
2	Z	0.43	0/44	0.84	0/57
2	a	0.41	0/44	0.95	0/57
2	b	0.42	0/44	1.10	0/57
2	c	0.41	0/44	1.32	0/57
2	d	0.40	0/44	1.06	0/57
2	e	0.45	0/44	1.05	0/57
2	f	0.53	0/31	1.16	0/39

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	0/19998	0.80	1/26998 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	2
1	F	0	1
1	I	0	1
1	J	0	3
1	K	0	2
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	4
1	P	0	4
2	Q	0	1
2	S	0	2
2	T	0	1
2	U	0	1
2	V	0	2
2	W	0	1
2	X	0	2
2	Y	0	1
2	Z	0	2
2	a	0	1
2	b	0	2
2	c	0	1
2	e	0	1
2	f	0	1
All	All	0	45

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	137	ARG	N-CA-C	-6.22	94.22	111.00

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Sidechain
1	B	137	ARG	Sidechain
1	C	16	ARG	Sidechain
1	D	16	ARG	Sidechain
1	D	96	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1159	0	1154	7	0
1	B	1165	0	1164	16	0
1	C	1192	0	1184	13	0
1	D	1167	0	1163	15	0
1	E	1166	0	1166	18	0
1	F	1161	0	1149	14	0
1	G	1170	0	1161	5	0
1	H	1182	0	1174	6	0
1	I	1164	0	1153	17	0
1	J	1180	0	1168	8	0
1	K	1167	0	1161	25	0
1	L	1202	0	1192	12	0
1	M	1161	0	1148	8	0
1	N	1163	0	1154	6	0
1	O	1180	0	1177	9	0
1	P	1142	0	1125	17	0
2	Q	59	0	48	1	0
2	R	59	0	48	1	0
2	S	46	0	32	0	0
2	T	59	0	48	1	0
2	U	59	0	48	0	0
2	V	59	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	59	0	48	1	0
2	X	46	0	32	2	0
2	Y	59	0	48	1	0
2	Z	59	0	48	2	0
2	a	59	0	48	0	0
2	b	59	0	48	0	0
2	c	59	0	48	0	0
2	d	59	0	48	0	0
2	e	59	0	48	0	0
2	f	46	0	32	0	0
3	B	12	0	13	1	0
3	I	24	0	26	0	0
3	N	12	0	13	0	0
3	P	12	0	13	0	0
3	S	12	0	13	0	0
4	A	24	0	0	0	0
4	B	24	0	0	0	0
4	C	15	0	0	1	0
4	D	18	0	0	2	0
4	E	29	0	0	2	0
4	F	22	0	0	0	0
4	G	18	0	0	1	0
4	H	20	0	0	2	0
4	I	16	0	0	1	0
4	J	24	0	0	1	0
4	K	19	0	0	0	0
4	L	23	0	0	1	0
4	M	19	0	0	1	0
4	N	17	0	0	1	0
4	O	14	0	0	0	0
4	P	15	0	0	0	0
4	Q	7	0	0	0	0
4	R	5	0	0	0	0
4	S	1	0	0	0	0
4	T	4	0	0	0	0
4	U	3	0	0	0	0
4	V	4	0	0	0	0
4	W	3	0	0	0	0
4	Y	2	0	0	0	0
4	Z	2	0	0	0	0
4	a	1	0	0	0	0
4	b	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	c	3	0	0	0	0
4	d	2	0	0	0	0
4	e	1	0	0	0	0
4	f	1	0	0	0	0
All	All	20056	0	19391	155	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 4.

The worst 5 of 155 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:B:34[B]:VAL:HG22	1:B:104:LEU:CD1	1.90	1.00
1:B:34[B]:VAL:CG2	1:B:104:LEU:CD1	2.41	0.98
1:A:15:HIS:CD2	1:A:104:LEU:HD12	2.10	0.85
1:I:72:LYS:CE	1:K:126:ASN:O	2.28	0.81
1:B:34[B]:VAL:HG22	1:B:104:LEU:HD11	1.63	0.80

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	138/145 (95%)	134 (97%)	4 (3%)	0	100	100
1	B	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
1	C	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
1	D	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
1	E	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
1	F	138/145 (95%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
1	H	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
1	I	138/145 (95%)	135 (98%)	3 (2%)	0	100	100
1	J	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
1	K	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
1	L	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
1	M	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
1	N	138/145 (95%)	133 (96%)	5 (4%)	0	100	100
1	O	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
1	P	136/145 (94%)	127 (93%)	9 (7%)	0	100	100
2	Q	4/7 (57%)	4 (100%)	0	0	100	100
2	R	4/7 (57%)	4 (100%)	0	0	100	100
2	S	2/7 (29%)	2 (100%)	0	0	100	100
2	T	4/7 (57%)	4 (100%)	0	0	100	100
2	U	4/7 (57%)	4 (100%)	0	0	100	100
2	V	4/7 (57%)	4 (100%)	0	0	100	100
2	W	4/7 (57%)	4 (100%)	0	0	100	100
2	X	2/7 (29%)	2 (100%)	0	0	100	100
2	Y	4/7 (57%)	4 (100%)	0	0	100	100
2	Z	4/7 (57%)	4 (100%)	0	0	100	100
2	a	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	b	4/7 (57%)	4 (100%)	0	0	100	100
2	c	4/7 (57%)	4 (100%)	0	0	100	100
2	d	4/7 (57%)	4 (100%)	0	0	100	100
2	e	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	f	2/7 (29%)	2 (100%)	0	0	100	100
All	All	2290/2432 (94%)	2224 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	129/134 (96%)	128 (99%)	1 (1%)	79	91
1	B	131/134 (98%)	130 (99%)	1 (1%)	79	91
1	C	133/134 (99%)	133 (100%)	0	100	100
1	D	130/134 (97%)	130 (100%)	0	100	100
1	E	131/134 (98%)	131 (100%)	0	100	100
1	F	129/134 (96%)	129 (100%)	0	100	100
1	G	130/134 (97%)	129 (99%)	1 (1%)	79	91
1	H	132/134 (98%)	131 (99%)	1 (1%)	79	91
1	I	129/134 (96%)	129 (100%)	0	100	100
1	J	131/134 (98%)	131 (100%)	0	100	100
1	K	130/134 (97%)	130 (100%)	0	100	100
1	L	134/134 (100%)	133 (99%)	1 (1%)	81	93
1	M	127/134 (95%)	126 (99%)	1 (1%)	79	91
1	N	129/134 (96%)	128 (99%)	1 (1%)	79	91
1	O	131/134 (98%)	130 (99%)	1 (1%)	79	91
1	P	126/134 (94%)	123 (98%)	3 (2%)	44	70
2	Q	4/4 (100%)	4 (100%)	0	100	100
2	R	4/4 (100%)	4 (100%)	0	100	100
2	S	3/4 (75%)	3 (100%)	0	100	100
2	T	4/4 (100%)	4 (100%)	0	100	100
2	U	4/4 (100%)	3 (75%)	1 (25%)	0	1
2	V	4/4 (100%)	4 (100%)	0	100	100
2	W	4/4 (100%)	3 (75%)	1 (25%)	0	1
2	X	3/4 (75%)	3 (100%)	0	100	100
2	Y	4/4 (100%)	4 (100%)	0	100	100
2	Z	4/4 (100%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	4/4 (100%)	4 (100%)	0	100	100
2	b	4/4 (100%)	4 (100%)	0	100	100
2	c	4/4 (100%)	4 (100%)	0	100	100
2	d	4/4 (100%)	4 (100%)	0	100	100
2	e	4/4 (100%)	4 (100%)	0	100	100
2	f	3/4 (75%)	3 (100%)	0	100	100
All	All	2143/2208 (97%)	2130 (99%)	13 (1%)	84	94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	142	MET
1	P	96	ARG
2	W	20	LEU
1	P	134	LYS
2	U	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	126	ASN
1	J	41	GLN
1	N	116	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	A1BIE	f	18	2	12,13,14	0.63	0	10,15,17	0.74	0
2	A1BIE	T	18	2	12,13,14	0.52	0	10,15,17	0.73	0
2	A1BIE	V	18	2	12,13,14	0.50	0	10,15,17	0.86	0
2	A1BIE	Z	18	2	12,13,14	0.50	0	10,15,17	0.67	0
2	A1BIE	b	18	2	12,13,14	0.57	0	10,15,17	0.75	0
2	A1BIE	X	18	2	12,13,14	0.57	0	10,15,17	0.59	0
2	A1BIE	U	18	2	12,13,14	0.54	0	10,15,17	0.56	0
2	A1BIE	d	18	2	12,13,14	0.55	0	10,15,17	1.09	0
2	A1BIE	e	18	2	12,13,14	0.75	0	10,15,17	0.74	0
2	A1BIE	Y	18	2	12,13,14	0.55	0	10,15,17	0.85	0
2	A1BIE	a	18	2	12,13,14	0.52	0	10,15,17	0.92	0
2	A1BIE	c	18	2	12,13,14	0.47	0	10,15,17	0.71	0
2	A1BIE	S	18	2	12,13,14	0.51	0	10,15,17	0.57	0
2	A1BIE	W	18	2	12,13,14	0.47	0	10,15,17	0.55	0
2	A1BIE	R	18	2	12,13,14	0.56	0	10,15,17	0.51	0
2	A1BIE	Q	18	2	12,13,14	0.43	0	10,15,17	0.93	0

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	A1BIE	f	18	2	-	4/13/14/16	-
2	A1BIE	T	18	2	-	3/13/14/16	-
2	A1BIE	V	18	2	-	3/13/14/16	-
2	A1BIE	Z	18	2	-	2/13/14/16	-
2	A1BIE	b	18	2	-	3/13/14/16	-
2	A1BIE	X	18	2	-	1/13/14/16	-
2	A1BIE	U	18	2	-	2/13/14/16	-
2	A1BIE	d	18	2	-	1/13/14/16	-
2	A1BIE	e	18	2	-	1/13/14/16	-
2	A1BIE	Y	18	2	-	4/13/14/16	-
2	A1BIE	a	18	2	-	5/13/14/16	-
2	A1BIE	c	18	2	-	1/13/14/16	-
2	A1BIE	S	18	2	-	3/13/14/16	-
2	A1BIE	W	18	2	-	4/13/14/16	-
2	A1BIE	R	18	2	-	2/13/14/16	-
2	A1BIE	Q	18	2	-	4/13/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	18	A1BIE	O-C-CA-CB
2	S	18	A1BIE	N-CA-CB-CG
2	S	18	A1BIE	C-CA-CB-CG
2	W	18	A1BIE	N-CA-CB-CG
2	a	18	A1BIE	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	18	A1BIE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands 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	$\# Z > 2$
3	MES	N	201	-	12,12,12	0.75	0	15,16,16	0.37	0
3	MES	S	101	-	12,12,12	0.76	0	15,16,16	0.37	0
3	MES	B	201	-	12,12,12	0.74	0	15,16,16	0.49	0
3	MES	I	201[B]	-	12,12,12	0.69	0	15,16,16	0.28	0
3	MES	I	201[A]	-	12,12,12	0.74	0	15,16,16	0.39	0
3	MES	P	201	-	12,12,12	0.78	0	15,16,16	0.42	0

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
3	MES	N	201	-	-	0/6/14/14	0/1/1/1
3	MES	S	101	-	-	1/6/14/14	0/1/1/1
3	MES	B	201	-	-	2/6/14/14	0/1/1/1
3	MES	I	201[B]	-	-	2/6/14/14	0/1/1/1
3	MES	I	201[A]	-	-	2/6/14/14	0/1/1/1
3	MES	P	201	-	-	2/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	201	MES	C8-C7-N4-C5
3	P	201	MES	N4-C7-C8-S
3	I	201[A]	MES	C8-C7-N4-C3
3	I	201[A]	MES	C8-C7-N4-C5
3	I	201[B]	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	MES	1	0

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	139/145 (95%)	-1.63	0 100 100	14, 29, 55, 73	1 (0%)
1	B	139/145 (95%)	-1.72	0 100 100	12, 26, 46, 56	3 (2%)
1	C	143/145 (98%)	-1.56	0 100 100	13, 32, 60, 85	1 (0%)
1	D	140/145 (96%)	-1.56	0 100 100	15, 31, 61, 78	1 (0%)
1	E	139/145 (95%)	-1.68	0 100 100	13, 27, 48, 68	3 (2%)
1	F	139/145 (95%)	-1.65	0 100 100	13, 30, 55, 79	1 (0%)
1	G	141/145 (97%)	-1.54	0 100 100	17, 32, 64, 77	0
1	H	142/145 (97%)	-1.58	0 100 100	18, 33, 59, 82	1 (0%)
1	I	140/145 (96%)	-1.43	0 100 100	22, 44, 81, 94	0
1	J	142/145 (97%)	-1.60	0 100 100	14, 30, 54, 72	0
1	K	140/145 (96%)	-1.44	0 100 100	15, 45, 90, 117	1 (0%)
1	L	143/145 (98%)	-1.61	0 100 100	13, 29, 57, 72	2 (1%)
1	M	141/145 (97%)	-1.54	0 100 100	22, 40, 64, 106	1 (0%)
1	N	140/145 (96%)	-1.53	0 100 100	22, 39, 65, 81	1 (0%)
1	O	140/145 (96%)	-1.42	0 100 100	17, 45, 85, 105	3 (2%)
1	P	138/145 (95%)	-1.42	0 100 100	26, 45, 85, 97	1 (0%)
2	Q	6/7 (85%)	-1.65	0 100 100	20, 24, 30, 33	0
2	R	6/7 (85%)	-1.58	0 100 100	22, 29, 31, 42	0
2	S	4/7 (57%)	-1.46	0 100 100	29, 33, 35, 37	1 (25%)
2	T	6/7 (85%)	-1.34	0 100 100	36, 38, 58, 68	0
2	U	6/7 (85%)	-1.65	0 100 100	23, 25, 32, 34	0
2	V	6/7 (85%)	-1.54	0 100 100	23, 25, 29, 31	0
2	W	6/7 (85%)	-1.33	0 100 100	39, 40, 52, 58	0
2	X	4/7 (57%)	-1.44	0 100 100	32, 36, 37, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9	
2	Y	6/7 (85%)	-1.33	0	100 100	40, 42, 76, 78	0
2	Z	6/7 (85%)	-1.33	0	100 100	33, 37, 76, 79	0
2	a	6/7 (85%)	-1.35	0	100 100	36, 41, 66, 75	0
2	b	6/7 (85%)	-1.25	0	100 100	33, 36, 77, 87	0
2	c	6/7 (85%)	-1.49	0	100 100	26, 32, 49, 57	0
2	d	6/7 (85%)	-1.66	0	100 100	29, 32, 43, 44	0
2	e	6/7 (85%)	-1.22	0	100 100	38, 43, 92, 95	0
2	f	4/7 (57%)	-1.52	0	100 100	37, 37, 40, 77	0
All	All	2336/2432 (96%)	-1.55	0	100 100	12, 34, 68, 117	21 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	A1BIE	Q	18	14/15	0.99	0.03	17,19,20,20	0
2	A1BIE	R	18	14/15	0.99	0.03	22,23,28,30	0
2	A1BIE	S	18	14/15	0.99	0.05	23,30,44,45	0
2	A1BIE	T	18	14/15	0.99	0.04	39,41,45,45	0
2	A1BIE	U	18	14/15	0.99	0.03	23,24,28,29	0
2	A1BIE	V	18	14/15	0.99	0.03	18,20,21,21	0
2	A1BIE	W	18	14/15	0.99	0.04	38,41,46,47	0
2	A1BIE	X	18	14/15	0.99	0.04	23,30,47,49	0
2	A1BIE	Y	18	14/15	0.99	0.05	43,56,62,65	0
2	A1BIE	Z	18	14/15	0.99	0.05	30,42,47,51	0
2	A1BIE	a	18	14/15	0.99	0.05	40,52,59,59	0
2	A1BIE	b	18	14/15	0.99	0.03	23,31,47,53	0
2	A1BIE	c	18	14/15	0.99	0.04	28,30,34,36	0
2	A1BIE	d	18	14/15	0.99	0.03	28,30,36,38	0
2	A1BIE	e	18	14/15	0.99	0.03	45,54,63,63	0
2	A1BIE	f	18	14/15	0.99	0.06	40,50,68,78	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
3	MES	N	201	12/12	0.96	0.07	86,90,106,112	0
3	MES	B	201	12/12	0.97	0.10	92,102,119,120	0
3	MES	S	101	12/12	0.97	0.07	96,108,129,133	0
3	MES	I	201[A]	12/12	0.98	0.06	51,56,72,81	12
3	MES	P	201	12/12	0.98	0.06	81,102,116,117	0
3	MES	I	201[B]	12/12	0.98	0.06	81,89,130,132	12

6.5 Other polymers [i](#)

There are no such residues in this entry.