



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:36 am BST

PDB ID : 2Q8D  
Title : Crystal structure of JMJ2D2A in ternary complex with histone H3-K36me2 and succinate  
Authors : Couture, J.-F.; Collazo, E.; Ortiz-Tello, P.; Brunzelle, J.S.; Trievel, R.C.  
Deposited on : 2007-06-10  
Resolution : 2.29 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

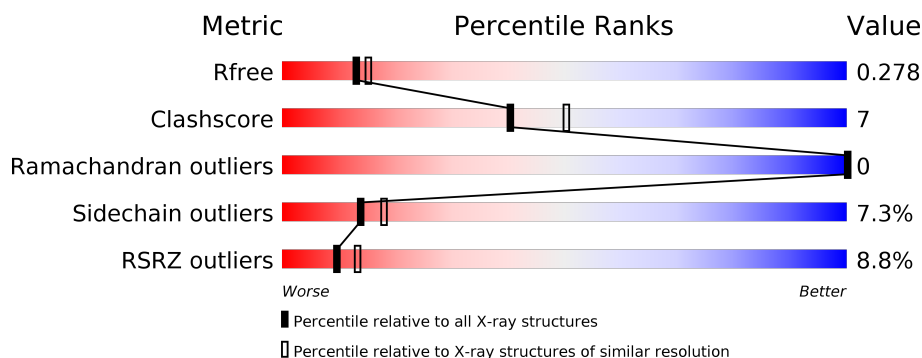
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	352	<div> <div>8%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	B	352	<div> <div>8%</div> <div>75%</div> <div>18%</div> <div>..</div> </div>
2	F	16	<div> <div>13%</div> <div>19%</div> <div>6%</div> <div>75%</div> </div>
2	G	16	<div> <div>19%</div> <div>31%</div> <div>69%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLY	F	36	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5916 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 JmjC domain-containing histone demethylation protein 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	1	0
			2824	1824	468	517	15			
1	B	338	Total	C	N	O	S	0	6	0
			2792	1804	474	498	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP O75164
A	0	SER	-	CLONING ARTIFACT	UNP O75164
B	-1	GLY	-	CLONING ARTIFACT	UNP O75164
B	0	SER	-	CLONING ARTIFACT	UNP O75164

- Molecule 2 is a protein called HISTONE 3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	4	Total	C	N	O	0	0	0
			26	17	5	4			
2	G	5	Total	C	N	O	0	0	0
			30	19	6	5			

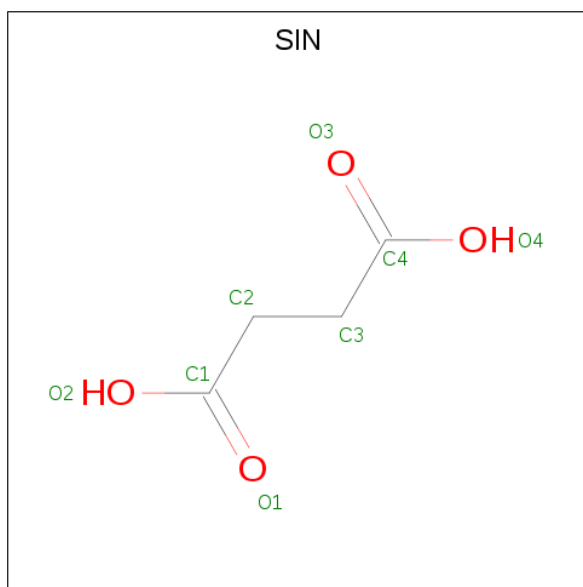
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

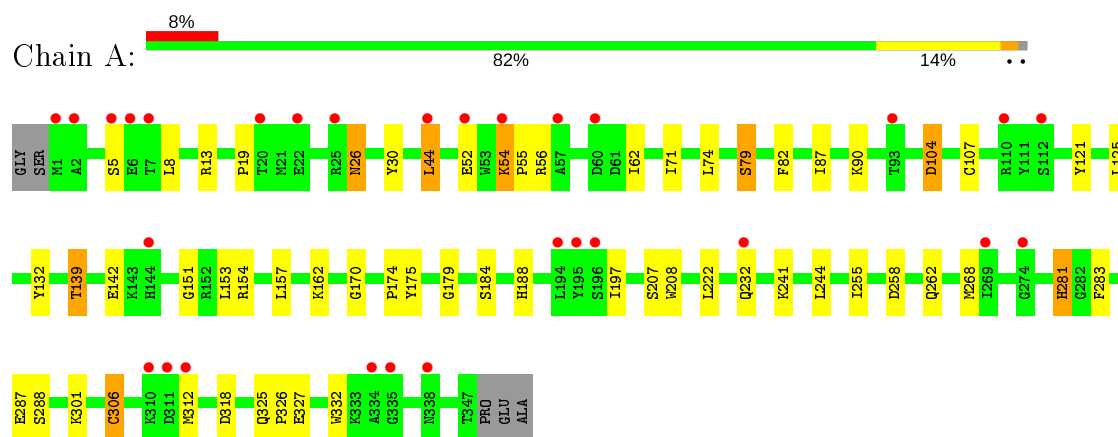
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total	O	0	0
			112	112		
6	B	112	Total	O	0	0
			112	112		

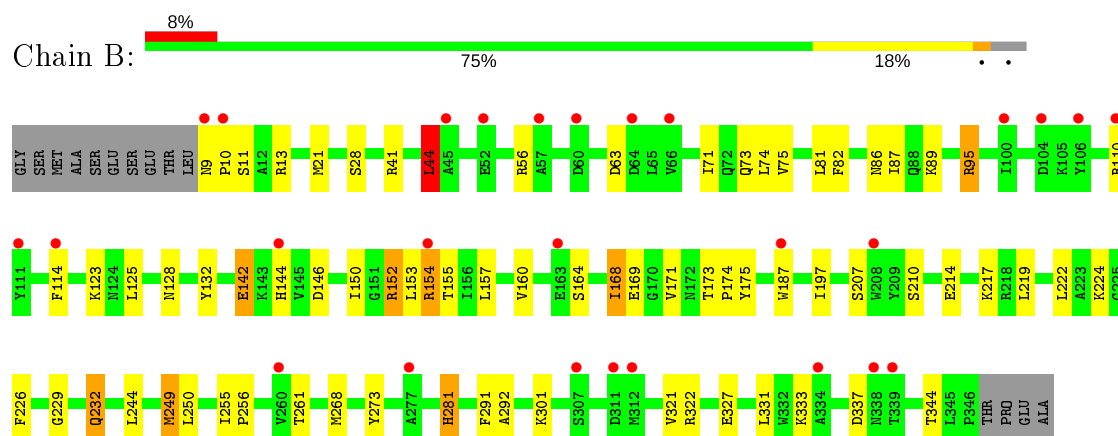
### 3 Residue-property plots [i](#)

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: JmjC domain-containing histone demethylation protein 3A



- Molecule 1: JmjC domain-containing histone demethylation protein 3A



- Molecule 2: HISTONE 3 peptide



- Molecule 2: HISTONE 3 peptide

Chain G:



ARG	LYS	SER	ALA	PRO	ALA	T32	G33	G34	V35	K36	LYS	PRO	HIS	ARG	TYR
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.86 Å   148.64 Å   57.35 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	37.80 – 2.29 37.87 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.80-2.29) 97.0 (37.87-2.29)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.204   ,   0.251 0.239   ,   0.278	Depositor DCC
$R_{free}$ test set	1927 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.53	0/2915	0.63	0/3951
1	B	0.55	2/2909 (0.1%)	0.70	3/3939 (0.1%)
2	F	0.89	0/14	0.61	0/17
2	G	0.78	0/18	0.62	0/22
All	All	0.55	2/5856 (0.0%)	0.67	3/7929 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	ARG	CZ-NH1	6.71	1.41	1.33
1	B	95	ARG	NE-CZ	5.83	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ARG	NE-CZ-NH2	-13.69	113.45	120.30
1	B	95	ARG	NE-CZ-NH1	12.91	126.76	120.30
1	B	44	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2824	0	2714	34	0
1	B	2792	0	2702	46	0
2	F	26	0	30	2	0
2	G	30	0	31	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	8	0	4	0	0
5	B	8	0	4	0	0
6	A	112	0	0	5	0
6	B	112	0	0	4	0
All	All	5916	0	5485	80	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 7.

All (80) 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:9:ASN:HB3	1:B:10:PRO:CD	1.74	1.17
1:B:9:ASN:CB	1:B:10:PRO:HD3	1.80	1.11
1:B:9:ASN:HB3	1:B:10:PRO:HD3	0.91	0.91
1:A:222:LEU:HD22	1:A:255:ILE:HD11	1.59	0.83
1:A:154:ARG:HD2	6:A:525:HOH:O	1.79	0.81
1:B:74:LEU:HD22	1:B:87:ILE:HD11	1.63	0.79
1:B:74:LEU:CD2	1:B:87:ILE:HD11	2.12	0.79
1:A:312:MET:HE3	6:A:583:HOH:O	1.83	0.78
1:A:139:THR:HG23	1:A:287:GLU:OE1	1.85	0.76
1:A:139:THR:HG21	6:A:541:HOH:O	1.85	0.75
1:A:222:LEU:HD22	1:A:255:ILE:CD1	2.17	0.73
1:B:168:ILE:HB	1:B:171:VAL:HB	1.70	0.72
1:B:322:ARG:HD2	6:B:603:HOH:O	1.94	0.67
1:B:160:VAL:O	1:B:164:SER:HB2	1.95	0.66
1:B:222:LEU:HD22	1:B:255:ILE:CD1	2.27	0.64
1:B:81:LEU:HD11	1:B:226:PHE:HB3	1.81	0.62
1:B:114[B]:PHE:CE1	1:B:261:THR:HG21	2.35	0.62
1:B:214:GLU:HG3	6:B:513:HOH:O	2.00	0.62
1:A:44:LEU:HD22	1:A:268:MET:HE3	1.83	0.60
1:A:139:THR:CG2	1:A:287:GLU:OE1	2.50	0.60
1:B:217:LYS:HD2	1:B:273:TYR:OH	2.02	0.59
1:A:107:CYS:HB2	6:A:586:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:SER:OG	2:F:36:MLY:HH21	2.04	0.57
1:A:207:SER:OG	1:A:281:HIS:HE1	1.87	0.57
1:B:152:ARG:HE	1:B:154:ARG:HH12	1.53	0.57
1:B:74:LEU:HD21	1:B:87:ILE:HD11	1.87	0.56
1:A:74:LEU:HD23	1:A:87:ILE:HD12	1.86	0.56
1:B:155:THR:HG21	1:B:291:PHE:HB2	1.88	0.55
1:B:207:SER:OG	1:B:281:HIS:HE1	1.91	0.54
1:B:169:GLU:HA	1:B:173:THR:OG1	2.10	0.52
1:A:104:ASP:N	1:A:104:ASP:OD1	2.40	0.52
1:A:44:LEU:HD22	1:A:268:MET:CE	2.39	0.52
1:B:63:ASP:HB3	1:B:95:ARG:HB2	1.94	0.50
1:B:114[B]:PHE:HE1	1:B:261:THR:HG21	1.76	0.49
1:B:75:VAL:HG11	1:B:125:LEU:HG	1.94	0.49
1:B:81:LEU:HD11	1:B:226:PHE:CG	2.48	0.48
1:A:82:PHE:HB2	1:A:244:LEU:HB2	1.96	0.48
1:A:79:SER:OG	1:A:79:SER:O	2.27	0.48
1:B:150:ILE:HG22	1:B:174:PRO:HB3	1.95	0.48
1:B:74:LEU:HD22	1:B:87:ILE:CD1	2.40	0.48
1:A:13:ARG:HG3	1:A:258:ASP:OD2	2.13	0.48
1:A:5:SER:HA	1:A:8:LEU:HD12	1.97	0.47
1:A:170:GLY:O	2:F:36:MLY:HH23	2.15	0.47
1:B:56:ARG:HA	1:B:142:GLU:HG3	1.97	0.46
1:B:44:LEU:HD22	1:B:268:MET:HE3	1.98	0.46
1:B:81:LEU:HD11	1:B:226:PHE:CB	2.47	0.45
1:B:301:LYS:NZ	1:B:337:ASP:OD1	2.50	0.45
1:A:56:ARG:HA	1:A:142:GLU:HG3	1.98	0.45
1:A:74:LEU:CD2	1:A:87:ILE:HD12	2.47	0.45
1:A:301:LYS:HE3	1:A:332:TRP:CD1	2.53	0.44
1:B:154:ARG:HG2	6:B:582:HOH:O	2.18	0.44
1:B:301:LYS:HD3	1:B:321:VAL:HG22	1.99	0.43
1:A:327:GLU:OE1	6:A:595:HOH:O	2.21	0.43
1:A:54:LYS:HA	1:A:55:PRO:HD3	1.84	0.43
1:B:255:ILE:HA	1:B:256:PRO:HD3	1.80	0.43
1:B:41:ARG:HD2	1:B:344:THR:HA	2.00	0.43
1:A:188:HIS:CD2	1:A:241:LYS:HE2	2.53	0.43
1:B:146:ASP:OD2	1:B:152:ARG:NH2	2.51	0.43
1:B:81:LEU:HG	1:B:249[B]:MET:SD	2.58	0.43
1:B:73:GLN:HG2	1:B:86:ASN:ND2	2.33	0.43
1:B:10:PRO:HA	1:B:13:ARG:HB2	1.99	0.43
1:B:9:ASN:ND2	6:B:523:HOH:O	2.52	0.43
1:A:153:LEU:HD11	1:A:197:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:CYS:SG	1:A:312:MET:HG3	2.59	0.42
1:B:155:THR:HB	1:B:292:ALA:O	2.19	0.42
1:A:26:ASN:C	1:A:26:ASN:HD22	2.23	0.42
1:B:44:LEU:HD12	1:B:210:SER:HB2	2.02	0.42
1:A:208:TRP:HE1	1:A:262:GLN:NE2	2.16	0.42
1:B:229:GLY:O	1:B:232:GLN:HG3	2.19	0.42
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.54	0.42
1:A:179:GLY:O	1:A:283:PHE:HA	2.20	0.42
1:B:82:PHE:HB2	1:B:244:LEU:HB2	2.02	0.42
1:B:142:GLU:HB2	1:B:144:HIS:CE1	2.55	0.41
1:B:187:TRP:CZ2	1:B:250:LEU:HD11	2.54	0.41
1:A:121:TYR:O	1:A:125:LEU:HB3	2.21	0.41
1:A:325:GLN:N	1:A:326:PRO:HD3	2.36	0.41
1:B:153:LEU:HD11	1:B:197:ILE:HG21	2.03	0.41
1:A:151:GLY:HA2	1:A:174:PRO:HG3	2.02	0.40
1:B:301:LYS:HD3	1:B:321:VAL:CG2	2.51	0.40
1:B:222:LEU:HD22	1:B:255:ILE:HD12	2.01	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	346/352 (98%)	341 (99%)	5 (1%)	0	100	100
1	B	342/352 (97%)	338 (99%)	4 (1%)	0	100	100
2	F	2/16 (12%)	2 (100%)	0	0	100	100
2	G	3/16 (19%)	2 (67%)	1 (33%)	0	100	100
All	All	693/736 (94%)	683 (99%)	10 (1%)	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	299/308 (97%)	280 (94%)	19 (6%)	17	23
1	B	298/308 (97%)	272 (91%)	26 (9%)	10	12
2	F	1/11 (9%)	1 (100%)	0	100	100
2	G	1/11 (9%)	1 (100%)	0	100	100
All	All	599/638 (94%)	554 (92%)	45 (8%)	14	17

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	44	LEU
1	A	52	GLU
1	A	54	LYS
1	A	62	ILE
1	A	71	ILE
1	A	79	SER
1	A	90	LYS
1	A	104	ASP
1	A	132	TYR
1	A	139	THR
1	A	157	LEU
1	A	162	LYS
1	A	175	TYR
1	A	184	SER
1	A	232	GLN
1	A	281	HIS
1	A	306	CYS
1	A	318	ASP
1	B	11	SER
1	B	21	MET
1	B	28	SER
1	B	44	LEU
1	B	71	ILE

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Mol	Chain	Res	Type
1	B	89	LYS
1	B	110	ARG
1	B	123	LYS
1	B	128[A]	ASN
1	B	128[B]	ASN
1	B	132	TYR
1	B	142	GLU
1	B	152	ARG
1	B	154	ARG
1	B	157	LEU
1	B	168	ILE
1	B	175	TYR
1	B	219	LEU
1	B	224	LYS
1	B	232	GLN
1	B	249[A]	MET
1	B	249[B]	MET
1	B	281	HIS
1	B	327	GLU
1	B	331	LEU
1	B	333	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	84	GLN
1	A	86	ASN
1	A	232	GLN
1	A	262	GLN
1	A	281	HIS
1	B	9	ASN
1	B	86	ASN
1	B	262	GLN
1	B	281	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	F	36	2	9,10,11	0.55	0	6,11,13	0.30	0
2	MLY	G	36	2	9,10,11	0.66	0	6,11,13	0.61	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	MLY	F	36	2	-	2/8/9/11	-
2	MLY	G	36	2	-	1/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	36	MLY	CE-CD-CG-CB
2	F	36	MLY	CA-CB-CG-CD
2	G	36	MLY	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	36	MLY	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
5	SIN	A	503	3	1,7,7	0.52	0	2,8,8	2.43	1 (50%)
5	SIN	B	504	3	1,7,7	0.30	0	2,8,8	1.30	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
5	SIN	A	503	3	-	0/1/5/5	-
5	SIN	B	504	3	-	0/1/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	SIN	C2-C3-C4	-3.21	107.29	112.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	347/352 (98%)	0.53	29 (8%)	11 15	28, 35, 47, 57	1 (0%)
1	B	338/352 (96%)	0.64	27 (7%)	12 16	25, 34, 50, 54	2 (0%)
2	F	3/16 (18%)	3.00	2 (66%)	0 0	71, 71, 71, 72	0
2	G	4/16 (25%)	2.91	3 (75%)	0 0	60, 61, 62, 62	0
All	All	692/736 (94%)	0.61	61 (8%)	10 13	25, 35, 50, 72	3 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	ASN	5.8
1	B	10	PRO	4.9
1	B	110	ARG	4.8
1	B	60	ASP	4.7
2	F	34	GLY	4.1
1	A	112	SER	4.1
1	A	1	MET	4.0
2	G	33	GLY	4.0
2	G	34	GLY	3.8
1	B	311	ASP	3.7
1	B	154	ARG	3.7
1	B	338	ASN	3.7
1	B	57	ALA	3.6
2	F	35	VAL	3.3
1	A	196	SER	3.2
1	A	52	GLU	3.0
1	A	335	GLY	3.0
1	A	57	ALA	3.0
1	A	2	ALA	2.9
1	B	114[A]	PHE	2.9
1	A	44	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	7	THR	2.8
1	B	307	SER	2.8
1	A	5	SER	2.7
1	A	334	ALA	2.7
1	A	25	ARG	2.6
1	B	163	GLU	2.6
1	A	311	ASP	2.6
1	A	93	THR	2.6
1	B	339	THR	2.6
1	A	338	ASN	2.5
1	B	52	GLU	2.5
1	A	110	ARG	2.5
1	B	277	ALA	2.4
1	B	187	TRP	2.4
1	A	310	LYS	2.4
1	A	274	GLY	2.4
2	G	32	THR	2.4
1	A	54	LYS	2.3
1	B	104	ASP	2.3
1	B	208	TRP	2.3
1	B	260	VAL	2.3
1	B	45	ALA	2.3
1	B	100	ILE	2.3
1	A	6	GLU	2.3
1	B	64	ASP	2.3
1	B	111	TYR	2.3
1	A	194	LEU	2.2
1	B	144	HIS	2.2
1	A	22	GLU	2.2
1	A	269	ILE	2.2
1	A	232	GLN	2.2
1	B	312	MET	2.1
1	B	106	TYR	2.1
1	A	312	MET	2.1
1	A	20	THR	2.1
1	B	334	ALA	2.1
1	B	66	VAL	2.1
1	A	195	TYR	2.1
1	A	144	HIS	2.0
1	A	60	ASP	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
2	MLY	F	36	11/12	0.55	0.42	64,69,71,71	0
2	MLY	G	36	11/12	0.80	0.22	49,53,58,58	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
5	SIN	B	504	8/8	0.86	0.20	31,35,36,37	0
5	SIN	A	503	8/8	0.88	0.55	24,28,30,31	8
3	NI	B	502	1/1	0.98	0.19	40,40,40,40	0
3	NI	A	501	1/1	0.98	0.16	39,39,39,39	0
4	ZN	B	506	1/1	0.99	0.05	36,36,36,36	0
4	ZN	A	505	1/1	0.99	0.07	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.