



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:22 PM GMT

PDB ID : 1T9C
Title : Crystal Structure Of Yeast Acetohydroxyacid Synthase In Complex With A
Sulfonylurea Herbicide, Sulfometuron methyl
Authors : McCourt, J.A.; Pang, S.S.; Guddat, L.W.; Duggleby, R.G.
Deposited on : 2004-05-16
Resolution : 2.34 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
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

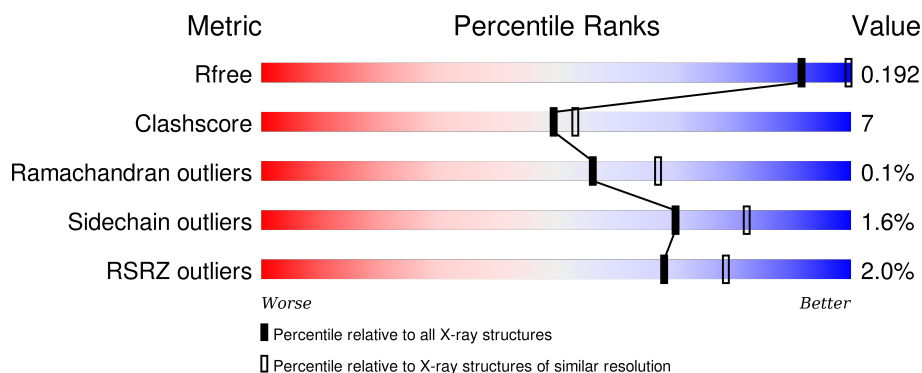
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


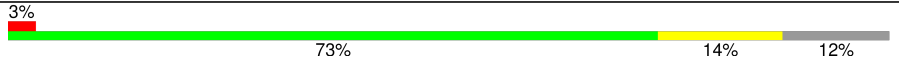
The reported resolution of this entry is 2.34 Å.

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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (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 ≥ 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	 75% 13% 12%
1	B	677	 3% 73% 14% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10410 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	6	0
			4546	2879	785	860	22			
1	B	593	Total	C	N	O	S	0	4	0
			4505	2856	776	851	22			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	CLONING ARTIFACT	UNP P07342
A	12	HIS	-	CLONING ARTIFACT	UNP P07342
A	13	HIS	-	CLONING ARTIFACT	UNP P07342
A	14	HIS	-	CLONING ARTIFACT	UNP P07342
A	15	HIS	-	CLONING ARTIFACT	UNP P07342
A	16	HIS	-	CLONING ARTIFACT	UNP P07342
A	17	HIS	-	CLONING ARTIFACT	UNP P07342
A	18	SER	-	CLONING ARTIFACT	UNP P07342
A	19	SER	-	CLONING ARTIFACT	UNP P07342
A	20	GLY	-	CLONING ARTIFACT	UNP P07342
A	21	LEU	-	CLONING ARTIFACT	UNP P07342
A	22	VAL	-	CLONING ARTIFACT	UNP P07342
A	23	PRO	-	CLONING ARTIFACT	UNP P07342
A	24	ARG	-	CLONING ARTIFACT	UNP P07342
A	25	GLY	-	CLONING ARTIFACT	UNP P07342
A	26	SER	-	CLONING ARTIFACT	UNP P07342
A	27	GLY	-	CLONING ARTIFACT	UNP P07342
A	28	MET	-	CLONING ARTIFACT	UNP P07342
A	29	LYS	-	CLONING ARTIFACT	UNP P07342
A	30	GLU	-	CLONING ARTIFACT	UNP P07342
A	31	THR	-	CLONING ARTIFACT	UNP P07342
A	32	ALA	-	CLONING ARTIFACT	UNP P07342
A	33	ALA	-	CLONING ARTIFACT	UNP P07342
A	34	ALA	-	CLONING ARTIFACT	UNP P07342
A	35	LYS	-	CLONING ARTIFACT	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	PHE	-	CLONING ARTIFACT	UNP P07342
A	37	GLU	-	CLONING ARTIFACT	UNP P07342
A	38	ARG	-	CLONING ARTIFACT	UNP P07342
A	39	GLN	-	CLONING ARTIFACT	UNP P07342
A	40	HIS	-	CLONING ARTIFACT	UNP P07342
A	41	MET	-	CLONING ARTIFACT	UNP P07342
A	42	ASP	-	CLONING ARTIFACT	UNP P07342
A	43	SER	-	CLONING ARTIFACT	UNP P07342
A	44	PRO	-	CLONING ARTIFACT	UNP P07342
A	45	ASP	-	CLONING ARTIFACT	UNP P07342
A	46	LEU	-	CLONING ARTIFACT	UNP P07342
A	47	GLY	-	CLONING ARTIFACT	UNP P07342
A	48	THR	-	CLONING ARTIFACT	UNP P07342
A	49	ASP	-	CLONING ARTIFACT	UNP P07342
A	50	ASP	-	CLONING ARTIFACT	UNP P07342
A	51	ASP	-	CLONING ARTIFACT	UNP P07342
A	52	ASP	-	CLONING ARTIFACT	UNP P07342
A	53	LYS	-	CLONING ARTIFACT	UNP P07342
A	54	ALA	-	CLONING ARTIFACT	UNP P07342
A	55	MET	-	CLONING ARTIFACT	UNP P07342
A	56	GLY	-	CLONING ARTIFACT	UNP P07342
A	57	SER	-	CLONING ARTIFACT	UNP P07342
B	11	MET	-	CLONING ARTIFACT	UNP P07342
B	12	HIS	-	CLONING ARTIFACT	UNP P07342
B	13	HIS	-	CLONING ARTIFACT	UNP P07342
B	14	HIS	-	CLONING ARTIFACT	UNP P07342
B	15	HIS	-	CLONING ARTIFACT	UNP P07342
B	16	HIS	-	CLONING ARTIFACT	UNP P07342
B	17	HIS	-	CLONING ARTIFACT	UNP P07342
B	18	SER	-	CLONING ARTIFACT	UNP P07342
B	19	SER	-	CLONING ARTIFACT	UNP P07342
B	20	GLY	-	CLONING ARTIFACT	UNP P07342
B	21	LEU	-	CLONING ARTIFACT	UNP P07342
B	22	VAL	-	CLONING ARTIFACT	UNP P07342
B	23	PRO	-	CLONING ARTIFACT	UNP P07342
B	24	ARG	-	CLONING ARTIFACT	UNP P07342
B	25	GLY	-	CLONING ARTIFACT	UNP P07342
B	26	SER	-	CLONING ARTIFACT	UNP P07342
B	27	GLY	-	CLONING ARTIFACT	UNP P07342
B	28	MET	-	CLONING ARTIFACT	UNP P07342
B	29	LYS	-	CLONING ARTIFACT	UNP P07342
B	30	GLU	-	CLONING ARTIFACT	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	CLONING ARTIFACT	UNP P07342
B	32	ALA	-	CLONING ARTIFACT	UNP P07342
B	33	ALA	-	CLONING ARTIFACT	UNP P07342
B	34	ALA	-	CLONING ARTIFACT	UNP P07342
B	35	LYS	-	CLONING ARTIFACT	UNP P07342
B	36	PHE	-	CLONING ARTIFACT	UNP P07342
B	37	GLU	-	CLONING ARTIFACT	UNP P07342
B	38	ARG	-	CLONING ARTIFACT	UNP P07342
B	39	GLN	-	CLONING ARTIFACT	UNP P07342
B	40	HIS	-	CLONING ARTIFACT	UNP P07342
B	41	MET	-	CLONING ARTIFACT	UNP P07342
B	42	ASP	-	CLONING ARTIFACT	UNP P07342
B	43	SER	-	CLONING ARTIFACT	UNP P07342
B	44	PRO	-	CLONING ARTIFACT	UNP P07342
B	45	ASP	-	CLONING ARTIFACT	UNP P07342
B	46	LEU	-	CLONING ARTIFACT	UNP P07342
B	47	GLY	-	CLONING ARTIFACT	UNP P07342
B	48	THR	-	CLONING ARTIFACT	UNP P07342
B	49	ASP	-	CLONING ARTIFACT	UNP P07342
B	50	ASP	-	CLONING ARTIFACT	UNP P07342
B	51	ASP	-	CLONING ARTIFACT	UNP P07342
B	52	ASP	-	CLONING ARTIFACT	UNP P07342
B	53	LYS	-	CLONING ARTIFACT	UNP P07342
B	54	ALA	-	CLONING ARTIFACT	UNP P07342
B	55	MET	-	CLONING ARTIFACT	UNP P07342
B	56	GLY	-	CLONING ARTIFACT	UNP P07342
B	57	SER	-	CLONING ARTIFACT	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).

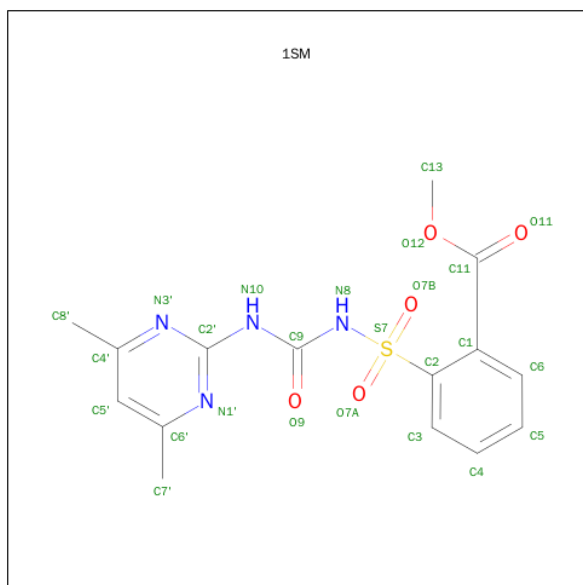
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

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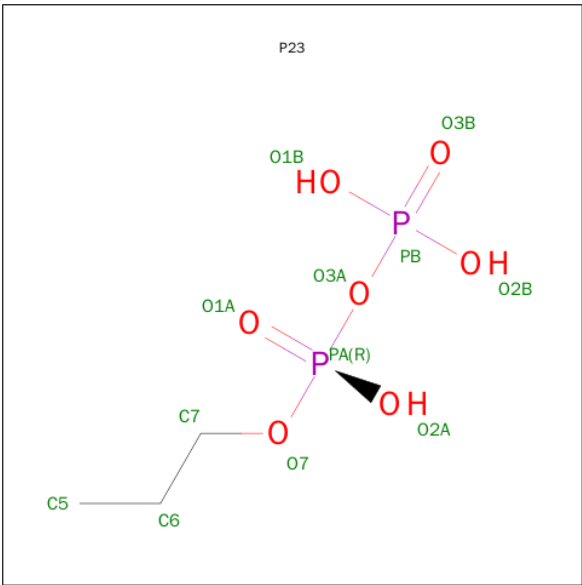
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is METHYL 2-([[(4,6-DIMETHYLPYRIMIDIN-2-YL)AMINO]CARBONYL}AMINO)SULFONYL]BENZOATE (three-letter code: 1SM) (formula: C₁₅H₁₆N₄O₅S).



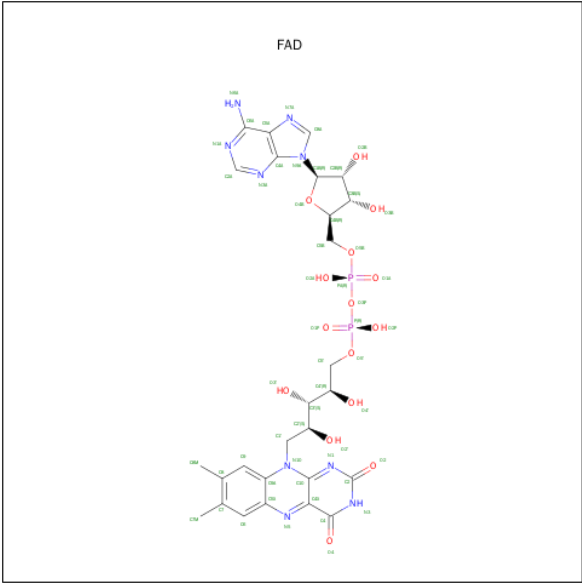
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			25	15	4	5	1		
4	B	1	Total	C	N	O	S	0	0
			25	15	4	5	1		

- Molecule 5 is PROPYL TRIHYDROGEN DIPHOSPHATE (three-letter code: P23) (formula: C₃H₁₀O₇P₂).



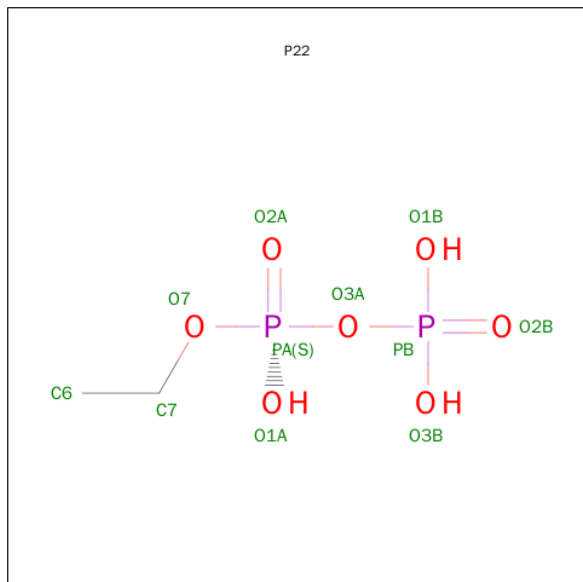
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			12	3	7	2		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 7 is ETHYL DIHYDROGEN DIPHOSPHATE (three-letter code: P22) (formula: $C_2H_8O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			11	2	7	2		

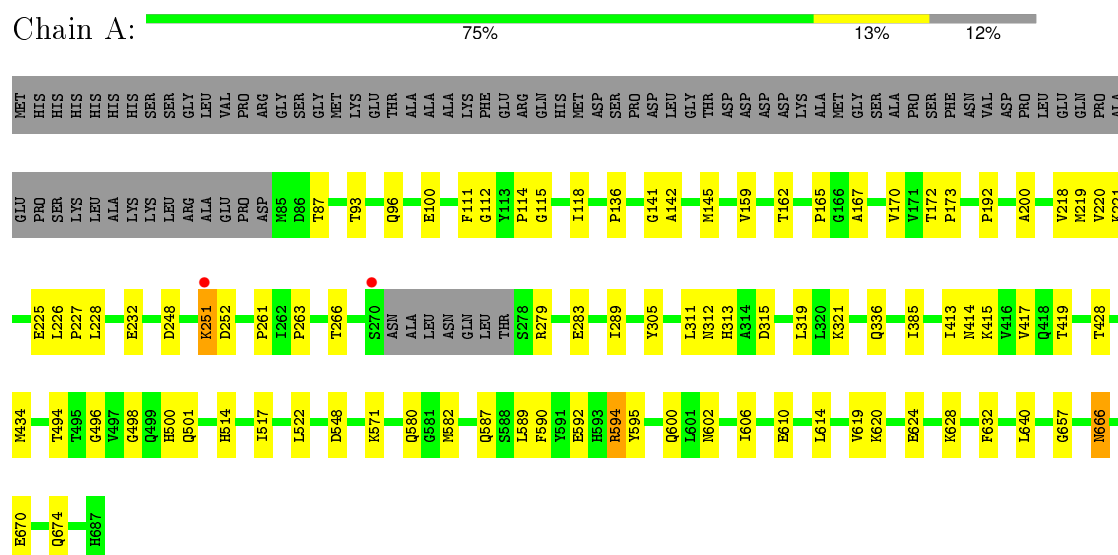
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	682	Total	O	0	0
			682	682		
8	B	494	Total	O	0	0
			494	494		

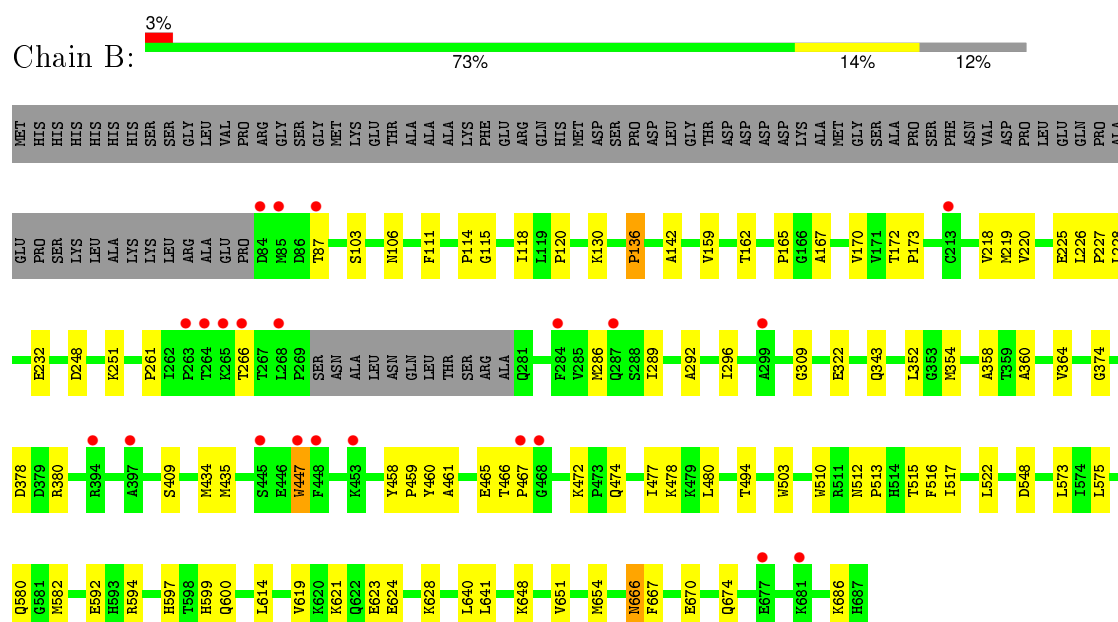
3 Residue-property plots

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, mitochondrial



- Molecule 1: Acetolactate synthase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.49 Å 154.49 Å 178.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.34 93.22 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.34) 96.7 (93.22-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.23 (at 2.34 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.162 , 0.191 0.166 , 0.192	Depositor DCC
R_{free} test set	8784 reflections (9.95%)	DCC
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 90495 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10410	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, K, 1SM, P23, P22, 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	0.33	0/4664	0.59	0/6326
1	B	0.33	2/4615 (0.0%)	0.55	0/6263
All	All	0.33	2/9279 (0.0%)	0.57	0/12589

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	592[A]	GLU	CD-OE2	5.69	1.31	1.25
1	B	592[B]	GLU	CD-OE2	5.69	1.31	1.25

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	4546	0	4530	69	0
1	B	4505	0	4485	65	0
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	25	0	15	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	25	0	15	6	0
5	B	12	0	7	2	0
6	A	53	0	31	0	0
6	B	53	0	31	1	0
7	A	11	0	5	1	0
8	A	682	0	0	11	0
8	B	494	0	0	5	0
All	All	10410	0	9119	130	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 7.

All (130) 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:619:VAL:HG22	1:B:628:LYS:HG2	1.43	0.96
1:A:313:HIS:HD2	1:A:315:ASP:H	1.24	0.85
1:A:251[A]:LYS:HE2	8:A:4547:HOH:O	1.77	0.83
1:B:87:THR:HG22	1:B:261:PRO:HB3	1.64	0.80
1:A:600:GLN:HE21	1:A:602:ASN:HD21	1.32	0.78
1:A:251[B]:LYS:HD3	4:B:1695:ISM:O7B	1.85	0.77
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.18	0.72
1:A:580:GLN:HE22	1:B:114:PRO:HG2	1.58	0.68
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.78	0.66
1:A:172:THR:HB	1:A:173:PRO:HD3	1.78	0.66
1:B:289:ILE:HG23	1:B:434:MET:HB2	1.78	0.66
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.79	0.65
1:A:251[B]:LYS:CD	4:B:1695:ISM:O7B	2.45	0.65
1:A:624:GLU:HG2	8:A:4378:HOH:O	1.96	0.64
1:A:385:ILE:HD11	1:A:417:VAL:HG13	1.80	0.61
1:B:172:THR:HB	1:B:173:PRO:HD3	1.82	0.61
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.82	0.61
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.82	0.61
1:A:414:ASN:ND2	1:A:419:THR:H	1.97	0.61
1:A:87:THR:HG22	1:A:261:PRO:HB3	1.84	0.59
1:B:580[A]:GLN:HG2	5:B:700:P23:H71	1.86	0.58
1:A:192:PRO:HG3	1:A:251[A]:LYS:HG2	1.86	0.58
1:A:219:MET:HE2	1:A:221:LYS:HD3	1.86	0.58
1:A:414:ASN:HD21	1:A:419:THR:H	1.52	0.58
1:A:413:ILE:HG22	8:A:4140:HOH:O	2.04	0.57
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ARG:NH2	8:B:4084:HOH:O	2.37	0.57
1:B:666:ASN:HB3	8:B:4303:HOH:O	2.06	0.56
1:A:228:LEU:O	1:A:232:GLU:HG3	2.06	0.56
1:A:93:THR:OG1	1:A:96:GLN:HG3	2.06	0.56
1:B:228:LEU:HB2	1:B:266:THR:HB	1.88	0.55
1:A:496:GLY:H	1:A:500:HIS:HE1	1.54	0.55
1:B:378:ASP:OD2	1:B:380:ARG:HB2	2.07	0.55
1:B:218:VAL:HG22	1:B:219:MET:N	2.22	0.55
4:A:695:1SM:O7B	1:B:251[A]:LYS:HD3	2.08	0.53
1:B:512:ASN:HB2	1:B:515:THR:HG21	1.90	0.53
1:B:670:GLU:O	1:B:674:GLN:HG3	2.09	0.53
1:A:415:LYS:HD2	8:B:4945:HOH:O	2.08	0.53
1:A:263:PRO:HB2	1:A:266:THR:HG23	1.92	0.52
1:A:606:ILE:O	1:A:610[B]:GLU:HB3	2.09	0.52
1:A:228:LEU:HB2	1:A:266:THR:HB	1.91	0.52
1:A:96:GLN:O	1:A:100[B]:GLU:HG2	2.09	0.52
1:B:322:GLU:OE2	1:B:435:MET:HG2	2.10	0.52
1:B:465:GLU:HG3	1:B:472:LYS:HG2	1.91	0.52
1:B:619:VAL:CG2	1:B:641:LEU:HD11	2.39	0.51
1:A:289:ILE:HG23	1:A:434:MET:HB2	1.91	0.51
1:A:666:ASN:ND2	8:A:4216:HOH:O	2.44	0.51
1:B:640:LEU:C	1:B:640:LEU:HD23	2.31	0.51
1:A:657:GLY:HA3	8:A:4909:HOH:O	2.11	0.51
1:A:167:ALA:O	1:A:170:VAL:HG22	2.10	0.51
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.93	0.50
4:A:695:1SM:O7B	1:B:251[B]:LYS:HD3	2.11	0.50
1:B:621:LYS:HE2	1:B:624:GLU:OE2	2.12	0.50
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.47	0.49
1:B:623:GLU:CD	1:B:623:GLU:H	2.16	0.48
1:A:251[B]:LYS:NZ	8:A:4036:HOH:O	2.30	0.48
1:A:118:ILE:HG13	1:A:118:ILE:O	2.13	0.48
1:A:600:GLN:HB2	8:B:4075:HOH:O	2.13	0.48
1:B:292:ALA:O	1:B:296:ILE:HG13	2.14	0.48
1:B:582[A]:MET:SD	6:B:1701:FAD:HM72	2.53	0.48
1:A:114:PRO:HG2	1:B:597:HIS:O	2.14	0.47
1:A:494:THR:HA	1:A:517:ILE:O	2.14	0.47
1:A:220:VAL:HG13	1:A:225:GLU:HG3	1.97	0.47
1:B:580[A]:GLN:HG2	5:B:700:P23:C7	2.44	0.47
1:B:599:HIS:HE1	1:B:648:LYS:NZ	2.11	0.47
1:A:592:GLU:HB2	1:A:594[A]:ARG:NH1	2.29	0.47
1:B:352:LEU:H	1:B:352:LEU:HD23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:O	1:A:159:VAL:HA	2.15	0.47
1:A:640:LEU:C	1:A:640:LEU:HD23	2.34	0.47
1:B:599:HIS:HE1	1:B:648:LYS:HZ2	1.62	0.46
1:A:200:ALA:HB1	4:B:1695:ISM:H5	1.97	0.46
1:A:218:VAL:HG22	1:A:219:MET:N	2.30	0.46
1:A:619:VAL:HB	1:A:628:LYS:HG3	1.98	0.46
1:B:582[A]:MET:HG2	4:B:1695:ISM:H5'	1.98	0.46
1:A:496:GLY:N	1:A:500:HIS:HE1	2.14	0.46
1:A:319:LEU:HD12	1:A:428:THR:CG2	2.46	0.46
1:A:620:LYS:NZ	8:A:4727:HOH:O	2.46	0.46
1:B:219:MET:HG3	1:B:248:ASP:HB3	1.98	0.46
1:A:587:GLN:NE2	1:A:595:TYR:HA	2.31	0.46
1:A:582[B]:MET:HG2	4:A:695:ISM:H7'1	1.97	0.45
1:A:251[B]:LYS:HE3	8:A:4036:HOH:O	2.16	0.45
1:B:358:ALA:HB3	1:B:458:TYR:HB3	1.98	0.45
1:B:466:THR:HB	1:B:467:PRO:HD2	1.98	0.45
1:B:666:ASN:ND2	1:B:667:PHE:H	2.15	0.45
1:B:621:LYS:HB3	1:B:623:GLU:OE1	2.16	0.45
1:A:319:LEU:HD12	1:A:428:THR:HG23	1.99	0.44
1:B:480:LEU:HD22	1:B:573:LEU:HD22	1.99	0.44
1:B:118:ILE:HG13	1:B:118:ILE:O	2.17	0.44
1:A:670:GLU:O	1:A:674:GLN:HG3	2.17	0.44
1:B:619:VAL:CG2	1:B:628:LYS:HG2	2.30	0.44
1:B:360:ALA:O	1:B:364:VAL:HG23	2.18	0.44
1:A:498:GLY:O	1:A:501:GLN:HB3	2.17	0.44
1:B:582[A]:MET:CG	4:B:1695:ISM:H5'	2.48	0.44
1:B:582[B]:MET:HG3	4:B:1695:ISM:H5'	1.99	0.44
1:B:115:GLY:HA3	1:B:162:THR:HB	2.00	0.44
1:A:336:GLN:OE1	1:A:336:GLN:HA	2.17	0.44
1:B:459:PRO:O	1:B:461:ALA:N	2.51	0.44
1:B:120:PRO:HG2	1:B:251[A]:LYS:HG3	2.00	0.43
1:B:228:LEU:O	1:B:232:GLU:HG3	2.19	0.43
1:B:494:THR:HG22	1:B:517:ILE:HB	2.00	0.43
1:B:447:TRP:HA	1:B:447:TRP:CE3	2.53	0.43
1:A:251[B]:LYS:CE	8:A:4036:HOH:O	2.66	0.43
1:B:409:SER:HB3	8:B:4679:HOH:O	2.18	0.43
1:A:219:MET:HG3	1:A:248:ASP:HB3	2.01	0.43
1:B:447:TRP:HA	1:B:447:TRP:HE3	1.84	0.42
1:A:311:LEU:O	1:A:514:HIS:HE1	2.01	0.42
1:A:313:HIS:CD2	1:A:315:ASP:H	2.16	0.42
1:A:251[A]:LYS:HG3	1:A:252:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:SER:HB2	1:B:130:LYS:HD2	2.02	0.42
1:A:589:LEU:HD23	1:A:590:PHE:CE1	2.55	0.42
1:A:582[A]:MET:HE1	8:A:4934:HOH:O	2.20	0.42
1:A:141:GLY:O	1:A:145:MET:HG3	2.19	0.42
1:B:309:GLY:HA3	1:B:374:GLY:HA3	2.00	0.42
1:B:220:VAL:HG13	1:B:225:GLU:HG3	2.02	0.41
1:A:321:LYS:NZ	8:A:4855:HOH:O	2.52	0.41
1:B:474:GLN:O	1:B:478:LYS:HG3	2.19	0.41
1:A:279:ARG:O	1:A:283:GLU:HG3	2.20	0.41
1:B:354:MET:O	1:B:654:MET:HA	2.21	0.41
1:B:512:ASN:HA	1:B:513:PRO:HD3	1.84	0.41
1:A:580:GLN:HG2	7:A:1702:P22:H71	2.02	0.41
1:B:477:ILE:HD11	1:B:575:LEU:HD11	2.02	0.41
1:A:312:ASN:HA	1:A:312:ASN:HD22	1.67	0.41
1:B:167:ALA:O	1:B:170:VAL:HG22	2.21	0.40
1:B:510:TRP:CH2	1:B:516:PHE:CD1	3.09	0.40
1:A:165:PRO:HD3	1:B:522:LEU:HG	2.03	0.40
1:B:503:TRP:CE2	1:B:651:VAL:HG22	2.57	0.40
1:B:111:PHE:O	1:B:159:VAL:HA	2.22	0.40
1:B:343:GLN:HG3	1:B:510:TRP:O	2.22	0.40
1:A:115:GLY:HA3	1:A:162:THR:HB	2.03	0.40
1:A:112:GLY:O	1:A:136:PRO:HD2	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	598/677 (88%)	586 (98%)	12 (2%)	0	100	100
1	B	593/677 (88%)	576 (97%)	16 (3%)	1 (0%)	52	61
All	All	1191/1354 (88%)	1162 (98%)	28 (2%)	1 (0%)	56	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	460	TYR

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%)	479 (98%)	8 (2%)	70	82
1	B	481/556 (86%)	472 (98%)	9 (2%)	65	78
All	All	968/1112 (87%)	951 (98%)	17 (2%)	70	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251[A]	LYS
1	A	251[B]	LYS
1	A	305	TYR
1	A	548	ASP
1	A	594[A]	ARG
1	A	594[B]	ARG
1	A	614	LEU
1	A	666	ASN
1	B	106	ASN
1	B	136	PRO
1	B	286	MET
1	B	447	TRP
1	B	548	ASP
1	B	600	GLN
1	B	614	LEU
1	B	666	ASN
1	B	686	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	127	ASN
1	A	312	ASN
1	A	313	HIS
1	A	414	ASN
1	A	500	HIS
1	A	512	ASN
1	A	554	ASN
1	A	580	GLN
1	A	587	GLN
1	A	602	ASN
1	A	666	ASN
1	B	106	ASN
1	B	126	HIS
1	B	127	ASN
1	B	312	ASN
1	B	452	ASN
1	B	514	HIS
1	B	554	ASN
1	B	587	GLN
1	B	599	HIS
1	B	602	ASN
1	B	666	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 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
7	P22	A	1702	3	8,10,10	2.29	5 (62%)	12,15,15	1.96	2 (16%)
4	1SM	A	695	-	26,26,26	7.60	15 (57%)	37,37,37	3.43	14 (37%)
6	FAD	A	701	-	48,58,58	2.64	21 (43%)	54,89,89	2.28	10 (18%)
4	1SM	B	1695	-	26,26,26	7.70	15 (57%)	37,37,37	3.46	14 (37%)
6	FAD	B	1701	-	48,58,58	2.77	22 (45%)	54,89,89	2.33	11 (20%)
5	P23	B	700	3	9,11,11	2.01	5 (55%)	14,16,16	2.28	5 (35%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	P22	A	1702	3	-	0/10/10/10	0/0/0/0
4	1SM	A	695	-	-	0/21/21/21	0/2/2/2
6	FAD	A	701	-	-	0/30/50/50	0/6/6/6
4	1SM	B	1695	-	-	0/21/21/21	0/2/2/2
6	FAD	B	1701	-	-	0/30/50/50	0/6/6/6
5	P23	B	700	3	-	0/11/11/11	0/0/0/0

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1695	1SM	C2'-N10	-6.47	1.31	1.39
4	A	695	1SM	C2'-N10	-6.39	1.31	1.39
6	A	701	FAD	C5'-C4'	-3.24	1.46	1.51
6	B	1701	FAD	C5'-C4'	-3.17	1.46	1.51
5	B	700	P23	PA-O2A	-3.11	1.41	1.54
4	A	695	1SM	C9-N8	-3.05	1.34	1.39
6	A	701	FAD	P-O2P	-2.94	1.42	1.54
7	A	1702	P22	PA-O2A	-2.85	1.40	1.51
4	A	695	1SM	C9-N10	-2.82	1.32	1.37
7	A	1702	P22	PA-O7	-2.82	1.46	1.59
4	B	1695	1SM	C9-N8	-2.81	1.34	1.39
6	B	1701	FAD	P-O2P	-2.81	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1695	ISM	C9-N10	-2.77	1.32	1.37
7	A	1702	P22	PB-O1B	-2.77	1.44	1.54
5	B	700	P23	PB-O1B	-2.73	1.44	1.54
5	B	700	P23	PA-O7	-2.70	1.46	1.59
6	B	1701	FAD	C8A-N7A	-2.47	1.29	1.34
5	B	700	P23	PB-O2B	-2.45	1.45	1.54
6	A	701	FAD	C8A-N7A	-2.36	1.30	1.34
7	A	1702	P22	PA-O1A	-2.30	1.45	1.54
6	A	701	FAD	PA-O2A	-2.26	1.45	1.54
6	B	1701	FAD	PA-O2A	-2.21	1.45	1.54
5	B	700	P23	PA-O1A	-2.12	1.43	1.51
6	B	1701	FAD	O2B-C2B	-2.04	1.38	1.43
6	A	701	FAD	C10-N10	2.01	1.41	1.39
6	A	701	FAD	C9A-N10	2.08	1.41	1.38
6	A	701	FAD	C10-N1	2.11	1.39	1.35
4	A	695	ISM	C2'-N3'	2.38	1.43	1.34
4	B	1695	ISM	C2'-N1'	2.41	1.43	1.34
6	B	1701	FAD	C8-C7	2.43	1.47	1.41
4	B	1695	ISM	C2'-N3'	2.46	1.43	1.34
6	B	1701	FAD	C9A-N10	2.49	1.42	1.38
4	A	695	ISM	C2'-N1'	2.50	1.43	1.34
6	A	701	FAD	C8-C7	2.53	1.47	1.41
7	A	1702	P22	O7-C7	2.55	1.59	1.44
6	B	1701	FAD	C10-N1	2.56	1.39	1.35
6	B	1701	FAD	C3B-C4B	2.61	1.60	1.53
6	B	1701	FAD	C10-N10	2.70	1.42	1.39
6	A	701	FAD	C9A-C5X	2.77	1.48	1.42
6	A	701	FAD	C3B-C4B	2.94	1.60	1.53
6	B	1701	FAD	C9A-C5X	2.99	1.48	1.42
6	B	1701	FAD	C4-C4X	3.07	1.47	1.41
6	A	701	FAD	C4X-N5	3.07	1.38	1.33
6	B	1701	FAD	C4X-N5	3.13	1.38	1.33
6	A	701	FAD	C1'-N10	3.17	1.51	1.48
6	A	701	FAD	C4-C4X	3.38	1.48	1.41
4	A	695	ISM	C3-C2	3.48	1.42	1.39
4	B	1695	ISM	C3-C2	3.55	1.43	1.39
6	A	701	FAD	C4X-C10	3.64	1.47	1.41
6	B	1701	FAD	C1'-N10	3.73	1.52	1.48
4	A	695	ISM	S7-N8	3.73	1.72	1.64
6	A	701	FAD	C5A-C4A	3.77	1.49	1.40
6	B	1701	FAD	C4X-C10	3.79	1.48	1.41
6	B	1701	FAD	O4'-C4'	3.98	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1701	FAD	O3'-C3'	4.03	1.52	1.43
6	A	701	FAD	O4'-C4'	4.09	1.52	1.43
4	B	1695	ISM	S7-N8	4.12	1.72	1.64
6	A	701	FAD	O3'-C3'	4.21	1.53	1.43
6	A	701	FAD	C2A-N3A	4.24	1.39	1.32
6	B	1701	FAD	C5A-C4A	4.25	1.50	1.40
4	A	695	ISM	C4'-N3'	4.30	1.43	1.34
4	A	695	ISM	C1-C2	4.33	1.44	1.40
4	B	1695	ISM	C4'-N3'	4.37	1.43	1.34
4	A	695	ISM	C5'-C4'	4.44	1.48	1.38
4	B	1695	ISM	C5'-C4'	4.48	1.48	1.38
4	A	695	ISM	C5'-C6'	4.53	1.48	1.38
4	A	695	ISM	C6'-N1'	4.56	1.44	1.34
6	A	701	FAD	C4-N3	4.59	1.41	1.33
4	B	1695	ISM	C6'-N1'	4.63	1.44	1.34
6	B	1701	FAD	C4-N3	4.71	1.41	1.33
4	A	695	ISM	O12-C11	4.83	1.44	1.33
4	B	1695	ISM	C5'-C6'	4.84	1.48	1.38
4	B	1695	ISM	O12-C11	4.87	1.44	1.33
6	B	1701	FAD	C2A-N3A	4.91	1.40	1.32
4	B	1695	ISM	C1-C2	5.07	1.45	1.40
6	A	701	FAD	C2A-N1A	5.80	1.44	1.33
6	B	1701	FAD	C2A-N1A	6.32	1.45	1.33
6	A	701	FAD	C4A-N3A	8.40	1.48	1.35
6	B	1701	FAD	C4A-N3A	8.89	1.48	1.35
4	B	1695	ISM	O7B-S7	24.66	1.70	1.43
4	A	695	ISM	O7B-S7	24.88	1.70	1.43
4	A	695	ISM	O7A-S7	25.46	1.71	1.43
4	B	1695	ISM	O7A-S7	26.12	1.72	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1695	ISM	C3-C2-S7	-10.29	104.85	117.39
4	A	695	ISM	C3-C2-S7	-10.22	104.94	117.39
6	B	1701	FAD	N3A-C2A-N1A	-6.76	123.72	128.89
6	A	701	FAD	N3A-C2A-N1A	-6.72	123.75	128.89
4	B	1695	ISM	C4'-C5'-C6'	-5.85	114.76	118.79
4	A	695	ISM	C4'-C5'-C6'	-5.70	114.86	118.79
6	A	701	FAD	C4X-C4-N3	-5.16	116.54	123.59
6	B	1701	FAD	C4X-C4-N3	-5.12	116.59	123.59
4	A	695	ISM	C2-C1-C11	-4.73	118.10	124.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1695	ISM	C2-C1-C11	-4.71	118.12	124.29
6	B	1701	FAD	C4X-C10-N10	-4.06	118.13	120.52
6	A	701	FAD	C4X-C10-N10	-3.54	118.44	120.52
6	A	701	FAD	C4-C4X-C10	-3.36	117.79	119.94
4	B	1695	ISM	O7B-S7-N8	-3.05	97.97	106.79
4	A	695	ISM	N3'-C2'-N1'	-3.04	121.54	126.22
4	B	1695	ISM	N3'-C2'-N1'	-2.92	121.73	126.22
6	B	1701	FAD	C4-C4X-C10	-2.91	118.08	119.94
4	A	695	ISM	O7B-S7-N8	-2.77	98.78	106.79
4	A	695	ISM	C8'-C4'-C5'	-2.74	118.07	121.75
4	B	1695	ISM	C8'-C4'-C5'	-2.68	118.15	121.75
6	A	701	FAD	O3'-C3'-C4'	-2.29	102.98	108.75
6	B	1701	FAD	O4B-C4B-C5B	-2.19	101.49	109.32
4	A	695	ISM	C7'-C6'-C5'	-2.09	118.94	121.75
6	B	1701	FAD	O3'-C3'-C4'	-2.09	103.48	108.75
4	B	1695	ISM	C7'-C6'-C5'	-2.06	118.99	121.75
6	A	701	FAD	O4B-C4B-C5B	-2.04	102.01	109.32
6	B	1701	FAD	C1'-C2'-C3'	2.08	115.76	109.82
4	B	1695	ISM	N8-C9-N10	2.12	117.98	114.55
7	A	1702	P22	O3B-PB-O1B	2.19	115.70	107.38
4	B	1695	ISM	N10-C2'-N1'	2.22	123.29	116.44
4	A	695	ISM	N10-C2'-N1'	2.30	123.56	116.44
5	B	700	P23	PA-O7-C7	2.35	134.92	121.50
4	A	695	ISM	C2-S7-N8	2.36	108.94	106.20
4	A	695	ISM	N8-C9-N10	2.45	118.53	114.55
4	B	1695	ISM	C2-S7-N8	2.51	109.11	106.20
6	B	1701	FAD	O2B-C2B-C3B	2.71	120.65	111.83
5	B	700	P23	O2B-PB-O1B	2.77	117.94	107.38
6	A	701	FAD	O2B-C2B-C3B	2.80	120.94	111.83
5	B	700	P23	O3A-PA-O7	2.81	110.38	102.94
4	A	695	ISM	C6-C1-C11	3.11	125.07	118.68
4	B	1695	ISM	C6-C1-C11	3.18	125.22	118.68
6	A	701	FAD	O3P-P-O5'	3.32	111.75	102.94
4	B	1695	ISM	O12-C11-C1	3.42	118.06	112.28
6	B	1701	FAD	O3P-P-O5'	3.43	112.03	102.94
4	A	695	ISM	O12-C11-C1	3.45	118.11	112.28
5	B	700	P23	O7-C7-C6	3.99	140.13	111.33
5	B	700	P23	C5-C6-C7	5.49	148.26	112.32
7	A	1702	P22	O7-C7-C6	5.74	149.81	111.23
6	A	701	FAD	C1B-N9A-C4A	6.93	137.40	126.94
6	B	1701	FAD	C1B-N9A-C4A	7.33	138.00	126.94
6	A	701	FAD	C4-N3-C2	8.00	122.17	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1701	FAD	C4-N3-C2	8.21	122.34	115.25
4	A	695	1SM	C2'-N10-C9	9.13	141.77	130.19
4	B	1695	1SM	C2'-N10-C9	9.36	142.06	130.19
4	A	695	1SM	C1-C2-S7	9.86	134.41	122.11
4	B	1695	1SM	C1-C2-S7	9.92	134.49	122.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1702	P 22	1	0
4	A	695	1SM	3	0
4	B	1695	1SM	6	0
6	B	1701	FAD	1	0
5	B	700	P 23	2	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, 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	596/677 (88%)	-0.27	2 (0%) 94 97	10, 18, 34, 72	1 (0%)
1	B	593/677 (87%)	0.12	22 (3%) 45 57	13, 32, 56, 82	0
All	All	1189/1354 (87%)	-0.07	24 (2%) 68 79	10, 23, 53, 82	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	LYS	4.7
1	B	266	THR	4.7
1	B	268	LEU	4.7
1	B	264	THR	3.8
1	B	84	ASP	3.3
1	B	397	ALA	3.1
1	B	448	PHE	3.0
1	A	270	SER	2.8
1	B	467	PRO	2.8
1	A	251[A]	LYS	2.6
1	B	87	THR	2.6
1	B	263	PRO	2.5
1	B	445	SER	2.4
1	B	447	TRP	2.4
1	B	299	ALA	2.4
1	B	284	PHE	2.3
1	B	468	GLY	2.2
1	B	681	LYS	2.2
1	B	213	CYS	2.2
1	B	287	GLN	2.1
1	B	453	LYS	2.1
1	B	85	MET	2.1
1	B	394	ARG	2.1
1	B	677	GLU	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(\AA^2)	Q<0.9
6	FAD	A	701	53/53	0.99	0.13	0.21	8,12,14,17	0
4	ISM	B	1695	25/25	0.95	0.17	0.16	30,33,36,38	0
6	FAD	B	1701	53/53	0.98	0.12	-0.02	25,28,32,33	0
5	P23	B	700	12/12	0.96	0.13	-0.25	19,26,34,38	0
4	ISM	A	695	25/25	0.98	0.12	-0.29	13,18,21,22	0
7	P22	A	1702	11/11	0.99	0.11	-0.50	11,13,20,22	0
3	MG	B	699	1/1	0.98	0.05	-2.50	21,21,21,21	0
2	K	B	696	1/1	1.00	0.05	-3.21	33,33,33,33	0
3	MG	A	1699	1/1	0.99	0.05	-3.63	11,11,11,11	0
2	K	A	1696	1/1	1.00	0.09	-4.87	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.