Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 04:47 PM EDT

PDB ID	:	3W2K
Title	:	Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-3-165
Authors	:	Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Shiba, T.; Sakamoto, K.; Suzuki, S.; Balogun, E.O.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
Deposited on	:	2012-11-29
Resolution	:	1.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

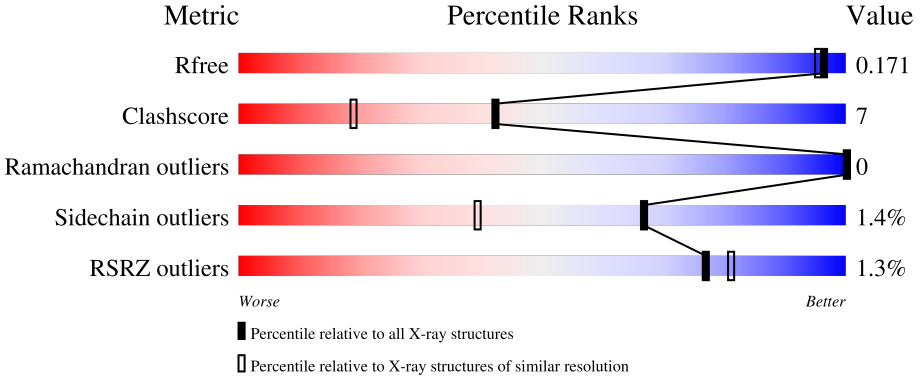
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	.% 87% 12%
1	B	313	2% 85% 13% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	410	-	-	X	-

2 Entry composition (i)

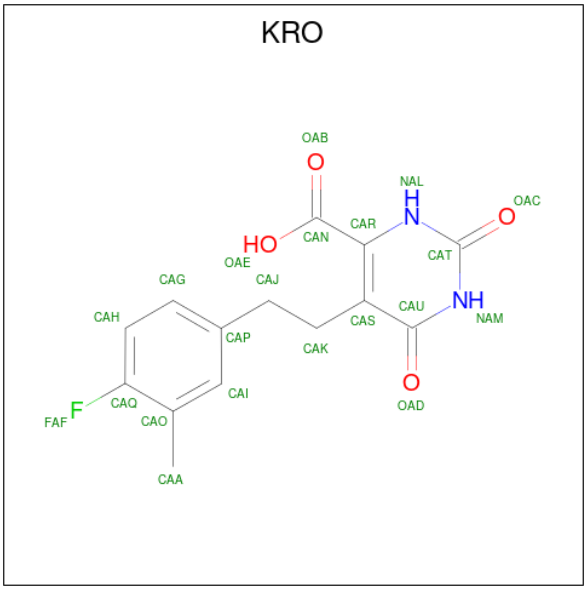
There are 6 unique types of molecules in this entry. The entry contains 5727 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

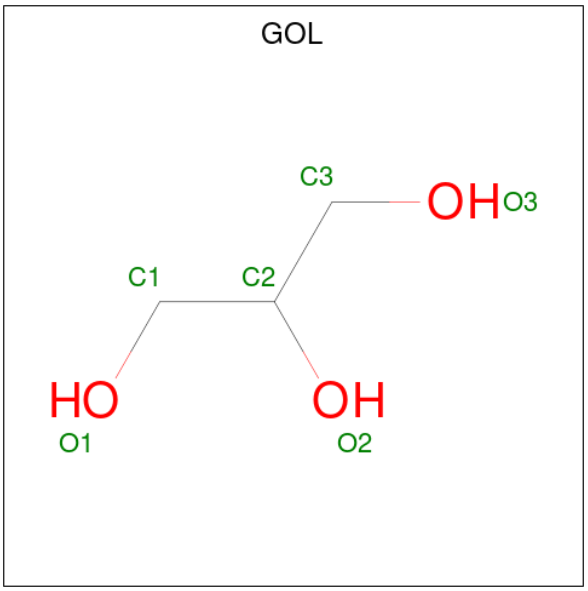
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2388	1530	396	444	18	0	0	0
1	B	313	2388	1530	396	444	18	0	0	0

- Molecule 2 is 5-[2-(4-fluoro-3-methylphenyl)ethyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: KRO) (formula: $C_{14}H_{13}FN_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	21	14	1	2	4	0	0
2	B	1	21	14	1	2	4	0	0

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



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

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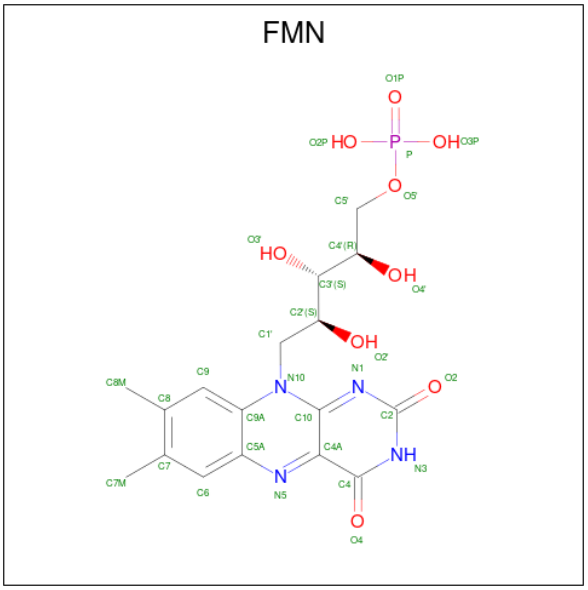
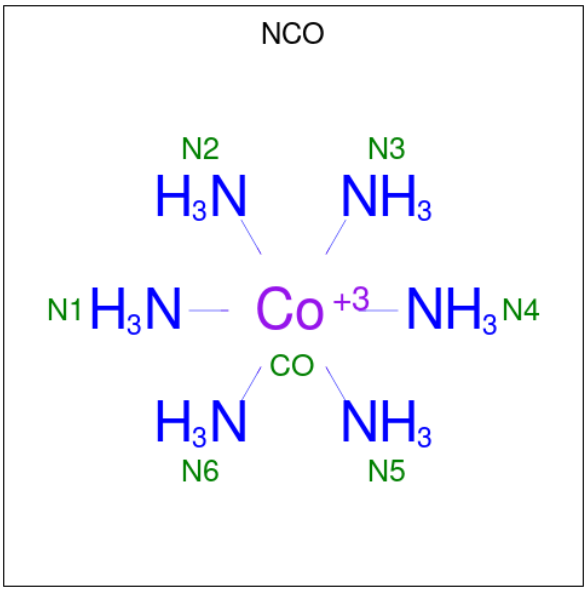
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	B	1	6	3	3		0	0
			Total	C	O			
3	B	1	6	3	3		0	0
			Total	C	O			
3	B	1	6	3	3		0	0
			Total	C	O			
3	B	1	6	3	3		0	0
			Total	C	O			
3	B	1	6	3	3		0	0
			Total	C	O			
3	B	1	6	3	3		0	0
			Total	C	O			
3	B	1	6	3	3		0	0
			Total	C	O			
3	B	1	6	3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

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 5 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).



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

- Molecule 6 is water.

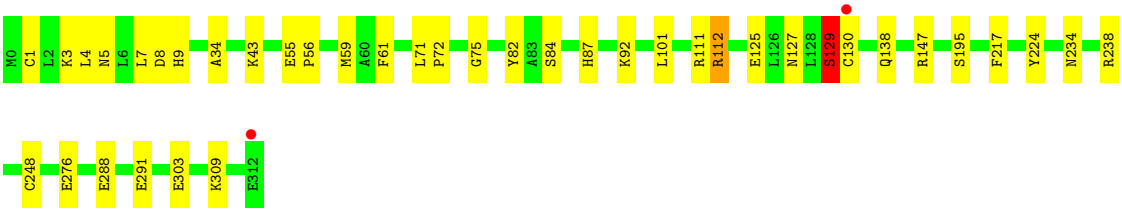
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	364	364	364	0	0
			Total	O		
6	B	344	344	344	0	0

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.

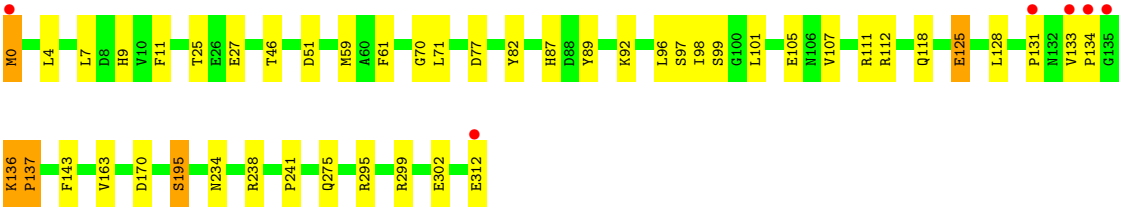
• Molecule 1: Dihydroorotate dehydrogenase (fumarate)

Chain A:



• Molecule 1: Dihydroorotate dehydrogenase (fumarate)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.06Å 71.98Å 128.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.66 – 1.54 34.66 – 1.54	Depositor EDS
% Data completeness (in resolution range)	83.2 (34.66-1.54) 83.3 (34.66-1.54)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.12 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.136 , 0.169 0.138 , 0.171	Depositor DCC
R_{free} test set	3970 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	11.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5727	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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 22.47 % 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 5.6644e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.38	15/2440 (0.6%)	1.16	5/3305 (0.2%)
1	B	1.30	7/2440 (0.3%)	1.13	10/3305 (0.3%)
All	All	1.34	22/4880 (0.5%)	1.14	15/6610 (0.2%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	GLU	CD-OE1	-7.98	1.16	1.25
1	A	129	SER	CB-OG	7.58	1.52	1.42
1	A	56	PRO	N-CD	6.30	1.56	1.47
1	B	134	PRO	N-CD	5.89	1.56	1.47
1	A	75	GLY	C-O	-5.83	1.14	1.23
1	B	195	SER	CB-OG	-5.82	1.34	1.42
1	A	72	PRO	N-CD	5.80	1.55	1.47
1	A	276	GLU	CD-OE1	5.75	1.31	1.25
1	A	84	SER	CB-OG	-5.64	1.34	1.42
1	A	248	CYS	C-O	-5.53	1.12	1.23
1	A	288	GLU	CD-OE1	-5.53	1.19	1.25
1	B	137	PRO	N-CD	5.51	1.55	1.47
1	A	125	GLU	CG-CD	5.29	1.59	1.51
1	A	55	GLU	CD-OE1	-5.28	1.19	1.25
1	B	105	GLU	CD-OE1	-5.24	1.19	1.25
1	B	27	GLU	CD-OE2	5.18	1.31	1.25
1	A	43	LYS	CE-NZ	5.16	1.61	1.49
1	B	125	GLU	CD-OE1	5.13	1.31	1.25
1	A	127	ASN	CG-OD1	-5.12	1.12	1.24
1	A	4	LEU	C-O	-5.10	1.13	1.23
1	A	224	TYR	CE1-CZ	-5.08	1.31	1.38
1	B	25	THR	C-O	-5.01	1.13	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	LYS	CD-CE-NZ	10.56	135.99	111.70
1	B	295	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	4	LEU	CB-CG-CD1	5.80	120.86	111.00
1	A	147	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	170	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	11	PHE	CB-CG-CD1	5.56	124.69	120.80
1	A	130	CYS	N-CA-CB	-5.54	100.62	110.60
1	B	77	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	51	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	299	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	112	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	77	ASP	CB-CG-OD1	5.24	123.01	118.30
1	B	136	LYS	C-N-CD	5.20	139.32	128.40
1	B	112	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	8	ASP	CB-CG-OD1	5.03	122.83	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	2388	0	2391	21	0
1	B	2388	0	2391	41	0
2	A	21	0	12	4	0
2	B	21	0	12	6	0
3	A	66	0	86	4	0
3	B	66	0	88	16	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0
5	A	7	0	0	0	0
6	A	364	0	0	8	0
6	B	344	0	0	11	0
All	All	5727	0	5018	69	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 7.

All (69) 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:118:GLN:HG3	6:B:837:HOH:O	1.48	1.09
1:A:61:PHE:CE1	3:A:407:GOL:H32	2.14	0.81
2:B:401:KRO:CAH	3:B:403:GOL:O3	2.30	0.80
1:B:136:LYS:HG3	1:B:137:PRO:HD2	1.66	0.75
1:B:9:HIS:CE1	3:B:410:GOL:H11	2.23	0.74
1:B:9:HIS:CE1	3:B:410:GOL:C1	2.72	0.72
1:A:129:SER:HA	1:A:138:GLN:OE1	1.90	0.72
1:A:71:LEU:HD22	2:A:401:KRO:H8	1.74	0.69
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.39	0.68
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.44	0.66
2:B:401:KRO:H12	3:B:403:GOL:O3	1.95	0.66
1:A:59:MET:HE3	6:A:626:HOH:O	1.94	0.66
1:A:291:GLU:CD	6:A:785:HOH:O	2.35	0.64
1:B:101:LEU:HD22	1:B:131:PRO:HG2	1.79	0.63
1:B:118:GLN:CG	6:B:837:HOH:O	2.23	0.63
1:B:101:LEU:HD22	1:B:131:PRO:CG	2.29	0.62
3:A:404:GOL:H32	6:A:572:HOH:O	2.00	0.62
1:B:9:HIS:ND1	3:B:410:GOL:H11	2.15	0.62
1:A:7:LEU:O	1:A:9:HIS:HD2	1.83	0.61
1:B:241:PRO:HA	3:B:404:GOL:H12	1.83	0.61
1:A:59:MET:CE	6:A:626:HOH:O	2.47	0.61
1:B:89:TYR:HB3	3:B:410:GOL:H2	1.84	0.60
1:B:96:LEU:CD2	1:B:98:ILE:HD11	2.32	0.59
1:B:136:LYS:HG3	1:B:137:PRO:CD	2.34	0.57
1:B:59:MET:HE3	6:B:618:HOH:O	2.03	0.57
1:B:70:GLY:HA2	2:B:401:KRO:H11	1.85	0.57
1:A:111:ARG:HD3	6:A:863:HOH:O	2.04	0.57
1:B:101:LEU:CD2	1:B:131:PRO:HG2	2.35	0.56
2:B:401:KRO:H9	6:B:802:HOH:O	2.06	0.56
1:B:9:HIS:ND1	3:B:410:GOL:C1	2.71	0.54
1:B:128:LEU:HD12	1:B:163:VAL:CG1	2.37	0.54
2:B:401:KRO:CAG	3:B:403:GOL:O3	2.56	0.54
1:A:101:LEU:HD21	2:A:401:KRO:H10	1.89	0.54
1:B:143:PHE:CE2	3:B:412:GOL:H31	2.42	0.54
1:A:87:HIS:HE1	1:A:92:LYS:O	1.92	0.53
1:B:133:VAL:O	1:B:136:LYS:HB2	2.08	0.53
1:B:128:LEU:HD12	1:B:163:VAL:HG11	1.90	0.53
3:B:410:GOL:H31	6:B:772:HOH:O	2.09	0.53
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.06	0.52
1:A:195:SER:HB3	6:A:793:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:HIS:HE1	1:B:92:LYS:O	1.92	0.52
1:B:59:MET:CE	6:B:618:HOH:O	2.58	0.52
1:A:112:ARG:NH2	6:A:806:HOH:O	2.41	0.51
1:B:0:MET:N	6:B:613:HOH:O	2.44	0.51
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.94	0.50
1:A:61:PHE:CZ	3:A:407:GOL:H32	2.47	0.50
1:B:111:ARG:NH2	6:B:787:HOH:O	2.30	0.49
1:A:71:LEU:CD2	2:A:401:KRO:H11	2.42	0.49
1:B:7:LEU:O	1:B:9:HIS:HD2	1.95	0.48
1:B:195:SER:HB3	6:B:786:HOH:O	2.12	0.48
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.96	0.47
1:B:61:PHE:CE1	3:B:406:GOL:H11	2.50	0.46
1:B:101:LEU:HD22	1:B:131:PRO:HG3	1.98	0.45
1:B:9:HIS:HE1	3:B:410:GOL:C1	2.26	0.45
1:B:97:SER:HA	1:B:125:GLU:O	2.17	0.44
1:B:128:LEU:CD1	1:B:163:VAL:CG1	2.94	0.44
1:B:46:THR:HG23	1:B:71:LEU:HD21	1.99	0.44
1:A:34:ALA:HB3	3:A:402:GOL:H12	2.00	0.44
2:B:401:KRO:CAA	6:B:802:HOH:O	2.64	0.44
1:B:96:LEU:CD2	1:B:98:ILE:CD1	2.97	0.43
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.13	0.43
1:B:107:VAL:O	1:B:111:ARG:HG3	2.20	0.42
1:A:71:LEU:HD23	2:A:401:KRO:H11	2.02	0.42
1:B:128:LEU:CD1	1:B:163:VAL:HG11	2.49	0.42
1:B:275:GLN:NE2	6:B:608:HOH:O	2.51	0.42
1:A:217:PHE:CE1	3:B:402:GOL:H12	2.55	0.41
1:B:143:PHE:CE2	3:B:412:GOL:C3	3.03	0.41
1:A:309:LYS:NZ	6:A:758:HOH:O	2.40	0.41
1:B:9:HIS:CE1	3:B:410:GOL:H12	2.56	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	311/313 (99%)	304 (98%)	7 (2%)	0	100	100
1	B	311/313 (99%)	304 (98%)	7 (2%)	0	100	100
All	All	622/626 (99%)	608 (98%)	14 (2%)	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	258/258 (100%)	255 (99%)	3 (1%)	71	47
1	B	258/258 (100%)	254 (98%)	4 (2%)	62	33
All	All	516/516 (100%)	509 (99%)	7 (1%)	67	39

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	5	ASN
1	A	129	SER
1	B	0	MET
1	B	99	SER
1	B	302	GLU
1	B	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	HIS
1	A	87	HIS
1	A	152	GLN
1	A	234	ASN
1	A	275	GLN

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Mol	Chain	Res	Type
1	B	9	HIS
1	B	87	HIS
1	B	152	GLN
1	B	215	GLN
1	B	234	ASN
1	B	275	GLN

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)

27 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	FMN	A	413	-	33,33,33	1.19	2 (6%)	48,50,50	1.31	6 (12%)
3	GOL	B	408	-	5,5,5	1.30	1 (20%)	5,5,5	1.22	1 (20%)
3	GOL	A	402	-	5,5,5	0.91	0	5,5,5	2.35	3 (60%)
3	GOL	A	407	-	5,5,5	1.55	1 (20%)	5,5,5	1.89	1 (20%)
2	KRO	A	401	-	21,22,22	3.04	10 (47%)	28,31,31	1.71	5 (17%)
3	GOL	A	409	-	5,5,5	0.84	0	5,5,5	0.49	0
3	GOL	B	406	-	5,5,5	0.69	0	5,5,5	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	403	-	5,5,5	0.75	0	5,5,5	0.49	0
3	GOL	B	411	-	5,5,5	0.38	0	5,5,5	0.65	0
3	GOL	A	404	-	5,5,5	0.47	0	5,5,5	0.45	0
2	KRO	B	401	-	21,22,22	2.74	8 (38%)	28,31,31	2.48	8 (28%)
3	GOL	A	406	-	5,5,5	0.95	0	5,5,5	1.30	1 (20%)
3	GOL	A	412	-	5,5,5	0.36	0	5,5,5	0.68	0
3	GOL	B	402	-	5,5,5	1.06	0	5,5,5	1.22	0
4	FMN	B	413	-	33,33,33	1.53	6 (18%)	48,50,50	1.21	5 (10%)
3	GOL	B	407	-	5,5,5	0.57	0	5,5,5	1.05	0
3	GOL	B	409	-	5,5,5	0.79	0	5,5,5	1.82	2 (40%)
3	GOL	A	408	-	5,5,5	0.50	0	5,5,5	0.95	0
5	NCO	A	414	-	6,6,6	3.34	6 (100%)	-		
3	GOL	B	404	-	5,5,5	0.57	0	5,5,5	0.72	0
3	GOL	A	411	-	5,5,5	0.72	0	5,5,5	0.36	0
3	GOL	B	412	-	5,5,5	0.79	0	5,5,5	0.48	0
3	GOL	A	410	-	5,5,5	0.26	0	5,5,5	0.95	0
3	GOL	B	410	-	5,5,5	0.40	0	5,5,5	0.85	0
3	GOL	B	405	-	5,5,5	0.54	0	5,5,5	0.86	0
3	GOL	A	405	-	5,5,5	1.32	1 (20%)	5,5,5	1.02	0
3	GOL	B	403	-	5,5,5	0.66	0	5,5,5	1.53	2 (40%)

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
4	FMN	A	413	-	-	1/18/18/18	0/3/3/3
3	GOL	B	408	-	-	0/4/4/4	-
3	GOL	A	402	-	-	1/4/4/4	-
3	GOL	A	407	-	-	2/4/4/4	-
2	KRO	A	401	-	-	4/9/9/9	0/2/2/2
3	GOL	A	409	-	-	2/4/4/4	-
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	B	411	-	-	0/4/4/4	-
3	GOL	A	404	-	-	3/4/4/4	-
2	KRO	B	401	-	-	3/9/9/9	0/2/2/2
3	GOL	A	406	-	-	0/4/4/4	-
3	GOL	A	412	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	402	-	-	0/4/4/4	-
4	FMN	B	413	-	-	1/18/18/18	0/3/3/3
3	GOL	B	407	-	-	2/4/4/4	-
3	GOL	B	409	-	-	0/4/4/4	-
3	GOL	A	408	-	-	0/4/4/4	-
3	GOL	B	404	-	-	4/4/4/4	-
3	GOL	A	411	-	-	0/4/4/4	-
3	GOL	B	412	-	-	0/4/4/4	-
3	GOL	A	410	-	-	2/4/4/4	-
3	GOL	B	410	-	-	2/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	KRO	CAJ-CAP	-8.36	1.27	1.51
2	B	401	KRO	CAJ-CAP	-7.92	1.28	1.51
2	B	401	KRO	CAA-CAO	-6.00	1.39	1.51
2	A	401	KRO	CAR-CAN	4.24	1.55	1.48
5	A	414	NCO	CO-N3	4.01	2.11	1.96
2	B	401	KRO	CAR-NAL	3.98	1.46	1.38
2	A	401	KRO	CAU-CAS	-3.81	1.38	1.44
2	A	401	KRO	CAK-CAS	-3.64	1.41	1.51
2	A	401	KRO	CAO-CAQ	3.63	1.42	1.37
5	A	414	NCO	CO-N6	3.54	2.09	1.96
2	A	401	KRO	CAR-NAL	3.40	1.45	1.38
2	A	401	KRO	CAI-CAO	-3.39	1.34	1.39
4	A	413	FMN	C5'-C4'	3.32	1.56	1.51
5	A	414	NCO	CO-N4	3.31	2.08	1.96
4	B	413	FMN	C1'-C2'	3.31	1.57	1.52
5	A	414	NCO	CO-N1	3.23	2.08	1.96
2	A	401	KRO	CAA-CAO	-3.15	1.44	1.51
4	B	413	FMN	C6-C7	-3.11	1.35	1.39
5	A	414	NCO	CO-N2	2.91	2.07	1.96
4	B	413	FMN	C4A-N5	2.90	1.36	1.30
5	A	414	NCO	CO-N5	2.90	2.07	1.96
3	A	407	GOL	O2-C2	-2.81	1.35	1.43
2	B	401	KRO	CAO-CAQ	2.81	1.41	1.37
3	B	408	GOL	O2-C2	2.73	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	KRO	CAT-NAM	2.72	1.42	1.37
2	B	401	KRO	CAU-CAS	-2.59	1.40	1.44
4	B	413	FMN	C4-N3	-2.50	1.34	1.38
2	A	401	KRO	OAE-CAN	-2.42	1.23	1.30
3	A	405	GOL	O2-C2	2.36	1.50	1.43
4	B	413	FMN	C5A-N5	-2.34	1.34	1.39
2	B	401	KRO	OAE-CAN	-2.31	1.23	1.30
2	B	401	KRO	OAD-CAU	2.27	1.27	1.23
4	B	413	FMN	C9-C8	2.23	1.42	1.39
4	A	413	FMN	C4A-N5	2.14	1.34	1.30
2	B	401	KRO	CAG-CAH	2.12	1.42	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	KRO	CAI-CAO-CAQ	8.48	121.46	116.06
2	A	401	KRO	CAJ-CAP-CAI	-5.14	112.11	120.54
2	B	401	KRO	CAN-CAR-CAS	4.75	127.23	122.74
4	A	413	FMN	O2-C2-N1	-3.94	115.30	121.83
2	B	401	KRO	CAS-CAU-NAM	3.58	118.36	115.69
2	B	401	KRO	CAH-CAQ-CAO	-3.57	119.28	124.08
2	A	401	KRO	CAN-CAR-CAS	3.43	125.98	122.74
3	A	402	GOL	O2-C2-C1	-3.39	94.17	109.12
3	A	407	GOL	C3-C2-C1	3.22	124.24	111.70
2	B	401	KRO	CAA-CAO-CAQ	-3.18	118.05	121.75
3	A	402	GOL	O2-C2-C3	-3.12	95.40	109.12
4	B	413	FMN	C7M-C7-C8	-3.03	114.53	120.74
4	B	413	FMN	C8M-C8-C7	2.91	126.71	120.74
2	A	401	KRO	CAG-CAP-CAI	2.87	122.56	118.54
2	B	401	KRO	NAM-CAT-NAL	2.84	120.36	115.80
4	B	413	FMN	C9-C8-C7	-2.81	115.64	119.67
3	B	409	GOL	C3-C2-C1	-2.79	100.85	111.70
2	A	401	KRO	CAI-CAO-CAQ	2.78	117.83	116.06
4	A	413	FMN	C9A-C9-C8	2.74	124.82	119.30
4	A	413	FMN	C9A-C5A-N5	-2.63	119.57	122.43
4	B	413	FMN	C7M-C7-C6	2.49	124.09	119.49
2	B	401	KRO	CAU-NAM-CAT	-2.47	122.79	126.34
3	B	403	GOL	C3-C2-C1	-2.39	102.40	111.70
3	A	402	GOL	C3-C2-C1	2.34	120.78	111.70
4	A	413	FMN	C4-C4A-N5	2.33	121.55	118.23
4	A	413	FMN	N3-C2-N1	2.33	123.95	119.38
2	A	401	KRO	CAH-CAG-CAP	-2.33	117.83	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	406	GOL	O3-C3-C2	2.31	121.30	110.20
4	B	413	FMN	O4-C4-C4A	-2.26	120.60	126.60
3	B	409	GOL	O2-C2-C3	2.16	118.64	109.12
3	B	403	GOL	O1-C1-C2	2.09	120.24	110.20
3	B	408	GOL	O2-C2-C3	2.08	118.27	109.12
2	B	401	KRO	CAO-CAI-CAP	-2.02	119.88	122.21
4	A	413	FMN	C9-C8-C7	-2.01	116.79	119.67

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	KRO	OAE-CAN-CAR-NAL
2	A	401	KRO	CAP-CAJ-CAK-CAS
2	B	401	KRO	OAE-CAN-CAR-NAL
3	A	402	GOL	O2-C2-C3-O3
3	A	405	GOL	O1-C1-C2-C3
3	A	407	GOL	C1-C2-C3-O3
3	A	409	GOL	O1-C1-C2-C3
3	A	412	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
3	B	410	GOL	C1-C2-C3-O3
3	B	410	GOL	O2-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
3	A	404	GOL	O1-C1-C2-C3
3	A	410	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
3	A	407	GOL	O2-C2-C3-O3
3	A	412	GOL	O2-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2
3	A	405	GOL	O1-C1-C2-O2
3	A	409	GOL	O1-C1-C2-O2
3	A	412	GOL	O1-C1-C2-O2
3	B	407	GOL	O1-C1-C2-O2
4	B	413	FMN	C4'-C5'-O5'-P
4	A	413	FMN	C4'-C5'-O5'-P
3	A	410	GOL	O2-C2-C3-O3
2	A	401	KRO	OAE-CAN-CAR-CAS
2	B	401	KRO	OAE-CAN-CAR-CAS
3	A	412	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	401	KRO	OAB-CAN-CAR-NAL
2	B	401	KRO	OAB-CAN-CAR-NAL
3	A	404	GOL	C1-C2-C3-O3

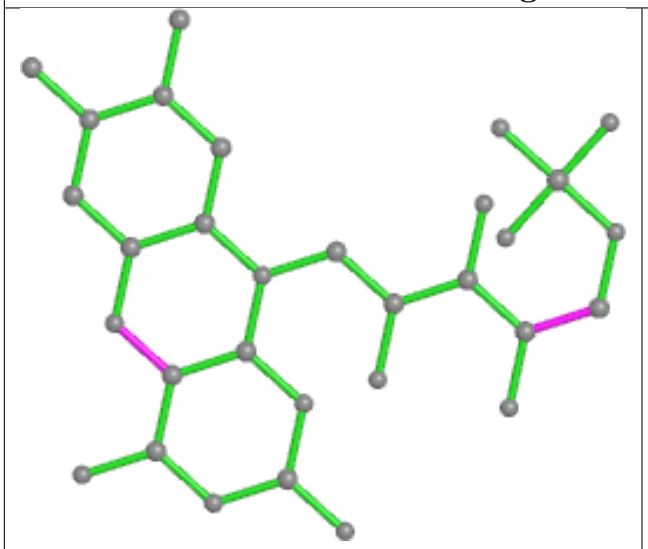
There are no ring outliers.

11 monomers are involved in 27 short contacts:

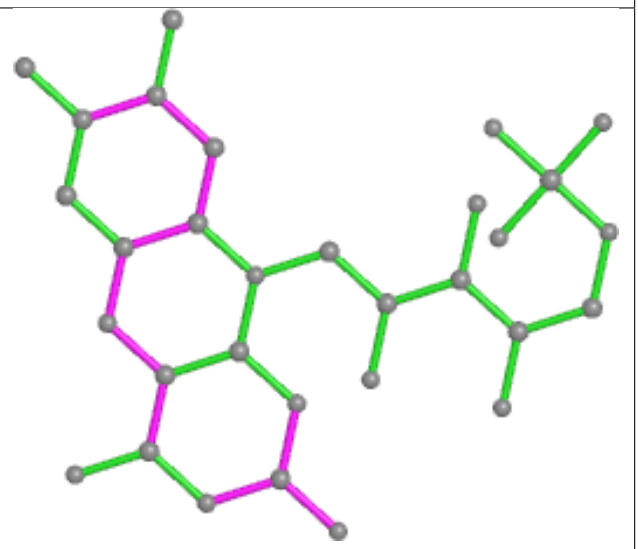
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	1	0
3	A	407	GOL	2	0
2	A	401	KRO	4	0
3	B	406	GOL	1	0
3	A	404	GOL	1	0
2	B	401	KRO	6	0
3	B	402	GOL	1	0
3	B	404	GOL	1	0
3	B	412	GOL	2	0
3	B	410	GOL	8	0
3	B	403	GOL	3	0

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.

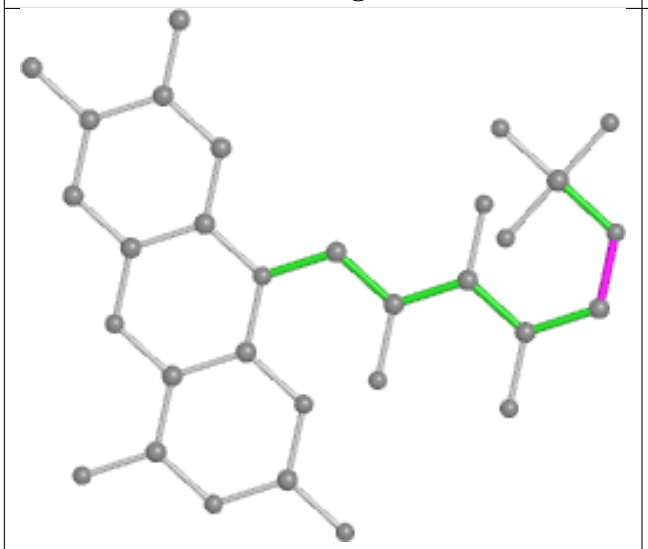
Ligand FMN A 413



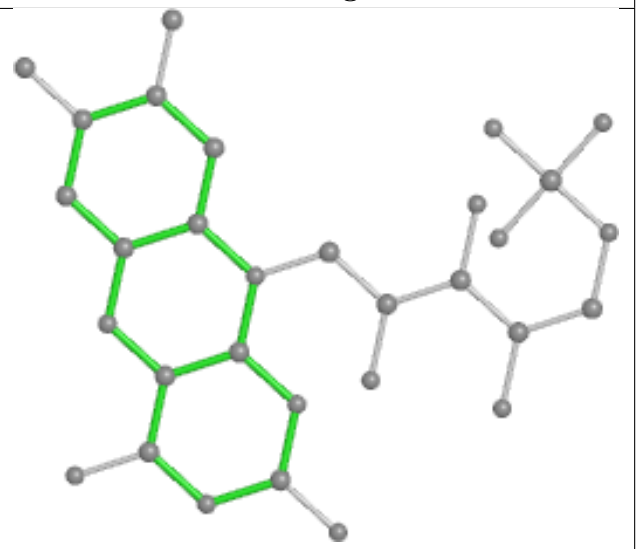
Bond lengths



Bond angles

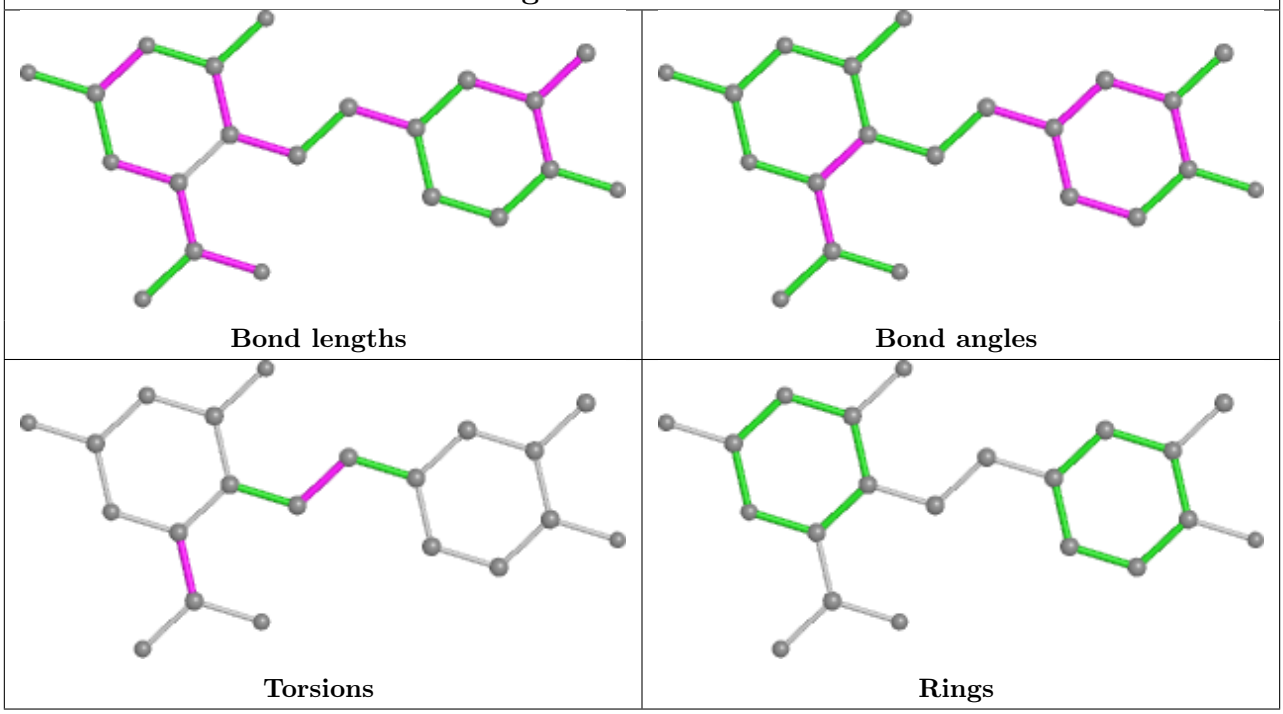


Torsions



Rings

Ligand KRO A 401



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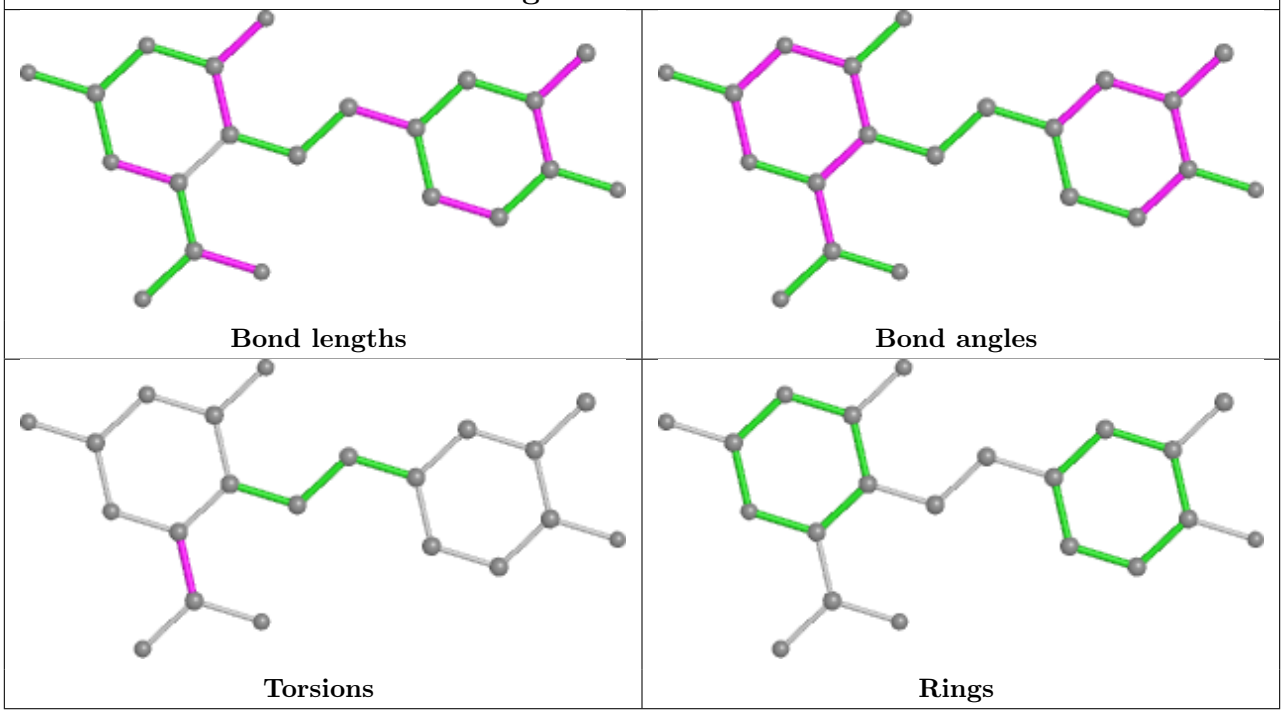
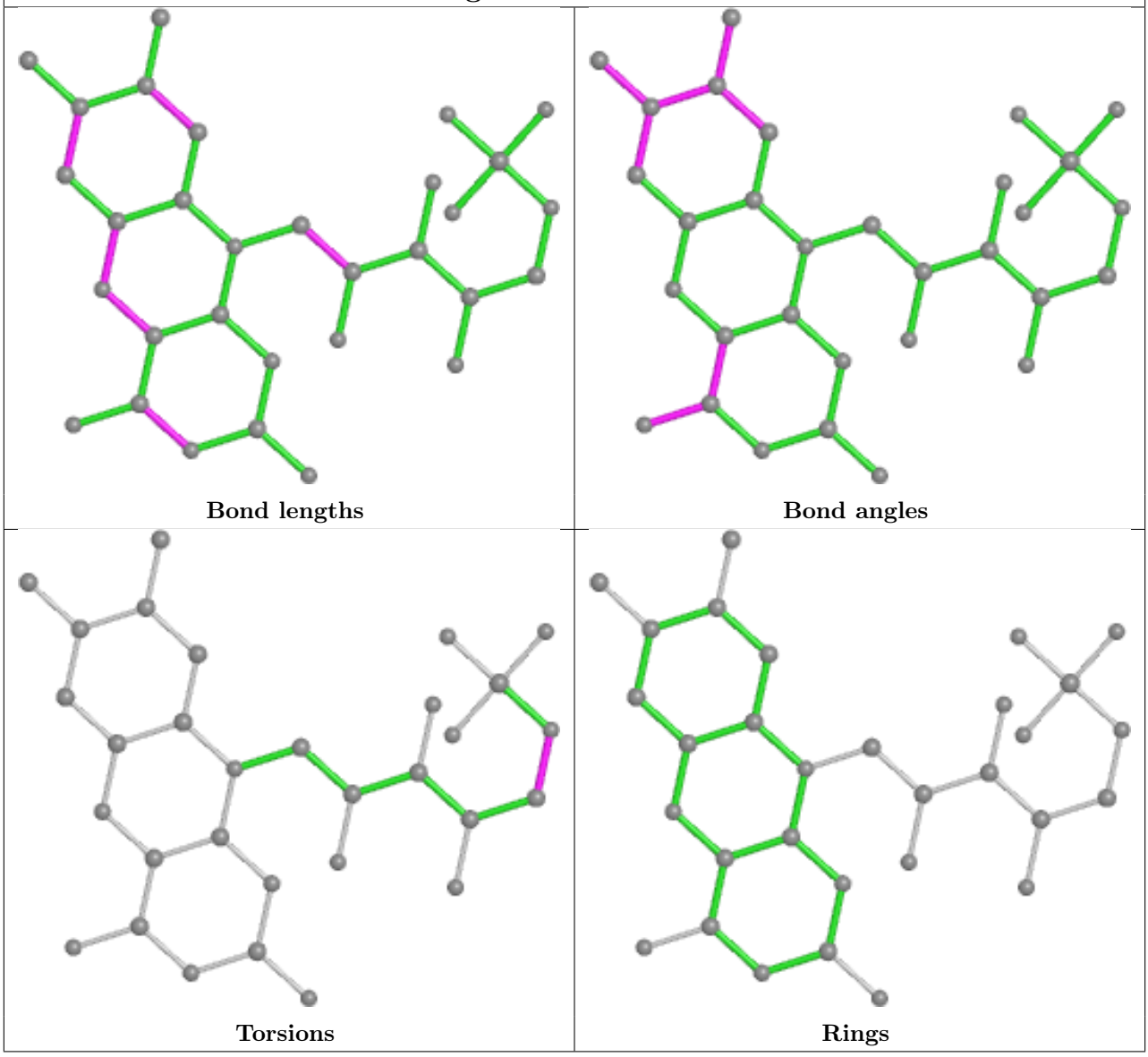


Ligand FMN B 413



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	313/313 (100%)	-0.32	2 (0%)	89	91	6, 11, 22, 51	0
1	B	313/313 (100%)	-0.25	6 (1%)	66	72	7, 12, 27, 53	0
All	All	626/626 (100%)	-0.28	8 (1%)	77	81	6, 11, 24, 53	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	VAL	4.8
1	B	312	GLU	4.2
1	A	312	GLU	4.1
1	B	134	PRO	3.5
1	B	131	PRO	3.2
1	B	0	MET	2.8
1	B	135	GLY	2.4
1	A	130	CYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

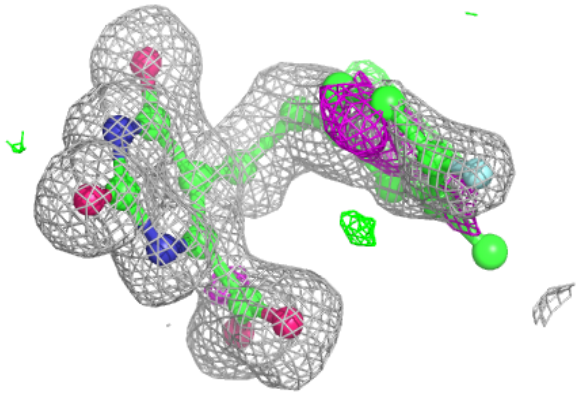
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

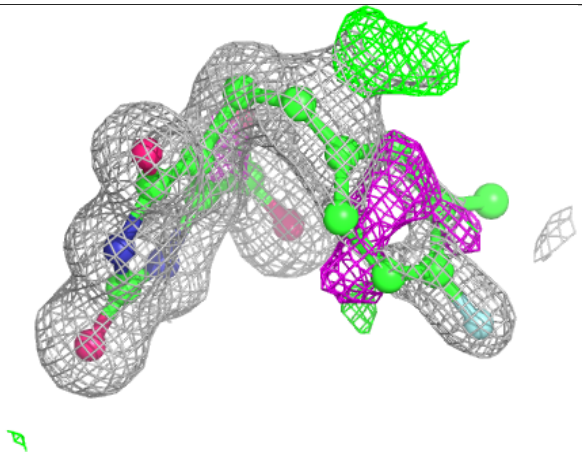
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	405	6/6	0.70	0.20	34,43,44,45	0
3	GOL	A	409	6/6	0.80	0.27	33,49,52,56	0
3	GOL	B	404	6/6	0.80	0.13	38,40,43,51	0
3	GOL	A	408	6/6	0.80	0.13	37,41,44,46	0
3	GOL	B	407	6/6	0.80	0.31	40,45,50,51	0
3	GOL	B	408	6/6	0.82	0.14	27,30,34,40	0
3	GOL	B	406	6/6	0.83	0.15	28,37,37,40	0
3	GOL	A	410	6/6	0.83	0.18	38,50,54,66	0
3	GOL	A	412	6/6	0.83	0.20	39,43,46,55	0
3	GOL	B	409	6/6	0.84	0.15	28,36,36,42	0
3	GOL	A	404	6/6	0.85	0.12	34,47,51,58	0
3	GOL	A	406	6/6	0.87	0.19	24,29,31,32	0
3	GOL	B	411	6/6	0.87	0.15	42,46,46,49	0
3	GOL	A	405	6/6	0.88	0.16	18,25,32,38	0
3	GOL	B	403	6/6	0.89	0.14	21,23,34,40	0
3	GOL	A	411	6/6	0.90	0.12	28,30,33,33	0
3	GOL	B	410	6/6	0.91	0.26	24,41,42,52	0
3	GOL	A	407	6/6	0.91	0.15	25,32,33,33	0
3	GOL	B	412	6/6	0.91	0.11	30,31,33,35	0
3	GOL	B	402	6/6	0.92	0.08	19,20,22,26	0
3	GOL	A	402	6/6	0.94	0.08	15,19,20,21	0
2	KRO	B	401	21/21	0.95	0.13	8,12,32,38	0
2	KRO	A	401	21/21	0.95	0.10	8,13,38,52	0
3	GOL	A	403	6/6	0.96	0.06	16,17,18,21	0
4	FMN	A	413	31/31	0.98	0.09	6,7,9,10	0
4	FMN	B	413	31/31	0.99	0.07	6,7,10,11	0
5	NCO	A	414	7/7	0.99	0.10	10,11,12,13	0

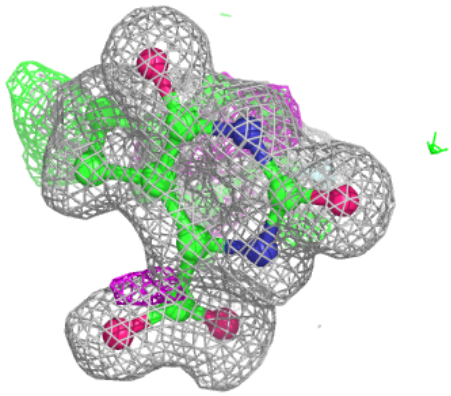
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KRO 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)

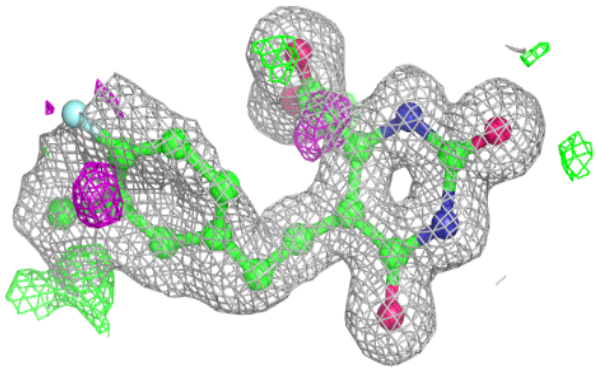


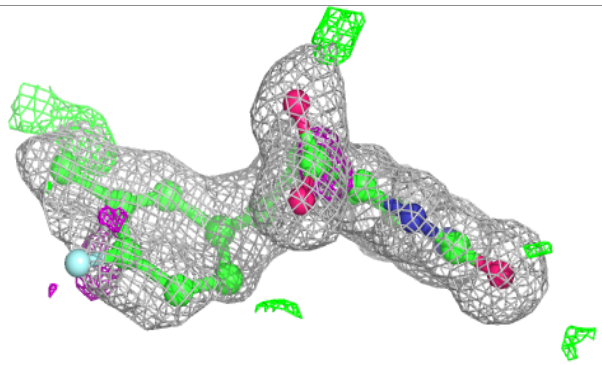


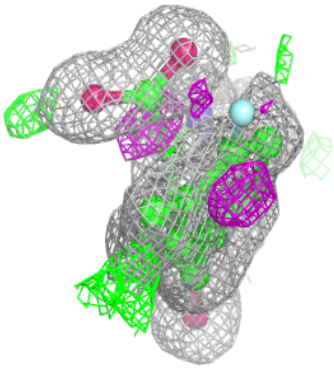


Electron density around KRO A 401:

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

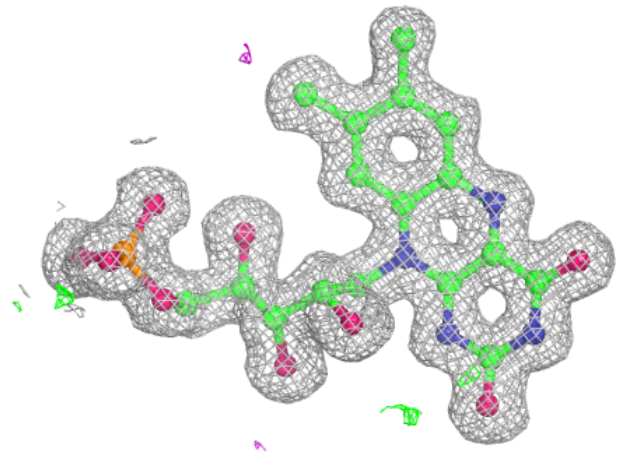


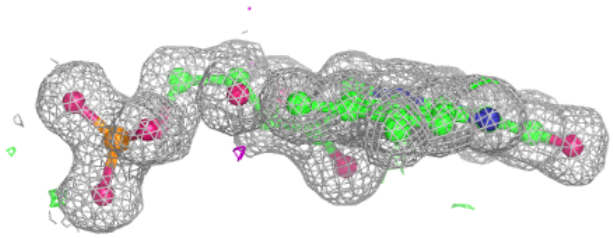


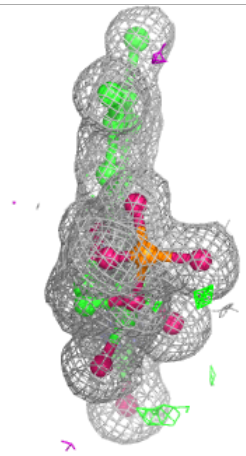


Electron density around FMN A 413:

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

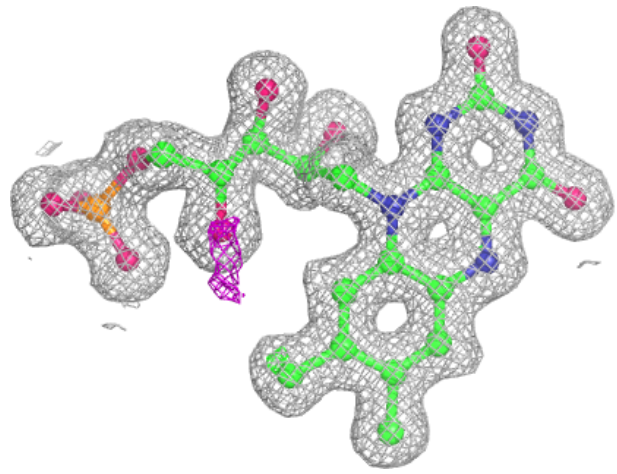


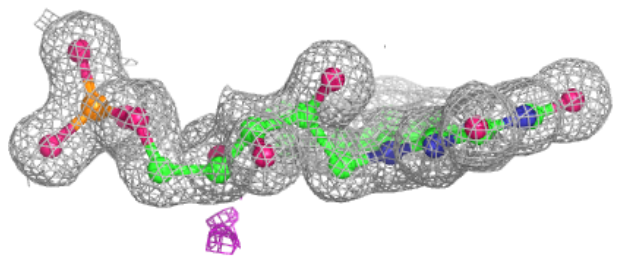


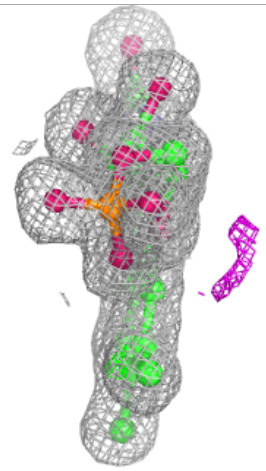


Electron density around FMN B 413:

$2mF_o$-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.