W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2016 – 03:43 PM EDT

PDB ID	:	5FEM
Title	:	Saccharomyces cerevisiae Acetohydroxyacid Synthase in complex with bensul-furon methyl
Authors	:	Guddat, L.W.; Lonhienne, T.
Deposited on	:	2015-12-17
Resolution	:	2.17 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027107

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 2.17 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.
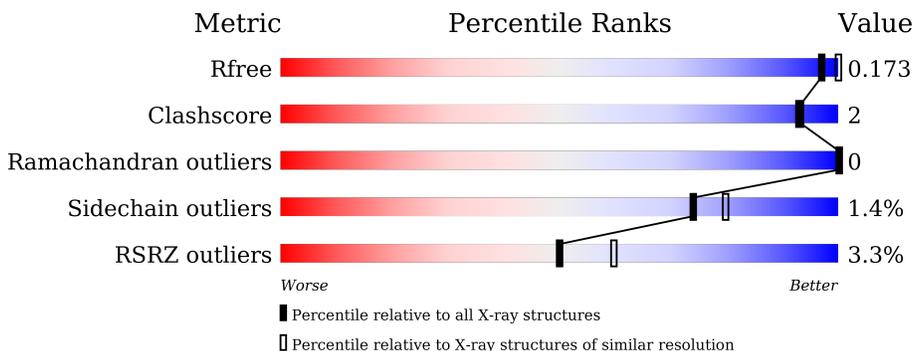
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 <=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	
1	B	677	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	704	-	-	-	X
2	MG	B	704	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9937 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	599	Total 4584	C 2901	N 795	O 866	S 22	0	4	0
1	B	599	Total 4578	C 2898	N 794	O 865	S 21	0	2	0

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	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
A	34	ALA	-	expression tag	UNP P07342
A	35	LYS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	expression tag	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
B	29	LYS	-	expression tag	UNP P07342
B	30	GLU	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
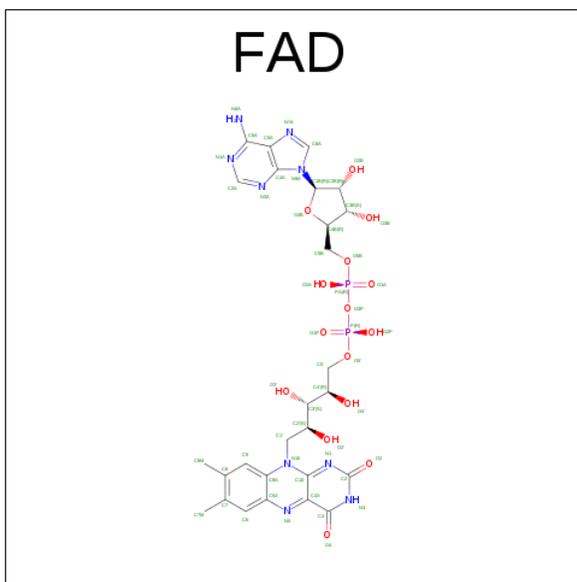
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is methyl 2-[(4,6-dimethoxypyrimidin-2-yl)carbamoylsulfamoylmethyl]benzoate (three-letter code: 60G) (formula: $C_{16}H_{18}N_4O_7S$).
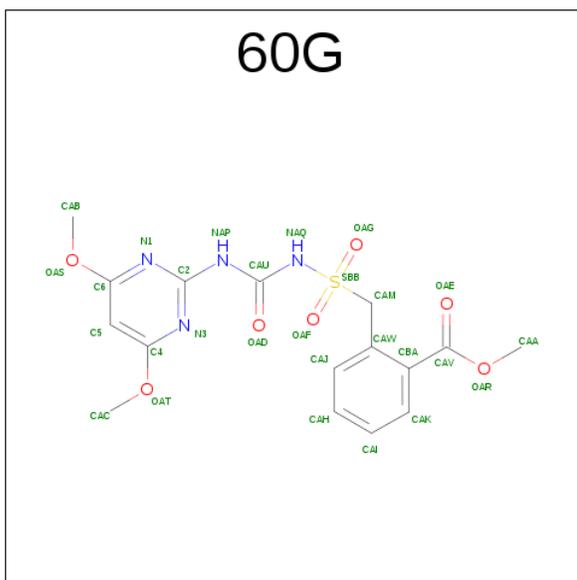

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).
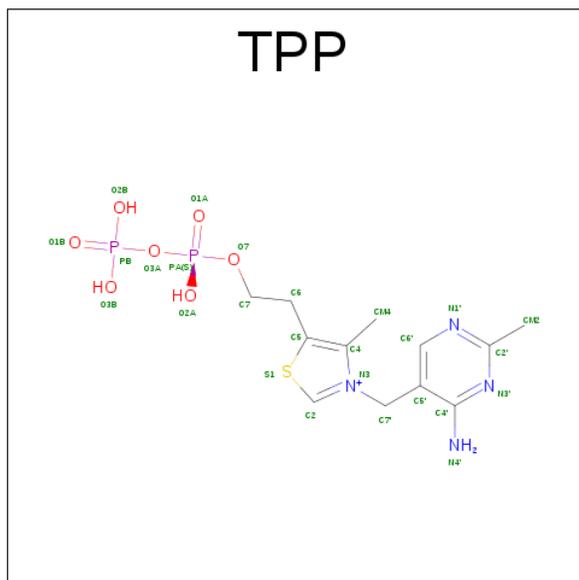
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	329	Total	O	0	0
			329	329		
6	B	228	Total	O	0	0
			228	228		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
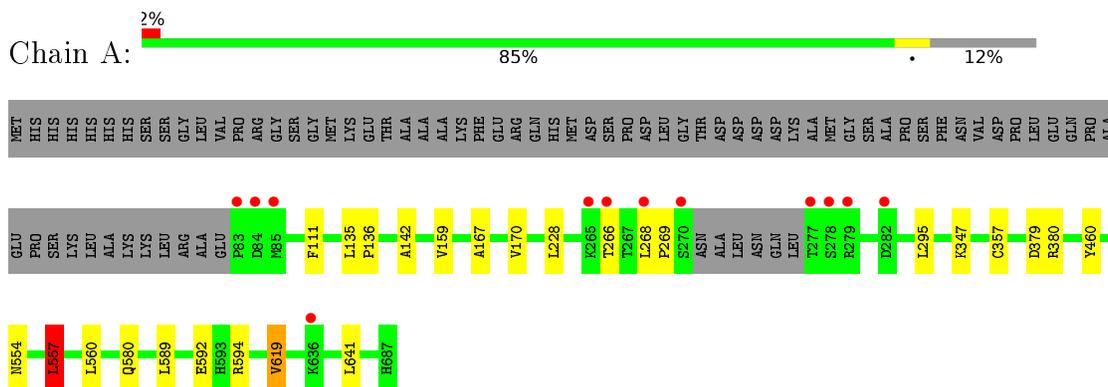
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial
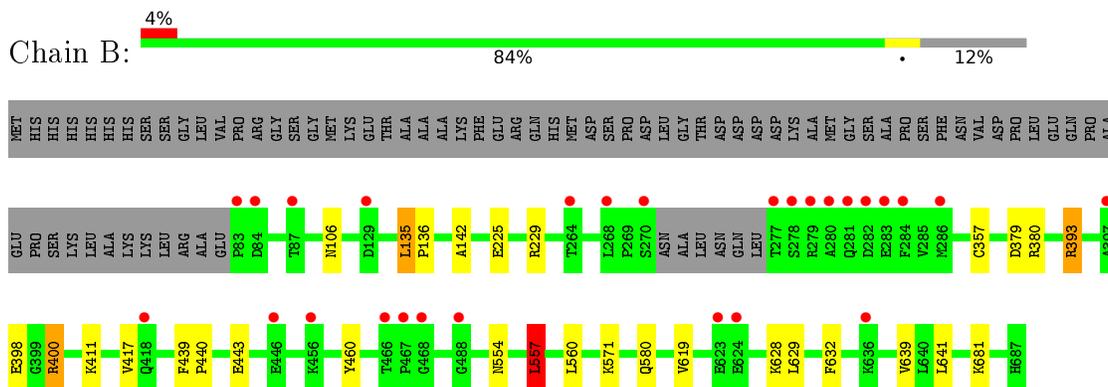
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.67Å 154.67Å 178.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.17 48.91 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-2.17) 99.7 (48.91-2.17)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.150 , 0.173 0.145 , 0.173	Depositor DCC
R_{free} test set	1999 reflections (1.75%)	DCC
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 114280 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9937	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 60G, FAD, TPP

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	0.32	0/4688	0.50	1/6358 (0.0%)
1	B	0.29	0/4679	0.47	2/6343 (0.0%)
All	All	0.30	0/9367	0.48	3/12701 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	557	LEU	CA-CB-CG	6.36	129.94	115.30
1	B	557	LEU	CA-CB-CG	6.04	129.20	115.30
1	B	135	LEU	CA-CB-CG	5.16	127.16	115.30

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	4584	0	4593	13	0
1	B	4578	0	4598	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	53	0	30	1	0
3	B	53	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	0	0	0
4	B	28	0	0	0	0
5	A	26	0	16	3	0
5	B	26	0	16	3	0
6	A	329	0	0	0	0
6	B	228	0	0	1	0
All	All	9937	0	9283	35	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 2.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:LYS:NZ	6:B:801:HOH:O	2.27	0.68
1:B:580:GLN:HB3	5:B:705:TPP:H61	1.81	0.63
1:A:379:ASP:OD1	1:A:380:ARG:NE	2.30	0.62
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.80	0.62
5:B:705:TPP:HN42	5:B:705:TPP:H2	1.65	0.61
1:A:554:ASN:HA	1:A:557:LEU:HD13	1.82	0.61
1:B:393:ARG:HH21	1:B:417:VAL:HG23	1.65	0.60
5:A:705:TPP:HN42	5:A:705:TPP:H2	1.66	0.59
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.85	0.59
5:B:705:TPP:C2	5:B:705:TPP:HN42	2.16	0.58
1:B:393:ARG:NH2	1:B:417:VAL:HG23	2.18	0.57
1:A:580:GLN:HB3	5:A:705:TPP:H61	1.85	0.56
5:A:705:TPP:HN42	5:A:705:TPP:C2	2.18	0.56
1:B:554:ASN:HA	1:B:557:LEU:HD13	1.87	0.56
1:B:571:LYS:HD2	1:B:639:VAL:HG12	1.89	0.54
1:A:592:GLU:OE1	1:A:594:ARG:NH2	2.43	0.51
1:B:357:CYS:HB3	1:B:460:TYR:CZ	2.47	0.49
1:B:379:ASP:OD1	1:B:380:ARG:NE	2.46	0.48
1:A:619[A]:VAL:CG2	1:A:641:LEU:HD11	2.44	0.47
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.95	0.47
1:A:357:CYS:HB3	1:A:460:TYR:CZ	2.49	0.47
1:A:619[A]:VAL:HG23	1:A:641:LEU:HD11	1.97	0.47
1:B:225:GLU:HG2	1:B:229:ARG:HG2	1.96	0.47
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.97	0.46
3:B:701:FAD:H9	3:B:701:FAD:H1'1	1.82	0.44
1:A:228:LEU:HB2	1:A:266:THR:HB	1.99	0.44
1:A:268:LEU:HA	1:A:269:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:O	1:B:632:PHE:HB3	2.18	0.44
1:B:439:PHE:HA	1:B:440:PRO:HD3	1.90	0.42
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.88	0.42
1:B:398:GLU:OE1	1:B:400:ARG:HD3	2.20	0.42
1:A:167:ALA:O	1:A:170:VAL:HG22	2.21	0.41
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.56	0.41
3:A:702:FAD:H9	3:A:702:FAD:H1'1	1.81	0.40
1:A:111:PHE:O	1:A:159:VAL:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/677 (88%)	592 (99%)	7 (1%)	0	100	100
1	B	597/677 (88%)	590 (99%)	7 (1%)	0	100	100
All	All	1196/1354 (88%)	1182 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	493/556 (89%)	486 (99%)	7 (1%)	74	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	493/556 (89%)	485 (98%)	8 (2%)	70	76
All	All	986/1112 (89%)	971 (98%)	15 (2%)	74	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	347	LYS
1	A	557	LEU
1	A	560	LEU
1	A	589	LEU
1	A	619[A]	VAL
1	A	619[B]	VAL
1	B	106	ASN
1	B	135	LEU
1	B	393	ARG
1	B	400	ARG
1	B	411	LYS
1	B	443	GLU
1	B	557	LEU
1	B	560	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	#$|Z| > 2$
3	FAD	A	702	-	52,58,58	2.19	12 (23%)	52,89,89	1.93	10 (19%)
4	60G	A	703	-	29,29,29	1.31	4 (13%)	37,40,40	3.11	14 (37%)
5	TPP	A	705	2	20,27,27	1.62	2 (10%)	27,40,40	1.74	7 (25%)
3	FAD	B	701	-	52,58,58	2.26	13 (25%)	52,89,89	1.80	8 (15%)
4	60G	B	703	-	29,29,29	1.41	6 (20%)	37,40,40	3.12	13 (35%)
5	TPP	B	705	2	20,27,27	1.61	2 (10%)	27,40,40	1.77	8 (29%)

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
3	FAD	A	702	-	-	0/30/50/50	0/6/6/6
4	60G	A	703	-	-	0/24/24/24	0/2/2/2
5	TPP	A	705	2	-	0/16/17/17	0/2/2/2
3	FAD	B	701	-	-	0/30/50/50	0/6/6/6
4	60G	B	703	-	-	0/24/24/24	0/2/2/2
5	TPP	B	705	2	-	0/16/17/17	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	FAD	O2'-C2'	-9.12	1.23	1.43
3	A	702	FAD	O2'-C2'	-8.83	1.23	1.43
5	A	705	TPP	C4-N3	-6.00	1.34	1.39
5	B	705	TPP	C4-N3	-5.72	1.34	1.39
3	B	701	FAD	C1'-N10	-5.71	1.42	1.48
3	A	702	FAD	C1'-N10	-5.18	1.42	1.48
3	A	702	FAD	C2B-C1B	-4.05	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	FAD	C2B-C1B	-3.98	1.47	1.53
4	B	703	60G	OAR-CAA	-2.80	1.38	1.45
4	A	703	60G	OAR-CAA	-2.73	1.38	1.45
3	B	701	FAD	O3'-C3'	-2.53	1.37	1.43
3	A	702	FAD	O3'-C3'	-2.42	1.37	1.43
3	B	701	FAD	C2B-C3B	-2.09	1.47	1.53
3	B	701	FAD	C7M-C7	2.01	1.55	1.51
3	A	702	FAD	C2-N1	2.01	1.42	1.38
4	B	703	60G	OAR-CAV	2.01	1.38	1.33
4	B	703	60G	C6-N1	2.01	1.36	1.33
4	A	703	60G	C6-N1	2.01	1.36	1.33
3	A	702	FAD	C7M-C7	2.04	1.55	1.51
4	B	703	60G	CAU-NAQ	2.24	1.43	1.39
3	B	701	FAD	C2-N1	2.36	1.43	1.38
3	B	701	FAD	C2'-C3'	2.42	1.58	1.53
4	A	703	60G	CAU-NAP	2.53	1.42	1.37
3	A	702	FAD	C2'-C3'	2.59	1.58	1.53
3	A	702	FAD	O4B-C1B	2.75	1.45	1.41
3	B	701	FAD	O4B-C1B	2.82	1.45	1.41
4	B	703	60G	CAU-NAP	2.84	1.42	1.37
5	A	705	TPP	C4'-N4'	2.86	1.41	1.34
3	A	702	FAD	C4-N3	2.95	1.38	1.33
5	B	705	TPP	C4'-N4'	3.02	1.42	1.34
3	B	701	FAD	C4-N3	3.21	1.38	1.33
4	A	703	60G	C2-NAP	3.27	1.42	1.38
4	B	703	60G	C2-NAP	3.80	1.43	1.38
3	B	701	FAD	C4X-N5	4.05	1.39	1.33
3	A	702	FAD	C4X-N5	4.09	1.39	1.33
3	A	702	FAD	C10-N1	4.45	1.43	1.35
3	B	701	FAD	C10-N1	4.61	1.43	1.35
3	A	702	FAD	C4-C4X	5.26	1.52	1.41
3	B	701	FAD	C4-C4X	5.27	1.52	1.41

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	60G	OAF-SBB-OAG	-9.18	103.32	119.31
4	A	703	60G	OAF-SBB-OAG	-9.16	103.35	119.31
3	A	702	FAD	N3A-C2A-N1A	-8.84	121.93	128.87
3	B	701	FAD	N3A-C2A-N1A	-7.97	122.61	128.87
4	A	703	60G	C5-C4-N3	-5.11	118.62	124.02
4	B	703	60G	C5-C4-N3	-5.06	118.66	124.02

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	703	60G	C5-C6-N1	-4.97	118.76	124.02
4	A	703	60G	C5-C6-N1	-4.80	118.94	124.02
3	B	701	FAD	N3-C2-N1	-4.07	120.84	127.69
3	A	702	FAD	N3-C2-N1	-3.98	120.98	127.69
4	B	703	60G	OAD-CAU-NAP	-3.97	117.52	123.59
4	A	703	60G	OAD-CAU-NAP	-3.69	117.94	123.59
5	A	705	TPP	N1'-C2'-N3'	-3.61	118.72	125.50
5	B	705	TPP	N1'-C2'-N3'	-3.60	118.74	125.50
5	B	705	TPP	CM4-C4-C5	-3.41	121.70	128.91
4	B	703	60G	N3-C2-N1	-3.29	121.26	126.19
4	A	703	60G	N3-C2-N1	-3.22	121.38	126.19
5	A	705	TPP	CM4-C4-C5	-3.08	122.40	128.91
3	A	702	FAD	C1B-N9A-C4A	-3.04	123.42	126.81
4	A	703	60G	C2-NAP-CAU	-2.67	126.71	130.21
5	A	705	TPP	C5'-C7'-N3	-2.64	108.73	113.37
4	A	703	60G	OAR-CAV-OAE	-2.63	118.00	123.45
3	B	701	FAD	C4X-C4-N3	-2.51	120.24	123.52
3	A	702	FAD	C4X-C4-N3	-2.49	120.27	123.52
3	A	702	FAD	C4B-O4B-C1B	-2.43	107.07	109.64
4	A	703	60G	CAU-NAQ-SBB	-2.41	118.22	123.69
4	B	703	60G	OAR-CAV-OAE	-2.35	118.57	123.45
3	B	701	FAD	C1B-N9A-C4A	-2.26	124.28	126.81
5	A	705	TPP	C5'-C6'-N1'	-2.14	120.12	123.86
4	B	703	60G	C2-NAP-CAU	-2.10	127.47	130.21
5	B	705	TPP	C5'-C7'-N3	-2.10	109.69	113.37
5	B	705	TPP	C5'-C6'-N1'	-2.09	120.22	123.86
3	A	702	FAD	C4-C4X-C10	-2.06	118.62	119.94
3	A	702	FAD	C1'-N10-C9A	2.10	121.26	118.83
5	B	705	TPP	C6-C5-S1	2.24	123.37	120.24
3	A	702	FAD	C4-C4X-N5	2.36	121.57	118.70
3	B	701	FAD	C4-C4X-N5	2.39	121.60	118.70
5	A	705	TPP	C5-C4-N3	2.41	113.09	107.78
3	B	701	FAD	C5X-C9A-N10	2.41	119.38	117.58
4	B	703	60G	NAP-C2-N1	2.41	124.08	116.43
3	B	701	FAD	C1'-N10-C9A	2.42	121.64	118.83
4	A	703	60G	NAP-C2-N1	2.51	124.40	116.43
5	B	705	TPP	C5-C4-N3	2.83	114.01	107.78
3	A	702	FAD	C5X-C9A-N10	2.84	119.71	117.58
5	B	705	TPP	CM2-C2'-N1'	3.08	120.85	117.05
5	A	705	TPP	C6'-N1'-C2'	3.18	121.96	115.92
5	B	705	TPP	C6'-N1'-C2'	3.20	122.00	115.92
5	A	705	TPP	CM2-C2'-N1'	3.41	121.26	117.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	60G	C2-N1-C6	4.34	118.78	114.92
4	A	703	60G	OAR-CAV-CBA	4.35	119.49	112.27
4	A	703	60G	NAQ-CAU-NAP	4.46	121.92	114.45
4	B	703	60G	C2-N1-C6	4.53	118.95	114.92
4	B	703	60G	OAR-CAV-CBA	4.57	119.85	112.27
4	B	703	60G	NAQ-CAU-NAP	4.66	122.27	114.45
3	A	702	FAD	C4-N3-C2	5.73	119.94	115.16
3	B	701	FAD	C4-N3-C2	5.77	119.97	115.16
4	A	703	60G	C4-C5-C6	6.13	120.34	115.22
4	B	703	60G	C4-C5-C6	6.57	120.71	115.22
4	B	703	60G	C2-N3-C4	7.57	121.65	114.92
4	A	703	60G	C2-N3-C4	7.89	121.94	114.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	FAD	1	0
5	A	705	TPP	3	0
3	B	701	FAD	1	0
5	B	705	TPP	3	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 (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	599/677 (88%)	-0.22	12 (2%)	68	75	15, 25, 46, 96	0
1	B	599/677 (88%)	0.00	27 (4%)	37	48	18, 34, 62, 104	0
All	All	1198/1354 (88%)	-0.11	39 (3%)	50	60	15, 29, 57, 104	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PRO	7.6
1	A	83	PRO	6.9
1	B	280	ALA	6.0
1	A	277	THR	5.9
1	B	279	ARG	5.7
1	B	270	SER	5.2
1	A	268	LEU	5.0
1	A	270	SER	4.6
1	B	268	LEU	4.4
1	B	467	PRO	4.3
1	B	281	GLN	4.2
1	B	87	THR	4.0
1	A	279	ARG	3.8
1	B	282	ASP	3.8
1	B	278	SER	3.8
1	B	284	PHE	3.6
1	B	283	GLU	3.5
1	B	277	THR	3.5
1	B	468	GLY	3.3
1	B	84	ASP	3.3
1	B	456	LYS	3.2
1	B	466	THR	3.2
1	A	265	LYS	3.1
1	A	84	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	418	GLN	2.8
1	B	129	ASP	2.7
1	B	636	LYS	2.7
1	B	264	THR	2.6
1	A	266	THR	2.6
1	B	446	GLU	2.4
1	A	278	SER	2.4
1	A	636	LYS	2.4
1	B	488	GLY	2.3
1	A	282	ASP	2.2
1	B	397	ALA	2.2
1	B	624	GLU	2.1
1	B	623	GLU	2.1
1	A	85	MET	2.0
1	B	286	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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(Å^2)	Q<0.9
2	MG	A	704	1/1	1.00	0.19	4.28	12,12,12,12	0
2	MG	B	704	1/1	0.99	0.13	3.40	19,19,19,19	0
2	MG	A	701	1/1	0.99	0.10	0.03	17,17,17,17	0
5	TPP	A	705	26/26	0.97	0.13	-0.17	16,20,36,50	0
3	FAD	A	702	53/53	0.99	0.11	-0.19	13,18,22,23	0
4	60G	A	703	28/28	0.97	0.11	-0.22	21,26,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	TPP	B	705	26/26	0.97	0.12	-0.41	17,23,48,54	0
3	FAD	B	701	53/53	0.97	0.09	-0.46	21,28,36,41	0
4	60G	B	703	28/28	0.96	0.09	-0.73	30,36,42,44	0
2	MG	B	702	1/1	0.98	0.07	-2.24	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.