



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 7, 2017 – 07:20 PM EST

PDB ID : 5INV
Title : Saccharomyces cerevisiae acetohydroxyacid synthase
Authors : Guddat, L.W.; Lonhienne, T.
Deposited on : 2016-03-07
Resolution : 2.28 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.

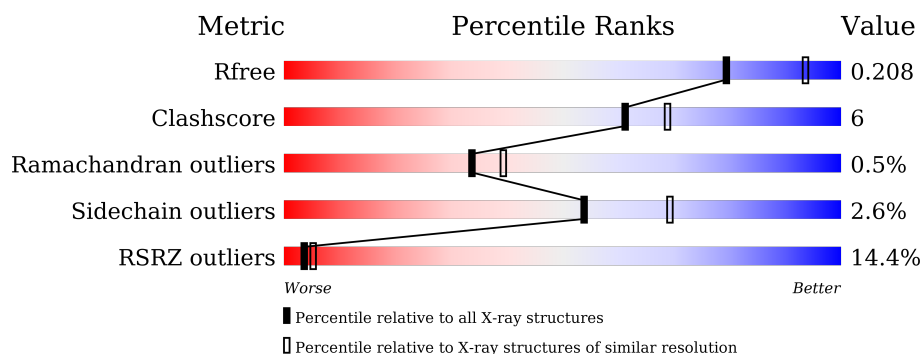
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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-20028442

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X-RAY DIFFRACTION

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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (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	677	<div> <div>4%</div> <div>73%</div> <div>6%</div> <div>21%</div> </div>
1	B	677	<div> <div>19%</div> <div>69%</div> <div>11%</div> <div>18%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OXY	A	704	-	-	-	X
5	OXY	A	706	-	-	-	X
5	OXY	B	706	-	-	X	X
5	OXY	B	708	-	-	-	X
6	CO2	A	707	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8818 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	538	Total	C	N	O	S	0	0	0
			4073	2581	701	772	19			
1	B	553	Total	C	N	O	S	0	0	0
			4188	2651	719	798	20			

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 POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0

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

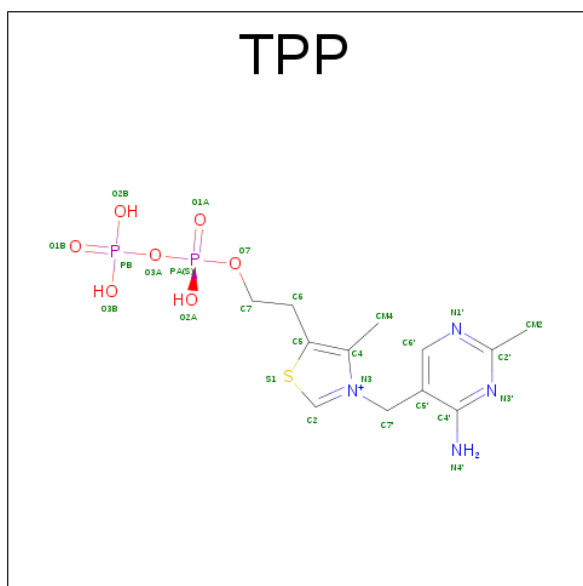
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

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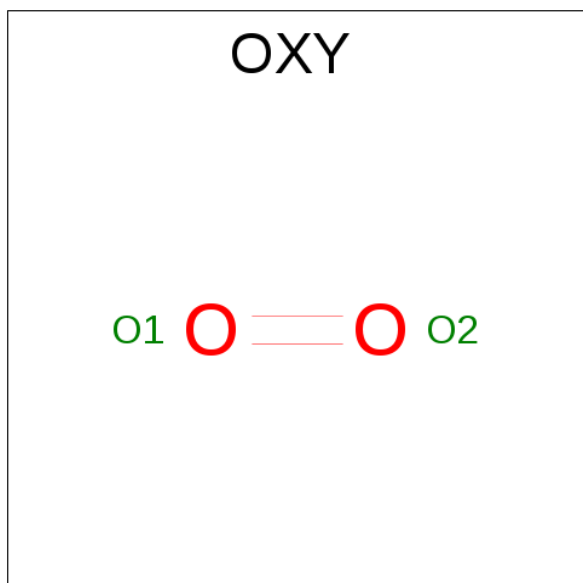
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



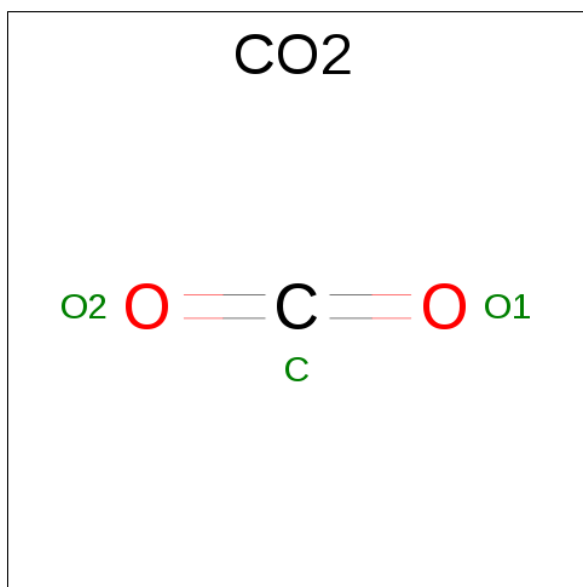
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



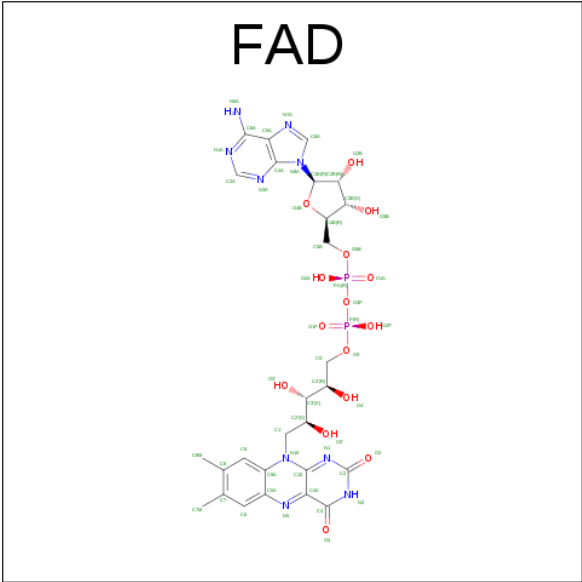
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	A	1	Total O 2 2	0	0
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

- Molecule 6 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO₂).



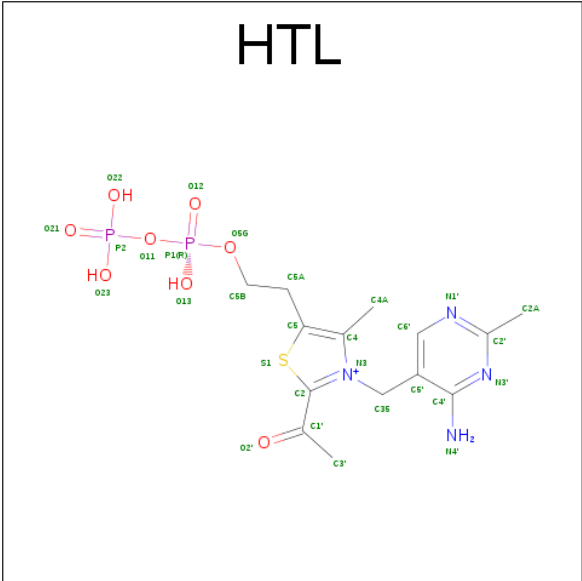
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



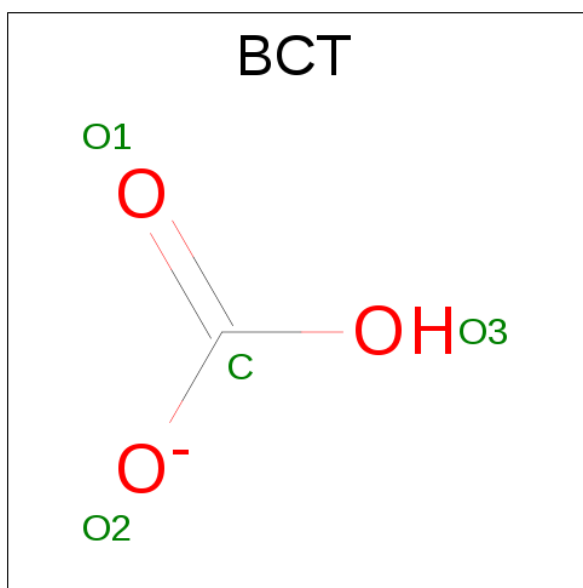
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
7	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: C₁₄H₂₁N₄O₈P₂S).



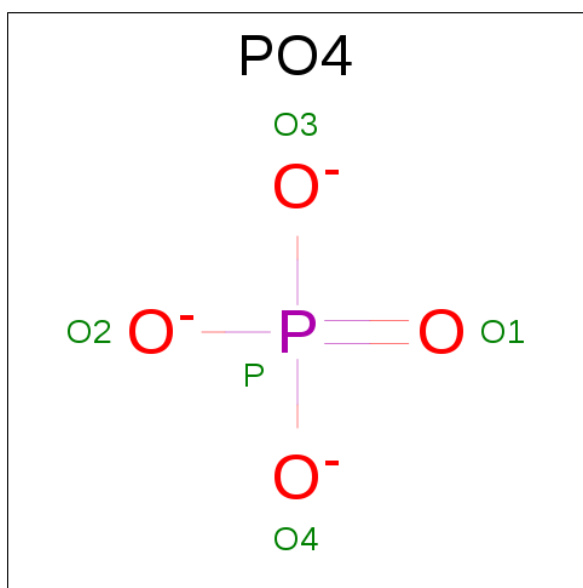
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		

- Molecule 9 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	228	Total 228	O 228	0	0
11	B	134	Total 134	O 134	0	0

D646	PRO
K647	VAL
K648	LEU
V649	PRO
	MET
	VAL
	ALA
	GLY
	GLY
	SER
	GLY
	LEU
	ASP
	GLU
	PHE
	ILE
	ASN
	PHE
	ASP
	PRO
	GLU
	VAL
	GLU
	ARG
	GLN
	GLN
	THR
	GLU
	LEU
	ARG
	HIS
	LYS
	ARG
	THR
	GLY
	GLY
	LYS
	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.90Å 108.77Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 2.28 47.95 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.31-2.28) 99.6 (47.95-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.168 , 0.199 0.184 , 0.208	Depositor DCC
R_{free} test set	1996 reflections (2.32%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8818	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, CO2, OXY, PO4, HTL, TPP, BCT, K, FAD

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	0.31	0/4154	0.46	0/5634
1	B	0.27	0/4269	0.47	0/5792
All	All	0.29	0/8423	0.46	0/11426

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	4073	0	4109	30	0
1	B	4188	0	4202	57	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	16	3	0
5	A	6	0	0	2	0
5	B	12	0	0	4	0
6	A	3	0	0	4	0
7	A	53	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	53	0	31	5	0
8	B	29	0	18	2	0
9	B	4	0	0	1	0
10	B	5	0	0	0	0
11	A	228	0	0	2	0
11	B	134	0	0	2	0
All	All	8818	0	8406	93	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 6.

The worst 5 of 93 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:A:201:PHE:CZ	7:B:712:FAD:HM82	1.99	0.98
1:A:385:ILE:O	1:A:393:ARG:NH2	2.19	0.75
1:B:295:LEU:HD11	1:B:401:GLY:HA2	1.71	0.71
1:B:330:PRO:HB2	1:B:349:LEU:HD11	1.73	0.70
1:A:151:ARG:NH1	1:A:518:THR:O	2.24	0.70

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)
1:B:129:ASP:OD2	1:B:472:LYS:NZ[4_477]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	532/677 (79%)	525 (99%)	6 (1%)	1 (0%)	52 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	545/677 (80%)	516 (95%)	25 (5%)	4 (1%)	26	30
All	All	1077/1354 (80%)	1041 (97%)	31 (3%)	5 (0%)	34	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	LYS
1	B	459	PRO
1	A	463	MET
1	B	390	PRO
1	B	398	GLU

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	439/556 (79%)	433 (99%)	6 (1%)	74	86
1	B	451/556 (81%)	434 (96%)	17 (4%)	40	53
All	All	890/1112 (80%)	867 (97%)	23 (3%)	54	69

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	384	ASN
1	B	400	ARG
1	B	614	LEU
1	B	393	ARG
1	B	411	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	290	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	TPP	A	703	3	20,27,27	1.68	2 (10%)	27,40,40	1.70	8 (29%)
5	OXY	A	704	-	1,1,1	0.11	0	0,0,0	0.00	-
5	OXY	A	705	-	1,1,1	0.03	0	0,0,0	0.00	-
5	OXY	A	706	-	1,1,1	0.02	0	0,0,0	0.00	-
6	CO2	A	707	-	2,2,2	1.11	0	1,1,1	0.63	0
7	FAD	A	708	-	52,58,58	2.17	18 (34%)	52,89,89	1.57	8 (15%)
8	HTL	B	703	3	24,30,30	4.30	11 (45%)	28,45,45	1.95	6 (21%)
9	BCT	B	704	-	0,3,3	0.00	-	0,3,3	0.00	-
5	OXY	B	705	-	1,1,1	0.08	0	0,0,0	0.00	-
5	OXY	B	706	-	1,1,1	0.11	0	0,0,0	0.00	-
5	OXY	B	707	-	1,1,1	0.07	0	0,0,0	0.00	-
5	OXY	B	708	-	1,1,1	0.03	0	0,0,0	0.00	-
5	OXY	B	709	-	1,1,1	0.01	0	0,0,0	0.00	-
5	OXY	B	710	-	1,1,1	0.03	0	0,0,0	0.00	-
10	PO4	B	711	-	4,4,4	0.70	0	6,6,6	0.23	0
7	FAD	B	712	-	52,58,58	1.44	12 (23%)	52,89,89	2.15	8 (15%)

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	TPP	A	703	3	-	0/16/17/17	0/2/2/2
5	OXY	A	704	-	-	0/0/0/0	0/0/0/0
5	OXY	A	705	-	-	0/0/0/0	0/0/0/0
5	OXY	A	706	-	-	0/0/0/0	0/0/0/0
6	CO2	A	707	-	-	0/0/0/0	0/0/0/0
7	FAD	A	708	-	-	0/30/50/50	0/6/6/6
8	HTL	B	703	3	-	0/16/21/21	0/2/2/2
9	BCT	B	704	-	-	0/0/0/0	0/0/0/0
5	OXY	B	705	-	-	0/0/0/0	0/0/0/0
5	OXY	B	706	-	-	0/0/0/0	0/0/0/0
5	OXY	B	707	-	-	0/0/0/0	0/0/0/0
5	OXY	B	708	-	-	0/0/0/0	0/0/0/0
5	OXY	B	709	-	-	0/0/0/0	0/0/0/0
5	OXY	B	710	-	-	0/0/0/0	0/0/0/0
10	PO4	B	711	-	-	0/0/0/0	0/0/0/0
7	FAD	B	712	-	-	0/30/50/50	0/6/6/6

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	703	HTL	C5-S1	-14.29	1.47	1.74
7	A	708	FAD	C1'-N10	-8.03	1.39	1.48
4	A	703	TPP	C4-N3	-6.02	1.34	1.39
7	A	708	FAD	C2B-C1B	-5.98	1.44	1.53
8	B	703	HTL	P2-O22	-3.83	1.41	1.54

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	712	FAD	N3A-C2A-N1A	-7.93	122.64	128.87
7	A	708	FAD	N3A-C2A-N1A	-6.08	124.09	128.87
7	B	712	FAD	C4-C4X-C10	-5.91	116.16	119.94
8	B	703	HTL	C5A-C5-C4	-3.78	123.11	127.34
7	B	712	FAD	C4X-C4-N3	-3.46	119.00	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	TPP	3	0
5	A	704	OXY	1	0
5	A	706	OXY	1	0
6	A	707	CO2	4	0
8	B	703	HTL	2	0
9	B	704	BCT	1	0
5	B	705	OXY	1	0
5	B	706	OXY	2	0
5	B	710	OXY	1	0
7	B	712	FAD	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 [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	538/677 (79%)	0.19	25 (4%) 36 44	30, 45, 91, 165	0
1	B	553/677 (81%)	1.22	132 (23%) 1 1	30, 57, 147, 174	0
All	All	1091/1354 (80%)	0.71	157 (14%) 3 5	30, 49, 136, 174	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	MET	9.4
1	B	402	GLY	9.3
1	B	460	TYR	9.0
1	B	296	ILE	8.7
1	B	394	ARG	7.8

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(\AA^2)	Q<0.9
5	OXY	B	706	2/2	0.90	0.45	10.32	80,80,80,85	0
5	OXY	B	708	2/2	0.67	0.33	4.68	114,114,114,114	0
5	OXY	A	704	2/2	0.89	0.24	3.72	80,80,80,90	0
5	OXY	A	706	2/2	0.91	0.25	2.39	89,89,89,90	0
7	FAD	B	712	53/53	0.93	0.20	0.97	20,20,20,20	0
7	FAD	A	708	53/53	0.95	0.16	0.77	20,20,20,20	0
4	TPP	A	703	26/26	0.89	0.18	0.22	30,60,71,536	0
8	HTL	B	703	29/29	0.92	0.16	-0.43	30,40,54,58	2
2	K	A	701	1/1	0.95	0.11	-0.59	51,51,51,51	0
2	K	B	701	1/1	0.98	0.08	-0.77	65,65,65,65	0
3	MG	A	702	1/1	0.92	0.12	-	65,65,65,65	0
3	MG	B	702	1/1	0.89	0.05	-	41,41,41,41	0
9	BCT	B	704	4/4	0.77	0.17	-	103,103,107,110	0
5	OXY	B	709	2/2	0.50	0.46	-	73,73,73,81	0
5	OXY	A	705	2/2	0.77	0.57	-	90,90,90,91	0
5	OXY	B	705	2/2	0.66	0.42	-	88,88,88,89	0
5	OXY	B	707	2/2	0.58	0.43	-	105,105,105,106	0
5	OXY	B	710	2/2	0.71	0.24	-	101,101,101,104	0
6	CO2	A	707	3/3	0.71	0.31	-	84,84,89,92	0
10	PO4	B	711	5/5	0.88	0.17	-	113,116,121,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.