Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:02 PM EDT

PDB ID	:	3W7R
Title	:	Structure of Human dihydroorotate dehydrogenase in complex with mii-4-097
Authors	:	Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Hashimoto, S.; Matsuoka, S.; Kuranaga, T.; Shiba, T.; Sakamoto, K.; Suzuki, S.; Balogun, E.O.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

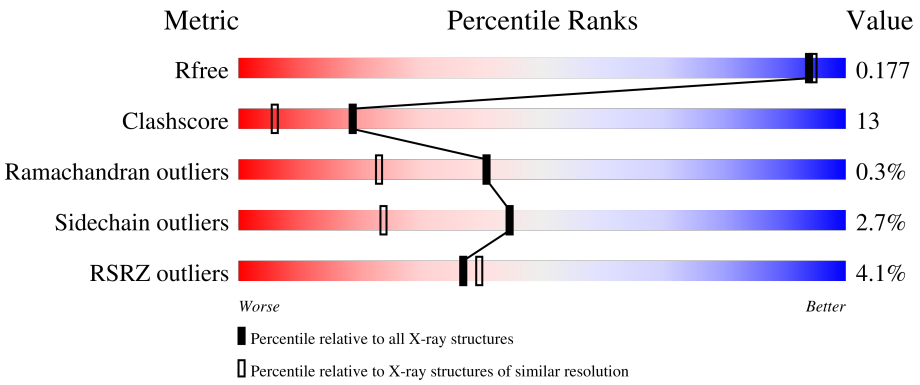
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.68 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}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	4% 76% 15% • • 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	GOL	A	410	-	X	-	-
6	GOL	A	431	-	-	X	-
7	ORO	A	432	-	X	-	-
8	SO4	A	435	-	-	X	-
9	ACT	A	438	-	-	X	-
9	ACT	A	443	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	367	2944	1837	546	556	5	5	16	0

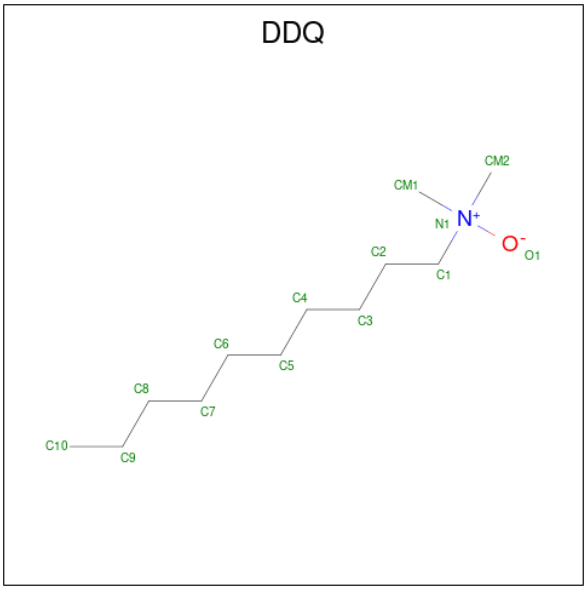
There are 23 discrepancies between the modelled and reference sequences:

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

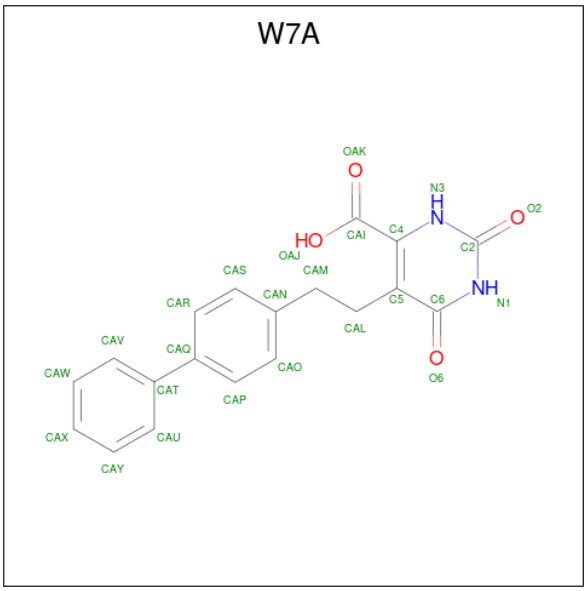
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0

- Molecule 3 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



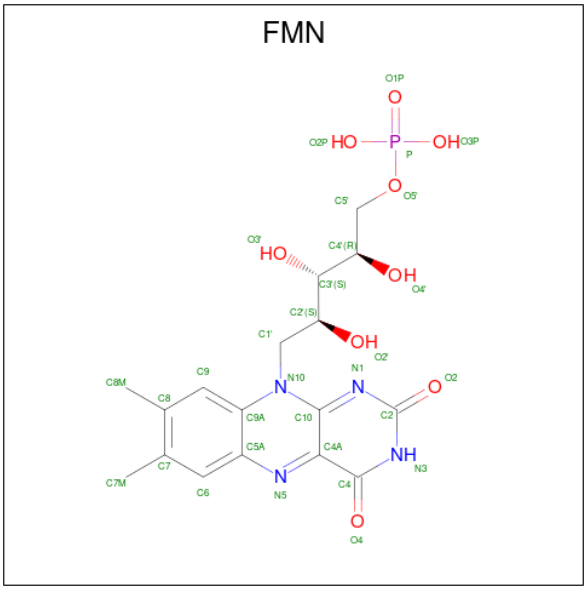
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	12	1	1	0	0
			Total	C	N	O		
3	A	1	14	12	1	1	0	0
			Total	C	N	O		
3	A	1	14	12	1	1	0	0
			Total	C	N	O		
3	A	1	14	12	1	1	0	0
			Total	C	N	O		
3	A	1	14	12	1	1	0	0
			Total	C	N	O		
3	A	1	14	12	1	1	0	0

- Molecule 4 is 2,6-dioxo-5-[2-(4-phenylphenyl)ethyl]-1,2,3,6- tetrahydropyrimidine-4-carboxy lic acid (three-letter code: W7A) (formula: $C_{19}H_{16}N_2O_4$).



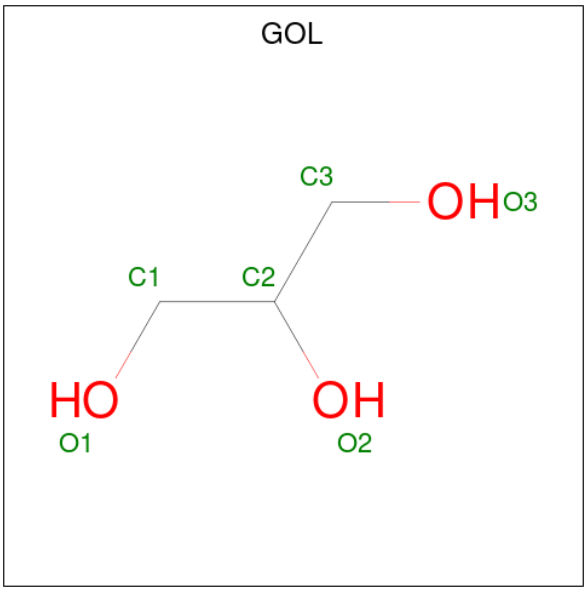
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	50	38	4	8	0	1

- Molecule 5 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		
5	A	1	31	17	4	9	1	0	0

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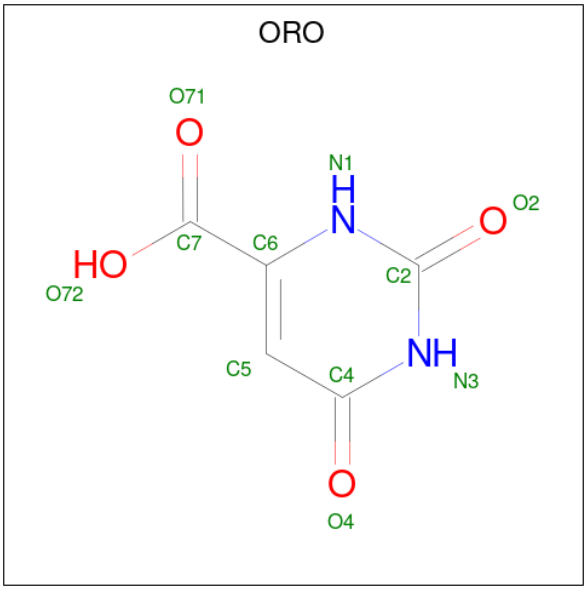
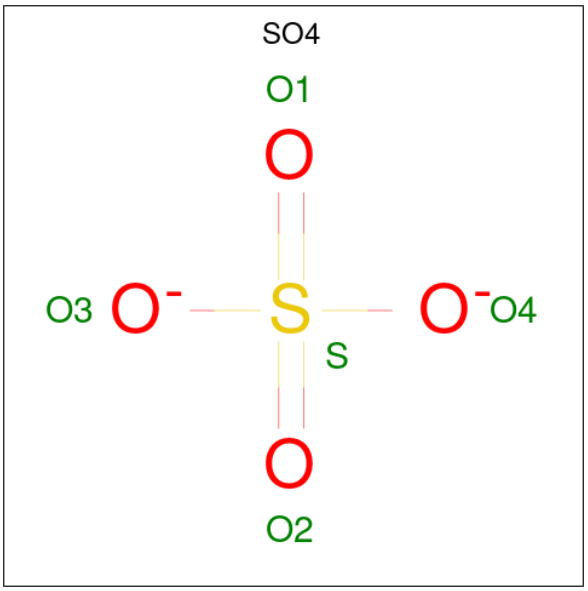
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3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

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



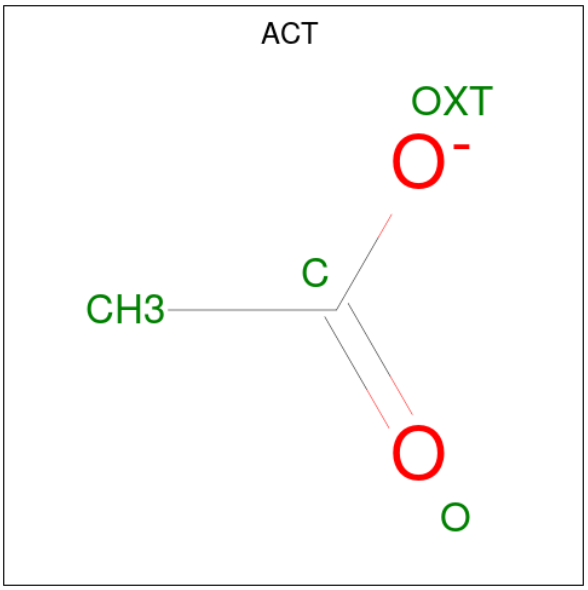
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	11	5	2	4	0	0

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



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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 10 is water.

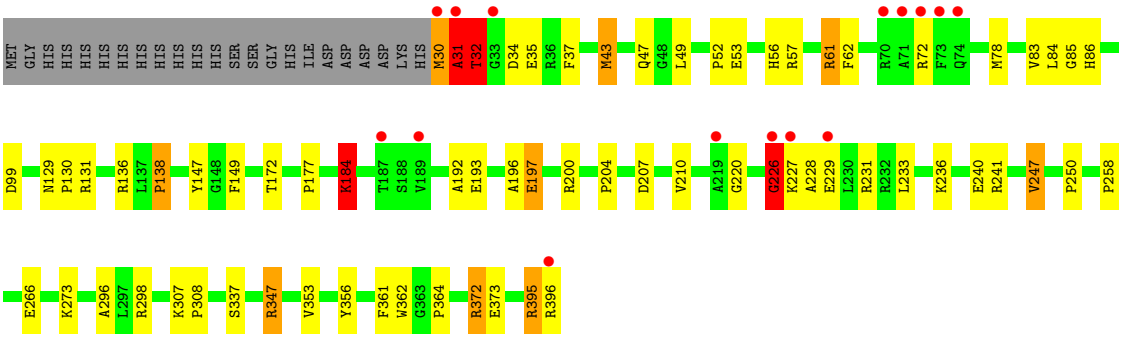
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	317	319	319	0	2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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	3387 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3626	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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: SO4, CL, GOL, FMN, W7A, DDQ, ACT, 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	1.51	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(^{o})	Ideal(^{o})
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	Peptide,Mainchain
1	A	31	ALA	Peptide,Mainchain
1	A	32[B]	THR	Mainchain
1	A	395	ARG	Mainchain

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	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:N	1:A:227[B]:LYS:HD3	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:61:ARG:HD3	6:A:414:GOL:H2	1.88	0.55
1:A:227[B]:LYS:HZ3	1:A:229:GLU:H	1.54	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:N	1:A:227[B]:LYS:CD	2.74	0.46
1:A:32[A]:THR:HG21	10:A:711:HOH:O	2.14	0.46
1:A:362[B]:TRP:CZ2	6:A:431:GOL:C2	2.69	0.46
4:A:408[A]:W7A:OAJ	4:A:408[A]:W7A:H4	2.17	0.45
8:A:435:SO4:O2	9:A:442:ACT:O	2.35	0.45
1:A:396[A]:ARG:NH2	1:A:396[A]:ARG:HG2	2.32	0.45
1:A:247:VAL:HB	10:A:578:HOH:O	2.16	0.44
1:A:43:MET:O	1:A:47[A]:GLN:HG3	2.18	0.44
1:A:220:GLY:H	6:A:415:GOL:H32	1.82	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%)	41 23

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%)	42 21

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

Sometimes 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 monosaccharides 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	$\#\|Z\| > 2$
6	GOL	A	414	-	5,5,5	0.26	0	5,5,5	0.44	0
6	GOL	A	424	-	5,5,5	0.52	0	5,5,5	1.12	0
8	SO4	A	434	-	4,4,4	0.70	0	6,6,6	0.75	0
4	W7A	A	408[B]	-	27,27,27	3.04	12 (44%)	35,37,37	2.77	9 (25%)
6	GOL	A	427	-	5,5,5	1.20	1 (20%)	5,5,5	1.30	1 (20%)
6	GOL	A	423	-	5,5,5	0.63	0	5,5,5	0.59	0
4	W7A	A	408[A]	-	27,27,27	2.35	9 (33%)	35,37,37	2.43	12 (34%)
3	DDQ	A	406	-	11,13,13	2.00	2 (18%)	12,15,15	0.94	1 (8%)
9	ACT	A	439	-	3,3,3	0.64	0	3,3,3	1.14	0
9	ACT	A	443	-	3,3,3	1.26	0	3,3,3	1.31	0
6	GOL	A	415	-	5,5,5	0.36	0	5,5,5	1.24	1 (20%)
6	GOL	A	419[B]	-	5,5,5	0.40	0	5,5,5	0.47	0
9	ACT	A	441	-	3,3,3	0.87	0	3,3,3	0.50	0
6	GOL	A	419[A]	-	5,5,5	0.36	0	5,5,5	0.51	0
8	SO4	A	433	-	4,4,4	0.80	0	6,6,6	0.62	0
5	FMN	A	409	-	33,33,33	1.59	8 (24%)	48,50,50	1.58	9 (18%)
7	ORO	A	432	-	10,11,11	2.89	5 (50%)	10,15,15	6.93	4 (40%)
6	GOL	A	417	-	5,5,5	1.18	0	5,5,5	1.32	1 (20%)
6	GOL	A	428	-	5,5,5	0.48	0	5,5,5	0.65	0
3	DDQ	A	407	-	11,13,13	2.42	1 (9%)	12,15,15	2.76	3 (25%)
6	GOL	A	412	-	5,5,5	0.34	0	5,5,5	0.61	0
3	DDQ	A	405	-	11,13,13	2.22	1 (9%)	12,15,15	0.90	1 (8%)
3	DDQ	A	404	-	11,13,13	2.21	2 (18%)	12,15,15	0.79	1 (8%)
9	ACT	A	442	-	3,3,3	0.82	0	3,3,3	0.74	0
6	GOL	A	411	-	5,5,5	0.50	0	5,5,5	1.10	0
6	GOL	A	430	-	5,5,5	0.32	0	5,5,5	1.19	0
6	GOL	A	425	-	5,5,5	0.44	0	5,5,5	2.95	2 (40%)
6	GOL	A	429	-	5,5,5	0.91	0	5,5,5	1.04	0
6	GOL	A	413	-	5,5,5	0.93	0	5,5,5	1.57	1 (20%)
6	GOL	A	421	-	5,5,5	0.71	0	5,5,5	2.07	1 (20%)
8	SO4	A	435	-	4,4,4	0.59	0	6,6,6	0.41	0
6	GOL	A	420	-	5,5,5	0.96	0	5,5,5	1.35	1 (20%)
9	ACT	A	440	-	3,3,3	0.67	0	3,3,3	1.43	0
9	ACT	A	437	-	3,3,3	1.08	0	3,3,3	0.31	0
6	GOL	A	418	-	5,5,5	0.71	0	5,5,5	0.56	0
6	GOL	A	410	-	5,5,5	1.26	1 (20%)	5,5,5	2.79	3 (60%)
9	ACT	A	438	-	3,3,3	0.71	0	3,3,3	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DDQ	A	402	-	11,13,13	1.84	1 (9%)	12,15,15	0.45	0
3	DDQ	A	403	-	11,13,13	2.19	2 (18%)	12,15,15	0.37	0
6	GOL	A	426	-	5,5,5	1.32	1 (20%)	5,5,5	1.40	1 (20%)
6	GOL	A	431	-	5,5,5	0.58	0	5,5,5	1.07	0
6	GOL	A	422	-	5,5,5	0.15	0	5,5,5	1.40	1 (20%)
8	SO4	A	436	-	4,4,4	0.51	0	6,6,6	0.93	0
6	GOL	A	416	-	5,5,5	0.59	0	5,5,5	0.63	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
6	GOL	A	414	-	-	2/4/4/4	-
6	GOL	A	424	-	-	4/4/4/4	-
4	W7A	A	408[B]	-	-	1/13/13/13	0/3/3/3
6	GOL	A	427	-	-	2/4/4/4	-
6	GOL	A	423	-	-	1/4/4/4	-
4	W7A	A	408[A]	-	-	1/13/13/13	0/3/3/3
3	DDQ	A	406	-	-	7/11/11/11	-
6	GOL	A	415	-	-	2/4/4/4	-
6	GOL	A	419[B]	-	-	4/4/4/4	-
6	GOL	A	419[A]	-	-	4/4/4/4	-
5	FMN	A	409	-	-	4/18/18/18	0/3/3/3
7	ORO	A	432	-	-	4/4/4/4	0/1/1/1
6	GOL	A	417	-	-	0/4/4/4	-
6	GOL	A	428	-	-	1/4/4/4	-
3	DDQ	A	407	-	-	4/11/11/11	-
6	GOL	A	412	-	-	4/4/4/4	-
3	DDQ	A	405	-	-	6/11/11/11	-
3	DDQ	A	404	-	-	5/11/11/11	-
6	GOL	A	411	-	-	4/4/4/4	-
6	GOL	A	430	-	-	4/4/4/4	-
6	GOL	A	425	-	-	0/4/4/4	-
6	GOL	A	429	-	-	4/4/4/4	-
6	GOL	A	413	-	-	0/4/4/4	-
6	GOL	A	421	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	420	-	-	4/4/4/4	-
6	GOL	A	418	-	-	3/4/4/4	-
6	GOL	A	410	-	-	2/4/4/4	-
3	DDQ	A	402	-	-	5/11/11/11	-
3	DDQ	A	403	-	-	4/11/11/11	-
6	GOL	A	426	-	-	3/4/4/4	-
6	GOL	A	431	-	-	0/4/4/4	-
6	GOL	A	422	-	-	2/4/4/4	-
6	GOL	A	416	-	-	0/4/4/4	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408[B]	W7A	CAL-C5	-8.93	1.28	1.51
3	A	407	DDQ	O1-N1	-7.81	1.23	1.42
3	A	405	DDQ	O1-N1	-6.96	1.25	1.42
7	A	432	ORO	C5-C4	6.88	1.44	1.37
3	A	404	DDQ	O1-N1	-6.67	1.25	1.42
3	A	403	DDQ	O1-N1	-6.48	1.26	1.42
3	A	406	DDQ	O1-N1	-6.09	1.27	1.42
4	A	408[B]	W7A	CAM-CAN	-5.84	1.35	1.51
3	A	402	DDQ	O1-N1	-5.75	1.28	1.42
4	A	408[A]	W7A	C4-CAI	-5.48	1.39	1.48
4	A	408[B]	W7A	CAT-CAQ	-5.46	1.36	1.49
4	A	408[A]	W7A	CAT-CAQ	-4.97	1.37	1.49
4	A	408[A]	W7A	C4-N3	-4.95	1.29	1.38
4	A	408[B]	W7A	C6-N1	-4.47	1.30	1.38
4	A	408[A]	W7A	OAJ-CAI	-4.18	1.19	1.30
4	A	408[B]	W7A	C4-CAI	-4.04	1.42	1.48
4	A	408[B]	W7A	C2-N1	-4.02	1.30	1.37
5	A	409	FMN	C4A-N5	3.91	1.39	1.30
7	A	432	ORO	C4-N3	3.48	1.39	1.33
4	A	408[B]	W7A	C2-N3	3.23	1.42	1.37
3	A	403	DDQ	C1-N1	-3.15	1.48	1.51
4	A	408[A]	W7A	O6-C6	-3.07	1.17	1.23
4	A	408[A]	W7A	CAM-CAN	-2.96	1.43	1.51
5	A	409	FMN	C5'-C4'	2.96	1.55	1.51
3	A	404	DDQ	C1-N1	-2.87	1.48	1.51
5	A	409	FMN	C6-C7	-2.81	1.35	1.39
4	A	408[B]	W7A	CAR-CAS	-2.78	1.34	1.38
4	A	408[B]	W7A	OAJ-CAI	-2.75	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	432	ORO	C5-C6	-2.69	1.33	1.40
7	A	432	ORO	C2-N3	-2.67	1.31	1.37
5	A	409	FMN	C4-N3	-2.60	1.34	1.38
6	A	426	GOL	O2-C2	2.57	1.50	1.43
5	A	409	FMN	O3'-C3'	2.41	1.48	1.43
5	A	409	FMN	O4-C4	2.39	1.28	1.23
4	A	408[B]	W7A	O2-C2	-2.38	1.18	1.23
4	A	408[A]	W7A	C4-C5	2.32	1.41	1.37
4	A	408[A]	W7A	C2-N1	-2.29	1.33	1.37
3	A	406	DDQ	C1-N1	-2.25	1.49	1.51
7	A	432	ORO	C6-N1	2.21	1.37	1.34
6	A	427	GOL	C3-C2	2.19	1.60	1.51
5	A	409	FMN	O2-C2	-2.12	1.20	1.24
5	A	409	FMN	C7M-C7	2.12	1.55	1.51
4	A	408[B]	W7A	CAV-CAT	-2.12	1.35	1.39
6	A	410	GOL	O1-C1	2.03	1.50	1.42
4	A	408[A]	W7A	CAL-C5	-2.01	1.46	1.51
4	A	408[B]	W7A	CAR-CAQ	-2.00	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	432	ORO	C2-N3-C4	18.16	126.57	114.49
4	A	408[B]	W7A	C5-C6-N1	11.54	124.47	115.70
7	A	432	ORO	C5-C4-N3	-9.45	113.11	124.16
4	A	408[A]	W7A	C5-C6-N1	7.81	121.64	115.70
7	A	432	ORO	C6-C5-C4	6.83	121.14	116.73
3	A	407	DDQ	CM2-N1-C1	-6.25	97.10	110.23
4	A	408[B]	W7A	C6-N1-C2	-6.16	117.89	126.37
6	A	425	GOL	C3-C2-C1	-5.90	90.16	111.80
3	A	407	DDQ	O1-N1-C1	-5.03	96.93	109.27
3	A	407	DDQ	CM1-N1-C1	-4.83	100.08	110.23
5	A	409	FMN	C9A-C5A-N5	-4.61	117.57	122.45
4	A	408[A]	W7A	CAP-CAO-CAN	4.60	127.04	121.00
4	A	408[A]	W7A	CAO-CAN-CAS	-4.51	111.53	118.23
6	A	421	GOL	O1-C1-C2	4.36	130.00	110.38
6	A	410	GOL	O1-C1-C2	-4.27	91.14	110.38
4	A	408[B]	W7A	N1-C2-N3	4.23	122.40	115.74
4	A	408[B]	W7A	OAJ-CAI-C4	4.19	123.37	116.73
5	A	409	FMN	C5A-C9A-N10	3.91	121.51	117.97
4	A	408[B]	W7A	O6-C6-N1	-3.90	112.78	120.11
5	A	409	FMN	C4-C4A-N5	3.80	123.46	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	408[A]	W7A	C6-N1-C2	-3.72	121.25	126.37
4	A	408[A]	W7A	CAI-C4-C5	3.55	129.26	123.88
4	A	408[A]	W7A	CAL-CAM-CAN	3.22	124.01	112.70
6	A	413	GOL	O2-C2-C3	3.15	122.22	109.18
6	A	410	GOL	O3-C3-C2	-3.10	96.41	110.38
6	A	410	GOL	O2-C2-C3	-3.07	96.45	109.18
3	A	406	DDQ	CM2-N1-C1	2.91	116.34	110.23
6	A	427	GOL	O2-C2-C3	2.73	120.46	109.18
4	A	408[B]	W7A	OAK-CAI-C4	-2.72	115.46	120.20
4	A	408[A]	W7A	CAL-C5-C6	2.72	120.29	116.64
6	A	417	GOL	O3-C3-C2	2.67	122.39	110.38
5	A	409	FMN	O4-C4-C4A	-2.60	119.67	126.53
6	A	425	GOL	O2-C2-C1	2.59	119.92	109.18
4	A	408[A]	W7A	CAL-C5-C4	2.57	124.67	119.56
4	A	408[A]	W7A	OAJ-CAI-C4	2.56	120.79	116.73
4	A	408[B]	W7A	CAL-C5-C6	2.42	119.88	116.64
6	A	415	GOL	O3-C3-C2	2.41	121.23	110.38
6	A	420	GOL	O1-C1-C2	-2.39	99.61	110.38
4	A	408[A]	W7A	O6-C6-N1	-2.39	115.63	120.11
6	A	422	GOL	O3-C3-C2	-2.35	99.78	110.38
3	A	405	DDQ	CM2-N1-C1	2.34	115.14	110.23
4	A	408[B]	W7A	CAP-CAO-CAN	2.23	123.92	121.00
4	A	408[A]	W7A	OAK-CAI-C4	-2.19	116.39	120.20
4	A	408[A]	W7A	CAS-CAR-CAQ	2.16	123.89	121.12
6	A	426	GOL	O2-C2-C3	2.15	118.09	109.18
5	A	409	FMN	C9-C9A-C5A	-2.15	116.23	120.03
5	A	409	FMN	C4-C4A-C10	-2.13	113.27	116.93
5	A	409	FMN	C10-N1-C2	2.12	121.44	116.85
5	A	409	FMN	C4A-C10-N10	-2.10	113.47	116.48
3	A	404	DDQ	CM1-N1-C1	2.09	114.63	110.23
7	A	432	ORO	N1-C2-N3	-2.06	117.76	121.62
4	A	408[B]	W7A	CAO-CAP-CAQ	-2.05	118.50	121.12
5	A	409	FMN	C6-C5A-C9A	2.02	121.82	119.05

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	DDQ	C2-C1-N1-CM1
3	A	407	DDQ	C2-C1-N1-CM2
6	A	411	GOL	O1-C1-C2-C3
6	A	412	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	415	GOL	O1-C1-C2-O2
6	A	415	GOL	O1-C1-C2-C3
6	A	418	GOL	C1-C2-C3-O3
6	A	419[A]	GOL	O1-C1-C2-C3
6	A	419[B]	GOL	O1-C1-C2-C3
6	A	419[B]	GOL	C1-C2-C3-O3
6	A	420	GOL	O1-C1-C2-C3
6	A	420	GOL	C1-C2-C3-O3
6	A	421	GOL	O1-C1-C2-O2
6	A	421	GOL	O1-C1-C2-C3
6	A	422	GOL	C1-C2-C3-O3
6	A	424	GOL	O1-C1-C2-C3
6	A	424	GOL	C1-C2-C3-O3
6	A	427	GOL	O1-C1-C2-C3
6	A	429	GOL	C1-C2-C3-O3
6	A	429	GOL	O2-C2-C3-O3
6	A	430	GOL	O1-C1-C2-C3
7	A	432	ORO	N1-C6-C7-O71
7	A	432	ORO	C5-C6-C7-O71
7	A	432	ORO	C5-C6-C7-O72
6	A	412	GOL	O2-C2-C3-O3
6	A	430	GOL	O2-C2-C3-O3
3	A	405	DDQ	C4-C5-C6-C7
5	A	409	FMN	O3'-C3'-C4'-C5'
7	A	432	ORO	N1-C6-C7-O72
5	A	409	FMN	O3'-C3'-C4'-O4'
6	A	410	GOL	O1-C1-C2-C3
6	A	411	GOL	C1-C2-C3-O3
6	A	412	GOL	O1-C1-C2-C3
6	A	414	GOL	C1-C2-C3-O3
6	A	419[A]	GOL	C1-C2-C3-O3
6	A	426	GOL	C1-C2-C3-O3
6	A	430	GOL	C1-C2-C3-O3
3	A	407	DDQ	C5-C6-C7-C8
6	A	411	GOL	O1-C1-C2-O2
6	A	418	GOL	O2-C2-C3-O3
6	A	419[A]	GOL	O1-C1-C2-O2
6	A	419[B]	GOL	O1-C1-C2-O2
6	A	419[B]	GOL	O2-C2-C3-O3
6	A	420	GOL	O1-C1-C2-O2
6	A	420	GOL	O2-C2-C3-O3
6	A	422	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	426	GOL	O2-C2-C3-O3
6	A	427	GOL	O1-C1-C2-O2
6	A	430	GOL	O1-C1-C2-O2
3	A	406	DDQ	C3-C4-C5-C6
3	A	403	DDQ	C6-C7-C8-C9
3	A	405	DDQ	C7-C8-C9-C10
3	A	404	DDQ	C6-C7-C8-C9
3	A	404	DDQ	C3-C4-C5-C6
3	A	406	DDQ	C4-C5-C6-C7
3	A	405	DDQ	C6-C7-C8-C9
6	A	411	GOL	O2-C2-C3-O3
6	A	424	GOL	O1-C1-C2-O2
6	A	424	GOL	O2-C2-C3-O3
6	A	429	GOL	O1-C1-C2-O2
4	A	408[B]	W7A	C5-CAL-CAM-CAN
5	A	409	FMN	C2'-C3'-C4'-O4'
3	A	403	DDQ	C4-C5-C6-C7
3	A	406	DDQ	C5-C6-C7-C8
3	A	404	DDQ	C1-C2-C3-C4
6	A	418	GOL	O1-C1-C2-O2
3	A	404	DDQ	C2-C3-C4-C5
4	A	408[A]	W7A	C5-CAL-CAM-CAN
6	A	428	GOL	O1-C1-C2-O2
3	A	406	DDQ	C6-C7-C8-C9
3	A	402	DDQ	C2-C3-C4-C5
3	A	402	DDQ	C2-C1-N1-CM1
3	A	405	DDQ	C2-C1-N1-CM2
3	A	407	DDQ	C2-C1-N1-CM1
3	A	406	DDQ	C1-C2-C3-C4
6	A	410	GOL	O2-C2-C3-O3
3	A	405	DDQ	C2-C1-N1-O1
5	A	409	FMN	C4'-C5'-O5'-P
6	A	414	GOL	O2-C2-C3-O3
3	A	406	DDQ	C7-C8-C9-C10
3	A	402	DDQ	C1-C2-C3-C4
6	A	426	GOL	O1-C1-C2-O2
6	A	429	GOL	O1-C1-C2-C3
6	A	412	GOL	O1-C1-C2-O2
6	A	423	GOL	O1-C1-C2-O2
3	A	402	DDQ	C5-C6-C7-C8
6	A	419[A]	GOL	O2-C2-C3-O3
3	A	404	DDQ	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	402	DDQ	C2-C1-N1-CM2
3	A	403	DDQ	C2-C1-N1-CM1
3	A	403	DDQ	C2-C1-N1-CM2
3	A	406	DDQ	C2-C3-C4-C5
3	A	407	DDQ	C6-C7-C8-C9

There are no ring outliers.

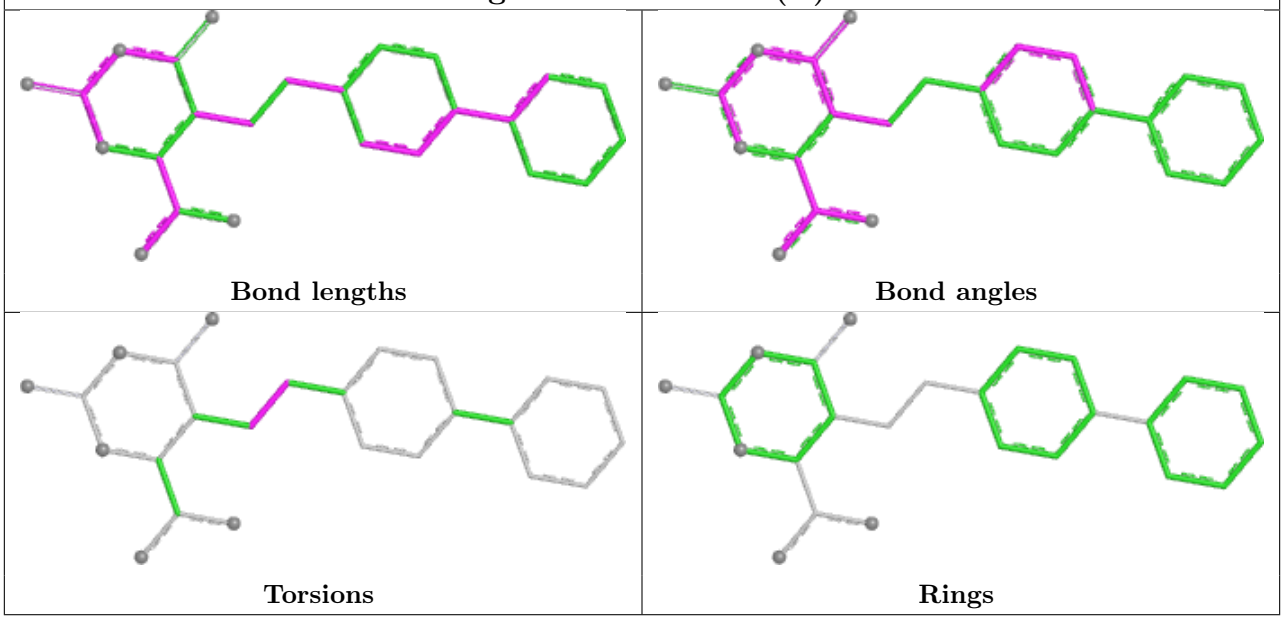
22 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	414	GOL	1	0
4	A	408[B]	W7A	2	0
6	A	427	GOL	1	0
6	A	423	GOL	1	0
4	A	408[A]	W7A	1	0
3	A	406	DDQ	3	0
9	A	439	ACT	1	0
6	A	415	GOL	2	0
6	A	419[B]	GOL	2	0
6	A	417	GOL	1	0
6	A	428	GOL	1	0
6	A	412	GOL	1	0
9	A	442	ACT	1	0
6	A	430	GOL	2	0
6	A	425	GOL	1	0
6	A	413	GOL	2	0
6	A	421	GOL	2	0
8	A	435	SO4	6	0
6	A	420	GOL	2	0
6	A	418	GOL	2	0
9	A	438	ACT	3	0
6	A	431	GOL	4	0

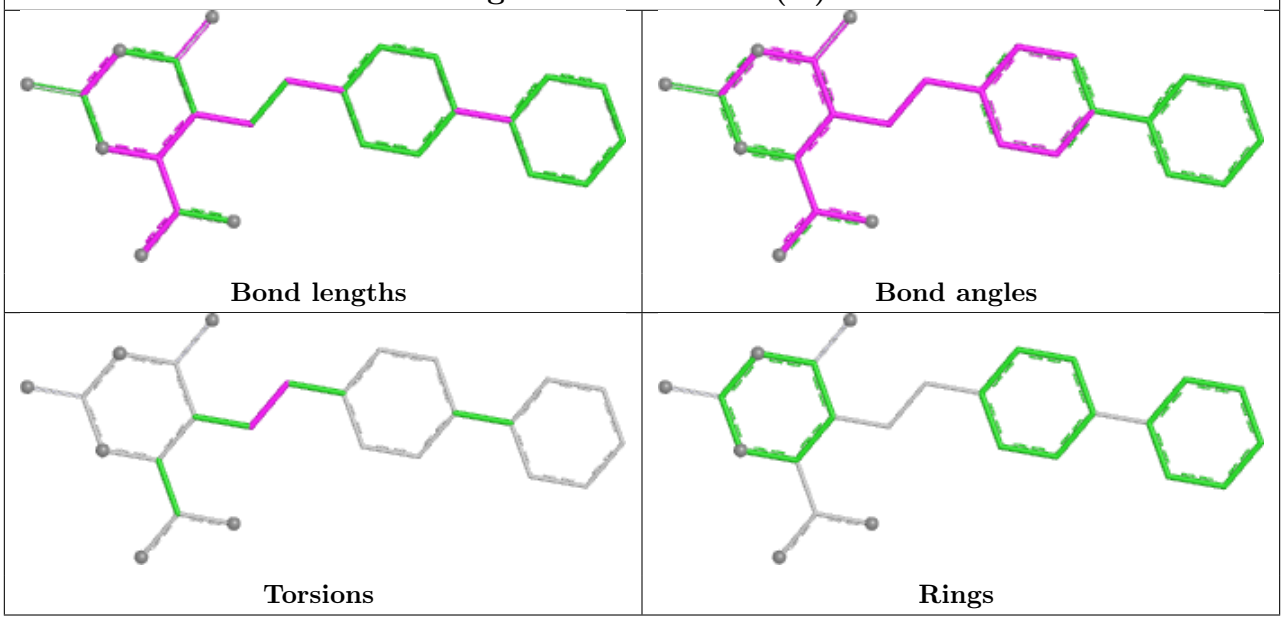
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

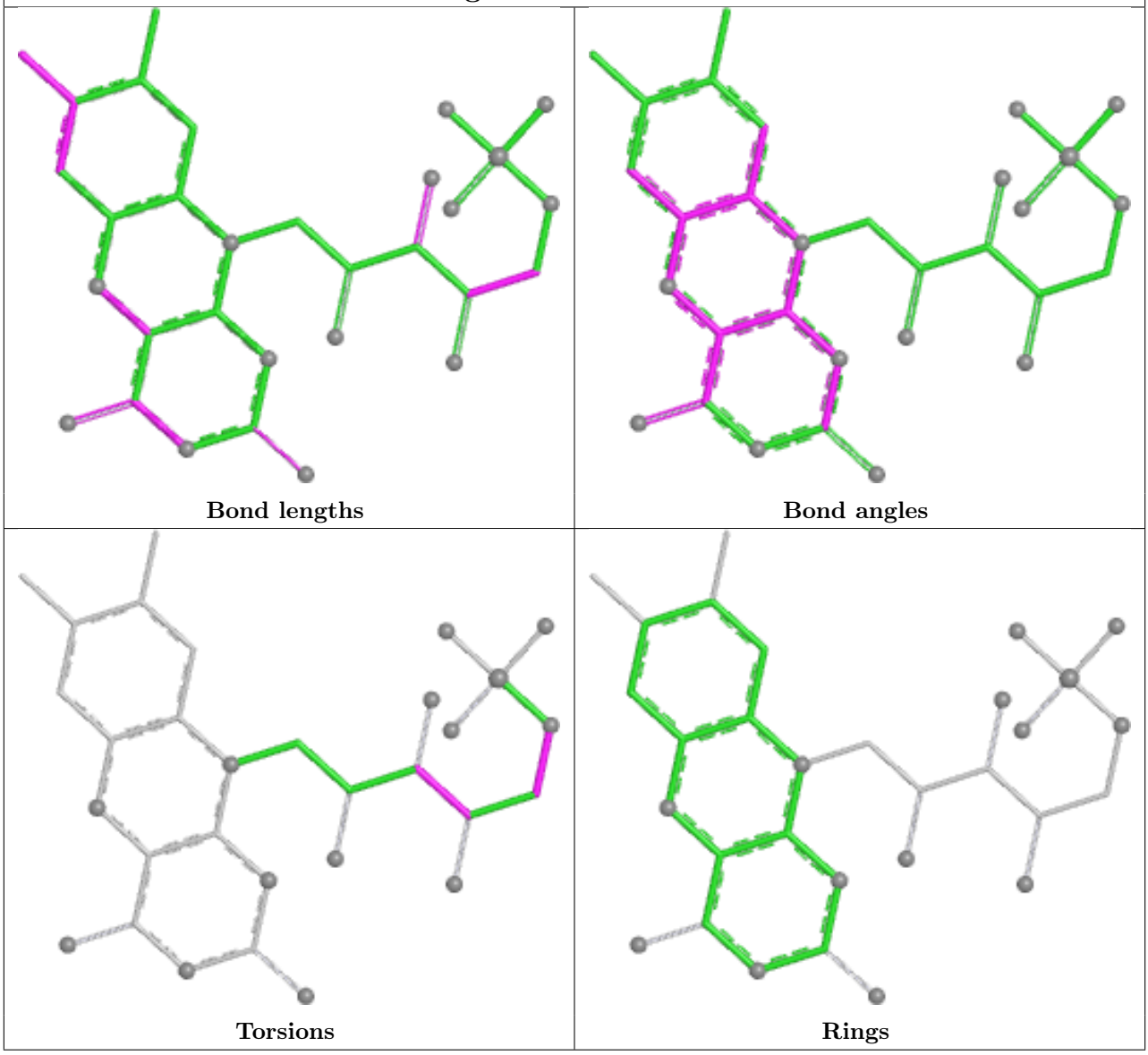
Ligand W7A A 408 (B)



Ligand W7A A 408 (A)



Ligand FMN A 409



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	196:ALA	C	197[A]:GLU	N	1.17

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	367/390 (94%)	-0.10	15 (4%) 37 39	7, 13, 33, 86	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ARG	8.4
1	A	30	MET	6.4
1	A	31	ALA	5.9
1	A	70	ARG	5.7
1	A	73	PHE	4.0
1	A	71	ALA	3.6
1	A	74	GLN	3.6
1	A	189	VAL	2.8
1	A	396[A]	ARG	2.7
1	A	229	GLU	2.6
1	A	227[A]	LYS	2.5
1	A	219	ALA	2.3
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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	DDQ	A	405	14/14	0.51	0.35	59,65,82,86	0
3	DDQ	A	403	14/14	0.56	0.38	62,74,86,95	0
3	DDQ	A	404	14/14	0.64	0.31	75,87,96,96	0
3	DDQ	A	406	14/14	0.65	0.39	45,66,81,82	0
6	GOL	A	412	6/6	0.68	0.15	61,61,68,70	0
6	GOL	A	427	6/6	0.72	0.30	31,37,44,46	0
9	ACT	A	441	4/4	0.72	0.15	56,61,64,65	0
6	GOL	A	419[A]	6/6	0.73	0.26	36,43,44,45	6
6	GOL	A	419[B]	6/6	0.73	0.26	55,57,59,59	6
6	GOL	A	426	6/6	0.74	0.27	33,45,54,57	0
9	ACT	A	443	4/4	0.75	0.43	39,42,43,50	0
3	DDQ	A	407	14/14	0.77	0.17	27,39,72,72	0
9	ACT	A	442	4/4	0.78	0.33	54,55,60,61	0
6	GOL	A	424	6/6	0.79	0.16	46,50,54,58	0
6	GOL	A	410	6/6	0.79	0.17	21,27,29,32	0
9	ACT	A	439	4/4	0.80	0.34	39,42,49,55	0
3	DDQ	A	402	14/14	0.80	0.28	52,59,70,71	0
6	GOL	A	418	6/6	0.81	0.26	33,51,54,59	0
6	GOL	A	422	6/6	0.82	0.17	33,52,57,61	0
6	GOL	A	413	6/6	0.82	0.12	26,42,43,45	0
6	GOL	A	425	6/6	0.82	0.21	26,35,41,42	0
6	GOL	A	430	6/6	0.83	0.37	51,54,58,61	0
6	GOL	A	423	6/6	0.83	0.28	61,68,75,79	0
9	ACT	A	440	4/4	0.83	0.22	41,53,55,57	0
6	GOL	A	421	6/6	0.84	0.19	29,43,50,55	0
6	GOL	A	416	6/6	0.85	0.22	33,42,49,51	0
6	GOL	A	420	6/6	0.86	0.23	33,41,48,51	0
6	GOL	A	429	6/6	0.88	0.21	28,38,52,53	0
6	GOL	A	411	6/6	0.88	0.14	35,43,45,51	0
8	SO4	A	434	5/5	0.88	0.32	50,57,63,68	0
6	GOL	A	415	6/6	0.88	0.15	37,51,59,60	0
6	GOL	A	414	6/6	0.89	0.26	53,56,60,65	0
9	ACT	A	437	4/4	0.90	0.18	33,50,50,58	0
6	GOL	A	428	6/6	0.90	0.12	49,57,58,58	0
6	GOL	A	417	6/6	0.90	0.16	22,40,46,47	0
8	SO4	A	436	5/5	0.91	0.28	48,50,61,61	0
6	GOL	A	431	6/6	0.92	0.13	25,41,50,51	0

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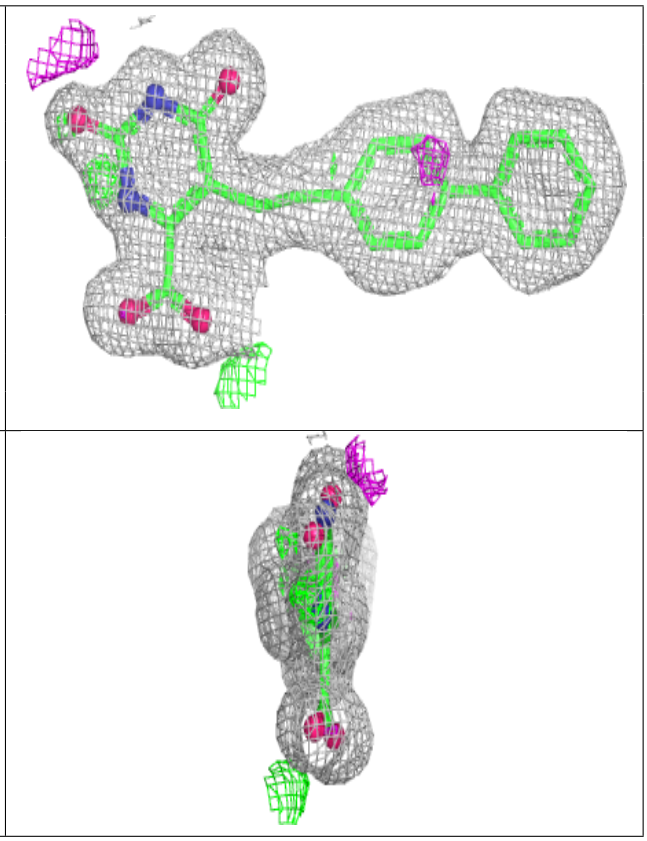
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	W7A	A	408[A]	25/25	0.94	0.09	11,13,20,22	25
4	W7A	A	408[B]	25/25	0.94	0.09	13,16,19,21	25
9	ACT	A	438	4/4	0.94	0.12	20,28,35,35	0
8	SO4	A	435	5/5	0.94	0.48	46,51,68,71	0
7	ORO	A	432	11/11	0.99	0.04	6,7,8,10	0
8	SO4	A	433	5/5	0.99	0.10	23,23,28,32	0
5	FMN	A	409	31/31	0.99	0.09	5,6,8,9	0
2	CL	A	401	1/1	0.99	0.03	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

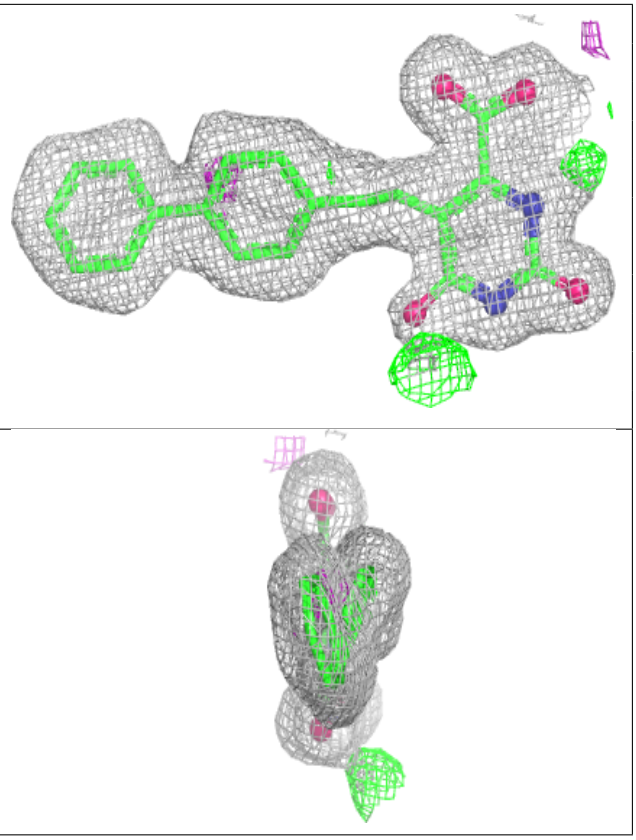
Electron density around W7A A 408 (A):

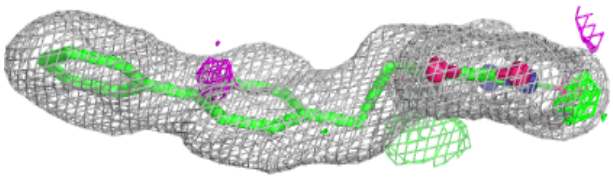
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around W7A A 408 (B):

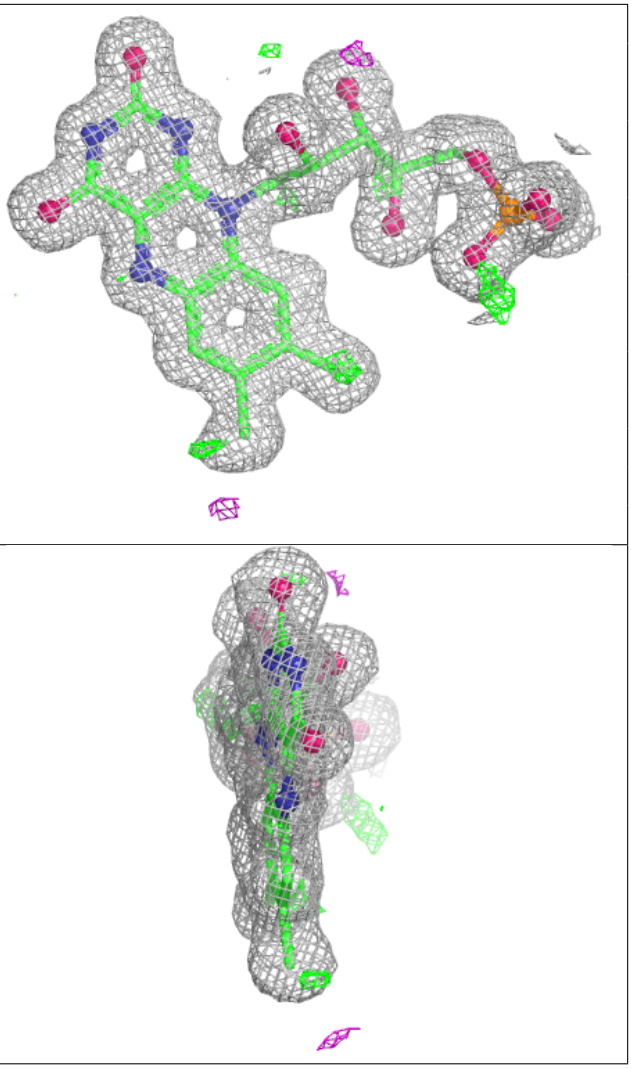
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around FMN A 409:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.