



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:48 PM GMT

PDB ID : 3W7R  
Title : Structure of Human dihydroorotate dehydrogenase in complex with mii-4-097  
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Deposited on : 2013-03-06  
Resolution : 1.68 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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-20026982

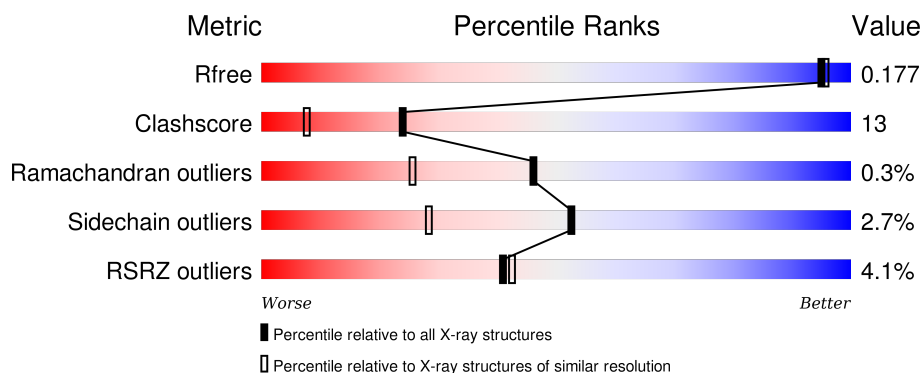
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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
3	DDQ	A	403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DDQ	A	404	-	-	-	X
3	DDQ	A	407	-	-	-	X
6	GOL	A	410	-	-	-	X
6	GOL	A	411	-	-	-	X
6	GOL	A	414	-	-	-	X
6	GOL	A	416	-	-	-	X
6	GOL	A	417	-	-	-	X
6	GOL	A	418	-	-	-	X
6	GOL	A	419[A]	-	-	-	X
6	GOL	A	419[B]	-	-	-	X
6	GOL	A	420	-	-	-	X
6	GOL	A	422	-	-	-	X
6	GOL	A	424	-	-	-	X
6	GOL	A	427	-	-	-	X
6	GOL	A	431	-	-	X	-
8	SO4	A	435	-	-	X	-
9	ACT	A	438	-	-	X	X
9	ACT	A	440	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3626 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	367	Total	C	N	O	S	5	16	0
			2944	1837	546	556	5			

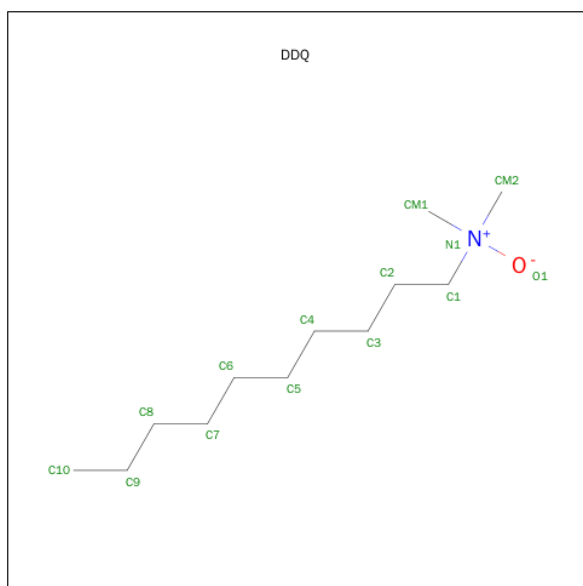
There are 23 discrepancies between the modelled and reference sequences:

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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

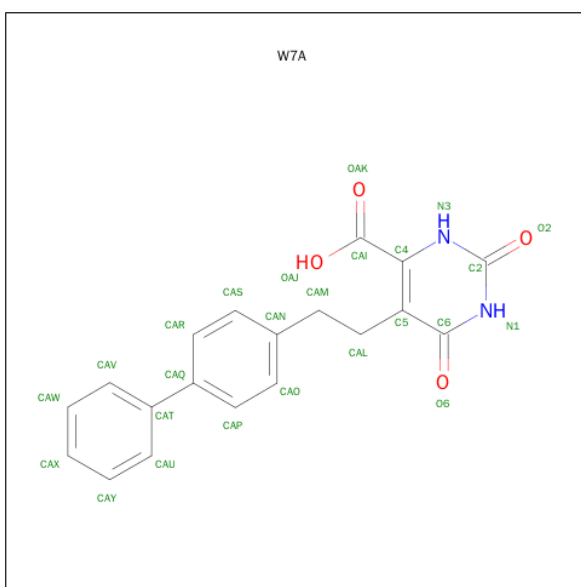
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: C<sub>12</sub>H<sub>27</sub>NO).



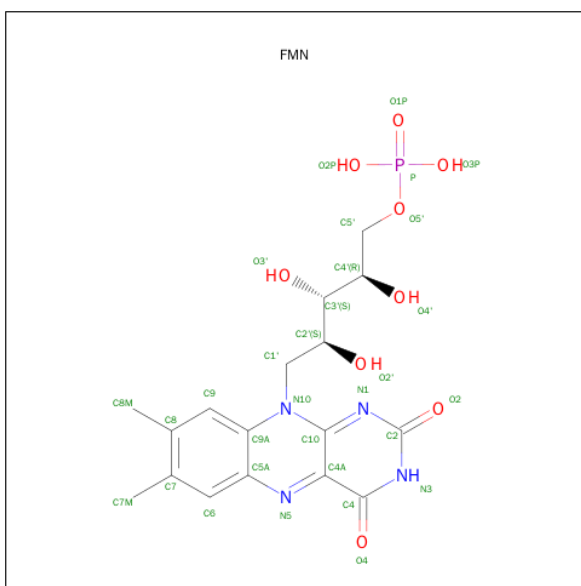
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 12 1 1	0	0
3	A	1	Total C N O 14 12 1 1	0	0
3	A	1	Total C N O 14 12 1 1	0	0
3	A	1	Total C N O 14 12 1 1	0	0
3	A	1	Total C N O 14 12 1 1	0	0
3	A	1	Total C N O 14 12 1 1	0	0

- Molecule 4 is 2,6-DIOXO-5-[2-(4-PHENYLPHENYL)ETHYL]-1,2,3,6- TETRAHYDROPYRIMIDINE-4-CARBOXYLIC ACID (three-letter code: W7A) (formula: C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			50	38	4	8		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



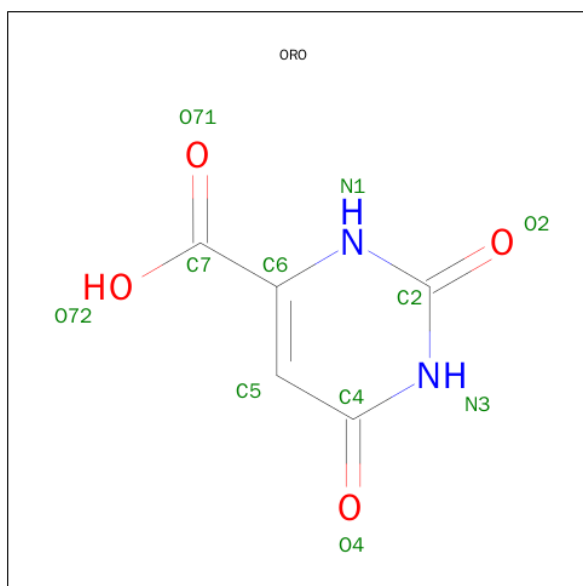
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	1
			12	6	6		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 7 is OROTIC ACID (three-letter code: ORO) (formula:  $C_5H_4N_2O_4$ ).



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

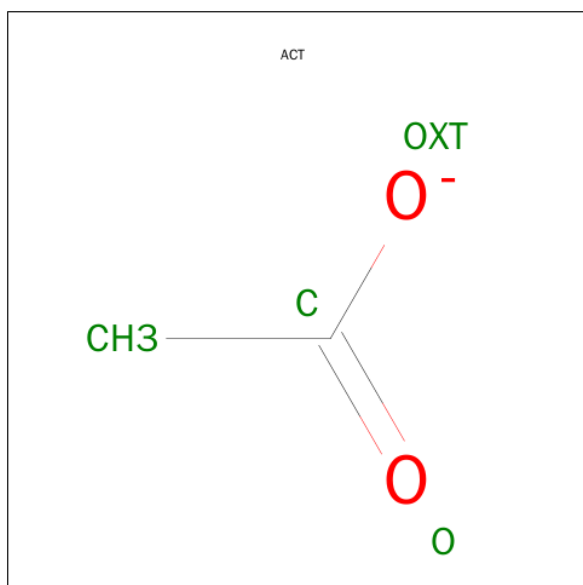
- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



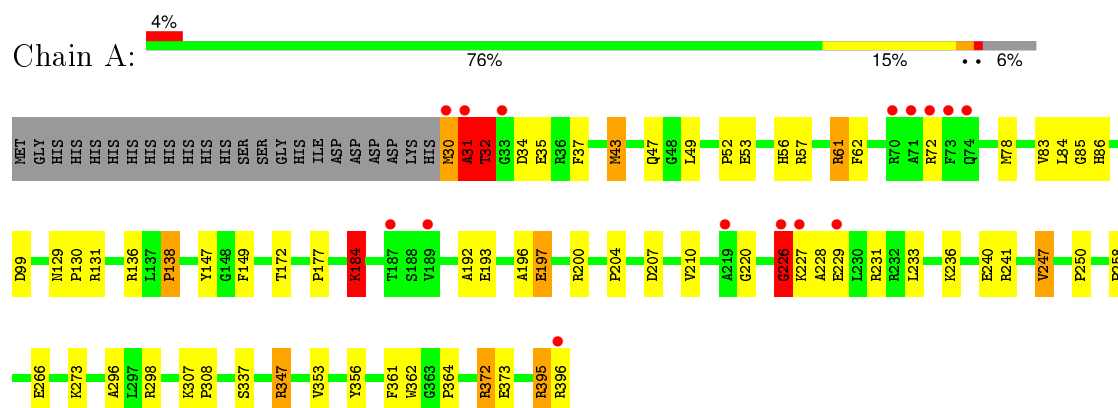
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	317	Total O 319 319	0	2



- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.45Å 90.45Å 123.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.34 – 1.68 36.34 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.34-1.68) 99.9 (36.34-1.68)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.79 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.140 , 0.172 0.148 , 0.177	Depositor DCC
$R_{free}$ test set	3386 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 60.5	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 66874 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL, DDQ, FMN, ORO, W7A, 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	1.51	18/2991 (0.6%)	1.25	13/4035 (0.3%)

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	11

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ALA	C-N	-7.05	1.17	1.34
1	A	266	GLU	CD-OE1	-6.38	1.18	1.25
1	A	258	PRO	N-CD	6.03	1.56	1.47
1	A	337[A]	SER	CB-OG	-6.01	1.34	1.42
1	A	337[B]	SER	CB-OG	-6.01	1.34	1.42
1	A	138	PRO	N-CD	5.78	1.55	1.47
1	A	177	PRO	N-CD	5.69	1.55	1.47
1	A	197[A]	GLU	C-N	-5.69	1.22	1.33
1	A	197[B]	GLU	C-N	-5.69	1.22	1.33
1	A	53	GLU	CD-OE1	5.60	1.31	1.25
1	A	308	PRO	N-CD	5.60	1.55	1.47
1	A	204	PRO	N-CD	5.40	1.55	1.47
1	A	250	PRO	N-CD	5.36	1.55	1.47
1	A	298	ARG	CZ-NH1	5.36	1.40	1.33
1	A	210	VAL	C-O	-5.26	1.13	1.23
1	A	62	PHE	CG-CD2	-5.22	1.30	1.38
1	A	147	TYR	CB-CG	-5.12	1.44	1.51
1	A	353	VAL	C-O	-5.04	1.13	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ALA	O-C-N	-18.26	93.49	122.70
1	A	226	GLY	O-C-N	-10.76	105.48	122.70
1	A	31	ALA	CA-C-N	9.55	138.21	117.20
1	A	347	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	372	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	226	GLY	CA-C-N	-5.45	105.21	117.20
1	A	43	MET	C-N-CD	5.45	139.84	128.40
1	A	99	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	A	395	ARG	O-C-N	-5.35	114.14	122.70
1	A	149	PHE	CB-CG-CD1	5.35	124.54	120.80
1	A	361	PHE	CB-CG-CD2	5.20	124.44	120.80
1	A	184	LYS	CD-CE-NZ	5.05	123.32	111.70
1	A	131	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	GLY	Mainchain,Peptide
1	A	31	ALA	Mainchain,Peptide
1	A	32[B]	THR	Mainchain
1	A	395	ARG	Mainchain

## 5.2 Too-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 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	2944	0	2975	78	0
2	A	1	0	0	0	0
3	A	84	0	162	3	0
4	A	50	0	30	3	0
5	A	31	0	19	0	0
6	A	138	0	184	25	0
7	A	11	0	3	0	0
8	A	20	0	0	6	0
9	A	28	0	21	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	319	0	0	17	0
All	All	3626	0	3394	88	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 13.

All (88) 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:227[B]:LYS:HG2	1:A:228:ALA:N	1.39	1.17
1:A:362[B]:TRP:CZ2	6:A:431:GOL:H2	1.84	1.11
1:A:362[B]:TRP:HZ2	6:A:431:GOL:H2	0.92	1.08
1:A:30:MET:HG3	1:A:31:ALA:H	1.23	0.99
1:A:362[B]:TRP:HZ2	6:A:431:GOL:C2	1.78	0.96
1:A:227[B]:LYS:CG	1:A:228:ALA:N	2.12	0.84
1:A:307:LYS:HD3	10:A:614:HOH:O	1.80	0.81
1:A:85:GLY:HA2	8:A:435:SO4:O4	1.81	0.79
1:A:273:LYS:HA	6:A:427:GOL:H2	1.64	0.79
1:A:307:LYS:CD	10:A:614:HOH:O	2.33	0.76
1:A:372:ARG:HG2	6:A:430:GOL:H12	1.68	0.75
1:A:30:MET:HG3	1:A:31:ALA:N	2.01	0.75
1:A:56:HIS:CE1	10:A:690:HOH:O	2.40	0.74
1:A:84:LEU:N	8:A:435:SO4:O1	2.24	0.71
1:A:32[A]:THR:HG22	1:A:35:GLU:HG3	1.74	0.69
1:A:227[B]:LYS:HG2	1:A:228:ALA:CA	2.23	0.68
1:A:85:GLY:CA	8:A:435:SO4:O4	2.42	0.68
1:A:37:PHE:HA	3:A:406:DDQ:HM12	1.77	0.67
1:A:184:LYS:HE2	10:A:714:HOH:O	1.94	0.66
4:A:408[B]:W7A:OAJ	4:A:408[B]:W7A:H5	1.93	0.66
1:A:227[B]:LYS:HD3	1:A:227[B]:LYS:N	2.11	0.66
1:A:227[B]:LYS:HD3	1:A:227[B]:LYS:H	1.60	0.66
1:A:347:ARG:NH2	1:A:396[B]:ARG:NH1	2.44	0.65
1:A:30:MET:CG	1:A:31:ALA:H	2.04	0.63
1:A:241:ARG:NH1	6:A:419[B]:GOL:H31	2.13	0.63
1:A:85:GLY:N	8:A:435:SO4:O4	2.31	0.63
1:A:56:HIS:HE1	10:A:690:HOH:O	1.78	0.62
6:A:412:GOL:H11	10:A:674:HOH:O	2.01	0.61
1:A:231:ARG:HH22	6:A:428:GOL:H2	1.66	0.61
1:A:347:ARG:HH21	1:A:396[B]:ARG:NH1	1.98	0.61
1:A:57:ARG:HH12	6:A:413:GOL:H2	1.67	0.59
1:A:57:ARG:NH1	6:A:413:GOL:H2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLY:H	6:A:415:GOL:H11	1.67	0.59
6:A:420:GOL:H2	10:A:783:HOH:O	2.02	0.59
1:A:207:ASP:OD1	9:A:438:ACT:CH3	2.52	0.58
1:A:207:ASP:OD1	9:A:438:ACT:H2	2.04	0.57
1:A:227[B]:LYS:HG2	1:A:228:ALA:CB	2.35	0.56
1:A:200:ARG:NH1	1:A:240[A]:GLU:CD	2.60	0.56
1:A:227[B]:LYS:HZ3	1:A:229:GLU:H	1.54	0.55
1:A:61:ARG:HD3	6:A:414:GOL:H2	1.88	0.55
1:A:200:ARG:HH11	1:A:240[A]:GLU:CD	2.11	0.54
1:A:86:HIS:HA	6:A:421:GOL:H2	1.90	0.54
3:A:406:DDQ:HM21	3:A:406:DDQ:C3	2.37	0.54
1:A:172:THR:O	6:A:421:GOL:H12	2.09	0.53
1:A:307:LYS:HG2	10:A:614:HOH:O	2.09	0.52
1:A:30:MET:HB3	1:A:372:ARG:HD2	1.92	0.52
1:A:362[B]:TRP:HE3	10:A:774:HOH:O	1.93	0.52
1:A:32[A]:THR:HG22	1:A:35:GLU:CG	2.41	0.51
1:A:30:MET:O	1:A:31:ALA:HB2	2.11	0.50
3:A:406:DDQ:HM21	3:A:406:DDQ:H32	1.94	0.50
1:A:200:ARG:NH1	1:A:240[A]:GLU:OE1	2.45	0.50
1:A:373:GLU:HG2	6:A:430:GOL:H31	1.93	0.49
1:A:307:LYS:CG	10:A:614:HOH:O	2.61	0.49
9:A:439:ACT:H2	10:A:583:HOH:O	2.12	0.48
1:A:347:ARG:NH2	1:A:396[B]:ARG:HH11	2.09	0.48
1:A:236:LYS:HE3	10:A:649:HOH:O	2.14	0.47
1:A:227[B]:LYS:HG3	10:A:790:HOH:O	2.14	0.47
1:A:227[B]:LYS:NZ	1:A:229:GLU:H	2.13	0.47
1:A:30:MET:HE3	6:A:423:GOL:H2	1.97	0.47
1:A:227[B]:LYS:CD	1:A:227[B]:LYS:N	2.74	0.46
1:A:362[B]:TRP:CZ2	6:A:431:GOL:C2	2.69	0.46
1:A:32[A]:THR:HG21	10:A:711:HOH:O	2.14	0.46
4:A:408[A]:W7A:H4	4:A:408[A]:W7A:OAJ	2.17	0.45
8:A:435:SO4:O2	9:A:442:ACT:O	2.35	0.45
1:A:396[A]:ARG:HG2	1:A:396[A]:ARG:NH2	2.32	0.45
1:A:247:VAL:HB	10:A:578:HOH:O	2.16	0.44
1:A:220:GLY:H	6:A:415:GOL:H32	1.82	0.44
1:A:43:MET:O	1:A:47[A]:GLN:HG3	2.18	0.44
1:A:32[A]:THR:HG23	1:A:34:ASP:H	1.82	0.44
1:A:364:PRO:O	6:A:425:GOL:H11	2.17	0.44
1:A:83:VAL:C	8:A:435:SO4:O1	2.57	0.43
1:A:52:PRO:HB3	4:A:408[B]:W7A:O2	2.19	0.43
1:A:52:PRO:HG3	1:A:136[A]:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:O	1:A:197[B]:GLU:HG3	2.19	0.43
1:A:32[A]:THR:CG2	1:A:35:GLU:H	2.31	0.42
1:A:241:ARG:CZ	6:A:419[B]:GOL:H31	2.49	0.42
1:A:296:ALA:HB2	6:A:417:GOL:H11	2.00	0.42
1:A:32[A]:THR:HG23	1:A:34:ASP:N	2.34	0.42
6:A:418:GOL:O3	10:A:776:HOH:O	2.20	0.42
6:A:420:GOL:O1	9:A:438:ACT:H1	2.20	0.41
1:A:129:ASN:HB3	1:A:130:PRO:HD2	2.02	0.41
1:A:192:ALA:HA	1:A:233:LEU:CD1	2.51	0.41
1:A:138:PRO:CD	6:A:418:GOL:H2	2.51	0.41
1:A:78:MET:HG3	10:A:747:HOH:O	2.21	0.41
1:A:226:GLY:C	1:A:227[B]:LYS:HZ3	2.25	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	380/390 (97%)	368 (97%)	11 (3%)	1 (0%)	46 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ALA

### 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	312/317 (98%)	303 (97%)	9 (3%)	50 25

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	32[A]	THR
1	A	32[B]	THR
1	A	49	LEU
1	A	61	ARG
1	A	72	ARG
1	A	184	LYS
1	A	247	VAL
1	A	356	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 45 ligands modelled in this entry, 1 is monoatomic - leaving 44 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	$\# Z  > 2$
3	DDQ	A	402	-	13,13,13	3.43	1 (7%)	14,15,15	0.69	1 (7%)
3	DDQ	A	403	-	13,13,13	3.92	1 (7%)	14,15,15	0.53	0
3	DDQ	A	404	-	13,13,13	4.06	1 (7%)	14,15,15	1.33	2 (14%)
3	DDQ	A	405	-	13,13,13	4.26	1 (7%)	14,15,15	1.42	2 (14%)
3	DDQ	A	406	-	13,13,13	3.78	2 (15%)	14,15,15	0.94	1 (7%)
3	DDQ	A	407	-	13,13,13	4.90	2 (15%)	14,15,15	4.81	6 (42%)
4	W7A	A	408[A]	-	22,27,27	1.95	6 (27%)	24,37,37	3.59	8 (33%)
4	W7A	A	408[B]	-	22,27,27	4.45	8 (36%)	24,37,37	1.76	5 (20%)
5	FMN	A	409	-	32,33,33	1.82	10 (31%)	34,50,50	3.86	10 (29%)
6	GOL	A	410	-	5,5,5	1.21	0	5,5,5	2.41	3 (60%)
6	GOL	A	411	-	5,5,5	0.45	0	5,5,5	1.01	0
6	GOL	A	412	-	5,5,5	0.30	0	5,5,5	0.52	0
6	GOL	A	413	-	5,5,5	0.90	0	5,5,5	1.40	1 (20%)
6	GOL	A	414	-	5,5,5	0.25	0	5,5,5	0.41	0
6	GOL	A	415	-	5,5,5	0.37	0	5,5,5	1.10	1 (20%)
6	GOL	A	416	-	5,5,5	0.56	0	5,5,5	0.57	0
6	GOL	A	417	-	5,5,5	1.12	0	5,5,5	1.24	1 (20%)
6	GOL	A	418	-	5,5,5	0.63	0	5,5,5	0.57	0
6	GOL	A	419[A]	-	5,5,5	0.30	0	5,5,5	0.48	0
6	GOL	A	419[B]	-	5,5,5	0.34	0	5,5,5	0.44	0
6	GOL	A	420	-	5,5,5	0.91	0	5,5,5	1.17	1 (20%)
6	GOL	A	421	-	5,5,5	0.67	0	5,5,5	1.85	1 (20%)
6	GOL	A	422	-	5,5,5	0.14	0	5,5,5	1.20	1 (20%)
6	GOL	A	423	-	5,5,5	0.67	0	5,5,5	0.44	0
6	GOL	A	424	-	5,5,5	0.51	0	5,5,5	0.92	0
6	GOL	A	425	-	5,5,5	0.40	0	5,5,5	2.54	2 (40%)
6	GOL	A	426	-	5,5,5	1.26	1 (20%)	5,5,5	1.26	1 (20%)
6	GOL	A	427	-	5,5,5	1.11	1 (20%)	5,5,5	1.22	1 (20%)
6	GOL	A	428	-	5,5,5	0.48	0	5,5,5	0.56	0
6	GOL	A	429	-	5,5,5	0.93	0	5,5,5	0.99	0
6	GOL	A	430	-	5,5,5	0.27	0	5,5,5	1.06	0
6	GOL	A	431	-	5,5,5	0.52	0	5,5,5	0.98	0
7	ORO	A	432	-	6,11,11	2.30	3 (50%)	6,15,15	7.49	5 (83%)
8	SO4	A	433	-	4,4,4	1.33	1 (25%)	6,6,6	0.71	0
8	SO4	A	434	-	4,4,4	0.84	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	A	435	-	4,4,4	1.40	1 (25%)	6,6,6	0.45	0
8	SO4	A	436	-	4,4,4	0.65	0	6,6,6	1.03	1 (16%)
9	ACT	A	437	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ACT	A	438	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ACT	A	439	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ACT	A	440	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ACT	A	441	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ACT	A	442	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ACT	A	443	-	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
3	DDQ	A	402	-	-	0/11/11/11	0/0/0/0
3	DDQ	A	403	-	-	0/11/11/11	0/0/0/0
3	DDQ	A	404	-	-	0/11/11/11	0/0/0/0
3	DDQ	A	405	-	-	0/11/11/11	0/0/0/0
3	DDQ	A	406	-	-	0/11/11/11	0/0/0/0
3	DDQ	A	407	-	-	0/11/11/11	0/0/0/0
4	W7A	A	408[A]	-	-	0/9/13/13	0/3/3/3
4	W7A	A	408[B]	-	-	0/9/13/13	0/3/3/3
5	FMN	A	409	-	-	0/18/18/18	0/3/3/3
6	GOL	A	410	-	-	0/4/4/4	0/0/0/0
6	GOL	A	411	-	-	0/4/4/4	0/0/0/0
6	GOL	A	412	-	-	0/4/4/4	0/0/0/0
6	GOL	A	413	-	-	0/4/4/4	0/0/0/0
6	GOL	A	414	-	-	0/4/4/4	0/0/0/0
6	GOL	A	415	-	-	0/4/4/4	0/0/0/0
6	GOL	A	416	-	-	0/4/4/4	0/0/0/0
6	GOL	A	417	-	-	0/4/4/4	0/0/0/0
6	GOL	A	418	-	-	0/4/4/4	0/0/0/0
6	GOL	A	419[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	419[B]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	420	-	-	0/4/4/4	0/0/0/0
6	GOL	A	421	-	-	0/4/4/4	0/0/0/0
6	GOL	A	422	-	-	0/4/4/4	0/0/0/0
6	GOL	A	423	-	-	0/4/4/4	0/0/0/0
6	GOL	A	424	-	-	0/4/4/4	0/0/0/0
6	GOL	A	425	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	426	-	-	0/4/4/4	0/0/0/0
6	GOL	A	427	-	-	0/4/4/4	0/0/0/0
6	GOL	A	428	-	-	0/4/4/4	0/0/0/0
6	GOL	A	429	-	-	0/4/4/4	0/0/0/0
6	GOL	A	430	-	-	0/4/4/4	0/0/0/0
6	GOL	A	431	-	-	0/4/4/4	0/0/0/0
7	ORO	A	432	-	-	0/0/4/4	0/1/1/1
8	SO4	A	433	-	-	0/0/0/0	0/0/0/0
8	SO4	A	434	-	-	0/0/0/0	0/0/0/0
8	SO4	A	435	-	-	0/0/0/0	0/0/0/0
8	SO4	A	436	-	-	0/0/0/0	0/0/0/0
9	ACT	A	437	-	-	0/0/0/0	0/0/0/0
9	ACT	A	438	-	-	0/0/0/0	0/0/0/0
9	ACT	A	439	-	-	0/0/0/0	0/0/0/0
9	ACT	A	440	-	-	0/0/0/0	0/0/0/0
9	ACT	A	441	-	-	0/0/0/0	0/0/0/0
9	ACT	A	442	-	-	0/0/0/0	0/0/0/0
9	ACT	A	443	-	-	0/0/0/0	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408[B]	W7A	CAL-C5	-17.67	1.28	1.52
3	A	407	DDQ	O1-N1	-17.32	1.23	1.39
3	A	405	DDQ	O1-N1	-15.18	1.25	1.39
3	A	404	DDQ	O1-N1	-14.47	1.25	1.39
3	A	403	DDQ	O1-N1	-13.98	1.26	1.39
3	A	406	DDQ	O1-N1	-13.02	1.27	1.39
3	A	402	DDQ	O1-N1	-12.15	1.28	1.39
4	A	408[B]	W7A	CAM-CAN	-5.69	1.35	1.51
4	A	408[B]	W7A	CAQ-CAT	-4.96	1.36	1.49
4	A	408[A]	W7A	CAQ-CAT	-4.51	1.37	1.49
4	A	408[A]	W7A	CAL-C5	-4.44	1.46	1.52
3	A	406	DDQ	CM1-N1	-3.60	1.43	1.49
4	A	408[B]	W7A	C2-N1	-3.52	1.30	1.38
4	A	408[A]	W7A	C4-N3	-3.47	1.29	1.34
7	A	432	ORO	C2-N3	-3.23	1.31	1.38
4	A	408[A]	W7A	CAM-CAN	-2.89	1.43	1.51
5	A	409	FMN	C10-N10	-2.77	1.35	1.39
5	A	409	FMN	C2-N1	-2.76	1.32	1.38
4	A	408[A]	W7A	O6-C6	-2.70	1.17	1.24
4	A	408[B]	W7A	C4-C5	-2.70	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	407	DDQ	CM2-N1	-2.63	1.45	1.49
7	A	432	ORO	C5-C6	-2.47	1.33	1.40
5	A	409	FMN	C6-C5A	-2.38	1.38	1.41
4	A	408[B]	W7A	CAS-CAR	-2.26	1.34	1.38
8	A	435	SO4	O2-S	-2.21	1.39	1.47
4	A	408[A]	W7A	C2-N1	-2.15	1.33	1.38
6	A	427	GOL	C3-C2	2.01	1.60	1.52
8	A	433	SO4	O4-S	2.02	1.54	1.47
5	A	409	FMN	C5A-N5	2.09	1.38	1.35
5	A	409	FMN	C9A-N10	2.09	1.41	1.38
4	A	408[B]	W7A	C2-N3	2.22	1.42	1.38
6	A	426	GOL	O2-C2	2.50	1.50	1.43
5	A	409	FMN	O3'-C3'	2.53	1.48	1.43
5	A	409	FMN	C5'-C4'	2.70	1.55	1.51
5	A	409	FMN	C4-C4A	2.84	1.47	1.41
7	A	432	ORO	C4-N3	3.28	1.39	1.33
5	A	409	FMN	C4A-N5	3.82	1.39	1.33
4	A	408[B]	W7A	C4-N3	4.30	1.41	1.34
5	A	409	FMN	C4A-C10	4.66	1.49	1.40

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	407	DDQ	O1-N1-C1	-11.86	96.93	110.27
5	A	409	FMN	C4-C4A-C10	-10.42	113.27	119.94
7	A	432	ORO	C5-C4-N3	-10.32	113.11	124.02
5	A	409	FMN	C4A-C10-N10	-9.70	113.47	120.52
4	A	408[A]	W7A	N1-C2-N3	-6.67	116.46	127.69
7	A	432	ORO	N3-C2-N1	-5.90	117.76	127.69
5	A	409	FMN	N3-C2-N1	-5.57	118.31	127.69
6	A	425	GOL	C3-C2-C1	-4.96	90.16	111.06
5	A	409	FMN	C4A-C4-N3	-4.54	117.59	123.52
4	A	408[B]	W7A	C5-C4-N3	-4.10	116.58	122.66
3	A	405	DDQ	O1-N1-CM2	-4.07	103.62	109.05
3	A	404	DDQ	O1-N1-C1	-4.03	105.74	110.27
4	A	408[A]	W7A	CAO-CAN-CAS	-4.02	111.53	118.15
3	A	407	DDQ	CM2-N1-C1	-3.93	97.10	109.77
6	A	410	GOL	O1-C1-C2	-3.72	91.14	109.97
4	A	408[B]	W7A	N1-C2-N3	-3.14	122.40	127.69
3	A	407	DDQ	CM1-N1-C1	-3.01	100.08	109.77
5	A	409	FMN	C9A-C5A-N5	-2.83	117.57	122.18
6	A	410	GOL	O3-C3-C2	-2.67	96.41	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	408[A]	W7A	C5-C4-N3	-2.59	118.81	122.66
6	A	410	GOL	O2-C2-C3	-2.50	96.45	108.47
3	A	402	DDQ	CM2-N1-CM1	-2.06	106.51	108.83
6	A	420	GOL	O1-C1-C2	-2.04	99.61	109.97
3	A	404	DDQ	O1-N1-CM1	-2.04	106.33	109.05
6	A	422	GOL	O3-C3-C2	-2.01	99.78	109.97
6	A	426	GOL	O2-C2-C3	2.00	118.09	108.47
3	A	406	DDQ	CM2-N1-C1	2.04	116.34	109.77
8	A	436	SO4	O4-S-O3	2.05	117.37	109.09
4	A	408[B]	W7A	CAP-CAO-CAN	2.06	123.92	121.02
6	A	415	GOL	O3-C3-C2	2.22	121.23	109.97
6	A	425	GOL	O2-C2-C1	2.38	119.92	108.47
3	A	405	DDQ	O1-N1-CM1	2.41	112.28	109.05
6	A	417	GOL	O3-C3-C2	2.45	122.39	109.97
5	A	409	FMN	C6-C5A-C9A	2.46	121.82	119.11
6	A	427	GOL	O2-C2-C3	2.50	120.46	108.47
5	A	409	FMN	C4A-N5-C5A	2.69	119.89	116.72
6	A	413	GOL	O2-C2-C3	2.86	122.22	108.47
7	A	432	ORO	C2-N1-C6	2.94	120.88	117.03
4	A	408[A]	W7A	CAL-CAM-CAN	3.25	124.01	113.27
4	A	408[B]	W7A	C6-N1-C2	3.28	117.89	115.16
5	A	409	FMN	C4-C4A-N5	3.92	123.46	118.70
6	A	421	GOL	O1-C1-C2	3.95	130.00	109.97
4	A	408[A]	W7A	CAP-CAO-CAN	4.28	127.04	121.02
4	A	408[A]	W7A	CAM-CAL-C5	4.28	119.99	112.47
4	A	408[B]	W7A	C2-N3-C4	4.39	120.08	115.68
5	A	409	FMN	C5A-C9A-N10	5.24	121.51	117.58
3	A	407	DDQ	O1-N1-CM2	6.11	117.22	109.05
3	A	407	DDQ	CM2-N1-CM1	6.82	116.53	108.83
7	A	432	ORO	C4-C5-C6	6.83	121.14	116.73
4	A	408[A]	W7A	C6-N1-C2	7.30	121.25	115.16
3	A	407	DDQ	O1-N1-CM1	8.54	120.46	109.05
4	A	408[A]	W7A	C2-N3-C4	11.01	126.71	115.68
7	A	432	ORO	C4-N3-C2	11.73	126.57	114.21
5	A	409	FMN	C4-N3-C2	12.97	125.98	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	DDQ	3	0
4	A	408[A]	W7A	1	0
4	A	408[B]	W7A	2	0
6	A	412	GOL	1	0
6	A	413	GOL	2	0
6	A	414	GOL	1	0
6	A	415	GOL	2	0
6	A	417	GOL	1	0
6	A	418	GOL	2	0
6	A	419[B]	GOL	2	0
6	A	420	GOL	2	0
6	A	421	GOL	2	0
6	A	423	GOL	1	0
6	A	425	GOL	1	0
6	A	427	GOL	1	0
6	A	428	GOL	1	0
6	A	430	GOL	2	0
6	A	431	GOL	4	0
8	A	435	SO4	6	0
9	A	438	ACT	3	0
9	A	439	ACT	1	0
9	A	442	ACT	1	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, 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	367/390 (94%)	-0.09	15 (4%) 41 42	7, 13, 33, 86	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ARG	8.5
1	A	30	MET	6.4
1	A	31	ALA	5.9
1	A	70	ARG	5.7
1	A	73	PHE	4.1
1	A	71	ALA	3.6
1	A	74	GLN	3.6
1	A	189	VAL	2.8
1	A	396[A]	ARG	2.6
1	A	229	GLU	2.6
1	A	227[A]	LYS	2.5
1	A	219	ALA	2.4
1	A	226	GLY	2.2
1	A	33	GLY	2.1
1	A	187	THR	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 ⓘ

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
6	GOL	A	419[B]	6/6	0.72	0.26	26.25	55,57,59,59	6
6	GOL	A	422	6/6	0.82	0.17	13.83	33,52,57,61	0
9	ACT	A	440	4/4	0.83	0.22	12.66	41,53,55,57	0
6	GOL	A	417	6/6	0.90	0.16	10.65	22,40,46,47	0
6	GOL	A	424	6/6	0.79	0.16	9.64	46,50,54,58	0
3	DDQ	A	404	14/14	0.64	0.31	7.67	75,87,96,96	0
6	GOL	A	419[A]	6/6	0.72	0.26	6.65	36,43,44,45	6
6	GOL	A	418	6/6	0.81	0.26	6.43	33,51,54,59	0
6	GOL	A	410	6/6	0.79	0.17	5.11	21,27,29,32	0
6	GOL	A	427	6/6	0.73	0.30	4.79	31,37,44,46	0
9	ACT	A	438	4/4	0.94	0.12	4.59	20,28,35,35	0
6	GOL	A	414	6/6	0.89	0.26	4.36	53,56,60,65	0
6	GOL	A	420	6/6	0.87	0.23	3.94	33,41,48,51	0
3	DDQ	A	407	14/14	0.77	0.17	2.72	27,39,72,72	0
3	DDQ	A	403	14/14	0.56	0.38	2.62	62,74,86,95	0
6	GOL	A	411	6/6	0.88	0.14	2.13	35,43,45,51	0
6	GOL	A	416	6/6	0.85	0.23	2.06	33,42,49,51	0
6	GOL	A	421	6/6	0.84	0.19	1.78	29,43,50,55	0
6	GOL	A	430	6/6	0.83	0.37	1.36	51,54,58,61	0
6	GOL	A	425	6/6	0.82	0.21	0.77	26,35,41,42	0
6	GOL	A	413	6/6	0.82	0.12	0.36	26,42,43,45	0
6	GOL	A	431	6/6	0.92	0.13	0.28	25,41,50,51	0
6	GOL	A	412	6/6	0.68	0.15	-0.08	61,61,68,70	0
5	FMN	A	409	31/31	0.99	0.09	-0.16	5,6,8,9	0
4	W7A	A	408[B]	25/25	0.94	0.09	-0.17	13,16,19,21	25
4	W7A	A	408[A]	25/25	0.94	0.09	-0.18	11,13,20,22	25
6	GOL	A	423	6/6	0.83	0.28	-0.26	61,68,75,79	0
6	GOL	A	415	6/6	0.88	0.15	-0.62	37,51,59,60	0
7	ORO	A	432	11/11	0.99	0.04	-1.33	6,7,8,10	0
3	DDQ	A	405	14/14	0.51	0.35	-	59,65,82,86	0
6	GOL	A	428	6/6	0.90	0.12	-	49,57,58,58	0
2	CL	A	401	1/1	0.99	0.03	-	17,17,17,17	0
8	SO4	A	436	5/5	0.91	0.28	-	48,50,61,61	0
8	SO4	A	435	5/5	0.94	0.48	-	46,51,68,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	ACT	A	437	4/4	0.90	0.18	-	33,50,50,58	0
9	ACT	A	439	4/4	0.80	0.34	-	39,42,49,55	0
6	GOL	A	426	6/6	0.75	0.27	-	33,45,54,57	0
6	GOL	A	429	6/6	0.88	0.21	-	28,38,52,53	0
9	ACT	A	441	4/4	0.72	0.15	-	56,61,64,65	0
8	SO4	A	433	5/5	0.99	0.10	-	23,23,28,32	0
8	SO4	A	434	5/5	0.88	0.33	-	50,57,63,68	0
9	ACT	A	442	4/4	0.78	0.33	-	54,55,60,61	0
3	DDQ	A	402	14/14	0.80	0.28	-	52,59,70,71	0
9	ACT	A	443	4/4	0.75	0.43	-	39,42,43,50	0
3	DDQ	A	406	14/14	0.65	0.39	-	45,66,81,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.