



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2014 – 06:35 PM EDT

PDB ID : 4ORM
Title : Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM338 (N-[3,5-difluoro-4-(trifluoromethyl)phenyl]-5-methyl-2-(trifluoromethyl)[1,2,4]triazolo[1,5-a]pyrimidin-7-amine)
Authors : Deng, X.; Phillips, M.A.
Deposited on : 2014-02-11
Resolution : 2.07 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

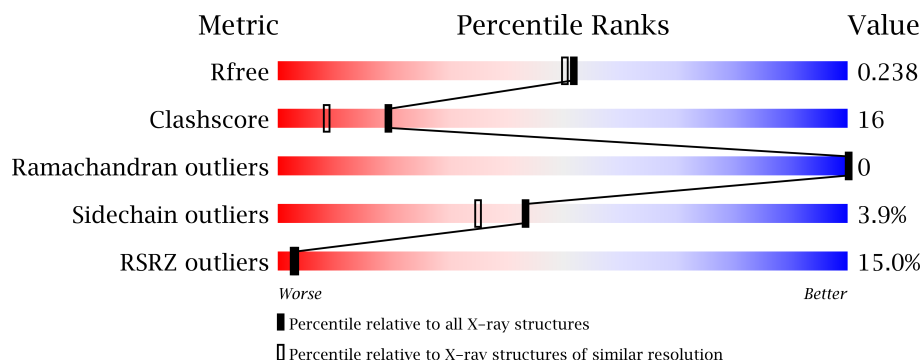
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance


The reported resolution of this entry is 2.07 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}	66092	1224 (2.08-2.04)
Clashscore	79885	1390 (2.08-2.04)
Ramachandran outliers	78287	1381 (2.08-2.04)
Sidechain outliers	78261	1381 (2.08-2.04)
RSRZ outliers	66119	1225 (2.08-2.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	401	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	SO4	A	1005	-	X
6	SO4	A	1006	-	X

2 Entry composition i

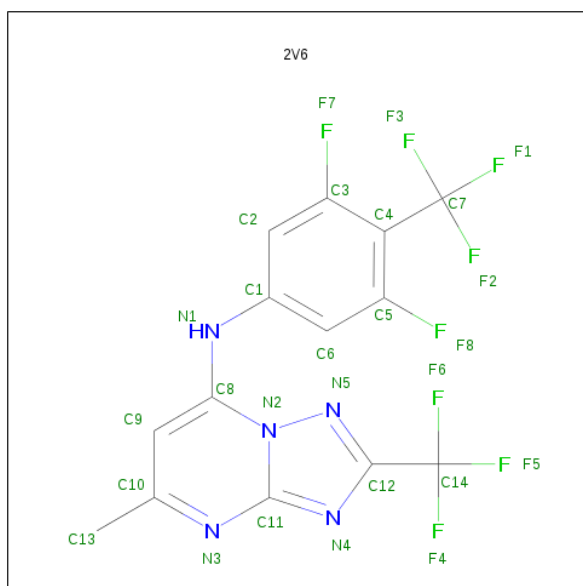
There are 7 unique types of molecules in this entry. The entry contains 3194 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

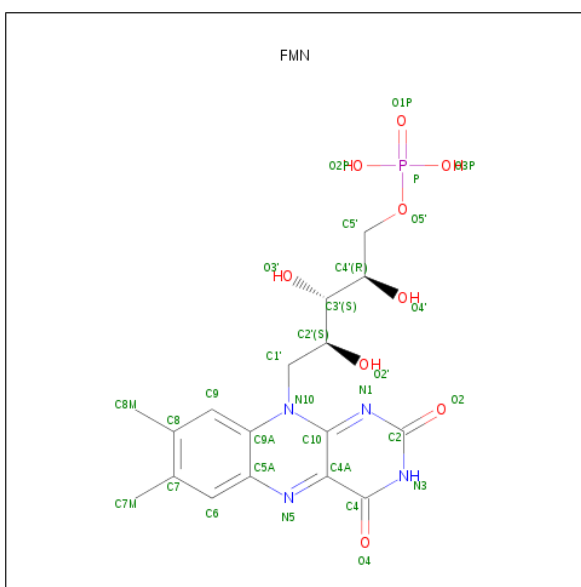
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	3	0
			2992	1911	500	564	17			

- Molecule 2 is N-[3,5-DIFLUORO-4-(TRIFLUOROMETHYL)PHENYL]-5-METHYL-2-(TRIFLUOROMETHYL)[1,2,4]TRIAZOLO[1,5-A]PYRIMIDIN-7-AMINE (three-letter code: 2V6) (formula: C₁₄H₇F₈N₅).



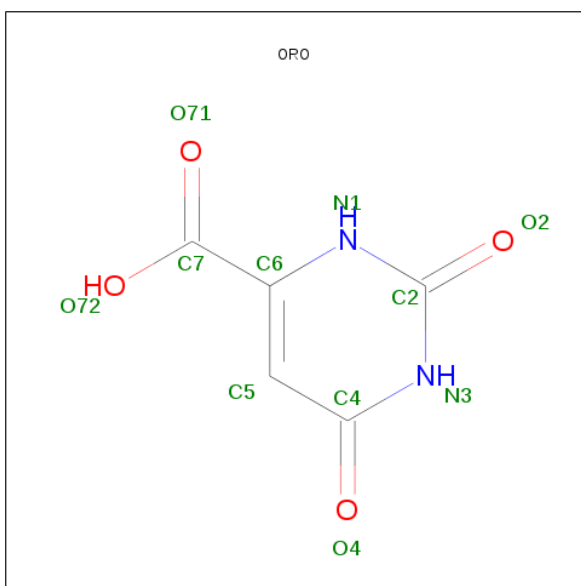
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			27	14	8	5		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



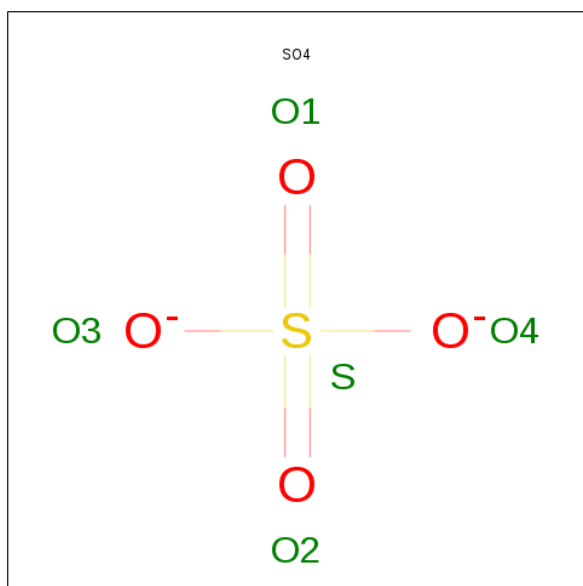
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

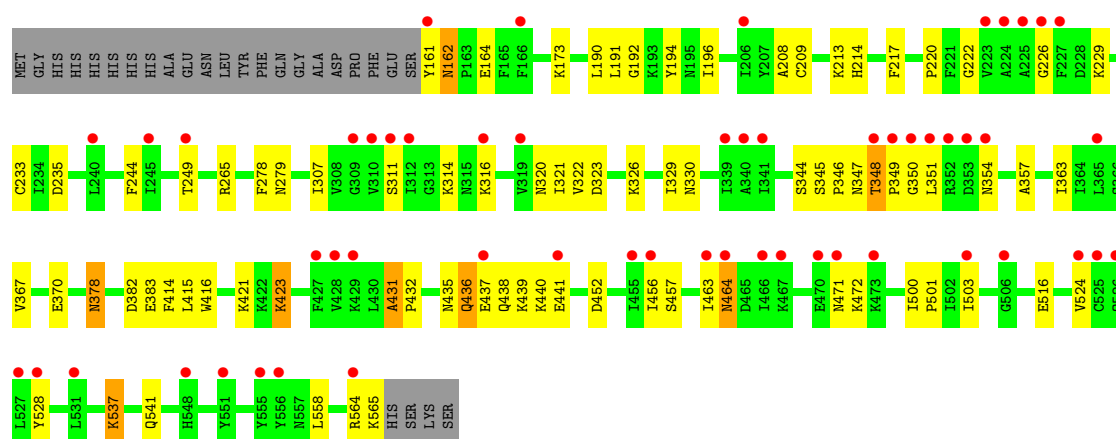
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	117	Total 117	O 117	0	0

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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	85.47Å 85.47Å 138.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.00 – 2.07 27.98 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.00-2.07) 99.1 (27.98-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.240 0.201 , 0.238	Depositor DCC
R_{free} test set	1832 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.9	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 36567 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3194	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, GOL, SO4, 2V6, ORO

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	1.06	2/3042 (0.1%)	0.93	4/4096 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	PRO	N-CD	5.30	1.55	1.47
1	A	432	PRO	N-CD	5.12	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	ILE	C-N-CD	5.87	140.73	128.40
1	A	431	ALA	C-N-CD	5.67	140.31	128.40
1	A	162	ASN	C-N-CD	5.63	140.22	128.40
1	A	348	THR	C-N-CD	5.45	139.85	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2992	0	3031	100	0
2	A	27	0	0	0	0
3	A	31	0	19	1	0
4	A	11	0	3	0	0
5	A	6	0	8	1	0
6	A	10	0	0	1	0
7	A	117	0	0	5	0
All	All	3194	0	3061	100	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (100) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:LYS:CD	1:A:370:GLU:HG3	1.86	1.04
1:A:321:ILE:HG21	1:A:354:ASN:HD21	1.25	1.02
1:A:326:LYS:HD2	1:A:370:GLU:HG3	1.03	1.01
1:A:326:LYS:HE3	1:A:370:GLU:HG2	1.44	0.97
1:A:326:LYS:HD2	1:A:370:GLU:CG	1.94	0.97
1:A:320:ASN:ND2	1:A:323:ASP:HB2	1.83	0.92
1:A:435:ASN:HD22	1:A:438:GLN:HG3	1.41	0.86
1:A:278:PHE:CD2	1:A:348:THR:HG23	2.10	0.86
1:A:278:PHE:CZ	1:A:345:SER:HB2	2.11	0.85
1:A:383:GLU:OE1	1:A:414:PHE:CZ	2.31	0.84
1:A:278:PHE:HD2	1:A:348:THR:HG23	1.44	0.82
1:A:320:ASN:HD22	1:A:323:ASP:HB2	1.43	0.81
1:A:278:PHE:CZ	1:A:345:SER:CB	2.65	0.80
1:A:321:ILE:HG13	1:A:322:VAL:H	1.45	0.80
1:A:321:ILE:CD1	1:A:363:ILE:HG12	2.11	0.80
1:A:278:PHE:HZ	1:A:345:SER:HB2	1.47	0.76
1:A:321:ILE:HG21	1:A:354:ASN:ND2	2.00	0.76
1:A:326:LYS:HE3	1:A:370:GLU:CG	2.16	0.76
1:A:191:LEU:HD22	1:A:196:ILE:HD11	1.70	0.74
1:A:346:PRO:HG2	1:A:347:ASN:CG	2.07	0.73
1:A:321:ILE:CG1	1:A:322:VAL:N	2.52	0.73
1:A:321:ILE:HG13	1:A:322:VAL:N	2.04	0.73
1:A:345:SER:OG	1:A:346:PRO:HD2	1.89	0.71
1:A:278:PHE:CD2	1:A:348:THR:CG2	2.75	0.70
1:A:321:ILE:HD11	1:A:322:VAL:HG23	1.73	0.69
1:A:217:PHE:CD1	1:A:307:ILE:HD12	2.29	0.67
1:A:435:ASN:O	1:A:439:LYS:HG3	1.92	0.67
1:A:383:GLU:OE1	1:A:414:PHE:CE1	2.47	0.67
1:A:357:ALA:HB2	1:A:441:GLU:HG3	1.77	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:LYS:CE	1:A:370:GLU:CG	2.73	0.66
1:A:346:PRO:HD2	1:A:347:ASN:H	1.59	0.66
1:A:321:ILE:HD12	1:A:322:VAL:N	2.10	0.65
1:A:321:ILE:HD11	1:A:363:ILE:HG12	1.78	0.65
1:A:346:PRO:CD	1:A:347:ASN:H	2.09	0.65
1:A:278:PHE:CE2	1:A:345:SER:CB	2.81	0.64
1:A:326:LYS:CD	1:A:370:GLU:CG	2.66	0.63
1:A:314:LYS:HG2	1:A:351:LEU:HD13	1.81	0.61
1:A:435:ASN:HD22	1:A:438:GLN:CG	2.10	0.61
1:A:278:PHE:HD2	1:A:348:THR:CG2	2.13	0.61
1:A:321:ILE:HD13	1:A:363:ILE:HG12	1.82	0.60
1:A:537:LYS:HD2	1:A:541:GLN:NE2	2.16	0.60
1:A:321:ILE:CD1	1:A:322:VAL:N	2.65	0.59
1:A:320:ASN:HB3	1:A:323:ASP:HB3	1.85	0.59
1:A:351:LEU:O	1:A:354:ASN:HB2	2.03	0.58
1:A:209[A]:CYS:SG	7:A:1185:HOH:O	2.57	0.57
1:A:278:PHE:HZ	1:A:345:SER:CB	2.11	0.57
1:A:164:GLU:OE2	6:A:1005:SO4:O2	2.23	0.56
1:A:346:PRO:CD	1:A:347:ASN:N	2.68	0.56
1:A:213:LYS:HB3	7:A:1134:HOH:O	2.05	0.56
1:A:322:VAL:O	1:A:326:LYS:HG2	2.06	0.56
1:A:321:ILE:HD11	1:A:363:ILE:CG1	2.36	0.55
1:A:435:ASN:HB2	1:A:438:GLN:HG3	1.90	0.54
1:A:357:ALA:HB2	1:A:441:GLU:CG	2.38	0.54
1:A:226:GLY:HA3	3:A:1002:FMN:N5	2.23	0.54
1:A:435:ASN:HB2	1:A:438:GLN:H	1.73	0.53
1:A:161:TYR:N	7:A:1178:HOH:O	2.42	0.52
1:A:471:ASN:CB	1:A:472:LYS:HD3	2.40	0.52
1:A:378:ASN:OD1	1:A:415:LEU:HD13	2.10	0.52
1:A:452:ASP:O	1:A:501:PRO:HD2	2.10	0.51
1:A:537:LYS:HD2	1:A:541:GLN:HE22	1.76	0.50
1:A:357:ALA:CB	1:A:441:GLU:HG3	2.42	0.50
1:A:321:ILE:CD1	1:A:363:ILE:CG1	2.87	0.50
1:A:346:PRO:HG2	1:A:347:ASN:ND2	2.26	0.49
1:A:278:PHE:CE2	1:A:345:SER:HB3	2.46	0.49
1:A:346:PRO:HG2	1:A:347:ASN:OD1	2.13	0.49
1:A:463:ILE:C	1:A:464:ASN:HD22	2.16	0.49
1:A:344:SER:HB2	1:A:431:ALA:HB2	1.93	0.49
1:A:350:GLY:O	1:A:351:LEU:HB3	2.13	0.49
1:A:516:GLU:OE1	7:A:1214:HOH:O	2.20	0.48
1:A:435:ASN:ND2	1:A:438:GLN:HG3	2.20	0.48
1:A:436:GLN:O	1:A:440:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:ILE:HD11	1:A:367:VAL:HG13	1.95	0.47
1:A:190:LEU:CD1	1:A:194:TYR:CE2	2.97	0.47
1:A:249:THR:HA	1:A:311:SER:HB3	1.95	0.47
1:A:321:ILE:HD12	1:A:322:VAL:CA	2.44	0.47
1:A:382:ASP:CG	5:A:1004:GOL:H32	2.36	0.47
1:A:416:TRP:CZ2	1:A:423:LYS:HB3	2.51	0.46
1:A:190:LEU:HD11	1:A:194:TYR:CE2	2.50	0.46
1:A:278:PHE:CE2	1:A:348:THR:HG23	2.50	0.46
1:A:278:PHE:CZ	1:A:345:SER:HB3	2.49	0.46
1:A:321:ILE:CD1	1:A:322:VAL:HG23	2.44	0.45
1:A:378:ASN:HB2	7:A:1126:HOH:O	2.16	0.45
1:A:190:LEU:CD1	1:A:194:TYR:HE2	2.30	0.44
1:A:330:ASN:HD22	1:A:330:ASN:HA	1.61	0.44
1:A:314:LYS:CD	1:A:351:LEU:HD13	2.49	0.43
1:A:192:GLY:HA3	1:A:233:CYS:SG	2.58	0.43
1:A:314:LYS:HE3	1:A:351:LEU:HB2	2.00	0.43
1:A:314:LYS:CG	1:A:351:LEU:HD13	2.47	0.43
1:A:222:GLY:HA3	1:A:244:PHE:CE1	2.54	0.43
1:A:321:ILE:HD12	1:A:322:VAL:HA	2.00	0.42
1:A:421:LYS:HA	1:A:421:LYS:HD2	1.83	0.42
1:A:435:ASN:ND2	1:A:438:GLN:CD	2.73	0.42
1:A:456:ILE:HA	1:A:457:SER:HA	1.88	0.42
1:A:229:LYS:HD3	1:A:279:ASN:O	2.19	0.42
1:A:503:ILE:HG13	1:A:524:VAL:HG12	2.02	0.42
1:A:208:ALA:O	1:A:220:PRO:HD3	2.19	0.41
1:A:213:LYS:HB3	1:A:214:HIS:H	1.62	0.41
1:A:437:GLU:HA	1:A:440:LYS:HD2	2.02	0.41
1:A:471:ASN:HB3	1:A:472:LYS:HD3	2.02	0.41
1:A:558:LEU:C	1:A:558:LEU:HD23	2.42	0.40

There are no symmetry-related clashes.

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	376/401 (94%)	367 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	335/354 (95%)	322 (96%)	13 (4%)	43	35

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	173	LYS
1	A	235	ASP
1	A	265	ARG
1	A	316	LYS
1	A	378	ASN
1	A	423	LYS
1	A	436	GLN
1	A	464	ASN
1	A	528	TYR
1	A	537	LYS
1	A	564	ARG
1	A	565	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	320	ASN
1	A	330	ASN
1	A	354	ASN
1	A	377	ASN
1	A	435	ASN
1	A	436	GLN

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Mol	Chain	Res	Type
1	A	450	ASN
1	A	464	ASN
1	A	541	GLN
1	A	548	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	2V6	A	1001	-	29,29,29	1.86	8 (27%)	46,46,46	3.52	19 (41%)
3	FMN	A	1002	-	33,33,33	1.67	8 (24%)	46,50,50	2.06	13 (28%)
4	ORO	A	1003	-	11,11,11	1.74	2 (18%)	11,15,15	2.92	7 (63%)
5	GOL	A	1004	-	5,5,5	0.66	0	5,5,5	1.58	1 (20%)
6	SO4	A	1005	-	4,4,4	0.61	0	6,6,6	0.32	0
6	SO4	A	1006	-	4,4,4	0.56	0	6,6,6	0.35	0

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	2V6	A	1001	-	-	0/16/16/16	0/3/3/3
3	FMN	A	1002	-	-	0/18/18/18	0/3/3/3
4	ORO	A	1003	-	-	0/4/4/4	0/1/1/1
5	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
6	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1006	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	FMN	O2-C2	4.39	1.27	1.21
4	A	1003	ORO	C5-C6	4.32	1.43	1.38
2	A	1001	2V6	C9-C8	4.08	1.47	1.40
3	A	1002	FMN	C4A-C10	3.65	1.48	1.41
2	A	1001	2V6	C4-C5	3.57	1.44	1.38
2	A	1001	2V6	C12-N5	-3.36	1.30	1.33
3	A	1002	FMN	C9A-N10	3.30	1.43	1.38
4	A	1003	ORO	O2-C2	2.82	1.25	1.21
2	A	1001	2V6	C9-C10	2.69	1.44	1.38
3	A	1002	FMN	C1'-N10	-2.59	1.45	1.48
3	A	1002	FMN	C9A-C5A	2.56	1.47	1.42
2	A	1001	2V6	C1-N1	-2.52	1.35	1.40
2	A	1001	2V6	C11-N4	-2.51	1.33	1.36
2	A	1001	2V6	C11-N3	2.45	1.35	1.32
3	A	1002	FMN	C8-C7	2.30	1.47	1.41
2	A	1001	2V6	C8-N2	-2.25	1.33	1.38
3	A	1002	FMN	P-O5'	2.02	1.67	1.60
3	A	1002	FMN	C4'-C3'	2.01	1.57	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	2V6	N1-C8-N2	18.16	127.66	113.56
2	A	1001	2V6	C9-C8-N1	-8.08	113.02	123.54
4	A	1003	ORO	C2-N1-C6	-5.72	118.77	123.46
4	A	1003	ORO	C4-N3-C2	-5.47	118.23	125.64
3	A	1002	FMN	C2-N1-C10	5.28	120.03	114.95
3	A	1002	FMN	C9A-N10-C10	-5.07	116.77	121.77
3	A	1002	FMN	C5A-C9A-N10	4.87	121.22	117.63
2	A	1001	2V6	C6-C5-C4	-4.54	119.87	124.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	FMN	C1'-N10-C9A	4.49	123.39	118.67
3	A	1002	FMN	C4A-N5-C5A	4.46	121.88	116.68
2	A	1001	2V6	C9-C10-N3	-3.70	117.94	122.58
2	A	1001	2V6	C14-C12-N4	3.66	126.64	118.08
2	A	1001	2V6	C11-N2-N5	3.44	113.58	110.57
2	A	1001	2V6	C5-C4-C3	3.31	119.58	115.46
3	A	1002	FMN	C2'-C1'-N10	-3.29	108.10	112.60
3	A	1002	FMN	P-O5'-C5'	2.97	126.22	118.63
2	A	1001	2V6	C2-C3-C4	-2.90	121.44	124.22
4	A	1003	ORO	O71-C7-C6	2.77	127.53	119.75
2	A	1001	2V6	C6-C1-C2	2.66	123.40	119.58
2	A	1001	2V6	C8-C9-C10	2.66	119.36	117.12
2	A	1001	2V6	C12-N5-N2	-2.65	98.68	102.32
2	A	1001	2V6	F5-C14-F6	2.65	115.69	105.67
2	A	1001	2V6	N4-C11-N2	-2.59	107.22	109.80
2	A	1001	2V6	N5-C12-N4	2.57	118.45	114.30
3	A	1002	FMN	O3P-P-O2P	2.51	116.81	107.38
4	A	1003	ORO	C4-C5-C6	2.51	119.39	116.84
3	A	1002	FMN	C4A-C10-N1	-2.51	119.47	123.00
3	A	1002	FMN	O3'-C3'-C2'	2.47	114.94	108.73
5	A	1004	GOL	O1-C1-C2	2.41	121.06	110.37
4	A	1003	ORO	C7-C6-N1	2.31	120.40	115.96
3	A	1002	FMN	C9A-C5A-N5	-2.29	119.00	122.39
2	A	1001	2V6	N3-C11-N2	2.24	124.07	122.30
3	A	1002	FMN	O2'-C2'-C3'	2.21	114.60	109.04
2	A	1001	2V6	C2-C1-N1	-2.19	113.44	120.32
2	A	1001	2V6	N4-C11-N3	2.16	128.63	128.15
2	A	1001	2V6	C10-N3-C11	2.14	119.63	117.54
4	A	1003	ORO	C5-C4-N3	2.09	120.76	117.59
3	A	1002	FMN	O3'-C3'-C4'	-2.04	103.61	108.73
2	A	1001	2V6	F5-C14-C12	-2.01	107.64	112.34
4	A	1003	ORO	C5-C6-C7	-2.00	119.72	124.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	375/401 (93%)	0.67	55 (14%) 3 3	30, 50, 86, 113	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	TYR	7.1
1	A	556	TYR	6.6
1	A	349	PRO	6.4
1	A	441	GLU	5.4
1	A	341	ILE	4.6
1	A	455	ILE	4.5
1	A	464	ASN	4.3
1	A	551	TYR	4.3
1	A	353	ASP	4.1
1	A	564	ARG	4.1
1	A	224	ALA	4.0
1	A	467	LYS	3.9
1	A	350	GLY	3.8
1	A	310	VAL	3.7
1	A	471	ASN	3.6
1	A	223	VAL	3.6
1	A	348	THR	3.2
1	A	473	LYS	3.1
1	A	463	ILE	3.1
1	A	437	GLU	3.0
1	A	340	ALA	2.9
1	A	351	LEU	2.9
1	A	528	TYR	2.8
1	A	225	ALA	2.8
1	A	311	SER	2.8
1	A	226	GLY	2.7
1	A	249	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	227	PHE	2.6
1	A	312	ILE	2.6
1	A	166	PHE	2.6
1	A	354	ASN	2.6
1	A	352	ARG	2.6
1	A	245	ILE	2.5
1	A	339	ILE	2.5
1	A	527	LEU	2.5
1	A	503	ILE	2.5
1	A	309	GLY	2.4
1	A	506	GLY	2.4
1	A	456	ILE	2.4
1	A	319	VAL	2.4
1	A	206	ILE	2.4
1	A	427	PHE	2.3
1	A	531	LEU	2.3
1	A	524	VAL	2.3
1	A	470	GLU	2.2
1	A	555	TYR	2.2
1	A	548	HIS	2.2
1	A	466	ILE	2.2
1	A	428	VAL	2.2
1	A	365	LEU	2.2
1	A	526	GLN	2.1
1	A	240	LEU	2.1
1	A	316	LYS	2.1
1	A	429	LYS	2.1
1	A	525	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	A	1006	5/5	0.37	6.40	30,30,30,30	0
6	SO4	A	1005	5/5	0.24	3.21	30,30,30,30	0
3	FMN	A	1002	31/31	0.23	0.40	33,38,42,44	0
4	ORO	A	1003	11/11	0.15	0.05	39,41,45,46	0
5	GOL	A	1004	6/6	0.10	-0.16	46,48,53,53	0
2	2V6	A	1001	27/27	0.14	-0.39	30,40,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.