Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2023 – 01:35 AM EDT

PDB ID	:	3W86
Title	:	Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with SH-1-96
Authors	:	Inaoka, D.K.; Hashimoto, S.; Rocha, J.R.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Kuranaga, T.; Shiba, T.; Balogun, E.O.; Sakamoto, K.; Suzuki, S.; Montanari, C.A.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
Deposited on	:	2013-03-12
Resolution	:	1.50 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 ⓘ 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 ⓘ) were used in the production of this report:

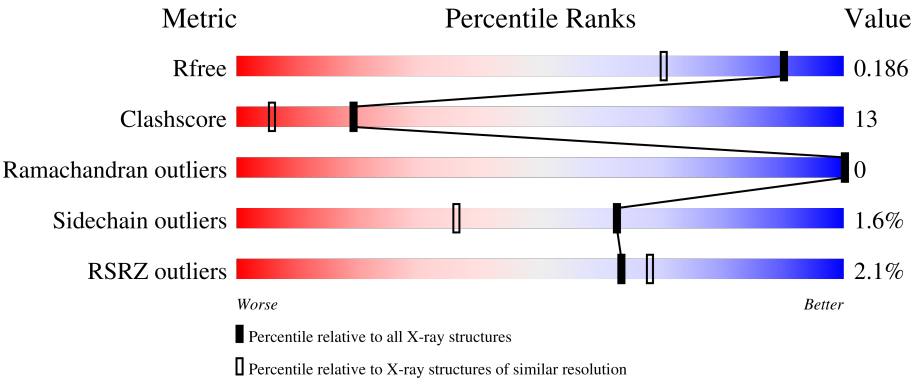
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	313	3% 80% 18%
1	B	313	% 85% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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
2	W86	B	401	-	-	X	-
6	EDO	A	415	-	-	X	-
6	EDO	A	418	-	-	X	-
6	EDO	A	419	-	-	X	-
6	EDO	A	420	-	-	X	-
6	EDO	A	425	-	-	X	-
6	EDO	B	418	-	-	-	X

2 Entry composition

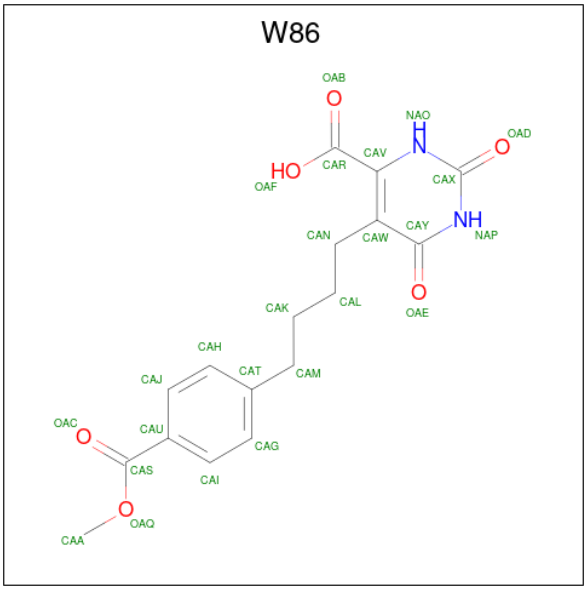
There are 8 unique types of molecules in this entry. The entry contains 6177 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (fumarate).

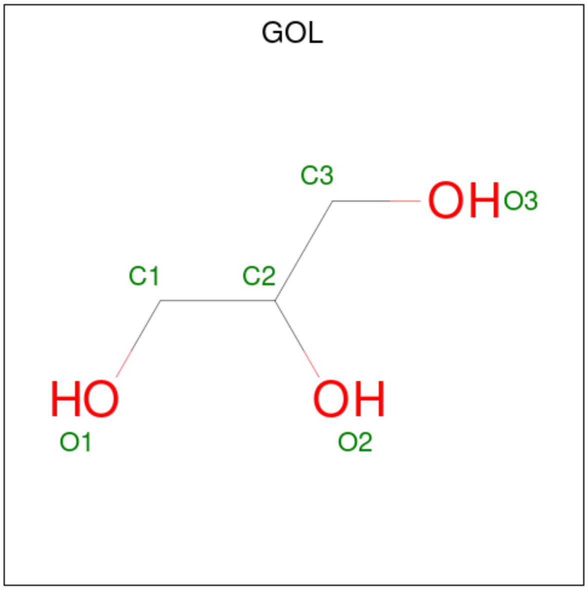
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	13	0
			2502	1598	418	468	18			
1	B	313	Total	C	N	O	S	0	12	0
			2493	1590	417	466	20			

- Molecule 2 is 5-{4-[4-(methoxycarbonyl)phenyl]butyl}-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: W86) (formula: $C_{17}H_{18}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	17	2	6		
2	B	1	Total	C	N	O	0	0
			25	17	2	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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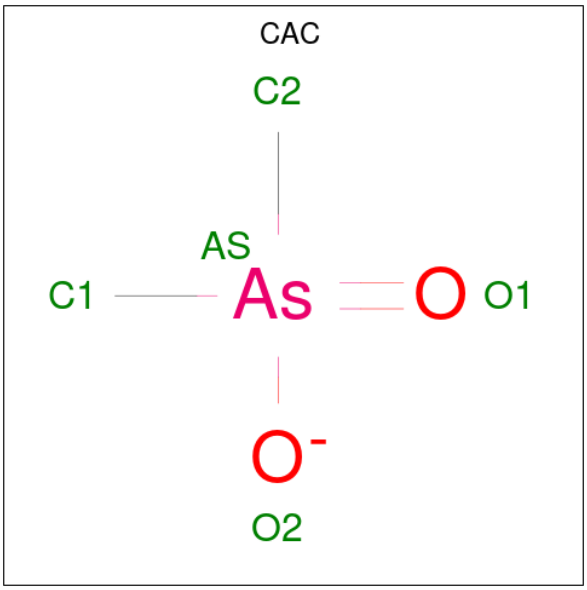
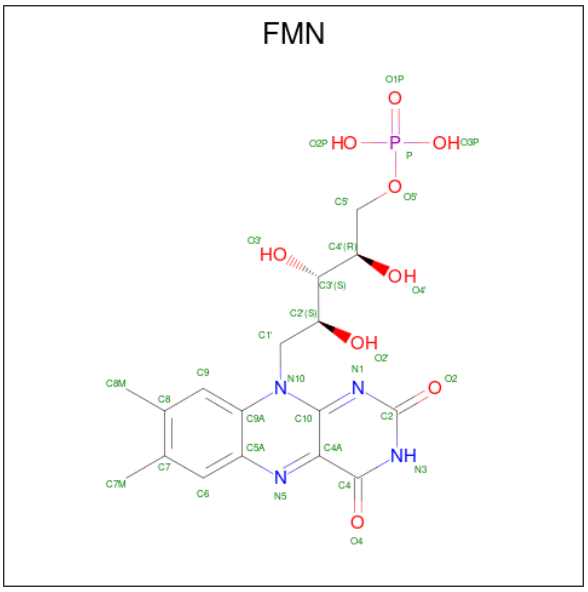
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 12 6 6	0	1
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



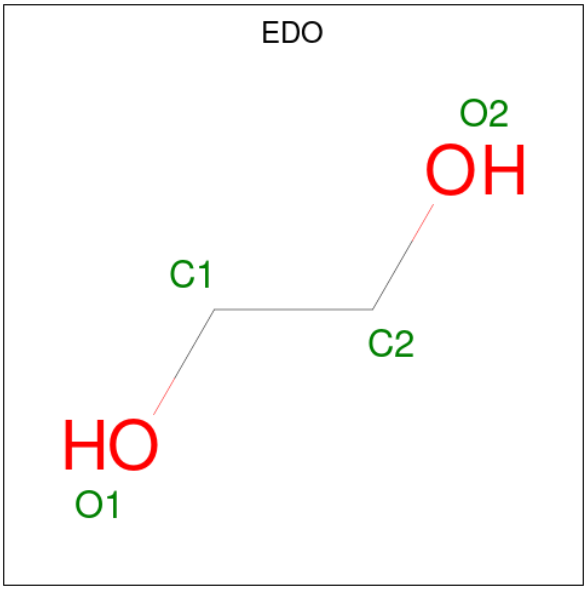
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total As C O 5 1 2 2	0	0
4	A	1	Total As C O 5 1 2 2	0	0

- 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		
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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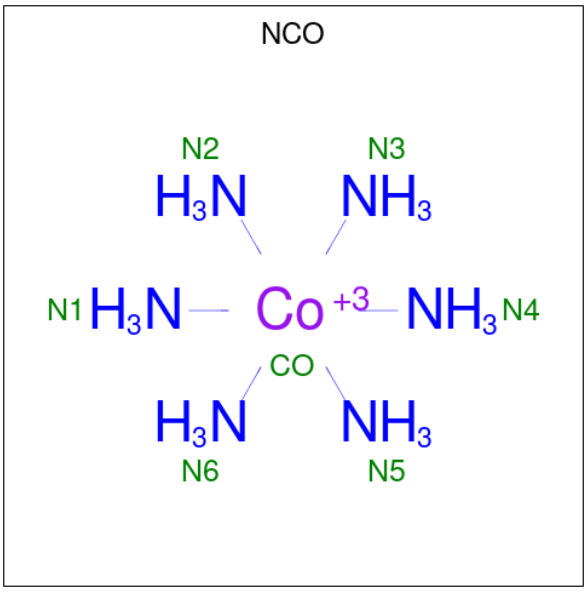
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0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

- Molecule 7 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Co N 7 1 6	0	0
7	A	1	Total Co N 14 2 12	0	1

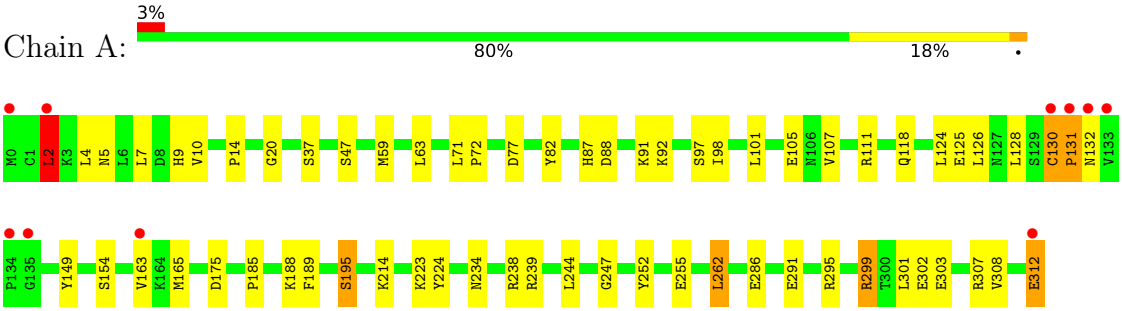
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	366	Total O 376 376	0	9
8	B	445	Total O 453 453	0	8

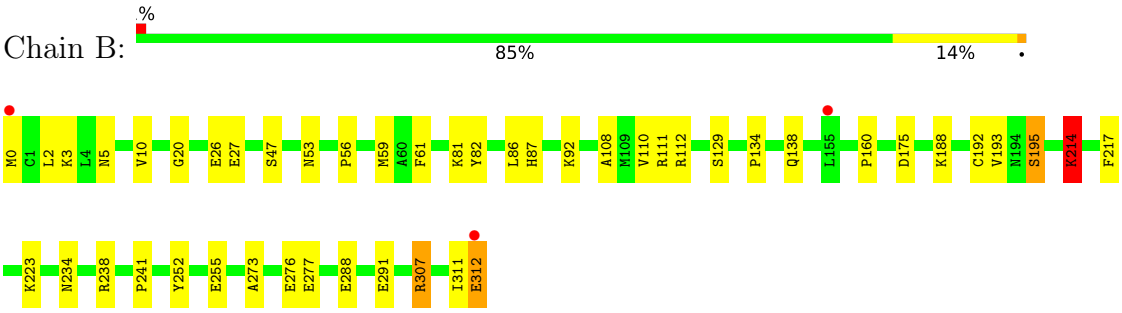
3 Residue-property plots (i)

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 (fumarate)



• Molecule 1: Dihydroorotate dehydrogenase (fumarate)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.89Å 71.51Å 129.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.64 – 1.50 31.64 – 1.50	Depositor EDS
% Data completeness (in resolution range)	87.2 (31.64-1.50) 87.3 (31.64-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.94 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.143 , 0.184 0.146 , 0.186	Depositor DCC
R_{free} test set	4454 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6177	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W86, FMN, GOL, NCO, CAC, EDO

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	1.23	5/2555 (0.2%)	1.17	10/3458 (0.3%)
1	B	1.31	12/2545 (0.5%)	1.09	7/3442 (0.2%)
All	All	1.27	17/5100 (0.3%)	1.13	17/6900 (0.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLU	CD-OE1	-8.16	1.16	1.25
1	B	3	LYS	CE-NZ	7.24	1.67	1.49
1	B	27	GLU	CD-OE1	-6.79	1.18	1.25
1	B	56	PRO	N-CD	6.72	1.57	1.47
1	A	247	GLY	C-O	-6.51	1.13	1.23
1	B	288	GLU	CD-OE1	-6.33	1.18	1.25
1	A	14	PRO	N-CD	5.87	1.56	1.47
1	B	195	SER	CB-OG	-5.72	1.34	1.42
1	B	288	GLU	CD-OE2	-5.65	1.19	1.25
1	B	110	VAL	C-N	-5.40	1.21	1.34
1	A	224	TYR	CE1-CZ	-5.37	1.31	1.38
1	B	291	GLU	CD-OE1	5.29	1.31	1.25
1	B	2	LEU	C-O	-5.23	1.13	1.23
1	A	131	PRO	N-CD	5.22	1.55	1.47
1	A	195	SER	CB-OG	-5.18	1.35	1.42
1	B	26	GLU	CD-OE2	-5.15	1.20	1.25
1	B	134	PRO	N-CD	5.11	1.55	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3	LYS	CD-CE-NZ	11.62	138.41	111.70
1	A	2	LEU	CB-CG-CD1	-11.59	91.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	LEU	O-C-N	-8.17	109.62	122.70
1	A	262	LEU	CB-CG-CD1	8.13	124.83	111.00
1	A	4	LEU	C-N-CA	6.85	138.82	121.70
1	A	175	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	299	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	252	TYR	CB-CG-CD2	5.71	124.43	121.00
1	A	88	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	239	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	77	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	112	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	307	ARG	CG-CD-NE	-5.28	100.72	111.80
1	B	214[A]	LYS	CD-CE-NZ	5.11	123.44	111.70
1	B	214[B]	LYS	CD-CE-NZ	5.11	123.44	111.70
1	B	214[C]	LYS	CD-CE-NZ	5.11	123.44	111.70
1	B	175	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2502	0	2488	72	0
1	B	2493	0	2489	40	0
2	A	25	0	17	7	0
2	B	25	0	17	13	0
3	A	54	0	72	1	0
3	B	72	0	96	8	0
4	A	10	0	0	1	0
5	A	31	0	19	1	0
5	B	31	0	19	1	0
6	A	56	0	84	29	0
6	B	28	0	42	11	0
7	A	21	0	0	0	0
8	A	376	0	0	15	0
8	B	453	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6177	0	5343	138	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 (138) 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:B:214[C]:LYS:HE2	2:B:401:W86:H16	1.21	1.13
1:B:214[C]:LYS:HE2	2:B:401:W86:CAA	1.79	1.12
2:A:401:W86:H15	2:A:401:W86:H17	1.40	1.01
1:A:128:LEU:CD1	1:A:163[B]:VAL:HG21	1.94	0.97
1:B:214[C]:LYS:CE	2:B:401:W86:CAA	2.47	0.92
1:B:277:GLU:HB2	6:B:416:EDO:H12	1.52	0.91
2:B:401:W86:H13	2:B:401:W86:H17	1.53	0.89
1:A:128:LEU:HD11	1:A:163[B]:VAL:HG21	1.55	0.87
6:B:419:EDO:C1	8:B:584:HOH:O	2.22	0.86
6:B:419:EDO:H12	8:B:584:HOH:O	1.78	0.83
2:B:401:W86:CAA	2:B:401:W86:H13	2.06	0.83
1:A:37:SER:O	6:A:419:EDO:H11	1.79	0.83
1:A:128:LEU:CD1	1:A:163[B]:VAL:CG2	2.58	0.81
1:B:214[C]:LYS:CE	2:B:401:W86:H18	2.11	0.79
1:B:214[C]:LYS:CE	2:B:401:W86:H16	2.05	0.79
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.32	0.78
1:B:59:MET:CE	8:B:602:HOH:O	2.31	0.78
1:A:299:ARG:HE	6:A:418:EDO:C1	2.00	0.74
1:B:111[B]:ARG:NH2	6:B:413:EDO:O1	2.21	0.73
1:A:128:LEU:HD12	1:A:163[B]:VAL:HG21	1.71	0.72
1:A:5[A]:ASN:ND2	1:A:10:VAL:HG22	2.05	0.72
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.38	0.71
1:B:129:SER:HB3	8:B:684:HOH:O	1.91	0.70
1:A:214[B]:LYS:NZ	8:A:690:HOH:O	2.24	0.69
1:A:303:GLU:OE2	6:A:418:EDO:H21	1.93	0.69
1:B:195:SER:HB3	8:B:685:HOH:O	1.92	0.68
1:B:214[C]:LYS:HE3	2:B:401:W86:H18	1.75	0.68
1:A:128:LEU:HD12	1:A:163[A]:VAL:CG1	2.24	0.67
2:A:401:W86:H15	2:A:401:W86:CAA	2.20	0.67
1:B:129:SER:HA	1:B:138:GLN:NE2	2.11	0.66
1:A:299:ARG:HE	6:A:418:EDO:H11	1.62	0.65
1:A:5[A]:ASN:HD21	1:A:10:VAL:HG22	1.61	0.64
1:A:308:VAL:O	6:A:413:EDO:C2	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.81	0.64
6:B:414:EDO:H11	8:B:537:HOH:O	1.97	0.64
1:A:128:LEU:HG	1:A:163[B]:VAL:HG23	1.79	0.63
1:A:91:LYS:O	6:A:419:EDO:H22	1.98	0.63
2:A:401:W86:H15	8:A:699:HOH:O	2.00	0.62
1:A:128:LEU:HD12	1:A:163[B]:VAL:CG2	2.29	0.62
6:A:424:EDO:H12	8:A:786:HOH:O	1.98	0.61
1:A:299:ARG:HH21	6:A:418:EDO:C2	2.13	0.61
1:A:128:LEU:CD1	1:A:163[A]:VAL:CG1	2.78	0.61
1:B:108:ALA:HB2	6:B:413:EDO:H22	1.83	0.61
1:A:154:SER:O	6:A:425:EDO:H21	2.01	0.61
1:B:214[B]:LYS:NZ	8:B:689[B]:HOH:O	2.34	0.60
1:B:307:ARG:NH2	8:B:852:HOH:O	2.33	0.60
1:A:59:MET:HE3	8:A:761:HOH:O	2.01	0.60
2:B:401:W86:CAA	2:B:401:W86:CAJ	2.80	0.60
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.83	0.60
1:A:128:LEU:HD12	1:A:163[A]:VAL:HG11	1.82	0.60
8:A:822:HOH:O	6:B:417:EDO:H21	2.00	0.60
2:B:401:W86:H13	8:B:688:HOH:O	2.02	0.60
1:B:312:GLU:N	1:B:312:GLU:OE2	2.36	0.59
4:A:410:CAC:C1	8:A:820:HOH:O	2.51	0.59
1:A:63:LEU:HD11	6:B:417:EDO:H22	1.85	0.59
3:B:411:GOL:C3	8:B:707:HOH:O	2.51	0.58
1:B:276:GLU:HB2	6:B:416:EDO:H22	1.86	0.58
1:A:302:GLU:OE1	6:A:422:EDO:O1	2.22	0.57
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG11	2.35	0.57
6:A:421:EDO:H12	8:B:900:HOH:O	2.04	0.57
1:A:291:GLU:OE2	1:A:295:ARG:NH1	2.37	0.57
1:B:59:MET:HE3	8:B:602:HOH:O	2.01	0.57
1:B:241:PRO:HA	3:B:410[B]:GOL:H31	1.86	0.56
1:A:87:HIS:HE1	1:A:92:LYS:O	1.87	0.56
1:A:299:ARG:NH2	6:A:418:EDO:O2	2.38	0.55
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG13	2.37	0.55
1:A:128:LEU:HG	1:A:163[B]:VAL:CG2	2.37	0.55
6:A:415:EDO:C2	6:A:425:EDO:H11	2.37	0.55
1:A:255:GLU:OE2	6:A:420:EDO:H21	2.06	0.54
1:A:195:SER:HB3	8:A:835:HOH:O	2.06	0.54
1:A:101:LEU:N	1:A:105:GLU:OE1	2.40	0.54
1:B:129:SER:CB	8:B:684:HOH:O	2.53	0.54
2:A:401:W86:H17	2:A:401:W86:CAI	2.26	0.53
2:A:401:W86:CAI	8:A:699:HOH:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:HH21	6:A:420:EDO:C1	2.22	0.53
1:A:185:PRO:HG2	6:A:415:EDO:H11	1.92	0.52
1:B:241:PRO:HA	3:B:410[A]:GOL:H31	1.92	0.52
1:A:2:LEU:HB2	1:A:286[A]:GLU:OE1	2.10	0.51
1:B:87:HIS:HE1	1:B:92:LYS:O	1.93	0.51
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.04	0.51
1:A:307:ARG:HH22	6:A:422:EDO:C2	2.24	0.50
1:A:149[A]:TYR:HE1	8:A:704:HOH:O	1.95	0.50
6:A:415:EDO:O1	6:A:425:EDO:C1	2.60	0.50
1:A:130:CYS:SG	1:A:131:PRO:HD2	2.52	0.49
1:A:223:LYS:HD3	6:A:421:EDO:H21	1.94	0.49
6:A:415:EDO:H21	6:A:425:EDO:H11	1.94	0.49
1:A:308:VAL:O	6:A:413:EDO:H21	2.12	0.49
1:A:188:LYS:HD2	8:A:791:HOH:O	2.13	0.49
1:A:163[A]:VAL:HG12	1:A:165:MET:SD	2.53	0.49
1:A:9:HIS:HE1	8:A:527:HOH:O	1.96	0.48
1:A:185:PRO:HG2	6:A:415:EDO:C1	2.42	0.48
1:A:132:ASN:HB2	8:A:595:HOH:O	2.13	0.48
1:A:312:GLU:N	1:A:312:GLU:CD	2.67	0.48
1:B:129:SER:HA	1:B:138:GLN:HE21	1.78	0.48
1:A:111[B]:ARG:NH1	8:A:793:HOH:O	2.28	0.48
6:A:416:EDO:H21	8:A:539:HOH:O	2.13	0.48
1:A:98[A]:ILE:HG13	1:A:126:LEU:HD12	1.94	0.47
1:B:5[B]:ASN:ND2	1:B:10:VAL:HG22	2.30	0.47
1:B:160:PRO:HB3	1:B:188:LYS:HG3	1.97	0.47
1:A:37:SER:O	6:A:419:EDO:C1	2.56	0.47
1:B:47[B]:SER:O	6:B:414:EDO:H12	2.16	0.46
1:A:128:LEU:CG	1:A:163[B]:VAL:CG2	2.93	0.46
1:B:61:PHE:CE1	3:B:405:GOL:H32	2.51	0.46
1:B:20:GLY:HA3	5:B:412:FMN:N5	2.31	0.46
1:A:98[A]:ILE:HG12	1:A:124:LEU:HD11	1.98	0.45
1:B:223:LYS:HG2	1:B:252:TYR:CE1	2.51	0.45
1:A:303:GLU:OE2	6:A:418:EDO:C2	2.62	0.45
1:A:20:GLY:HA3	5:A:412:FMN:N5	2.32	0.45
1:A:128:LEU:HG	1:A:163[A]:VAL:HG13	1.97	0.45
1:A:91:LYS:O	6:A:419:EDO:C2	2.64	0.45
1:B:81[B]:LYS:HE2	1:B:86:LEU:HD11	1.98	0.44
1:B:217:PHE:CE1	3:B:402:GOL:H31	2.52	0.44
1:A:2:LEU:HD11	1:A:301:LEU:HD21	1.99	0.44
1:A:255:GLU:OE2	6:A:420:EDO:C2	2.66	0.44
1:A:128:LEU:HD11	1:A:163[B]:VAL:CG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:411:GOL:H31	8:B:707:HOH:O	2.13	0.44
1:A:214[B]:LYS:HD2	2:A:401:W86:CAA	2.48	0.44
1:B:273:ALA:HB1	6:B:416:EDO:H11	2.01	0.43
3:B:411:GOL:O3	3:B:411:GOL:O1	2.37	0.43
1:A:312:GLU:OE2	1:A:312:GLU:CA	2.66	0.43
1:B:214[C]:LYS:HE3	2:B:401:W86:CAA	2.36	0.43
1:A:97:SER:HA	1:A:125:GLU:O	2.20	0.42
1:A:163[A]:VAL:CG1	1:A:165:MET:SD	3.07	0.42
1:A:295:ARG:NH2	6:A:420:EDO:H22	2.34	0.42
2:A:401:W86:CAA	2:A:401:W86:CAI	2.89	0.42
1:B:53:ASN:HD21	2:B:401:W86:CAA	2.33	0.42
1:B:241:PRO:HA	3:B:410[B]:GOL:C3	2.49	0.42
1:B:311:ILE:O	1:B:312:GLU:HB2	2.20	0.42
3:A:404:GOL:O3	8:A:523[B]:HOH:O	2.22	0.41
2:B:401:W86:CAJ	8:B:688:HOH:O	2.63	0.41
1:A:7:LEU:O	1:A:9:HIS:HD2	2.04	0.41
1:A:47:SER:HB3	6:A:426:EDO:H12	2.02	0.41
1:A:312:GLU:N	1:A:312:GLU:OE2	2.53	0.41
1:B:192:CYS:HA	1:B:193:VAL:HA	1.91	0.41
1:A:189:PHE:HA	1:A:244:LEU:O	2.21	0.41
1:A:71:LEU:N	1:A:72:PRO:CD	2.84	0.41
1:A:107:VAL:O	1:A:111[B]:ARG:HG3	2.20	0.41
1:B:312:GLU:OE2	1:B:312:GLU:CA	2.68	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	324/313 (104%)	315 (97%)	9 (3%)	0	100	100
1	B	323/313 (103%)	312 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	647/626 (103%)	627 (97%)	20 (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	271/258 (105%)	266 (98%)	5 (2%)	59 30
1	B	271/258 (105%)	265 (98%)	6 (2%)	52 22
All	All	542/516 (105%)	531 (98%)	11 (2%)	62 25

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	118	GLN
1	A	130	CYS
1	A	262	LEU
1	A	312	GLU
1	B	0[A]	MET
1	B	0[B]	MET
1	B	214[A]	LYS
1	B	214[B]	LYS
1	B	214[C]	LYS
1	B	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	87	HIS
1	A	138	GLN
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	234	ASN
1	A	275	GLN
1	B	87	HIS
1	B	118	GLN
1	B	138	GLN
1	B	234	ASN

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)

51 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	$\#\|Z\| > 2$
6	EDO	B	418	-	3,3,3	0.58	0	2,2,2	0.31	0
2	W86	B	401	-	25,26,26	1.66	7 (28%)	32,35,35	2.05	6 (18%)
6	EDO	A	418	-	3,3,3	0.44	0	2,2,2	0.52	0
6	EDO	A	422	-	3,3,3	0.35	0	2,2,2	0.68	0
2	W86	A	401	-	25,26,26	1.87	6 (24%)	32,35,35	1.75	6 (18%)
7	NCO	A	428[A]	-	6,6,6	1.01	0	-		
7	NCO	A	427	-	6,6,6	1.76	2 (33%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	424	-	3,3,3	0.55	0	2,2,2	0.96	0
3	GOL	A	402[B]	-	5,5,5	0.91	0	5,5,5	0.79	0
3	GOL	B	403	-	5,5,5	0.88	0	5,5,5	1.32	0
6	EDO	B	413	-	3,3,3	0.53	0	2,2,2	0.16	0
6	EDO	B	415	-	3,3,3	0.33	0	2,2,2	1.25	0
6	EDO	A	414	-	3,3,3	0.47	0	2,2,2	0.19	0
3	GOL	B	410[B]	-	5,5,5	0.46	0	5,5,5	0.56	0
5	FMN	B	412	-	33,33,33	1.09	2 (6%)	48,50,50	1.19	5 (10%)
6	EDO	A	417	-	3,3,3	0.48	0	2,2,2	0.71	0
3	GOL	B	407	-	5,5,5	0.77	0	5,5,5	1.27	0
3	GOL	B	404[B]	-	5,5,5	0.36	0	5,5,5	0.81	0
3	GOL	B	409	-	5,5,5	0.26	0	5,5,5	0.54	0
4	CAC	A	411	-	0,4,4	-	-	0,6,6	-	-
6	EDO	A	419	-	3,3,3	0.33	0	2,2,2	0.64	0
6	EDO	A	425	-	3,3,3	0.37	0	2,2,2	0.22	0
6	EDO	B	414	-	3,3,3	1.58	0	2,2,2	1.10	0
6	EDO	A	423	-	3,3,3	0.92	0	2,2,2	0.37	0
3	GOL	A	408	-	5,5,5	0.52	0	5,5,5	1.07	0
4	CAC	A	410	-	0,4,4	-	-	0,6,6	-	-
7	NCO	A	428[B]	-	6,6,6	1.01	0	-		
6	EDO	B	417	-	3,3,3	0.69	0	2,2,2	0.74	0
3	GOL	B	405	-	5,5,5	1.18	1 (20%)	5,5,5	1.17	0
3	GOL	A	407	-	5,5,5	0.61	0	5,5,5	0.48	0
3	GOL	A	406	-	5,5,5	0.28	0	5,5,5	0.52	0
6	EDO	A	416	-	3,3,3	0.71	0	2,2,2	1.13	0
6	EDO	B	416	-	3,3,3	0.59	0	2,2,2	0.33	0
6	EDO	A	415	-	3,3,3	0.42	0	2,2,2	0.76	0
3	GOL	A	403	-	5,5,5	0.78	0	5,5,5	0.77	0
3	GOL	A	405	-	5,5,5	0.63	0	5,5,5	0.84	0
3	GOL	A	409	-	5,5,5	0.44	0	5,5,5	0.39	0
3	GOL	B	408	-	5,5,5	1.21	1 (20%)	5,5,5	1.67	1 (20%)
6	EDO	B	419	-	3,3,3	0.57	0	2,2,2	0.53	0
3	GOL	B	411	-	5,5,5	0.56	0	5,5,5	0.67	0
6	EDO	A	421	-	3,3,3	0.80	0	2,2,2	0.46	0
3	GOL	B	406	-	5,5,5	0.89	0	5,5,5	1.12	1 (20%)
3	GOL	A	402[A]	-	5,5,5	0.94	0	5,5,5	0.70	0
3	GOL	A	404	-	5,5,5	0.88	0	5,5,5	1.86	1 (20%)
5	FMN	A	412	-	33,33,33	1.36	2 (6%)	48,50,50	1.31	8 (16%)
3	GOL	B	410[A]	-	5,5,5	0.33	0	5,5,5	0.94	0
6	EDO	A	413	-	3,3,3	0.74	0	2,2,2	1.44	0
3	GOL	B	404[A]	-	5,5,5	0.35	0	5,5,5	0.58	0
6	EDO	A	420	-	3,3,3	0.32	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	426	-	3,3,3	0.62	0	2,2,2	0.26	0
3	GOL	B	402	-	5,5,5	0.56	0	5,5,5	0.93	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	EDO	B	418	-	-	0/1/1/1	-
2	W86	B	401	-	-	4/17/17/17	0/2/2/2
6	EDO	A	418	-	-	1/1/1/1	-
6	EDO	A	422	-	-	1/1/1/1	-
2	W86	A	401	-	-	3/17/17/17	0/2/2/2
6	EDO	A	424	-	-	1/1/1/1	-
3	GOL	A	402[B]	-	-	0/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
6	EDO	B	413	-	-	1/1/1/1	-
6	EDO	B	415	-	-	0/1/1/1	-
6	EDO	A	414	-	-	1/1/1/1	-
3	GOL	B	410[B]	-	-	2/4/4/4	-
5	FMN	B	412	-	-	1/18/18/18	0/3/3/3
6	EDO	A	417	-	-	0/1/1/1	-
3	GOL	B	407	-	-	0/4/4/4	-
3	GOL	B	404[B]	-	-	4/4/4/4	-
3	GOL	B	409	-	-	2/4/4/4	-
6	EDO	A	419	-	-	1/1/1/1	-
6	EDO	A	425	-	-	1/1/1/1	-
6	EDO	B	414	-	-	1/1/1/1	-
6	EDO	A	423	-	-	1/1/1/1	-
3	GOL	A	408	-	-	2/4/4/4	-
6	EDO	B	417	-	-	1/1/1/1	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	A	407	-	-	0/4/4/4	-
3	GOL	A	406	-	-	4/4/4/4	-
6	EDO	A	416	-	-	1/1/1/1	-
6	EDO	B	416	-	-	0/1/1/1	-
6	EDO	A	415	-	-	0/1/1/1	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	405	-	-	0/4/4/4	-
3	GOL	A	409	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	408	-	-	2/4/4/4	-
6	EDO	B	419	-	-	1/1/1/1	-
3	GOL	B	411	-	-	0/4/4/4	-
6	EDO	A	421	-	-	1/1/1/1	-
3	GOL	B	406	-	-	2/4/4/4	-
3	GOL	A	402[A]	-	-	0/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
5	FMN	A	412	-	-	1/18/18/18	0/3/3/3
3	GOL	B	410[A]	-	-	2/4/4/4	-
6	EDO	A	413	-	-	1/1/1/1	-
3	GOL	B	404[A]	-	-	2/4/4/4	-
6	EDO	A	420	-	-	0/1/1/1	-
6	EDO	A	426	-	-	1/1/1/1	-
3	GOL	B	402	-	-	0/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	412	FMN	C1'-C2'	-4.23	1.46	1.52
2	A	401	W86	OAQ-CAS	4.18	1.42	1.33
2	A	401	W86	CAM-CAT	-4.17	1.39	1.51
2	B	401	W86	OAQ-CAS	3.90	1.42	1.33
5	A	412	FMN	C4-N3	-3.72	1.31	1.38
2	A	401	W86	CAU-CAS	-3.59	1.41	1.50
2	B	401	W86	CAI-CAG	2.92	1.44	1.38
5	B	412	FMN	C4-N3	-2.73	1.33	1.38
2	B	401	W86	CAY-NAP	2.71	1.43	1.38
2	A	401	W86	CAV-CAR	-2.66	1.44	1.48
5	B	412	FMN	O4-C4	2.54	1.28	1.23
2	B	401	W86	CAV-NAO	2.48	1.43	1.38
2	B	401	W86	CAJ-CAH	2.44	1.43	1.38
7	A	427	NCO	CO-N5	2.40	2.05	1.96
2	B	401	W86	CAG-CAT	2.40	1.44	1.38
2	B	401	W86	CAU-CAS	-2.33	1.44	1.50
3	B	408	GOL	O1-C1	2.26	1.51	1.42
2	A	401	W86	OAQ-CAA	-2.24	1.40	1.45
2	A	401	W86	OAF-CAR	-2.09	1.24	1.30
7	A	427	NCO	CO-N3	2.09	2.04	1.96
3	B	405	GOL	O2-C2	-2.01	1.37	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	W86	CAA-OAQ-CAS	7.94	131.13	115.83
2	A	401	W86	OAQ-CAS-CAU	5.41	120.55	112.34
2	B	401	W86	OAQ-CAS-CAU	4.33	118.90	112.34
2	A	401	W86	CAA-OAQ-CAS	4.18	123.90	115.83
2	B	401	W86	CAJ-CAH-CAT	3.68	126.09	121.03
2	A	401	W86	CAR-CAV-CAW	3.56	126.11	122.74
3	A	404	GOL	O3-C3-C2	3.31	126.06	110.20
3	B	408	GOL	O2-C2-C1	3.25	123.45	109.12
5	A	412	FMN	O4-C4-C4A	-3.05	118.50	126.60
5	B	412	FMN	C4-C4A-N5	2.96	122.45	118.23
2	B	401	W86	OAQ-CAS-OAC	-2.94	117.70	123.45
2	A	401	W86	CAY-NAP-CAX	-2.80	122.31	126.34
5	B	412	FMN	C4A-C10-N10	2.74	120.48	116.48
5	A	412	FMN	C6-C5A-C9A	-2.65	115.19	118.94
5	A	412	FMN	O2-C2-N1	-2.63	117.48	121.83
5	B	412	FMN	O4-C4-C4A	-2.58	119.76	126.60
5	A	412	FMN	C6-C5A-N5	2.54	122.96	118.51
2	A	401	W86	CAW-CAY-NAP	2.54	117.58	115.69
2	B	401	W86	CAG-CAT-CAH	-2.46	114.30	118.17
5	A	412	FMN	N3-C2-N1	2.46	124.20	119.38
5	A	412	FMN	O4-C4-N3	2.34	124.61	120.12
5	A	412	FMN	C7M-C7-C6	2.29	123.73	119.49
5	A	412	FMN	C4-C4A-N5	2.26	121.45	118.23
2	B	401	W86	CAN-CAW-CAV	2.23	123.94	119.57
5	B	412	FMN	O2-C2-N1	-2.21	118.17	121.83
3	B	406	GOL	O1-C1-C2	2.11	120.31	110.20
2	A	401	W86	NAP-CAX-NAO	2.07	119.12	115.80
5	B	412	FMN	C10-C4A-N5	-2.06	120.48	124.86

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	W86	OAF-CAR-CAV-NAO
2	A	401	W86	CAU-CAS-OAQ-CAA
2	A	401	W86	OAC-CAS-OAQ-CAA
2	B	401	W86	OAF-CAR-CAV-NAO
3	A	404	GOL	C1-C2-C3-O3
3	A	406	GOL	O1-C1-C2-C3
3	A	408	GOL	O1-C1-C2-C3
3	A	409	GOL	O1-C1-C2-C3
3	A	409	GOL	C1-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	404[A]	GOL	O1-C1-C2-C3
3	B	404[B]	GOL	C1-C2-C3-O3
3	B	404[B]	GOL	O2-C2-C3-O3
3	B	406	GOL	C1-C2-C3-O3
3	B	408	GOL	C1-C2-C3-O3
3	B	410[A]	GOL	C1-C2-C3-O3
3	B	410[B]	GOL	O1-C1-C2-O2
3	B	410[B]	GOL	O1-C1-C2-C3
2	B	401	W86	OAC-CAS-OAQ-CAA
2	B	401	W86	CAU-CAS-OAQ-CAA
3	A	406	GOL	C1-C2-C3-O3
3	B	403	GOL	O1-C1-C2-C3
3	A	406	GOL	O1-C1-C2-O2
3	A	408	GOL	O1-C1-C2-O2
3	A	409	GOL	O1-C1-C2-O2
3	A	409	GOL	O2-C2-C3-O3
3	B	404[A]	GOL	O1-C1-C2-O2
3	B	408	GOL	O2-C2-C3-O3
3	B	410[A]	GOL	O2-C2-C3-O3
6	A	416	EDO	O1-C1-C2-O2
6	B	414	EDO	O1-C1-C2-O2
6	B	417	EDO	O1-C1-C2-O2
3	B	409	GOL	O1-C1-C2-O2
6	A	414	EDO	O1-C1-C2-O2
6	B	419	EDO	O1-C1-C2-O2
3	B	406	GOL	O2-C2-C3-O3
5	A	412	FMN	C4'-C5'-O5'-P
5	B	412	FMN	C4'-C5'-O5'-P
6	A	418	EDO	O1-C1-C2-O2
6	A	419	EDO	O1-C1-C2-O2
6	A	423	EDO	O1-C1-C2-O2
3	B	403	GOL	O2-C2-C3-O3
3	B	404[B]	GOL	O1-C1-C2-O2
3	B	409	GOL	O1-C1-C2-C3
6	A	413	EDO	O1-C1-C2-O2
6	A	422	EDO	O1-C1-C2-O2
6	A	424	EDO	O1-C1-C2-O2
6	A	426	EDO	O1-C1-C2-O2
3	A	404	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
6	B	413	EDO	O1-C1-C2-O2
3	B	404[B]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	406	GOL	O2-C2-C3-O3
2	B	401	W86	OAB-CAR-CAV-NAO
6	A	421	EDO	O1-C1-C2-O2
6	A	425	EDO	O1-C1-C2-O2

There are no ring outliers.

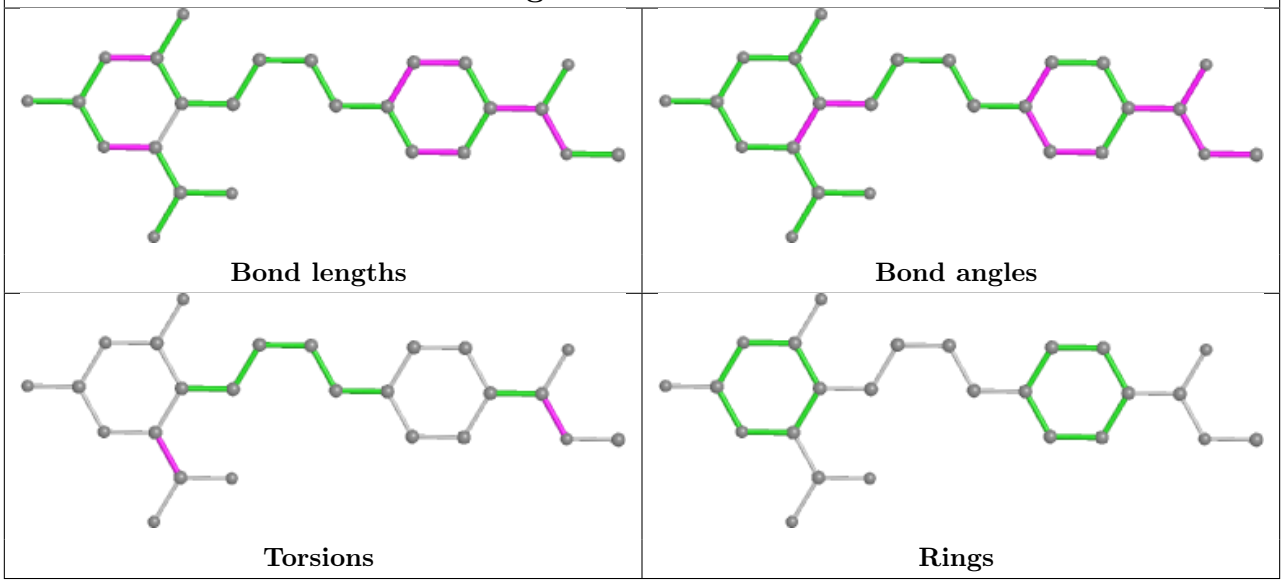
27 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	W86	13	0
6	A	418	EDO	6	0
6	A	422	EDO	2	0
2	A	401	W86	7	0
6	A	424	EDO	1	0
6	B	413	EDO	2	0
3	B	410[B]	GOL	2	0
5	B	412	FMN	1	0
6	A	419	EDO	4	0
6	A	425	EDO	4	0
6	B	414	EDO	2	0
4	A	410	CAC	1	0
6	B	417	EDO	2	0
3	B	405	GOL	1	0
6	A	416	EDO	1	0
6	B	416	EDO	3	0
6	A	415	EDO	5	0
6	B	419	EDO	2	0
3	B	411	GOL	3	0
6	A	421	EDO	2	0
3	A	404	GOL	1	0
5	A	412	FMN	1	0
3	B	410[A]	GOL	1	0
6	A	413	EDO	2	0
6	A	420	EDO	4	0
6	A	426	EDO	1	0
3	B	402	GOL	1	0

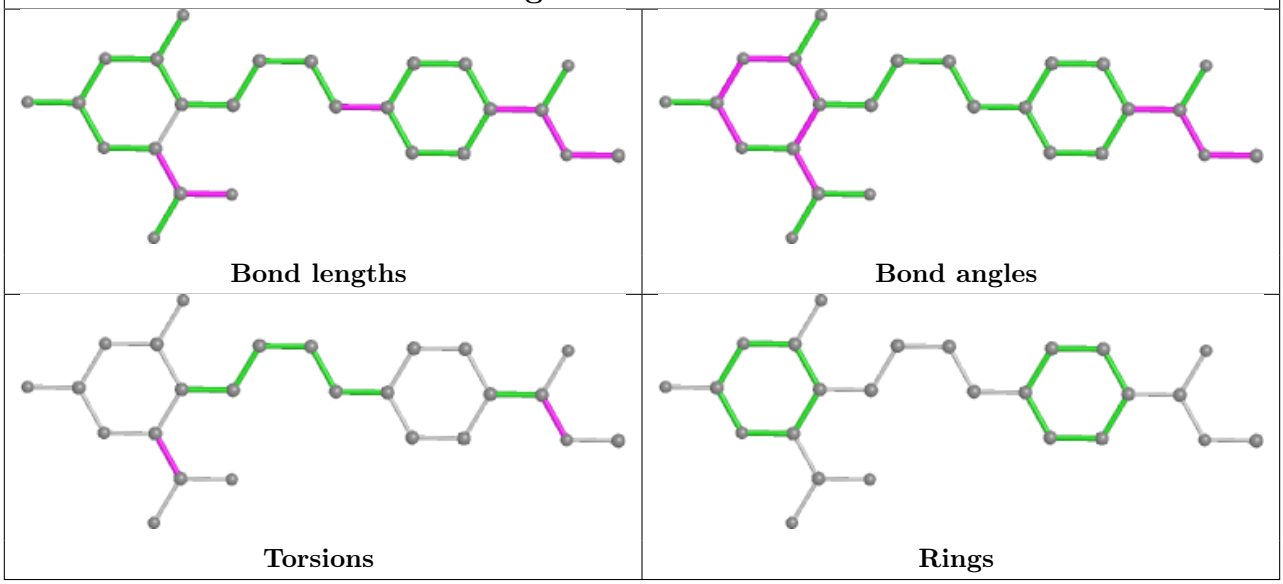
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

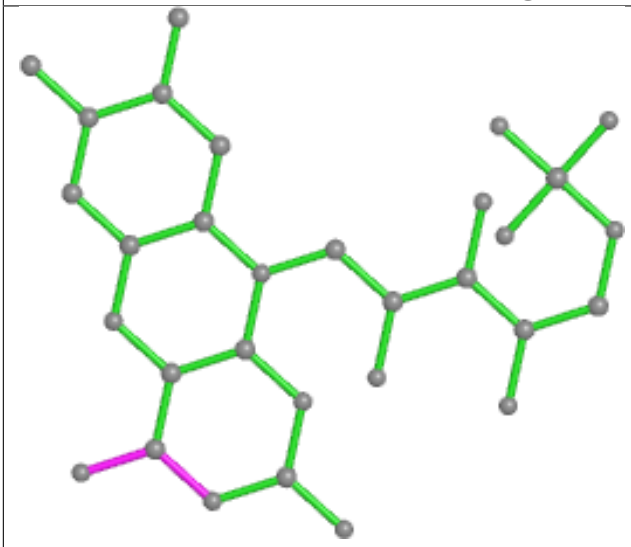
Ligand W86 B 401



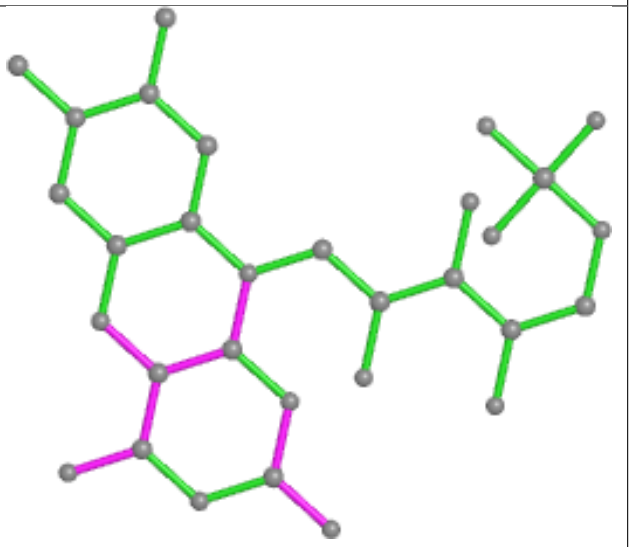
Ligand W86 A 401



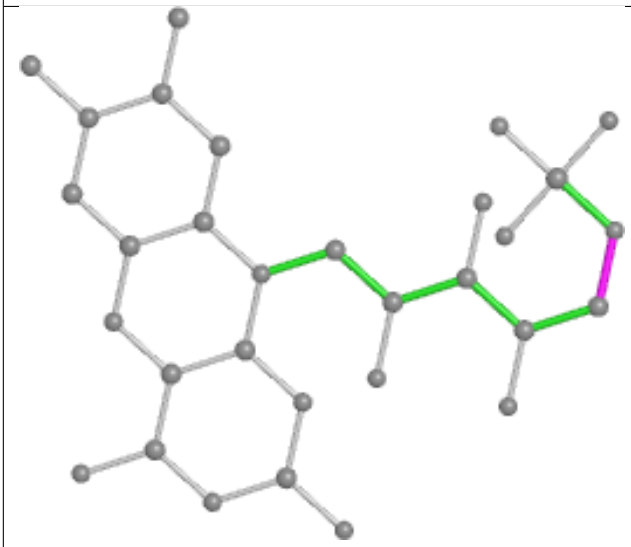
Ligand FMN B 412



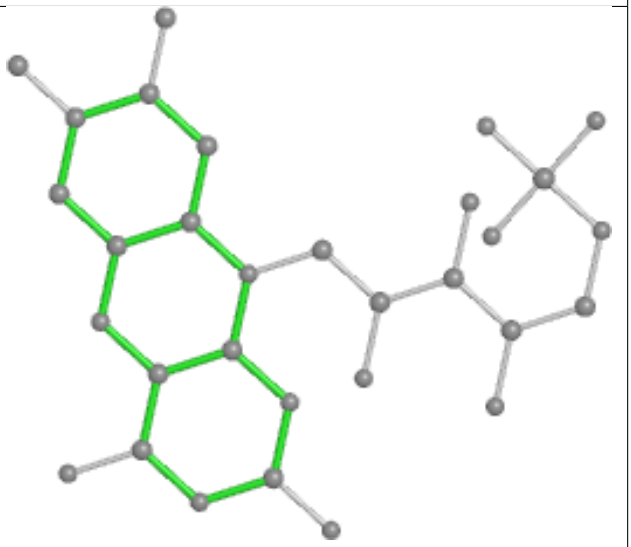
Bond lengths



Bond angles

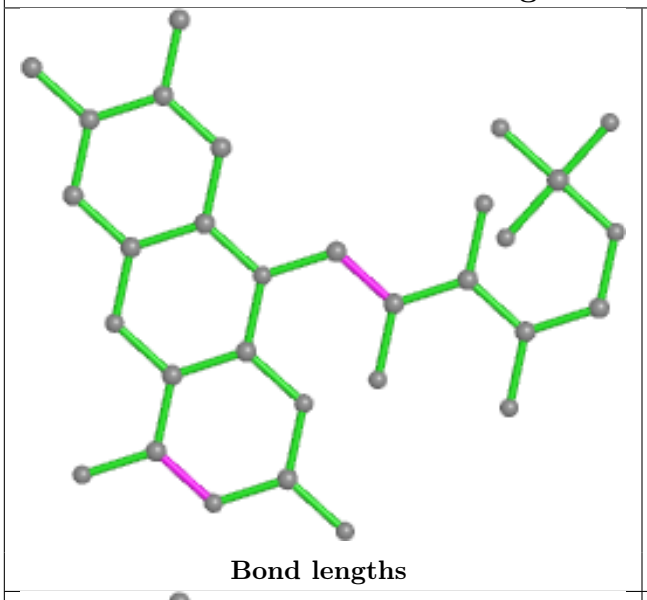


Torsions

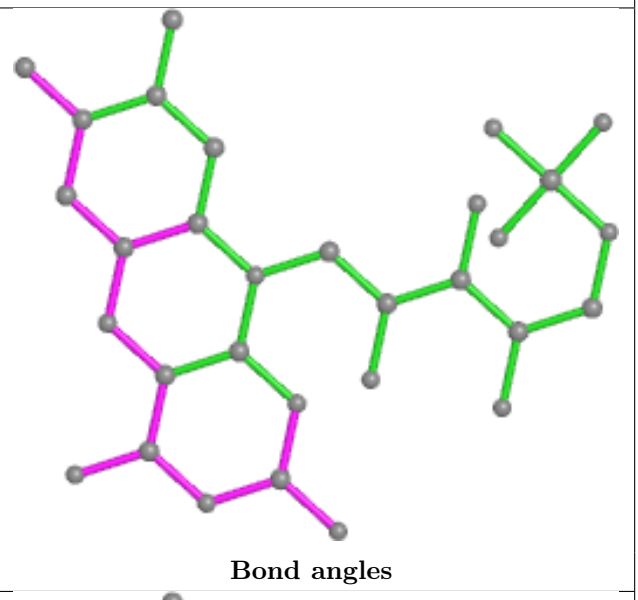


Rings

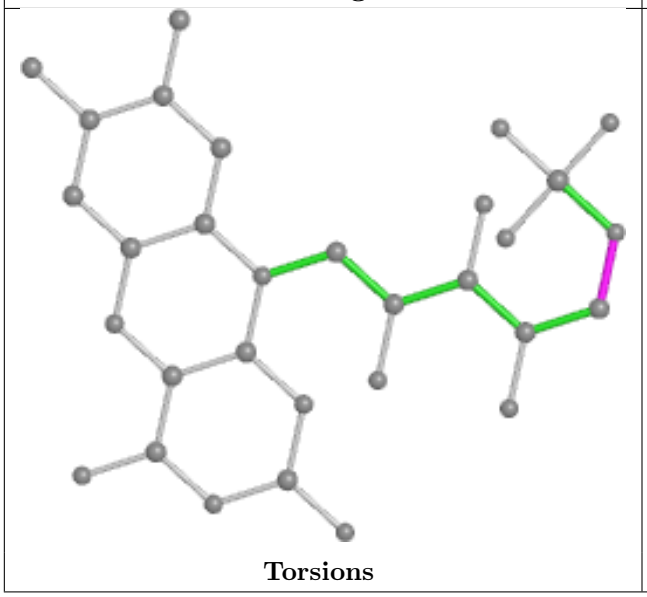
Ligand FMN A 412



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	313/313 (100%)	0.04	10 (3%) 47 52	8, 13, 29, 47	0
1	B	313/313 (100%)	-0.11	3 (0%) 82 85	9, 13, 23, 42	0
All	All	626/626 (100%)	-0.04	13 (2%) 63 68	8, 13, 26, 47	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	5.2
1	A	134	PRO	5.0
1	A	133	VAL	4.7
1	B	312	GLU	3.9
1	A	312	GLU	3.9
1	A	130	CYS	3.8
1	A	132	ASN	3.7
1	A	135	GLY	3.5
1	A	0	MET	3.2
1	A	2	LEU	3.1
1	A	163[A]	VAL	2.4
1	B	0[A]	MET	2.2
1	B	155	LEU	2.2

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

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

6.3 Carbohydrates

There are no 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, 95^{th} 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
6	EDO	A	426	4/4	0.65	0.24	48,49,52,53	0
6	EDO	A	423	4/4	0.66	0.36	43,43,44,44	0
6	EDO	A	421	4/4	0.66	0.40	35,38,39,39	0
3	GOL	B	403	6/6	0.69	0.20	27,30,34,35	0
6	EDO	B	418	4/4	0.71	0.41	45,46,46,51	0
6	EDO	B	414	4/4	0.72	0.24	30,31,33,41	0
3	GOL	B	408	6/6	0.74	0.27	28,37,38,39	0
3	GOL	B	410[B]	6/6	0.75	0.20	28,35,37,42	6
3	GOL	A	409	6/6	0.75	0.33	40,47,54,66	0
3	GOL	B	410[A]	6/6	0.75	0.20	33,38,39,43	6
3	GOL	B	406	6/6	0.76	0.15	31,35,42,44	0
6	EDO	A	418	4/4	0.77	0.23	41,43,45,50	0
3	GOL	A	407	6/6	0.78	0.23	36,37,45,51	0
3	GOL	A	406	6/6	0.80	0.25	36,48,51,52	0
6	EDO	B	415	4/4	0.81	0.14	33,37,38,40	0
6	EDO	A	422	4/4	0.81	0.31	49,51,52,53	0
3	GOL	B	411	6/6	0.82	0.43	26,34,39,41	0
3	GOL	B	404[B]	6/6	0.83	0.21	29,30,33,33	6
3	GOL	B	404[A]	6/6	0.83	0.21	38,42,44,47	6
6	EDO	A	413	4/4	0.84	0.21	27,35,36,40	0
6	EDO	A	414	4/4	0.84	0.23	49,54,56,57	0
6	EDO	B	419	4/4	0.85	0.31	34,35,36,38	0
3	GOL	B	402	6/6	0.86	0.14	25,28,31,34	0
6	EDO	A	425	4/4	0.87	0.34	34,35,36,37	0
3	GOL	A	404	6/6	0.87	0.15	25,31,40,42	0
6	EDO	A	420	4/4	0.88	0.19	32,33,38,40	0
6	EDO	A	417	4/4	0.88	0.15	34,34,39,42	0
3	GOL	A	405	6/6	0.89	0.15	25,31,32,33	0
3	GOL	A	408	6/6	0.89	0.21	32,35,37,48	0
6	EDO	A	416	4/4	0.90	0.27	29,34,36,39	0
6	EDO	A	419	4/4	0.90	0.23	30,30,32,35	0
3	GOL	B	407	6/6	0.90	0.18	20,22,25,26	0
6	EDO	A	415	4/4	0.91	0.33	30,31,33,36	0
6	EDO	B	417	4/4	0.91	0.28	32,35,38,39	0
3	GOL	B	409	6/6	0.91	0.16	34,45,47,47	0
3	GOL	B	405	6/6	0.91	0.14	26,29,30,30	0
6	EDO	B	416	4/4	0.92	0.20	24,24,24,27	0

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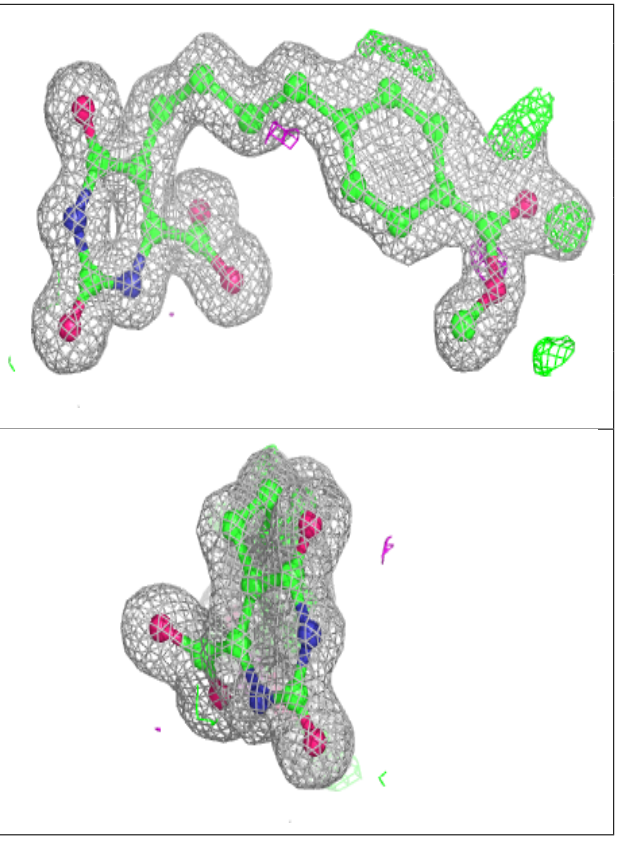
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	W86	B	401	25/25	0.93	0.10	10,12,25,29	0
6	EDO	A	424	4/4	0.93	0.18	20,32,34,36	0
2	W86	A	401	25/25	0.94	0.11	10,13,36,43	0
4	CAC	A	410	5/5	0.95	0.24	17,20,22,26	0
4	CAC	A	411	5/5	0.95	0.35	30,37,41,41	0
6	EDO	B	413	4/4	0.95	0.18	30,30,31,32	0
7	NCO	A	428[A]	7/7	0.95	0.17	20,21,23,23	7
7	NCO	A	428[B]	7/7	0.95	0.17	20,20,22,23	7
3	GOL	A	403	6/6	0.96	0.07	19,22,22,25	0
3	GOL	A	402[A]	6/6	0.97	0.09	11,13,14,14	6
3	GOL	A	402[B]	6/6	0.97	0.09	15,16,18,18	6
5	FMN	B	412	31/31	0.98	0.08	8,9,10,10	0
5	FMN	A	412	31/31	0.98	0.07	8,9,11,11	0
7	NCO	A	427	7/7	0.99	0.09	11,11,14,15	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.

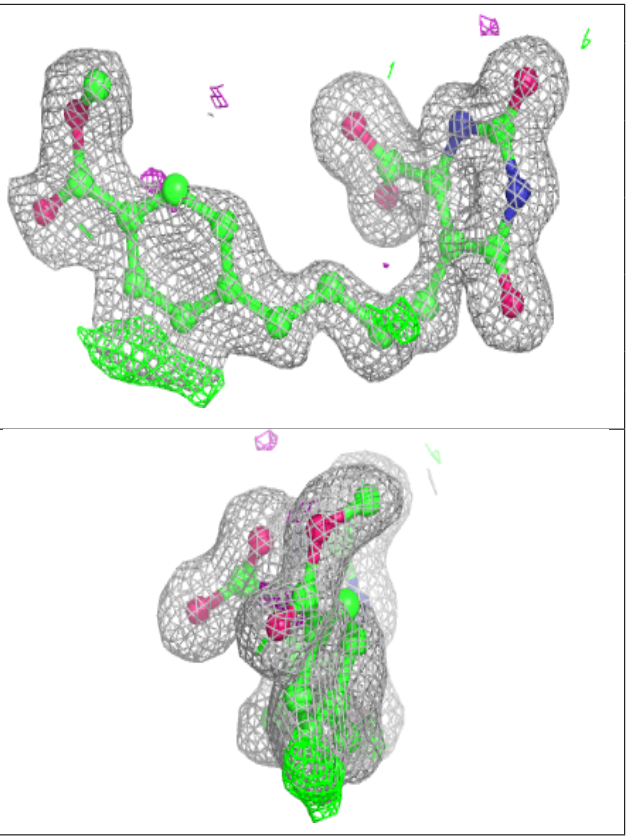
Electron density around W86 B 401:

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



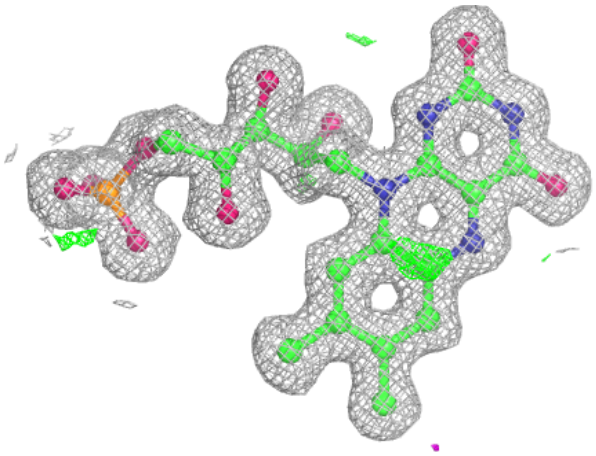
Electron density around W86 A 401:

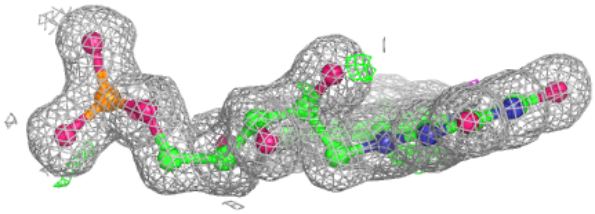
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

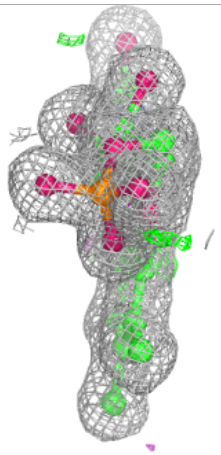


Electron density around FMN B 412:

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

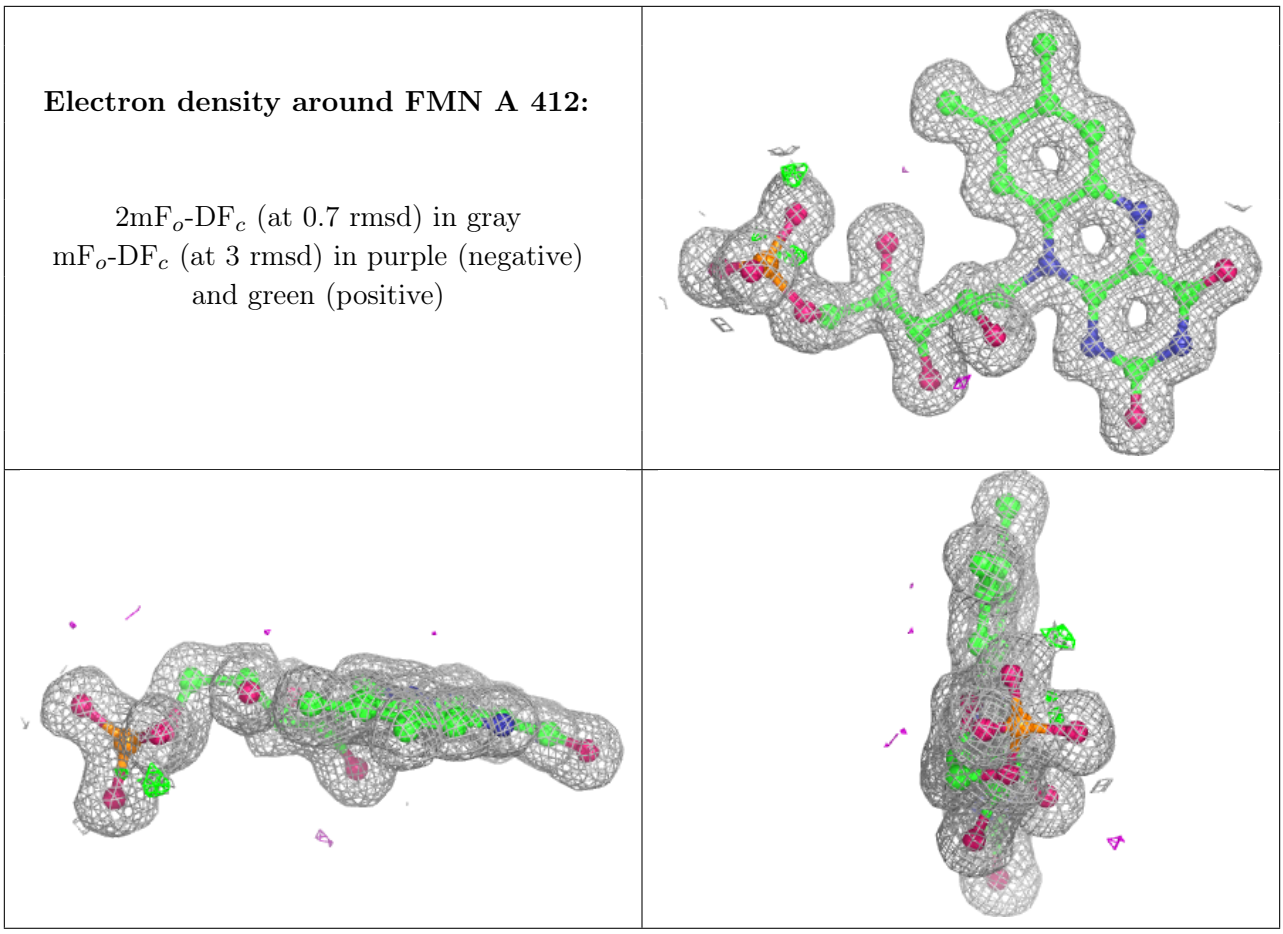






Electron density around FMN A 412:

$2mF_o$-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

There are no such residues in this entry.