wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 01:59 PM EDT

PDB ID	:	2R4J
Title	:	Crystal structure of Escherichia coli SeMet substituted Glycerol-3-phosphate Dehydrogenase in complex with DHAP
Authors	:	Yeh, J.I.; Du, S.; Chinte, U.
Deposited on	:	2007-08-31
Resolution	:	1.96 Å(reported)

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

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

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

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

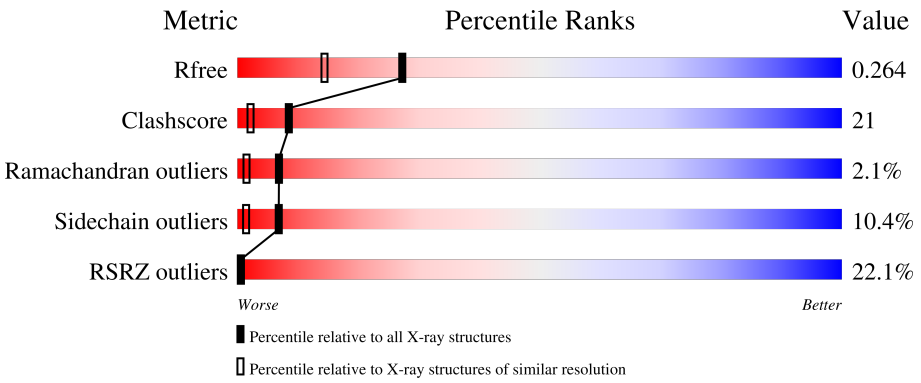
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	501	22% 67% 26% 5% •
1	B	501	21% 65% 27% 6% ••

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	A	1949	-	-	-	X
2	BOG	A	1950	-	-	-	X
2	BOG	A	800	-	-	-	X
2	BOG	B	800	-	-	-	X
3	PO4	B	801	-	-	-	X
5	EDO	A	1956	-	-	-	X
5	EDO	A	1957	-	-	X	-
5	EDO	A	1958	-	-	X	-
5	EDO	A	1959	-	-	X	-
5	EDO	B	806	-	-	-	X
5	EDO	B	807	-	-	X	-
5	EDO	B	813	-	-	X	-
5	EDO	B	817	-	-	-	X
6	IMD	A	1960	-	-	X	-
6	IMD	A	1961	-	-	X	-
6	IMD	A	1963	-	-	X	-
6	IMD	A	1966	-	-	X	-
7	13P	A	1968	-	X	-	-
7	13P	B	816	-	X	X	-
8	BCN	A	1969	-	-	-	X
8	BCN	B	820	-	-	-	X
8	BCN	B	821	-	-	-	X
9	TAM	B	812	-	-	X	X

2 Entry composition (i)

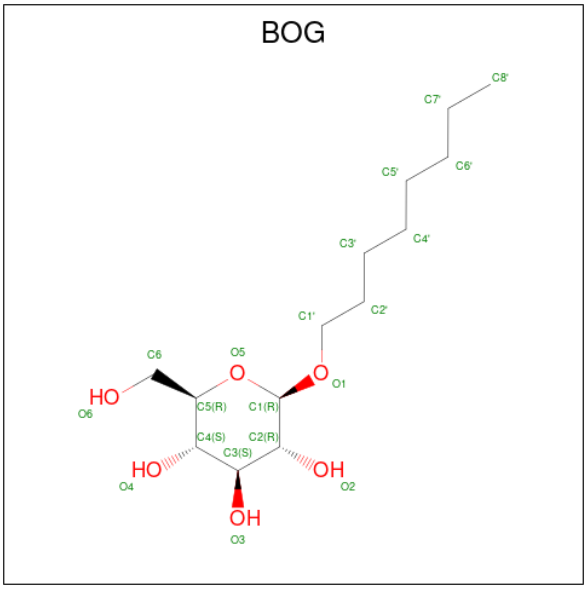
There are 10 unique types of molecules in this entry. The entry contains 8645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aerobic glycerol-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	494	3953	2510	703	727	6	7	0	0	0
1	B	497	3981	2527	710	731	6	7	0	0	0

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	20	14	6	0	0
2	A	1	20	14	6	0	0
2	A	1	20	14	6	0	0
2	A	1	20	14	6	0	0

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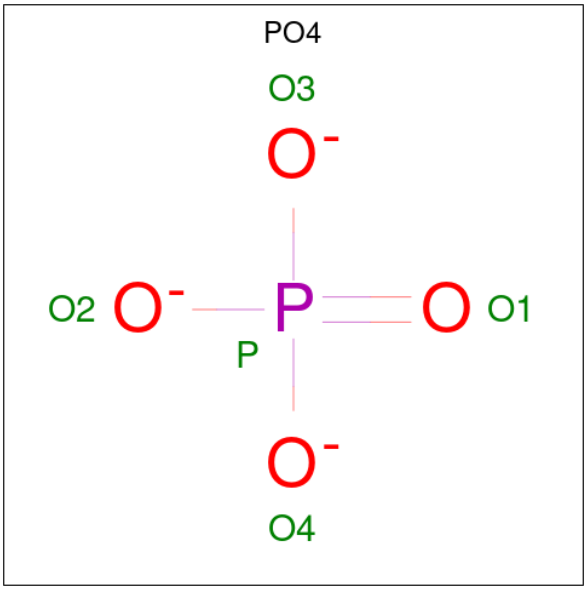
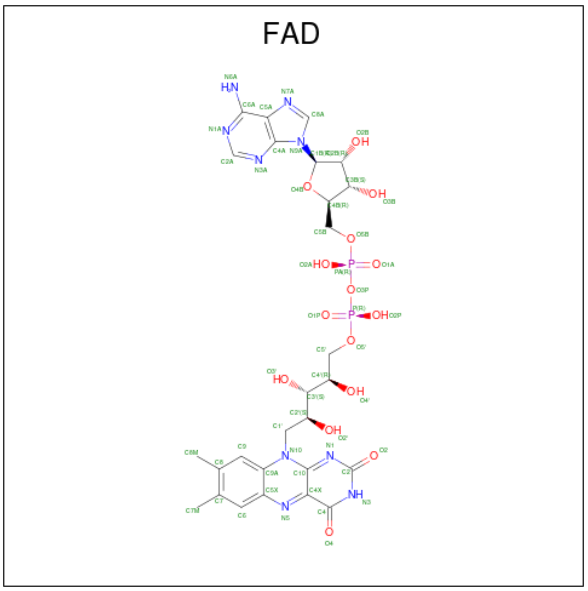
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	20	14	6	0	0
			Total	C	O		
2	B	1	20	14	6	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



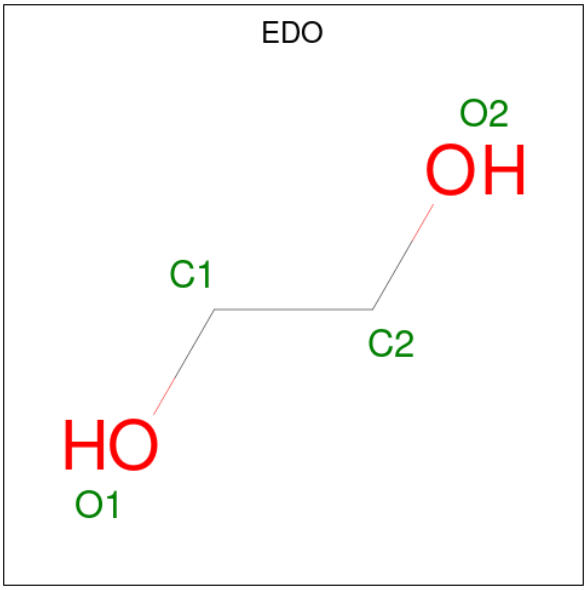
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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



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

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

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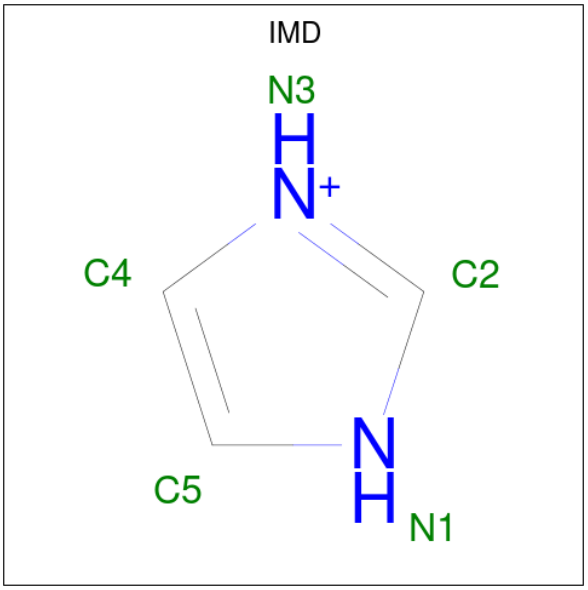
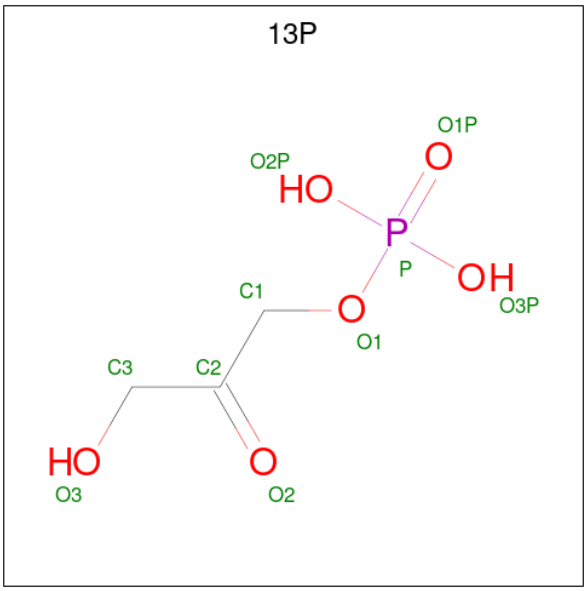
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



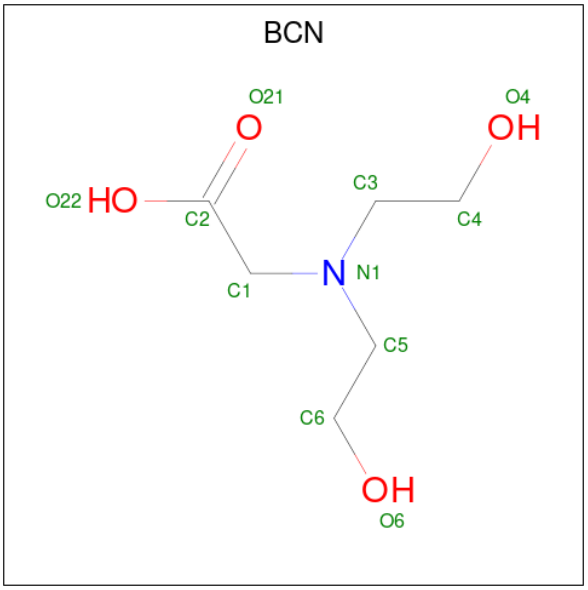
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	B	1	5	3	2	0	0

- Molecule 7 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
7	A	1	10	3	6	1	0	0
			Total	C	O	P		
7	B	1	10	3	6	1	0	0

- Molecule 8 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	11	6	1	4	0	0
			Total	C	N	O		
8	B	1	11	6	1	4	0	0

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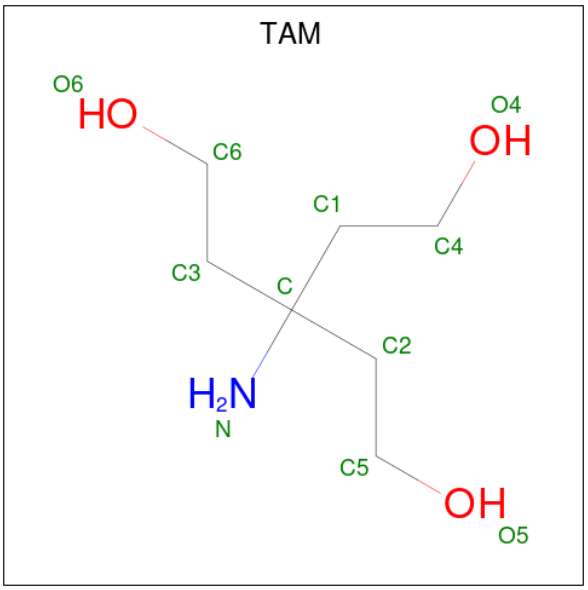
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	11	6	1	4	0	0

- Molecule 9 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	B	1	11	7	1	3	0	0

- Molecule 10 is water.

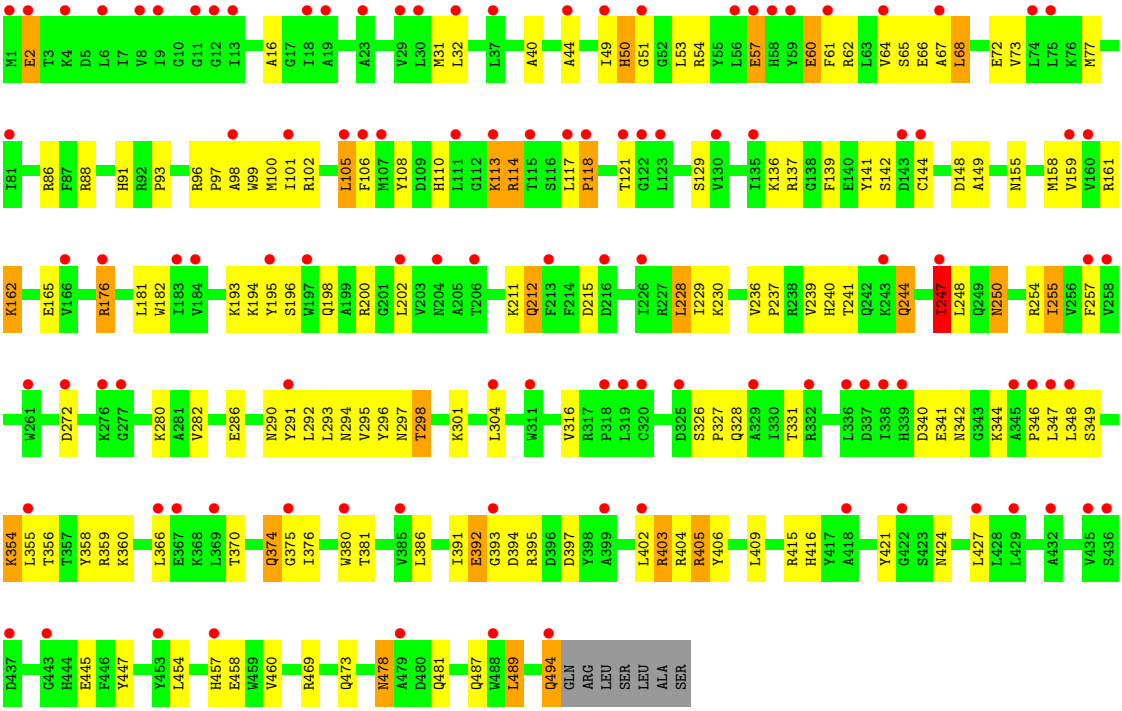
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	140	140	140	0	0
10	B	137	137	137	0	0

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.

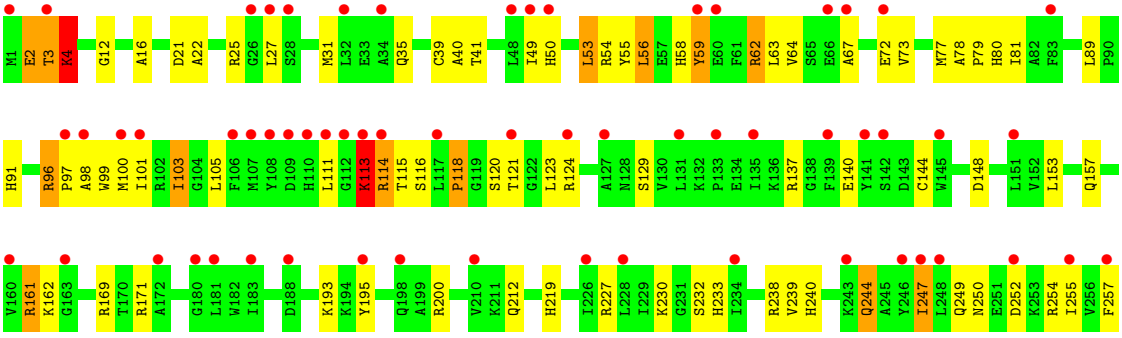
• Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase

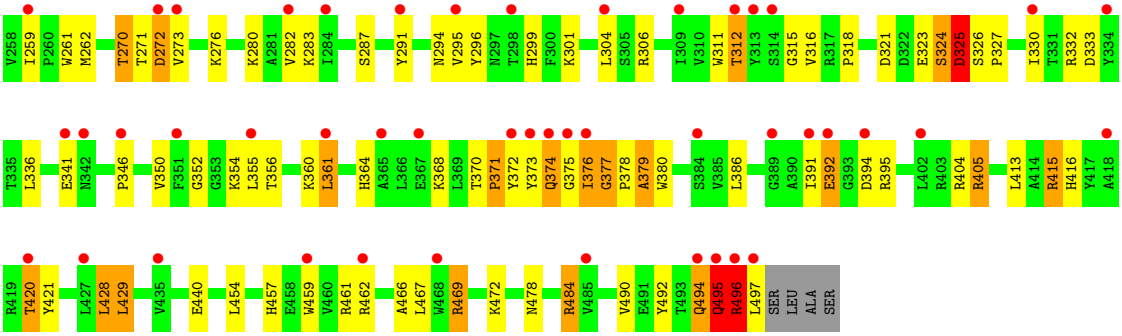
Chain A:



• Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase

Chain B:




V258 I259 P260 W261 M262 T270 T271 D272 V273 K276 K280 A281 V282 K283 I284 S287 Y291 N294 V295 Y296 N297 T298 H299 F300 K301 L304 S305 R306 I309 V310 W311 T312 Y313 S314 G315 V316 R317 P318 D321 D322 E323 S324 D325 S326 P327 I330 T331 R332 D333 Y334
T335 L336 E341 N342 P346 V350 F351 G352 G353 K354 L355 T356 K360 L361 H364 A365 L366 E367 K368 L369 T370 P371 Y372 Y373 Q374 G375 I376 G377 P378 A379 W380 S384 V385 L386 G389 A390 I391 E392 G393 D394 R395 L402 R403 R404 R405 L413 A414 R415 H416 Y417 A418
R419 T420 Y421 L427 L428 L429 V435 E440 L454 H457 E458 W459 V460 R461 R462 A466 L467 W468 R469 K472 N478 R484 V485 V490 E491 Y492 T493 Q494 Q495 R496 L497 SER LEU ALA SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	113.92Å 114.14Å 193.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.96 40.32 – 1.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-1.96) 91.0 (40.32-1.96)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	133.85 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.263 0.220 , 0.264	Depositor DCC
R_{free} test set	4126 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.450 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8645	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, BCN, IMD, BOG, EDO, TAM, PO4, 13P

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	1.10	4/4041 (0.1%)	1.03	6/5461 (0.1%)
1	B	1.12	2/4069 (0.0%)	1.05	12/5498 (0.2%)
All	All	1.11	6/8110 (0.1%)	1.04	18/10959 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	VAL	C-O	5.60	1.33	1.23
1	A	447	TYR	CD2-CE2	5.58	1.47	1.39
1	A	165	GLU	CB-CG	5.50	1.62	1.52
1	B	12	GLY	N-CA	-5.27	1.38	1.46
1	A	236	VAL	CB-CG2	5.19	1.63	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	247	ILE	CB-CA-C	-5.74	100.11	111.60
1	A	355	LEU	CB-CG-CD1	-5.71	101.28	111.00
1	B	148	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	355	LEU	CA-CB-CG	5.60	128.17	115.30

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	3953	0	3903	144	0
1	B	3981	0	3935	177	0
2	A	80	0	112	7	0
2	B	40	0	56	9	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	31	0	0
5	A	44	0	66	28	0
5	B	60	0	90	24	0
6	A	25	0	25	21	0
6	B	5	0	5	1	0
7	A	10	0	5	0	0
7	B	10	0	5	4	0
8	A	11	0	12	1	0
8	B	22	0	24	5	0
9	B	11	0	17	7	0
10	A	140	0	0	9	0
10	B	137	0	0	13	0
All	All	8645	0	8317	347	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 21.

The worst 5 of 347 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:27:LEU:HD21	1:B:376:ILE:CD1	1.54	1.37
1:B:374:GLN:CB	1:B:375:GLY:HA3	1.59	1.27
1:B:467:LEU:HA	10:B:938:HOH:O	1.37	1.22
5:B:813:EDO:H22	10:B:869:HOH:O	1.37	1.20
1:B:428:LEU:HD12	1:B:428:LEU:O	1.36	1.20

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	492/501 (98%)	456 (93%)	30 (6%)	6 (1%)	13 4
1	B	495/501 (99%)	454 (92%)	26 (5%)	15 (3%)	4 0
All	All	987/1002 (98%)	910 (92%)	56 (6%)	21 (2%)	7 1

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	LYS
1	A	118	PRO
1	B	113	LYS
1	B	118	PRO
1	B	324	SER

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	413/412 (100%)	377 (91%)	36 (9%)	10 2
1	B	416/412 (101%)	366 (88%)	50 (12%)	5 1
All	All	829/824 (101%)	743 (90%)	86 (10%)	7 1

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	244	GLN

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Mol	Chain	Res	Type
1	B	361	LEU
1	B	255	ILE
1	B	312	THR
1	B	404	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	GLN
1	B	249	GLN
1	B	244	GLN
1	B	294	ASN
1	A	250	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)

48 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	805	-	3,3,3	0.52	0	2,2,2	0.66	0
6	IMD	A	1961	-	3,5,5	0.37	0	4,5,5	0.60	0
8	BCN	B	820	-	10,10,10	1.01	0	11,11,11	2.20	3 (27%)
5	EDO	A	1954	-	3,3,3	0.55	0	2,2,2	0.29	0
5	EDO	B	814	-	3,3,3	0.72	0	2,2,2	0.21	0
5	EDO	A	1953	-	3,3,3	0.62	0	2,2,2	0.91	0
2	BOG	A	700	-	20,20,20	0.77	1 (5%)	25,25,25	1.14	2 (8%)
9	TAM	B	812	-	10,10,10	1.04	0	12,12,12	2.58	7 (58%)
5	EDO	B	809	-	3,3,3	0.56	0	2,2,2	0.41	0
2	BOG	A	800	-	20,20,20	0.64	1 (5%)	25,25,25	1.56	5 (20%)
2	BOG	A	1949	-	20,20,20	0.98	1 (5%)	25,25,25	0.92	1 (4%)
5	EDO	B	818	-	3,3,3	0.53	0	2,2,2	0.31	0
5	EDO	A	1955	-	3,3,3	0.66	0	2,2,2	0.39	0
5	EDO	B	807	-	3,3,3	0.97	0	2,2,2	0.55	0
2	BOG	A	1950	-	20,20,20	0.98	1 (5%)	25,25,25	1.68	5 (20%)
5	EDO	B	803	-	3,3,3	0.80	0	2,2,2	0.72	0
5	EDO	A	1964	-	3,3,3	0.53	0	2,2,2	0.47	0
5	EDO	A	1959	-	3,3,3	0.66	0	2,2,2	0.51	0
5	EDO	A	1965	-	3,3,3	0.59	0	2,2,2	0.64	0
5	EDO	B	810	-	3,3,3	0.56	0	2,2,2	0.44	0
4	FAD	A	600	-	54,58,58	1.94	22 (40%)	71,89,89	1.57	15 (21%)
2	BOG	B	700	-	20,20,20	0.82	1 (5%)	25,25,25	1.09	2 (8%)
8	BCN	B	821	-	10,10,10	1.16	1 (10%)	11,11,11	2.25	4 (36%)
5	EDO	B	817	-	3,3,3	0.62	0	2,2,2	0.33	0
5	EDO	B	804	-	3,3,3	0.50	0	2,2,2	0.87	0
5	EDO	A	1958	-	3,3,3	0.49	0	2,2,2	0.25	0
5	EDO	B	813	-	3,3,3	0.25	0	2,2,2	0.83	0
7	13P	B	816	-	9,9,9	4.34	6 (66%)	10,12,12	3.70	4 (40%)
5	EDO	B	808	-	3,3,3	0.83	0	2,2,2	0.35	0
3	PO4	B	801	-	4,4,4	0.51	0	6,6,6	1.02	0
5	EDO	B	811	-	3,3,3	0.29	0	2,2,2	0.77	0
6	IMD	A	1967	-	3,5,5	0.55	0	4,5,5	0.49	0
5	EDO	A	1957	-	3,3,3	1.08	0	2,2,2	0.77	0
5	EDO	B	802	-	3,3,3	0.93	0	2,2,2	0.82	0
6	IMD	A	1966	-	3,5,5	0.41	0	4,5,5	1.12	0
7	13P	A	1968	-	9,9,9	4.45	6 (66%)	10,12,12	4.01	4 (40%)
5	EDO	B	815	-	3,3,3	0.34	0	2,2,2	0.88	0
4	FAD	B	600	-	54,58,58	2.00	18 (33%)	71,89,89	1.99	19 (26%)
3	PO4	A	1951	-	4,4,4	0.69	0	6,6,6	0.72	0
5	EDO	A	1962	-	3,3,3	0.52	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	A	1956	-	3,3,3	0.48	0	2,2,2	0.24	0
5	EDO	B	806	-	3,3,3	1.10	0	2,2,2	0.31	0
6	IMD	A	1960	-	3,5,5	0.34	0	4,5,5	0.92	0
6	IMD	A	1963	-	3,5,5	0.52	0	4,5,5	0.49	0
6	IMD	B	819	-	3,5,5	0.46	0	4,5,5	0.44	0
8	BCN	A	1969	-	10,10,10	1.03	0	11,11,11	2.05	4 (36%)
5	EDO	A	1952	-	3,3,3	0.71	0	2,2,2	0.21	0
2	BOG	B	800	-	20,20,20	0.57	0	25,25,25	1.22	2 (8%)

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	805	-	-	1/1/1/1	-
6	IMD	A	1961	-	-	-	0/1/1/1
8	BCN	B	820	-	-	7/10/10/10	-
5	EDO	A	1954	-	-	0/1/1/1	-
5	EDO	B	814	-	-	0/1/1/1	-
5	EDO	A	1953	-	-	0/1/1/1	-
2	BOG	A	700	-	-	7/11/31/31	0/1/1/1
9	TAM	B	812	-	-	5/12/12/12	-
5	EDO	B	809	-	-	1/1/1/1	-
2	BOG	A	800	-	-	8/11/31/31	0/1/1/1
2	BOG	A	1949	-	-	6/11/31/31	0/1/1/1
5	EDO	B	818	-	-	1/1/1/1	-
5	EDO	A	1955	-	-	1/1/1/1	-
5	EDO	B	807	-	-	1/1/1/1	-
2	BOG	A	1950	-	-	5/11/31/31	0/1/1/1
5	EDO	B	803	-	-	1/1/1/1	-
5	EDO	A	1964	-	-	1/1/1/1	-
5	EDO	A	1959	-	-	0/1/1/1	-
5	EDO	A	1965	-	-	1/1/1/1	-
5	EDO	B	810	-	-	1/1/1/1	-
4	FAD	A	600	-	-	5/30/50/50	0/6/6/6
2	BOG	B	700	-	-	5/11/31/31	0/1/1/1
8	BCN	B	821	-	-	7/10/10/10	-
5	EDO	B	817	-	-	1/1/1/1	-
5	EDO	B	804	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1958	-	-	1/1/1/1	-
5	EDO	B	813	-	-	1/1/1/1	-
7	13P	B	816	-	-	7/8/8/8	-
5	EDO	B	808	-	-	1/1/1/1	-
5	EDO	B	811	-	-	1/1/1/1	-
6	IMD	A	1967	-	-	-	0/1/1/1
5	EDO	A	1957	-	-	1/1/1/1	-
5	EDO	B	802	-	-	1/1/1/1	-
7	13P	A	1968	-	-	7/8/8/8	-
6	IMD	A	1966	-	-	-	0/1/1/1
5	EDO	B	815	-	-	1/1/1/1	-
4	FAD	B	600	-	-	0/30/50/50	0/6/6/6
5	EDO	A	1962	-	-	1/1/1/1	-
5	EDO	A	1956	-	-	1/1/1/1	-
5	EDO	B	806	-	-	1/1/1/1	-
6	IMD	A	1960	-	-	-	0/1/1/1
6	IMD	A	1963	-	-	-	0/1/1/1
6	IMD	B	819	-	-	-	0/1/1/1
8	BCN	A	1969	-	-	5/10/10/10	-
5	EDO	A	1952	-	-	0/1/1/1	-
2	BOG	B	800	-	-	6/11/31/31	0/1/1/1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	816	13P	O1-C1	8.37	1.51	1.43
7	A	1968	13P	O1-C1	7.95	1.51	1.43
7	A	1968	13P	O2-C2	6.41	1.33	1.21
7	B	816	13P	C1-C2	5.90	1.61	1.50
7	B	816	13P	O2-C2	5.69	1.31	1.21

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1968	13P	O3P-P-O1	-8.90	83.48	106.67
7	B	816	13P	O3P-P-O1	-8.01	85.77	106.67
7	B	816	13P	O2P-P-O1	6.43	123.44	106.67
7	A	1968	13P	O2P-P-O1	6.28	123.05	106.67
4	B	600	FAD	N3A-C2A-N1A	-5.47	121.25	128.67

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	BOG	O5-C1-O1-C1'
2	A	800	BOG	C2'-C1'-O1-C1
4	A	600	FAD	N10-C1'-C2'-O2'
4	A	600	FAD	O4'-C4'-C5'-O5'
7	A	1968	13P	C1-O1-P-O2P

There are no ring outliers.

36 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1961	IMD	5	0
8	B	820	BCN	2	0
5	A	1953	EDO	2	0
2	A	700	BOG	1	0
9	B	812	TAM	7	0
2	A	800	BOG	5	0
5	A	1955	EDO	2	0
5	B	807	EDO	7	0
2	A	1950	BOG	1	0
5	B	803	EDO	2	0
5	A	1964	EDO	1	0
5	A	1959	EDO	7	0
5	A	1965	EDO	3	0
5	B	810	EDO	2	0
4	A	600	FAD	1	0
2	B	700	BOG	2	0
8	B	821	BCN	3	0
5	B	817	EDO	1	0
5	B	804	EDO	1	0
5	A	1958	EDO	4	0
5	B	813	EDO	6	0
7	B	816	13P	4	0
5	B	808	EDO	2	0
5	B	811	EDO	3	0
5	A	1957	EDO	6	0
5	B	802	EDO	1	0
6	A	1966	IMD	4	0
5	B	815	EDO	1	0
5	A	1962	EDO	1	0
5	A	1956	EDO	3	0
5	B	806	EDO	1	0

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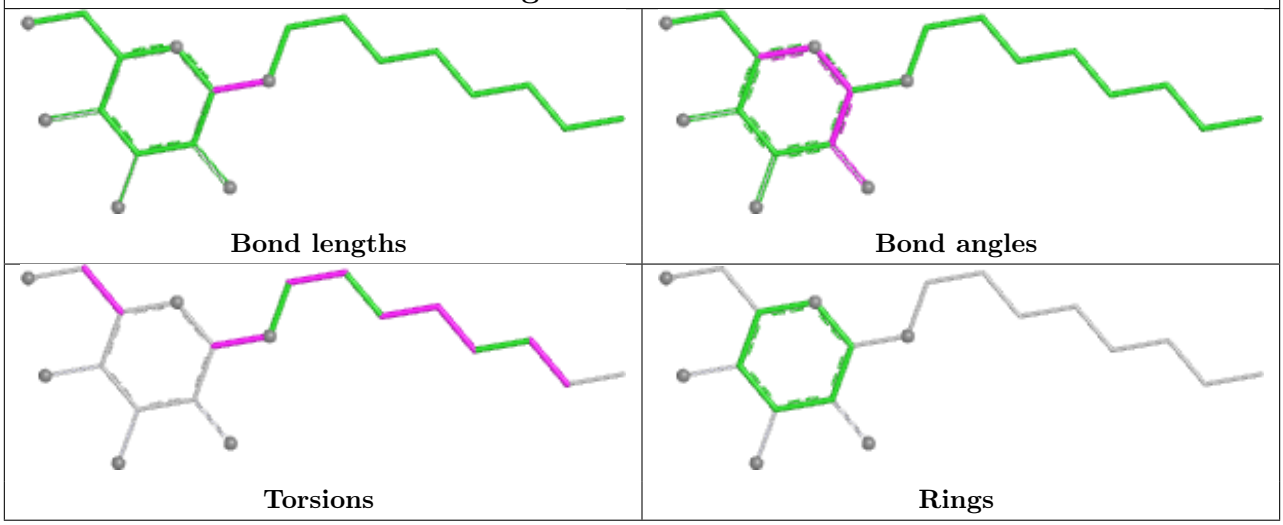
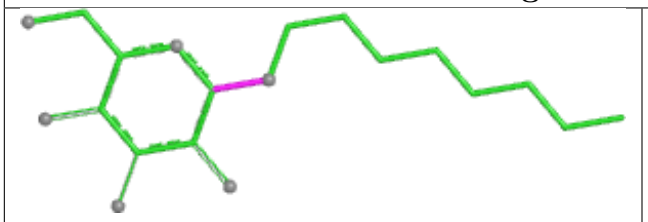
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1960	IMD	4	0
6	A	1963	IMD	8	0
6	B	819	IMD	1	0
8	A	1969	BCN	1	0
2	B	800	BOG	7	0

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.

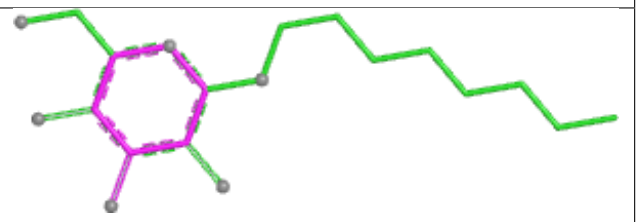
Ligand BOG A 700



Ligand BOG A 800

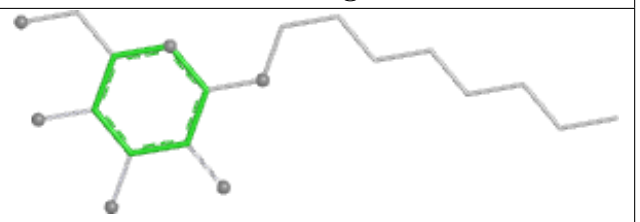


Bond lengths



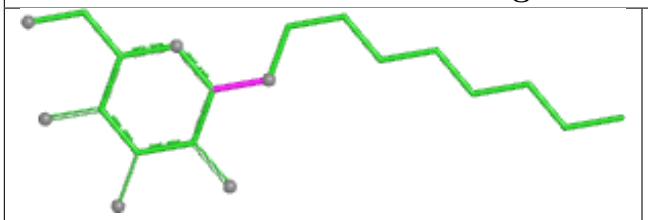
Bond angles

Torsions

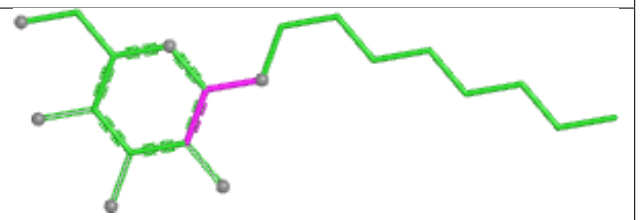


Rings

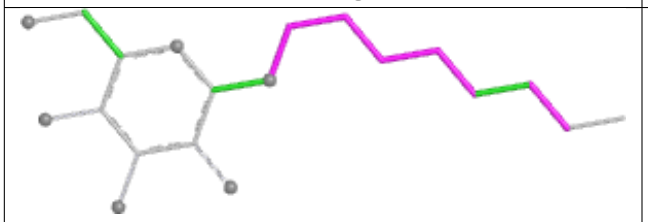
Ligand BOG A 1949



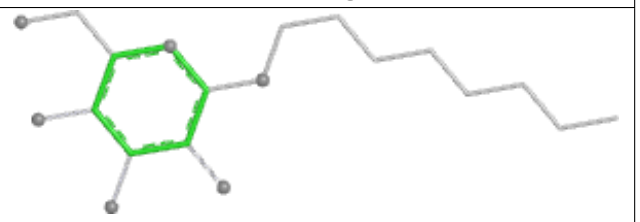
Bond lengths



Bond angles

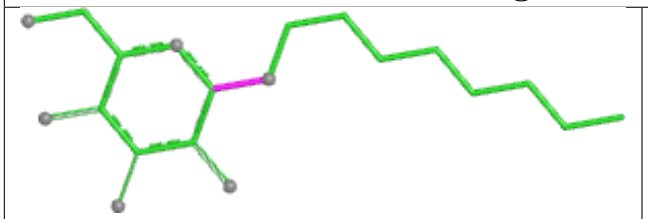


Torsions

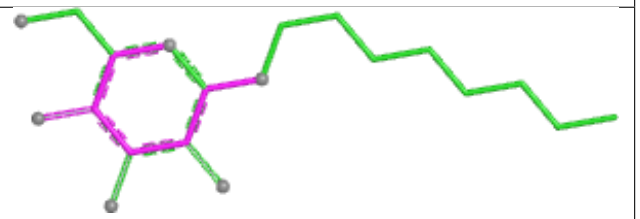


Rings

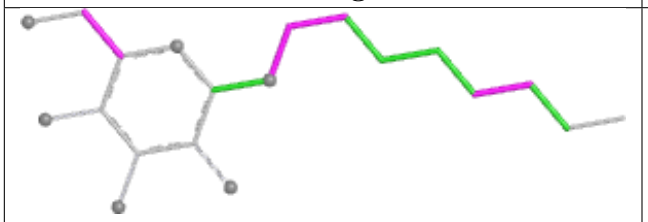
Ligand BOG A 1950



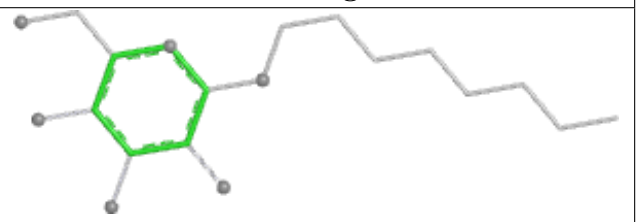
Bond lengths



Bond angles

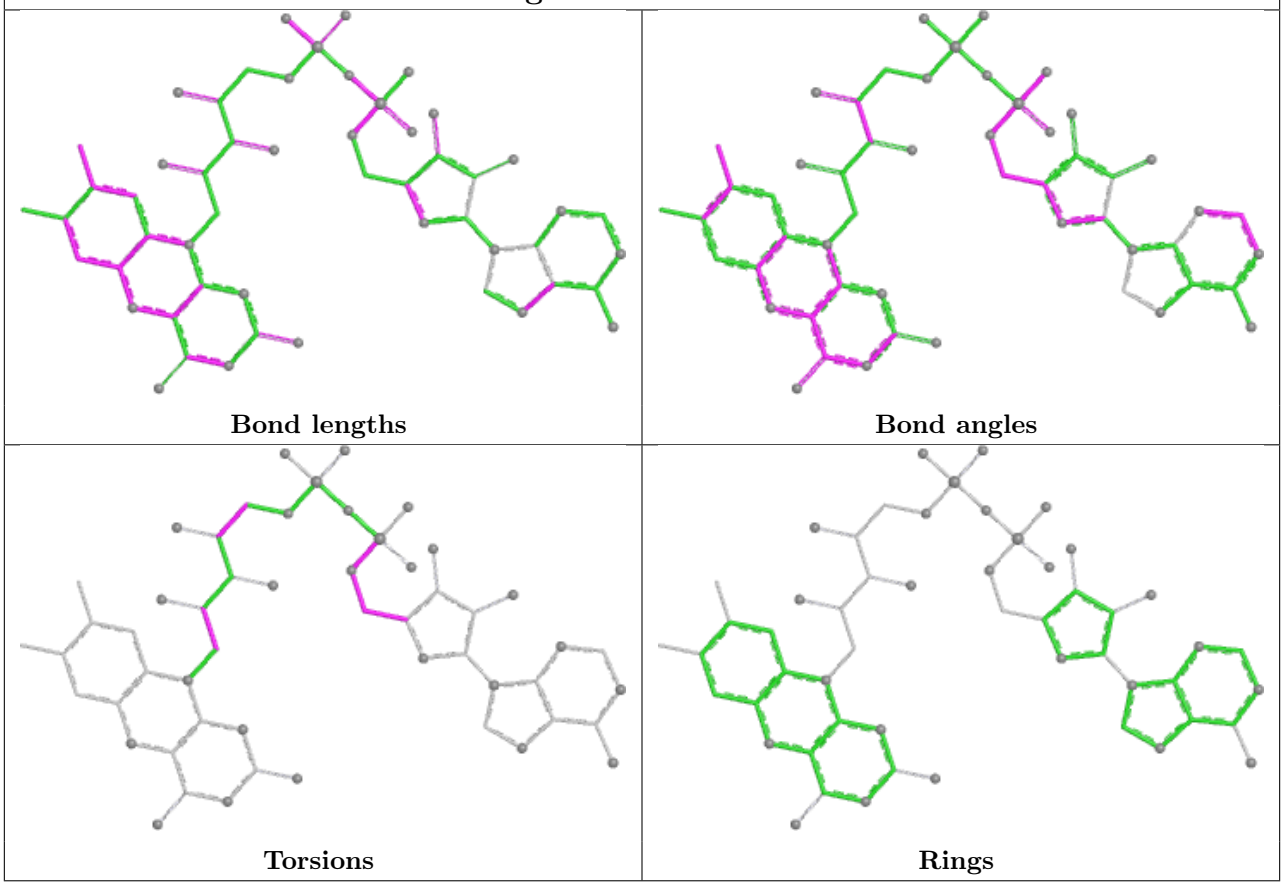


Torsions

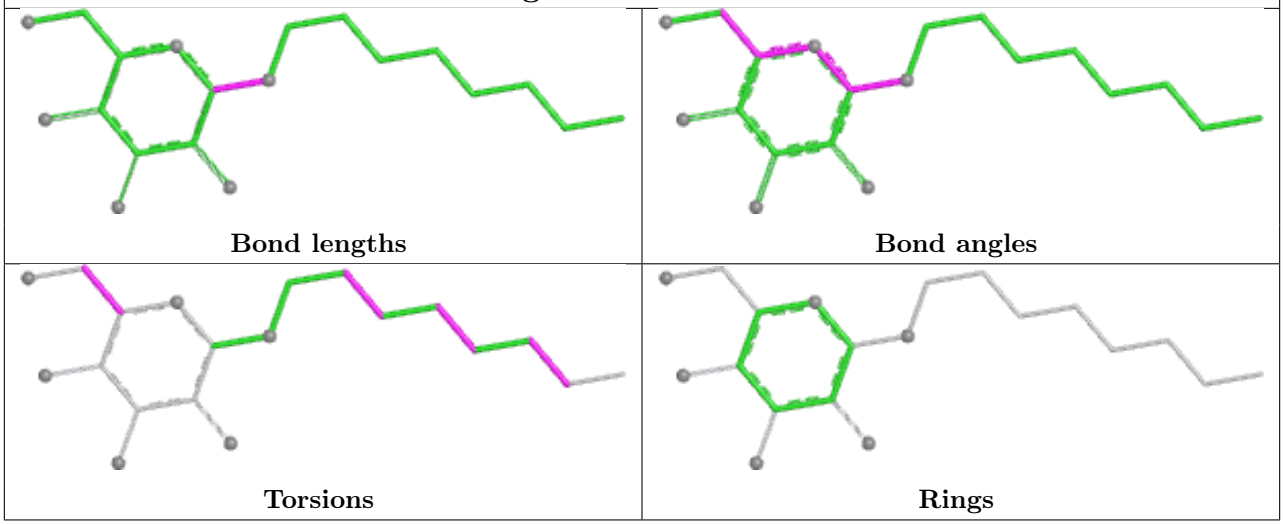


Rings

Ligand FAD A 600



Ligand BOG B 700



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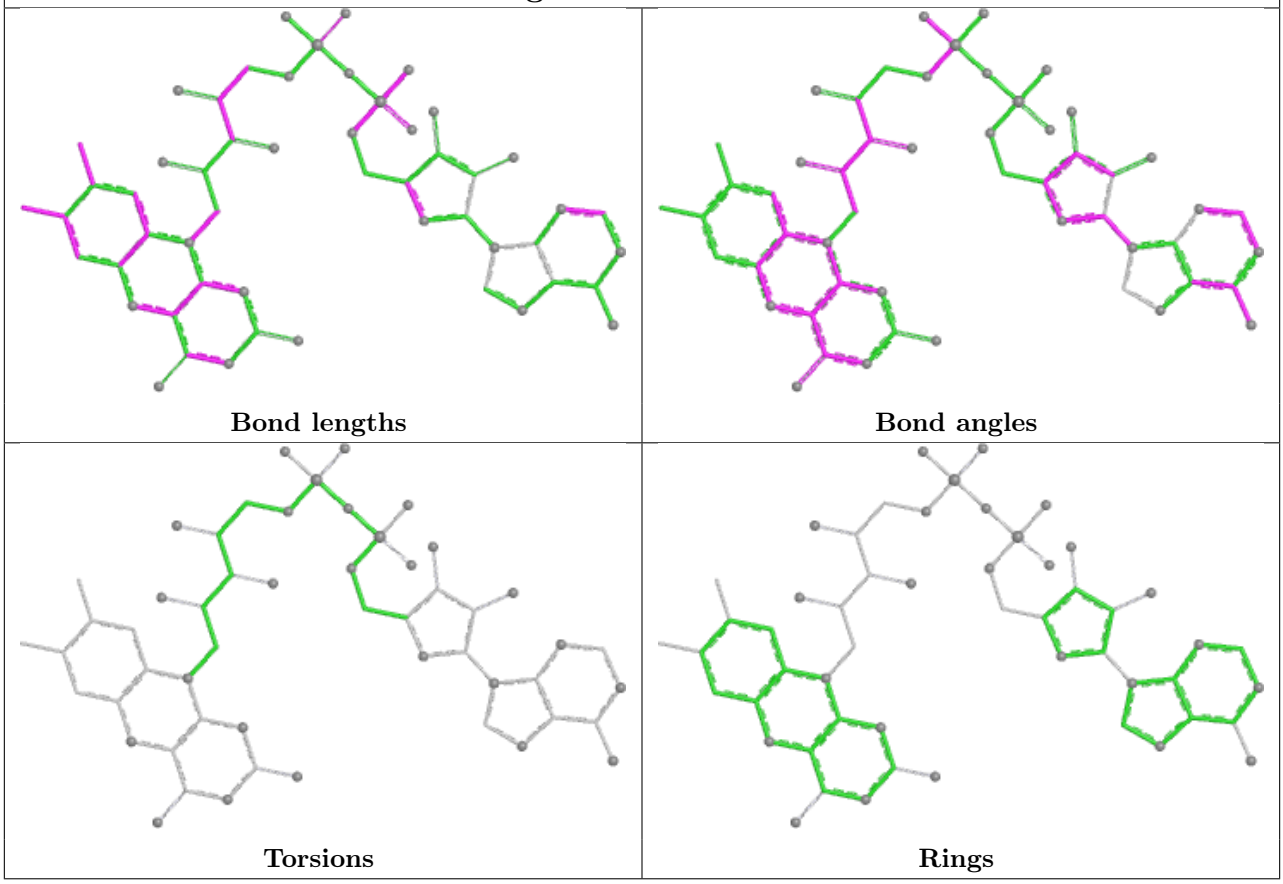
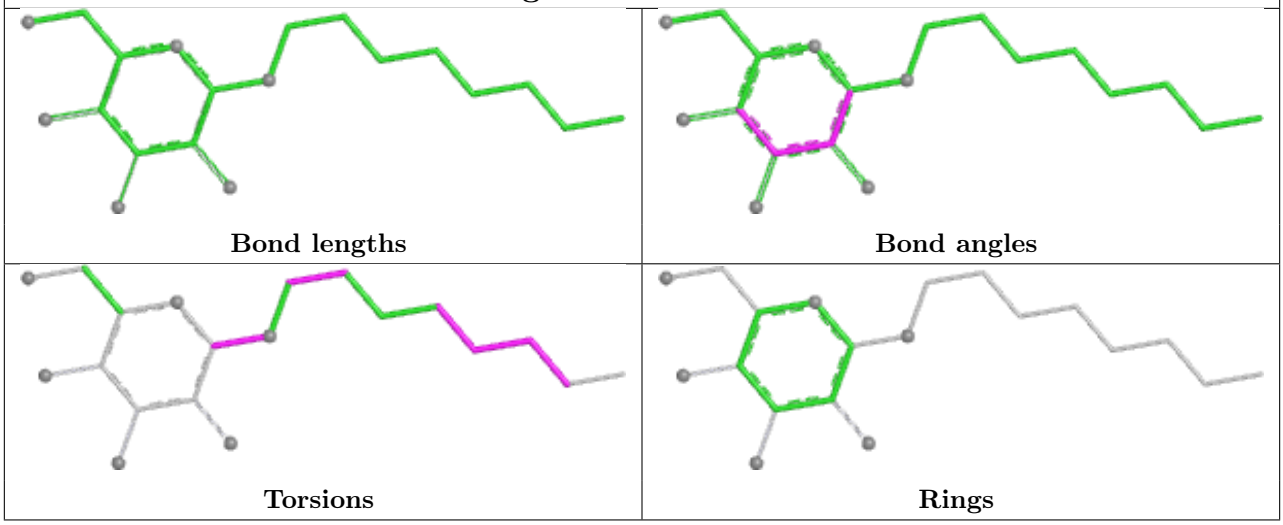


Ligand BOG B 800



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	487/501 (97%)	1.40	109 (22%)	0	0	20, 41, 65, 84	0
1	B	490/501 (97%)	1.45	107 (21%)	0	0	19, 41, 66, 98	0
All	All	977/1002 (97%)	1.42	216 (22%)	0	0	19, 41, 66, 98	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	LYS	11.3
1	B	494	GLN	9.3
1	B	59	TYR	8.4
1	A	1	MET	8.0
1	B	106	PHE	6.7

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
2	BOG	A	800	20/20	0.02	1.70	131,136,138,138	0
2	BOG	A	1949	20/20	0.10	0.55	92,95,97,97	0
2	BOG	A	1950	20/20	0.12	0.67	90,93,94,95	0
8	BCN	A	1969	11/11	0.20	0.60	63,76,79,79	0
5	EDO	B	806	4/4	0.35	0.63	34,45,50,55	0
2	BOG	B	800	20/20	0.42	0.66	133,136,139,140	0
9	TAM	B	812	11/11	0.45	0.49	56,63,66,70	0
5	EDO	B	809	4/4	0.47	0.19	65,66,67,68	0
2	BOG	A	700	20/20	0.51	0.31	86,91,94,94	0
5	EDO	B	807	4/4	0.52	0.22	46,47,50,52	0
8	BCN	B	821	11/11	0.52	0.45	58,64,70,70	0
5	EDO	A	1964	4/4	0.52	0.20	64,66,66,67	0
6	IMD	A	1960	5/5	0.53	0.37	58,58,60,60	0
5	EDO	B	802	4/4	0.56	0.37	38,44,48,50	0
5	EDO	B	808	4/4	0.63	0.30	52,56,57,60	0
8	BCN	B	820	11/11	0.64	0.47	64,69,72,74	0
6	IMD	B	819	5/5	0.66	0.18	78,78,79,81	0
6	IMD	A	1961	5/5	0.67	0.25	73,73,74,74	0
6	IMD	A	1966	5/5	0.68	0.24	70,70,72,72	0
5	EDO	B	818	4/4	0.70	0.21	72,75,75,75	0
5	EDO	A	1956	4/4	0.71	0.49	41,44,50,54	0
5	EDO	B	805	4/4	0.71	0.20	63,64,64,68	0
5	EDO	B	810	4/4	0.71	0.26	53,53,54,58	0
3	PO4	B	801	5/5	0.76	0.52	68,68,70,71	0
5	EDO	B	804	4/4	0.76	0.22	49,49,51,52	0
5	EDO	B	814	4/4	0.76	0.23	54,56,56,56	0
6	IMD	A	1963	5/5	0.76	0.19	42,47,49,50	0
5	EDO	B	817	4/4	0.76	0.74	55,62,65,66	0
5	EDO	A	1957	4/4	0.77	0.17	43,48,48,49	0
5	EDO	A	1954	4/4	0.77	0.15	64,65,65,66	0
5	EDO	A	1965	4/4	0.80	0.24	37,37,42,42	0
5	EDO	A	1952	4/4	0.81	0.23	63,63,64,64	0
7	13P	B	816	10/10	0.81	0.24	28,40,45,45	0
5	EDO	B	803	4/4	0.81	0.23	47,49,52,53	0
7	13P	A	1968	10/10	0.83	0.23	28,38,43,44	0
2	BOG	B	700	20/20	0.83	0.30	63,71,77,79	0
5	EDO	B	813	4/4	0.83	0.25	36,39,41,43	0
5	EDO	A	1955	4/4	0.84	0.30	38,50,50,52	0
5	EDO	A	1953	4/4	0.85	0.22	32,45,46,47	0
6	IMD	A	1967	5/5	0.85	0.19	63,64,65,67	0
5	EDO	A	1962	4/4	0.85	0.16	70,71,72,74	0
5	EDO	B	815	4/4	0.88	0.17	54,57,59,62	0
3	PO4	A	1951	5/5	0.89	0.15	84,84,84,85	0

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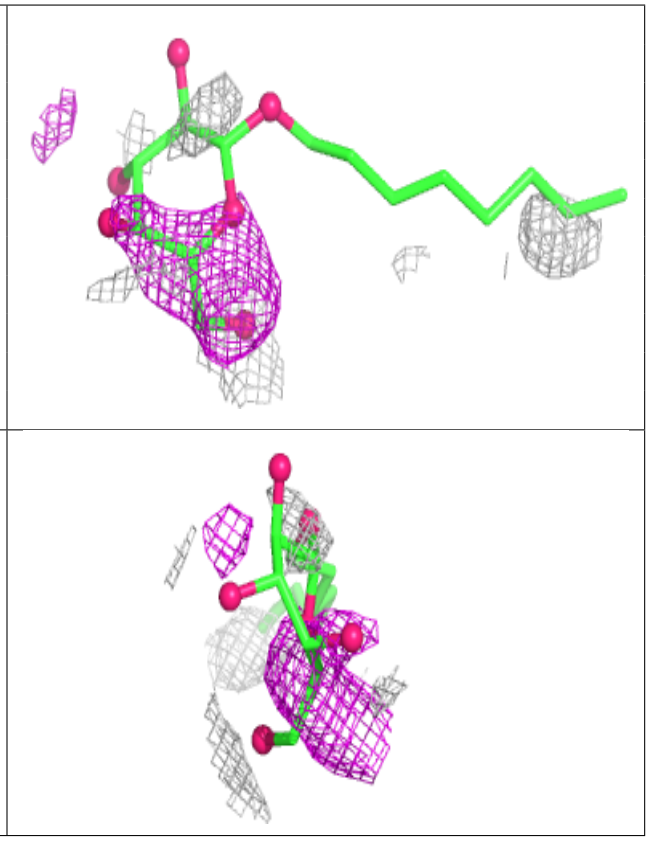
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1959	4/4	0.90	0.14	43,48,49,52	0
4	FAD	B	600	53/53	0.90	0.15	19,25,29,32	0
5	EDO	B	811	4/4	0.91	0.28	36,43,44,49	0
5	EDO	A	1958	4/4	0.92	0.36	32,34,40,46	0
4	FAD	A	600	53/53	0.92	0.16	18,26,29,36	0

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.

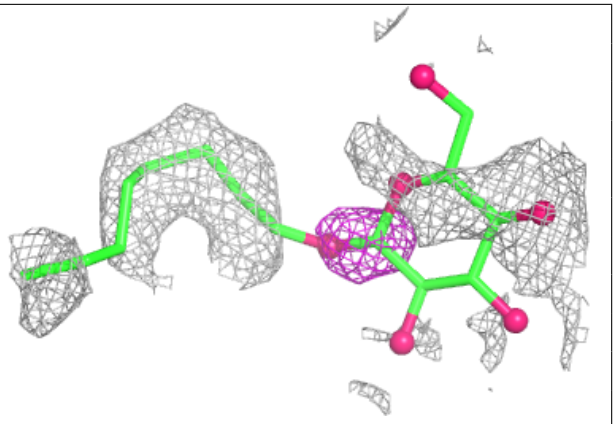
Electron density around BOG A 800:

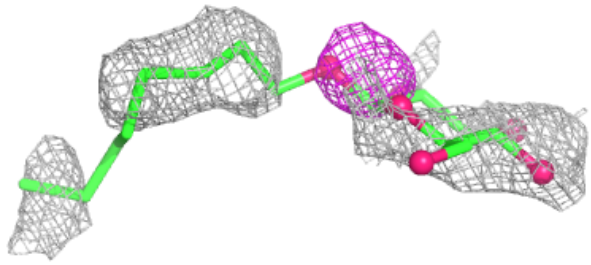
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

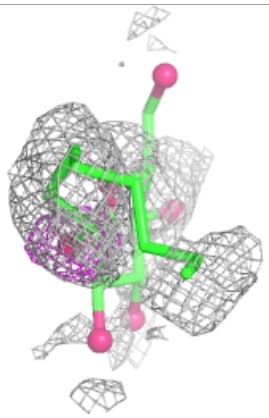


Electron density around BOG A 1949:

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

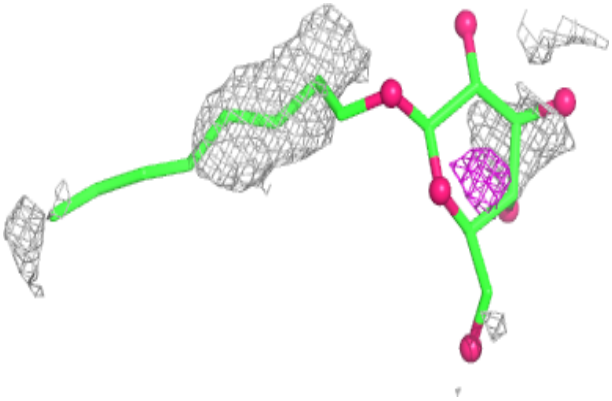


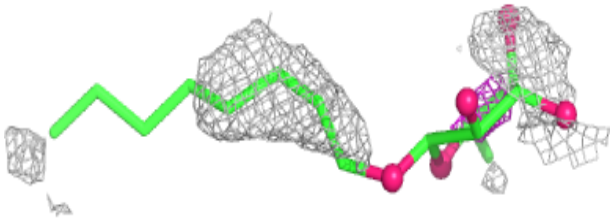




Electron density around BOG A 1950:

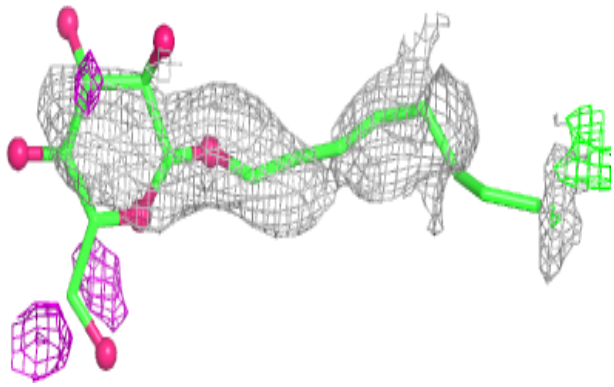
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

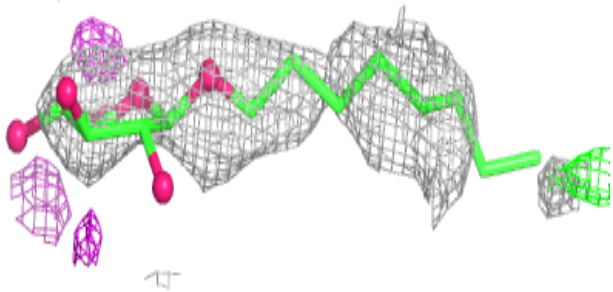


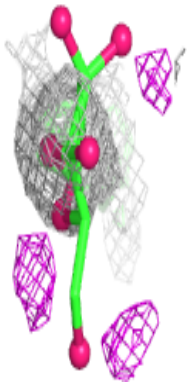


Electron density around BOG B 800:

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

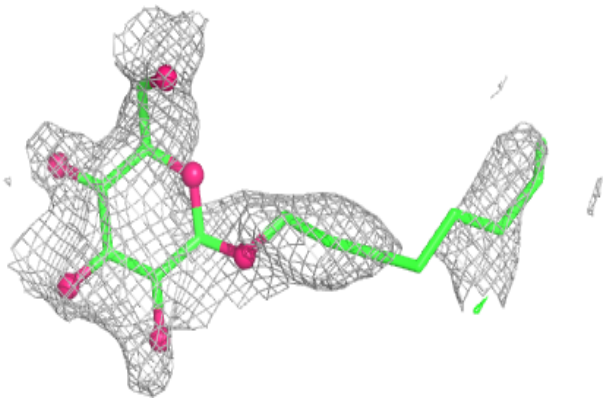


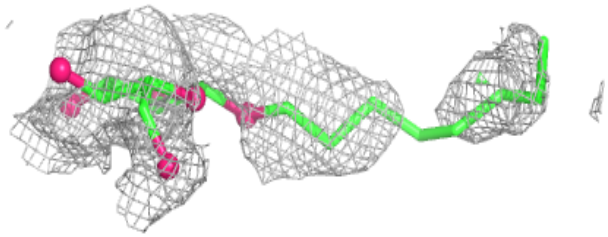


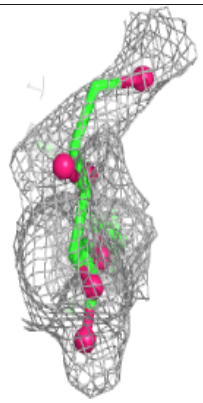


Electron density around BOG A 700:

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

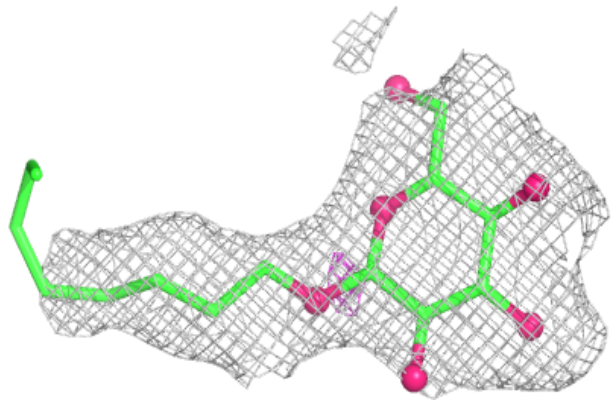


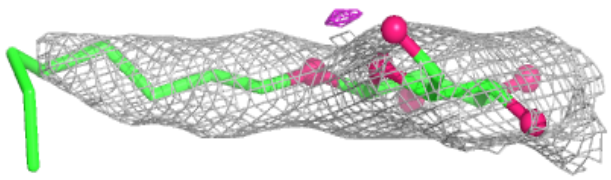


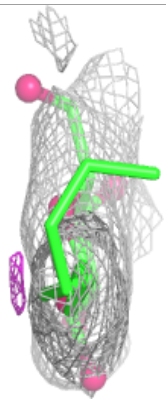


Electron density around BOG B 700:

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

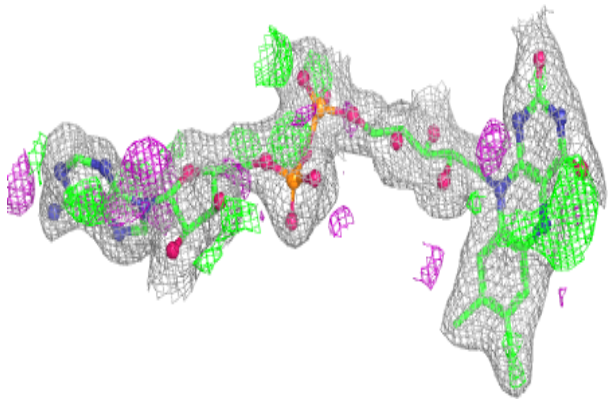


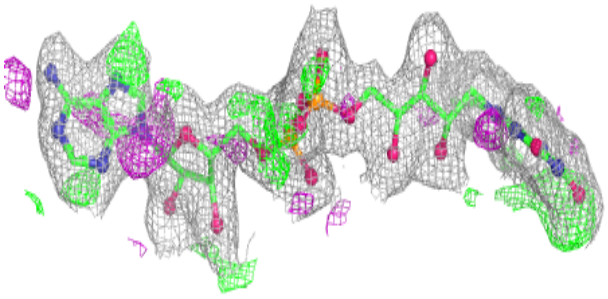


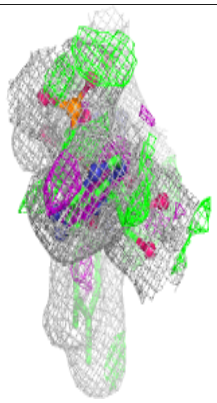


Electron density around FAD B 600:

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

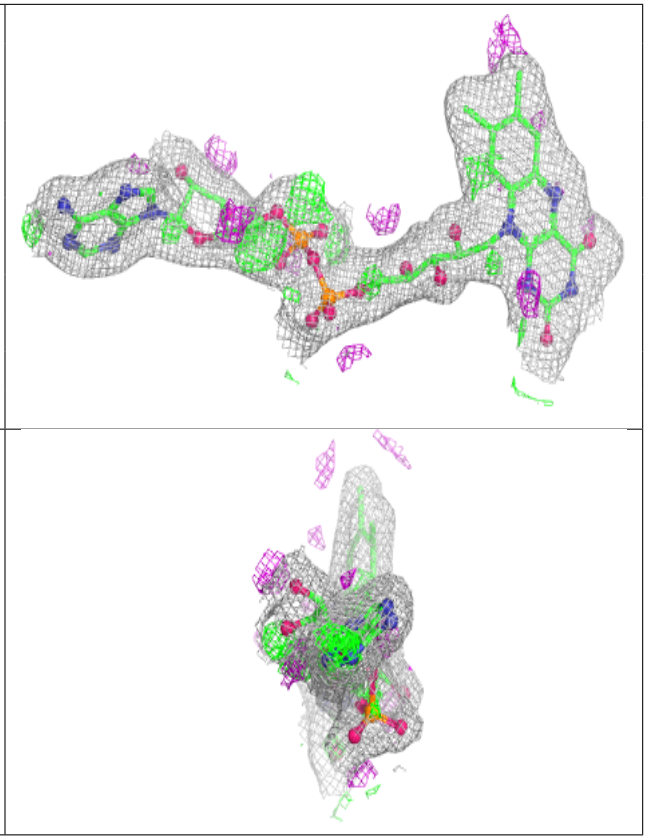






Electron density around FAD A 600:

$2mF_o$-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.