Full wwPDB X-ray Structure Validation Report (i)

Jul 10, 2016 – 11:28 PM EDT

PDB ID	:	5HIN
Title	:	Crystal structure of human dihydroorotate dehydrogenase (DHODH) with 18L compound
Authors	:	Huang, J.; Wu, D.; Lu, Q.; Yao, X.
Deposited on	:	2016-01-12
Resolution	:	1.60 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-20027790
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-20027790

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 1.60 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	Percentile Ranks	Value
Rfree		0.188
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		0.7%
RSRZ outliers		6.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
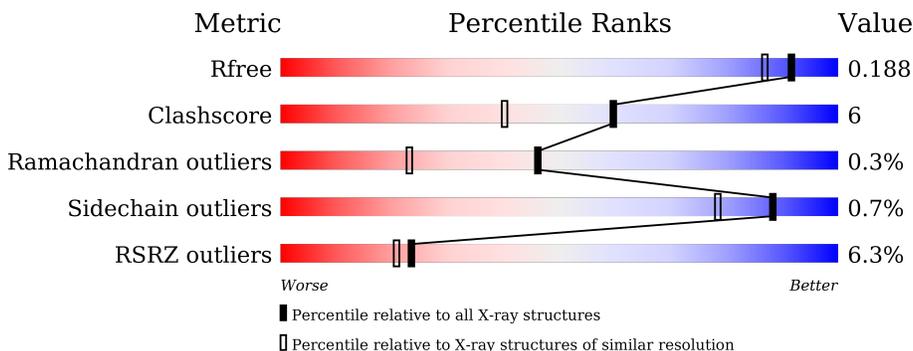
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	390	6% 78% 14% · 6%

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
6	ACT	A	410	-	-	X	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3100 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 Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total 2807	C 1760	N 519	O 524	S 4	0	3	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q02127
A	8	GLY	-	expression tag	UNP Q02127
A	9	HIS	-	expression tag	UNP Q02127
A	10	HIS	-	expression tag	UNP Q02127
A	11	HIS	-	expression tag	UNP Q02127
A	12	HIS	-	expression tag	UNP Q02127
A	13	HIS	-	expression tag	UNP Q02127
A	14	HIS	-	expression tag	UNP Q02127
A	15	HIS	-	expression tag	UNP Q02127
A	16	HIS	-	expression tag	UNP Q02127
A	17	HIS	-	expression tag	UNP Q02127
A	18	HIS	-	expression tag	UNP Q02127
A	19	SER	-	expression tag	UNP Q02127
A	20	SER	-	expression tag	UNP Q02127
A	21	GLY	-	expression tag	UNP Q02127
A	22	HIS	-	expression tag	UNP Q02127
A	23	ILE	-	expression tag	UNP Q02127
A	24	ASP	-	expression tag	UNP Q02127
A	25	ASP	-	expression tag	UNP Q02127
A	26	ASP	-	expression tag	UNP Q02127
A	27	ASP	-	expression tag	UNP Q02127
A	28	LYS	-	expression tag	UNP Q02127
A	29	HIS	-	expression tag	UNP Q02127

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
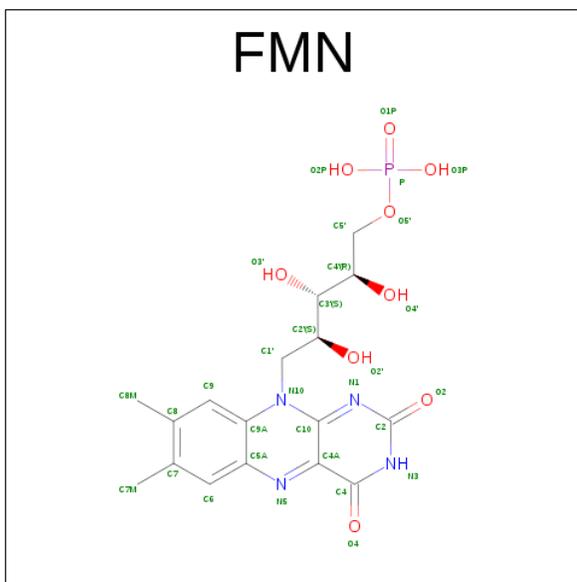
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0

• Molecule 3 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).
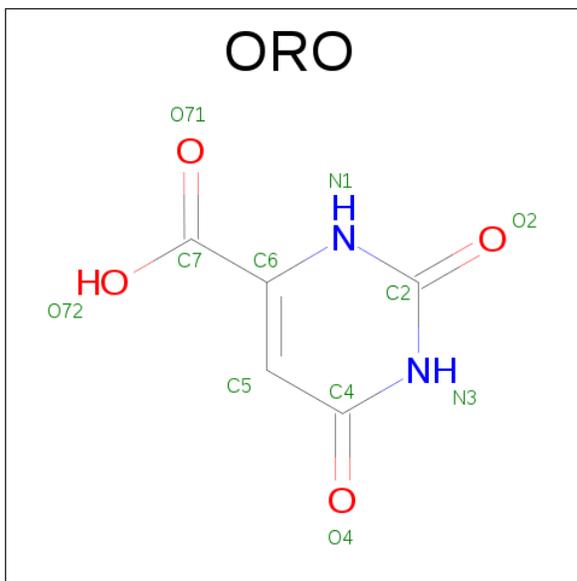
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	5	2	4	0	0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
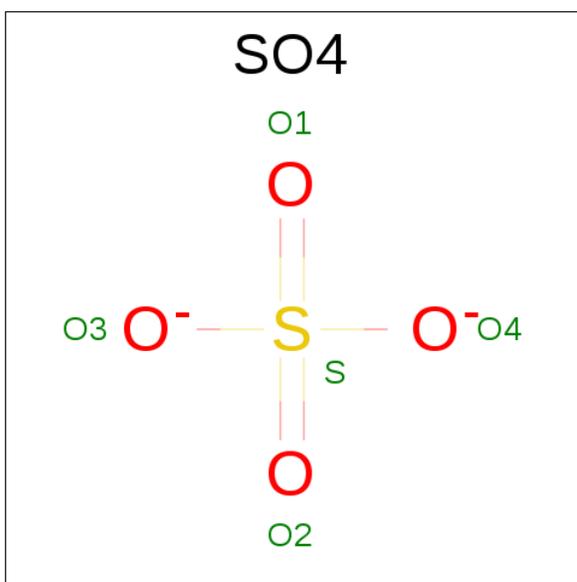
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0

- Molecule 5 is methyl (2Z)-(3-{4-[(4-tert-butylphenyl)carbamoyl]phenyl}-4-oxo-1,3-thiazolidin-2-ylidene)(cyano)acetate (three-letter code: 1KL) (formula: $C_{24}H_{23}N_3O_4S$).
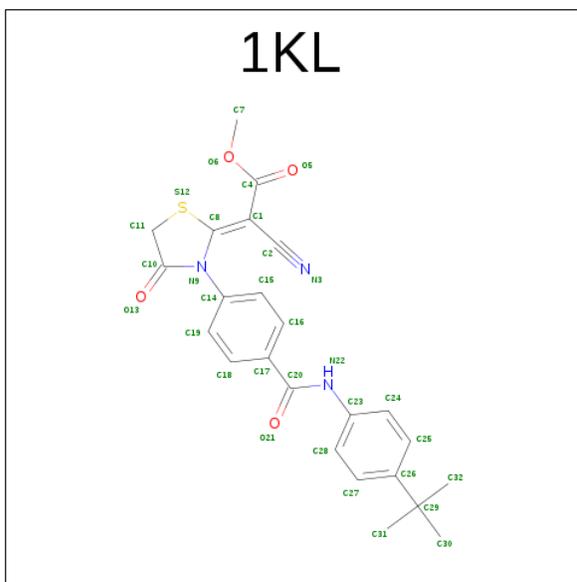
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	32	24	3	4	1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
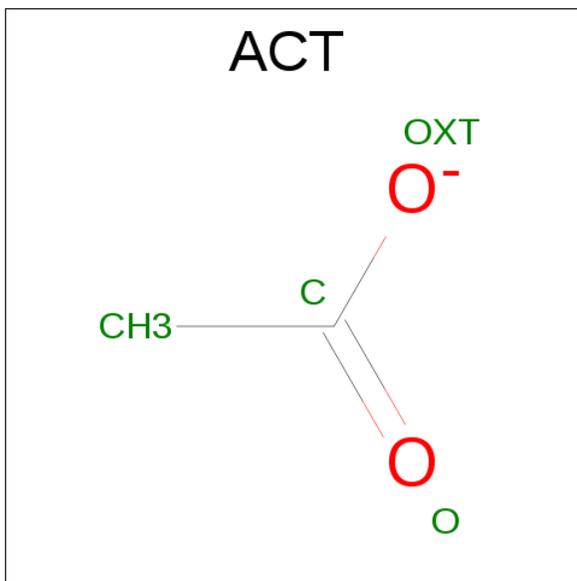
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	186	Total O 186 186	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: Dihydroorotate dehydrogenase (quinone), mitochondrial
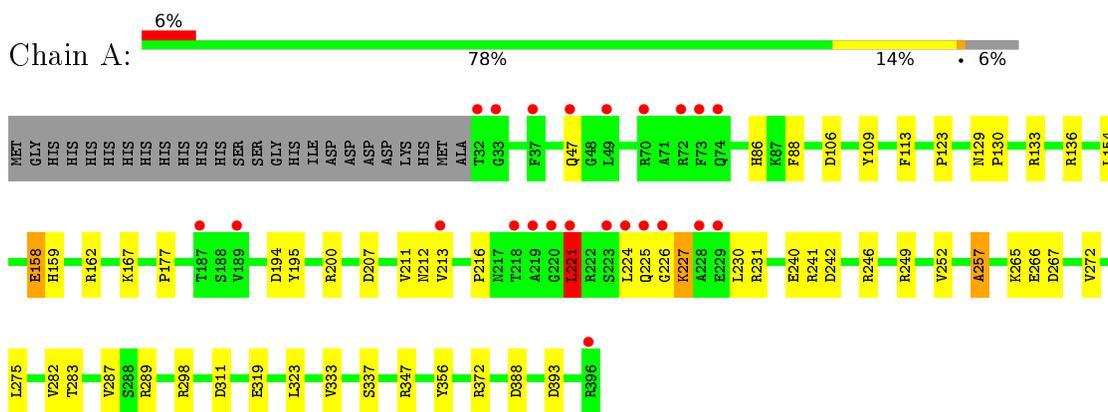
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.73Å 90.73Å 122.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.56 – 1.60 28.56 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.56-1.60) 99.7 (28.56-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	8.97 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.163 , 0.182 0.168 , 0.188	Depositor DCC
R_{free} test set	2001 reflections (2.66%)	DCC
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 55.1	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3100	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: FMN, ORO, ACT, SO4, 1KL

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	1.38	10/2865 (0.3%)	1.46	34/3870 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	SER	CB-OG	-7.94	1.31	1.42
1	A	266	GLU	CD-OE2	-6.66	1.18	1.25
1	A	319	GLU	CG-CD	6.11	1.61	1.51
1	A	212	ASN	N-CA	-5.95	1.34	1.46
1	A	257	ALA	N-CA	-5.45	1.35	1.46
1	A	267	ASP	CB-CG	5.35	1.62	1.51
1	A	195	TYR	CZ-OH	5.29	1.46	1.37
1	A	323	LEU	CA-CB	-5.21	1.41	1.53
1	A	133	ARG	NE-CZ	5.02	1.39	1.33
1	A	212	ASN	CG-OD1	-5.01	1.12	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	133	ARG	NE-CZ-NH1	-9.31	115.65	120.30
1	A	227	LYS	N-CA-C	9.06	135.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	ASP	CB-CG-OD1	8.92	126.33	118.30
1	A	347	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	275	LEU	CB-CG-CD1	7.89	124.42	111.00
1	A	319	GLU	OE1-CD-OE2	-7.43	114.39	123.30
1	A	207	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	207	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	372	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	289	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	231	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	167	LYS	CD-CE-NZ	-6.66	96.37	111.70
1	A	113	PHE	CB-CG-CD2	6.46	125.33	120.80
1	A	298	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	A	241	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	A	221	LEU	CB-CG-CD1	6.32	121.75	111.00
1	A	393	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	109	TYR	CG-CD2-CE2	6.14	126.21	121.30
1	A	252	VAL	CG1-CB-CG2	-5.92	101.42	110.90
1	A	393	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	388	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	A	106	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	372	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	194	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	246	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	333	VAL	CA-CB-CG1	5.25	118.77	110.90
1	A	113	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	A	231	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	319	GLU	CG-CD-OE2	5.13	128.56	118.30
1	A	242	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	162	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	272	VAL	CG1-CB-CG2	5.10	119.06	110.90
1	A	158	GLU	OE1-CD-OE2	-5.03	117.26	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLU	Sidechain

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	2807	0	2879	30	0
2	A	31	0	19	0	0
3	A	11	0	3	0	0
4	A	25	0	0	0	0
5	A	32	0	0	3	0
6	A	8	0	6	3	0
7	A	186	0	0	2	0
All	All	3100	0	2907	33	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 6.

All (33) 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:47:GLN:HG3	1:A:136:ARG:CZ	1.46	1.41
1:A:47:GLN:HG3	1:A:136:ARG:NH1	1.70	1.06
1:A:47:GLN:CG	1:A:136:ARG:CZ	2.35	1.03
1:A:47:GLN:HG3	1:A:136:ARG:NH2	1.92	0.84
1:A:47:GLN:CG	1:A:136:ARG:NH1	2.45	0.79
1:A:221:LEU:HD23	1:A:224:LEU:HD12	1.68	0.73
1:A:200:ARG:NH1	1:A:240:GLU:OE2	2.23	0.71
1:A:213:VAL:HA	1:A:221:LEU:HD21	1.74	0.69
1:A:226:GLY:O	1:A:230:LEU:HB2	1.96	0.64
5:A:408:1KL:S12	5:A:408:1KL:O5	2.57	0.62
1:A:47:GLN:CD	1:A:136:ARG:NE	2.53	0.62
1:A:159:HIS:HD2	7:A:671:HOH:O	1.82	0.62
1:A:216:PRO:HB3	1:A:287:VAL:CG1	2.33	0.59
1:A:226:GLY:O	1:A:230:LEU:CB	2.52	0.58
1:A:200:ARG:HH11	1:A:240:GLU:CD	2.06	0.58
1:A:200:ARG:NH1	1:A:240:GLU:CD	2.57	0.57
5:A:408:1KL:C14	5:A:408:1KL:C2	2.85	0.54
1:A:211:VAL:HG12	1:A:213:VAL:HG13	1.89	0.54
1:A:225:GLN:HE22	1:A:257:ALA:H	1.56	0.51
1:A:265:LYS:NZ	6:A:410:ACT:CH3	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASN:HB3	1:A:130:PRO:HD2	1.93	0.50
1:A:221:LEU:C	1:A:221:LEU:CD2	2.80	0.50
1:A:86:HIS:HB3	7:A:537:HOH:O	2.14	0.47
1:A:221:LEU:CD2	1:A:221:LEU:O	2.63	0.47
1:A:123:PRO:HA	1:A:154:LEU:HG	1.98	0.46
1:A:265:LYS:NZ	6:A:410:ACT:H1	2.30	0.46
1:A:221:LEU:C	1:A:221:LEU:HD22	2.37	0.45
1:A:47:GLN:CD	1:A:136:ARG:CZ	2.84	0.44
1:A:282:VAL:HA	1:A:283:THR:HA	1.83	0.43
5:A:408:1KL:C15	5:A:408:1KL:C2	2.97	0.43
1:A:47:GLN:OE1	1:A:136:ARG:CD	2.68	0.42
1:A:265:LYS:HZ2	6:A:410:ACT:CH3	2.34	0.40
1:A:88:PHE:CE2	1:A:177:PRO:HG2	2.57	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	367/390 (94%)	354 (96%)	12 (3%)	1 (0%)	46	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	LYS

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	299/317 (94%)	297 (99%)	2 (1%)	88	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	A	356	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	225	GLN

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)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FMN	A	401	-	32,33,33	1.59	9 (28%)	34,50,50	2.78	11 (32%)
3	ORO	A	402	-	6,11,11	2.01	2 (33%)	6,15,15	4.80	5 (83%)
4	SO4	A	403	-	4,4,4	0.93	0	6,6,6	0.57	0
4	SO4	A	404	-	4,4,4	0.51	0	6,6,6	0.52	0
4	SO4	A	405	-	4,4,4	1.22	0	6,6,6	0.97	0
4	SO4	A	406	-	4,4,4	0.85	0	6,6,6	0.44	0
4	SO4	A	407	-	4,4,4	0.56	0	6,6,6	1.46	1 (16%)
5	1KL	A	408	-	33,34,34	2.37	10 (30%)	43,49,49	2.10	12 (27%)
6	ACT	A	409	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	A	410	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	401	-	-	0/18/18/18	0/3/3/3
3	ORO	A	402	-	-	0/0/4/4	0/1/1/1
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
4	SO4	A	404	-	-	0/0/0/0	0/0/0/0
4	SO4	A	405	-	-	0/0/0/0	0/0/0/0
4	SO4	A	406	-	-	0/0/0/0	0/0/0/0
4	SO4	A	407	-	-	0/0/0/0	0/0/0/0
5	1KL	A	408	-	-	0/28/43/43	0/3/3/3
6	ACT	A	409	-	-	0/0/0/0	0/0/0/0
6	ACT	A	410	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	408	1KL	C10-N9	-6.80	1.31	1.40
5	A	408	1KL	C2-C1	-6.37	1.30	1.43
5	A	408	1KL	C11-S12	-3.89	1.74	1.80
5	A	408	1KL	C23-N22	-3.13	1.35	1.41
5	A	408	1KL	C8-N9	-3.09	1.34	1.39
3	A	402	ORO	C2-N3	-2.99	1.31	1.38
2	A	401	FMN	C2-N1	-2.94	1.32	1.38
3	A	402	ORO	C2-N1	-2.78	1.32	1.38
2	A	401	FMN	C10-N10	-2.13	1.36	1.39
2	A	401	FMN	C2-N3	-2.13	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	P-O1P	-2.10	1.44	1.50
2	A	401	FMN	P-O2P	-2.04	1.47	1.54
5	A	408	1KL	C16-C17	-2.03	1.36	1.39
2	A	401	FMN	C10-N1	-2.02	1.32	1.35
2	A	401	FMN	C9A-C5A	2.06	1.46	1.42
5	A	408	1KL	O13-C10	2.67	1.29	1.23
2	A	401	FMN	C4A-C10	2.94	1.46	1.40
5	A	408	1KL	C2-N3	3.01	1.20	1.14
5	A	408	1KL	C14-N9	3.28	1.49	1.44
5	A	408	1KL	C11-C10	3.38	1.56	1.50
2	A	401	FMN	C4-C4A	3.44	1.48	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	C4-C4A-C10	-7.18	115.35	119.94
3	A	402	ORO	C5-C4-N3	-6.14	117.52	124.02
2	A	401	FMN	C4A-C4-N3	-4.53	117.60	123.52
3	A	402	ORO	N3-C2-N1	-4.45	120.20	127.69
2	A	401	FMN	N3-C2-N1	-4.10	120.78	127.69
5	A	408	1KL	C14-N9-C10	-3.83	116.08	122.94
5	A	408	1KL	O13-C10-C11	-3.20	116.86	123.37
5	A	408	1KL	C27-C26-C25	-2.96	113.57	117.95
5	A	408	1KL	C10-C11-S12	-2.57	104.45	107.46
5	A	408	1KL	O21-C20-C17	-2.10	117.35	120.95
5	A	408	1KL	C28-C23-C24	-2.07	116.18	119.06
2	A	401	FMN	O2'-C2'-C1'	-2.04	104.90	109.93
2	A	401	FMN	O4'-C4'-C3'	2.07	114.28	108.96
2	A	401	FMN	C1'-N10-C9A	2.10	121.27	118.83
5	A	408	1KL	O6-C4-C1	2.12	115.81	111.45
2	A	401	FMN	C5A-C9A-N10	2.37	119.35	117.58
5	A	408	1KL	C10-N9-C8	2.40	120.19	116.14
3	A	402	ORO	C2-N1-C6	2.55	120.37	117.03
2	A	401	FMN	C6-C5A-N5	2.86	122.48	118.92
4	A	407	SO4	O2-S-O1	2.88	119.21	109.59
3	A	402	ORO	C4-C5-C6	3.00	118.67	116.73
5	A	408	1KL	C25-C26-C29	3.07	127.38	121.61
5	A	408	1KL	C27-C28-C23	3.40	124.12	120.30
5	A	408	1KL	C24-C25-C26	3.85	126.30	121.26
2	A	401	FMN	C4A-N5-C5A	3.91	121.33	116.72
2	A	401	FMN	C4-C4A-N5	4.16	123.76	118.70
3	A	402	ORO	C4-N3-C2	7.96	122.59	114.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	408	1KL	O13-C10-N9	8.15	131.81	123.92
2	A	401	FMN	C4-N3-C2	9.97	123.47	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	1KL	3	0
6	A	410	ACT	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	365/390 (93%)	-0.02	23 (6%)	23	21	10, 17, 41, 87	5 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ARG	6.2
1	A	219	ALA	5.8
1	A	225	GLN	5.6
1	A	189	VAL	5.5
1	A	70	ARG	5.5
1	A	223	SER	5.2
1	A	224	LEU	5.2
1	A	226	GLY	4.5
1	A	213	VAL	4.2
1	A	74	GLN	4.1
1	A	47	GLN	4.1
1	A	32	THR	3.9
1	A	396	ARG	3.7
1	A	220	GLY	3.4
1	A	218	THR	3.2
1	A	228	ALA	3.1
1	A	49	LEU	2.7
1	A	33	GLY	2.6
1	A	221	LEU	2.6
1	A	73	PHE	2.5
1	A	37	PHE	2.3
1	A	187	THR	2.1
1	A	229	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(Å^2)	Q<0.9
6	ACT	A	410	4/4	0.77	0.20	<mark>7.90</mark>	23,31,32,38	0
5	1KL	A	408	32/32	0.94	0.08	-0.21	16,20,31,35	0
2	FMN	A	401	31/31	0.97	0.09	-0.24	8,10,12,13	0
3	ORO	A	402	11/11	0.97	0.07	-0.72	11,11,15,15	0
4	SO4	A	403	5/5	0.99	0.10	-	26,26,34,37	0
4	SO4	A	406	5/5	0.90	0.32	-	41,70,73,75	0
4	SO4	A	405	5/5	0.93	0.28	-	33,50,56,58	0
4	SO4	A	404	5/5	0.93	0.31	-	63,71,80,92	0
6	ACT	A	409	4/4	0.70	0.18	-	45,50,51,65	0
4	SO4	A	407	5/5	0.94	0.27	-	53,62,65,72	0

6.5 Other polymers (i)

There are no such residues in this entry.