



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 06:17 PM EST

PDB ID : 5WKC  
Title : Saccharomyces cerevisiae acetohydroxyacid synthase in complex with the herbicide penoxsulam  
Authors : Guddat, W.L.; Lonhienne, G.T.  
Deposited on : 2017-07-25  
Resolution : 2.33 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (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

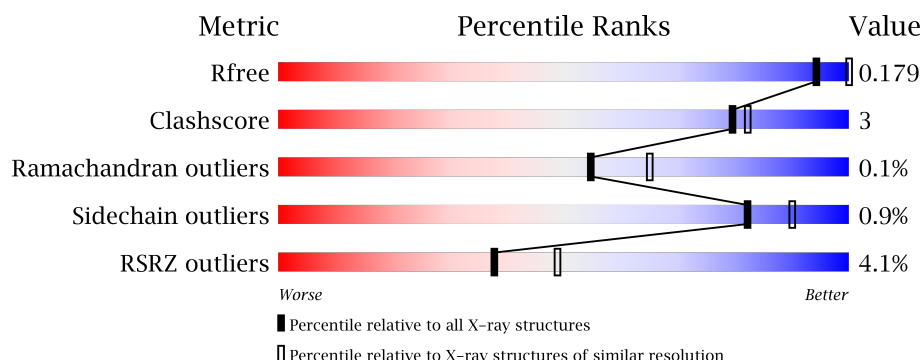
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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. 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	677	<div> <div>3%</div> <div>82%</div> <div>5%</div> <div>13%</div> </div>
1	B	677	<div> <div>0%</div> <div>82%</div> <div>6%</div> <div>12%</div> </div>
1	E	677	<div> <div>9%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
2	D	677	<div> <div>0%</div> <div>83%</div> <div>5%</div> <div>12%</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
6	F50	A	704	-	-	X	X
6	F50	B	705	-	-	X	X
6	F50	E	705	-	-	X	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19824 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 Acetolactate synthase catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	3	0
			4526	2866	784	854	22			
1	B	598	Total	C	N	O	S	0	4	0
			4580	2898	792	868	22			
1	E	592	Total	C	N	O	S	0	2	0
			4528	2868	782	856	22			

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP P07342
A	12	HIS	-	expression tag	UNP P07342
A	13	HIS	-	expression tag	UNP P07342
A	14	HIS	-	expression tag	UNP P07342
A	15	HIS	-	expression tag	UNP P07342
A	16	HIS	-	expression tag	UNP P07342
A	17	HIS	-	expression tag	UNP P07342
A	18	SER	-	expression tag	UNP P07342
A	19	SER	-	expression tag	UNP P07342
A	20	GLY	-	expression tag	UNP P07342
A	21	LEU	-	expression tag	UNP P07342
A	22	VAL	-	expression tag	UNP P07342
A	23	PRO	-	expression tag	UNP P07342
A	24	ARG	-	expression tag	UNP P07342
A	25	GLY	-	expression tag	UNP P07342
A	26	SER	-	expression tag	UNP P07342
A	27	GLY	-	expression tag	UNP P07342
A	28	MET	-	expression tag	UNP P07342
A	29	LYS	-	expression tag	UNP P07342
A	30	GLU	-	expression tag	UNP P07342
A	31	THR	-	expression tag	UNP P07342
A	32	ALA	-	expression tag	UNP P07342
A	33	ALA	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	expression tag	UNP P07342
A	35	LYS	-	expression tag	UNP P07342
A	36	PHE	-	expression tag	UNP P07342
A	37	GLU	-	expression tag	UNP P07342
A	38	ARG	-	expression tag	UNP P07342
A	39	GLN	-	expression tag	UNP P07342
A	40	HIS	-	expression tag	UNP P07342
A	41	MET	-	expression tag	UNP P07342
A	42	ASP	-	expression tag	UNP P07342
A	43	SER	-	expression tag	UNP P07342
A	44	PRO	-	expression tag	UNP P07342
A	45	ASP	-	expression tag	UNP P07342
A	46	LEU	-	expression tag	UNP P07342
A	47	GLY	-	expression tag	UNP P07342
A	48	THR	-	expression tag	UNP P07342
A	49	ASP	-	expression tag	UNP P07342
A	50	ASP	-	expression tag	UNP P07342
A	51	ASP	-	expression tag	UNP P07342
A	52	ASP	-	expression tag	UNP P07342
A	53	LYS	-	expression tag	UNP P07342
A	54	ALA	-	expression tag	UNP P07342
A	55	MET	-	expression tag	UNP P07342
A	56	GLY	-	expression tag	UNP P07342
A	57	SER	-	expression tag	UNP P07342
B	11	MET	-	initiating methionine	UNP P07342
B	12	HIS	-	expression tag	UNP P07342
B	13	HIS	-	expression tag	UNP P07342
B	14	HIS	-	expression tag	UNP P07342
B	15	HIS	-	expression tag	UNP P07342
B	16	HIS	-	expression tag	UNP P07342
B	17	HIS	-	expression tag	UNP P07342
B	18	SER	-	expression tag	UNP P07342
B	19	SER	-	expression tag	UNP P07342
B	20	GLY	-	expression tag	UNP P07342
B	21	LEU	-	expression tag	UNP P07342
B	22	VAL	-	expression tag	UNP P07342
B	23	PRO	-	expression tag	UNP P07342
B	24	ARG	-	expression tag	UNP P07342
B	25	GLY	-	expression tag	UNP P07342
B	26	SER	-	expression tag	UNP P07342
B	27	GLY	-	expression tag	UNP P07342
B	28	MET	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	LYS	-	expression tag	UNP P07342
B	30	GLU	-	expression tag	UNP P07342
B	31	THR	-	expression tag	UNP P07342
B	32	ALA	-	expression tag	UNP P07342
B	33	ALA	-	expression tag	UNP P07342
B	34	ALA	-	expression tag	UNP P07342
B	35	LYS	-	expression tag	UNP P07342
B	36	PHE	-	expression tag	UNP P07342
B	37	GLU	-	expression tag	UNP P07342
B	38	ARG	-	expression tag	UNP P07342
B	39	GLN	-	expression tag	UNP P07342
B	40	HIS	-	expression tag	UNP P07342
B	41	MET	-	expression tag	UNP P07342
B	42	ASP	-	expression tag	UNP P07342
B	43	SER	-	expression tag	UNP P07342
B	44	PRO	-	expression tag	UNP P07342
B	45	ASP	-	expression tag	UNP P07342
B	46	LEU	-	expression tag	UNP P07342
B	47	GLY	-	expression tag	UNP P07342
B	48	THR	-	expression tag	UNP P07342
B	49	ASP	-	expression tag	UNP P07342
B	50	ASP	-	expression tag	UNP P07342
B	51	ASP	-	expression tag	UNP P07342
B	52	ASP	-	expression tag	UNP P07342
B	53	LYS	-	expression tag	UNP P07342
B	54	ALA	-	expression tag	UNP P07342
B	55	MET	-	expression tag	UNP P07342
B	56	GLY	-	expression tag	UNP P07342
B	57	SER	-	expression tag	UNP P07342
E	11	MET	-	initiating methionine	UNP P07342
E	12	HIS	-	expression tag	UNP P07342
E	13	HIS	-	expression tag	UNP P07342
E	14	HIS	-	expression tag	UNP P07342
E	15	HIS	-	expression tag	UNP P07342
E	16	HIS	-	expression tag	UNP P07342
E	17	HIS	-	expression tag	UNP P07342
E	18	SER	-	expression tag	UNP P07342
E	19	SER	-	expression tag	UNP P07342
E	20	GLY	-	expression tag	UNP P07342
E	21	LEU	-	expression tag	UNP P07342
E	22	VAL	-	expression tag	UNP P07342
E	23	PRO	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
E	24	ARG	-	expression tag	UNP P07342
E	25	GLY	-	expression tag	UNP P07342
E	26	SER	-	expression tag	UNP P07342
E	27	GLY	-	expression tag	UNP P07342
E	28	MET	-	expression tag	UNP P07342
E	29	LYS	-	expression tag	UNP P07342
E	30	GLU	-	expression tag	UNP P07342
E	31	THR	-	expression tag	UNP P07342
E	32	ALA	-	expression tag	UNP P07342
E	33	ALA	-	expression tag	UNP P07342
E	34	ALA	-	expression tag	UNP P07342
E	35	LYS	-	expression tag	UNP P07342
E	36	PHE	-	expression tag	UNP P07342
E	37	GLU	-	expression tag	UNP P07342
E	38	ARG	-	expression tag	UNP P07342
E	39	GLN	-	expression tag	UNP P07342
E	40	HIS	-	expression tag	UNP P07342
E	41	MET	-	expression tag	UNP P07342
E	42	ASP	-	expression tag	UNP P07342
E	43	SER	-	expression tag	UNP P07342
E	44	PRO	-	expression tag	UNP P07342
E	45	ASP	-	expression tag	UNP P07342
E	46	LEU	-	expression tag	UNP P07342
E	47	GLY	-	expression tag	UNP P07342
E	48	THR	-	expression tag	UNP P07342
E	49	ASP	-	expression tag	UNP P07342
E	50	ASP	-	expression tag	UNP P07342
E	51	ASP	-	expression tag	UNP P07342
E	52	ASP	-	expression tag	UNP P07342
E	53	LYS	-	expression tag	UNP P07342
E	54	ALA	-	expression tag	UNP P07342
E	55	MET	-	expression tag	UNP P07342
E	56	GLY	-	expression tag	UNP P07342
E	57	SER	-	expression tag	UNP P07342

- Molecule 2 is a protein called Acetolactate synthase catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	596	Total	C	N	O	S	0	1	0
			4553	2880	789	862	22			

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	11	MET	-	initiating methionine	UNP P07342
D	12	HIS	-	expression tag	UNP P07342
D	13	HIS	-	expression tag	UNP P07342
D	14	HIS	-	expression tag	UNP P07342
D	15	HIS	-	expression tag	UNP P07342
D	16	HIS	-	expression tag	UNP P07342
D	17	HIS	-	expression tag	UNP P07342
D	18	SER	-	expression tag	UNP P07342
D	19	SER	-	expression tag	UNP P07342
D	20	GLY	-	expression tag	UNP P07342
D	21	LEU	-	expression tag	UNP P07342
D	22	VAL	-	expression tag	UNP P07342
D	23	PRO	-	expression tag	UNP P07342
D	24	ARG	-	expression tag	UNP P07342
D	25	GLY	-	expression tag	UNP P07342
D	26	SER	-	expression tag	UNP P07342
D	27	GLY	-	expression tag	UNP P07342
D	28	MET	-	expression tag	UNP P07342
D	29	LYS	-	expression tag	UNP P07342
D	30	GLU	-	expression tag	UNP P07342
D	31	THR	-	expression tag	UNP P07342
D	32	ALA	-	expression tag	UNP P07342
D	33	ALA	-	expression tag	UNP P07342
D	34	ALA	-	expression tag	UNP P07342
D	35	LYS	-	expression tag	UNP P07342
D	36	PHE	-	expression tag	UNP P07342
D	37	GLU	-	expression tag	UNP P07342
D	38	ARG	-	expression tag	UNP P07342
D	39	GLN	-	expression tag	UNP P07342
D	40	HIS	-	expression tag	UNP P07342
D	41	MET	-	expression tag	UNP P07342
D	42	ASP	-	expression tag	UNP P07342
D	43	SER	-	expression tag	UNP P07342
D	44	PRO	-	expression tag	UNP P07342
D	45	ASP	-	expression tag	UNP P07342
D	46	LEU	-	expression tag	UNP P07342
D	47	GLY	-	expression tag	UNP P07342
D	48	THR	-	expression tag	UNP P07342
D	49	ASP	-	expression tag	UNP P07342
D	50	ASP	-	expression tag	UNP P07342
D	51	ASP	-	expression tag	UNP P07342
D	52	ASP	-	expression tag	UNP P07342
D	53	LYS	-	expression tag	UNP P07342

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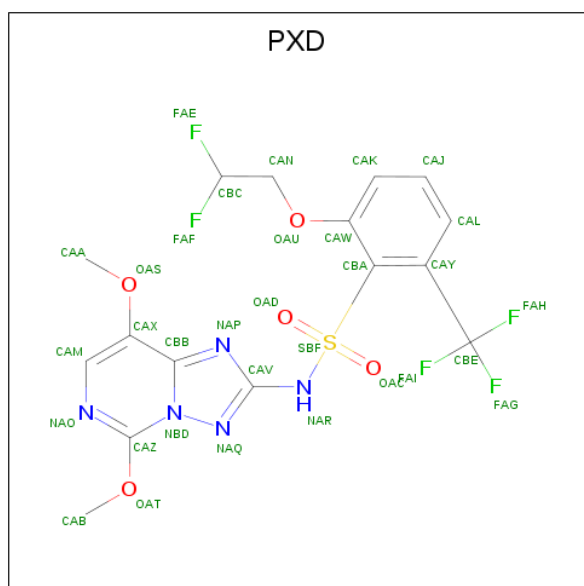
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Chain	Residue	Modelled	Actual	Comment	Reference
D	54	ALA	-	expression tag	UNP P07342
D	55	MET	-	expression tag	UNP P07342
D	56	GLY	-	expression tag	UNP P07342
D	57	SER	-	expression tag	UNP P07342

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is 2-(2,2-difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide (three-letter code: PXD) (formula: C<sub>16</sub>H<sub>14</sub>F<sub>5</sub>N<sub>5</sub>O<sub>5</sub>S).



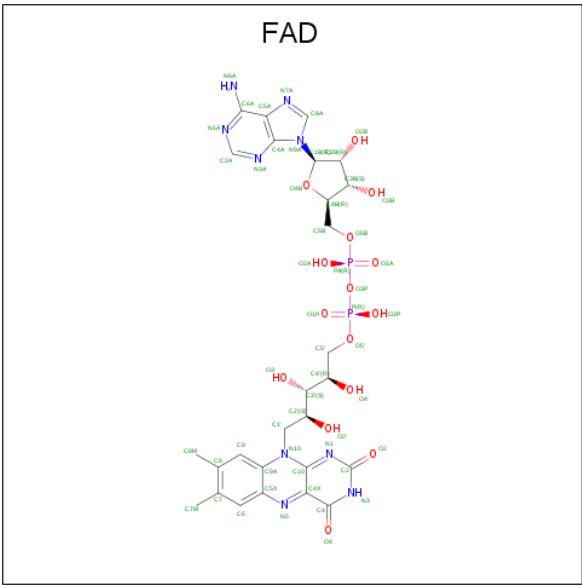
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O S 32 16 5 5 5 1	0	0
4	B	1	Total C F N O S 32 16 5 5 5 1	0	0
4	E	1	Total C F N O S 32 16 5 5 5 1	0	0

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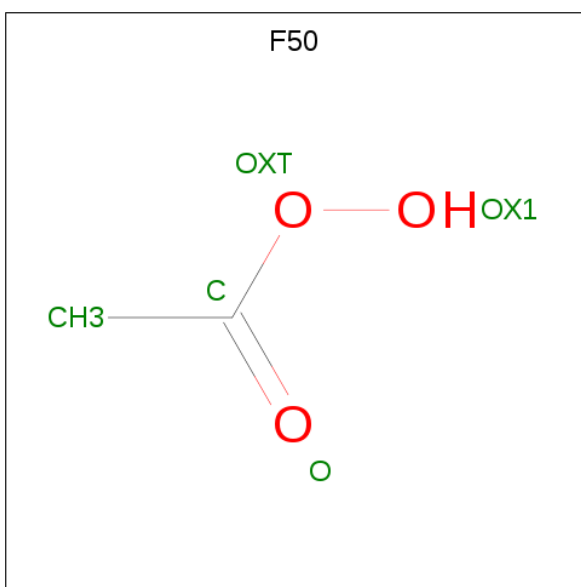
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	F	N	O	S	0	0
			32	16	5	5	5	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



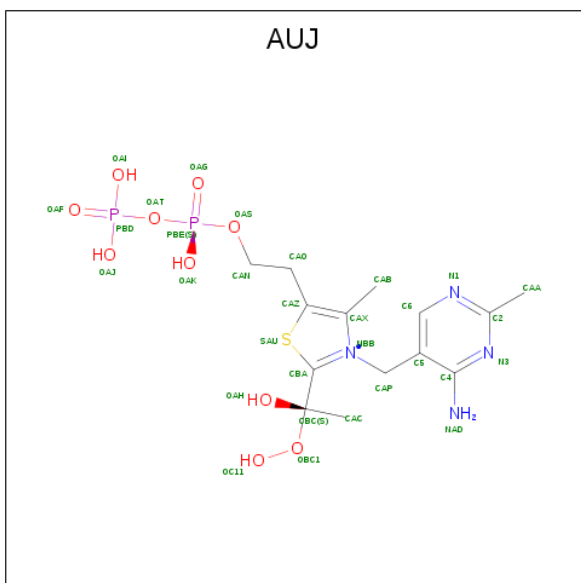
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is ETHANEPEROXOIC ACID (three-letter code: F50) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>3</sub>).



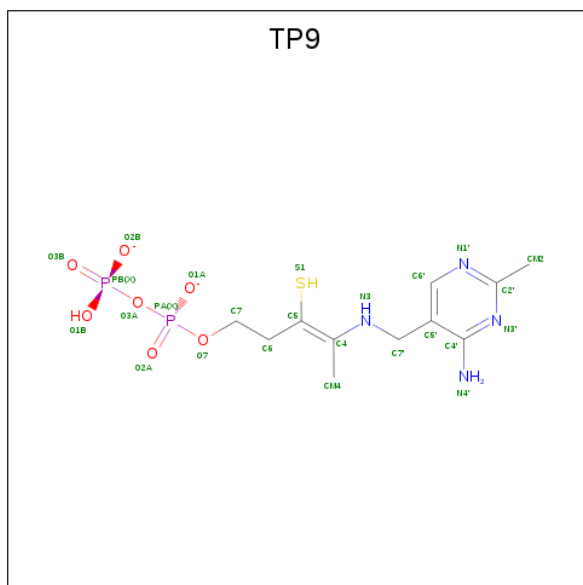
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	C 2	O 3	0	0
6	B	1	Total 5	C 2	O 3	0	0
6	E	1	Total 5	C 2	O 3	0	0

- Molecule 7 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 {S})-1-(dioxidanyl)-1-oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: AUJ) (formula: C<sub>14</sub>H<sub>23</sub>N<sub>4</sub>O<sub>10</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	S	0	0
			31	14	4	10	2	1		

- Molecule 8 is (3Z)-4-[[[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]AMINO}-3-MERCAPTOPENT-3-EN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: TP9) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	S	0	0
			25	11	4	7	2	1		
8	E	1	Total	C	N	O	P	S	0	0
			25	11	4	7	2	1		
8	D	1	Total	C	N	O	P	S	0	0
			25	11	4	7	2	1		

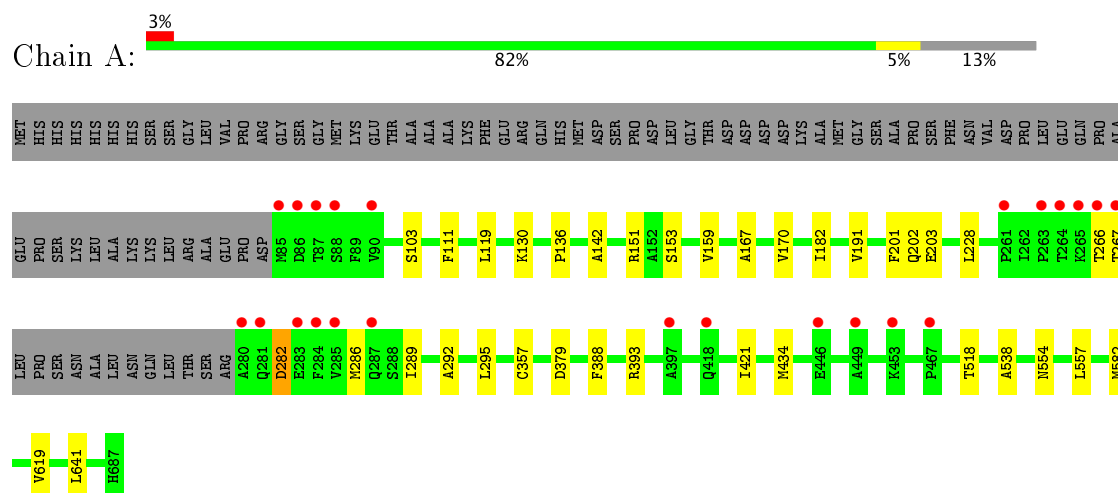
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	260	Total	O	0	0
			260	260		
9	B	357	Total	O	0	0
			357	357		
9	E	177	Total	O	0	0
			177	177		
9	D	378	Total	O	0	0
			378	378		

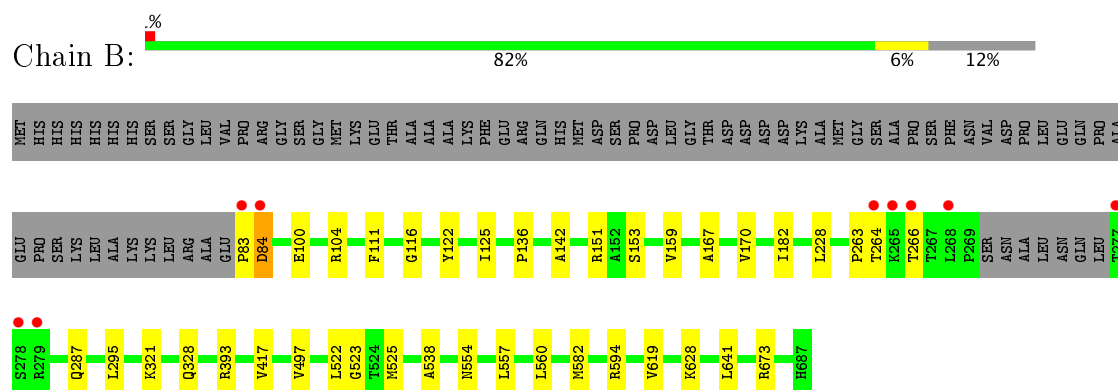
### 3 Residue-property plots [i](#)

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.

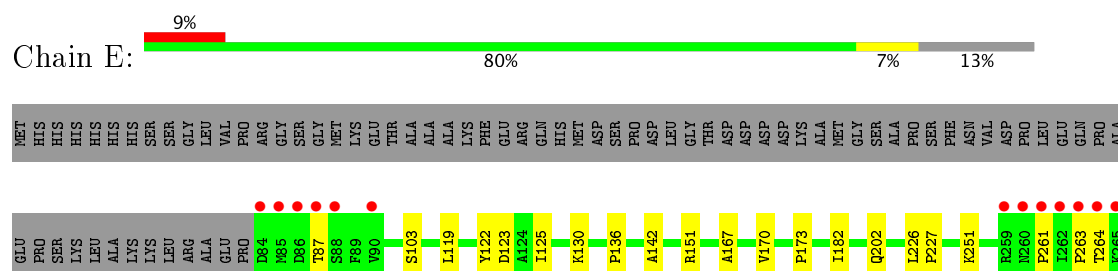
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

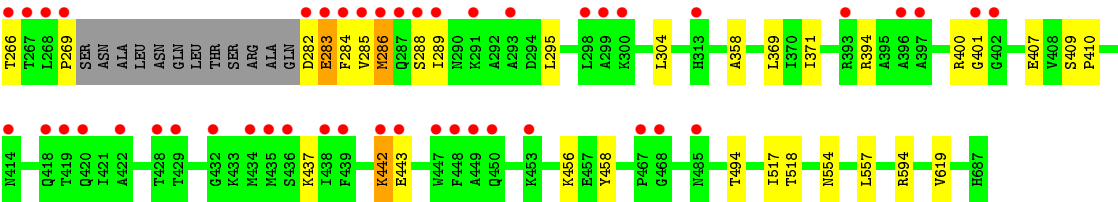


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

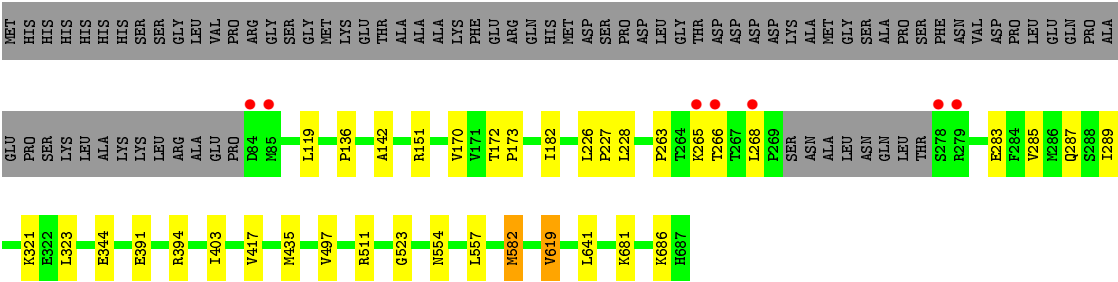
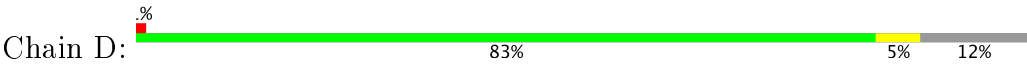


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





• Molecule 2: Acetolactate synthase catalytic subunit, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.21Å 218.21Å 361.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 2.33 48.79 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.79-2.33) 99.9 (48.79-2.33)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.150 , 0.180 0.148 , 0.179	Depositor DCC
$R_{free}$ test set	1994 reflections (1.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19824	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 2.04% 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: MG, F50, AUJ, FAD, SME, TP9, PXD

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	0.35	0/4630	0.44	0/6276
1	B	0.34	0/4688	0.46	0/6356
1	E	0.28	0/4629	0.44	0/6275
2	D	0.36	0/4641	0.45	0/6291
All	All	0.33	0/18588	0.45	0/25198

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	4526	0	4542	20	0
1	B	4580	0	4591	30	0
1	E	4528	0	4544	32	0
2	D	4553	0	4559	25	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	0	1	0
4	D	32	0	0	0	0
4	E	32	0	0	0	0
5	A	53	0	30	1	0
5	B	53	0	30	0	0
5	D	53	0	30	1	0
5	E	53	0	30	2	0
6	A	5	0	4	5	0
6	B	5	0	4	4	0
6	E	5	0	4	5	0
7	A	31	0	0	1	0
8	B	25	0	17	3	0
8	D	25	0	17	3	0
8	E	25	0	17	3	0
9	A	260	0	0	2	0
9	B	357	0	0	4	1
9	D	378	0	0	3	0
9	E	177	0	0	2	1
All	All	19824	0	18419	117	1

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 3.

All (117) 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)
6:A:704:F50:HH33	8:D:704:TP9:S1	1.83	1.17
6:A:704:F50:HH31	2:D:582[A]:MET:HG2	1.49	0.93
8:B:704:TP9:S1	6:E:705:F50:HH33	2.11	0.90
2:D:151:ARG:HD3	2:D:182:ILE:HD12	1.57	0.87
6:A:704:F50:CH3	8:D:704:TP9:S1	2.64	0.85
1:A:388:PHE:O	1:A:393:ARG:NH1	2.10	0.84
6:B:705:F50:HH33	8:E:704:TP9:S1	2.17	0.84
1:E:295:LEU:HD21	1:E:401:GLY:HA2	1.62	0.79
1:B:84:ASP:OD2	1:B:264:THR:OG1	1.99	0.79
1:B:151:ARG:HD3	1:B:182:ILE:HD12	1.70	0.72
1:B:393:ARG:HG3	1:B:393:ARG:HH11	1.57	0.70
1:E:282:ASP:O	1:E:285:VAL:N	2.14	0.70
2:D:344:GLU:HG3	2:D:511:ARG:HE	1.57	0.70
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.77	0.67
1:E:87:THR:HG22	1:E:261:PRO:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:NH2	9:B:802:HOH:O	2.29	0.65
6:A:704:F50:CH3	2:D:582[A]:MET:HG2	2.24	0.64
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.80	0.64
1:A:103:SER:HB2	1:A:130:LYS:HD3	1.80	0.64
1:B:83:PRO:O	1:B:84:ASP:HB3	1.98	0.63
2:D:151:ARG:NH2	9:D:802:HOH:O	2.32	0.63
1:E:285:VAL:O	1:E:289:ILE:HG13	1.99	0.63
1:B:673:ARG:NH2	9:B:803:HOH:O	2.33	0.62
1:A:151:ARG:NH2	1:A:518:THR:O	2.32	0.62
1:E:151:ARG:NH2	1:E:518:THR:O	2.33	0.62
1:E:136:PRO:HG3	1:E:142:ALA:HB2	1.81	0.61
1:E:251:LYS:NZ	9:E:804:HOH:O	2.33	0.61
2:D:136:PRO:HG3	2:D:142:ALA:HB2	1.84	0.60
2:D:321:LYS:NZ	9:D:803:HOH:O	2.35	0.59
6:A:704:F50:C	8:D:704:TP9:HN3	2.16	0.59
4:B:702:PXD:CAM	6:E:705:F50:HH31	2.32	0.59
1:B:582[A]:MET:HG2	6:E:705:F50:CH3	2.32	0.58
2:D:283:GLU:OE1	9:D:801:HOH:O	2.17	0.58
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.86	0.57
1:B:263:PRO:HB2	1:B:266:THR:HG23	1.85	0.57
1:E:456:LYS:HD2	1:E:456:LYS:N	2.19	0.57
1:E:554:ASN:HA	1:E:557:LEU:HD23	1.86	0.57
2:D:554:ASN:HA	2:D:557:LEU:HD23	1.86	0.56
1:E:103[B]:SER:HB2	1:E:130:LYS:HD3	1.88	0.56
1:A:379:ASP:OD1	9:A:801:HOH:O	2.18	0.56
1:E:151:ARG:HD3	1:E:182:ILE:HD12	1.89	0.54
1:E:103[A]:SER:HB2	1:E:130:LYS:HD3	1.89	0.54
1:B:594:ARG:NH1	1:E:123:ASP:OD1	2.40	0.54
1:B:328:GLN:NE2	9:B:801:HOH:O	2.28	0.52
1:B:228:LEU:HB2	1:B:266:THR:HB	1.91	0.52
2:D:263:PRO:HB2	2:D:266:THR:HG23	1.92	0.52
2:D:228:LEU:HB2	2:D:266:THR:HB	1.91	0.52
2:D:403:ILE:HD12	2:D:417:VAL:HG11	1.91	0.50
1:B:554:ASN:HA	1:B:557:LEU:HD23	1.94	0.50
1:B:393:ARG:HH22	1:B:417:VAL:HG23	1.78	0.48
1:E:594:ARG:NH2	9:E:806:HOH:O	2.46	0.48
6:B:705:F50:CH3	8:E:704:TP9:S1	2.95	0.48
1:A:357:CYS:SG	9:A:1052:HOH:O	2.60	0.48
1:E:122:TYR:HA	1:E:125:ILE:HG12	1.96	0.48
8:B:704:TP9:HN3	6:E:705:F50:C	2.27	0.48
1:B:153:SER:HB3	1:B:538:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLY:N	6:B:705:F50:OX1	2.36	0.47
2:D:686:LYS:HE3	2:D:686:LYS:HB2	1.65	0.47
1:E:282:ASP:OD1	1:E:283:GLU:N	2.48	0.47
1:A:554:ASN:HA	1:A:557:LEU:HD23	1.97	0.47
1:E:286:MET:SD	1:E:437:LYS:NZ	2.88	0.47
1:B:525:MET:SD	8:B:704:TP9:H61	2.54	0.46
1:B:122:TYR:HA	1:B:125:ILE:HG12	1.98	0.46
2:D:619:VAL:HG23	2:D:641:LEU:HD11	1.96	0.46
1:E:167:ALA:O	1:E:170:VAL:HG22	2.15	0.46
1:A:619:VAL:HG23	1:A:641:LEU:HD11	1.96	0.46
2:D:285:VAL:O	2:D:289:ILE:HG13	2.15	0.46
1:A:582[A]:MET:HG2	7:A:705:AUJ:CAC	2.45	0.46
2:D:323:LEU:HA	2:D:435:MET:HE1	1.98	0.45
6:B:705:F50:C	8:E:704:TP9:HN3	2.30	0.45
1:B:167:ALA:O	1:B:170:VAL:HG22	2.18	0.44
1:E:407:GLU:OE2	5:E:703:FAD:O2B	2.33	0.44
1:A:228:LEU:HB2	1:A:266:THR:HB	1.99	0.44
2:D:681:LYS:HB2	2:D:681:LYS:HE3	1.67	0.44
1:B:100:GLU:HB3	1:B:104:ARG:HH21	1.81	0.44
2:D:323:LEU:HD13	2:D:435:MET:HE3	1.99	0.44
1:E:358:ALA:HB3	1:E:458:TYR:HB3	2.01	0.43
5:E:703:FAD:H9	5:E:703:FAD:H1'1	1.76	0.43
1:A:282:ASP:OD1	1:A:282:ASP:N	2.51	0.43
1:B:111:PHE:O	1:B:159:VAL:HA	2.19	0.43
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.29	0.42
1:B:522:LEU:O	1:E:202:GLN:HG2	2.19	0.42
1:B:619:VAL:HG22	1:B:628:LYS:HG3	2.00	0.42
1:E:304:LEU:HD23	1:E:371:ILE:HB	2.01	0.42
1:B:582[A]:MET:HG2	6:E:705:F50:HH31	2.01	0.42
1:A:191:VAL:HG11	1:A:203:GLU:HB2	2.02	0.42
1:E:226:LEU:HB3	1:E:227:PRO:HD3	2.02	0.42
1:B:497:VAL:HG21	1:B:523:GLY:C	2.40	0.42
2:D:497:VAL:HG21	2:D:523:GLY:C	2.39	0.42
1:A:295:LEU:HD12	1:A:421:ILE:HD12	2.00	0.42
1:E:494:THR:HG22	1:E:517:ILE:HB	2.02	0.42
1:A:151:ARG:HD3	1:A:182:ILE:HD12	2.00	0.42
1:A:153:SER:HB3	1:A:538:ALA:HB1	2.01	0.42
2:D:170:VAL:C	2:D:173:PRO:HD2	2.41	0.42
2:D:172:THR:HB	2:D:173:PRO:HD3	2.01	0.42
1:A:289:ILE:HG23	1:A:434:MET:HB2	2.02	0.41
2:D:268:LEU:HD23	2:D:268:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:ASP:O	1:E:284:PHE:N	2.54	0.41
2:D:226:LEU:HB3	2:D:227:PRO:HD3	2.01	0.41
1:A:201:PHE:CE2	1:A:202:GLN:HG3	2.54	0.41
1:A:292:ALA:HB2	1:A:421:ILE:HG21	2.02	0.41
1:B:393:ARG:HG3	1:B:393:ARG:NH1	2.30	0.41
1:E:295:LEU:HD22	1:E:369:LEU:HD13	2.02	0.41
5:D:703:FAD:H9	5:D:703:FAD:H1'1	1.76	0.41
5:A:703:FAD:H8A	5:A:703:FAD:H2B	1.91	0.41
1:E:263:PRO:HB2	1:E:266:THR:HG23	2.02	0.41
1:E:442:LYS:HB2	1:E:443:GLU:H	1.59	0.41
2:D:151:ARG:HD3	2:D:182:ILE:CD1	2.40	0.41
1:E:282:ASP:C	1:E:284:PHE:N	2.72	0.41
1:A:167:ALA:O	1:A:170:VAL:HG22	2.20	0.41
1:A:111:PHE:O	1:A:159:VAL:HA	2.21	0.41
1:B:321:LYS:NZ	9:B:810:HOH:O	2.53	0.41
1:B:295:LEU:HA	1:B:295:LEU:HD23	1.82	0.40
1:E:394:ARG:HH21	1:E:400:ARG:NH2	2.19	0.40
2:D:391:GLU:OE2	2:D:394:ARG:NH1	2.54	0.40
1:E:409:SER:HA	1:E:410:PRO:HD3	1.95	0.40
1:E:170:VAL:C	1:E:173:PRO:HD2	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1097:HOH:O	9:E:806:HOH:O[3_775]	2.19	0.01

## 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	590/677 (87%)	581 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	598/677 (88%)	589 (98%)	8 (1%)	1 (0%)	51	59
1	E	590/677 (87%)	577 (98%)	11 (2%)	2 (0%)	44	51
2	D	592/677 (87%)	585 (99%)	7 (1%)	0	100	100
All	All	2370/2708 (88%)	2332 (98%)	35 (2%)	3 (0%)	55	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	442	LYS
1	E	283	GLU
1	B	84	ASP

### 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	487/556 (88%)	483 (99%)	4 (1%)	85	91
1	B	494/556 (89%)	492 (100%)	2 (0%)	93	96
1	E	488/556 (88%)	482 (99%)	6 (1%)	75	86
2	D	488/555 (88%)	482 (99%)	6 (1%)	75	86
All	All	1957/2223 (88%)	1939 (99%)	18 (1%)	82	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	267	THR
1	A	282	ASP
1	A	286	MET
1	B	287	GLN
1	B	560	LEU
1	E	119	LEU
1	E	264	THR

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Mol	Chain	Res	Type
1	E	269	PRO
1	E	286	MET
1	E	288	SER
1	E	619	VAL
2	D	119	LEU
2	D	265	LYS
2	D	287	GLN
2	D	582[A]	MET
2	D	582[B]	MET
2	D	619	VAL

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

Mol	Chain	Res	Type
1	A	202	GLN
1	B	202	GLN
1	E	202	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	SME	D	502	2	8,8,9	1.38	2 (25%)	6,9,11	5.42	3 (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	SME	D	502	2	-	0/5/7/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	SME	CB-CA	-2.67	1.50	1.53
2	D	502	SME	OE-S	-2.09	1.44	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	SME	OE-S-CG	4.85	119.39	106.03
2	D	502	SME	OE-S-CE	6.12	118.71	106.20
2	D	502	SME	CE-S-CG	10.41	121.39	97.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	$\# Z  > 2$
4	PXD	A	702	-	27,34,34	3.39	13 (48%)	32,51,51	2.98	14 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FAD	A	703	-	51,58,58	2.12	11 (21%)	54,89,89	1.67	8 (14%)
6	F50	A	704	-	3,4,4	1.90	1 (33%)	2,4,4	2.66	1 (50%)
7	AUJ	A	705	3	27,32,32	3.71	13 (48%)	28,49,49	2.39	11 (39%)
4	PXD	B	702	-	27,34,34	3.37	13 (48%)	32,51,51	2.67	12 (37%)
5	FAD	B	703	-	51,58,58	2.52	20 (39%)	54,89,89	1.66	9 (16%)
8	TP9	B	704	3	22,25,25	2.72	11 (50%)	25,36,36	1.98	8 (32%)
6	F50	B	705	-	3,4,4	1.69	1 (33%)	2,4,4	3.52	1 (50%)
4	PXD	D	702	-	27,34,34	3.79	13 (48%)	32,51,51	2.91	12 (37%)
5	FAD	D	703	-	51,58,58	2.09	11 (21%)	54,89,89	1.65	7 (12%)
8	TP9	D	704	3	22,25,25	2.83	10 (45%)	25,36,36	2.08	7 (28%)
4	PXD	E	702	-	27,34,34	3.08	13 (48%)	32,51,51	2.60	12 (37%)
5	FAD	E	703	-	51,58,58	2.14	11 (21%)	54,89,89	1.63	8 (14%)
8	TP9	E	704	3	22,25,25	2.51	11 (50%)	25,36,36	2.17	9 (36%)
6	F50	E	705	-	3,4,4	1.63	1 (33%)	2,4,4	2.64	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
4	PXD	A	702	-	-	0/24/26/26	0/3/3/3
5	FAD	A	703	-	-	0/28/50/50	0/6/6/6
6	F50	A	704	-	-	0/0/2/2	0/0/0/0
7	AUJ	A	705	3	-	0/18/42/42	0/2/2/2
4	PXD	B	702	-	-	0/24/26/26	0/3/3/3
5	FAD	B	703	-	-	0/28/50/50	0/6/6/6
8	TP9	B	704	3	-	0/16/22/22	0/1/1/1
6	F50	B	705	-	-	0/0/2/2	0/0/0/0
4	PXD	D	702	-	-	0/24/26/26	0/3/3/3
5	FAD	D	703	-	-	0/28/50/50	0/6/6/6
8	TP9	D	704	3	-	0/16/22/22	0/1/1/1
4	PXD	E	702	-	-	0/24/26/26	0/3/3/3
5	FAD	E	703	-	-	0/28/50/50	0/6/6/6
8	TP9	E	704	3	-	0/16/22/22	0/1/1/1
6	F50	E	705	-	-	0/0/2/2	0/0/0/0

All (153) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	PXD	OAC-SBF	-13.31	1.29	1.43
7	A	705	AUJ	CAZ-SAU	-12.40	1.72	1.83
4	A	702	PXD	OAC-SBF	-10.53	1.32	1.43
4	B	702	PXD	OAC-SBF	-9.92	1.32	1.43
4	E	702	PXD	OAC-SBF	-9.62	1.33	1.43
5	B	703	FAD	C1'-N10	-8.30	1.39	1.48
5	E	703	FAD	C1'-N10	-6.27	1.41	1.48
5	D	703	FAD	C1'-N10	-6.19	1.42	1.48
5	B	703	FAD	C2B-C1B	-6.19	1.43	1.53
4	B	702	PXD	OAD-SBF	-6.04	1.37	1.43
5	A	703	FAD	C1'-N10	-6.00	1.42	1.48
7	A	705	AUJ	C4-N3	-5.73	1.26	1.35
8	D	704	TP9	PB-O3A	-5.68	1.50	1.60
7	A	705	AUJ	CAP-NBB	-5.49	1.40	1.47
4	A	702	PXD	OAD-SBF	-5.48	1.37	1.43
8	B	704	TP9	PB-O3A	-5.24	1.51	1.60
4	D	702	PXD	FAE-CBC	-5.14	1.25	1.35
4	D	702	PXD	OAD-SBF	-5.05	1.38	1.43
4	A	702	PXD	FAE-CBC	-4.60	1.26	1.35
5	B	703	FAD	O3'-C3'	-4.53	1.32	1.43
8	E	704	TP9	PB-O3A	-4.50	1.52	1.60
4	A	702	PXD	SBF-NAR	-4.41	1.55	1.63
7	A	705	AUJ	PBD-OAF	-4.28	1.36	1.50
4	D	702	PXD	CAV-NAP	-4.27	1.28	1.34
5	E	703	FAD	C2B-C1B	-4.15	1.47	1.53
4	D	702	PXD	SBF-NAR	-4.13	1.56	1.63
8	D	704	TP9	PA-O1A	-4.13	1.34	1.55
5	A	703	FAD	C2B-C1B	-4.11	1.47	1.53
5	D	703	FAD	C2B-C1B	-4.10	1.47	1.53
4	B	702	PXD	FAE-CBC	-4.10	1.27	1.35
8	D	704	TP9	PB-O1B	-4.05	1.38	1.54
4	B	702	PXD	CAV-NAP	-4.03	1.28	1.34
8	B	704	TP9	PB-O2B	-4.02	1.38	1.54
7	A	705	AUJ	PBD-OAI	-4.01	1.38	1.54
8	B	704	TP9	PA-O2A	-4.00	1.35	1.50
7	A	705	AUJ	PBE-OAG	-3.90	1.36	1.50
8	E	704	TP9	PB-O2B	-3.84	1.39	1.54
7	A	705	AUJ	PBD-OAT	-3.81	1.53	1.60
4	E	702	PXD	FAE-CBC	-3.80	1.28	1.35
7	A	705	AUJ	C2-N1	-3.79	1.28	1.34
4	B	702	PXD	SBF-NAR	-3.70	1.57	1.63
7	A	705	AUJ	CBA-SAU	-3.66	1.72	1.82
4	A	702	PXD	CAV-NAP	-3.63	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	PXD	OAU-CAN	-3.57	1.33	1.44
5	B	703	FAD	O4-C4	-3.53	1.15	1.24
4	D	702	PXD	FAH-CBE	-3.50	1.20	1.32
4	A	702	PXD	CBA-SBF	-3.49	1.72	1.79
7	A	705	AUJ	PBE-OAK	-3.49	1.37	1.55
4	E	702	PXD	CAV-NAP	-3.44	1.29	1.34
8	B	704	TP9	PB-O3B	-3.41	1.39	1.50
4	E	702	PXD	SBF-NAR	-3.40	1.57	1.63
5	B	703	FAD	C8A-N7A	-3.40	1.28	1.34
8	E	704	TP9	PA-O1A	-3.38	1.38	1.55
8	D	704	TP9	PA-O2A	-3.37	1.38	1.50
4	B	702	PXD	CBA-SBF	-3.37	1.73	1.79
5	B	703	FAD	PA-O2A	-3.32	1.38	1.55
4	E	702	PXD	OAD-SBF	-3.28	1.40	1.43
4	B	702	PXD	OAU-CAN	-3.24	1.34	1.44
5	B	703	FAD	P-O2P	-3.24	1.38	1.55
4	B	702	PXD	FAH-CBE	-3.18	1.21	1.32
8	B	704	TP9	PA-O1A	-3.15	1.39	1.55
4	E	702	PXD	CBA-SBF	-3.09	1.73	1.79
4	A	702	PXD	FAH-CBE	-3.04	1.21	1.32
5	B	703	FAD	C2B-C3B	-2.99	1.45	1.53
4	E	702	PXD	FAH-CBE	-2.93	1.22	1.32
5	E	703	FAD	O3'-C3'	-2.86	1.36	1.43
4	E	702	PXD	OAU-CAN	-2.84	1.35	1.44
4	D	702	PXD	OAT-CAB	-2.83	1.34	1.42
4	A	702	PXD	FAG-CBE	-2.82	1.22	1.32
8	B	704	TP9	C4'-N3'	-2.79	1.30	1.35
5	A	703	FAD	O3'-C3'	-2.77	1.36	1.43
5	B	703	FAD	C4X-C10	-2.75	1.36	1.41
5	D	703	FAD	O3'-C3'	-2.74	1.36	1.43
8	D	704	TP9	PB-O2B	-2.68	1.43	1.54
8	D	704	TP9	PB-O3B	-2.62	1.41	1.50
4	A	702	PXD	OAU-CAN	-2.61	1.36	1.44
5	B	703	FAD	O2'-C2'	-2.59	1.37	1.43
8	E	704	TP9	PB-O3B	-2.56	1.42	1.50
8	B	704	TP9	PB-O1B	-2.46	1.44	1.54
8	D	704	TP9	PA-O7	-2.45	1.48	1.59
4	D	702	PXD	CBA-SBF	-2.45	1.74	1.79
8	B	704	TP9	PA-O7	-2.42	1.48	1.59
4	D	702	PXD	FAG-CBE	-2.42	1.24	1.32
5	B	703	FAD	C4A-N3A	-2.41	1.32	1.35
5	B	703	FAD	C9A-C5X	-2.40	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	704	TP9	PB-O1B	-2.39	1.45	1.54
4	B	702	PXD	FAG-CBE	-2.39	1.24	1.32
8	D	704	TP9	C4'-N3'	-2.37	1.31	1.35
4	E	702	PXD	FAG-CBE	-2.37	1.24	1.32
4	A	702	PXD	OAT-CAB	-2.36	1.35	1.42
4	E	702	PXD	OAT-CAB	-2.33	1.35	1.42
5	B	703	FAD	C3B-C4B	-2.33	1.46	1.53
5	E	703	FAD	C2B-C3B	-2.33	1.47	1.53
5	B	703	FAD	C5'-C4'	-2.33	1.48	1.51
7	A	705	AUJ	C6-C5	-2.31	1.32	1.37
5	A	703	FAD	C2B-C3B	-2.30	1.47	1.53
8	E	704	TP9	C4'-N3'	-2.30	1.31	1.35
4	B	702	PXD	OAT-CAB	-2.27	1.36	1.42
8	E	704	TP9	C7'-N3	-2.26	1.41	1.46
5	B	703	FAD	PA-O1A	-2.24	1.42	1.50
8	E	704	TP9	PA-O7	-2.24	1.49	1.59
8	E	704	TP9	PA-O2A	-2.24	1.42	1.50
5	D	703	FAD	C2B-C3B	-2.22	1.47	1.53
8	B	704	TP9	C7'-N3	-2.20	1.41	1.46
5	B	703	FAD	O4B-C4B	-2.17	1.40	1.45
5	B	703	FAD	C5A-N7A	-2.16	1.32	1.39
8	B	704	TP9	O7-C7	-2.12	1.36	1.44
5	B	703	FAD	C2A-N1A	-2.11	1.29	1.33
8	D	704	TP9	O7-C7	-2.11	1.36	1.44
8	E	704	TP9	C4'-N4'	2.03	1.39	1.34
5	E	703	FAD	C2'-C3'	2.15	1.57	1.53
5	D	703	FAD	C2'-C3'	2.18	1.57	1.53
5	A	703	FAD	C2'-C3'	2.28	1.58	1.53
5	A	703	FAD	C2-N1	2.37	1.42	1.38
5	E	703	FAD	C2-N1	2.44	1.43	1.38
5	D	703	FAD	C2-N1	2.46	1.43	1.38
5	D	703	FAD	O4B-C1B	2.54	1.44	1.41
6	E	705	F50	OXT-C	2.56	1.43	1.36
6	B	705	F50	OXT-C	2.57	1.43	1.36
5	A	703	FAD	O4B-C1B	2.64	1.44	1.41
7	A	705	AUJ	C2-N3	2.70	1.39	1.34
5	E	703	FAD	O4B-C1B	2.90	1.45	1.41
6	A	704	F50	OXT-C	2.95	1.44	1.36
7	A	705	AUJ	C5-C4	2.99	1.49	1.42
5	D	703	FAD	C4-N3	3.03	1.38	1.33
5	E	703	FAD	C4-N3	3.11	1.38	1.33
4	A	702	PXD	CAV-NAR	3.15	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	703	FAD	C4-N3	3.16	1.38	1.33
4	B	702	PXD	CAV-NAR	3.55	1.42	1.39
4	E	702	PXD	CAV-NAR	3.92	1.43	1.39
4	D	702	PXD	CBB-NAP	4.06	1.37	1.33
5	D	703	FAD	C4X-N5	4.07	1.39	1.33
5	B	703	FAD	C4-C4X	4.16	1.49	1.41
5	E	703	FAD	C4X-N5	4.21	1.39	1.33
5	A	703	FAD	C4X-N5	4.40	1.39	1.33
4	D	702	PXD	OAT-CAZ	4.47	1.40	1.33
4	D	702	PXD	CAV-NAR	4.56	1.43	1.39
4	E	702	PXD	CBB-NAP	4.71	1.37	1.33
4	B	702	PXD	OAT-CAZ	5.06	1.41	1.33
5	B	703	FAD	C10-N1	5.06	1.40	1.33
4	A	702	PXD	CBB-NAP	5.08	1.38	1.33
4	A	702	PXD	OAT-CAZ	5.14	1.41	1.33
4	B	702	PXD	CBB-NAP	5.39	1.38	1.33
4	E	702	PXD	OAT-CAZ	5.49	1.41	1.33
5	D	703	FAD	C4-C4X	5.49	1.51	1.41
5	E	703	FAD	C4-C4X	5.71	1.52	1.41
5	A	703	FAD	C4-C4X	5.80	1.52	1.41
8	B	704	TP9	C4-N3	6.27	1.40	1.32
8	E	704	TP9	C4-N3	6.53	1.40	1.32
8	D	704	TP9	C4-N3	6.97	1.41	1.32
5	D	703	FAD	C10-N1	7.29	1.43	1.33
5	A	703	FAD	C10-N1	7.31	1.43	1.33
5	E	703	FAD	C10-N1	7.38	1.43	1.33

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	702	PXD	OAD-SBF-OAC	-7.93	109.40	119.55
4	D	702	PXD	OAD-SBF-OAC	-7.60	109.83	119.55
5	D	703	FAD	N3A-C2A-N1A	-7.50	122.32	128.86
5	A	703	FAD	N3A-C2A-N1A	-7.50	122.32	128.86
5	E	703	FAD	N3A-C2A-N1A	-7.35	122.46	128.86
4	A	702	PXD	OAD-SBF-OAC	-5.57	112.42	119.55
4	B	702	PXD	OAD-SBF-OAC	-5.43	112.61	119.55
5	B	703	FAD	N3A-C2A-N1A	-4.60	124.86	128.86
4	D	702	PXD	OAU-CAW-CAK	-4.54	114.22	124.00
5	B	703	FAD	C4A-C5A-N7A	-4.19	105.36	109.41
8	E	704	TP9	C7'-N3-C4	-4.14	120.03	125.96
8	D	704	TP9	O1A-PA-O2A	-3.99	91.63	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	PXD	CAX-CAM-NAO	-3.73	117.46	122.93
4	A	702	PXD	OAU-CAW-CAK	-3.73	115.97	124.00
8	D	704	TP9	C5'-C6'-N1'	-3.50	117.96	123.87
4	B	702	PXD	OAU-CAW-CAK	-3.47	116.54	124.00
8	B	704	TP9	C5'-C6'-N1'	-3.45	118.03	123.87
4	B	702	PXD	CAX-CAM-NAO	-3.28	118.12	122.93
4	E	702	PXD	OAU-CAW-CAK	-3.28	116.94	124.00
8	E	704	TP9	C5'-C6'-N1'	-3.26	118.36	123.87
7	A	705	AUJ	CBA-SAU-CAZ	-3.21	91.06	94.02
5	E	703	FAD	C4A-C5A-N7A	-3.17	106.34	109.41
5	A	703	FAD	C4A-C5A-N7A	-3.13	106.39	109.41
4	E	702	PXD	CAX-CAM-NAO	-3.11	118.37	122.93
4	A	702	PXD	CAX-CAM-NAO	-3.04	118.48	122.93
5	D	703	FAD	C4A-C5A-N7A	-3.03	106.48	109.41
7	A	705	AUJ	C5-C6-N1	-2.64	119.40	123.87
4	E	702	PXD	CAW-CBA-SBF	-2.61	116.88	120.87
4	A	702	PXD	OAD-SBF-NAR	-2.58	100.17	106.74
8	B	704	TP9	O1A-PA-O2A	-2.56	99.04	112.28
4	A	702	PXD	CAW-CBA-SBF	-2.39	117.22	120.87
5	E	703	FAD	C4X-C4-N3	-2.27	120.25	123.48
7	A	705	AUJ	OAK-PBE-OAG	-2.27	100.54	112.28
8	E	704	TP9	C7'-C5'-C4'	-2.26	120.26	122.45
5	B	703	FAD	C1B-N9A-C4A	-2.26	122.73	126.64
5	B	703	FAD	C4X-C4-N3	-2.26	120.27	123.48
8	B	704	TP9	O2B-PB-O3B	-2.24	101.72	110.50
4	B	702	PXD	OAD-SBF-NAR	-2.24	101.04	106.74
5	D	703	FAD	C4X-C4-N3	-2.23	120.31	123.48
5	A	703	FAD	C4X-C4-N3	-2.21	120.34	123.48
5	A	703	FAD	C4B-O4B-C1B	-2.14	107.50	109.77
4	E	702	PXD	CAL-CAJ-CAK	-2.14	117.24	120.24
5	E	703	FAD	C4B-O4B-C1B	-2.05	107.59	109.77
8	B	704	TP9	O7-C7-C6	2.01	117.27	108.70
8	E	704	TP9	N4'-C4'-N3'	2.09	120.09	117.00
4	A	702	PXD	OAU-CAW-CBA	2.10	120.04	116.68
4	E	702	PXD	OAD-SBF-CBA	2.15	111.98	108.85
5	E	703	FAD	C5X-C9A-N10	2.26	119.33	117.66
5	B	703	FAD	C4-C4X-N5	2.26	121.16	118.68
4	B	702	PXD	CAJ-CAL-CAY	2.28	124.14	119.95
7	A	705	AUJ	C6-C5-C4	2.31	118.75	115.68
5	B	703	FAD	N6A-C6A-N1A	2.31	123.34	118.77
8	D	704	TP9	N4'-C4'-N3'	2.34	120.46	117.00
8	E	704	TP9	O7-C7-C6	2.35	118.69	108.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	705	AUJ	CAA-C2-N1	2.36	119.72	117.06
5	D	703	FAD	C4-C4X-N5	2.43	121.34	118.68
7	A	705	AUJ	C6-N1-C2	2.45	120.11	115.88
4	D	702	PXD	OAU-CAW-CBA	2.47	120.62	116.68
4	E	702	PXD	CAJ-CAL-CAY	2.47	124.48	119.95
7	A	705	AUJ	CAP-NBB-CBA	2.50	124.95	116.21
5	A	703	FAD	C5X-C9A-N10	2.52	119.53	117.66
4	E	702	PXD	CAA-OAS-CAX	2.55	121.39	117.77
4	A	702	PXD	CAY-CBA-SBF	2.57	125.61	119.82
4	B	702	PXD	FAG-CBE-CAY	2.58	117.35	112.69
4	D	702	PXD	CAY-CBA-SBF	2.68	125.86	119.82
5	E	703	FAD	C1'-N10-C9A	2.68	120.80	118.35
5	D	703	FAD	C5X-C9A-N10	2.74	119.69	117.66
4	B	702	PXD	CAB-OAT-CAZ	2.76	119.92	117.44
8	E	704	TP9	CM4-C4-N3	2.78	121.13	118.04
5	E	703	FAD	C4-C4X-N5	2.78	121.73	118.68
5	D	703	FAD	C1'-N10-C9A	2.80	120.92	118.35
4	B	702	PXD	CAY-CBA-SBF	2.82	126.17	119.82
8	D	704	TP9	O7-C7-C6	2.84	120.78	108.70
5	A	703	FAD	C4-C4X-N5	2.87	121.82	118.68
4	A	702	PXD	CAJ-CAL-CAY	2.98	125.42	119.95
8	B	704	TP9	CM4-C4-N3	3.05	121.44	118.04
5	A	703	FAD	C1'-N10-C9A	3.10	121.18	118.35
4	D	702	PXD	CAJ-CAL-CAY	3.10	125.64	119.95
4	D	702	PXD	FAG-CBE-CAY	3.11	118.29	112.69
4	A	702	PXD	CAB-OAT-CAZ	3.17	120.29	117.44
8	D	704	TP9	C7-C6-C5	3.17	122.58	112.61
6	E	705	F50	OXT-C-CH3	3.23	117.17	111.10
6	A	704	F50	OXT-C-CH3	3.24	117.19	111.10
4	E	702	PXD	CAY-CBA-SBF	3.32	127.30	119.82
8	E	704	TP9	C6'-C5'-C4'	3.55	120.40	115.68
8	B	704	TP9	C6'-C5'-C4'	3.58	120.44	115.68
8	B	704	TP9	C7-C6-C5	3.64	124.06	112.61
4	E	702	PXD	CAK-CAW-CBA	3.65	123.95	119.02
4	A	702	PXD	CAK-CAW-CBA	3.66	123.96	119.02
5	B	703	FAD	C5X-C9A-N10	3.69	120.40	117.66
4	A	702	PXD	FAG-CBE-CAY	3.69	119.35	112.69
4	A	702	PXD	CAA-OAS-CAX	3.72	123.06	117.77
4	D	702	PXD	CAA-OAS-CAX	3.78	123.15	117.77
4	D	702	PXD	CAB-OAT-CAZ	3.83	120.88	117.44
8	B	704	TP9	C5'-C7'-N3	3.96	121.73	113.00
4	B	702	PXD	CAA-OAS-CAX	4.02	123.48	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	705	AUJ	CAO-CAZ-SAU	4.03	123.97	112.62
5	B	703	FAD	C1'-N10-C9A	4.08	122.09	118.35
8	D	704	TP9	C6'-C5'-C4'	4.08	121.11	115.68
4	B	702	PXD	CAK-CAW-CBA	4.13	124.59	119.02
4	D	702	PXD	CAM-NAO-CAZ	4.18	119.40	114.92
4	E	702	PXD	CAM-NAO-CAZ	4.29	119.53	114.92
8	D	704	TP9	C5'-C7'-N3	4.38	122.65	113.00
8	E	704	TP9	C7-C6-C5	4.47	126.67	112.61
4	A	702	PXD	CAM-NAO-CAZ	4.52	119.77	114.92
4	D	702	PXD	CAK-CAW-CBA	4.53	125.14	119.02
7	A	705	AUJ	CAX-CAZ-SAU	4.60	111.64	104.81
8	E	704	TP9	C5'-C7'-N3	4.66	123.26	113.00
4	B	702	PXD	CAM-NAO-CAZ	4.74	120.01	114.92
6	B	705	F50	OXT-C-CH3	4.81	120.12	111.10
7	A	705	AUJ	CAP-NBB-CAX	5.02	123.72	114.36
5	B	703	FAD	C4-N3-C2	5.37	119.86	115.16
5	A	703	FAD	C4-N3-C2	5.45	119.92	115.16
5	E	703	FAD	C4-N3-C2	5.52	119.99	115.16
5	D	703	FAD	C4-N3-C2	5.58	120.04	115.16
7	A	705	AUJ	CAO-CAZ-CAX	5.97	124.39	116.14
4	E	702	PXD	CBA-SBF-NAR	6.31	113.42	106.60
4	B	702	PXD	CBA-SBF-NAR	7.73	114.96	106.60
4	D	702	PXD	CBA-SBF-NAR	7.99	115.23	106.60
4	A	702	PXD	CBA-SBF-NAR	10.35	117.79	106.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	FAD	1	0
6	A	704	F50	5	0
7	A	705	AUJ	1	0
4	B	702	PXD	1	0
8	B	704	TP9	3	0
6	B	705	F50	4	0
5	D	703	FAD	1	0
8	D	704	TP9	3	0
5	E	703	FAD	2	0
8	E	704	TP9	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	705	F50	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	591/677 (87%)	-0.08	23 (3%) 40 51	20, 34, 59, 97	0
1	B	598/677 (88%)	-0.23	9 (1%) 74 82	19, 28, 47, 97	0
1	E	592/677 (87%)	0.33	59 (9%) 8 12	23, 44, 83, 128	0
2	D	595/677 (87%)	-0.23	7 (1%) 79 86	16, 26, 47, 77	0
All	All	2376/2708 (87%)	-0.05	98 (4%) 38 49	16, 32, 66, 128	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	268	LEU	7.3
1	E	264	THR	6.4
2	D	268	LEU	5.9
1	A	264	THR	5.7
1	E	284	PHE	5.7
1	B	83	PRO	5.4
1	A	265	LYS	5.0
1	E	286	MET	5.0
1	E	263	PRO	4.8
1	A	284	PHE	4.6
1	E	84	ASP	4.5
1	B	268	LEU	4.4
1	A	263	PRO	4.4
1	E	266	THR	4.3
1	E	287	GLN	4.2
1	E	87	THR	4.2
1	E	265	LYS	4.2
1	A	267	THR	4.1
1	E	435	MET	4.1
2	D	279	ARG	4.0
2	D	265	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	269	PRO	4.0
1	E	85	MET	4.0
1	E	267	THR	4.0
1	E	283	GLU	4.0
1	E	418	GLN	3.9
1	A	266	THR	3.8
1	E	439	PHE	3.6
1	E	438	ILE	3.6
1	A	87	THR	3.6
1	E	442	LYS	3.3
1	A	280	ALA	3.3
1	A	283	GLU	3.3
1	E	436	SER	3.2
1	E	419	THR	3.2
1	A	467	PRO	3.1
1	E	448	PHE	3.1
1	A	449	ALA	3.1
1	E	396	ALA	3.0
1	B	277	THR	3.0
1	E	468	GLY	3.0
1	E	86	ASP	3.0
1	E	432	GLY	3.0
1	B	279	ARG	3.0
1	A	86	ASP	3.0
1	E	285	VAL	2.9
1	E	447	TRP	2.9
1	E	397	ALA	2.9
1	E	401	GLY	2.9
1	E	88	SER	2.8
1	E	262	ILE	2.8
1	A	85	MET	2.8
1	E	298	LEU	2.8
1	E	90	VAL	2.8
1	E	299	ALA	2.8
1	E	288	SER	2.7
1	B	84	ASP	2.7
2	D	266	THR	2.7
1	E	260	ASN	2.6
2	D	85	MET	2.6
1	E	261	PRO	2.6
1	B	265	LYS	2.6
1	E	293	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	266	THR	2.5
2	D	84	ASP	2.5
1	E	467	PRO	2.5
1	A	397	ALA	2.5
1	A	261	PRO	2.4
1	E	414	ASN	2.4
1	A	281	GLN	2.4
1	E	289	ILE	2.4
1	E	429	THR	2.4
1	A	418	GLN	2.4
1	E	485	ASN	2.3
1	E	420	GLN	2.3
1	A	285	VAL	2.3
1	B	278	SER	2.3
1	B	264	THR	2.3
1	E	450	GLN	2.2
1	A	446	GLU	2.2
1	E	393	ARG	2.2
1	E	300	LYS	2.2
1	E	453	LYS	2.2
1	A	453	LYS	2.2
2	D	278	SER	2.2
1	A	287	GLN	2.2
1	E	428	THR	2.1
1	E	313	HIS	2.1
1	E	282	ASP	2.1
1	A	90	VAL	2.1
1	E	443	GLU	2.1
1	E	402	GLY	2.1
1	E	291	LYS	2.1
1	E	259	ARG	2.1
1	E	434	MET	2.0
1	E	422	ALA	2.0
1	A	88	SER	2.0
1	E	449	ALA	2.0

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

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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SME	D	502	9/10	0.98	0.12	-	22,23,38,63	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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	F50	B	705	5/5	0.87	0.35	8.27	27,30,35,35	5
6	F50	A	704	5/5	0.89	0.32	5.81	22,39,43,43	5
6	F50	E	705	5/5	0.93	0.29	3.74	38,39,42,43	5
5	FAD	D	703	53/53	0.98	0.14	0.12	13,20,24,33	0
8	TP9	D	704	25/25	0.97	0.14	-0.06	14,20,26,39	0
7	AUJ	A	705	31/31	0.97	0.15	-0.23	15,24,37,38	3
8	TP9	E	704	25/25	0.97	0.14	-0.30	22,26,34,40	0
5	FAD	A	703	53/53	0.97	0.10	-0.34	21,29,34,36	0
8	TP9	B	704	25/25	0.97	0.14	-0.35	17,24,29,40	0
5	FAD	B	703	53/53	0.98	0.11	-0.36	16,24,27,30	0
4	PXD	D	702	32/32	0.97	0.11	-0.54	15,27,45,55	0
5	FAD	E	703	53/53	0.96	0.11	-0.55	32,39,50,50	0
4	PXD	E	702	32/32	0.96	0.10	-0.76	33,38,60,66	0
4	PXD	B	702	32/32	0.97	0.11	-0.84	21,31,48,54	0
4	PXD	A	702	32/32	0.96	0.11	-0.86	23,30,52,58	0
3	MG	A	701	1/1	0.98	0.09	-1.46	23,23,23,23	0
3	MG	E	701	1/1	0.96	0.07	-2.20	26,26,26,26	0
3	MG	B	701	1/1	0.97	0.06	-2.43	23,23,23,23	0
3	MG	D	701	1/1	0.96	0.07	-3.14	20,20,20,20	0

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

There are no such residues in this entry.