Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 09:52 AM EDT

PDB ID	:	4H2P
Title	:	Tetrameric form of 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase (MHPCO)
Authors	:	Kobayashi, J.; Yoshida, H.; Mikami, B.; Hayashi, H.; Kamitori, S.; Yagi, T.
Deposited on	:	2012-09-13
Resolution	:	1.98 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:

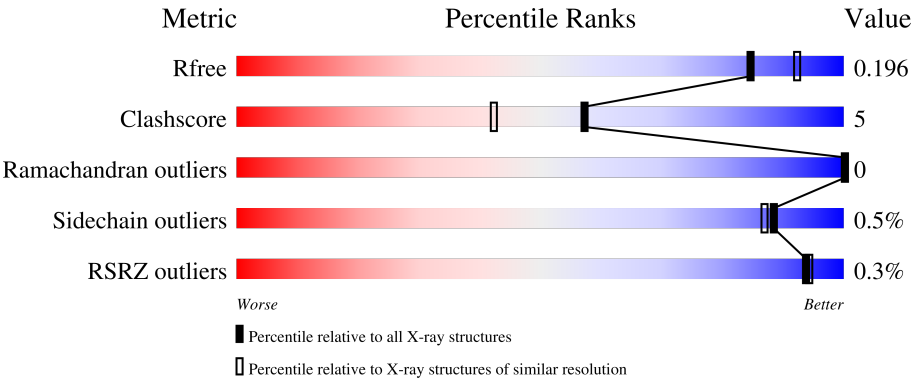
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	379	89% 9%
1	B	379	87% 10%
1	C	379	89% 9%
1	D	379	89% 9%

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
5	EDO	A	405	-	-	X	-

2 Entry composition

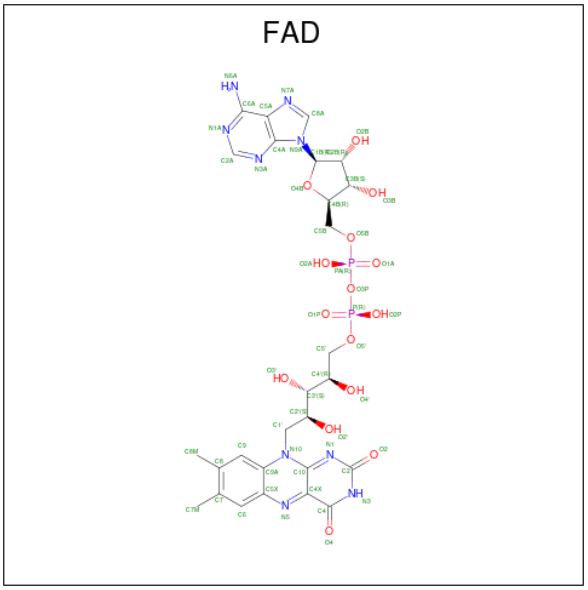
There are 9 unique types of molecules in this entry. The entry contains 13768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	9	0
			2914	1842	515	542	15			
1	B	371	Total	C	N	O	S	0	9	0
			2917	1844	515	543	15			
1	C	370	Total	C	N	O	S	0	9	0
			2915	1841	517	542	15			
1	D	369	Total	C	N	O	S	0	10	0
			2911	1837	515	544	15			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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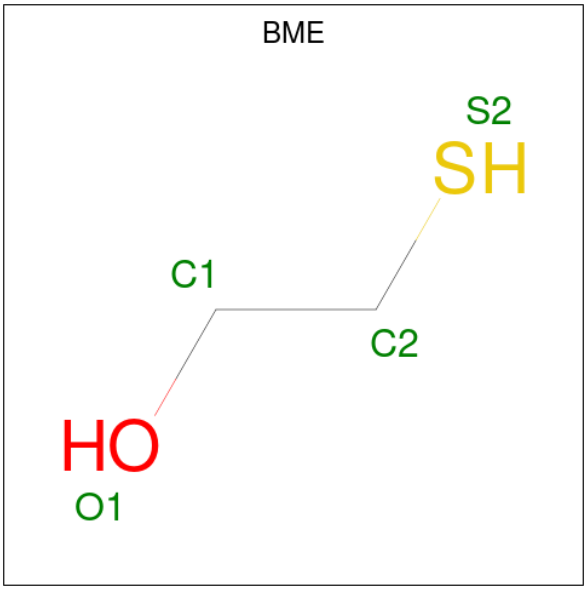
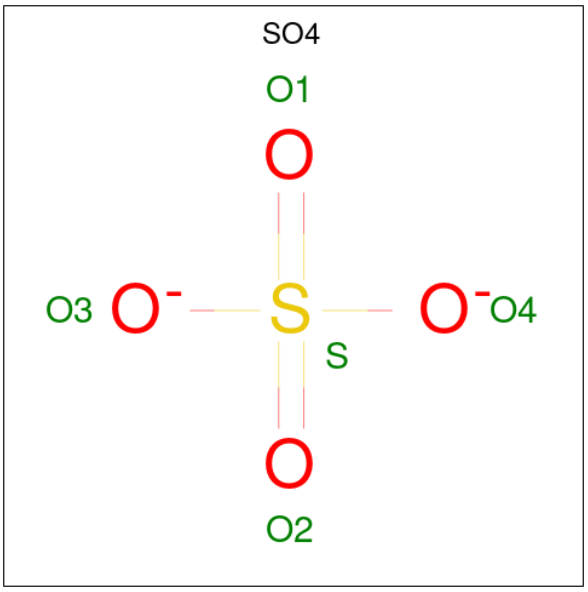
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



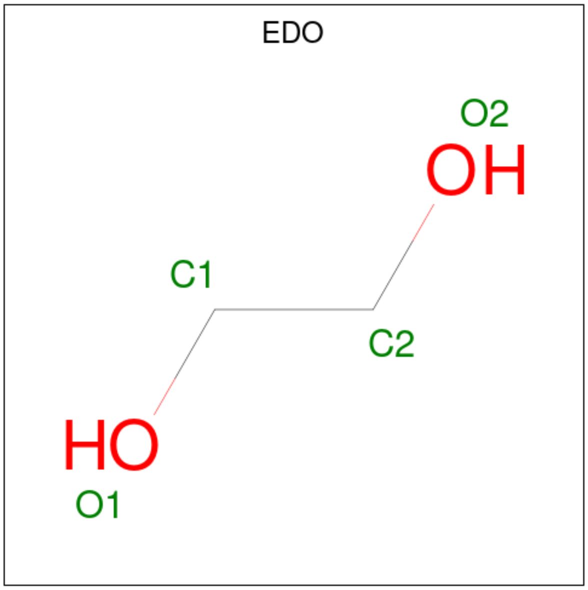
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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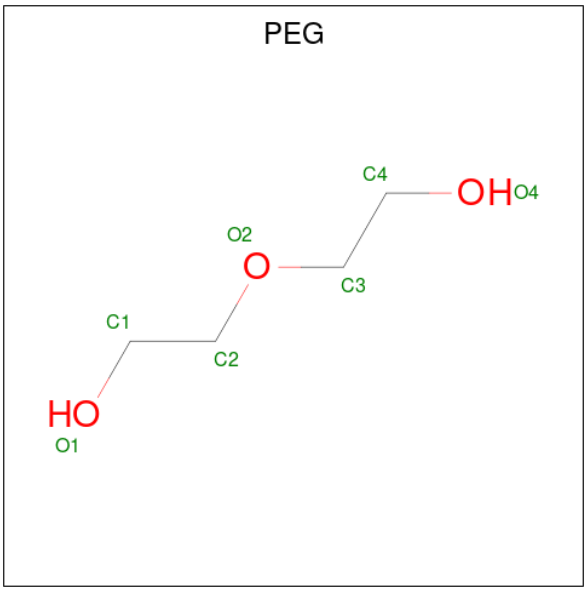
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	1
			14	8	6		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	1
			14	8	6		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	1
			14	8	6		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

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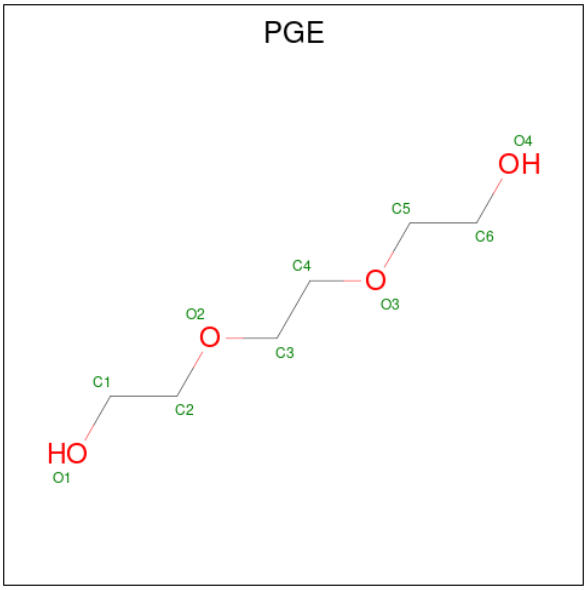
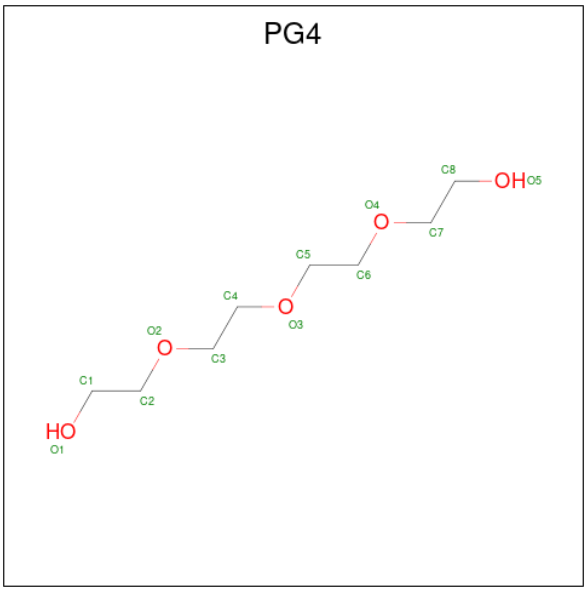
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 14 8 6	0	1
6	D	1	Total C O 7 4 3	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0
7	B	1	Total C O 10 6 4	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 13 8 5	0	0
8	C	1	Total C O 13 8 5	0	0
8	D	1	Total C O 13 8 5	0	0

- Molecule 9 is water.

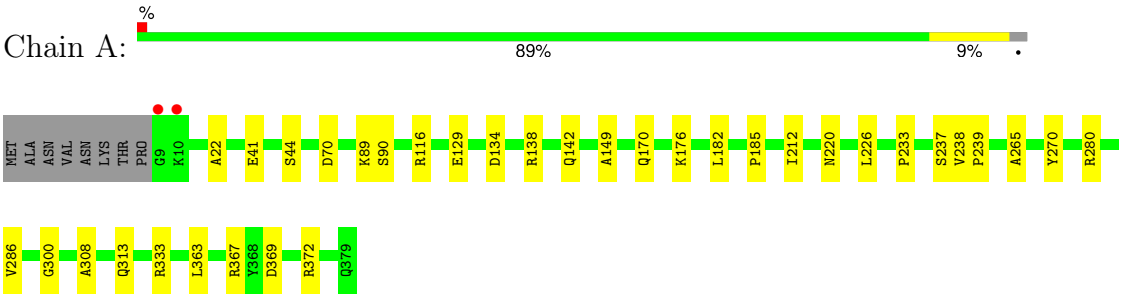
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	379	Total O 379 379	0	0
9	B	372	Total O 372 372	0	0
9	C	316	Total O 316 316	0	0
9	D	311	Total O 311 311	0	0

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.

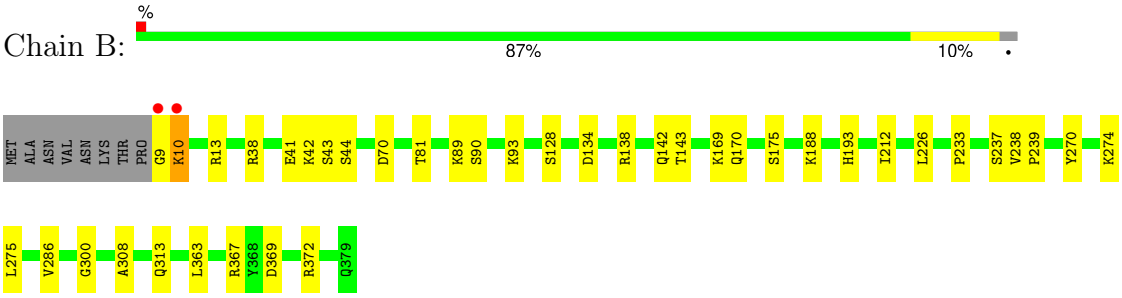
• Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase

Chain A:



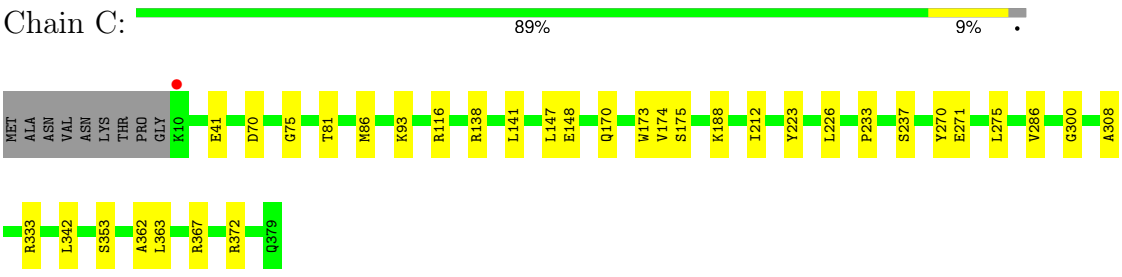
• Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase

Chain B:



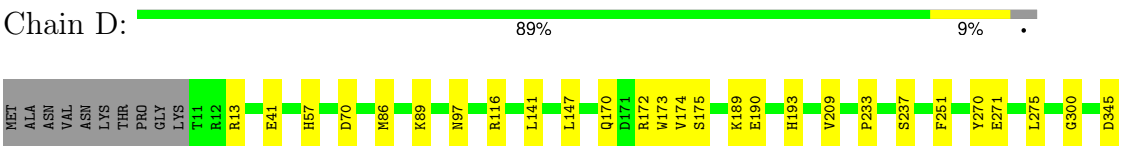
• Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase

Chain C:



• Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase

Chain D:




N349
S353
L363
R367
R372
W377
P378
Q379

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.84Å 103.84Å 452.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.91 – 1.98 49.10 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.91-1.98) 97.5 (49.10-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.68 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.172 , 0.200 0.169 , 0.196	Depositor DCC
R_{free} test set	9859 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13768	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: FAD, SO4, PEG, EDO, PGE, BME, PG4

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	0.37	0/3011	0.55	0/4087
1	B	0.37	0/3010	0.55	0/4085
1	C	0.34	0/3008	0.53	0/4082
1	D	0.34	0/3011	0.53	0/4087
All	All	0.36	0/12040	0.54	0/16341

There are no bond length outliers.

There are no bond angle outliers.

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	2914	0	2896	31	0
1	B	2917	0	2900	36	0
1	C	2915	0	2897	22	0
1	D	2911	0	2887	31	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	A	4	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	5	2	0
3	C	4	0	5	1	0
3	D	4	0	5	1	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	20	0	0	0	0
5	A	32	0	48	7	0
5	B	60	0	90	13	0
5	C	52	0	78	2	0
5	D	60	0	90	9	0
6	A	56	0	80	6	0
6	B	63	0	90	8	0
6	C	35	0	50	6	0
6	D	28	0	40	4	0
7	A	10	0	14	0	0
7	B	10	0	14	0	0
8	B	13	0	18	2	0
8	C	13	0	18	0	0
8	D	13	0	18	0	0
9	A	379	0	0	1	0
9	B	372	0	0	1	0
9	C	316	0	0	0	0
9	D	311	0	0	0	0
All	All	13768	0	12372	121	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 5.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:H	5:A:405:EDO:H11	1.32	0.93
1:B:313:GLN:HE21	6:B:425:PEG:H12	1.32	0.90
1:C:188:LYS:H	5:C:418:EDO:H12	1.42	0.85
1:B:188:LYS:H	5:B:409:EDO:H22	1.48	0.79
1:C:116:ARG:HH22	5:C:406:EDO:H12	1.48	0.78
1:B:143:THR:HG23	5:B:412:EDO:H11	1.66	0.77
1:A:89:LYS:HD2	6:C:420:PEG:H41	1.70	0.74
1:C:70:ASP:OD2	1:D:372:ARG:NH2	2.21	0.74
1:A:44:SER:H	5:A:409:EDO:H21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HH22	5:D:407:EDO:H21	1.57	0.69
1:A:233:PRO:O	1:A:237[A]:SER:OG	2.10	0.69
1:C:75:GLY:H	6:C:421:PEG:H12	1.56	0.69
1:C:233:PRO:O	1:C:237[A]:SER:OG	2.10	0.68
1:B:89:LYS:HD2	6:B:427:PEG:H12	1.75	0.68
1:A:142:GLN:HB3	5:A:405:EDO:H12	1.75	0.68
1:B:212:ILE:HG12	1:B:226:LEU:HD22	1.76	0.67
1:D:193:HIS:H	6:D:424:PEG:H32	1.59	0.67
1:B:367:ARG:HH22	8:B:430:PG4:H42	1.61	0.65
1:C:81[A]:THR:HG21	1:C:93:LYS:HB3	1.78	0.65
1:D:189:LYS:H	5:D:421:EDO:H22	1.61	0.65
1:B:13:ARG:HH12	6:B:422:PEG:H21	1.61	0.64
1:D:300:GLY:HA3	2:D:401:FAD:H1'2	1.78	0.63
1:B:233:PRO:O	1:B:237[A]:SER:OG	2.17	0.63
1:B:142:GLN:HB3	5:B:412:EDO:H22	1.81	0.62
1:A:372:ARG:NH2	1:B:70:ASP:OD2	2.29	0.62
1:B:286[B]:VAL:HG11	1:B:308:ALA:HB2	1.82	0.62
1:C:372:ARG:NH2	1:D:70:ASP:OD2	2.32	0.62
1:D:233:PRO:O	1:D:237[A]:SER:OG	2.17	0.62
1:D:345[B]:ASP:OD1	1:D:349:ASN:ND2	2.33	0.61
1:B:367:ARG:HH12	8:B:430:PG4:H52	1.66	0.61
1:A:313:GLN:HE21	6:A:417:PEG:H31	1.66	0.60
1:D:116:ARG:HH22	5:D:409:EDO:H21	1.65	0.60
1:D:377:TRP:HE1	6:D:423[A]:PEG:H21	1.65	0.60
1:D:209:VAL:HG21	5:D:414:EDO:H12	1.84	0.59
1:A:212:ILE:HG12	1:A:226:LEU:HD22	1.84	0.59
1:C:174:VAL:HG22	1:C:271:GLU:HG2	1.83	0.58
3:B:402:BME:H11	6:B:423:PEG:H41	1.85	0.58
1:C:300:GLY:HA3	2:C:401:FAD:H1'2	1.86	0.57
1:C:75:GLY:N	6:C:421:PEG:H12	2.19	0.57
1:A:129:GLU:H	5:A:405:EDO:C1	2.10	0.57
5:B:411:EDO:H21	1:D:89:LYS:HE2	1.87	0.56
1:A:116:ARG:HH22	5:A:412:EDO:H11	1.71	0.55
1:A:70:ASP:OD2	1:B:372:ARG:NH2	2.37	0.55
1:B:193:HIS:H	6:B:426:PEG:H41	1.71	0.55
1:B:38:ARG:HH12	6:B:422:PEG:H41	1.73	0.54
1:A:90:SER:H	6:C:420:PEG:C4	2.21	0.54
1:B:128:SER:HA	5:B:412:EDO:H12	1.90	0.54
1:A:286[B]:VAL:HG11	1:A:308:ALA:HB2	1.89	0.53
1:B:81[B]:THR:HG21	1:B:93:LYS:HB3	1.91	0.53
1:D:174:VAL:HG22	1:D:271:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:PHE:CE1	5:D:411:EDO:H11	2.44	0.52
1:A:300:GLY:HA3	2:A:401:FAD:H1'2	1.91	0.52
1:B:44:SER:H	5:B:418:EDO:H22	1.75	0.51
1:D:41:GLU:OE2	2:D:401:FAD:O3B	2.23	0.51
1:A:134:ASP:HB3	1:A:138:ARG:HB2	1.92	0.51
1:B:270:TYR:CG	3:B:402:BME:H22	2.46	0.50
1:B:188:LYS:N	5:B:409:EDO:H22	2.23	0.50
1:A:270:TYR:CG	3:A:402:BME:H22	2.46	0.50
1:B:300:GLY:HA3	2:B:401:FAD:H1'2	1.93	0.50
1:D:270:TYR:CG	3:D:402:BME:H22	2.47	0.50
1:A:41:GLU:OE2	2:A:401:FAD:O3B	2.28	0.50
1:C:41:GLU:OE2	2:C:401:FAD:O3B	2.22	0.50
1:C:286[B]:VAL:HG11	1:C:308:ALA:HB2	1.93	0.50
1:C:363:LEU:O	1:C:367:ARG:HG3	2.11	0.50
1:A:369:ASP:OD2	1:A:372:ARG:HD3	2.13	0.49
1:D:367:ARG:HH12	5:D:416:EDO:H22	1.77	0.49
1:A:313:GLN:HG2	6:A:417:PEG:H22	1.95	0.49
1:A:185:PRO:HD3	6:A:415:PEG:H42	1.95	0.48
1:A:372:ARG:HH21	5:B:413:EDO:H11	1.78	0.48
1:D:363:LEU:O	1:D:367:ARG:HG3	2.14	0.48
1:A:170:GLN:HG2	9:A:716:HOH:O	2.13	0.48
2:D:401:FAD:H9	2:D:401:FAD:H1'1	1.60	0.47
1:A:182:LEU:HD21	1:A:265:ALA:HB2	1.96	0.47
1:A:149:ALA:N	6:A:418[A]:PEG:H21	2.28	0.47
1:B:188:LYS:HB3	5:B:409:EDO:H11	1.97	0.47
1:A:129:GLU:N	5:A:405:EDO:H11	2.14	0.46
1:A:313:GLN:HE21	6:A:417:PEG:C3	2.28	0.46
1:B:274:LYS:HG2	5:B:408:EDO:H22	1.98	0.46
1:C:141:LEU:HD11	1:C:147:LEU:HD11	1.98	0.46
1:B:41:GLU:OE2	2:B:401:FAD:O3B	2.26	0.46
1:D:57:HIS:CD2	6:D:423[B]:PEG:H21	2.51	0.46
1:B:363:LEU:O	1:B:367:ARG:HG3	2.15	0.45
1:C:86:MET:CE	1:C:353:SER:HB2	2.45	0.45
1:C:170:GLN:HB3	1:C:275:LEU:HD22	1.97	0.45
1:B:169:LYS:HG3	5:B:416:EDO:H12	1.98	0.45
1:B:175:SER:HB3	1:B:270:TYR:HB2	1.98	0.45
1:B:170:GLN:HG2	9:B:639:HOH:O	2.15	0.45
1:C:86:MET:HE1	1:C:353:SER:HB2	1.97	0.45
1:A:220:ASN:HB2	6:A:413:PEG:H31	1.97	0.45
1:B:9:GLY:HA2	1:B:10:LYS:HA	1.57	0.45
1:D:190:GLU:OE1	1:D:190:GLU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ALA:HB1	1:A:286[B]:VAL:HG12	1.99	0.45
1:D:86:MET:HE1	1:D:353:SER:HB2	1.99	0.45
1:D:141:LEU:HD11	1:D:147:LEU:HD11	1.99	0.45
1:D:173:TRP:CH2	1:D:175[B]:SER:HB3	2.52	0.45
1:D:173:TRP:CH2	1:D:175[A]:SER:HB2	2.52	0.45
1:D:172:ARG:HH22	5:D:420:EDO:H11	1.81	0.44
1:D:170:GLN:HB3	1:D:275:LEU:HD22	1.99	0.44
1:D:251:PHE:CD1	5:D:411:EDO:H11	2.52	0.44
1:B:43:SER:HB2	5:B:418:EDO:H22	1.99	0.44
1:A:238:VAL:HA	1:A:239:PRO:C	2.39	0.43
1:B:369:ASP:OD2	1:B:372:ARG:HD3	2.19	0.43
1:C:173:TRP:CH2	1:C:175[A]:SER:HB2	2.53	0.43
1:B:170:GLN:HB3	1:B:275:LEU:HD22	2.01	0.43
1:A:142:GLN:CB	5:A:405:EDO:H12	2.44	0.43
6:B:425:PEG:H42	6:B:425:PEG:H22	1.78	0.43
1:C:212:ILE:HG12	1:C:226:LEU:HD22	2.00	0.43
1:C:342:LEU:HD23	1:C:362:ALA:HA	2.00	0.42
1:B:134:ASP:HB3	1:B:138:ARG:HB2	2.01	0.42
1:D:377:TRP:HE1	6:D:423[B]:PEG:H21	1.82	0.42
2:B:401:FAD:H9	2:B:401:FAD:H1'1	1.60	0.42
1:D:86:MET:CE	1:D:353:SER:HB2	2.49	0.42
1:C:270:TYR:CG	3:C:402:BME:H22	2.55	0.42
1:A:363:LEU:O	1:A:367:ARG:HG3	2.20	0.41
1:C:138:ARG:HG2	1:C:148:GLU:HG2	2.02	0.41
6:C:420:PEG:H31	6:C:420:PEG:H11	1.76	0.41
1:B:42:LYS:HZ1	5:B:420:EDO:C2	2.34	0.41
1:B:90:SER:H	6:B:427:PEG:C1	2.34	0.41
6:C:421:PEG:O4	1:D:97:ASN:HB3	2.21	0.41
1:B:238:VAL:HA	1:B:239:PRO:C	2.42	0.40
1:D:13:ARG:HH12	5:D:407:EDO:H12	1.85	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	378/379 (100%)	367 (97%)	11 (3%)	0	100	100
1	B	378/379 (100%)	366 (97%)	12 (3%)	0	100	100
1	C	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
1	D	377/379 (100%)	367 (97%)	10 (3%)	0	100	100
All	All	1510/1516 (100%)	1465 (97%)	45 (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	307/305 (101%)	304 (99%)	3 (1%)	76	73
1	B	307/305 (101%)	306 (100%)	1 (0%)	92	92
1	C	307/305 (101%)	305 (99%)	2 (1%)	84	83
1	D	307/305 (101%)	307 (100%)	0	100	100
All	All	1228/1220 (101%)	1222 (100%)	6 (0%)	88	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	280	ARG
1	A	333	ARG
1	B	10	LYS
1	C	223	TYR
1	C	333	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	220	ASN
1	B	313	GLN
1	D	349	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)

102 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	$\#\|Z\| > 2$
5	EDO	B	417	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	A	410	-	3,3,3	0.39	0	2,2,2	0.63	0
5	EDO	B	411	-	3,3,3	0.45	0	2,2,2	0.33	0
6	PEG	A	416[B]	-	6,6,6	0.49	0	5,5,5	0.18	0
5	EDO	C	412	-	3,3,3	0.47	0	2,2,2	0.30	0
7	PGE	B	429	-	9,9,9	0.53	0	8,8,8	0.21	0
6	PEG	C	421	-	6,6,6	0.42	0	5,5,5	0.69	0
5	EDO	A	407	-	3,3,3	0.46	0	2,2,2	0.39	0
2	FAD	A	401	-	54,58,58	1.84	10 (18%)	71,89,89	2.23	19 (26%)
4	SO4	D	405	-	4,4,4	0.26	0	6,6,6	0.07	0
5	EDO	C	415	-	3,3,3	0.42	0	2,2,2	0.44	0
6	PEG	B	422	-	6,6,6	0.47	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	411	-	3,3,3	0.45	0	2,2,2	0.25	0
6	PEG	C	423	-	6,6,6	0.53	0	5,5,5	0.17	0
5	EDO	D	419	-	3,3,3	0.44	0	2,2,2	0.45	0
6	PEG	A	414	-	6,6,6	0.47	0	5,5,5	0.37	0
5	EDO	D	407	-	3,3,3	0.46	0	2,2,2	0.31	0
2	FAD	D	401	-	54,58,58	1.90	11 (20%)	71,89,89	2.35	19 (26%)
5	EDO	A	405	-	3,3,3	0.32	0	2,2,2	0.52	0
6	PEG	A	413	-	6,6,6	0.48	0	5,5,5	0.26	0
5	EDO	D	414	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	B	408	-	3,3,3	0.47	0	2,2,2	0.31	0
7	PGE	A	419	-	9,9,9	0.49	0	8,8,8	0.28	0
5	EDO	D	421	-	3,3,3	0.43	0	2,2,2	0.32	0
6	PEG	D	424	-	6,6,6	0.50	0	5,5,5	0.38	0
6	PEG	A	418[A]	-	6,6,6	0.50	0	5,5,5	0.48	0
5	EDO	D	416	-	3,3,3	0.42	0	2,2,2	0.32	0
8	PG4	C	424	-	12,12,12	0.54	0	11,11,11	0.14	0
5	EDO	C	406	-	3,3,3	0.43	0	2,2,2	0.38	0
6	PEG	C	422	-	6,6,6	0.48	0	5,5,5	0.22	0
6	PEG	A	415	-	6,6,6	0.45	0	5,5,5	0.33	0
5	EDO	D	412	-	3,3,3	0.45	0	2,2,2	0.38	0
4	SO4	C	405	-	4,4,4	0.26	0	6,6,6	0.19	0
6	PEG	D	423[B]	-	6,6,6	0.44	0	5,5,5	0.52	0
5	EDO	D	415	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	B	420	-	3,3,3	0.42	0	2,2,2	0.35	0
6	PEG	A	417	-	6,6,6	0.53	0	5,5,5	0.22	0
5	EDO	C	410	-	3,3,3	0.46	0	2,2,2	0.20	0
4	SO4	A	404	-	4,4,4	0.28	0	6,6,6	0.08	0
5	EDO	D	411	-	3,3,3	0.46	0	2,2,2	0.25	0
6	PEG	C	420	-	6,6,6	0.30	0	5,5,5	0.69	0
5	EDO	C	407	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	B	415	-	3,3,3	0.45	0	2,2,2	0.34	0
4	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.25	0
6	PEG	B	426	-	6,6,6	0.53	0	5,5,5	0.19	0
4	SO4	A	403	-	4,4,4	0.31	0	6,6,6	0.21	0
5	EDO	C	416	-	3,3,3	0.47	0	2,2,2	0.35	0
5	EDO	C	411	-	3,3,3	0.43	0	2,2,2	0.44	0
5	EDO	D	408	-	3,3,3	0.48	0	2,2,2	0.31	0
5	EDO	C	414	-	3,3,3	0.45	0	2,2,2	0.37	0
6	PEG	D	422	-	6,6,6	0.59	0	5,5,5	0.23	0
5	EDO	C	417	-	3,3,3	0.32	0	2,2,2	0.67	0
4	SO4	D	406	-	4,4,4	0.28	0	6,6,6	0.16	0
6	PEG	B	424[A]	-	6,6,6	0.52	0	5,5,5	0.22	0
5	EDO	B	418	-	3,3,3	0.40	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	B	412	-	3,3,3	0.38	0	2,2,2	0.39	0
6	PEG	A	418[B]	-	6,6,6	0.47	0	5,5,5	0.31	0
4	SO4	D	403	-	4,4,4	0.24	0	6,6,6	0.23	0
4	SO4	B	405	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	B	403	-	4,4,4	0.27	0	6,6,6	0.16	0
5	EDO	C	409	-	3,3,3	0.52	0	2,2,2	0.21	0
5	EDO	B	416	-	3,3,3	0.29	0	2,2,2	0.55	0
3	BME	C	402	-	3,3,3	0.31	0	2,2,2	0.29	0
4	SO4	D	404	-	4,4,4	0.26	0	6,6,6	0.12	0
2	FAD	C	401	-	54,58,58	1.90	11 (20%)	71,89,89	2.35	19 (26%)
5	EDO	B	406	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	A	412	-	3,3,3	0.43	0	2,2,2	0.49	0
4	SO4	C	404	-	4,4,4	0.26	0	6,6,6	0.10	0
3	BME	A	402	-	3,3,3	0.22	0	2,2,2	0.46	0
5	EDO	B	413	-	3,3,3	0.47	0	2,2,2	0.37	0
6	PEG	B	425	-	6,6,6	0.55	0	5,5,5	0.56	0
3	BME	B	402	-	3,3,3	0.28	0	2,2,2	0.24	0
5	EDO	A	408	-	3,3,3	0.43	0	2,2,2	0.33	0
5	EDO	A	406	-	3,3,3	0.46	0	2,2,2	0.40	0
6	PEG	A	416[A]	-	6,6,6	0.48	0	5,5,5	0.15	0
5	EDO	B	409	-	3,3,3	0.41	0	2,2,2	0.43	0
3	BME	D	402	-	3,3,3	0.21	0	2,2,2	0.42	0
6	PEG	C	419	-	6,6,6	0.46	0	5,5,5	0.43	0
5	EDO	C	413	-	3,3,3	0.46	0	2,2,2	0.27	0
6	PEG	B	428	-	6,6,6	0.52	0	5,5,5	0.20	0
6	PEG	B	424[B]	-	6,6,6	0.46	0	5,5,5	0.19	0
5	EDO	D	418	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	D	417	-	3,3,3	0.46	0	2,2,2	0.37	0
6	PEG	B	421	-	6,6,6	0.51	0	5,5,5	0.55	0
8	PG4	B	430	-	12,12,12	0.49	0	11,11,11	0.48	0
5	EDO	B	419	-	3,3,3	0.42	0	2,2,2	0.50	0
5	EDO	C	418	-	3,3,3	0.51	0	2,2,2	0.18	0
5	EDO	D	409	-	3,3,3	0.41	0	2,2,2	0.44	0
5	EDO	B	407	-	3,3,3	0.46	0	2,2,2	0.24	0
2	FAD	B	401	-	54,58,58	1.83	10 (18%)	71,89,89	2.33	20 (28%)
6	PEG	B	427	-	6,6,6	0.31	0	5,5,5	0.62	0
6	PEG	B	423	-	6,6,6	0.44	0	5,5,5	0.47	0
5	EDO	B	414	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	D	420	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	B	410	-	3,3,3	0.45	0	2,2,2	0.36	0
4	SO4	B	404	-	4,4,4	0.28	0	6,6,6	0.08	0
8	PG4	D	425	-	12,12,12	0.52	0	11,11,11	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	409	-	3,3,3	0.40	0	2,2,2	0.41	0
5	EDO	C	408	-	3,3,3	0.48	0	2,2,2	0.26	0
6	PEG	D	423[A]	-	6,6,6	0.52	0	5,5,5	0.19	0
5	EDO	D	410	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	D	413	-	3,3,3	0.49	0	2,2,2	0.25	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
5	EDO	B	417	-	-	0/1/1/1	-
5	EDO	A	410	-	-	0/1/1/1	-
5	EDO	B	411	-	-	1/1/1/1	-
6	PEG	A	416[B]	-	-	1/4/4/4	-
5	EDO	C	412	-	-	1/1/1/1	-
7	PGE	B	429	-	-	1/7/7/7	-
6	PEG	C	421	-	-	3/4/4/4	-
5	EDO	A	407	-	-	0/1/1/1	-
2	FAD	A	401	-	-	1/30/50/50	0/6/6/6
5	EDO	C	415	-	-	1/1/1/1	-
6	PEG	B	422	-	-	1/4/4/4	-
5	EDO	A	411	-	-	0/1/1/1	-
6	PEG	C	423	-	-	0/4/4/4	-
5	EDO	D	419	-	-	1/1/1/1	-
6	PEG	A	414	-	-	3/4/4/4	-
5	EDO	D	407	-	-	0/1/1/1	-
2	FAD	D	401	-	-	1/30/50/50	0/6/6/6
5	EDO	A	405	-	-	1/1/1/1	-
6	PEG	A	413	-	-	1/4/4/4	-
5	EDO	D	414	-	-	0/1/1/1	-
5	EDO	B	408	-	-	1/1/1/1	-
7	PGE	A	419	-	-	2/7/7/7	-
5	EDO	D	421	-	-	0/1/1/1	-
6	PEG	D	424	-	-	2/4/4/4	-
6	PEG	A	418[A]	-	-	0/4/4/4	-
5	EDO	D	416	-	-	0/1/1/1	-
8	PG4	C	424	-	-	0/10/10/10	-
5	EDO	C	406	-	-	1/1/1/1	-
6	PEG	C	422	-	-	1/4/4/4	-
6	PEG	A	415	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	412	-	-	0/1/1/1	-
6	PEG	D	423[B]	-	-	1/4/4/4	-
5	EDO	D	415	-	-	1/1/1/1	-
5	EDO	B	420	-	-	0/1/1/1	-
6	PEG	A	417	-	-	1/4/4/4	-
5	EDO	C	410	-	-	1/1/1/1	-
5	EDO	D	411	-	-	0/1/1/1	-
6	PEG	C	420	-	-	3/4/4/4	-
5	EDO	C	407	-	-	1/1/1/1	-
5	EDO	B	415	-	-	1/1/1/1	-
6	PEG	B	426	-	-	3/4/4/4	-
5	EDO	C	416	-	-	1/1/1/1	-
5	EDO	C	411	-	-	0/1/1/1	-
5	EDO	D	408	-	-	0/1/1/1	-
5	EDO	C	414	-	-	0/1/1/1	-
6	PEG	D	422	-	-	0/4/4/4	-
5	EDO	C	417	-	-	1/1/1/1	-
6	PEG	B	424[A]	-	-	0/4/4/4	-
5	EDO	B	418	-	-	0/1/1/1	-
5	EDO	B	412	-	-	1/1/1/1	-
6	PEG	A	418[B]	-	-	2/4/4/4	-
5	EDO	C	409	-	-	0/1/1/1	-
5	EDO	B	416	-	-	0/1/1/1	-
3	BME	C	402	-	-	0/1/1/1	-
5	EDO	B	406	-	-	0/1/1/1	-
2	FAD	C	401	-	-	1/30/50/50	0/6/6/6
5	EDO	A	412	-	-	1/1/1/1	-
3	BME	A	402	-	-	0/1/1/1	-
5	EDO	B	413	-	-	1/1/1/1	-
6	PEG	B	425	-	-	3/4/4/4	-
3	BME	B	402	-	-	0/1/1/1	-
5	EDO	A	408	-	-	0/1/1/1	-
5	EDO	A	406	-	-	1/1/1/1	-
6	PEG	A	416[A]	-	-	0/4/4/4	-
5	EDO	B	409	-	-	1/1/1/1	-
3	BME	D	402	-	-	0/1/1/1	-
6	PEG	C	419	-	-	3/4/4/4	-
5	EDO	C	413	-	-	0/1/1/1	-
6	PEG	B	428	-	-	2/4/4/4	-
6	PEG	B	424[B]	-	-	0/4/4/4	-
5	EDO	D	418	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	417	-	-	0/1/1/1	-
6	PEG	B	421	-	-	3/4/4/4	-
8	PG4	B	430	-	-	5/10/10/10	-
5	EDO	B	419	-	-	1/1/1/1	-
5	EDO	C	418	-	-	1/1/1/1	-
5	EDO	D	409	-	-	1/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
2	FAD	B	401	-	-	1/30/50/50	0/6/6/6
6	PEG	B	427	-	-	1/4/4/4	-
6	PEG	B	423	-	-	3/4/4/4	-
5	EDO	B	414	-	-	1/1/1/1	-
5	EDO	D	420	-	-	0/1/1/1	-
5	EDO	B	410	-	-	0/1/1/1	-
8	PG4	D	425	-	-	4/10/10/10	-
5	EDO	A	409	-	-	1/1/1/1	-
5	EDO	C	408	-	-	1/1/1/1	-
6	PEG	D	423[A]	-	-	0/4/4/4	-
5	EDO	D	410	-	-	0/1/1/1	-
5	EDO	D	413	-	-	0/1/1/1	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	C8M-C8	-5.67	1.40	1.51
2	B	401	FAD	C7M-C7	-5.60	1.40	1.51
2	C	401	FAD	C2A-N3A	5.43	1.40	1.32
2	C	401	FAD	C8M-C8	-5.43	1.40	1.51
2	D	401	FAD	C7M-C7	-5.42	1.40	1.51
2	A	401	FAD	C7M-C7	-5.30	1.41	1.51
2	A	401	FAD	C8M-C8	-5.20	1.41	1.51
2	B	401	FAD	C8M-C8	-5.19	1.41	1.51
2	D	401	FAD	C2A-N3A	5.15	1.40	1.32
2	C	401	FAD	C7M-C7	-5.04	1.41	1.51
2	A	401	FAD	C4X-N5	4.77	1.41	1.30
2	B	401	FAD	C4X-N5	4.72	1.40	1.30
2	A	401	FAD	C2A-N3A	4.65	1.39	1.32
2	C	401	FAD	C4X-N5	4.55	1.40	1.30
2	D	401	FAD	C4X-N5	4.24	1.39	1.30
2	B	401	FAD	C2A-N3A	4.23	1.38	1.32
2	A	401	FAD	C10-N1	3.50	1.40	1.33
2	D	401	FAD	C9A-N10	-3.32	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FAD	C9A-N10	-3.21	1.35	1.41
2	B	401	FAD	C10-N1	3.17	1.39	1.33
2	C	401	FAD	C9A-N10	-3.14	1.35	1.41
2	A	401	FAD	C9A-N10	-3.14	1.35	1.41
2	D	401	FAD	C2A-N1A	3.07	1.39	1.33
2	C	401	FAD	C10-N1	3.06	1.39	1.33
2	D	401	FAD	C10-N1	2.88	1.39	1.33
2	C	401	FAD	C2A-N1A	2.79	1.38	1.33
2	B	401	FAD	C2A-N1A	2.75	1.38	1.33
2	C	401	FAD	C1'-C2'	2.74	1.56	1.52
2	A	401	FAD	C2A-N1A	2.73	1.38	1.33
2	C	401	FAD	O4B-C4B	2.68	1.50	1.45
2	B	401	FAD	O4B-C4B	2.67	1.50	1.45
2	D	401	FAD	O4B-C4B	2.57	1.50	1.45
2	D	401	FAD	C5'-C4'	2.54	1.55	1.51
2	B	401	FAD	C6A-C5A	-2.38	1.34	1.43
2	A	401	FAD	C6A-C5A	-2.37	1.34	1.43
2	D	401	FAD	PA-O3P	2.33	1.62	1.59
2	A	401	FAD	C1'-C2'	2.25	1.55	1.52
2	B	401	FAD	PA-O3P	2.22	1.61	1.59
2	D	401	FAD	C6A-C5A	-2.22	1.35	1.43
2	C	401	FAD	C6A-C5A	-2.22	1.35	1.43
2	A	401	FAD	C2-N1	2.14	1.41	1.36
2	C	401	FAD	C5'-C4'	2.08	1.54	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FAD	O4B-C4B-C5B	-9.85	77.78	109.33
2	D	401	FAD	O4B-C4B-C5B	-9.71	78.23	109.33
2	C	401	FAD	O4B-C4B-C5B	-9.64	78.46	109.33
2	A	401	FAD	O4B-C4B-C5B	-9.15	80.02	109.33
2	C	401	FAD	N3A-C2A-N1A	-8.06	117.73	128.67
2	D	401	FAD	N3A-C2A-N1A	-7.96	117.87	128.67
2	B	401	FAD	N3A-C2A-N1A	-7.87	117.98	128.67
2	A	401	FAD	N3A-C2A-N1A	-7.63	118.32	128.67
2	B	401	FAD	O4B-C4B-C3B	-7.09	91.08	105.15
2	D	401	FAD	O4B-C4B-C3B	-6.90	91.45	105.15
2	C	401	FAD	O4B-C4B-C3B	-6.84	91.57	105.15
2	A	401	FAD	O4B-C4B-C3B	-6.50	92.25	105.15
2	D	401	FAD	C5B-C4B-C3B	5.62	135.46	115.21
2	A	401	FAD	C5B-C4B-C3B	5.40	134.66	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	FAD	C5B-C4B-C3B	5.28	134.22	115.21
2	B	401	FAD	C5B-C4B-C3B	5.24	134.09	115.21
2	B	401	FAD	C4-N3-C2	-3.48	119.47	125.64
2	D	401	FAD	O3B-C3B-C2B	3.48	122.96	111.82
2	B	401	FAD	C5X-C9A-N10	3.28	120.93	117.97
2	A	401	FAD	C5X-C9A-N10	3.23	120.89	117.97
2	C	401	FAD	C5X-C9A-N10	3.21	120.87	117.97
2	D	401	FAD	C5X-C9A-N10	3.20	120.86	117.97
2	D	401	FAD	C4-N3-C2	-3.18	120.00	125.64
2	D	401	FAD	O5B-C5B-C4B	-3.16	98.25	108.99
2	A	401	FAD	C9A-C5X-N5	-3.14	119.12	122.45
2	B	401	FAD	C9A-C5X-N5	-3.13	119.13	122.45
2	C	401	FAD	C4-N3-C2	-3.12	120.10	125.64
2	C	401	FAD	O3B-C3B-C2B	3.11	121.80	111.82
2	D	401	FAD	C2B-C3B-C4B	-3.10	96.61	102.61
2	C	401	FAD	O5B-C5B-C4B	-3.10	98.44	108.99
2	D	401	FAD	C9A-C5X-N5	-3.07	119.19	122.45
2	B	401	FAD	O3B-C3B-C2B	3.07	121.65	111.82
2	A	401	FAD	C4-N3-C2	-3.06	120.20	125.64
2	C	401	FAD	C2B-C3B-C4B	-3.00	96.81	102.61
2	C	401	FAD	C9A-C5X-N5	-2.97	119.31	122.45
2	D	401	FAD	O2B-C2B-C3B	-2.96	102.34	111.82
2	C	401	FAD	O2B-C2B-C3B	-2.92	102.46	111.82
2	B	401	FAD	O5B-C5B-C4B	-2.88	99.18	108.99
2	A	401	FAD	C2B-C3B-C4B	-2.80	97.19	102.61
2	A	401	FAD	O5B-C5B-C4B	-2.78	99.52	108.99
2	C	401	FAD	C4X-C4-N3	2.73	120.21	113.25
2	C	401	FAD	C4X-C10-N10	2.73	120.39	116.48
2	B	401	FAD	O2B-C2B-C3B	-2.72	103.08	111.82
2	D	401	FAD	C4X-C10-N10	2.70	120.34	116.48
2	D	401	FAD	C4X-C4-N3	2.70	120.12	113.25
2	A	401	FAD	C4X-C4-N3	2.69	120.10	113.25
2	A	401	FAD	O2B-C2B-C3B	-2.64	103.35	111.82
2	B	401	FAD	C4X-C4-N3	2.60	119.87	113.25
2	B	401	FAD	C10-C4X-N5	-2.52	119.66	124.81
2	C	401	FAD	C10-C4X-N5	-2.47	119.76	124.81
2	D	401	FAD	C10-C4X-N5	-2.47	119.77	124.81
2	B	401	FAD	C4-C4X-C10	2.40	121.04	116.93
2	A	401	FAD	C10-C4X-N5	-2.38	119.95	124.81
2	B	401	FAD	C4X-C10-N10	2.35	119.85	116.48
2	D	401	FAD	C4X-C10-N1	-2.34	118.84	124.59
2	A	401	FAD	O3B-C3B-C2B	2.33	119.27	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	FAD	C4X-C10-N1	-2.32	118.90	124.59
2	A	401	FAD	C4X-C10-N1	-2.27	119.04	124.59
2	B	401	FAD	O4'-C4'-C3'	2.26	114.54	109.25
2	C	401	FAD	C5'-C4'-C3'	-2.24	108.00	112.22
2	B	401	FAD	C4X-C10-N1	-2.23	119.13	124.59
2	C	401	FAD	PA-O5B-C5B	2.21	133.99	121.35
2	B	401	FAD	C2B-C3B-C4B	-2.20	98.36	102.61
2	D	401	FAD	C10-N1-C2	2.20	121.61	116.85
2	A	401	FAD	PA-O5B-C5B	2.17	133.81	121.35
2	A	401	FAD	C4-C4X-C10	2.17	120.66	116.93
2	C	401	FAD	O3'-C3'-C2'	2.17	113.86	108.93
2	D	401	FAD	O4-C4-C4X	-2.15	120.86	126.53
2	C	401	FAD	C10-N1-C2	2.14	121.47	116.85
2	B	401	FAD	O4-C4-C4X	-2.12	120.93	126.53
2	A	401	FAD	O4-C4-C4X	-2.09	121.03	126.53
2	D	401	FAD	PA-O5B-C5B	2.07	133.23	121.35
2	B	401	FAD	PA-O5B-C5B	2.03	133.00	121.35
2	D	401	FAD	O4'-C4'-C3'	2.03	113.99	109.25
2	A	401	FAD	O4'-C4'-C3'	2.02	113.98	109.25
2	A	401	FAD	C4X-C10-N10	2.02	119.37	116.48
2	B	401	FAD	C1'-N10-C9A	-2.01	116.72	120.63

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	425	PEG	C4-C3-O2-C2
6	A	415	PEG	O2-C3-C4-O4
7	A	419	PGE	O1-C1-C2-O2
8	D	425	PG4	O2-C3-C4-O3
8	B	430	PG4	O3-C5-C6-O4
6	B	423	PEG	O1-C1-C2-O2
6	D	424	PEG	O1-C1-C2-O2
8	D	425	PG4	O1-C1-C2-O2
6	B	425	PEG	O1-C1-C2-O2
6	D	423[B]	PEG	O2-C3-C4-O4
2	A	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B
6	B	428	PEG	O1-C1-C2-O2
5	B	411	EDO	O1-C1-C2-O2
5	C	408	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	401	FAD	O4B-C4B-C5B-O5B
8	B	430	PG4	O2-C3-C4-O3
6	A	416[B]	PEG	O2-C3-C4-O4
8	D	425	PG4	O4-C7-C8-O5
5	A	405	EDO	O1-C1-C2-O2
5	B	409	EDO	O1-C1-C2-O2
5	C	407	EDO	O1-C1-C2-O2
6	B	425	PEG	C1-C2-O2-C3
6	C	420	PEG	O1-C1-C2-O2
6	A	414	PEG	C1-C2-O2-C3
8	B	430	PG4	C4-C3-O2-C2
6	A	413	PEG	C4-C3-O2-C2
6	B	426	PEG	O2-C3-C4-O4
5	B	412	EDO	O1-C1-C2-O2
5	D	418	EDO	O1-C1-C2-O2
6	A	414	PEG	C4-C3-O2-C2
8	D	425	PG4	C8-C7-O4-C6
6	C	421	PEG	C1-C2-O2-C3
6	B	421	PEG	O2-C3-C4-O4
6	B	427	PEG	O2-C3-C4-O4
8	B	430	PG4	O4-C7-C8-O5
6	A	414	PEG	O2-C3-C4-O4
7	B	429	PGE	O3-C5-C6-O4
6	D	424	PEG	C4-C3-O2-C2
6	A	418[B]	PEG	C4-C3-O2-C2
6	C	419	PEG	C1-C2-O2-C3
5	B	408	EDO	O1-C1-C2-O2
5	B	413	EDO	O1-C1-C2-O2
5	B	415	EDO	O1-C1-C2-O2
5	C	410	EDO	O1-C1-C2-O2
5	C	412	EDO	O1-C1-C2-O2
5	C	416	EDO	O1-C1-C2-O2
6	C	420	PEG	O2-C3-C4-O4
8	B	430	PG4	C3-C4-O3-C5
6	B	423	PEG	C1-C2-O2-C3
6	B	421	PEG	O1-C1-C2-O2
6	B	423	PEG	C4-C3-O2-C2
6	C	422	PEG	C1-C2-O2-C3
6	B	426	PEG	O1-C1-C2-O2
6	A	418[B]	PEG	C1-C2-O2-C3
5	B	419	EDO	O1-C1-C2-O2
5	C	415	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	C	419	PEG	O2-C3-C4-O4
6	A	417	PEG	C4-C3-O2-C2
6	C	419	PEG	C4-C3-O2-C2
5	A	406	EDO	O1-C1-C2-O2
5	B	414	EDO	O1-C1-C2-O2
5	C	406	EDO	O1-C1-C2-O2
5	D	409	EDO	O1-C1-C2-O2
5	D	415	EDO	O1-C1-C2-O2
5	D	419	EDO	O1-C1-C2-O2
6	B	428	PEG	O2-C3-C4-O4
6	C	421	PEG	O2-C3-C4-O4
6	A	415	PEG	C4-C3-O2-C2
5	C	418	EDO	O1-C1-C2-O2
6	C	421	PEG	C4-C3-O2-C2
6	B	426	PEG	C1-C2-O2-C3
5	A	409	EDO	O1-C1-C2-O2
5	A	412	EDO	O1-C1-C2-O2
5	C	417	EDO	O1-C1-C2-O2
7	A	419	PGE	O3-C5-C6-O4
6	C	420	PEG	C1-C2-O2-C3
6	B	422	PEG	C4-C3-O2-C2
6	B	421	PEG	C1-C2-O2-C3

There are no ring outliers.

43 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	411	EDO	1	0
6	C	421	PEG	3	0
2	A	401	FAD	2	0
6	B	422	PEG	2	0
5	D	407	EDO	2	0
2	D	401	FAD	3	0
5	A	405	EDO	5	0
6	A	413	PEG	1	0
5	D	414	EDO	1	0
5	B	408	EDO	1	0
5	D	421	EDO	1	0
6	D	424	PEG	1	0
6	A	418[A]	PEG	1	0
5	D	416	EDO	1	0
5	C	406	EDO	1	0

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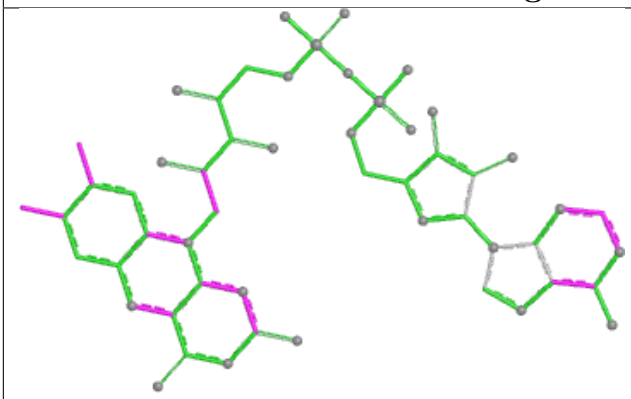
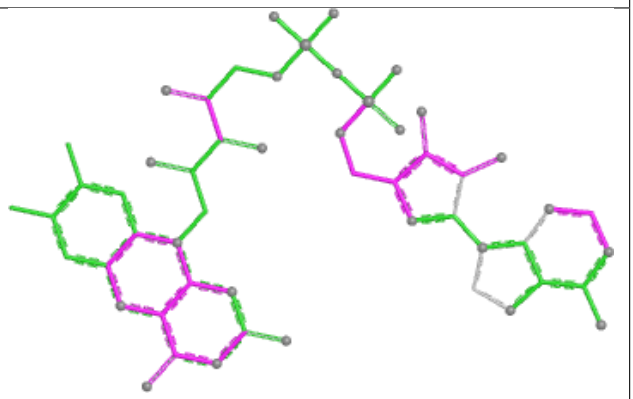
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	415	PEG	1	0
6	D	423[B]	PEG	2	0
5	B	420	EDO	1	0
6	A	417	PEG	3	0
5	D	411	EDO	2	0
6	C	420	PEG	3	0
6	B	426	PEG	1	0
5	B	418	EDO	2	0
5	B	412	EDO	3	0
5	B	416	EDO	1	0
3	C	402	BME	1	0
2	C	401	FAD	2	0
5	A	412	EDO	1	0
3	A	402	BME	1	0
5	B	413	EDO	1	0
6	B	425	PEG	2	0
3	B	402	BME	2	0
5	B	409	EDO	3	0
3	D	402	BME	1	0
8	B	430	PG4	2	0
5	C	418	EDO	1	0
5	D	409	EDO	1	0
2	B	401	FAD	3	0
6	B	427	PEG	2	0
6	B	423	PEG	1	0
5	D	420	EDO	1	0
5	A	409	EDO	1	0
6	D	423[A]	PEG	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.

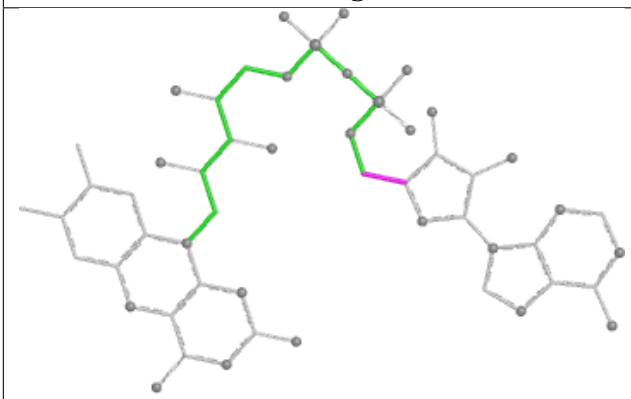
Ligand FAD A 401



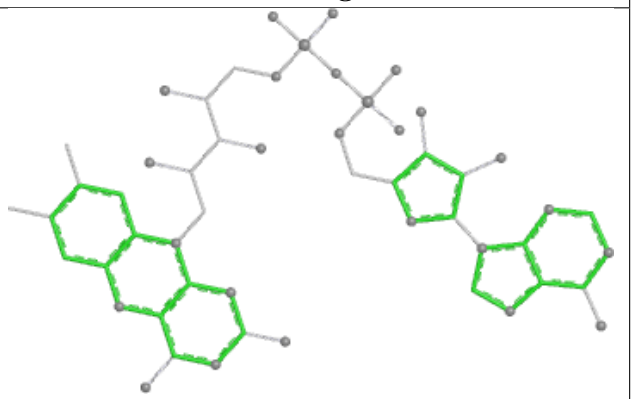
Bond lengths



Bond angles

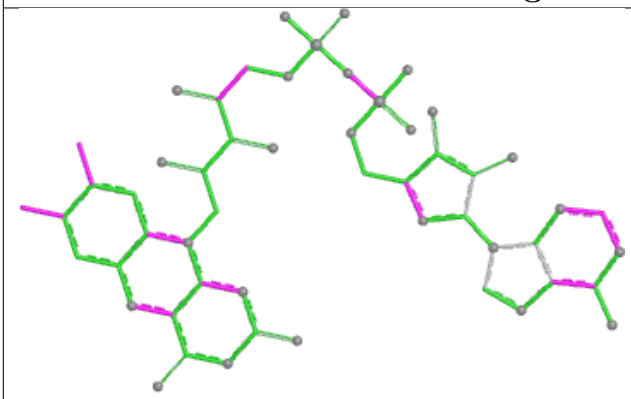


Torsions

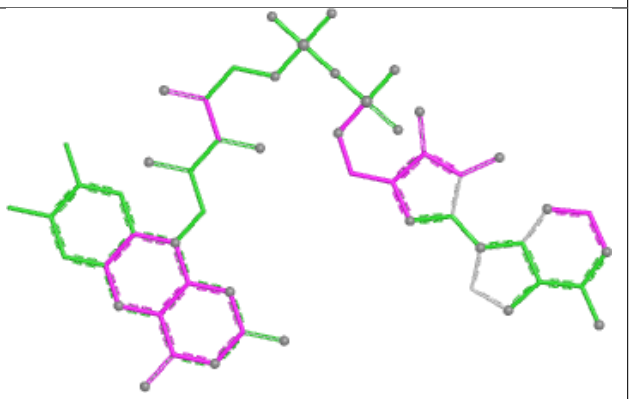


Rings

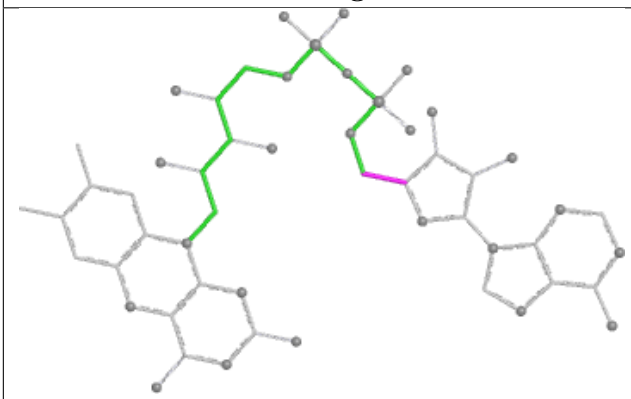
Ligand FAD D 401



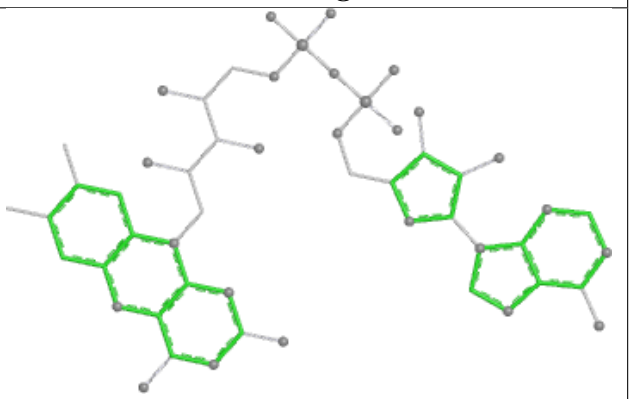
Bond lengths



Bond angles

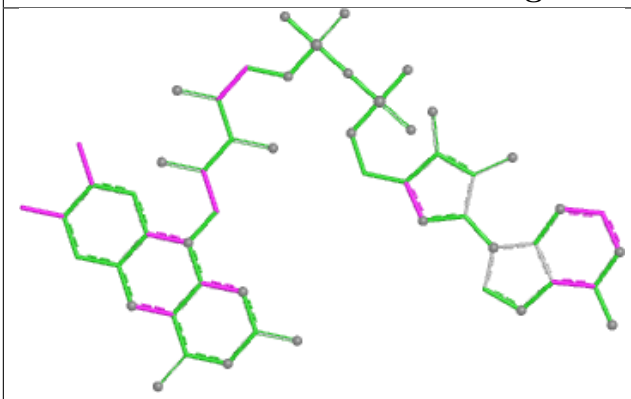


Torsions

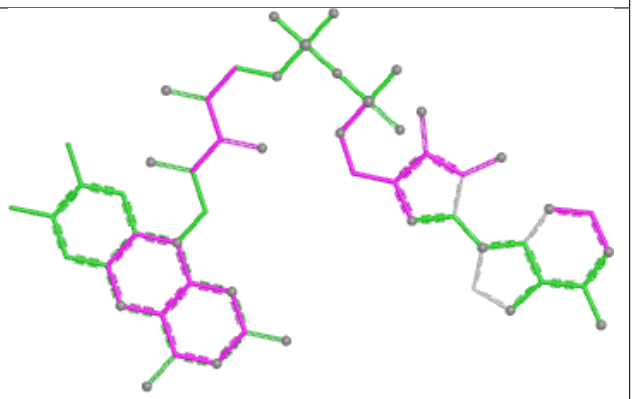


Rings

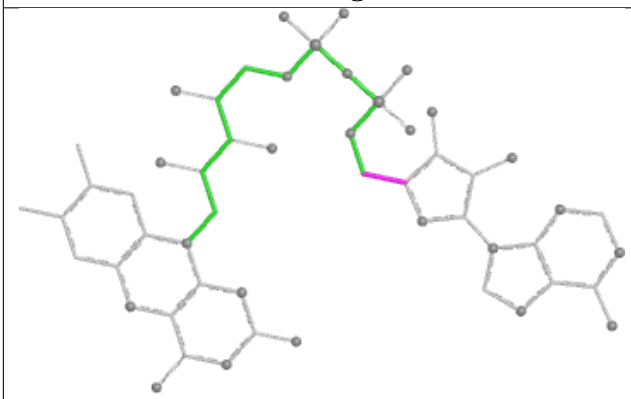
Ligand FAD C 401



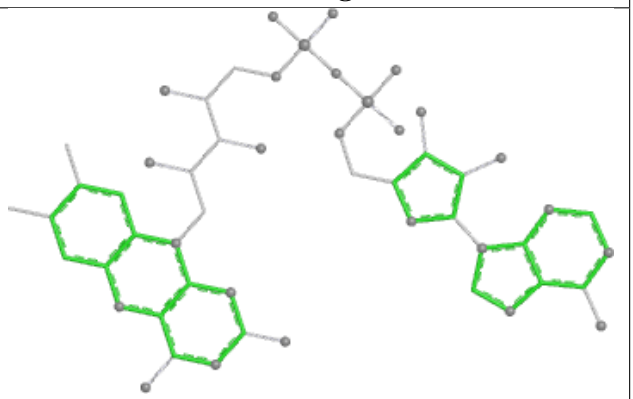
Bond lengths



Bond angles

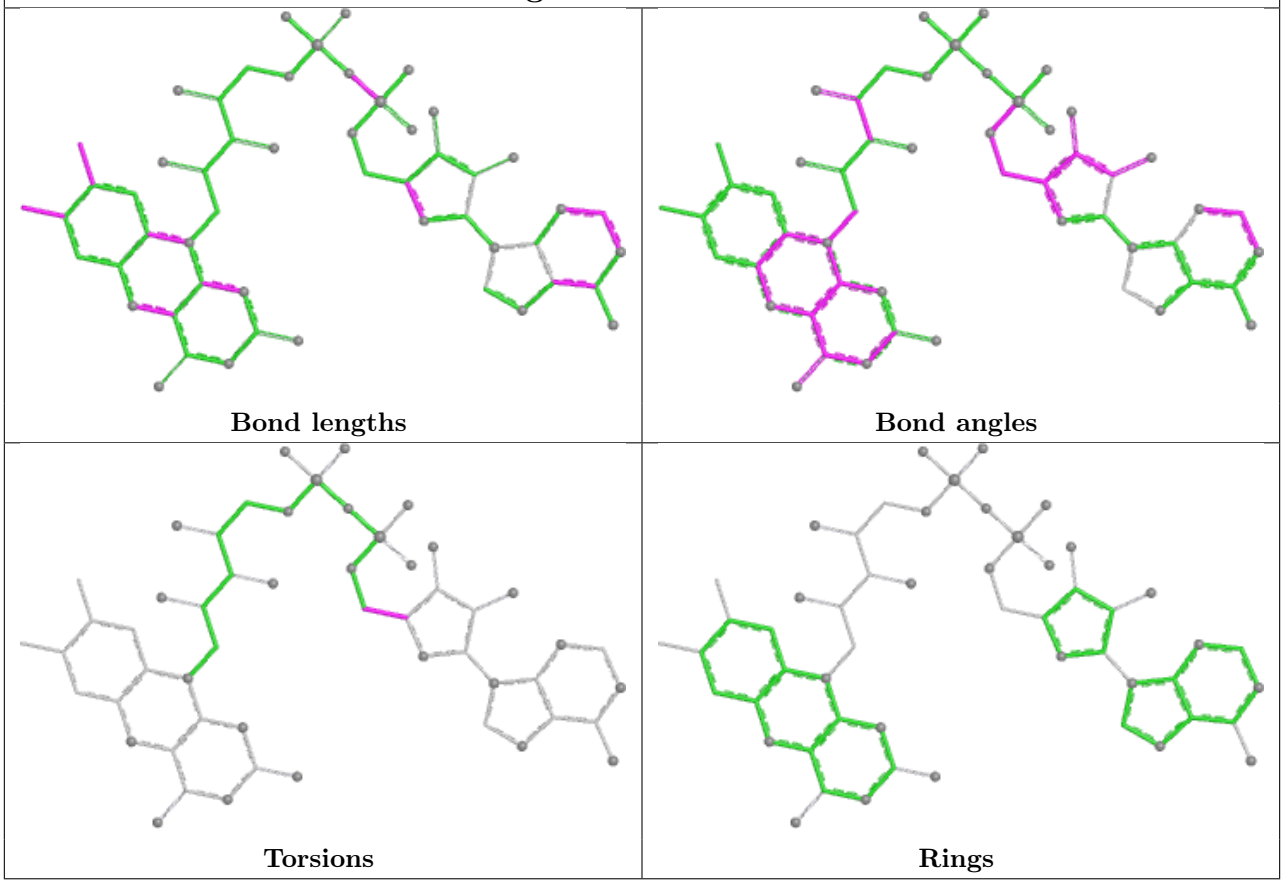


Torsions



Rings

Ligand FAD B 401



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

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	371/379 (97%)	-0.04	2 (0%)	91	91	12, 19, 34, 84	0
1	B	371/379 (97%)	-0.04	2 (0%)	91	91	12, 19, 34, 81	0
1	C	370/379 (97%)	-0.01	1 (0%)	94	94	14, 23, 39, 78	0
1	D	369/379 (97%)	-0.04	0	100	100	15, 23, 38, 52	0
All	All	1481/1516 (97%)	-0.03	5 (0%)	94	94	12, 21, 37, 84	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	LYS	5.4
1	A	10	LYS	3.3
1	A	9	GLY	2.3
1	B	9	GLY	2.2
1	C	10	LYS	2.1

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

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	PEG	D	422	7/7	0.68	0.21	43,46,50,51	0
6	PEG	D	424	7/7	0.68	0.21	44,49,58,61	0
5	EDO	D	413	4/4	0.70	0.19	44,47,53,57	0
6	PEG	B	422	7/7	0.71	0.21	60,62,73,78	0
7	PGE	B	429	10/10	0.71	0.21	43,54,63,65	0
5	EDO	B	413	4/4	0.72	0.38	45,47,57,57	0
8	PG4	B	430	13/13	0.72	0.29	33,49,59,62	0
5	EDO	D	407	4/4	0.73	0.25	61,70,71,75	0
6	PEG	C	423	7/7	0.75	0.16	45,47,55,58	0
5	EDO	C	409	4/4	0.76	0.31	44,44,47,56	0
6	PEG	B	424[A]	7/7	0.76	0.23	37,41,46,50	7
6	PEG	B	424[B]	7/7	0.76	0.23	35,41,46,50	7
5	EDO	B	407	4/4	0.76	0.22	47,54,55,59	0
5	EDO	B	420	4/4	0.76	0.17	50,52,58,66	0
5	EDO	D	415	4/4	0.76	0.18	40,43,50,50	0
6	PEG	A	418[A]	7/7	0.76	0.26	37,39,43,43	7
6	PEG	A	418[B]	7/7	0.76	0.26	32,38,41,43	7
5	EDO	B	415	4/4	0.77	0.17	40,50,51,53	0
6	PEG	B	428	7/7	0.78	0.24	42,50,53,54	0
6	PEG	D	423[A]	7/7	0.78	0.27	24,33,40,44	7
6	PEG	D	423[B]	7/7	0.78	0.27	25,32,41,42	7
6	PEG	A	417	7/7	0.80	0.35	31,42,50,51	0
3	BME	B	402	4/4	0.80	0.18	30,32,44,47	0
5	EDO	C	406	4/4	0.80	0.23	47,53,53,54	0
5	EDO	B	408	4/4	0.80	0.29	37,45,48,51	0
6	PEG	B	423	7/7	0.80	0.33	41,50,57,64	0
5	EDO	C	410	4/4	0.81	0.15	45,46,47,55	0
6	PEG	A	414	7/7	0.81	0.13	48,53,57,61	0
5	EDO	C	407	4/4	0.81	0.22	53,60,61,61	0
5	EDO	D	408	4/4	0.81	0.29	50,53,53,57	0
6	PEG	B	425	7/7	0.81	0.27	27,46,52,52	0
3	BME	D	402	4/4	0.81	0.24	36,37,47,53	0
6	PEG	C	419	7/7	0.81	0.24	40,56,61,64	0
5	EDO	B	417	4/4	0.82	0.28	48,50,52,63	0
5	EDO	D	418	4/4	0.82	0.11	53,58,62,64	0
3	BME	C	402	4/4	0.82	0.28	33,34,50,51	0
5	EDO	D	410	4/4	0.82	0.18	52,53,56,58	0
5	EDO	A	408	4/4	0.82	0.17	45,51,55,56	0
5	EDO	A	411	4/4	0.83	0.13	44,47,55,60	0
5	EDO	C	411	4/4	0.83	0.18	42,50,55,65	0
5	EDO	C	414	4/4	0.83	0.10	45,50,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	C	422	7/7	0.84	0.15	51,58,65,68	0
6	PEG	A	413	7/7	0.84	0.23	43,47,55,58	0
6	PEG	B	426	7/7	0.84	0.23	45,47,53,62	0
6	PEG	C	420	7/7	0.84	0.16	27,31,41,49	0
8	PG4	D	425	13/13	0.84	0.20	34,45,55,56	0
6	PEG	B	421	7/7	0.85	0.30	38,49,54,55	0
5	EDO	A	406	4/4	0.85	0.10	44,48,48,52	0
6	PEG	A	415	7/7	0.85	0.20	36,44,50,50	0
5	EDO	C	415	4/4	0.85	0.20	45,47,53,65	0
6	PEG	C	421	7/7	0.85	0.24	34,38,46,53	0
5	EDO	D	419	4/4	0.85	0.11	42,52,53,58	0
8	PG4	C	424	13/13	0.85	0.22	34,45,52,53	0
5	EDO	C	413	4/4	0.85	0.11	48,48,52,57	0
7	PGE	A	419	10/10	0.86	0.14	44,47,58,59	0
5	EDO	D	420	4/4	0.86	0.29	45,45,52,58	0
5	EDO	A	407	4/4	0.86	0.15	47,47,48,50	0
5	EDO	B	411	4/4	0.86	0.30	38,42,42,65	0
4	SO4	B	404	5/5	0.86	0.23	45,53,72,75	0
6	PEG	A	416[A]	7/7	0.87	0.20	32,40,44,51	7
6	PEG	A	416[B]	7/7	0.87	0.20	38,40,44,51	7
6	PEG	B	427	7/7	0.87	0.17	28,31,40,53	0
5	EDO	D	412	4/4	0.87	0.23	54,55,56,56	0
4	SO4	C	405	5/5	0.87	0.30	54,72,89,91	0
4	SO4	D	406	5/5	0.87	0.27	68,71,87,92	0
5	EDO	D	414	4/4	0.88	0.24	44,52,53,53	0
5	EDO	C	416	4/4	0.88	0.11	46,51,53,57	0
5	EDO	B	414	4/4	0.88	0.44	41,41,43,45	0
5	EDO	B	406	4/4	0.88	0.18	36,40,41,43	0
4	SO4	B	405	5/5	0.89	0.25	49,65,90,90	0
5	EDO	A	410	4/4	0.89	0.17	29,29,39,51	0
5	EDO	C	408	4/4	0.89	0.26	40,41,45,45	0
5	EDO	D	411	4/4	0.89	0.29	33,40,40,48	0
5	EDO	B	418	4/4	0.89	0.20	24,43,47,47	0
5	EDO	B	409	4/4	0.89	0.17	29,34,47,49	0
5	EDO	D	417	4/4	0.90	0.26	46,49,50,57	0
5	EDO	B	410	4/4	0.90	0.20	49,53,55,55	0
5	EDO	C	412	4/4	0.90	0.11	47,50,54,55	0
5	EDO	B	419	4/4	0.90	0.08	42,42,45,50	0
5	EDO	C	418	4/4	0.90	0.16	22,40,42,49	0
5	EDO	D	409	4/4	0.91	0.10	50,51,51,55	0
4	SO4	C	404	5/5	0.91	0.21	60,65,74,81	0
5	EDO	B	416	4/4	0.91	0.16	26,32,37,44	0

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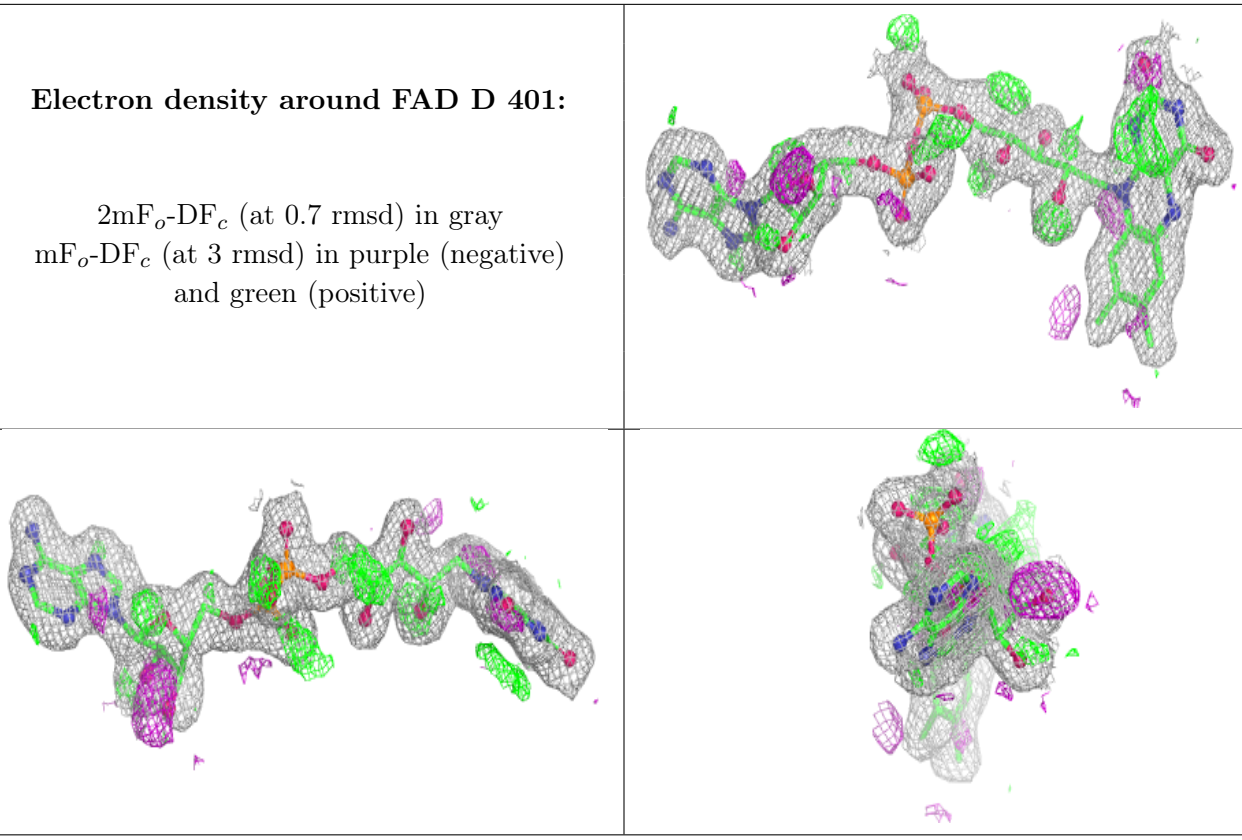
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	D	416	4/4	0.92	0.11	50,51,55,55	0
5	EDO	A	412	4/4	0.92	0.12	42,42,45,51	0
3	BME	A	402	4/4	0.92	0.15	33,36,46,48	0
4	SO4	D	405	5/5	0.93	0.23	57,60,73,78	0
5	EDO	B	412	4/4	0.93	0.38	26,33,35,45	0
5	EDO	A	409	4/4	0.93	0.12	23,39,47,47	0
5	EDO	D	421	4/4	0.93	0.16	31,39,41,49	0
5	EDO	C	417	4/4	0.93	0.14	29,33,44,58	0
5	EDO	A	405	4/4	0.94	0.22	24,36,37,45	0
2	FAD	D	401	53/53	0.94	0.12	14,19,24,26	0
2	FAD	A	401	53/53	0.95	0.12	10,16,22,22	0
2	FAD	B	401	53/53	0.95	0.11	10,16,21,23	0
2	FAD	C	401	53/53	0.95	0.12	14,19,25,27	0
4	SO4	A	404	5/5	0.96	0.18	51,56,67,69	0
4	SO4	B	403	5/5	0.97	0.14	26,33,44,46	0
4	SO4	C	403	5/5	0.97	0.11	28,32,44,49	0
4	SO4	D	403	5/5	0.98	0.10	26,32,45,45	0
4	SO4	D	404	5/5	0.98	0.19	51,59,63,70	0
4	SO4	A	403	5/5	0.99	0.09	24,31,45,46	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.

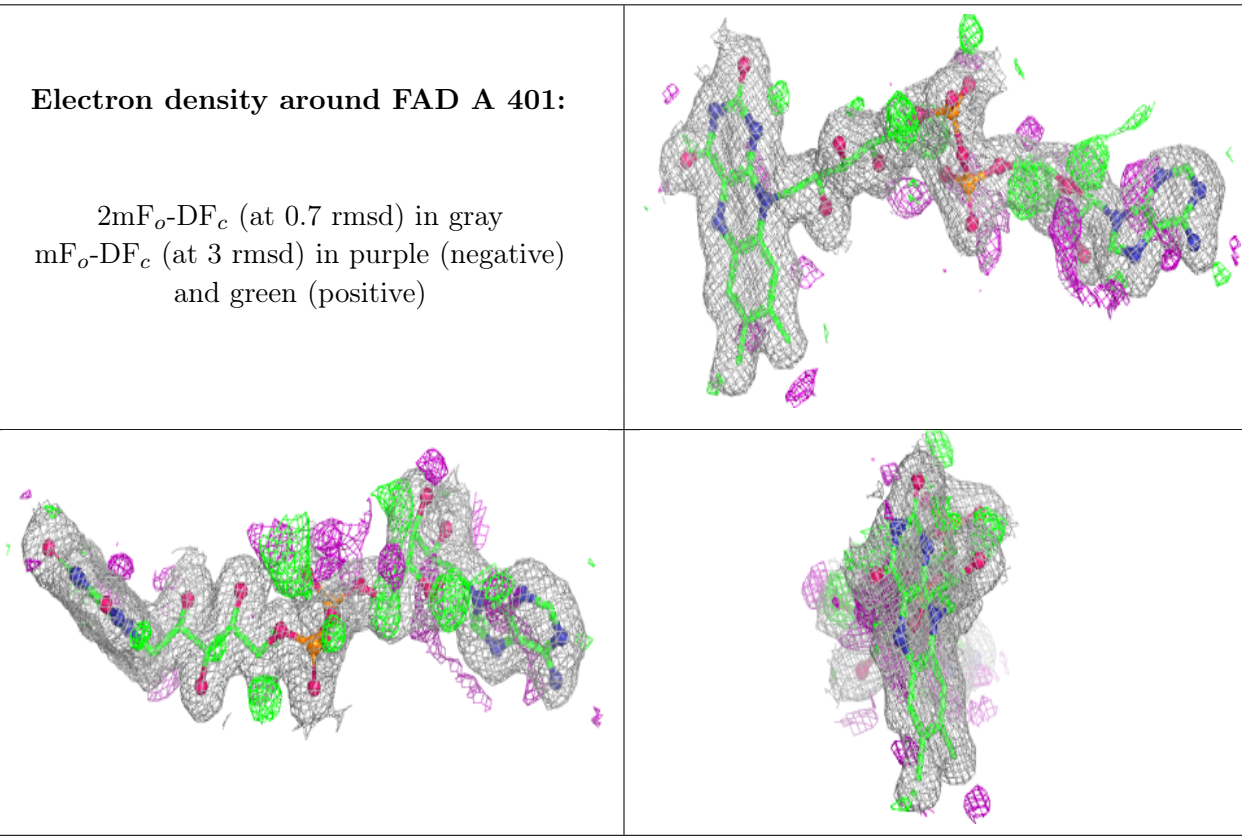
Electron density around FAD D 401:

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



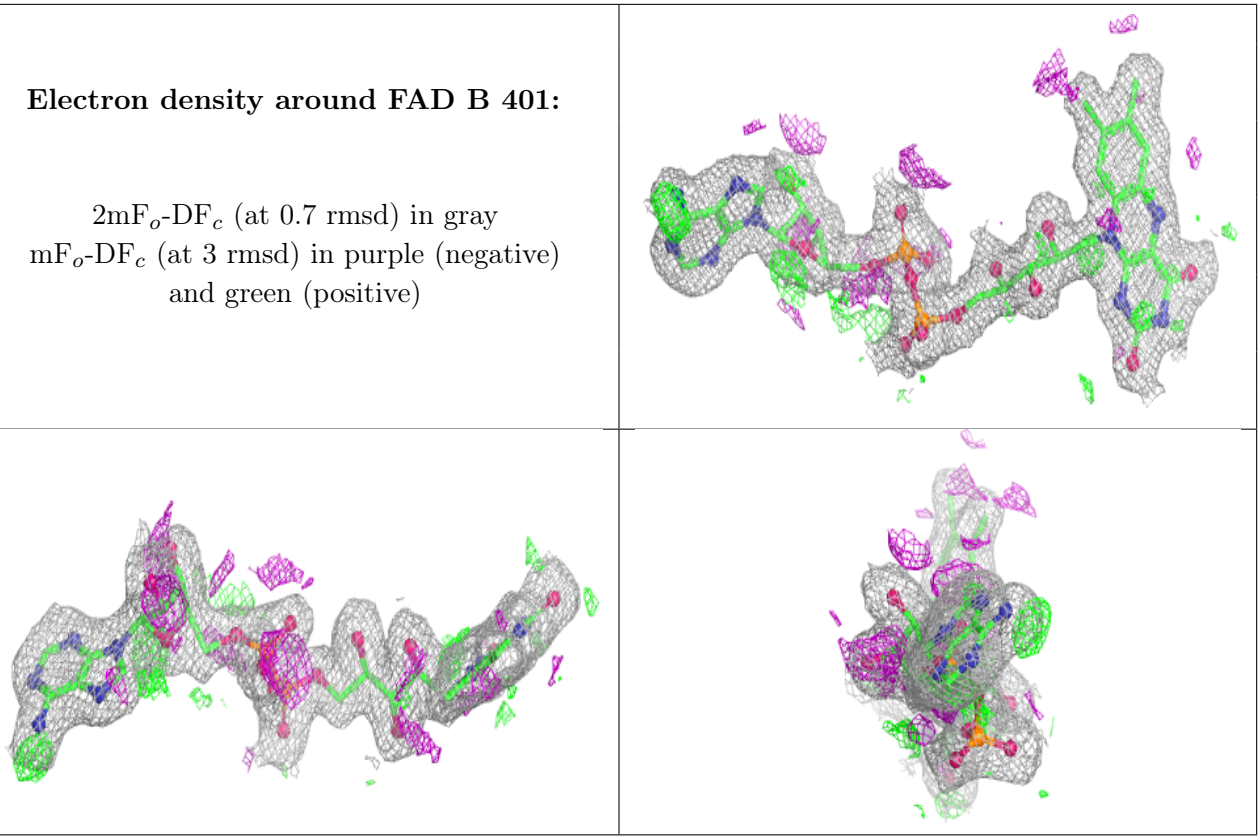
Electron density around FAD A 401:

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



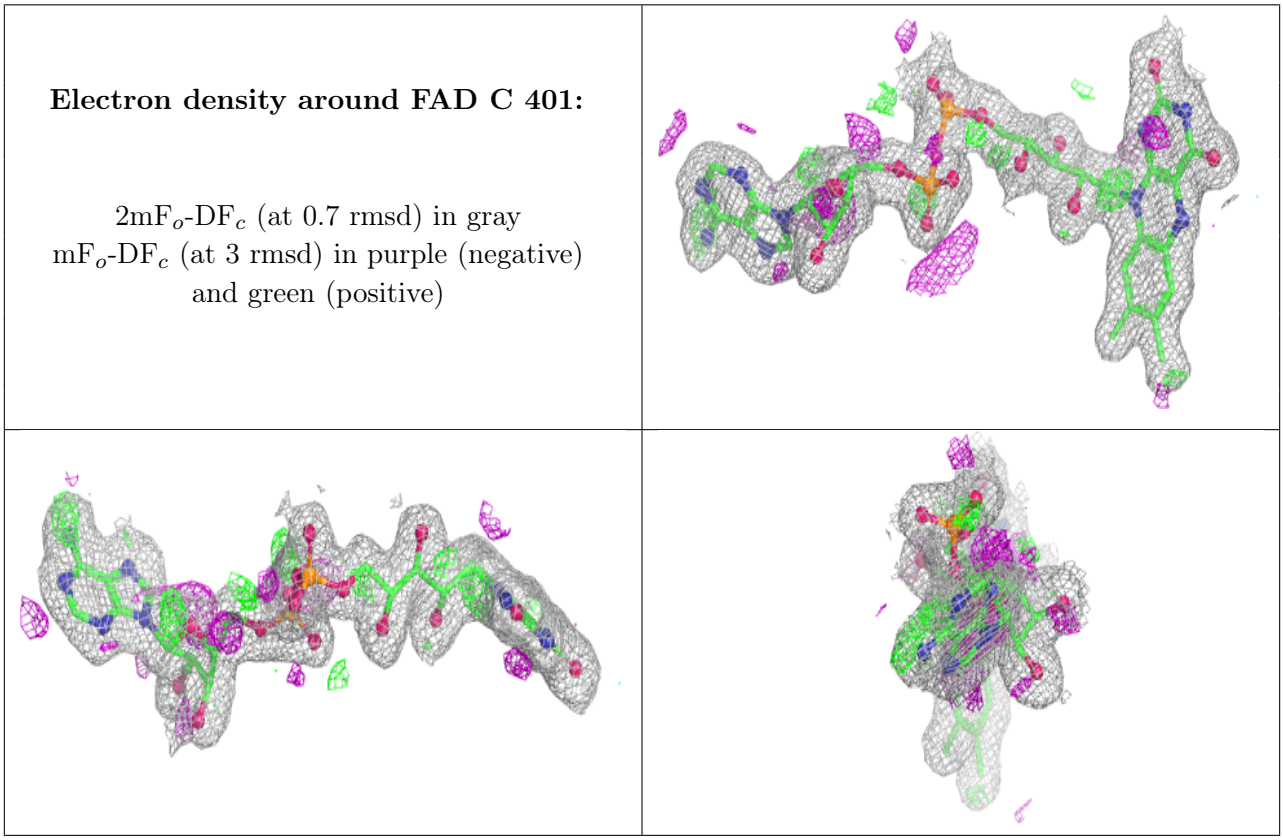
Electron density around FAD B 401:

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



Electron density around FAD C 401:

$2mF_o$-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.