



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 04:28 PM EST

PDB ID : 5H2Z  
Title : Crystal structure of Human Dihydroorotate Dehydrogenase (DHODH) with 7GF  
Authors : Wu, D.; Huang, J.  
Deposited on : 2016-10-19  
Resolution : 1.58 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

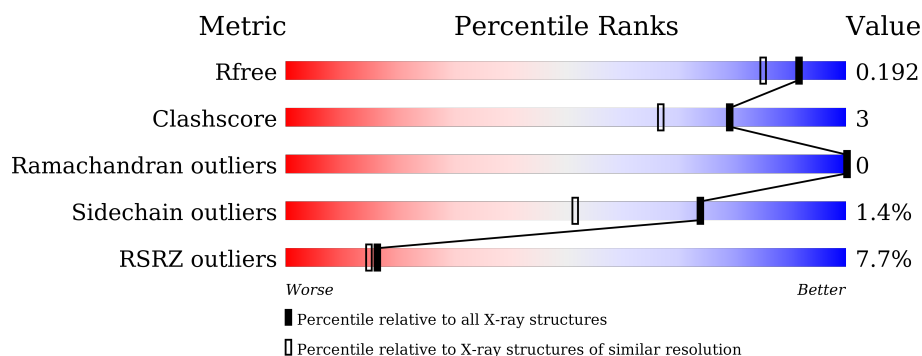
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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  $\geq 3$ , 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	390	

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	ACT	A	406	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2998 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.

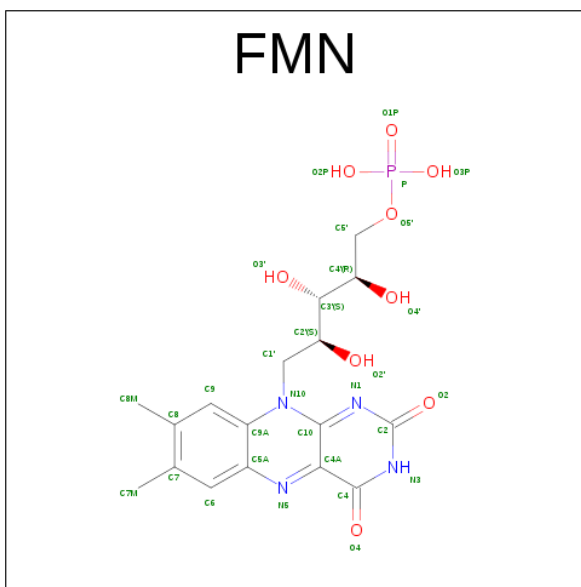
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	1	0
			2784	1747	514	519	4			

There are 23 discrepancies between the modelled and reference sequences:

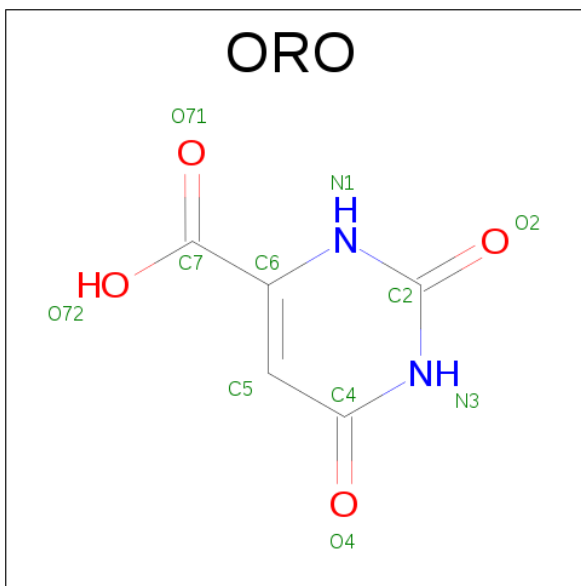
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q02127
A	8	GLY	-	expression tag	UNP Q02127
A	9	HIS	-	expression tag	UNP Q02127
A	10	HIS	-	expression tag	UNP Q02127
A	11	HIS	-	expression tag	UNP Q02127
A	12	HIS	-	expression tag	UNP Q02127
A	13	HIS	-	expression tag	UNP Q02127
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<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

- Molecule 3 is OROTIC ACID (three-letter code: ORO) (formula:  $C_5H_4N_2O_4$ ).



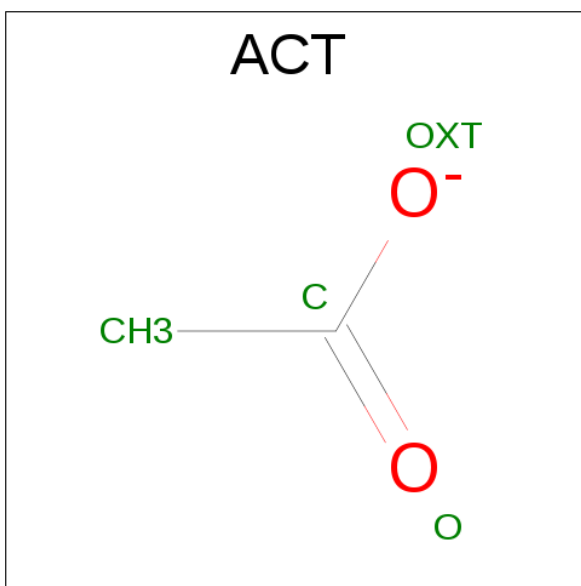
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



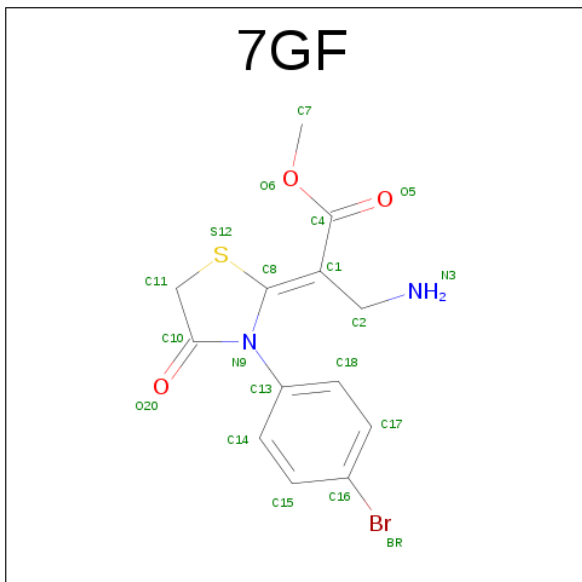
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 6 is methyl (2Z)-3-azanyl-2-[3-(4-bromophenyl)-4-oxidanylidene-1,3-thiazolidin-2-ylidene]propanoate (three-letter code: 7GF) (formula:  $C_{13}H_{13}BrN_2O_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
6	A	1	20	1	13	2	3	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	134	Total	O	0	0
			134	134		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.88Å 90.88Å 123.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.40 – 1.58 36.40 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.40-1.58) 99.9 (36.40-1.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.170 , 0.186 0.182 , 0.192	Depositor DCC
$R_{free}$ test set	4024 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ORO, 7GF, SO4, ACT

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	1.55	17/2833 (0.6%)	1.69	43/3830 (1.1%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	GLU	CD-OE1	23.46	1.51	1.25
1	A	266	GLU	CG-CD	13.85	1.72	1.51
1	A	136	ARG	CZ-NH2	-9.59	1.20	1.33
1	A	200	ARG	CD-NE	-7.64	1.33	1.46
1	A	344	GLU	CD-OE2	7.28	1.33	1.25
1	A	214	SER	CB-OG	-7.17	1.32	1.42
1	A	319	GLU	CD-OE1	7.04	1.33	1.25
1	A	313	SER	CB-OG	-6.62	1.33	1.42
1	A	160	ARG	CZ-NH1	6.25	1.41	1.33
1	A	319	GLU	CG-CD	5.63	1.60	1.51
1	A	53	GLU	CD-OE1	5.62	1.31	1.25
1	A	99	ASP	N-CA	5.48	1.57	1.46
1	A	246	ARG	C-O	5.43	1.33	1.23
1	A	160	ARG	CZ-NH2	-5.37	1.26	1.33
1	A	333	VAL	CB-CG1	-5.33	1.41	1.52
1	A	267	ASP	CB-CG	5.17	1.62	1.51
1	A	136	ARG	CD-NE	-5.02	1.38	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ARG	NE-CZ-NH1	31.18	135.89	120.30
1	A	136	ARG	NE-CZ-NH2	-28.79	105.90	120.30
1	A	266	GLU	CG-CD-OE2	-12.71	92.88	118.30
1	A	266	GLU	OE1-CD-OE2	11.61	137.23	123.30
1	A	160	ARG	NE-CZ-NH2	10.34	125.47	120.30
1	A	311	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	347	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	A	207	ASP	CB-CG-OD2	9.09	126.48	118.30
1	A	298	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	A	136	ARG	CD-NE-CZ	7.71	134.40	123.60
1	A	53	GLU	OE1-CD-OE2	-7.55	114.24	123.30
1	A	267	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	A	133	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	A	207	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	A	259	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	249	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	162	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	272	VAL	CG1-CB-CG2	6.89	121.92	110.90
1	A	318	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	113	PHE	CB-CG-CD2	6.66	125.46	120.80
1	A	275	LEU	CB-CG-CD1	6.66	122.32	111.00
1	A	99	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	A	266	GLU	CA-CB-CG	6.60	127.91	113.40
1	A	58	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	164	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	160	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
1	A	372	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	213	VAL	CA-CB-CG2	-5.83	102.15	110.90
1	A	341	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	266	GLU	CG-CD-OE1	5.68	129.67	118.30
1	A	245	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	A	289	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	393	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	395	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	160	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	307	LYS	CD-CE-NZ	5.46	124.26	111.70
1	A	275	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	158	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	A	200	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	53	GLU	CG-CD-OE2	5.28	128.86	118.30
1	A	117	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	113	PHE	CB-CG-CD1	-5.14	117.20	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PHE	CD1-CE1-CZ	5.00	126.10	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	ARG	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	2784	0	2850	18	0
2	A	31	0	19	0	0
3	A	11	0	3	1	0
4	A	10	0	0	0	0
5	A	8	0	6	3	0
6	A	20	0	0	2	0
7	A	134	0	0	1	0
All	All	2998	0	2878	20	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 3.

All (20) 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:261:THR:OG1	5:A:406:ACT:H2	1.82	0.78
1:A:315:GLN:HE22	1:A:318:ARG:HE	1.33	0.77
1:A:145:ASN:OD1	3:A:402:ORO:H5	1.87	0.74
1:A:32:THR:HB	1:A:72:ARG:NH1	2.11	0.65
1:A:261:THR:HG1	5:A:406:ACT:H2	1.62	0.64
1:A:200:ARG:HH11	1:A:240:GLU:CD	2.06	0.59
6:A:407:7GF:S12	6:A:407:7GF:O5	2.63	0.57
1:A:200:ARG:NH1	1:A:240:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLN:NE2	1:A:318:ARG:HE	2.03	0.54
1:A:200:ARG:NH1	1:A:240:GLU:CD	2.61	0.54
1:A:173:GLU:HG3	7:A:573:HOH:O	2.10	0.51
1:A:224:LEU:HD23	1:A:229:GLU:OE1	2.12	0.49
1:A:189:VAL:O	1:A:189:VAL:HG12	2.13	0.49
1:A:160:ARG:HH21	5:A:405:ACT:H3	1.80	0.47
6:A:407:7GF:C2	6:A:407:7GF:C13	2.94	0.46
1:A:192:ALA:HB1	1:A:236:LYS:HD3	1.98	0.45
1:A:123:PRO:HA	1:A:154:LEU:HG	1.99	0.44
1:A:211:VAL:HG12	1:A:213:VAL:HG13	2.00	0.43
1:A:32:THR:HB	1:A:72:ARG:CZ	2.49	0.42
1:A:129:ASN:HB3	1:A:130:PRO:HD2	2.03	0.41

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	363/390 (93%)	353 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	295/317 (93%)	291 (99%)	4 (1%)	74 52

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	78	MET
1	A	247	VAL
1	A	356	TYR

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

Mol	Chain	Res	Type
1	A	315	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	1.87	10 (31%)	34,50,50	4.27	10 (29%)
3	ORO	A	402	-	6,11,11	1.49	1 (16%)	6,15,15	4.59	4 (66%)
4	SO4	A	403	-	4,4,4	1.20	0	6,6,6	0.90	0
4	SO4	A	404	-	4,4,4	1.60	1 (25%)	6,6,6	0.80	0
5	ACT	A	405	-	0,3,3	0.00	-	0,3,3	0.00	-
5	ACT	A	406	-	0,3,3	0.00	-	0,3,3	0.00	-
6	7GF	A	407	-	20,21,21	2.45	10 (50%)	21,29,29	3.25	11 (52%)

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
5	ACT	A	405	-	-	0/0/0/0	0/0/0/0
5	ACT	A	406	-	-	0/0/0/0	0/0/0/0
6	7GF	A	407	-	-	0/12/29/29	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	7GF	C11-S12	-5.10	1.71	1.80
6	A	407	7GF	C2-N3	-3.97	1.20	1.48
2	A	401	FMN	C10-N10	-3.04	1.35	1.39
6	A	407	7GF	C10-N9	-3.03	1.36	1.40
6	A	407	7GF	C8-N9	-3.02	1.34	1.39
2	A	401	FMN	C2-N1	-2.90	1.32	1.38
2	A	401	FMN	C10-N1	-2.78	1.30	1.35
6	A	407	7GF	C17-C16	-2.62	1.32	1.38
2	A	401	FMN	C6-C5A	-2.23	1.38	1.41
6	A	407	7GF	C15-C14	2.01	1.42	1.38
6	A	407	7GF	C17-C18	2.10	1.42	1.38
2	A	401	FMN	C5A-N5	2.14	1.38	1.35
2	A	401	FMN	C2-N3	2.33	1.43	1.38
4	A	404	SO4	O2-S	2.44	1.55	1.47
2	A	401	FMN	C5'-C4'	2.92	1.56	1.51
2	A	401	FMN	O4-C4	3.23	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	7GF	BR-C16	3.24	1.97	1.90
6	A	407	7GF	C11-C10	3.35	1.56	1.50
6	A	407	7GF	O20-C10	3.50	1.31	1.23
3	A	402	ORO	C2-N1	3.57	1.45	1.38
2	A	401	FMN	C1'-N10	3.62	1.52	1.48
2	A	401	FMN	C4A-C10	4.19	1.48	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	C4-C4A-C10	-15.53	110.00	119.94
2	A	401	FMN	C4A-C10-N10	-10.35	113.00	120.52
3	A	402	ORO	N3-C2-N1	-7.23	115.51	127.69
2	A	401	FMN	N3-C2-N1	-6.92	116.04	127.69
6	A	407	7GF	C10-C11-S12	-5.10	101.50	107.46
6	A	407	7GF	C13-N9-C10	-4.98	114.04	122.94
6	A	407	7GF	C14-C15-C16	-4.08	113.33	119.17
2	A	401	FMN	C1'-N10-C9A	-3.72	114.51	118.83
6	A	407	7GF	BR-C16-C15	-3.29	114.30	119.29
6	A	407	7GF	BR-C16-C17	-3.27	114.33	119.29
6	A	407	7GF	O5-C4-C1	-2.60	119.38	125.04
6	A	407	7GF	C18-C17-C16	-2.54	115.54	119.17
3	A	402	ORO	C5-C4-N3	-2.23	121.66	124.02
2	A	401	FMN	C4A-N5-C5A	2.00	119.08	116.72
3	A	402	ORO	C4-C5-C6	2.03	118.04	116.73
6	A	407	7GF	O6-C4-C1	2.21	116.17	112.29
2	A	401	FMN	O4'-C4'-C3'	2.25	114.76	108.96
6	A	407	7GF	C13-N9-C8	2.27	128.98	125.12
2	A	401	FMN	C6-C5A-N5	2.35	121.84	118.92
2	A	401	FMN	C7-C6-C5A	3.03	125.84	120.90
6	A	407	7GF	C17-C16-C15	5.21	130.91	121.39
2	A	401	FMN	C4-C4A-N5	5.78	125.73	118.70
3	A	402	ORO	C4-N3-C2	7.83	122.46	114.21
6	A	407	7GF	C11-C10-N9	8.81	114.73	111.41
2	A	401	FMN	C4-N3-C2	11.20	124.50	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	ORO	1	0
5	A	405	ACT	1	0
5	A	406	ACT	2	0
6	A	407	7GF	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	364/390 (93%)	0.24	28 (7%) 16 15	11, 21, 41, 86	11 (3%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	VAL	10.8
1	A	213	VAL	9.1
1	A	362	TRP	6.1
1	A	72	ARG	6.0
1	A	212	ASN	5.9
1	A	70	ARG	5.5
1	A	32	THR	5.3
1	A	219	ALA	5.1
1	A	73	PHE	5.0
1	A	189	VAL	4.8
1	A	134	VAL	4.5
1	A	71	ALA	4.4
1	A	74	GLN	4.3
1	A	33	GLY	4.2
1	A	226	GLY	4.2
1	A	187	THR	3.7
1	A	224	LEU	3.2
1	A	223	SER	3.1
1	A	229	GLU	3.1
1	A	94	ILE	2.7
1	A	77	ASP	2.5
1	A	210	VAL	2.5
1	A	225	GLN	2.5
1	A	313	SER	2.3
1	A	95	ALA	2.3
1	A	220	GLY	2.1
1	A	37	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	A	404	5/5	0.95	0.22	1.93	37,41,49,58	0
2	FMN	A	401	31/31	0.99	0.11	-0.12	13,14,16,17	0
6	7GF	A	407	20/20	0.98	0.07	-0.13	18,28,33,38	0
3	ORO	A	402	11/11	0.99	0.04	-0.69	11,15,19,20	0
5	ACT	A	405	4/4	0.88	0.13	-	42,43,47,61	0
4	SO4	A	403	5/5	0.98	0.14	-	30,33,43,46	0
5	ACT	A	406	4/4	0.92	0.18	-	32,34,50,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.