



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:28 PM BST

PDB ID : 3W87  
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with SH-1-103  
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 : 1.43 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

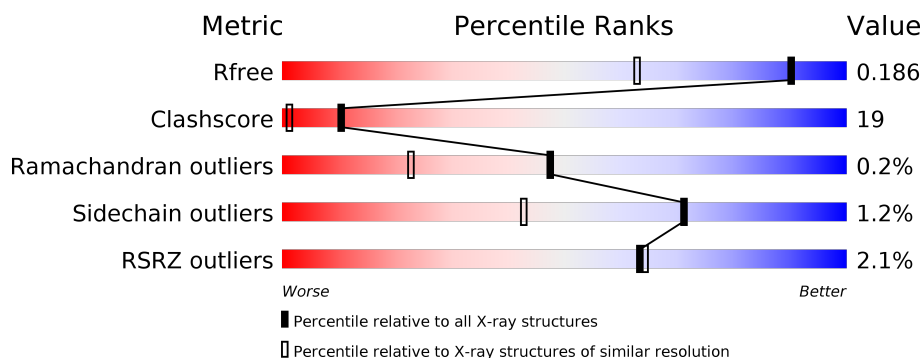
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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 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  $\leq 5\%$ . 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	314	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	314	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>

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	EDO	A	423	-	-	X	-
6	EDO	A	424	-	-	X	-
6	EDO	A	427	-	-	-	X
6	EDO	A	428	-	-	X	-
6	EDO	A	431	-	X	X	-
6	EDO	B	417	-	-	X	-
6	EDO	B	419	-	-	X	-
6	EDO	B	420	-	-	X	-
6	EDO	B	422	-	-	X	-
6	EDO	B	425	-	X	X	-
7	PEG	A	432	-	-	X	-
7	PEG	A	433	-	X	X	-
7	PEG	B	427	-	-	X	-



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.

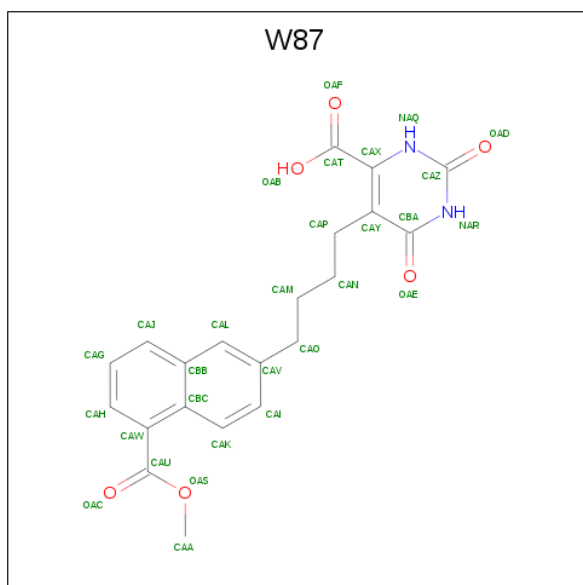
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (fumarate).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	18	0
			2540	1618	425	478	19			
1	B	314	Total	C	N	O	S	0	15	0
			2522	1603	423	477	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q4D3W2
B	-1	SER	-	EXPRESSION TAG	UNP Q4D3W2

- Molecule 2 is 5-{4-[5-(methoxycarbonyl)naphthalen-2-yl]butyl}-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: W87) (formula: C<sub>21</sub>H<sub>20</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	21	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			58	42	4	12		

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



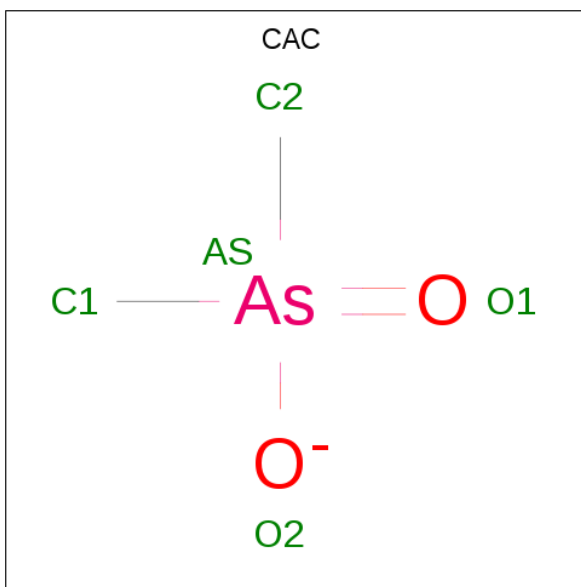
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

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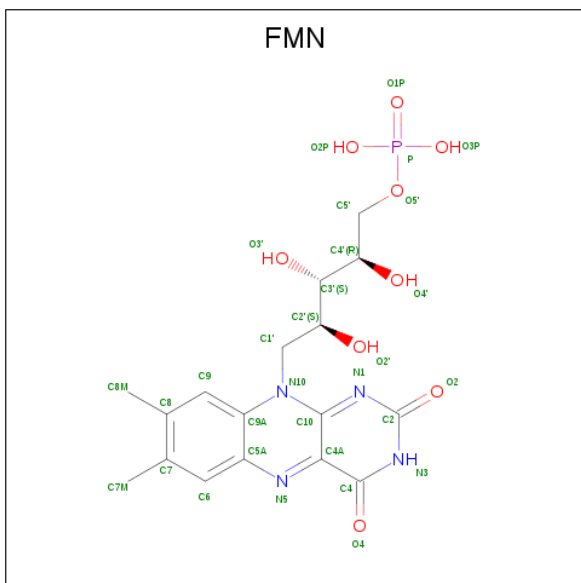
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



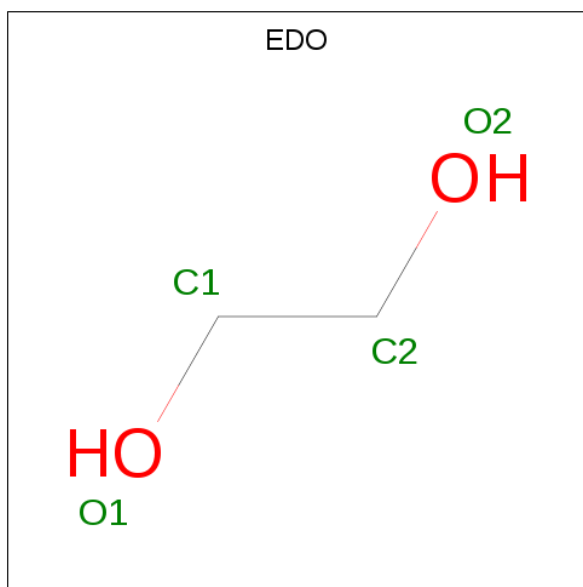
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

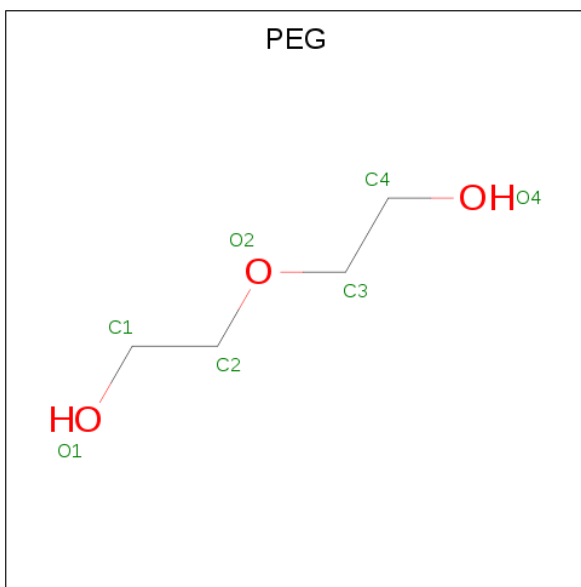
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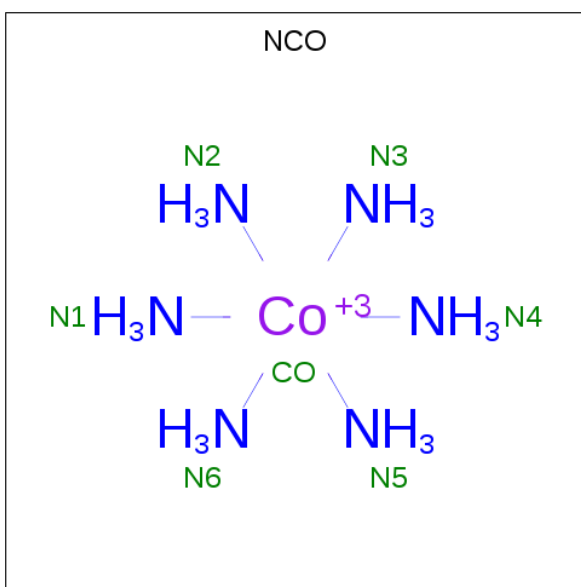
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula:  $\text{CoH}_{18}\text{N}_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Co	N	0	0
			7	1	6		

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

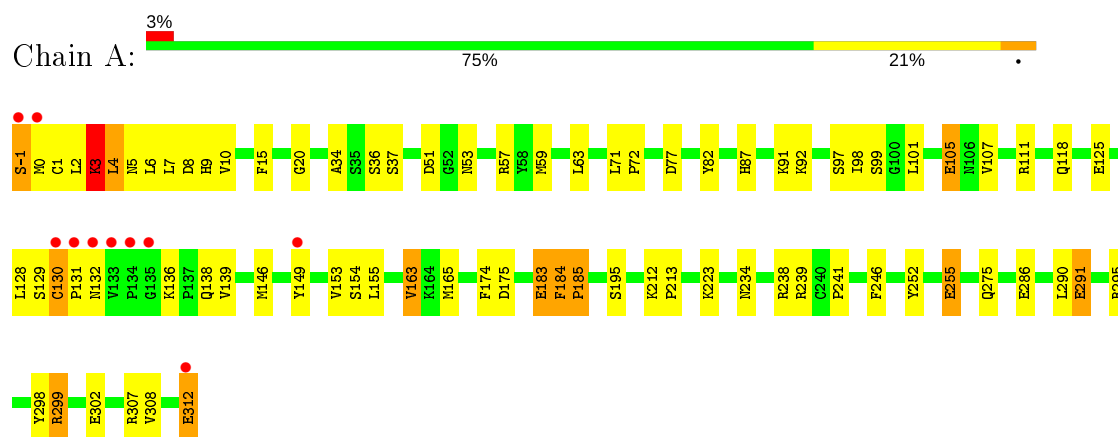
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	377	Total	O	0	9
			386	386		
9	B	444	Total	O	0	6
			450	450		

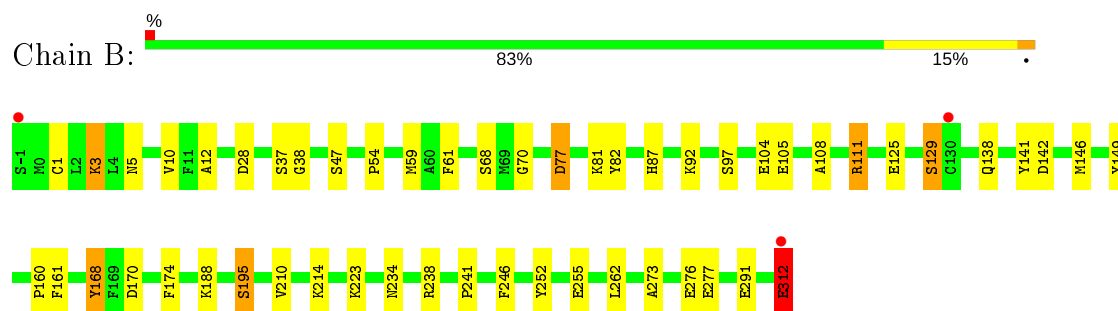
### 3 Residue-property plots

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.93Å 71.48Å 129.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.98 – 1.43 39.21 – 1.43	Depositor EDS
% Data completeness (in resolution range)	97.3 (36.98-1.43) 97.4 (39.21-1.43)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.39 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.153 , 0.187 0.152 , 0.186	Depositor DCC
$R_{free}$ test set	5704 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3903e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, W87, EDO, FMN, NCO, CAC, PEG

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	1.41	15/2591 (0.6%)	1.30	19/3506 (0.5%)
1	B	1.39	12/2574 (0.5%)	1.30	19/3482 (0.5%)
All	All	1.40	27/5165 (0.5%)	1.30	38/6988 (0.5%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	LYS	CE-NZ	14.96	1.86	1.49
1	B	1	CYS	CB-SG	-12.48	1.61	1.82
1	B	3	LYS	CD-CE	8.12	1.71	1.51
1	B	195	SER	CB-OG	-7.68	1.32	1.42
1	B	291	GLU	CG-CD	7.31	1.62	1.51
1	B	255	GLU	CD-OE1	-7.28	1.17	1.25
1	A	129	SER	CB-OG	7.14	1.51	1.42
1	A	255	GLU	CD-OE1	-7.04	1.18	1.25
1	A	6	LEU	CA-CB	6.78	1.69	1.53
1	A	129	SER	CA-C	6.74	1.70	1.52
1	B	146	MET	SD-CE	-6.27	1.42	1.77
1	B	312	GLU	CD-OE1	5.89	1.32	1.25
1	A	99	SER	CB-OG	-5.74	1.34	1.42
1	B	291	GLU	CD-OE1	5.68	1.31	1.25
1	A	129	SER	CA-CB	5.65	1.61	1.52
1	A	163[A]	VAL	CB-CG1	-5.57	1.41	1.52
1	A	163[B]	VAL	CB-CG1	-5.57	1.41	1.52
1	A	36	SER	CB-OG	-5.54	1.35	1.42
1	A	136	LYS	N-CA	5.49	1.57	1.46
1	B	149	TYR	CG-CD1	5.46	1.46	1.39
1	A	15	PHE	CD2-CE2	5.40	1.50	1.39
1	B	61	PHE	CB-CG	-5.25	1.42	1.51
1	B	105	GLU	CD-OE1	-5.18	1.20	1.25
1	A	291	GLU	CD-OE1	5.18	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	GLU	CG-CD	5.09	1.59	1.51
1	A	153	VAL	CB-CG1	-5.04	1.42	1.52
1	A	185	PRO	N-CA	-5.04	1.38	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LYS	CD-CE-NZ	13.46	142.67	111.70
1	B	146	MET	CG-SD-CE	-9.20	85.48	100.20
1	B	77	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	A	105	GLU	OE1-CD-OE2	-8.41	113.20	123.30
1	B	1	CYS	N-CA-CB	-8.03	96.15	110.60
1	B	142	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	174	PHE	CB-CG-CD2	-7.42	115.61	120.80
1	A	299	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	111[A]	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	B	111[B]	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	B	111[A]	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	111[B]	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	4[A]	LEU	CB-CG-CD1	6.97	122.86	111.00
1	A	4[B]	LEU	CB-CG-CD1	6.97	122.86	111.00
1	A	77	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	51	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	246	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	A	3	LYS	CA-CB-CG	6.67	128.08	113.40
1	A	146	MET	CG-SD-CE	-6.25	90.19	100.20
1	A	3	LYS	CB-CG-CD	-6.24	95.36	111.60
1	A	129	SER	CB-CA-C	6.12	121.74	110.10
1	B	168	TYR	CG-CD1-CE1	-6.07	116.44	121.30
1	B	174	PHE	CB-CG-CD1	5.97	124.98	120.80
1	B	174	PHE	CB-CG-CD2	-5.88	116.68	120.80
1	B	141	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	262	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	A	175	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	239	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	184	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	A	57	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	239	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	149	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	129	SER	CB-CA-C	5.32	120.21	110.10
1	A	183	GLU	OE1-CD-OE2	-5.28	116.97	123.30
1	B	246	PHE	CB-CG-CD2	-5.12	117.21	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	161	PHE	CB-CG-CD2	5.09	124.36	120.80
1	A	184	PHE	CB-CG-CD2	5.02	124.31	120.80

There are no chirality outliers.

There are no planarity outliers.

## 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	2540	0	2524	118	0
1	B	2522	0	2501	57	0
2	A	29	0	19	1	0
2	B	58	0	38	3	0
3	A	90	0	119	12	0
3	B	78	0	102	9	0
4	A	10	0	0	2	0
4	B	10	0	0	0	0
5	A	31	0	19	1	0
5	B	31	0	19	0	0
6	A	56	0	84	33	0
6	B	40	0	59	34	0
7	A	14	0	19	21	0
7	B	7	0	10	8	0
8	A	21	0	0	4	0
9	A	386	0	0	24	0
9	B	450	0	0	23	0
All	All	6373	0	5513	207	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 19.

All (207) 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:3:LYS:NZ	1:B:3:LYS:CE	1.86	1.38
1:A:2:LEU:HD12	1:A:286:GLU:HG3	1.18	1.09
1:A:128:LEU:CD1	1:A:163[B]:VAL:HG21	1.85	1.06
1:A:1:CYS:HB2	7:A:433:PEG:H22	1.26	1.06
6:B:420:EDO:H21	9:B:874:HOH:O	1.54	1.05
1:A:5[A]:ASN:ND2	1:A:10[A]:VAL:HG22	1.73	1.04
1:A:4[B]:LEU:C	1:A:4[B]:LEU:HD12	1.73	1.01
1:A:312[A]:GLU:N	1:A:312[A]:GLU:OE2	1.94	1.01
8:A:434:NCO:N4	9:A:655:HOH:O	1.91	1.01
1:A:2:LEU:HD12	1:A:286:GLU:CG	1.92	1.00
1:B:81:LYS:HE2	9:B:920:HOH:O	1.63	0.97
1:A:5[A]:ASN:HD21	1:A:10[A]:VAL:HG22	1.28	0.96
1:A:5[B]:ASN:HB3	6:A:431:EDO:C2	1.96	0.94
1:A:2:LEU:CD1	1:A:286:GLU:HG3	1.97	0.94
1:A:312[A]:GLU:HG3	9:B:748:HOH:O	1.67	0.93
1:B:277:GLU:HB2	6:B:419:EDO:H12	1.51	0.93
1:A:5[A]:ASN:HB3	6:A:431:EDO:C2	1.99	0.92
1:A:128:LEU:HD12	1:A:163[B]:VAL:HG21	1.52	0.91
1:A:2:LEU:HB2	7:A:433:PEG:H12	1.51	0.91
1:A:138[B]:GLN:HG2	1:B:170:ASP:OD2	1.68	0.90
1:B:54:PRO:HG2	6:B:423:EDO:H21	1.52	0.90
6:B:423:EDO:H11	9:B:527:HOH:O	1.75	0.86
1:A:91:LYS:O	6:A:423:EDO:H22	1.76	0.85
1:A:185:PRO:HG2	6:A:420:EDO:H12	1.60	0.83
1:A:2:LEU:H	7:A:433:PEG:C2	1.91	0.83
1:A:138[B]:GLN:CG	1:B:170:ASP:OD2	2.28	0.82
1:A:5[B]:ASN:HB3	6:A:431:EDO:H21	1.62	0.81
3:A:410:GOL:H12	9:A:809:HOH:O	1.80	0.80
1:B:59:MET:CE	9:B:602:HOH:O	2.30	0.79
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.31	0.79
1:A:128:LEU:CD1	1:A:163[B]:VAL:CG2	2.61	0.78
1:A:5[A]:ASN:HB3	6:A:431:EDO:H21	1.66	0.78
1:A:128:LEU:HD11	1:A:163[B]:VAL:HG21	1.66	0.78
1:B:47[B]:SER:O	6:B:417:EDO:H12	1.85	0.77
1:A:130[B]:CYS:SG	1:A:139:VAL:HG23	2.23	0.77
1:A:312[A]:GLU:CG	9:B:748:HOH:O	2.30	0.76
1:B:188:LYS:HE3	9:B:927:HOH:O	1.83	0.76
1:B:37:SER:O	6:B:425:EDO:H22	1.86	0.75
1:B:195:SER:HB3	9:B:679:HOH:O	1.87	0.75
1:A:291:GLU:OE2	1:A:295:ARG:NH1	2.20	0.74
8:A:434:NCO:N5	9:A:626:HOH:O	2.19	0.74
1:A:4[B]:LEU:CD1	1:A:4[B]:LEU:C	2.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68[B]:SER:OG	1:B:214[B]:LYS:NZ	2.20	0.74
3:B:413:GOL:H11	9:B:938:HOH:O	1.86	0.73
1:A:1:CYS:CB	7:A:433:PEG:H22	2.12	0.73
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.35	0.72
1:A:1:CYS:HB2	7:A:433:PEG:C2	2.14	0.72
1:A:128:LEU:HD12	1:A:163[A]:VAL:CG1	2.19	0.72
1:A:3:LYS:N	7:A:433:PEG:H21	2.06	0.71
1:B:129:SER:HA	1:B:138:GLN:NE2	2.06	0.70
1:A:128:LEU:HD12	1:A:163[A]:VAL:HG11	1.73	0.70
1:A:-1:SER:N	1:A:299:ARG:HA	2.06	0.70
1:A:312[A]:GLU:CA	1:A:312[A]:GLU:OE2	2.40	0.69
1:A:138[A]:GLN:HG3	9:A:868:HOH:O	1.94	0.68
1:A:128:LEU:HG	1:A:163[B]:VAL:HG23	1.75	0.68
1:A:4[B]:LEU:O	1:A:4[B]:LEU:HD12	1.93	0.68
1:A:5[A]:ASN:HD21	1:A:10[A]:VAL:CG2	2.06	0.68
2:B:401[A]:W87:H14	2:B:401[A]:W87:OAC	1.94	0.68
1:B:195:SER:OG	3:B:403:GOL:H11	1.93	0.68
1:A:185:PRO:HG2	6:A:420:EDO:C1	2.24	0.67
1:A:184:PHE:CE1	3:A:411:GOL:H32	2.30	0.67
1:A:128:LEU:CD1	1:A:163[A]:VAL:CG1	2.73	0.66
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.79	0.66
1:A:255:GLU:OE2	6:A:424:EDO:H21	1.94	0.66
1:B:129:SER:HB3	9:B:678:HOH:O	1.96	0.66
1:B:214[C]:LYS:NZ	6:B:422:EDO:H11	2.11	0.65
1:A:128:LEU:HG	1:A:163[B]:VAL:CG2	2.26	0.65
7:A:432:PEG:H21	9:A:874:HOH:O	1.97	0.65
1:B:276:GLU:HB2	6:B:419:EDO:H22	1.79	0.65
1:B:273:ALA:HB1	6:B:419:EDO:H11	1.79	0.65
1:A:149:TYR:HE1	9:A:691:HOH:O	1.80	0.64
1:A:2:LEU:H	7:A:433:PEG:C1	2.12	0.63
1:A:3:LYS:HG3	7:A:433:PEG:O2	1.98	0.63
4:A:415:CAC:C1	9:A:795:HOH:O	2.46	0.63
1:A:63:LEU:HD11	6:B:420:EDO:H22	1.81	0.63
1:A:183:GLU:HB3	3:A:411:GOL:H12	1.80	0.62
1:A:312[A]:GLU:OE2	1:A:312[A]:GLU:HA	2.00	0.62
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG11	2.29	0.62
6:B:421:EDO:H11	9:B:585:HOH:O	2.00	0.62
1:A:5[B]:ASN:HB3	6:A:431:EDO:O2	2.00	0.62
1:B:59:MET:HE3	9:B:602:HOH:O	1.95	0.62
1:A:307:ARG:HH22	6:A:426:EDO:H22	1.65	0.62
1:B:92:LYS:HB3	6:B:425:EDO:H11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401[B]:W87:OAS	2:B:401[B]:W87:H14	2.01	0.61
1:A:132:ASN:HB2	9:A:590:HOH:O	2.00	0.60
1:A:5[A]:ASN:HB3	6:A:431:EDO:O2	2.02	0.60
1:A:2:LEU:N	7:A:433:PEG:C2	2.63	0.60
1:A:275:GLN:O	8:A:434:NCO:N3	2.33	0.60
1:A:2:LEU:CD1	1:A:286:GLU:CG	2.70	0.60
3:B:413:GOL:H32	6:B:420:EDO:O2	2.02	0.59
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.85	0.59
8:A:434:NCO:N2	9:A:712:HOH:O	2.32	0.59
1:A:107:VAL:O	1:A:111[B]:ARG:HG3	2.04	0.58
1:A:154:SER:O	6:A:428:EDO:H21	2.03	0.58
1:B:87:HIS:HE1	1:B:92:LYS:O	1.86	0.58
1:B:210:VAL:HA	3:B:411:GOL:H31	1.85	0.58
1:A:37:SER:O	6:A:423:EDO:H11	2.03	0.58
1:B:111[B]:ARG:NH2	7:B:427:PEG:H21	2.19	0.57
1:A:3:LYS:HG3	7:A:433:PEG:C3	2.34	0.57
1:B:111[B]:ARG:NH2	7:B:427:PEG:C2	2.67	0.57
1:A:98[A]:ILE:O	1:A:98[A]:ILE:HG13	2.05	0.56
1:A:238:ARG:NH2	6:A:418:EDO:H22	2.21	0.56
1:A:128:LEU:HD12	1:A:163[B]:VAL:CG2	2.28	0.56
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG13	2.36	0.56
1:A:298:TYR:HE1	6:A:427:EDO:H22	1.70	0.56
1:A:155:LEU:HA	6:A:428:EDO:H21	1.87	0.55
1:A:195:SER:HB3	9:A:808:HOH:O	2.06	0.55
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.05	0.55
1:B:277:GLU:CB	6:B:419:EDO:H12	2.31	0.55
1:B:47[B]:SER:O	6:B:417:EDO:C1	2.54	0.55
1:A:241:PRO:HB3	3:A:413:GOL:H12	1.87	0.55
1:B:108:ALA:HA	7:B:427:PEG:H12	1.89	0.55
1:B:241:PRO:HA	3:B:409:GOL:H31	1.89	0.54
1:A:2:LEU:N	7:A:433:PEG:H21	2.21	0.54
1:A:3:LYS:CG	7:A:433:PEG:H31	2.36	0.54
1:A:183:GLU:O	3:A:411:GOL:H31	2.08	0.54
7:A:433:PEG:H11	9:A:653:HOH:O	2.06	0.54
1:B:92:LYS:HE2	6:B:425:EDO:H11	1.89	0.53
1:A:212:LYS:NZ	1:B:312:GLU:HG2	2.23	0.53
1:A:87:HIS:HE1	1:A:92:LYS:O	1.90	0.53
1:B:12:ALA:HB3	6:B:425:EDO:H21	1.90	0.53
1:A:128:LEU:CG	1:A:163[B]:VAL:CG2	2.87	0.53
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.02	0.53
1:A:5[A]:ASN:ND2	1:A:10[A]:VAL:CG2	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HG	1:A:163[A]:VAL:HG13	1.91	0.52
6:A:421:EDO:H21	9:A:535:HOH:O	2.09	0.52
2:A:401:W87:OAC	2:A:401:W87:H14	2.09	0.52
1:A:91:LYS:O	6:A:423:EDO:C2	2.54	0.52
4:A:416:CAC:C2	6:A:427:EDO:O1	2.58	0.52
1:B:104:GLU:HB3	7:B:427:PEG:H31	1.92	0.52
1:A:308:VAL:O	6:A:418:EDO:H21	2.10	0.51
1:A:2:LEU:H	7:A:433:PEG:H21	1.72	0.51
1:A:3:LYS:HG3	7:A:433:PEG:H31	1.93	0.51
1:A:130[A]:CYS:SG	1:A:131:PRO:HD2	2.51	0.51
1:B:38:GLY:HA2	6:B:425:EDO:H22	1.92	0.50
1:A:295:ARG:HH21	6:A:424:EDO:C1	2.23	0.50
3:B:410:GOL:C3	9:B:697:HOH:O	2.60	0.49
1:A:7:LEU:O	1:A:9:HIS:HD2	1.96	0.49
1:B:214[C]:LYS:HZ3	6:B:422:EDO:H11	1.76	0.49
1:B:5[B]:ASN:ND2	1:B:10:VAL:HG22	2.28	0.49
1:B:77:ASP:H	6:B:417:EDO:H11	1.78	0.48
1:B:37:SER:O	6:B:425:EDO:C2	2.59	0.48
1:A:10[B]:VAL:O	3:A:409:GOL:H11	2.15	0.47
1:A:34:ALA:HB3	3:A:402[A]:GOL:H11	1.97	0.47
3:A:403:GOL:O1	6:B:422:EDO:H12	2.15	0.46
1:A:59:MET:HE3	9:A:739:HOH:O	2.15	0.46
1:A:275:GLN:NE2	9:A:589:HOH:O	2.48	0.46
7:A:432:PEG:H12	1:B:168:TYR:HA	1.97	0.46
6:B:421:EDO:C1	9:B:585:HOH:O	2.59	0.46
1:A:9:HIS:HE1	9:A:523:HOH:O	1.99	0.46
6:A:420:EDO:O1	6:A:428:EDO:C1	2.64	0.46
1:B:108:ALA:CB	7:B:427:PEG:H12	2.46	0.45
1:A:307:ARG:HH22	6:A:426:EDO:C2	2.29	0.45
1:B:77:ASP:H	6:B:417:EDO:C1	2.30	0.45
1:A:37:SER:O	6:A:423:EDO:C1	2.66	0.44
1:B:160:PRO:HB2	6:B:426:EDO:H22	1.98	0.44
1:B:223:LYS:HD3	6:B:420:EDO:H12	1.99	0.44
6:B:423:EDO:C1	9:B:527:HOH:O	2.47	0.44
6:B:417:EDO:H11	9:B:539:HOH:O	2.16	0.44
1:A:92:LYS:HE2	6:A:423:EDO:H11	1.99	0.44
1:A:149:TYR:CE1	9:A:691:HOH:O	2.56	0.44
1:B:47[A]:SER:O	6:B:417:EDO:H12	2.17	0.43
7:A:432:PEG:H32	9:A:786:HOH:O	2.17	0.43
1:B:97:SER:HA	1:B:125:GLU:O	2.18	0.43
6:A:430:EDO:H11	9:A:580:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLY:HA2	2:B:401[B]:W87:CAK	2.47	0.43
1:A:5[A]:ASN:HD22	6:A:431:EDO:C2	2.31	0.43
1:B:129:SER:CB	9:B:678:HOH:O	2.60	0.43
6:B:417:EDO:C2	9:B:539:HOH:O	2.66	0.43
1:A:163[A]:VAL:HG12	1:A:165:MET:SD	2.59	0.43
1:B:104:GLU:CA	7:B:427:PEG:H31	2.49	0.43
6:B:418:EDO:H11	9:B:760:HOH:O	2.19	0.42
1:A:138[A]:GLN:CG	9:A:868:HOH:O	2.61	0.42
1:A:8[B]:ASP:N	6:A:431:EDO:O1	2.39	0.42
1:A:98[A]:ILE:O	1:A:98[A]:ILE:CG1	2.68	0.42
1:A:3:LYS:CG	7:A:433:PEG:C3	2.96	0.42
1:B:223:LYS:HG2	1:B:252:TYR:CE1	2.54	0.42
3:B:408:GOL:H32	9:B:659:HOH:O	2.19	0.42
1:B:108:ALA:CA	7:B:427:PEG:H12	2.48	0.42
1:A:101:LEU:N	1:A:105:GLU:OE1	2.48	0.42
1:A:128:LEU:O	9:A:868:HOH:O	2.21	0.42
1:B:214[C]:LYS:HZ2	6:B:422:EDO:C1	2.32	0.42
6:B:417:EDO:H22	9:B:539:HOH:O	2.19	0.42
1:A:2:LEU:HG	1:A:290:LEU:HD21	2.01	0.42
1:A:155:LEU:HA	6:A:428:EDO:C2	2.48	0.42
1:A:295:ARG:NH2	6:A:424:EDO:H22	2.35	0.42
1:A:71:LEU:N	1:A:72:PRO:CD	2.83	0.42
3:B:410:GOL:H31	9:B:697:HOH:O	2.19	0.42
7:B:427:PEG:H41	9:B:811:HOH:O	2.19	0.42
1:A:20:GLY:HA3	5:A:417:FMN:N5	2.35	0.41
1:A:10[A]:VAL:O	3:A:409:GOL:H11	2.20	0.41
1:A:97:SER:HA	1:A:125:GLU:O	2.20	0.41
6:A:425:EDO:H21	9:A:633:HOH:O	2.20	0.41
1:B:241:PRO:HA	3:B:409:GOL:C3	2.50	0.41
1:A:-1:SER:H3	1:A:299:ARG:HA	1.80	0.41
1:A:308:VAL:O	6:A:418:EDO:C2	2.68	0.41
1:A:295:ARG:HH21	6:A:424:EDO:H12	1.85	0.41
1:A:223[B]:LYS:HG3	1:A:252:TYR:CE1	2.56	0.41
3:A:414:GOL:C3	9:A:747:HOH:O	2.69	0.41
1:A:138[B]:GLN:HG3	1:B:170:ASP:OD2	2.16	0.41
1:A:59:MET:CE	9:A:739:HOH:O	2.68	0.41
3:A:414:GOL:H32	9:A:747:HOH:O	2.21	0.41
3:A:406[B]:GOL:H2	1:B:238:ARG:HB3	2.03	0.41
7:A:432:PEG:H41	7:A:432:PEG:H21	1.42	0.41
7:A:432:PEG:H22	7:A:432:PEG:H42	1.64	0.40
1:B:77:ASP:HB2	6:B:417:EDO:H21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:HB3	1:A:213:PRO:HG3	2.04	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	329/314 (105%)	318 (97%)	10 (3%)	1 (0%)	41	19
1	B	328/314 (104%)	316 (96%)	12 (4%)	0	100	100
All	All	657/628 (105%)	634 (96%)	22 (3%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	MET

### 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	277/259 (107%)	270 (98%)	7 (2%)	47	13
1	B	275/259 (106%)	274 (100%)	1 (0%)	91	80
All	All	552/518 (107%)	544 (99%)	8 (1%)	71	37

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	3	LYS
1	A	118	GLN
1	A	130[A]	CYS
1	A	130[B]	CYS
1	A	312[A]	GLU
1	A	312[B]	GLU
1	B	312	GLU

Some 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	151	GLN
1	A	234	ASN
1	A	275	GLN
1	B	87	HIS
1	B	118	GLN
1	B	138	GLN
1	B	234	ASN
1	B	275	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

67 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
4	CAC	A	415	-	0,4,4	0.00	-	0,6,6	0.00	-
6	EDO	A	424	-	3,3,3	0.61	0	2,2,2	0.36	0
7	PEG	A	433	-	6,6,6	1.02	1 (16%)	5,5,5	2.24	1 (20%)
3	GOL	A	409	-	5,5,5	0.80	0	5,5,5	1.42	1 (20%)
6	EDO	A	419	-	3,3,3	0.53	0	2,2,2	0.42	0
6	EDO	A	430	-	3,3,3	0.90	0	2,2,2	0.68	0
4	CAC	B	414	-	0,4,4	0.00	-	0,6,6	0.00	-
6	EDO	A	431	-	3,3,3	1.66	1 (33%)	2,2,2	1.67	1 (50%)
6	EDO	B	425	-	3,3,3	1.28	1 (33%)	2,2,2	2.04	1 (50%)
3	GOL	B	411	-	5,5,5	0.51	0	5,5,5	1.10	0
3	GOL	A	407	-	5,5,5	0.38	0	5,5,5	0.42	0
2	W87	A	401	-	27,31,31	1.86	4 (14%)	30,43,43	2.45	13 (43%)
7	PEG	A	432	-	6,6,6	1.05	1 (16%)	5,5,5	1.10	0
3	GOL	A	403	-	5,5,5	0.62	0	5,5,5	1.09	0
6	EDO	B	426	-	3,3,3	0.82	0	2,2,2	0.69	0
8	NCO	A	435[A]	-	6,6,6	2.39	3 (50%)	-	-	-
6	EDO	B	419	-	3,3,3	0.65	0	2,2,2	0.54	0
8	NCO	A	434	-	6,6,6	5.15	6 (100%)	-	-	-
6	EDO	A	420	-	3,3,3	0.64	0	2,2,2	0.81	0
3	GOL	A	405	-	5,5,5	0.94	0	5,5,5	1.25	1 (20%)
3	GOL	B	408	-	5,5,5	0.50	0	5,5,5	0.67	0
7	PEG	B	427	-	6,6,6	1.24	1 (16%)	5,5,5	1.78	1 (20%)
2	W87	B	401[A]	-	27,31,31	1.86	6 (22%)	30,43,43	2.20	8 (26%)
3	GOL	A	408	-	5,5,5	0.46	0	5,5,5	0.70	0
6	EDO	B	424	-	3,3,3	0.60	0	2,2,2	0.29	0
6	EDO	B	420	-	3,3,3	0.97	0	2,2,2	0.97	0
6	EDO	A	425	-	3,3,3	0.68	0	2,2,2	0.38	0
2	W87	B	401[B]	-	27,31,31	1.70	5 (18%)	30,43,43	2.01	5 (16%)
8	NCO	A	435[B]	-	6,6,6	2.46	4 (66%)	-	-	-
6	EDO	A	421	-	3,3,3	0.38	0	2,2,2	2.04	1 (50%)
3	GOL	B	405[B]	-	5,5,5	0.35	0	5,5,5	1.16	0
3	GOL	B	404	-	5,5,5	1.26	1 (20%)	5,5,5	0.99	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	403	-	5,5,5	0.57	0	5,5,5	0.87	0
3	GOL	B	405[A]	-	5,5,5	0.71	0	5,5,5	0.82	0
3	GOL	A	402[B]	-	5,5,5	1.28	0	5,5,5	1.02	0
6	EDO	B	422	-	3,3,3	0.68	0	2,2,2	0.30	0
6	EDO	A	426	-	3,3,3	0.53	0	2,2,2	0.20	0
3	GOL	A	402[A]	-	5,5,5	1.02	0	5,5,5	0.41	0
3	GOL	A	411	-	5,5,5	0.56	0	5,5,5	1.30	1 (20%)
6	EDO	A	427	-	3,3,3	0.83	0	2,2,2	0.14	0
6	EDO	B	417	-	3,3,3	1.28	0	2,2,2	1.37	0
3	GOL	A	413	-	5,5,5	0.73	0	5,5,5	0.77	0
6	EDO	A	423	-	3,3,3	0.52	0	2,2,2	0.47	0
3	GOL	B	413	-	5,5,5	0.40	0	5,5,5	1.13	0
6	EDO	B	423	-	3,3,3	0.48	0	2,2,2	0.64	0
3	GOL	B	406	-	5,5,5	0.98	0	5,5,5	1.40	1 (20%)
4	CAC	B	415	-	0,4,4	0.00	-	0,6,6	0.00	-
6	EDO	B	418	-	3,3,3	0.31	0	2,2,2	1.05	0
3	GOL	B	402	-	5,5,5	0.65	0	5,5,5	0.64	0
3	GOL	B	409	-	5,5,5	0.89	0	5,5,5	0.88	0
3	GOL	A	414	-	5,5,5	0.39	0	5,5,5	0.36	0
4	CAC	A	416	-	0,4,4	0.00	-	0,6,6	0.00	-
3	GOL	A	410	-	5,5,5	0.38	0	5,5,5	0.62	0
6	EDO	A	422	-	3,3,3	0.37	0	2,2,2	1.10	0
3	GOL	A	406[B]	-	5,5,5	0.22	0	5,5,5	0.67	0
3	GOL	A	406[A]	-	5,5,5	0.50	0	5,5,5	0.44	0
5	FMN	A	417	-	31,33,33	1.66	4 (12%)	40,50,50	2.30	4 (10%)
3	GOL	A	412	-	5,5,5	0.56	0	5,5,5	0.70	0
3	GOL	B	412	-	5,5,5	0.37	0	5,5,5	0.79	0
6	EDO	A	428	-	3,3,3	0.51	0	2,2,2	0.61	0
5	FMN	B	416	-	31,33,33	1.39	2 (6%)	40,50,50	1.88	7 (17%)
6	EDO	A	429	-	3,3,3	0.41	0	2,2,2	0.80	0
3	GOL	A	404	-	5,5,5	0.83	0	5,5,5	2.20	3 (60%)
6	EDO	A	418	-	3,3,3	0.88	0	2,2,2	0.35	0
6	EDO	B	421	-	3,3,3	0.84	0	2,2,2	0.55	0
3	GOL	B	407	-	5,5,5	0.45	0	5,5,5	0.83	0
3	GOL	B	410	-	5,5,5	0.25	0	5,5,5	0.79	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	A	424	-	-	0/1/1/1	-
7	PEG	A	433	-	-	4/4/4/4	-
3	GOL	A	409	-	-	0/4/4/4	-
6	EDO	A	419	-	-	0/1/1/1	-
6	EDO	A	430	-	-	1/1/1/1	-
6	EDO	A	431	-	-	1/1/1/1	-
6	EDO	B	425	-	-	1/1/1/1	-
3	GOL	B	411	-	-	2/4/4/4	-
3	GOL	A	407	-	-	1/4/4/4	-
2	W87	A	401	-	-	4/13/17/17	0/3/3/3
7	PEG	A	432	-	-	2/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
6	EDO	B	426	-	-	0/1/1/1	-
6	EDO	B	419	-	-	0/1/1/1	-
3	GOL	B	413	-	-	3/4/4/4	-
6	EDO	A	420	-	-	0/1/1/1	-
3	GOL	A	405	-	-	0/4/4/4	-
3	GOL	B	408	-	-	2/4/4/4	-
7	PEG	B	427	-	-	3/4/4/4	-
2	W87	B	401[A]	-	-	6/13/17/17	0/3/3/3
3	GOL	A	408	-	-	3/4/4/4	-
6	EDO	B	424	-	-	1/1/1/1	-
6	EDO	B	420	-	-	1/1/1/1	-
6	EDO	A	425	-	-	0/1/1/1	-
2	W87	B	401[B]	-	-	10/13/17/17	0/3/3/3
6	EDO	A	421	-	-	1/1/1/1	-
3	GOL	B	405[B]	-	-	3/4/4/4	-
3	GOL	B	404	-	-	0/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
3	GOL	B	405[A]	-	-	1/4/4/4	-
3	GOL	A	402[B]	-	-	0/4/4/4	-
6	EDO	B	422	-	-	1/1/1/1	-
6	EDO	A	426	-	-	1/1/1/1	-
3	GOL	A	402[A]	-	-	0/4/4/4	-
3	GOL	A	411	-	-	4/4/4/4	-
6	EDO	A	427	-	-	1/1/1/1	-
6	EDO	B	417	-	-	0/1/1/1	-
3	GOL	A	413	-	-	4/4/4/4	-
6	EDO	A	423	-	-	1/1/1/1	-
6	EDO	B	423	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	422	-	-	1/1/1/1	-
3	GOL	B	406	-	-	0/4/4/4	-
6	EDO	B	418	-	-	0/1/1/1	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	B	409	-	-	4/4/4/4	-
3	GOL	A	414	-	-	3/4/4/4	-
3	GOL	A	410	-	-	4/4/4/4	-
3	GOL	A	406[B]	-	-	1/4/4/4	-
3	GOL	A	406[A]	-	-	4/4/4/4	-
5	FMN	A	417	-	-	1/18/18/18	0/3/3/3
3	GOL	A	412	-	-	0/4/4/4	-
3	GOL	B	412	-	-	0/4/4/4	-
6	EDO	A	428	-	-	0/1/1/1	-
5	FMN	B	416	-	-	2/18/18/18	0/3/3/3
6	EDO	A	429	-	-	1/1/1/1	-
3	GOL	A	404	-	-	2/4/4/4	-
6	EDO	A	418	-	-	1/1/1/1	-
6	EDO	B	421	-	-	1/1/1/1	-
3	GOL	B	407	-	-	3/4/4/4	-
3	GOL	B	410	-	-	0/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	434	NCO	CO-N5	7.71	2.24	1.96
5	A	417	FMN	C4A-C10	6.87	1.45	1.38
8	A	434	NCO	CO-N3	6.11	2.18	1.96
2	B	401[B]	W87	OAS-CAU	6.08	1.46	1.33
2	B	401[A]	W87	OAS-CAU	6.03	1.46	1.33
2	A	401	W87	OAS-CAU	5.27	1.45	1.33
8	A	434	NCO	CO-N4	5.18	2.15	1.96
2	A	401	W87	CBA-NAR	4.44	1.40	1.33
8	A	435[A]	NCO	CO-N5	4.34	2.12	1.96
8	A	434	NCO	CO-N2	4.15	2.11	1.96
5	B	416	FMN	C4A-C10	4.00	1.42	1.38
8	A	434	NCO	CO-N6	3.49	2.09	1.96
8	A	435[B]	NCO	CO-N6	3.29	2.08	1.96
5	B	416	FMN	C4-C4A	-3.04	1.36	1.41
8	A	435[B]	NCO	CO-N1	3.00	2.07	1.96
5	A	417	FMN	C6-C5A	-2.93	1.37	1.41
8	A	435[B]	NCO	CO-N4	2.71	2.06	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	W87	CAL-CBB	-2.68	1.35	1.42
8	A	435[B]	NCO	CO-N5	2.66	2.06	1.96
8	A	435[A]	NCO	CO-N6	2.65	2.06	1.96
3	B	404	GOL	O2-C2	-2.63	1.35	1.43
2	B	401[B]	W87	OAE-CBA	2.54	1.30	1.24
2	B	401[A]	W87	OAE-CBA	2.53	1.30	1.24
8	A	434	NCO	CO-N1	2.50	2.05	1.96
5	A	417	FMN	C1'-N10	2.39	1.50	1.48
2	A	401	W87	CAX-NAQ	2.38	1.38	1.34
2	B	401[A]	W87	CBA-NAR	2.35	1.37	1.33
2	B	401[B]	W87	CBA-NAR	2.33	1.37	1.33
6	A	431	EDO	O2-C2	2.32	1.54	1.42
2	B	401[B]	W87	CAK-CAI	2.30	1.41	1.36
2	B	401[B]	W87	CAZ-NAR	-2.29	1.33	1.38
2	B	401[A]	W87	CAZ-NAR	-2.26	1.33	1.38
8	A	435[A]	NCO	CO-N3	2.25	2.04	1.96
6	B	425	EDO	O1-C1	-2.21	1.30	1.42
7	B	427	PEG	O2-C2	2.16	1.51	1.42
7	A	433	PEG	O2-C3	2.15	1.51	1.42
2	B	401[A]	W87	CAL-CBB	-2.15	1.37	1.42
2	B	401[A]	W87	CBC-CBB	-2.06	1.39	1.43
7	A	432	PEG	O4-C4	-2.04	1.31	1.42
5	A	417	FMN	C5A-N5	2.03	1.38	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	417	FMN	C4-C4A-C10	-8.51	114.32	119.95
5	A	417	FMN	C4-N3-C2	8.10	121.98	115.14
2	B	401[A]	W87	CBA-NAR-CAZ	8.09	121.97	115.14
2	B	401[B]	W87	CBA-NAR-CAZ	8.01	121.91	115.14
2	A	401	W87	CBA-NAR-CAZ	7.42	121.41	115.14
5	B	416	FMN	C4-N3-C2	6.45	120.59	115.14
5	B	416	FMN	C4-C4A-C10	-5.22	116.50	119.95
7	A	433	PEG	C3-O2-C2	4.92	134.59	113.29
2	A	401	W87	CAO-CAV-CAL	-4.85	111.01	121.04
5	A	417	FMN	C4A-C10-N10	-4.76	115.41	120.30
5	A	417	FMN	C10-C4A-N5	4.32	124.25	121.26
2	B	401[B]	W87	OAS-CAU-CAW	4.02	119.09	111.75
2	B	401[A]	W87	CAO-CAV-CAL	-3.84	113.09	121.04
3	A	404	GOL	O3-C3-C2	3.66	127.73	110.20
2	A	401	W87	CAJ-CBB-CAL	-3.58	115.70	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	416	FMN	C1'-N10-C10	3.52	121.56	118.41
2	B	401[A]	W87	OAS-CAU-CAW	3.45	118.05	111.75
5	B	416	FMN	C4A-N5-C5A	3.40	120.17	116.77
2	A	401	W87	CAI-CAV-CAL	3.34	125.33	118.85
2	A	401	W87	CAJ-CBB-CBC	3.28	123.44	119.12
2	A	401	W87	CAI-CAK-CBC	-3.26	116.59	121.13
5	B	416	FMN	C4-C4A-N5	3.19	122.24	118.60
2	B	401[A]	W87	CAM-CAO-CAV	2.95	124.78	113.68
6	A	421	EDO	O1-C1-C2	-2.84	91.45	111.91
7	B	427	PEG	O2-C2-C1	2.79	122.33	110.07
2	A	401	W87	CAG-CAJ-CBB	-2.77	116.11	120.44
6	B	425	EDO	O2-C2-C1	-2.68	92.61	111.91
2	A	401	W87	CAM-CAN-CAP	2.60	123.88	113.76
2	A	401	W87	CAK-CBC-CBB	2.59	121.24	117.89
2	B	401[A]	W87	CAZ-NAQ-CAX	2.53	118.55	115.24
2	B	401[B]	W87	CAZ-NAQ-CAX	2.51	118.52	115.24
3	B	406	GOL	O1-C1-C2	2.48	122.09	110.20
2	B	401[A]	W87	CAA-OAS-CAU	2.34	120.35	115.83
3	A	411	GOL	O3-C3-C2	2.31	121.29	110.20
2	B	401[A]	W87	CAJ-CBB-CBC	2.30	122.14	119.12
2	B	401[B]	W87	CAA-OAS-CAU	2.29	120.24	115.83
3	A	405	GOL	O2-C2-C1	2.25	119.03	109.12
2	A	401	W87	OAS-CAU-CAW	2.25	115.85	111.75
2	A	401	W87	CAZ-NAQ-CAX	2.24	118.16	115.24
2	A	401	W87	CAK-CBC-CAW	-2.21	119.91	123.31
3	A	404	GOL	O2-C2-C1	2.20	118.83	109.12
5	B	416	FMN	C4A-C4-N3	-2.15	120.49	123.43
5	B	416	FMN	C9A-N10-C10	-2.13	119.12	121.91
3	A	409	GOL	C3-C2-C1	-2.12	103.47	111.70
6	A	431	EDO	O2-C2-C1	2.07	126.78	111.91
2	B	401[A]	W87	CAO-CAV-CAI	2.06	126.43	121.23
2	A	401	W87	CAP-CAY-CBA	-2.03	116.82	120.95
3	A	404	GOL	O2-C2-C3	2.03	118.07	109.12
2	B	401[B]	W87	CAI-CAK-CBC	-2.01	118.34	121.13

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	411	GOL	O1-C1-C2-O2
3	B	411	GOL	O1-C1-C2-C3
3	B	413	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	413	GOL	O1-C1-C2-C3
3	B	408	GOL	O1-C1-C2-C3
2	B	401[A]	W87	CAW-CAU-OAS-CAA
3	A	408	GOL	C1-C2-C3-O3
3	A	413	GOL	C1-C2-C3-O3
3	B	405[B]	GOL	C1-C2-C3-O3
3	B	405[B]	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	A	411	GOL	C1-C2-C3-O3
3	B	409	GOL	C1-C2-C3-O3
3	A	414	GOL	C1-C2-C3-O3
3	A	414	GOL	O2-C2-C3-O3
3	A	410	GOL	O1-C1-C2-O2
3	A	410	GOL	O1-C1-C2-C3
3	A	410	GOL	C1-C2-C3-O3
3	A	406[A]	GOL	O1-C1-C2-O2
3	A	406[A]	GOL	O1-C1-C2-C3
3	A	404	GOL	C1-C2-C3-O3
3	B	407	GOL	C1-C2-C3-O3
2	B	401[B]	W87	CAW-CAU-OAS-CAA
7	A	432	PEG	C4-C3-O2-C2
2	B	401[A]	W87	OAC-CAU-OAS-CAA
2	B	401[B]	W87	OAC-CAU-OAS-CAA
3	B	403	GOL	O1-C1-C2-O2
3	A	406[A]	GOL	O2-C2-C3-O3
2	B	401[A]	W87	CAN-CAM-CAO-CAV
7	A	433	PEG	O1-C1-C2-O2
7	A	432	PEG	O1-C1-C2-O2
3	B	413	GOL	C1-C2-C3-O3
3	A	413	GOL	O1-C1-C2-C3
3	A	411	GOL	O1-C1-C2-C3
3	B	409	GOL	O1-C1-C2-C3
3	A	414	GOL	O1-C1-C2-C3
3	A	406[A]	GOL	C1-C2-C3-O3
3	B	408	GOL	O1-C1-C2-O2
3	A	413	GOL	O2-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	B	409	GOL	O1-C1-C2-O2
3	A	410	GOL	O2-C2-C3-O3
2	B	401[A]	W87	CAO-CAM-CAN-CAP
2	A	401	W87	CAN-CAM-CAO-CAV

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Mol	Chain	Res	Type	Atoms
7	A	433	PEG	O2-C3-C4-O4
6	B	425	EDO	O1-C1-C2-O2
6	B	424	EDO	O1-C1-C2-O2
6	A	426	EDO	O1-C1-C2-O2
6	A	427	EDO	O1-C1-C2-O2
6	A	423	EDO	O1-C1-C2-O2
6	A	422	EDO	O1-C1-C2-O2
6	A	429	EDO	O1-C1-C2-O2
6	B	421	EDO	O1-C1-C2-O2
3	A	408	GOL	O2-C2-C3-O3
3	A	413	GOL	O1-C1-C2-O2
2	A	401	W87	CAO-CAM-CAN-CAP
3	A	407	GOL	O1-C1-C2-O2
7	B	427	PEG	C4-C3-O2-C2
5	A	417	FMN	C4'-C5'-O5'-P
5	B	416	FMN	C4'-C5'-O5'-P
7	B	427	PEG	O2-C3-C4-O4
6	A	431	EDO	O1-C1-C2-O2
6	B	422	EDO	O1-C1-C2-O2
6	A	418	EDO	O1-C1-C2-O2
3	B	405[A]	GOL	O2-C2-C3-O3
3	A	411	GOL	O2-C2-C3-O3
3	A	406[B]	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2
3	B	407	GOL	O1-C1-C2-O2
7	A	433	PEG	C4-C3-O2-C2
6	B	423	EDO	O1-C1-C2-O2
7	B	427	PEG	O1-C1-C2-O2
2	B	401[B]	W87	CAN-CAM-CAO-CAV
3	A	411	GOL	O1-C1-C2-O2
2	B	401[A]	W87	CAM-CAO-CAV-CAI
2	A	401	W87	CAM-CAO-CAV-CAI
7	A	433	PEG	C1-C2-O2-C3
2	B	401[B]	W87	OAS-CAU-CAW-CAH
2	B	401[B]	W87	OAS-CAU-CAW-CBC
2	A	401	W87	CAM-CAO-CAV-CAL
6	A	421	EDO	O1-C1-C2-O2
2	B	401[A]	W87	CAM-CAO-CAV-CAL
3	B	405[B]	GOL	O1-C1-C2-O2
2	B	401[B]	W87	CAO-CAM-CAN-CAP
2	B	401[B]	W87	CAM-CAO-CAV-CAL
2	B	401[B]	W87	CAM-CAO-CAV-CAI

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Mol	Chain	Res	Type	Atoms
6	A	430	EDO	O1-C1-C2-O2
3	B	409	GOL	O2-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
2	B	401[B]	W87	OAC-CAU-CAW-CAH
5	B	416	FMN	O3'-C3'-C4'-C5'
6	B	420	EDO	O1-C1-C2-O2
2	B	401[B]	W87	OAC-CAU-CAW-CBC
3	A	408	GOL	O1-C1-C2-O2

There are no ring outliers.

44 monomers are involved in 125 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	415	CAC	1	0
6	A	424	EDO	4	0
7	A	433	PEG	16	0
3	A	409	GOL	2	0
6	A	430	EDO	1	0
6	A	431	EDO	8	0
6	B	425	EDO	6	0
3	B	411	GOL	1	0
2	A	401	W87	1	0
7	A	432	PEG	5	0
3	A	403	GOL	1	0
6	B	426	EDO	1	0
6	B	419	EDO	4	0
8	A	434	NCO	4	0
6	A	420	EDO	3	0
3	B	408	GOL	1	0
7	B	427	PEG	8	0
2	B	401[A]	W87	1	0
6	B	420	EDO	4	0
6	A	425	EDO	1	0
2	B	401[B]	W87	2	0
6	A	421	EDO	1	0
3	B	403	GOL	1	0
6	B	422	EDO	4	0
6	A	426	EDO	2	0
3	A	402[A]	GOL	1	0
3	A	411	GOL	3	0
6	A	427	EDO	2	0
6	B	417	EDO	9	0

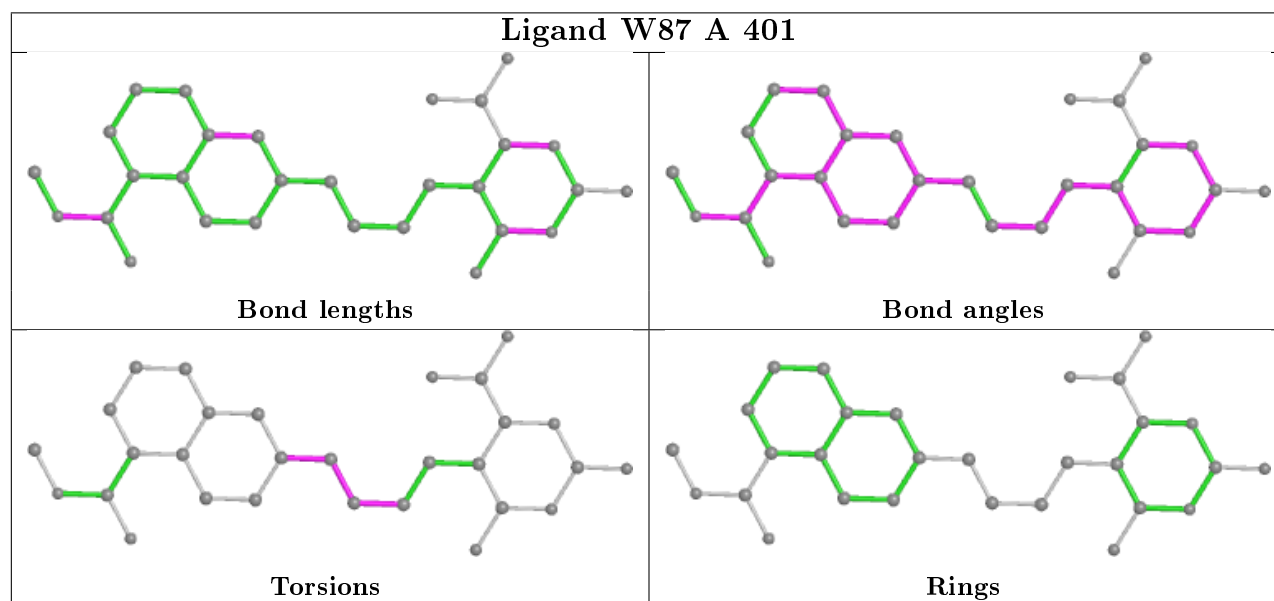
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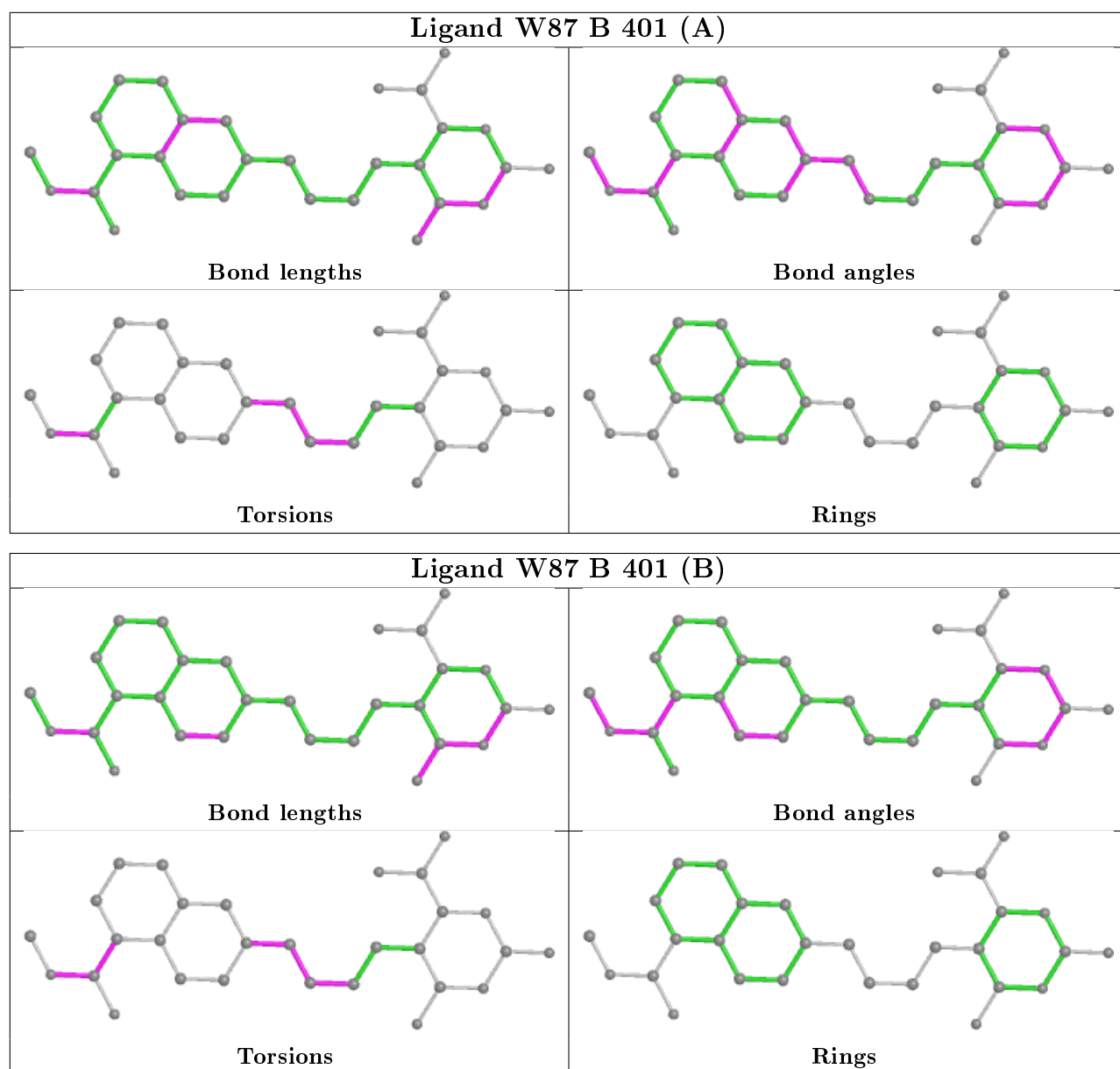


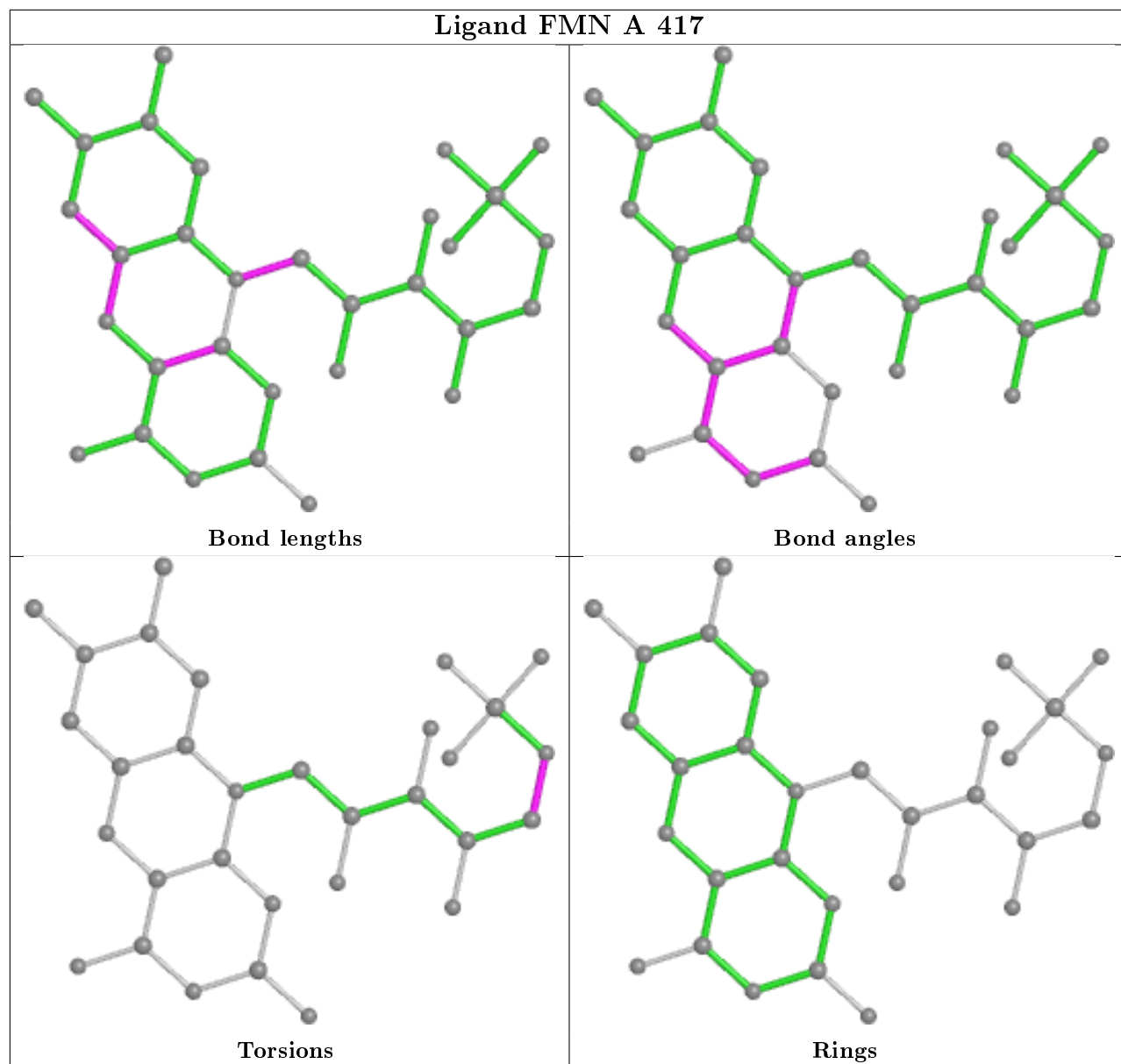
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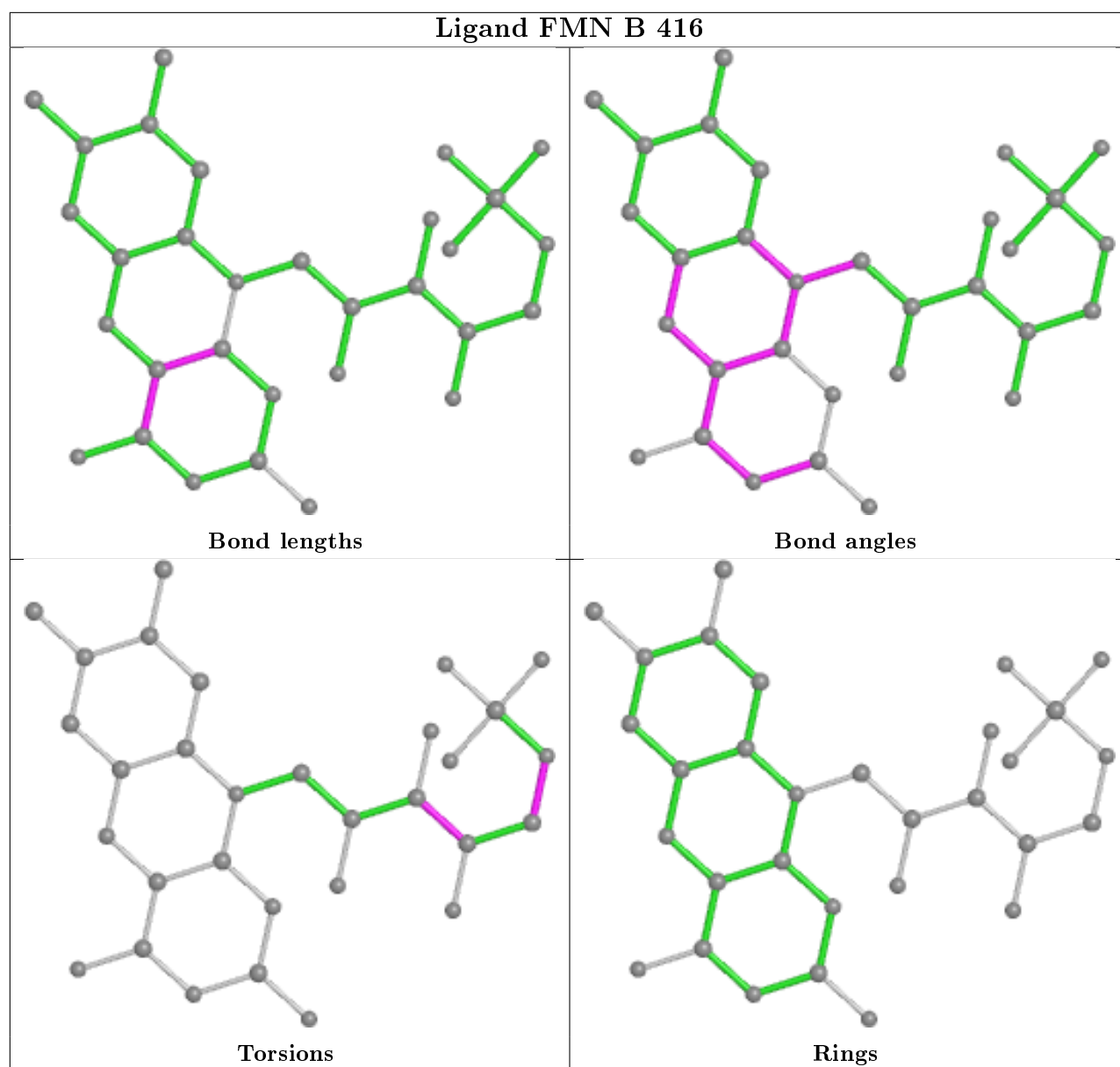
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	413	GOL	1	0
6	A	423	EDO	5	0
3	B	413	GOL	2	0
6	B	423	EDO	3	0
6	B	418	EDO	1	0
3	B	409	GOL	2	0
3	A	414	GOL	2	0
4	A	416	CAC	1	0
3	A	410	GOL	1	0
3	A	406[B]	GOL	1	0
5	A	417	FMN	1	0
6	A	428	EDO	4	0
6	A	418	EDO	3	0
6	B	421	EDO	2	0
3	B	410	GOL	2	0

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 than 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.









## 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	314/314 (100%)	-0.21	10 (3%) 47 48	4, 9, 24, 41	0
1	B	314/314 (100%)	-0.39	3 (0%) 82 82	4, 8, 19, 36	0
All	All	628/628 (100%)	-0.30	13 (2%) 63 64	4, 8, 21, 41	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	5.6
1	A	133	VAL	5.4
1	A	-1	SER	5.3
1	A	135	GLY	4.8
1	A	134	PRO	4.7
1	B	-1	SER	4.7
1	B	312	GLU	3.6
1	A	130[A]	CYS	3.5
1	A	312[A]	GLU	3.1
1	A	132	ASN	2.9
1	A	0	MET	2.6
1	A	149	TYR	2.5
1	B	130[A]	CYS	2.2

### 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 ⓘ

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<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	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	410	6/6	0.40	0.26	50,56,58,62	0
4	CAC	B	415	5/5	0.55	0.36	169,169,169,169	0
3	GOL	B	412	6/6	0.62	0.21	49,50,50,51	0
6	EDO	A	427	4/4	0.63	0.43	39,48,48,52	0
6	EDO	A	419	4/4	0.65	0.13	53,53,54,55	0
6	EDO	A	426	4/4	0.67	0.24	53,54,54,55	0
6	EDO	B	424	4/4	0.68	0.16	47,47,50,51	0
6	EDO	B	422	4/4	0.71	0.25	41,42,43,44	0
3	GOL	A	407	6/6	0.75	0.24	38,51,54,55	0
3	GOL	A	408	6/6	0.76	0.21	29,35,40,48	0
6	EDO	A	425	4/4	0.76	0.24	33,35,37,39	0
3	GOL	B	403	6/6	0.77	0.20	20,34,36,37	0
6	EDO	A	429	4/4	0.78	0.17	51,52,52,53	0
3	GOL	B	405[A]	6/6	0.80	0.18	14,18,18,27	6
3	GOL	B	405[B]	6/6	0.80	0.18	22,28,31,36	6
6	EDO	B	421	4/4	0.80	0.21	33,34,40,41	0
6	EDO	A	431	4/4	0.81	0.14	17,23,29,31	0
3	GOL	B	409	6/6	0.82	0.19	29,35,36,43	0
3	GOL	A	414	6/6	0.82	0.28	33,48,49,52	0
3	GOL	A	412	6/6	0.83	0.29	31,42,44,45	0
3	GOL	B	411	6/6	0.83	0.34	26,32,35,40	0
6	EDO	A	430	4/4	0.83	0.19	30,36,38,40	0
7	PEG	A	433	7/7	0.83	0.23	18,21,32,38	0
6	EDO	B	420	4/4	0.86	0.22	27,31,32,33	0
6	EDO	B	418	4/4	0.86	0.16	35,37,39,41	0
7	PEG	B	427	7/7	0.86	0.22	20,25,26,26	0
3	GOL	A	406[A]	6/6	0.87	0.16	35,37,38,41	6
3	GOL	A	413	6/6	0.87	0.17	29,38,42,43	0
3	GOL	A	405	6/6	0.87	0.19	19,24,29,31	0
3	GOL	B	413	6/6	0.87	0.36	27,46,48,51	0
3	GOL	A	406[B]	6/6	0.87	0.16	16,26,27,28	6
3	GOL	B	406	6/6	0.88	0.15	16,20,21,23	0
3	GOL	A	403	6/6	0.88	0.11	22,22,25,30	0
6	EDO	A	428	4/4	0.88	0.36	34,35,36,37	0
3	GOL	B	408	6/6	0.88	0.20	27,41,42,43	0
6	EDO	B	417	4/4	0.88	0.24	17,23,23,32	0
3	GOL	B	407	6/6	0.88	0.18	28,37,39,48	0

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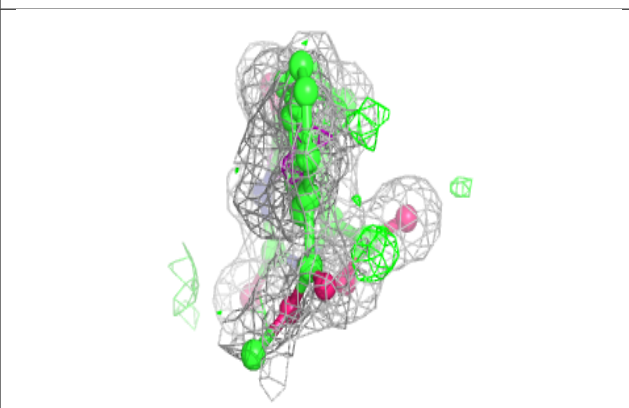
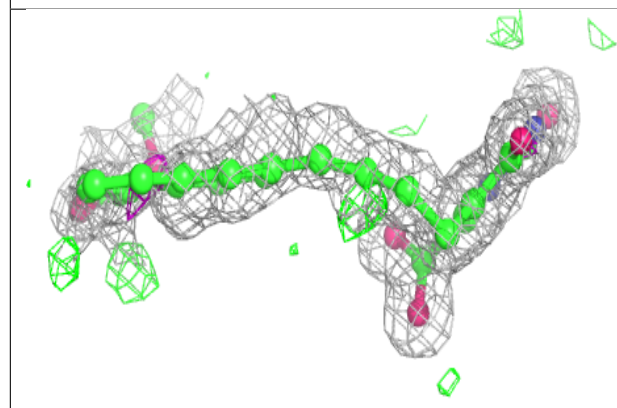
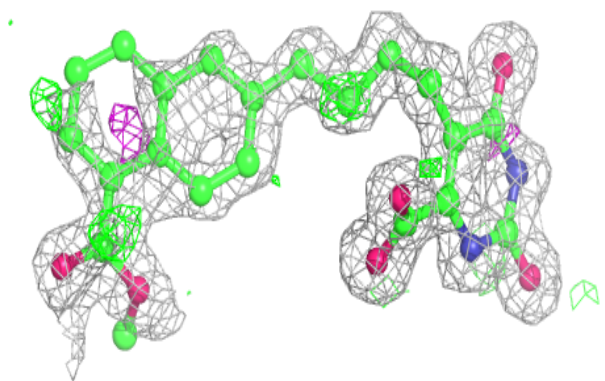
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	418	4/4	0.89	0.23	15,24,30,31	0
6	EDO	A	424	4/4	0.89	0.20	30,30,37,40	0
3	GOL	A	409	6/6	0.89	0.16	23,25,30,38	0
3	GOL	A	404	6/6	0.90	0.16	19,23,33,33	0
3	GOL	A	411	6/6	0.90	0.48	25,41,44,52	0
3	GOL	B	410	6/6	0.90	0.42	20,39,42,43	0
6	EDO	A	423	4/4	0.91	0.23	20,27,28,35	0
6	EDO	B	423	4/4	0.91	0.29	22,29,34,35	0
6	EDO	A	422	4/4	0.91	0.13	31,32,36,37	0
3	GOL	B	404	6/6	0.91	0.15	22,23,24,25	0
6	EDO	A	421	4/4	0.92	0.27	22,28,33,34	0
6	EDO	B	426	4/4	0.92	0.20	25,31,33,35	0
4	CAC	A	415	5/5	0.92	0.28	11,18,21,21	0
6	EDO	A	420	4/4	0.93	0.25	27,28,30,35	0
4	CAC	A	416	5/5	0.93	0.41	33,35,43,44	0
6	EDO	B	419	4/4	0.94	0.19	19,20,22,23	0
8	NCO	A	435[B]	7/7	0.94	0.35	14,25,29,30	7
2	W87	B	401[B]	29/29	0.94	0.15	5,9,24,29	29
2	W87	A	401	29/29	0.94	0.12	5,16,32,34	0
8	NCO	A	435[A]	7/7	0.94	0.35	16,26,28,29	7
2	W87	B	401[A]	29/29	0.94	0.15	5,11,27,29	29
6	EDO	B	425	4/4	0.95	0.21	18,21,21,24	0
7	PEG	A	432	7/7	0.95	0.14	11,23,26,30	0
8	NCO	A	434	7/7	0.96	0.31	7,14,18,19	0
3	GOL	A	402[A]	6/6	0.96	0.10	8,9,10,10	6
3	GOL	A	402[B]	6/6	0.96	0.10	8,11,11,11	6
4	CAC	B	414	5/5	0.96	0.20	10,16,19,19	0
3	GOL	B	402	6/6	0.96	0.07	15,15,18,18	0
5	FMN	A	417	31/31	0.99	0.07	3,4,6,6	0
5	FMN	B	416	31/31	0.99	0.08	3,4,6,6	0

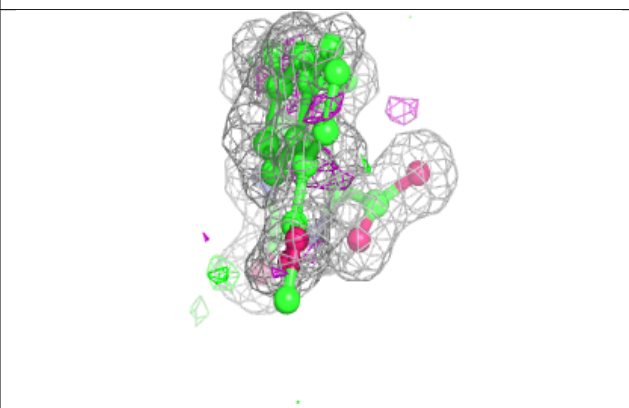
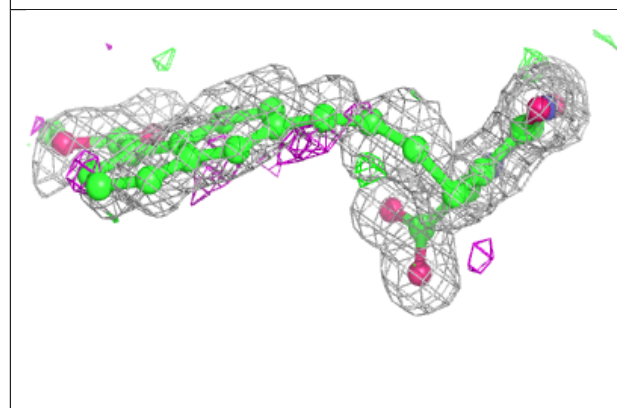
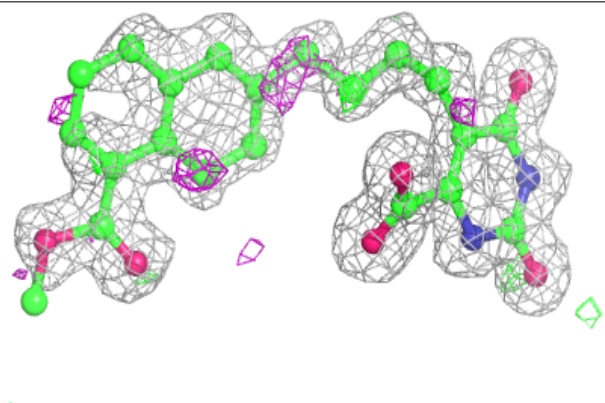
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around W87 B 401 (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 W87 A 401:**

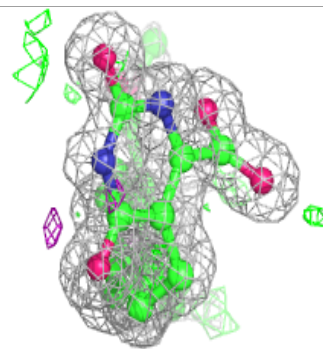
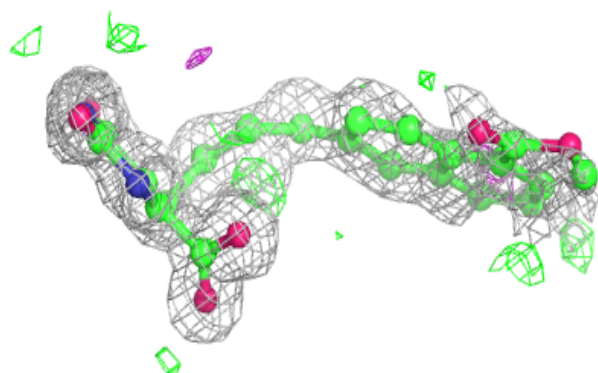
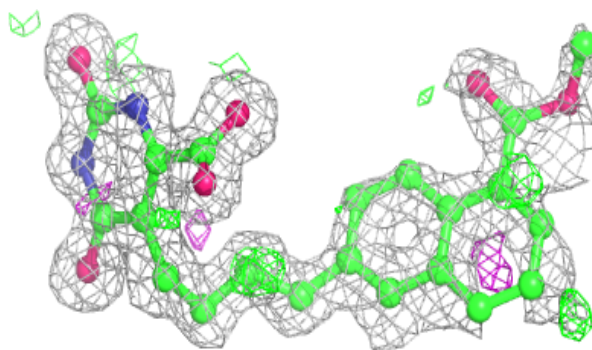
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





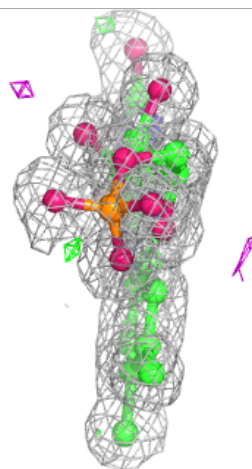
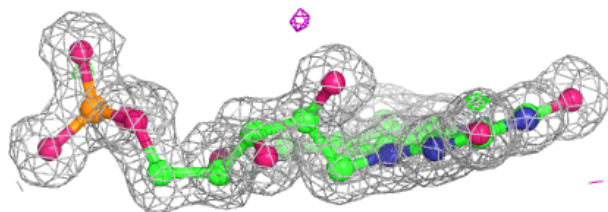
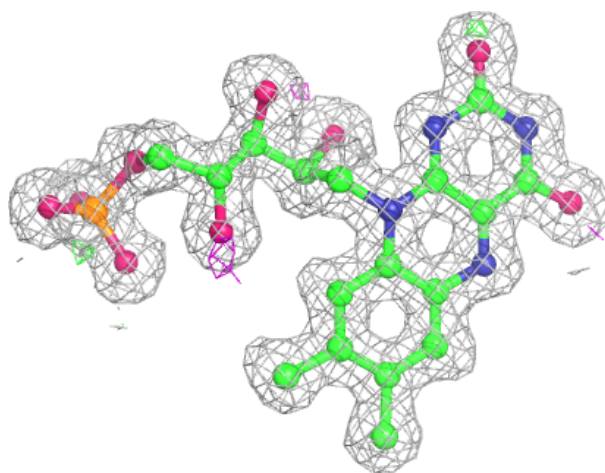
**Electron density around W87 B 401 (A):**

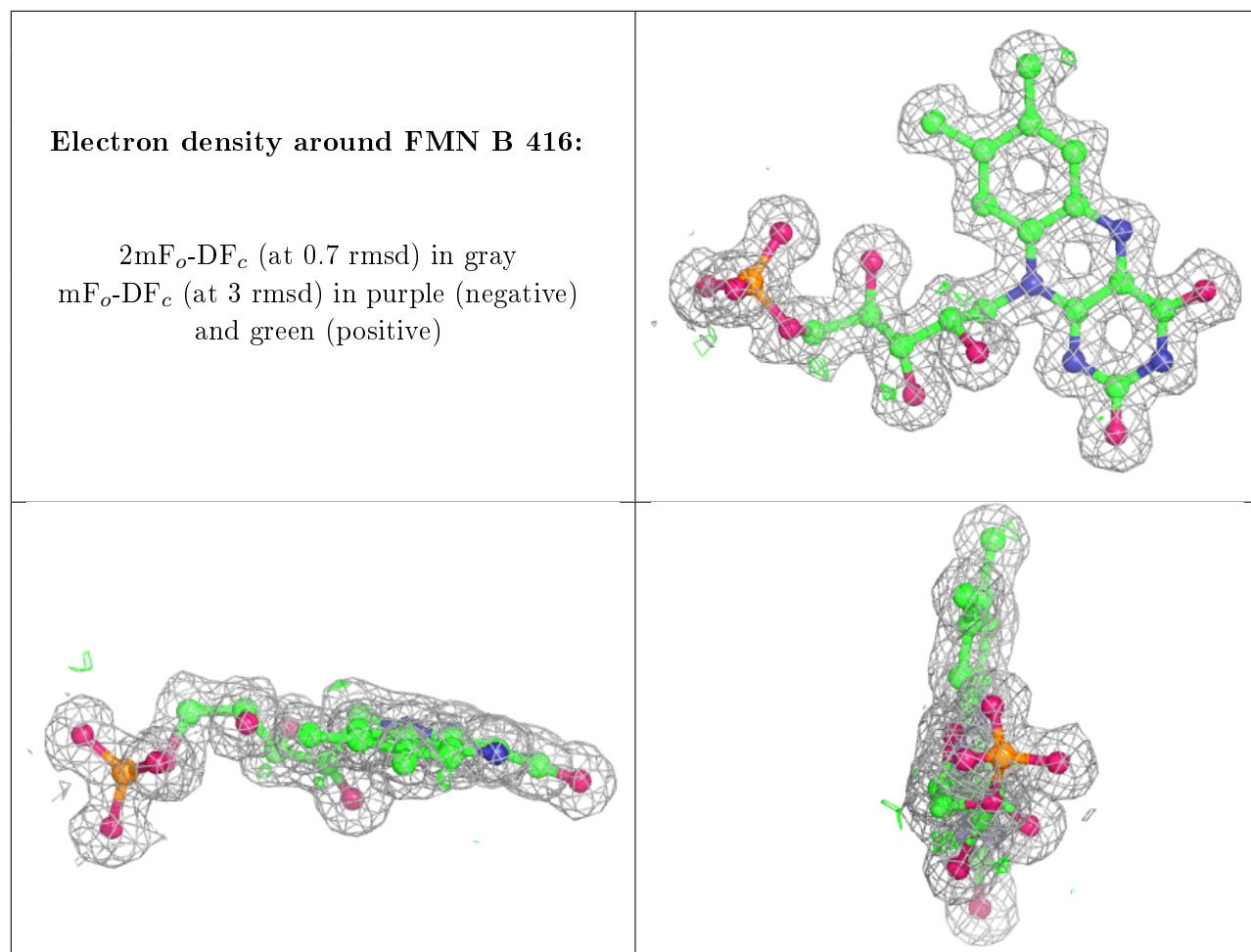
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN A 417:**

$2mF_o-DF_c$  (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.