



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:30 am BST

PDB ID : 5Z8N  
Title : Crystal structure of Arabidopsis thaliana EBS C-terminal deletion construct  
in complex with an H3K4me2 peptide  
Authors : Yang, Z.; Du, J.  
Deposited on : 2018-01-31  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

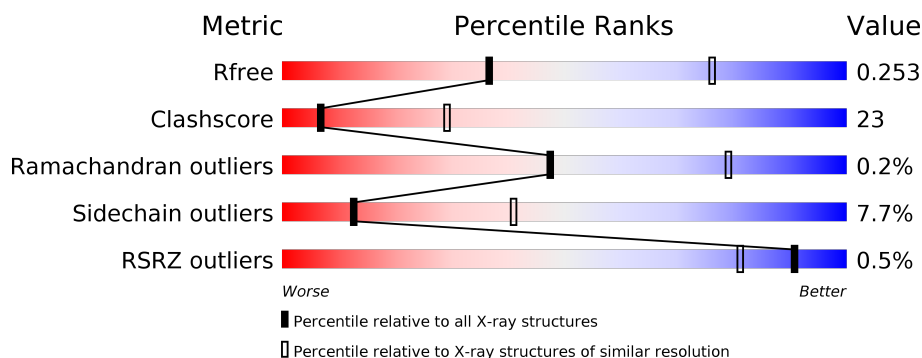
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	199	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 63%, yellow 25%, orange 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>63%</span> <span>25%</span> <span>• 8%</span> </div> </div>
1	B	199	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 59%, yellow 28%, orange 5%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>59%</span> <span>28%</span> <span>5% 9%</span> </div> </div>
1	C	199	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 25%, orange 7%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>61%</span> <span>25%</span> <span>7% 8%</span> </div> </div>
2	P	15	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 27%, yellow 7%, grey 67%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>27%</span> <span>7%</span> <span>67%</span> </div> </div>
2	Q	15	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 20%, yellow 27%, grey 53%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>20%</span> <span>27%</span> <span>53%</span> </div> </div>
2	R	15	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 20%, yellow 20%, orange 7%, grey 53%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>20%</span> <span>20%</span> <span>7% 53%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4544 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 Chromatin remodeling protein EBS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1463	916	258	274	15			
1	B	182	Total	C	N	O	S	0	0	0
			1459	914	257	273	15			
1	C	183	Total	C	N	O	S	0	0	0
			1463	916	258	274	15			

- Molecule 2 is a protein called H3K4me2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			43	26	10	7			
2	Q	7	Total	C	N	O	0	0	0
			55	33	12	10			
2	R	7	Total	C	N	O	0	0	0
			55	33	12	10			

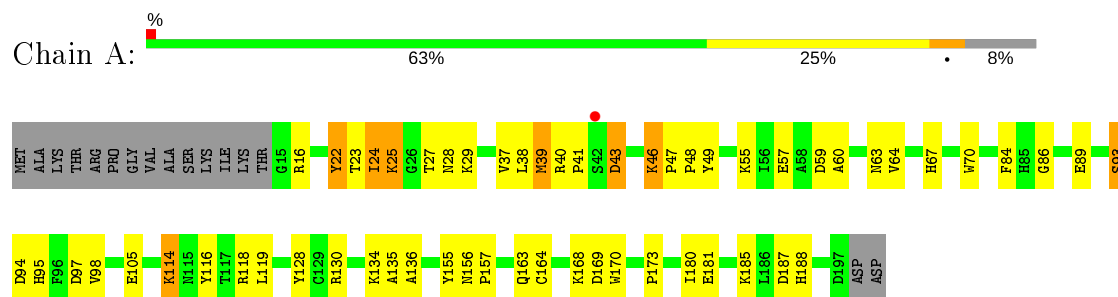
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

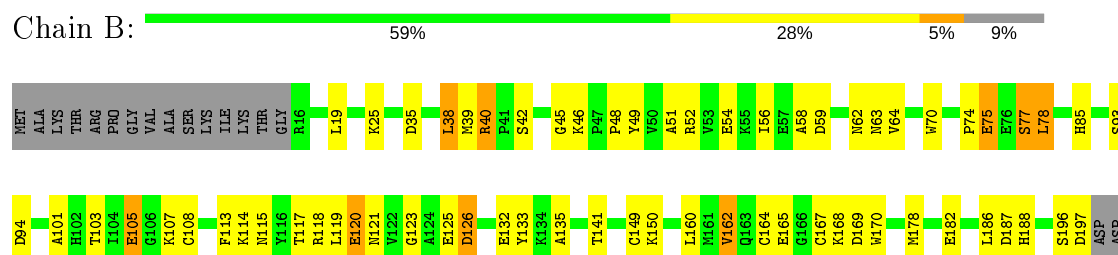
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

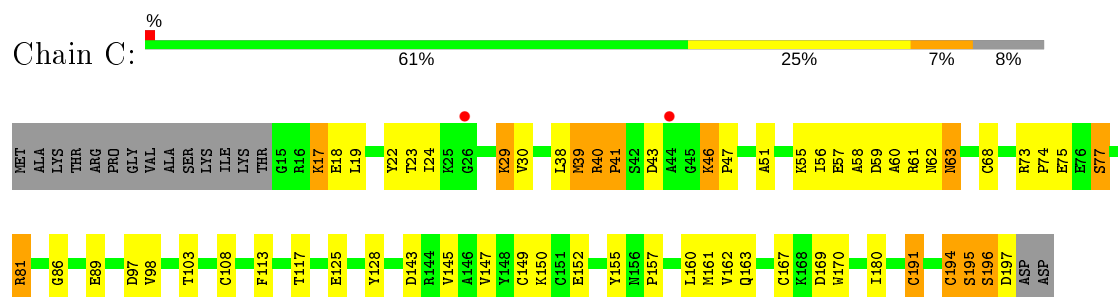
#### • Molecule 1: Chromatin remodeling protein EBS



#### • Molecule 1: Chromatin remodeling protein EBS




#### • Molecule 1: Chromatin remodeling protein EBS



#### • Molecule 2: H3K4me2 peptide




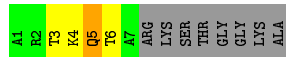
- Molecule 2: H3K4me2 peptide

Chain Q:  20% 27% 53%



- Molecule 2: H3K4me2 peptide

Chain R:  20% 20% 7% 53%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.46 Å   75.70 Å   80.36 Å 90.00°   115.41°   90.00°	Depositor
Resolution (Å)	40.99 – 3.10 40.99 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.99-3.10) 99.1 (40.99-3.09)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 3.12 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.213 , 0.252 0.214 , 0.253	Depositor DCC
$R_{free}$ test set	739 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.8	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MLY

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	0.34	0/1499	0.54	0/2023
1	B	0.46	0/1495	0.56	0/2018
1	C	0.45	0/1499	0.55	0/2023
2	P	0.21	0/31	0.49	0/40
2	Q	0.46	0/43	0.79	0/57
2	R	0.34	0/43	0.75	0/57
All	All	0.42	0/4610	0.56	0/6218

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](#)

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	1463	0	1390	72	0
1	B	1459	0	1388	56	0
1	C	1463	0	1391	78	0
2	P	43	0	50	3	0
2	Q	55	0	62	4	0
2	R	55	0	62	8	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
All	All	4544	0	4343	206	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 23.

All (206) 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:C:40:ARG:HG2	1:C:103:THR:HG23	1.19	1.12
1:B:77:SER:HB3	1:B:133:TYR:CZ	1.86	1.11
1:C:61:ARG:HB2	1:C:63:ASN:HD21	0.98	1.09
1:C:40:ARG:HG2	1:C:103:THR:CG2	1.93	0.99
1:C:19:LEU:HD11	1:C:58:ALA:HB3	1.42	0.98
1:A:46:LYS:HG3	1:A:47:PRO:HD2	1.49	0.94
1:C:61:ARG:HB2	1:C:63:ASN:ND2	1.82	0.94
1:B:59:ASP:CB	1:B:63:ASN:HB2	1.98	0.93
1:C:19:LEU:HD11	1:C:58:ALA:CB	1.98	0.92
1:A:27:THR:HG22	1:A:29:LYS:HE2	1.51	0.91
1:C:17:LYS:HD2	1:C:17:LYS:O	1.71	0.90
1:A:27:THR:O	1:A:27:THR:HG22	1.73	0.89
1:B:59:ASP:HB2	1:B:63:ASN:HB2	1.51	0.89
1:B:59:ASP:HB3	1:B:63:ASN:H	1.41	0.86
1:B:115:ASN:O	1:B:119:LEU:HD13	1.79	0.82
1:C:46:LYS:NZ	1:C:73:ARG:HH12	1.78	0.81
1:A:114:LYS:HD2	1:A:114:LYS:H	1.46	0.81
1:A:22:TYR:HE1	1:A:64:VAL:HG21	1.44	0.80
1:A:118:ARG:HH22	1:B:78:LEU:CD2	1.97	0.78
1:A:118:ARG:HH22	1:B:78:LEU:HD21	1.48	0.77
1:C:63:ASN:ND2	1:C:63:ASN:H	1.84	0.76
1:A:40:ARG:HB3	1:A:105:GLU:OE2	1.87	0.75
1:A:27:THR:HG22	1:A:29:LYS:HG2	1.69	0.74
1:B:46:LYS:N	1:B:46:LYS:HE2	2.03	0.73
1:B:77:SER:HB3	1:B:133:TYR:CE1	2.23	0.73
1:B:39:MET:HE3	1:B:103:THR:OG1	1.90	0.71
1:C:61:ARG:CB	1:C:63:ASN:HD21	1.92	0.70
1:B:59:ASP:HB3	1:B:63:ASN:N	2.06	0.70
1:C:40:ARG:O	1:C:40:ARG:HG3	1.91	0.70
1:A:40:ARG:N	1:A:105:GLU:OE2	2.25	0.69
1:C:47:PRO:HB2	1:C:73:ARG:HH21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:OE1	1:A:105:GLU:N	2.26	0.69
1:A:27:THR:O	1:A:27:THR:CG2	2.39	0.69
1:C:19:LEU:CD1	1:C:58:ALA:CB	2.73	0.67
1:C:160:LEU:HB2	2:R:5:GLN:NE2	2.09	0.67
1:C:169:ASP:OD1	1:C:170:TRP:N	2.28	0.67
1:A:93:SER:HG	1:A:95:HIS:H	1.41	0.67
1:A:93:SER:OG	1:A:94:ASP:N	2.24	0.66
1:C:47:PRO:HD2	1:C:73:ARG:NH2	2.10	0.66
1:A:169:ASP:OD1	1:A:170:TRP:N	2.29	0.66
1:A:86:GLY:H	1:A:89:GLU:HG3	1.61	0.66
1:B:120:GLU:OE1	1:B:121:ASN:HB3	1.96	0.65
1:B:39:MET:CE	1:B:103:THR:OG1	2.44	0.65
1:B:132:GLU:HB2	1:B:141:THR:HB	1.79	0.65
1:A:27:THR:HG22	1:A:29:LYS:CG	2.27	0.64
1:A:93:SER:OG	1:A:95:HIS:N	2.24	0.64
1:B:77:SER:HB3	1:B:133:TYR:CE2	2.33	0.64
1:A:181:GLU:N	1:A:181:GLU:OE1	2.31	0.63
1:A:41:PRO:HA	1:A:49:TYR:HE2	1.63	0.63
1:B:75:GLU:H	1:B:75:GLU:CD	2.00	0.63
1:B:59:ASP:OD1	1:B:63:ASN:HB2	1.99	0.62
1:B:187:ASP:OD1	1:B:188:HIS:N	2.32	0.62
1:B:19:LEU:HD11	1:B:58:ALA:HB2	1.79	0.62
1:C:46:LYS:NZ	1:C:73:ARG:NH1	2.48	0.62
1:A:27:THR:O	1:A:28:ASN:HB3	2.00	0.61
1:A:22:TYR:CE1	1:A:64:VAL:HG21	2.30	0.60
1:C:160:LEU:HD22	1:C:180:ILE:HG23	1.84	0.60
1:A:24:ILE:HG23	1:A:24:ILE:O	2.00	0.60
1:A:22:TYR:HE2	1:A:24:ILE:HA	1.66	0.59
1:A:27:THR:O	1:A:29:LYS:HE2	2.02	0.59
1:A:86:GLY:N	1:A:89:GLU:HG3	2.16	0.59
1:C:46:LYS:HZ2	1:C:73:ARG:HH12	1.49	0.59
1:A:43:ASP:OD1	1:A:43:ASP:N	2.35	0.59
1:C:75:GLU:H	1:C:75:GLU:CD	2.06	0.59
1:C:162:VAL:HG12	2:R:3:THR:HG22	1.83	0.59
1:B:94:ASP:OD1	1:B:94:ASP:N	2.36	0.59
1:B:114:LYS:HE2	1:B:118:ARG:NH1	2.17	0.58
1:C:63:ASN:HD22	1:C:63:ASN:H	1.49	0.58
1:C:46:LYS:HZ3	1:C:73:ARG:HH12	1.50	0.58
1:A:116:TYR:HA	1:A:119:LEU:HD23	1.85	0.58
1:A:38:LEU:O	1:A:105:GLU:OE1	2.21	0.58
1:C:39:MET:HG3	1:C:103:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:HB2	1:B:63:ASN:CB	2.28	0.57
1:B:169:ASP:OD1	1:B:170:TRP:N	2.36	0.57
1:B:35:ASP:OD2	1:B:107:LYS:NZ	2.30	0.57
1:A:22:TYR:CD2	1:A:23:THR:N	2.73	0.57
1:A:27:THR:CG2	1:A:29:LYS:HE2	2.30	0.57
1:A:16:ARG:HD3	1:A:59:ASP:HA	1.86	0.56
1:C:75:GLU:CD	1:C:81:ARG:HH11	2.09	0.56
1:B:196:SER:OG	1:B:197:ASP:N	2.38	0.56
1:C:167:CYS:HB2	1:C:169:ASP:H	1.71	0.56
1:C:97:ASP:OD1	1:C:98:VAL:N	2.39	0.56
1:A:97:ASP:OD1	1:A:98:VAL:N	2.37	0.55
1:C:51:ALA:HB1	1:C:68:CYS:HB2	1.87	0.55
1:A:24:ILE:HD12	1:A:25:LYS:N	2.21	0.55
1:C:41:PRO:HB2	1:C:46:LYS:HB3	1.89	0.55
1:C:74:PRO:HA	1:C:77:SER:OG	2.07	0.55
1:C:170:TRP:CZ3	2:R:4:MLY:HG3	2.42	0.55
1:B:160:LEU:HB2	2:Q:5:GLN:OE1	2.07	0.55
1:C:160:LEU:HB2	2:R:5:GLN:HE21	1.73	0.54
1:B:165:GLU:O	1:B:168:LYS:NZ	2.39	0.54
1:C:19:LEU:HD11	1:C:58:ALA:HB2	1.83	0.53
1:B:38:LEU:HB3	1:B:48:PRO:HB2	1.90	0.53
1:B:40:ARG:NE	1:B:105:GLU:HG3	2.24	0.53
1:C:47:PRO:O	1:C:73:ARG:NH2	2.42	0.53
1:C:125:GLU:N	1:C:125:GLU:OE1	2.41	0.53
1:B:59:ASP:CG	1:B:63:ASN:HB2	2.29	0.53
1:B:123:GLY:N	1:B:126:ASP:OD2	2.41	0.53
1:C:19:LEU:CD1	1:C:58:ALA:HB2	2.38	0.52
1:C:18:GLU:HA	1:C:56:ILE:O	2.09	0.52
1:A:118:ARG:NH1	1:B:75:GLU:O	2.42	0.52
1:C:23:THR:HG22	1:C:30:VAL:HG22	1.91	0.52
1:B:46:LYS:N	1:B:46:LYS:CD	2.73	0.51
1:B:46:LYS:N	1:B:46:LYS:CE	2.73	0.51
1:C:59:ASP:CG	1:C:60:ALA:H	2.13	0.51
1:B:46:LYS:HE2	1:B:46:LYS:H	1.75	0.51
1:A:59:ASP:OD2	1:A:60:ALA:N	2.42	0.50
1:A:164:CYS:O	1:A:168:LYS:HA	2.12	0.50
1:A:22:TYR:CD2	1:A:22:TYR:C	2.85	0.50
1:A:187:ASP:OD1	1:A:188:HIS:N	2.45	0.50
1:A:25:LYS:HE2	1:A:27:THR:OG1	2.11	0.50
1:A:89:GLU:HG2	1:A:128:TYR:CZ	2.47	0.49
1:A:70:TRP:O	1:A:93:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LEU:HD11	1:C:108:CYS:HB3	1.95	0.49
1:B:115:ASN:O	1:B:119:LEU:CD1	2.57	0.49
1:A:134:LYS:HE3	1:A:136:ALA:HB3	1.95	0.48
1:B:121:ASN:OD1	1:B:121:ASN:N	2.46	0.48
1:C:38:LEU:CD1	1:C:108:CYS:HB3	2.43	0.48
1:B:51:ALA:HB2	1:B:70:TRP:CZ3	2.49	0.48
1:C:170:TRP:CD1	2:R:4:MLY:HH22	2.49	0.48
1:C:46:LYS:HZ2	1:C:73:ARG:NH1	2.08	0.48
1:B:186:LEU:O	2:Q:1:ALA:N	2.42	0.48
1:A:25:LYS:HE2	1:A:25:LYS:HB3	1.59	0.47
1:B:162:VAL:HG12	2:Q:3:THR:HG22	1.95	0.47
1:A:40:ARG:CB	1:A:105:GLU:OE2	2.62	0.47
1:C:61:ARG:O	1:C:62:ASN:HB2	2.15	0.47
1:B:164:CYS:HB3	1:B:167:CYS:HB2	1.97	0.47
1:A:173:PRO:HG2	1:A:180:ILE:HD13	1.97	0.47
1:C:46:LYS:HZ3	1:C:73:ARG:NH1	2.11	0.47
1:C:143:ASP:N	1:C:143:ASP:OD2	2.48	0.47
1:C:18:GLU:N	1:C:57:GLU:HG2	2.30	0.47
1:A:24:ILE:HG22	1:A:29:LYS:HB2	1.97	0.46
1:A:89:GLU:OE1	1:A:130:ARG:NE	2.37	0.46
1:C:150:LYS:HD2	1:C:150:LYS:O	2.15	0.46
1:B:38:LEU:HD11	1:B:108:CYS:HB3	1.98	0.46
1:B:52:ARG:NH1	1:B:54:GLU:OE2	2.48	0.46
1:C:155:TYR:CE2	1:C:157:PRO:HA	2.50	0.46
1:C:163:GLN:HB2	1:C:170:TRP:CE3	2.51	0.46
1:B:45:GLY:C	1:B:46:LYS:HE2	2.35	0.46
1:C:149:CYS:SG	1:C:150:LYS:N	2.88	0.46
1:B:113:PHE:O	1:B:117:THR:HG23	2.17	0.45
1:C:191:CYS:HB3	1:C:194:CYS:H	1.80	0.45
1:A:155:TYR:CZ	1:A:157:PRO:HA	2.51	0.45
1:C:117:THR:HA	2:R:6:THR:HG21	1.99	0.45
1:A:24:ILE:CG2	1:A:29:LYS:HB2	2.46	0.45
1:C:41:PRO:HG3	1:C:46:LYS:O	2.16	0.45
1:A:181:GLU:O	1:A:185:LYS:HG2	2.17	0.45
1:C:147:VAL:CG2	1:C:152:GLU:C	2.85	0.45
1:C:41:PRO:O	1:C:43:ASP:N	2.45	0.45
1:A:22:TYR:CE2	1:A:23:THR:O	2.70	0.44
1:C:18:GLU:HA	1:C:57:GLU:HA	1.99	0.44
1:C:39:MET:HG3	1:C:103:THR:CG2	2.47	0.44
1:C:17:LYS:HD2	1:C:17:LYS:C	2.36	0.44
1:C:195:SER:O	1:C:196:SER:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG23	1:A:39:MET:HE3	2.00	0.44
1:B:178:MET:HG3	1:B:182:GLU:HB2	1.99	0.44
1:C:191:CYS:HB2	1:C:194:CYS:HB2	2.00	0.44
2:Q:5:GLN:HG3	2:Q:6:THR:N	2.32	0.44
1:C:147:VAL:HG22	1:C:152:GLU:C	2.39	0.44
1:B:133:TYR:CE2	1:B:135:ALA:HA	2.53	0.43
1:B:114:LYS:HE2	1:B:118:ARG:HH12	1.80	0.43
1:B:149:CYS:SG	1:B:150:LYS:N	2.91	0.43
1:C:160:LEU:HD11	2:R:3:THR:HB	2.00	0.43
1:C:81:ARG:HE	1:C:81:ARG:HB2	1.65	0.43
1:A:163:GLN:NE2	1:A:168:LYS:HG2	2.34	0.43
1:C:46:LYS:HD3	1:C:73:ARG:HH22	1.83	0.43
1:A:40:ARG:HG3	1:A:40:ARG:O	2.18	0.43
1:A:55:LYS:HB3	1:A:67:HIS:HB2	2.00	0.42
1:A:170:TRP:CZ3	2:P:4:MLY:HG2	2.54	0.42
1:C:59:ASP:CG	1:C:60:ALA:N	2.72	0.42
1:C:89:GLU:HG2	1:C:128:TYR:CZ	2.54	0.42
1:A:38:LEU:HD22	1:A:48:PRO:HG2	2.00	0.42
1:A:70:TRP:HE1	1:A:97:ASP:HB2	1.84	0.42
1:A:41:PRO:HB3	1:A:49:TYR:CE2	2.54	0.42
1:B:38:LEU:HD22	1:B:48:PRO:HG2	2.01	0.42
1:B:19:LEU:HD12	1:B:56:ILE:HG22	2.01	0.42
1:A:59:ASP:HB3	1:A:63:ASN:OD1	2.19	0.42
1:A:27:THR:O	1:A:29:LYS:HG2	2.19	0.42
1:B:39:MET:HE3	1:B:39:MET:HB3	1.74	0.42
1:C:160:LEU:HG	1:C:161:MET:N	2.34	0.42
1:A:27:THR:HG22	1:A:29:LYS:CE	2.36	0.41
1:C:74:PRO:O	1:C:77:SER:OG	2.37	0.41
1:B:49:TYR:HB3	1:B:70:TRP:CZ3	2.55	0.41
1:C:163:GLN:HB2	1:C:170:TRP:CZ3	2.54	0.41
1:C:75:GLU:N	1:C:75:GLU:CD	2.73	0.41
1:A:134:LYS:HD2	1:A:135:ALA:N	2.35	0.41
1:C:22:TYR:CE2	1:C:24:ILE:HA	2.55	0.41
1:A:84:PHE:HA	1:A:156:ASN:HB2	2.03	0.41
1:A:155:TYR:CZ	2:P:4:MLY:HD3	2.55	0.41
1:B:74:PRO:HB3	1:B:85:HIS:ND1	2.35	0.41
1:A:16:ARG:NH1	1:A:57:GLU:OE2	2.53	0.41
1:C:29:LYS:HA	1:C:29:LYS:HD3	1.49	0.41
1:C:81:ARG:HG3	1:C:81:ARG:O	2.19	0.41
1:C:86:GLY:N	1:C:89:GLU:HG3	2.36	0.41
1:C:40:ARG:CG	1:C:103:THR:CG2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HD2	1:A:25:LYS:O	2.20	0.41
1:A:46:LYS:HG3	1:A:47:PRO:CD	2.36	0.41
2:P:4:MLY:HD2	2:P:4:MLY:HH13	1.68	0.41
1:B:93:SER:HA	1:B:133:TYR:O	2.20	0.40
2:R:4:MLY:HH13	2:R:4:MLY:HD2	1.65	0.40
1:C:113:PHE:O	1:C:117:THR:HG23	2.22	0.40
1:A:114:LYS:O	1:A:118:ARG:HG3	2.21	0.40
1:A:24:ILE:O	1:A:27:THR:HB	2.22	0.40
1:B:64:VAL:HG12	1:B:101:ALA:HB2	2.03	0.40
1:C:43:ASP:HB2	1:C:46:LYS:HB2	2.04	0.40
1:A:37:VAL:CG2	1:A:39:MET:HE3	2.51	0.40

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	181/199 (91%)	178 (98%)	3 (2%)	0	100	100
1	B	180/199 (90%)	175 (97%)	5 (3%)	0	100	100
1	C	181/199 (91%)	172 (95%)	8 (4%)	1 (1%)	25	59
2	P	2/15 (13%)	2 (100%)	0	0	100	100
2	Q	4/15 (27%)	4 (100%)	0	0	100	100
2	R	4/15 (27%)	3 (75%)	1 (25%)	0	100	100
All	All	552/642 (86%)	534 (97%)	17 (3%)	1 (0%)	47	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	PRO

### 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	156/169 (92%)	148 (95%)	8 (5%)	24	56
1	B	156/169 (92%)	143 (92%)	13 (8%)	11	38
1	C	156/169 (92%)	141 (90%)	15 (10%)	8	31
2	P	3/9 (33%)	3 (100%)	0	100	100
2	Q	4/9 (44%)	4 (100%)	0	100	100
2	R	4/9 (44%)	3 (75%)	1 (25%)	0	2
All	All	479/534 (90%)	442 (92%)	37 (8%)	13	41

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	TYR
1	A	24	ILE
1	A	25	LYS
1	A	39	MET
1	A	43	ASP
1	A	46	LYS
1	A	93	SER
1	A	114	LYS
1	B	25	LYS
1	B	38	LEU
1	B	40	ARG
1	B	42	SER
1	B	62	ASN
1	B	75	GLU
1	B	77	SER
1	B	78	LEU
1	B	105	GLU
1	B	120	GLU
1	B	125	GLU
1	B	126	ASP
1	B	162	VAL
1	C	17	LYS

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Mol	Chain	Res	Type
1	C	29	LYS
1	C	39	MET
1	C	40	ARG
1	C	46	LYS
1	C	55	LYS
1	C	63	ASN
1	C	77	SER
1	C	81	ARG
1	C	145	VAL
1	C	191	CYS
1	C	194	CYS
1	C	195	SER
1	C	196	SER
1	C	197	ASP
2	R	5	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	63	ASN
2	R	5	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	MLY	Q	4	2	9,10,11	0.58	0	6,11,13	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLY	P	4	2	9,10,11	0.54	0	6,11,13	0.91	0
2	MLY	R	4	2	9,10,11	0.57	0	6,11,13	1.16	1 (16%)

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	MLY	Q	4	2	-	1/8/9/11	-
2	MLY	P	4	2	-	6/8/9/11	-
2	MLY	R	4	2	-	4/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	4	MLY	CH2-NZ-CH1	-2.17	104.11	109.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	4	MLY	N-CA-CB-CG
2	P	4	MLY	C-CA-CB-CG
2	P	4	MLY	O-C-CA-CB
2	R	4	MLY	CD-CE-NZ-CH1
2	P	4	MLY	CD-CE-NZ-CH1
2	P	4	MLY	CE-CD-CG-CB
2	Q	4	MLY	CE-CD-CG-CB
2	R	4	MLY	CA-CB-CG-CD
2	R	4	MLY	CE-CD-CG-CB
2	R	4	MLY	CD-CE-NZ-CH2
2	P	4	MLY	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	4	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	4	MLY	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	183/199 (91%)	-0.02	1 (0%) 91 81	51, 80, 124, 157	0
1	B	182/199 (91%)	-0.01	0 100 100	50, 83, 121, 163	0
1	C	183/199 (91%)	0.09	2 (1%) 80 64	59, 89, 132, 178	0
2	P	4/15 (26%)	0.66	0 100 100	89, 96, 97, 103	0
2	Q	6/15 (40%)	0.02	0 100 100	77, 82, 85, 98	0
2	R	6/15 (40%)	-0.12	0 100 100	71, 77, 79, 94	0
All	All	564/642 (87%)	0.02	3 (0%) 91 81	50, 84, 125, 178	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	ALA	4.3
1	A	42	SER	3.5
1	C	26	GLY	2.1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLY	Q	4	11/12	0.91	0.29	57,67,81,82	0
2	MLY	R	4	11/12	0.92	0.26	57,68,81,81	0
2	MLY	P	4	11/12	0.93	0.31	52,66,89,91	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	C	302	1/1	0.93	0.19	86,86,86,86	0
3	ZN	B	302	1/1	0.93	0.18	85,85,85,85	0
3	ZN	A	302	1/1	0.98	0.20	83,83,83,83	0
3	ZN	A	301	1/1	0.98	0.20	76,76,76,76	0
3	ZN	C	301	1/1	0.99	0.17	79,79,79,79	0
3	ZN	B	301	1/1	0.99	0.16	65,65,65,65	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.