



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 5, 2018 – 10:40 PM 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

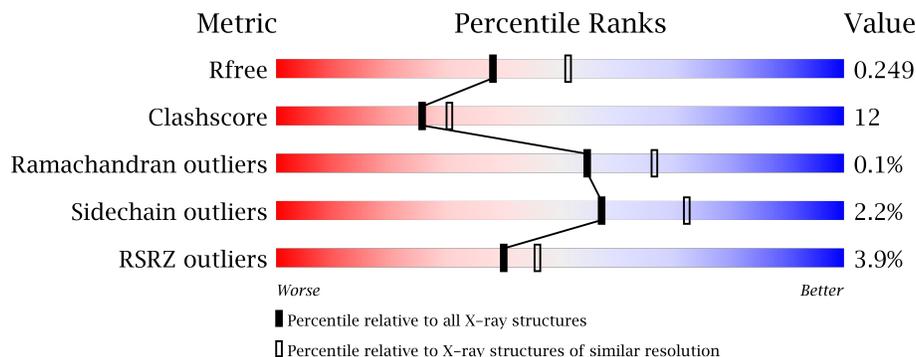
1 Overall quality at a glance

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}	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	216	
1	E	216	
2	B	206	
3	C	216	
3	G	216	

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Mol	Chain	Length	Quality of chain
4	D	206	 <p>.% 76% 22% .</p>
5	F	206	 <p>3% 78% 20% ..</p>
5	H	206	 <p>2% 79% 17% ..</p>

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	1627	1044	272	308	3	0	0	0
1	E	175	1440	936	235	267	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
E	-17	MET	-	expression tag	UNP P17122
E	-16	LYS	-	expression tag	UNP P17122
E	-15	SER	-	expression tag	UNP P17122
E	-14	SER	-	expression tag	UNP P17122
E	-13	HIS	-	expression tag	UNP P17122
E	-12	HIS	-	expression tag	UNP P17122

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-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
E	0	ASN	-	expression tag	UNP P17122
E	1	ALA	-	expression tag	UNP P17122

- Molecule 2 is a protein called Protein ZIP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	206	1735	1131	279	316	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	197	1625	1046	267	309	3	0	0	0
3	G	174	1411	910	236	262	3	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASN	-	expression tag	UNP P17122
C	-5	LEU	-	expression tag	UNP P17122
C	-4	TYR	-	expression tag	UNP P17122
C	-3	PHE	-	expression tag	UNP P17122
C	-2	GLN	-	expression tag	UNP P17122
C	-1	SER	-	expression tag	UNP P17122
C	0	ASN	-	expression tag	UNP P17122
C	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

- Molecule 4 is a protein called Protein ZIP2.

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

- Molecule 5 is a protein called Protein ZIP2.

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

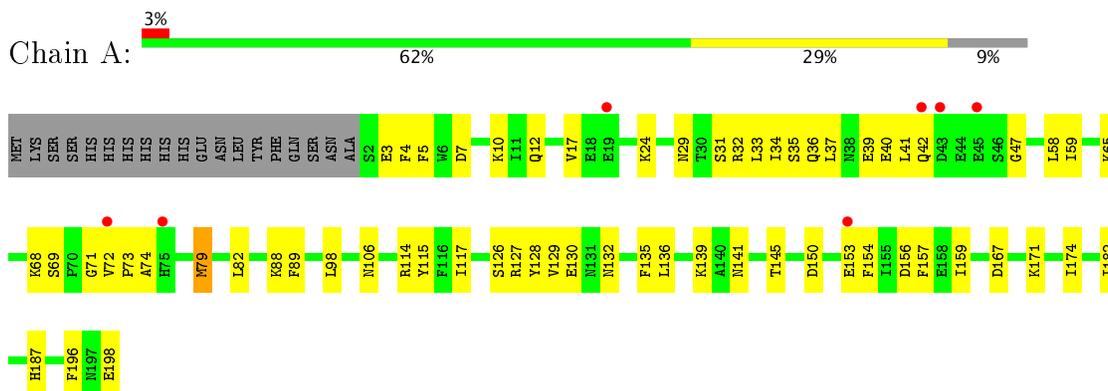
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	26	Total O 26 26	0	0
6	B	50	Total O 50 50	0	0
6	C	25	Total O 25 25	0	0
6	D	57	Total O 57 57	0	0
6	E	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	H	26	Total O 26 26	0	0

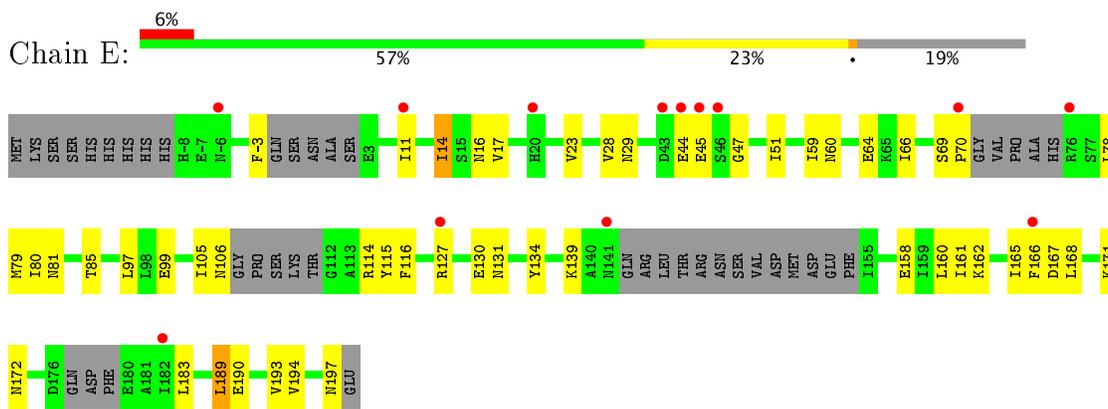
3 Residue-property plots [i](#)

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.

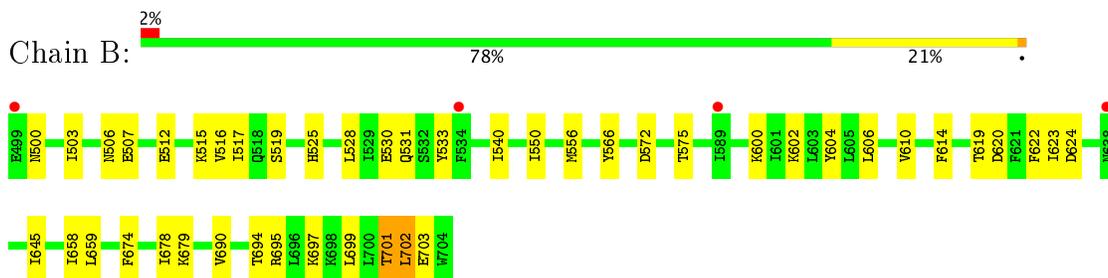
- Molecule 1: Sporulation-specific protein 16



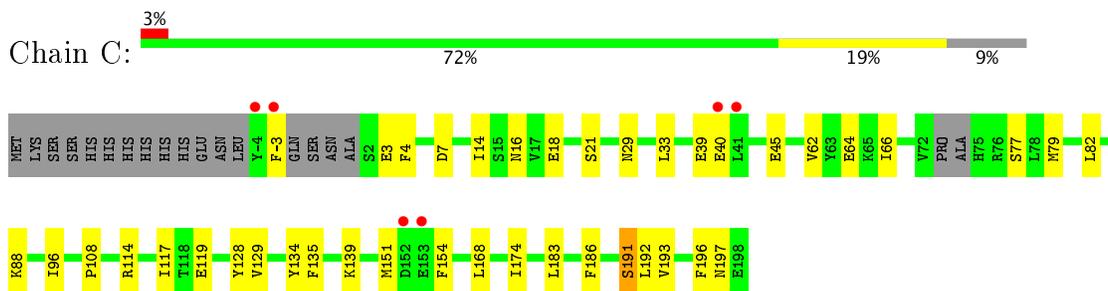
- Molecule 1: Sporulation-specific protein 16



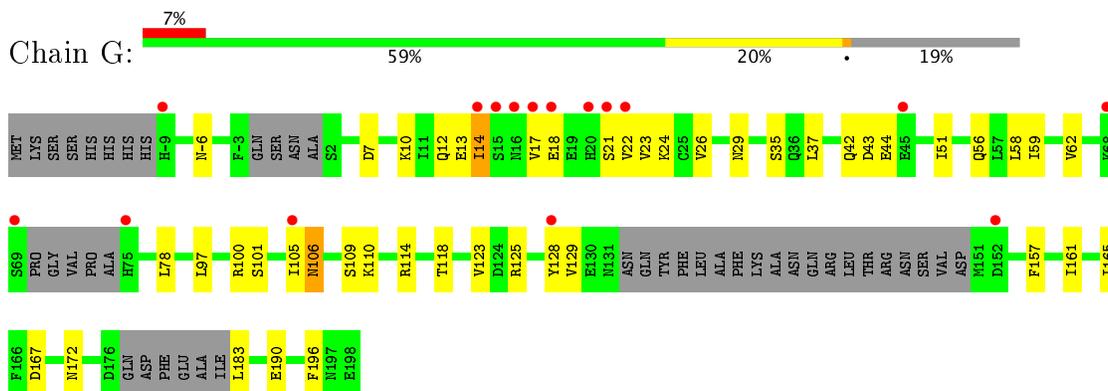
- Molecule 2: Protein ZIP2



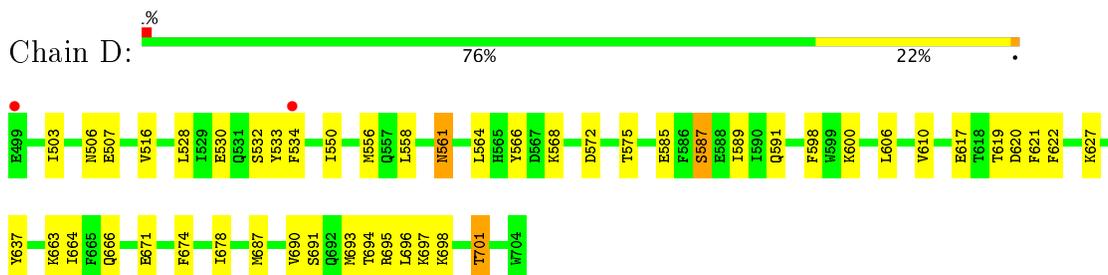
- Molecule 3: Sporulation-specific protein 16



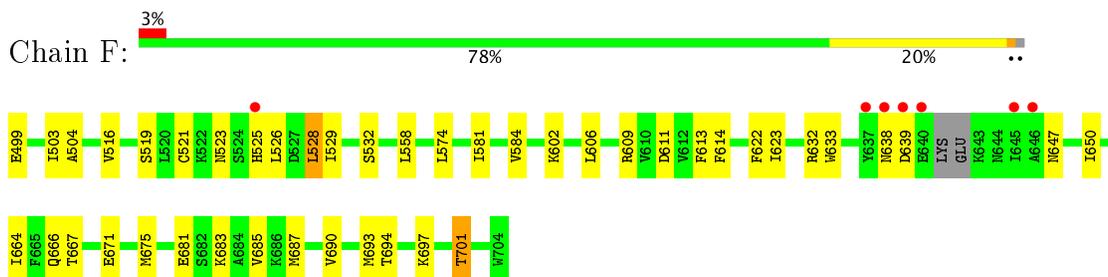
- Molecule 3: Sporulation-specific protein 16



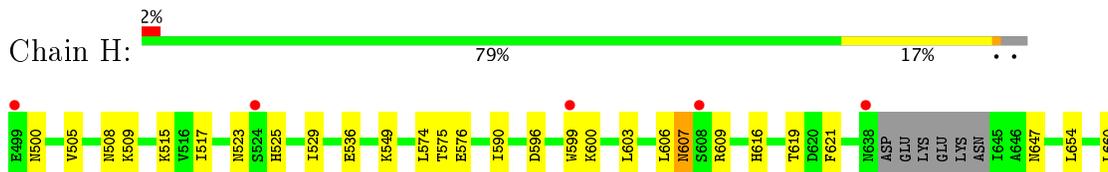
- Molecule 4: Protein ZIP2



- Molecule 5: Protein ZIP2



- Molecule 5: Protein ZIP2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.40Å 63.59Å 199.04Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	57.09 – 2.29 99.52 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.3 (57.09-2.29) 98.4 (99.52-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.196 , 0.250 0.194 , 0.249	Depositor DCC
R_{free} test set	4810 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	43.2	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13182	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² 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: MLY, M0H

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	0.38	0/1647	0.53	0/2230
1	E	0.36	0/1452	0.50	0/1961
2	B	0.45	0/1728	0.57	0/2331
3	C	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	H	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	C	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	C	14	ILE	Peptide

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	1627	0	1613	55	0
1	E	1440	0	1420	52	0
2	B	1735	0	1743	46	0
3	C	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	H	1678	0	1681	32	0
6	A	26	0	0	1	0
6	B	50	0	0	3	0
6	C	25	0	0	6	0
6	D	57	0	0	6	0
6	E	9	0	0	2	0
6	F	22	0	0	0	0
6	G	9	0	0	0	0
6	H	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	Interatomic distance (Å)	Clash overlap (Å)
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	Percentiles	
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	B	200/206 (97%)	191 (96%)	9 (4%)	0	100	100
3	C	191/216 (88%)	185 (97%)	5 (3%)	1 (0%)	32	38
3	G	164/216 (76%)	158 (96%)	5 (3%)	1 (1%)	28	33
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	H	193/206 (94%)	189 (98%)	4 (2%)	0	100	100
All	All	1500/1688 (89%)	1456 (97%)	42 (3%)	2 (0%)	55	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	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	Percentiles	
1	A	184/202 (91%)	180 (98%)	4 (2%)	57	72
1	E	159/202 (79%)	156 (98%)	3 (2%)	62	77
2	B	190/190 (100%)	187 (98%)	3 (2%)	68	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	184/203 (91%)	179 (97%)	5 (3%)	50	65
3	G	158/203 (78%)	154 (98%)	4 (2%)	53	68
4	D	189/189 (100%)	185 (98%)	4 (2%)	59	73
5	F	186/191 (97%)	183 (98%)	3 (2%)	68	81
5	H	184/191 (96%)	179 (97%)	5 (3%)	50	65
All	All	1434/1571 (91%)	1403 (98%)	31 (2%)	57	72

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

Mol	Chain	Res	Type
4	D	691	SER
1	E	160	LEU
5	H	666	GLN
4	D	701	THR
1	E	189	LEU

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

Mol	Chain	Res	Type
4	D	666	GLN
1	E	16	ASN
3	G	67	GLN
2	B	531	GLN
3	G	12	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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	MLY	A	24	1	10,10,11	0.80	0	8,11,13	1.10	0
2	M0H	B	521	2	5,7,8	1.10	0	2,7,9	1.78	1 (50%)
2	MLY	B	600	2	10,10,11	0.67	0	8,11,13	0.83	0
2	MLY	B	627	2	10,10,11	0.70	0	8,11,13	1.00	0
2	MLY	B	663	2	10,10,11	0.92	0	8,11,13	0.86	0
4	M0H	D	521	4	5,7,8	0.90	0	2,7,9	0.99	0
4	MLY	D	568	4	10,10,11	0.81	0	8,11,13	1.04	1 (12%)
4	MLY	D	600	4	10,10,11	0.88	1 (10%)	8,11,13	0.90	0
4	MLY	D	627	4	10,10,11	0.66	0	8,11,13	1.07	0
4	MLY	D	663	4	10,10,11	0.98	1 (10%)	8,11,13	0.85	0
1	MLY	E	24	1	10,10,11	0.64	0	8,11,13	1.12	1 (12%)
5	M0H	F	521	5	5,7,8	0.83	0	2,7,9	2.39	1 (50%)
5	MLY	F	549	5	10,10,11	0.74	0	8,11,13	1.02	0
5	MLY	F	600	5	10,10,11	1.01	1 (10%)	8,11,13	0.98	0
5	M0H	H	521	5	5,7,8	1.09	0	2,7,9	0.83	0
5	MLY	H	549	5	10,10,11	0.57	0	8,11,13	1.23	0
5	MLY	H	600	5	10,10,11	0.83	0	8,11,13	1.35	1 (12%)

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
1	MLY	A	24	1	-	0/7/9/11	0/0/0/0
2	M0H	B	521	2	-	0/5/6/8	0/0/0/0
2	MLY	B	600	2	-	0/7/9/11	0/0/0/0
2	MLY	B	627	2	-	0/7/9/11	0/0/0/0
2	MLY	B	663	2	-	0/7/9/11	0/0/0/0
4	M0H	D	521	4	-	0/5/6/8	0/0/0/0
4	MLY	D	568	4	-	0/7/9/11	0/0/0/0
4	MLY	D	600	4	-	0/7/9/11	0/0/0/0
4	MLY	D	627	4	-	0/7/9/11	0/0/0/0
4	MLY	D	663	4	-	0/7/9/11	0/0/0/0
1	MLY	E	24	1	-	0/7/9/11	0/0/0/0
5	M0H	F	521	5	-	0/5/6/8	0/0/0/0
5	MLY	F	549	5	-	0/7/9/11	0/0/0/0
5	MLY	F	600	5	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	M0H	H	521	5	-	0/5/6/8	0/0/0/0
5	MLY	H	549	5	-	0/7/9/11	0/0/0/0
5	MLY	H	600	5	-	0/7/9/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	600	MLY	CA-C	2.41	1.53	1.50
4	D	663	MLY	CA-C	2.42	1.53	1.50
5	F	600	MLY	CA-C	2.43	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	600	MLY	CB-CA-C	-2.88	106.91	111.65
4	D	568	MLY	O-C-CA	-2.49	118.13	125.02
1	E	24	MLY	O-C-CA	-2.03	119.41	125.02
2	B	521	M0H	CB-SG-CD	2.24	105.79	102.06
5	F	521	M0H	CB-SG-CD	3.25	107.47	102.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	196/216 (90%)	0.21	7 (3%) 43 49	31, 53, 112, 155	0
1	E	174/216 (80%)	0.43	13 (7%) 15 19	35, 60, 116, 150	0
2	B	202/206 (98%)	0.03	4 (1%) 65 71	27, 41, 64, 134	0
3	C	197/216 (91%)	0.14	6 (3%) 51 57	30, 52, 97, 117	0
3	G	174/216 (80%)	0.49	16 (9%) 10 12	35, 61, 129, 164	0
4	D	201/206 (97%)	0.02	2 (0%) 82 85	28, 41, 68, 117	0
5	F	201/206 (97%)	0.19	7 (3%) 44 50	29, 47, 94, 211	0
5	H	197/206 (95%)	0.07	5 (2%) 58 64	28, 44, 75, 111	0
All	All	1542/1688 (91%)	0.19	60 (3%) 40 46	27, 50, 100, 211	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	17	VAL	14.6
5	F	638	ASN	7.6
1	A	45	GLU	7.1
5	F	639	ASP	6.7
1	E	44	GLU	5.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	M0H	B	521	8/9	0.95	0.10	-	39,47,53,56	0
4	MLY	D	568	11/12	0.96	0.24	-	31,37,80,81	0
4	MLY	D	627	11/12	0.95	0.15	-	34,37,63,65	0
2	MLY	B	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	600	11/12	0.98	0.13	-	29,33,42,46	0
4	MLY	D	663	11/12	0.97	0.17	-	32,41,71,75	0
2	MLY	B	600	11/12	0.97	0.13	-	34,42,47,50	0
1	MLY	E	24	11/12	0.95	0.21	-	58,65,69,76	0
5	MLY	H	549	11/12	0.98	0.16	-	30,37,67,71	0
1	MLY	A	24	11/12	0.95	0.14	-	36,51,65,69	0
4	M0H	D	521	8/9	0.95	0.12	-	40,45,65,67	0
5	M0H	H	521	8/9	0.92	0.12	-	46,57,64,69	0
5	MLY	F	549	11/12	0.97	0.12	-	32,36,66,69	0
5	M0H	F	521	8/9	0.94	0.12	-	42,47,55,63	0
2	MLY	B	627	11/12	0.97	0.17	-	28,31,50,50	0
5	MLY	H	600	11/12	0.95	0.16	-	30,48,56,59	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.