Full wwPDB X-ray Structure Validation Report (i)

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)

The following versions of software and data (see references (i)) 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

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 2.28 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.
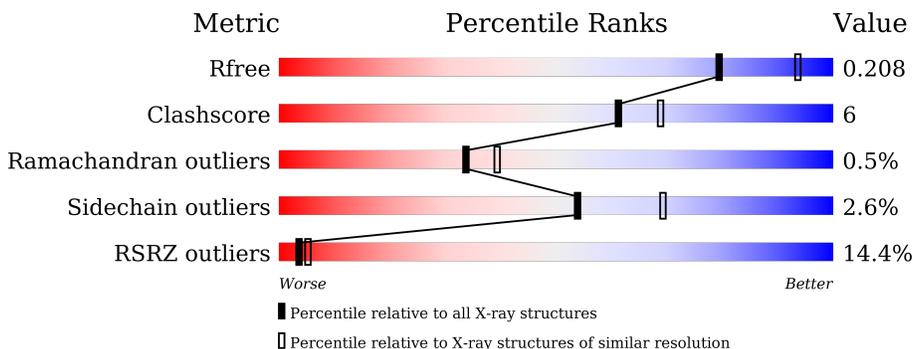
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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 <=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
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 (i)

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	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

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

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

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

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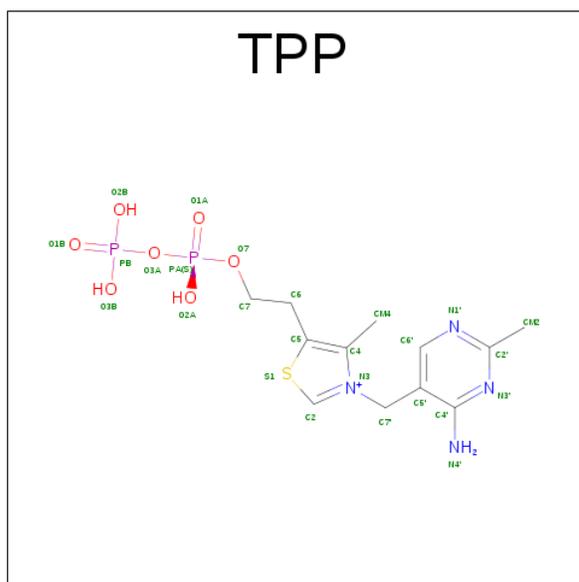
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).
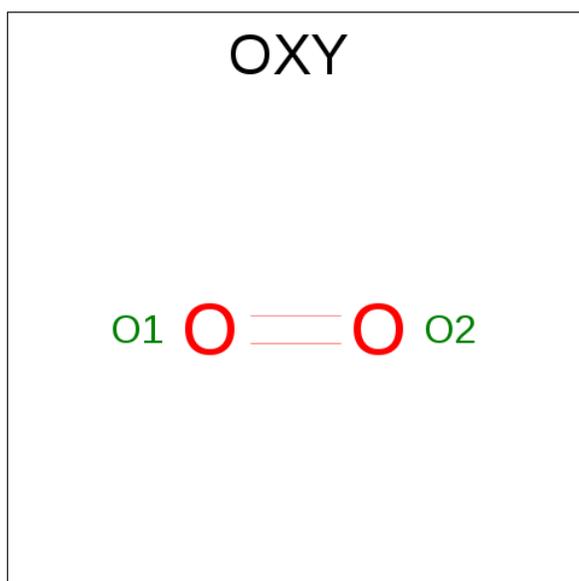
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total O 2 2		0	0
5	A	1	Total O 2 2		0	0
5	A	1	Total O 2 2		0	0
5	B	1	Total O 2 2		0	0
5	B	1	Total O 2 2		0	0
5	B	1	Total O 2 2		0	0
5	B	1	Total O 2 2		0	0
5	B	1	Total O 2 2		0	0
5	B	1	Total O 2 2		0	0

- Molecule 6 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO_2).
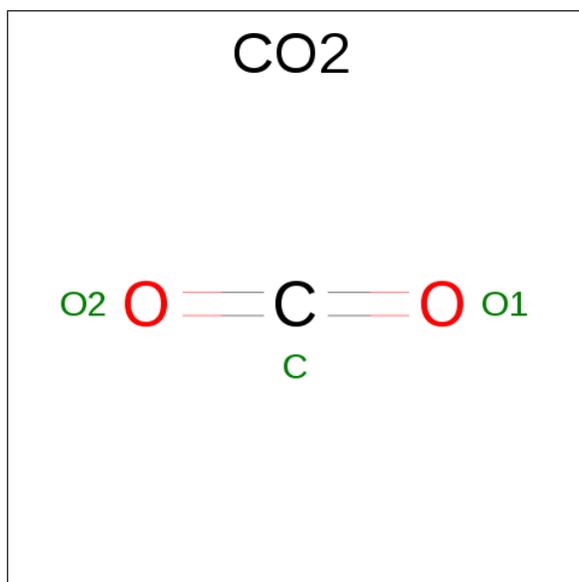
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total C O 3 1 2			0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
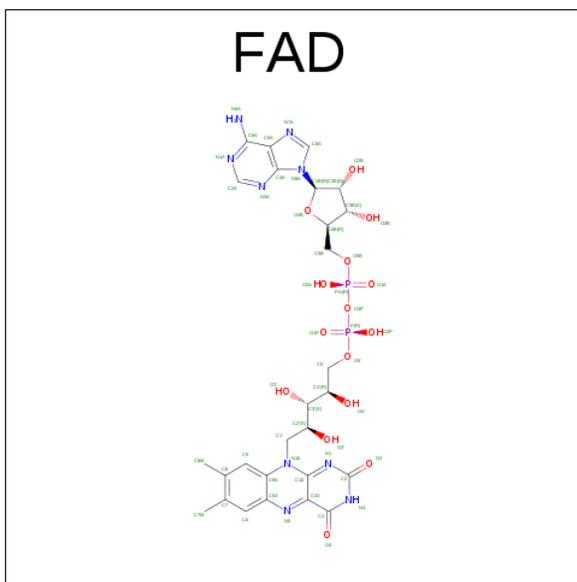
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
7	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$).

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

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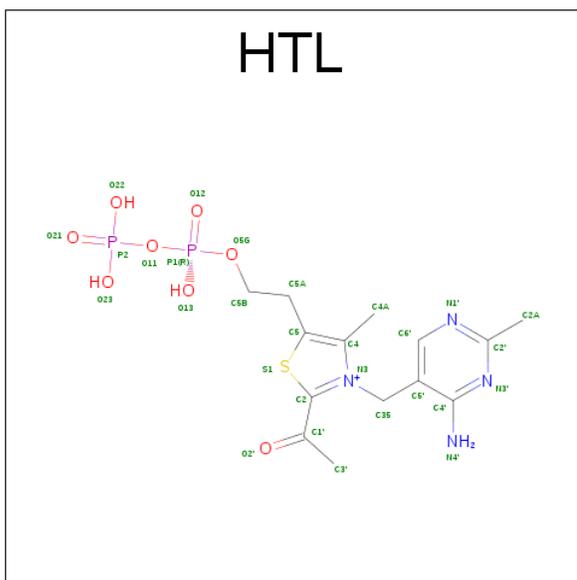
- Molecule 9 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).
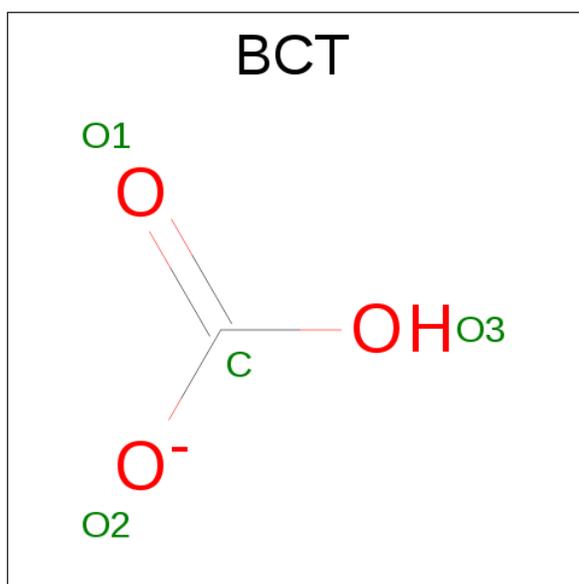
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	4	1	3	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
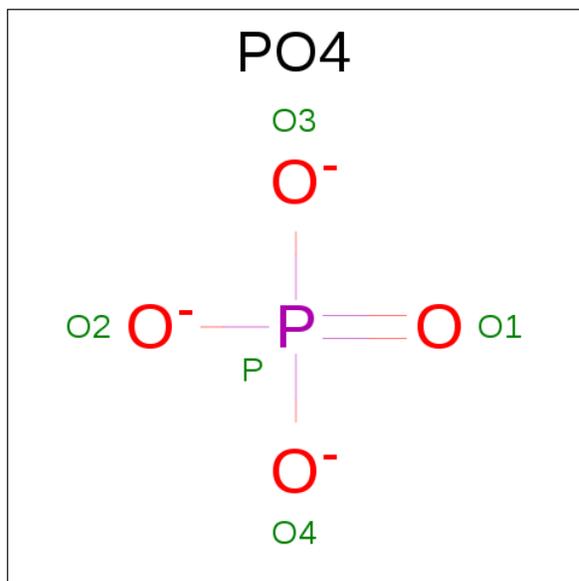
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
10	B	1	5	4	1	0	0

- 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

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

Chain A:

• Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

Chain B:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< |L| > = 0.49, < L^2 > = 0.33$	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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.

All (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
1:B:326:ARG:NH2	1:B:438:ILE:O	2.25	0.69
5:B:710:OXY:O2	11:B:801:HOH:O	2.11	0.68
1:B:162:THR:OG1	5:B:706:OXY:O1	2.12	0.67
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.77	0.67
1:A:376:ARG:NH2	11:A:801:HOH:O	2.25	0.65
1:B:292:ALA:HB2	1:B:421:ILE:HG21	1.79	0.64
1:B:325:ASP:OD1	1:B:347:LYS:NZ	2.31	0.64
1:B:395:ALA:HA	1:B:400:ARG:HB3	1.81	0.61
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.82	0.61
1:A:201:PHE:CE1	7:B:712:FAD:HM82	2.36	0.61
1:B:296:ILE:HG22	1:B:369:LEU:HD21	1.83	0.60
1:A:292:ALA:HB3	1:A:434:MET:HE1	1.83	0.60
6:A:707:CO2:O2	5:B:705:OXY:O1	2.21	0.58
1:B:296:ILE:HD11	1:B:438:ILE:HG23	1.85	0.58
1:B:146:ALA:HB3	1:B:184:MET:HE2	1.86	0.57
1:A:201:PHE:CE2	1:A:202:GLN:HG3	2.39	0.57
1:A:201:PHE:HZ	7:B:712:FAD:HM82	1.64	0.57
1:B:361:ASN:N	1:B:361:ASN:OD1	2.37	0.57
1:B:472:LYS:NZ	1:B:646:ASP:OD2	2.35	0.56
1:B:299:ALA:O	1:B:444:ARG:NH2	2.39	0.55
1:A:202:GLN:NE2	5:A:704:OXY:O2	2.38	0.55
1:B:294:ASP:HA	1:B:297:ASN:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:707:CO2:C	8:B:703:HTL:C1'	2.86	0.54
1:B:286:MET:O	1:B:290:ASN:ND2	2.41	0.54
1:A:494:THR:HG22	1:A:517:ILE:HB	1.90	0.53
1:B:381:VAL:HG22	7:B:712:FAD:O2	2.08	0.53
1:B:395:ALA:HB1	1:B:401:GLY:N	2.24	0.52
1:B:301:LYS:HD2	1:B:447:TRP:CE3	2.45	0.52
1:B:416:VAL:HG12	1:B:417:VAL:HG23	1.92	0.52
1:A:116:GLY:H	6:A:707:CO2:C	2.23	0.52
1:B:300:LYS:HB3	1:B:368:ASP:OD2	2.10	0.51
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.92	0.51
1:B:99:ASN:HD22	1:B:125:ILE:HD13	1.76	0.51
1:B:413:ILE:HD13	1:B:422:ALA:HB1	1.91	0.51
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.41	0.51
1:A:201:PHE:CE1	7:B:712:FAD:C8M	2.94	0.51
1:B:296:ILE:O	1:B:299:ALA:HB2	2.11	0.50
1:A:465:GLU:HG2	1:A:472:LYS:HG2	1.93	0.50
1:B:382:THR:HG22	1:B:388:PHE:HE1	1.76	0.49
1:B:292:ALA:HB1	1:B:404:ILE:HD13	1.93	0.49
1:B:560:LEU:HG	1:B:614:LEU:HD21	1.93	0.49
1:B:342:ASP:OD2	1:B:511:ARG:NH2	2.37	0.49
1:A:619:VAL:HG22	1:A:628:LYS:HG3	1.95	0.48
4:A:703:TPP:H2	4:A:703:TPP:HN42	1.78	0.48
1:B:582:MET:HG2	11:B:801:HOH:O	2.13	0.48
1:B:385:ILE:HD12	1:B:385:ILE:H	1.78	0.48
1:A:251:LYS:NZ	11:A:807:HOH:O	2.43	0.48
6:A:707:CO2:O1	8:B:703:HTL:O2'	2.32	0.47
1:B:362:LEU:HD21	1:B:450:GLN:OE1	2.15	0.47
1:B:361:ASN:O	1:B:365:GLN:HG2	2.16	0.46
1:A:410:PRO:HG3	1:A:424:GLU:OE2	2.15	0.46
1:B:388:PHE:CD2	1:B:389:ALA:HB2	2.50	0.46
1:B:388:PHE:HA	1:B:389:ALA:HA	1.59	0.45
1:B:411:LYS:H	1:B:411:LYS:HD2	1.79	0.45
4:A:703:TPP:C2	4:A:703:TPP:HN42	2.29	0.45
1:A:472:LYS:NZ	1:A:646:ASP:OD2	2.42	0.45
1:B:301:LYS:HB3	1:B:367:ALA:HA	1.99	0.45
1:B:384:ASN:N	1:B:384:ASN:OD1	2.39	0.45
1:B:202:GLN:NE2	5:B:706:OXY:O2	2.50	0.44
4:A:703:TPP:H7'2	9:B:704:BCT:O3	2.17	0.44
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.53	0.43
1:B:296:ILE:HD11	1:B:438:ILE:HD12	2.01	0.43
1:B:297:ASN:ND2	1:B:437:LYS:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:HA	1:A:269:PRO:HD3	1.93	0.42
1:B:389:ALA:HA	1:B:390:PRO:HD3	1.90	0.42
1:B:621:LYS:HE3	1:B:621:LYS:HB2	1.86	0.42
1:B:393:ARG:HG2	1:B:393:ARG:O	2.19	0.42
1:B:585:GLN:HG2	1:B:586:TRP:HD1	1.84	0.42
1:A:263:PRO:HB2	1:A:266:THR:HG23	2.00	0.42
1:A:465:GLU:OE2	1:A:472:LYS:N	2.39	0.42
1:A:165:PRO:HD3	1:B:522:LEU:HG	2.01	0.42
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.87	0.42
1:B:151:ARG:HD2	1:B:182:ILE:CD1	2.50	0.41
1:B:290:ASN:HD22	1:B:437:LYS:NZ	2.18	0.41
1:B:382:THR:HG22	1:B:388:PHE:CE1	2.55	0.41
1:B:360:ALA:O	1:B:364:VAL:HG23	2.20	0.41
1:A:554:ASN:HA	1:A:557:LEU:HD23	2.02	0.41
1:B:300:LYS:O	1:B:301:LYS:HD3	2.19	0.41
1:A:201:PHE:CD2	1:A:202:GLN:HG3	2.55	0.41
1:A:260:ASN:HA	1:A:261:PRO:HD3	1.98	0.41
1:B:184:MET:O	1:B:244:PRO:HA	2.21	0.41
1:B:444:ARG:HH11	1:B:444:ARG:HB3	1.85	0.41
1:B:444:ARG:HB3	1:B:444:ARG:NH1	2.36	0.41
1:B:268:LEU:HA	1:B:269:PRO:HD3	1.89	0.40
1:A:600:GLN:NE2	5:A:706:OXY:O1	2.41	0.40
1:B:368:ASP:OD1	1:B:369:LEU:N	2.54	0.40
1:A:172:THR:HB	1:A:173:PRO:HD3	2.03	0.40
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.03	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)
1:B:129:ASP:OD2	1:B:472:LYS:NZ[4_477]	2.18	0.02

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

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	CYS
1	A	376	ARG
1	A	411	LYS
1	A	460	TYR
1	A	555	MET
1	A	645	VAL
1	B	296	ILE
1	B	352	LEU

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Mol	Chain	Res	Type
1	B	357	CYS
1	B	361	ASN
1	B	384	ASN
1	B	393	ARG
1	B	400	ARG
1	B	411	LYS
1	B	435	MET
1	B	442	LYS
1	B	443	GLU
1	B	450	GLN
1	B	460	TYR
1	B	560	LEU
1	B	600	GLN
1	B	614	LEU
1	B	649	VAL

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 (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 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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
8	B	703	HTL	P1-O13	-3.61	1.39	1.55
8	B	703	HTL	C5'-C4'	-3.56	1.36	1.42
7	A	708	FAD	O3'-C3'	-3.40	1.35	1.43
7	A	708	FAD	C2B-C3B	-2.94	1.45	1.53
7	B	712	FAD	C2B-C1B	-2.89	1.49	1.53
7	B	712	FAD	C2-N3	-2.84	1.32	1.38
7	A	708	FAD	C4X-C10	-2.82	1.35	1.40
8	B	703	HTL	P2-O23	-2.69	1.45	1.54
7	A	708	FAD	PA-O2A	-2.47	1.44	1.55
7	A	708	FAD	C10-N10	-2.41	1.36	1.39
7	B	712	FAD	C2-N1	-2.40	1.33	1.38
7	B	712	FAD	C1'-N10	-2.33	1.45	1.48
8	B	703	HTL	P2-O21	-2.32	1.43	1.50
7	A	708	FAD	P-O2P	-2.30	1.45	1.55
7	A	708	FAD	O4B-C4B	-2.29	1.39	1.45
7	B	712	FAD	C6-C5X	-2.28	1.38	1.41
7	B	712	FAD	PA-O2A	-2.21	1.45	1.55
7	A	708	FAD	C3B-C4B	-2.13	1.47	1.53
7	A	708	FAD	O2'-C2'	-2.12	1.38	1.43
8	B	703	HTL	P1-O12	-2.10	1.43	1.51
7	B	712	FAD	P-O2P	-2.08	1.46	1.55
7	A	708	FAD	C8A-N7A	-2.07	1.30	1.34
7	A	708	FAD	O4-C4	-2.07	1.19	1.24
7	A	708	FAD	C5'-C4'	-2.03	1.48	1.51
7	A	708	FAD	C9A-C5X	-2.01	1.38	1.42
7	B	712	FAD	O4B-C4B	-2.01	1.40	1.45
7	A	708	FAD	C4X-N5	2.22	1.36	1.33
7	B	712	FAD	C9A-C5X	2.34	1.47	1.42
7	B	712	FAD	C4-C4X	2.37	1.46	1.41
7	B	712	FAD	C4X-C10	2.55	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	712	FAD	C8-C7	2.68	1.48	1.41
7	A	708	FAD	C10-N1	2.89	1.40	1.35
4	A	703	TPP	C4'-N4'	3.13	1.42	1.34
8	B	703	HTL	C4'-N4'	3.27	1.42	1.34
7	A	708	FAD	C4-C4X	4.24	1.49	1.41
8	B	703	HTL	O2'-C1'	4.90	1.39	1.22
8	B	703	HTL	C4-N3	7.69	1.57	1.39
8	B	703	HTL	C2-N3	8.63	1.45	1.35

All (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
7	A	708	FAD	N3-C2-N1	-3.42	121.94	127.69
4	A	703	TPP	N1'-C2'-N3'	-3.41	119.10	125.50
4	A	703	TPP	CM4-C4-C5	-3.09	122.37	128.91
7	B	712	FAD	N3-C2-N1	-2.94	122.74	127.69
7	A	708	FAD	C1B-N9A-C4A	-2.87	123.60	126.81
7	A	708	FAD	C4X-C4-N3	-2.40	120.39	123.52
8	B	703	HTL	N1'-C2'-N3'	-2.37	121.05	125.50
8	B	703	HTL	C5'-C6'-N1'	-2.21	120.01	123.86
4	A	703	TPP	C5'-C6'-N1'	-2.17	120.06	123.86
4	A	703	TPP	C5'-C7'-N3	-2.15	109.59	113.37
7	A	708	FAD	C6-C5X-C9A	2.01	121.33	119.11
7	B	712	FAD	C2A-N1A-C6A	2.09	122.49	118.77
4	A	703	TPP	C6-C5-S1	2.13	123.22	120.24
4	A	703	TPP	C5-C4-N3	2.70	113.73	107.78
7	A	708	FAD	C5X-C9A-N10	2.74	119.63	117.58
4	A	703	TPP	CM2-C2'-N1'	3.01	120.77	117.05
4	A	703	TPP	C6'-N1'-C2'	3.03	121.67	115.92
8	B	703	HTL	C2A-C2'-N1'	3.12	120.90	117.05
7	A	708	FAD	C1'-N10-C9A	3.16	122.49	118.83
7	B	712	FAD	C4X-N5-C5X	3.39	120.72	116.72
8	B	703	HTL	C6'-C5'-C4'	3.42	120.47	115.65
7	B	712	FAD	C4-C4X-N5	3.63	123.11	118.70
7	A	708	FAD	C4-N3-C2	4.31	118.75	115.16
8	B	703	HTL	C5A-C5-S1	6.11	128.79	120.24
7	B	712	FAD	C4-N3-C2	7.98	121.81	115.16

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(Å²)	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

All (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
1	B	396	ALA	7.7
1	B	362	LEU	7.7
1	B	444	ARG	7.3
1	B	649	VAL	7.1
1	B	390	PRO	7.0
1	B	449	ALA	6.9
1	B	590	PHE	6.9
1	B	451	ILE	6.9
1	B	366	ASN	6.7
1	B	441	VAL	6.6
1	B	448	PHE	6.6
1	B	303	VAL	6.4
1	B	368	ASP	6.2
1	B	447	TRP	6.1
1	B	293	ALA	6.0
1	B	367	ALA	6.0
1	B	392	ALA	5.9
1	B	299	ALA	5.5
1	B	439	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	324	SER	5.3
1	B	397	ALA	5.3
1	B	595	TYR	5.3
1	B	363	ALA	5.2
1	A	458	TYR	5.2
1	B	416	VAL	5.1
1	B	438	ILE	5.1
1	B	330	PRO	5.0
1	B	370	ILE	5.0
1	A	461	ALA	4.7
1	B	285	VAL	4.7
1	B	459	PRO	4.7
1	B	364	VAL	4.7
1	B	419	THR	4.7
1	B	276	LEU	4.7
1	B	589	LEU	4.6
1	B	325	ASP	4.6
1	B	445	SER	4.6
1	A	456	LYS	4.6
1	A	462	TYR	4.5
1	B	466	THR	4.5
1	B	391	GLU	4.4
1	B	398	GLU	4.4
1	B	446	GLU	4.4
1	B	329	ILE	4.4
1	B	388	PHE	4.4
1	B	418	GLN	4.3
1	B	326	ARG	4.3
1	B	387	LYS	4.3
1	B	294	ASP	4.2
1	B	442	LYS	4.2
1	B	403	ILE	4.2
1	B	463	MET	4.2
1	B	395	ALA	4.2
1	B	297	ASN	4.2
1	B	400	ARG	4.1
1	B	286	MET	4.1
1	B	277	THR	4.1
1	B	458	TYR	4.0
1	A	467	PRO	4.0
1	B	302	PRO	4.0
1	B	462	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	383	GLY	4.0
1	B	369	LEU	4.0
1	B	298	LEU	4.0
1	B	287	GLN	4.0
1	B	284	PHE	3.9
1	B	360	ALA	3.9
1	B	384	ASN	3.8
1	B	279	ARG	3.7
1	A	268	LEU	3.7
1	B	290	ASN	3.7
1	B	417	VAL	3.7
1	B	401	GLY	3.7
1	A	265	LYS	3.6
1	B	443	GLU	3.6
1	B	435	MET	3.6
1	B	283	GLU	3.6
1	B	328	GLN	3.6
1	B	393	ARG	3.5
1	A	83	PRO	3.5
1	B	385	ILE	3.4
1	B	359	THR	3.4
1	B	436	SER	3.4
1	A	466	THR	3.4
1	B	321	LYS	3.3
1	B	347	LYS	3.3
1	B	278	SER	3.2
1	B	280	ALA	3.2
1	B	420	GLN	3.1
1	B	467	PRO	3.1
1	B	457	GLU	3.1
1	B	413	ILE	3.1
1	B	292	ALA	3.1
1	A	596	SER	3.1
1	B	421	ILE	3.0
1	B	386	SER	3.0
1	B	341	PHE	2.9
1	A	270	SER	2.9
1	B	170	VAL	2.8
1	B	322	GLU	2.8
1	A	84	ASP	2.8
1	A	597	HIS	2.8
1	B	348	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	365	GLN	2.7
1	B	379	ASP	2.7
1	B	464	GLU	2.6
1	B	410	PRO	2.6
1	B	399	GLY	2.6
1	B	185	VAL	2.5
1	B	301	LYS	2.5
1	B	159	VAL	2.5
1	B	404	ILE	2.5
1	B	349	LEU	2.5
1	B	647	LYS	2.5
1	A	168	THR	2.4
1	B	291	LYS	2.4
1	B	173	PRO	2.4
1	A	460	TYR	2.4
1	A	170	VAL	2.4
1	B	412	ASN	2.4
1	B	411	LYS	2.4
1	A	469	SER	2.4
1	B	414	ASN	2.4
1	B	323	LEU	2.3
1	B	346	PRO	2.3
1	B	171	VAL	2.3
1	B	468	GLY	2.3
1	A	354	MET	2.3
1	B	174	MET	2.2
1	B	450	GLN	2.2
1	B	289	ILE	2.2
1	B	213	CYS	2.2
1	A	468	GLY	2.2
1	B	430	ASN	2.2
1	B	184	MET	2.2
1	A	459	PRO	2.2
1	A	171	VAL	2.2
1	B	161	VAL	2.2
1	B	522	LEU	2.2
1	A	209	ILE	2.2
1	B	646	ASP	2.2
1	A	648	LYS	2.1
1	A	387	LYS	2.1
1	B	172	THR	2.1
1	B	175	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	127	ASN	2.1
1	B	431	LEU	2.1
1	B	511	ARG	2.1
1	B	331	VAL	2.1
1	B	415	LYS	2.1
1	B	111	PHE	2.1
1	B	209	ILE	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(Å²)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
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.