

# wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 06:36 AM EST

PDB ID : 6BZF

Title: Structure of S. cerevisiae Zip2:Spo16 complex, C2 form

Authors : Arora, K.; Corbett, K.D.

Deposited on : 2017-12-23

Resolution : 2.29 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 (i) 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 (1)) 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 : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

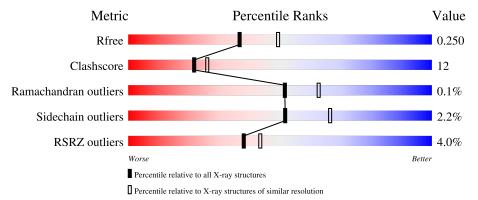
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.29 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
$R_{free}$	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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% 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 chai	n			
1	٨	016	4%				
1	A	216	62%		29%		9%
1	E	216	57%	23%		19%	_
			2%				
2	В	206	78%			21%	
			3%				
3	С	216	72%		19%	g	9%
			7%				
3	G	216	59%	20%	•	19%	



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			1 0		
Mol	Chain	Length	Quality of chain		
	-	200	<u>%</u>		
4	D	206	76%	22%	•
			3%		
5	F	206	78%	20%	•••
			2%		
5	Н	206	79%	17%	



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13182 atoms, of which 1 is hydrogen 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 Sporulation-specific protein 16.

$\mathbf{Mol}$	Chain	Residues		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace
1	A	197	Total 1627	C 1044	11	O 308	S 3	0	0	0
1	E	175	Total 1440	C 936		O 267	S 2	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP P17122
A	-16	LYS	-	expression tag	UNP P17122
A	-15	SER	-	expression tag	UNP P17122
A	-14	SER	-	expression tag	UNP P17122
A	-13	HIS	-	expression tag	UNP P17122
A	-12	HIS	-	expression tag	UNP P17122
A	-11	HIS	-	expression tag	UNP P17122
A	-10	HIS	-	expression tag	UNP P17122
A	-9	HIS	-	expression tag	UNP P17122
A	-8	HIS	-	expression tag	UNP P17122
A	-7	GLU	-	expression tag	UNP P17122
A	-6	ASN	-	expression tag	UNP P17122
A	-5	LEU	-	expression tag	UNP P17122
A	-4	TYR	-	expression tag	UNP P17122
A	-3	PHE	-	expression tag	UNP P17122
A	-2	GLN	-	expression tag	UNP P17122
A	-1	SER	-	expression tag	UNP P17122
A	0	ASN	-	expression tag	UNP P17122
A	1	ALA	-	expression tag	UNP P17122
Е	-17	MET	-	expression tag	UNP P17122
Е	-16	LYS	-	expression tag	UNP P17122
Е	-15	SER	-	expression tag	UNP P17122
Е	-14	SER	-	expression tag	UNP P17122
Е	-13	HIS	-	expression tag	UNP P17122
Е	-12	HIS	-	expression tag	UNP P17122



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Chain	Residue	Modelled	Actual	Comment	Reference
Е	-11	HIS	-	expression tag	UNP P17122
E	-10	HIS	-	expression tag	UNP P17122
E	-9	HIS	-	expression tag	UNP P17122
E	-8	HIS	-	expression tag	UNP P17122
E	-7	GLU	-	expression tag	UNP P17122
E	-6	ASN	-	expression tag	UNP P17122
E	-5	LEU	_	expression tag	UNP P17122
E	-4	TYR	-	expression tag	UNP P17122
E	-3	PHE	_	expression tag	UNP P17122
E	-2	GLN	-	expression tag	UNP P17122
E	-1	SER	-	expression tag	UNP P17122
Е	0	ASN	-	expression tag	UNP P17122
E	1	ALA	-	expression tag	UNP P17122

• Molecule 2 is a protein called Protein ZIP2.

$\mathbf{Mol}$	Chain	Residues		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace
9	В	206	Total	С	N	О	S	0	0	0
2	Ъ	200	1735	1131	279	316	9	0	U	

• Molecule 3 is a protein called Sporulation-specific protein 16.

Mol	Chain	Residues		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace
2	С	197	Total	С	N	О	S	0	0	0
		191	1625	1046	267	309	3	0	0	U
9	С	174	Total	С	N	О	S	0	0	0
3	3 G	174	1411	910	236	262	3	0	U	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-17	MET	-	expression tag	UNP P17122
С	-16	LYS	-	expression tag	UNP P17122
С	-15	SER	-	expression tag	UNP P17122
С	-14	SER	-	expression tag	UNP P17122
С	-13	HIS	-	expression tag	UNP P17122
С	-12	HIS	-	expression tag	UNP P17122
С	-11	HIS	_	expression tag	UNP P17122
С	-10	HIS	-	expression tag	UNP P17122
С	-9	HIS	-	expression tag	UNP P17122
С	-8	HIS	-	expression tag	UNP P17122
С	-7	GLU	_	expression tag	UNP P17122



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Chain	Residue	Modelled	Actual	Comment	Reference
С	-6	ASN	-	expression tag	UNP P17122
С	-5	LEU	-	expression tag	UNP P17122
С	-4	TYR	-	expression tag	UNP P17122
С	-3	PHE	-	expression tag	UNP P17122
С	-2	GLN	-	expression tag	UNP P17122
С	-1	SER	-	expression tag	UNP P17122
С	0	ASN	-	expression tag	UNP P17122
С	1	ALA	-	expression tag	UNP P17122
G	-17	MET	-	expression tag	UNP P17122
G	-16	LYS	-	expression tag	UNP P17122
G	-15	SER	-	expression tag	UNP P17122
G	-14	SER	-	expression tag	UNP P17122
G	-13	HIS	-	expression tag	UNP P17122
G	-12	HIS	-	expression tag	UNP P17122
G	-11	HIS	-	expression tag	UNP P17122
G	-10	HIS	-	expression tag	UNP P17122
G	-9	HIS	-	expression tag	UNP P17122
G	-8	HIS	-	expression tag	UNP P17122
G	-7	GLU	-	expression tag	UNP P17122
G	-6	ASN	-	expression tag	UNP P17122
G	-5	LEU	-	expression tag	UNP P17122
G	-4	TYR	-	expression tag	UNP P17122
G	-3	PHE	-	expression tag	UNP P17122
G	-2	GLN	-	expression tag	UNP P17122
G	-1	SER		expression tag	UNP P17122
G	0	ASN	-	expression tag	UNP P17122
G	1	ALA	-	expression tag	UNP P17122

 $\bullet$  Molecule 4 is a protein called Protein ZIP2.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
4	D	206	Total 1737	C 1133	N 279	O 316	S 9	0	0	0

• Molecule 5 is a protein called Protein ZIP2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	204	Total C H N O S 1705 1112 1 274 309 9	0	0	0
5	Н	200	Total C N O S 1678 1096 270 303 9	0	0	0



#### • Molecule 6 is water.

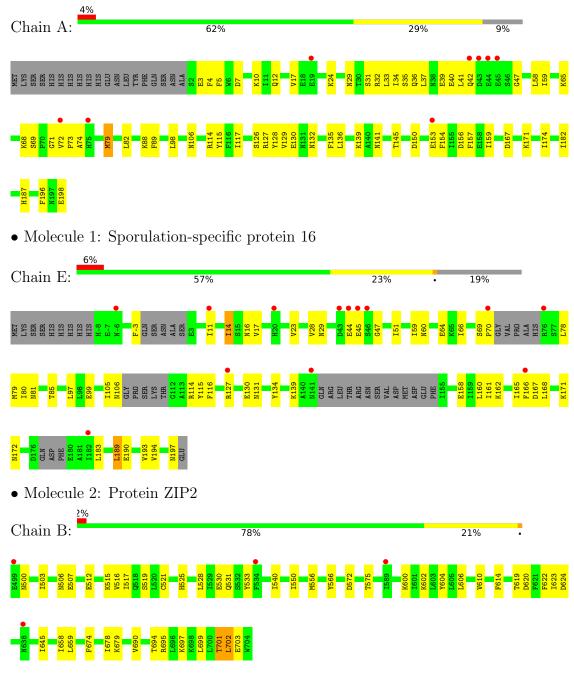
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	26	Total O 26 26	0	0
6	В	50	Total O 50 50	0	0
6	С	25	Total O 25 25	0	0
6	D	57	Total O 57 57	0	0
6	Е	9	Total O 9 9	0	0
6	F	22	Total O 22 22	0	0
6	G	9	Total O 9 9	0	0
6	Н	26	Total O 26 26	0	0



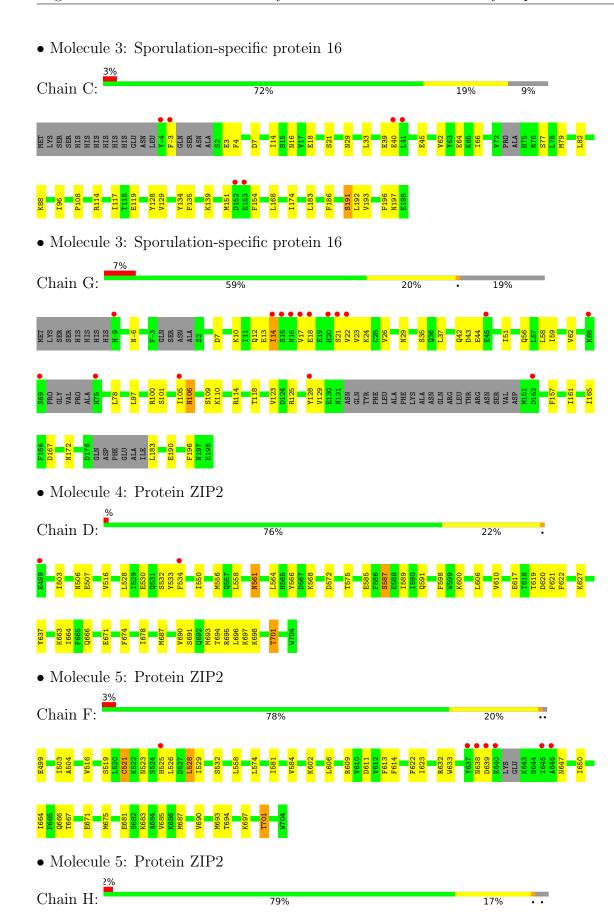
# 3 Residue-property plots (i)

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 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.

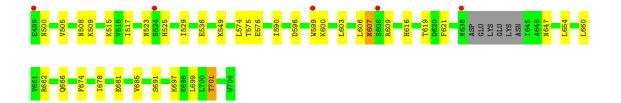
• Molecule 1: Sporulation-specific protein 16













## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	169.40Å 63.59Å 199.04Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.60^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	57.09 - 2.29	Depositor
Resolution (A)	99.52 - 2.29	EDS
% Data completeness	98.3 (57.09-2.29)	Depositor
(in resolution range)	98.4 (99.52-2.29)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$< I/\sigma(I) > 1$	1.46 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
D D	0.196 , 0.250	Depositor
$R, R_{free}$	0.196 , $0.250$	DCC
$R_{free}$ test set	4807 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34 , 42.7	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	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 22.93 % 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 5.1553e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: M0H, 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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.38	0/1647	0.53	0/2230
1	Е	0.36	0/1452	0.50	0/1961
2	В	0.45	0/1728	0.57	0/2331
3	С	0.39	0/1654	0.51	0/2235
3	G	0.36	0/1434	0.51	0/1937
4	D	0.45	0/1719	0.56	0/2320
5	F	0.42	0/1707	0.55	0/2303
5	Н	0.42	0/1681	0.56	0/2267
All	All	0.41	0/13022	0.54	0/17584

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
3	С	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	С	14	ILE	Peptide



#### 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	1627	0	1613	55	0
1	Е	1440	0	1420	52	0
2	В	1735	0	1743	46	0
3	С	1625	0	1602	36	0
3	G	1411	0	1387	44	0
4	D	1737	0	1746	52	0
5	F	1704	1	1700	47	0
5	Н	1678	0	1681	32	0
6	A	26	0	0	1	0
6	В	50	0	0	3	0
6	С	25	0	0	6	0
6	D	57	0	0	6	0
6	Е	9	0	0	2	0
6	F	22	0	0	0	0
6	G	9	0	0	0	0
6	Н	26	0	0	0	0
All	All	13181	1	12892	307	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 12.

The worst 5 of 307 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \AA) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:E:193:VAL:HG12	5:F:675:MET:HE1	1.06	1.03
3:C:79:MET:HE2	4:D:606:LEU:HD11	1.52	0.92
1:E:193:VAL:CG1	5:F:675:MET:HE1	1.98	0.89
3:G:56:GLN:HG2	3:G:105:ILE:HD11	1.57	0.86
1:A:37:LEU:HD23	1:A:41:LEU:HD12	1.58	0.86

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	Perce	$\mathbf{ntiles}$
1	A	194/216 (90%)	188 (97%)	6 (3%)	0	100	100
1	E	162/216 (75%)	158 (98%)	4 (2%)	0	100	100
2	В	200/206~(97%)	191 (96%)	9 (4%)	0	100	100
3	С	191/216 (88%)	185 (97%)	5 (3%)	1 (0%)	29	34
3	G	164/216 (76%)	158 (96%)	5 (3%)	1 (1%)	25	29
4	D	199/206 (97%)	193 (97%)	6 (3%)	0	100	100
5	F	197/206 (96%)	194 (98%)	3 (2%)	0	100	100
5	Н	193/206 (94%)	189 (98%)	4 (2%)	0	100	100
All	All	1500/1688 (89%)	1456 (97%)	42 (3%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	88	LYS
3	G	14	ILE

#### 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	Percent	iles
1	A	184/202~(91%)	180 (98%)	4 (2%)	52 6	66
1	E	159/202~(79%)	156 (98%)	3 (2%)	57 7	'1
2	В	190/190 (100%)	187 (98%)	3 (2%)	62 7	6



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Analysed	Rotameric	Outliers	Percer	$_{ m tiles}$
3	$\mathbf{C}$	184/203 (91%)	179 (97%)	5 (3%)	44	59
3	G	158/203 (78%)	154 (98%)	4 (2%)	47	62
4	D	189/189 (100%)	185 (98%)	4 (2%)	53	68
5	F	186/191 (97%)	183 (98%)	3 (2%)	62	76
5	Н	184/191 (96%)	179 (97%)	5 (3%)	44	59
All	All	1434/1571 (91%)	1403 (98%)	31 (2%)	52	66

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	691	SER
5	Н	607	ASN
1	Е	160	LEU
5	Н	691	SER
3	G	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	12	GLN
3	G	67	GLN
5	Н	647	ASN
3	G	106	ASN
4	D	666	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)

17 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	В	ond leng	$\operatorname{gths}$	В	ond ang	gles
WIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLY	В	627	2	9,10,11	0.54	0	6,11,13	0.97	0
5	MLY	F	600	5	9,10,11	0.72	0	6,11,13	0.76	0
1	MLY	Е	24	1	9,10,11	0.58	0	6,11,13	0.85	0
5	M0H	Н	521	5	5,7,8	0.87	0	2,7,9	0.78	0
2	MLY	В	600	2	9,10,11	0.46	0	6,11,13	0.66	0
5	MLY	Н	600	5	9,10,11	0.73	0	6,11,13	0.84	0
4	MLY	D	568	4	9,10,11	0.63	0	6,11,13	0.64	0
4	MLY	D	600	4	9,10,11	0.48	0	6,11,13	0.73	0
1	MLY	A	24	1	9,10,11	0.58	0	6,11,13	1.12	0
4	MLY	D	663	4	9,10,11	0.68	0	6,11,13	0.76	0
2	MLY	В	663	2	9,10,11	0.76	0	6,11,13	0.72	0
5	M0H	F	521	5	5,7,8	0.72	0	2,7,9	2.37	1 (50%)
5	MLY	F	549	5	9,10,11	0.57	0	6,11,13	0.92	0
4	M0H	D	521	4	5,7,8	0.78	0	2,7,9	0.93	0
4	MLY	D	627	4	9,10,11	0.48	0	6,11,13	0.96	0
5	MLY	Н	549	5	9,10,11	0.48	0	6,11,13	1.19	0
2	МОН	В	521	2	5,7,8	1.04	0	2,7,9	1.75	1 (50%)

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	В	627	2	-	1/8/9/11	-
5	MLY	F	600	5	-	7/8/9/11	-
1	MLY	Е	24	1	-	1/8/9/11	-
5	M0H	Н	521	5	-	1/5/6/8	-
2	MLY	В	600	2	-	1/8/9/11	-
5	MLY	Н	600	5	-	2/8/9/11	1
4	MLY	D	568	4	-	5/8/9/11	-
4	MLY	D	600	4	-	2/8/9/11	-
1	MLY	A	24	1	-	4/8/9/11	-
4	MLY	D	663	4	-	2/8/9/11	-
2	MLY	В	663	2	-	2/8/9/11	-
5	M0H	F	521	5	-	1/5/6/8	-
5	MLY	F	549	5	-	1/8/9/11	
4	МОН	D	521	4	-	2/5/6/8	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLY	D	627	4	-	2/8/9/11	-
5	MLY	Н	549	5	-	0/8/9/11	-
2	M0H	В	521	2	-	3/5/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	F	521	M0H	CB-SG-CD	3.25	107.47	102.06
2	В	521	M0H	CB-SG-CD	2.24	105.79	102.06

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	568	MLY	C-CA-CB-CG
4	D	627	MLY	C-CA-CB-CG
5	F	600	MLY	N-CA-CB-CG
5	F	600	MLY	C-CA-CB-CG
1	A	24	MLY	CD-CE-NZ-CH2

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	600	MLY	2	0
5	Н	600	MLY	4	0
4	D	568	MLY	3	0
4	D	600	MLY	1	0
1	A	24	MLY	1	0
4	D	663	MLY	5	0
5	F	521	M0H	2	0
4	D	627	MLY	1	0
5	Н	549	MLY	1	0

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 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,  $95^{th}$  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>	#RSRZ>	-2	$ ext{OWAB}( ext{Å}^2)$	Q < 0.9
1	A	$196/216\ (90\%)$	0.21	8 (4%) 37	42	31, 53, 112, 155	0
1	E	174/216~(80%)	0.44	13 (7%) 14	18	35, 60, 116, 150	0
2	В	$202/206\ (98\%)$	0.03	4 (1%) 65	70	27, 41, 64, 134	0
3	С	197/216~(91%)	0.14	6 (3%) 50	56	30, 52, 97, 117	0
3	G	174/216~(80%)	0.50	16 (9%) 9	11	35, 61, 129, 164	0
4	D	$201/206\ (97\%)$	0.02	2 (0%) 82	86	28, 41, 68, 117	0
5	F	$201/206\ (97\%)$	0.19	7 (3%) 44	49	29, 47, 94, 211	0
5	Н	197/206~(95%)	0.07	5 (2%) 57	63	28, 44, 75, 111	0
All	All	1542/1688~(91%)	0.19	61 (3%) 38	43	27, 50, 100, 211	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	17	VAL	14.6
5	F	638	ASN	7.5
1	A	45	GLU	7.1
5	F	639	ASP	6.6
1	Е	44	GLU	5.7

### 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	M0H	Н	521	8/9	0.92	0.12	46,57,64,69	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	M0H	F	521	8/9	0.94	0.12	42,47,55,63	0
4	M0H	D	521	8/9	0.95	0.12	40,45,65,67	0
4	MLY	D	627	11/12	0.95	0.15	34,37,63,65	0
1	MLY	Ε	24	11/12	0.95	0.21	58,65,69,76	0
1	MLY	A	24	11/12	0.95	0.14	36,51,65,69	0
2	M0H	В	521	8/9	0.95	0.10	39,47,53,56	0
5	MLY	Н	600	11/12	0.95	0.16	30,48,56,59	0
2	MLY	В	663	11/12	0.96	0.15	33,36,68,68	0
5	MLY	F	600	11/12	0.96	0.15	37,46,53,54	0
4	MLY	D	663	11/12	0.96	0.17	32,41,71,75	0
4	MLY	D	568	11/12	0.96	0.24	31,37,80,81	0
2	MLY	В	627	11/12	0.97	0.17	28,31,50,50	0
2	MLY	В	600	11/12	0.97	0.13	34,42,47,50	0
5	MLY	F	549	11/12	0.97	0.12	32,36,66,69	0
5	MLY	Н	549	11/12	0.98	0.16	30,37,67,71	0
4	MLY	D	600	11/12	0.98	0.13	29,33,42,46	0

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

