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

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

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

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

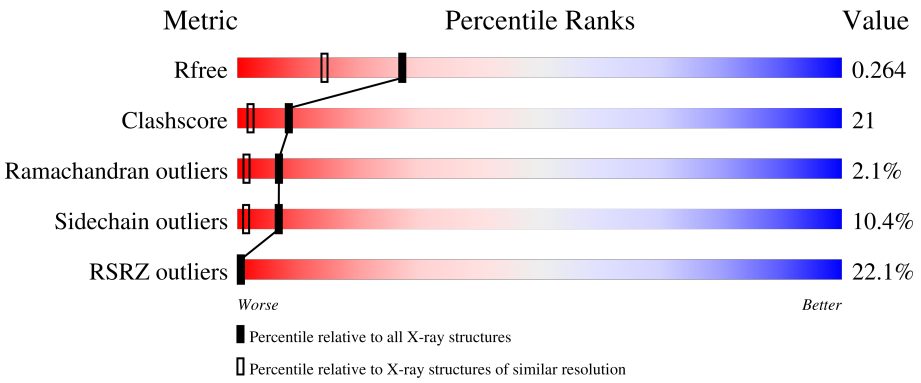
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

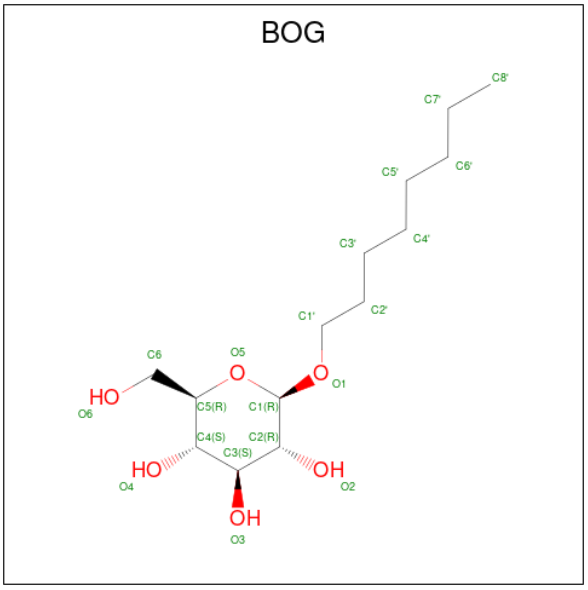
There are 10 unique types of molecules in this entry. The entry contains 8645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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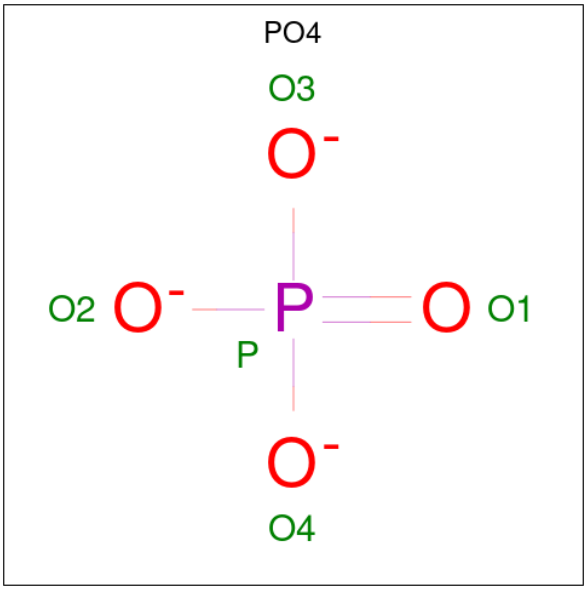
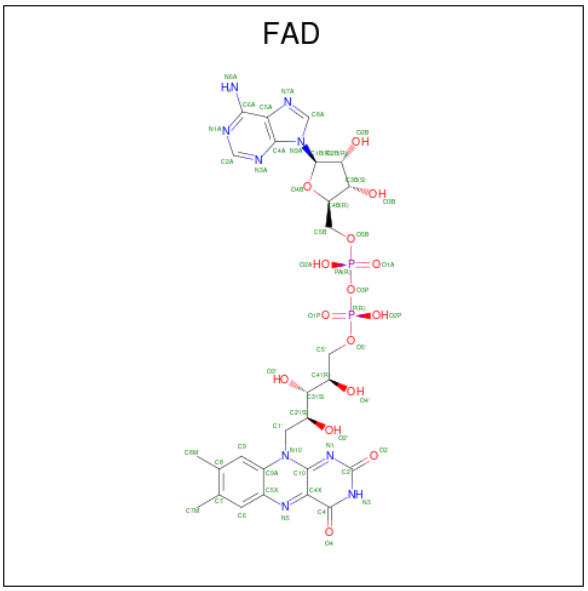
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	20	14	6	0	0
			Total	C	O		
2	B	1	20	14	6	0	0

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



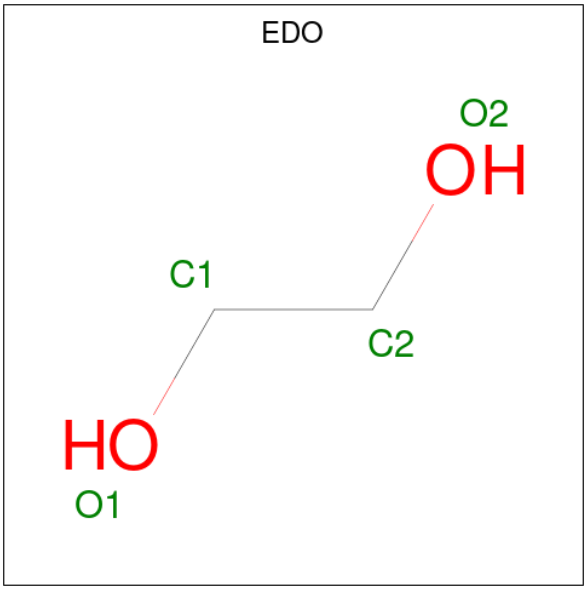
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0

- 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
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0

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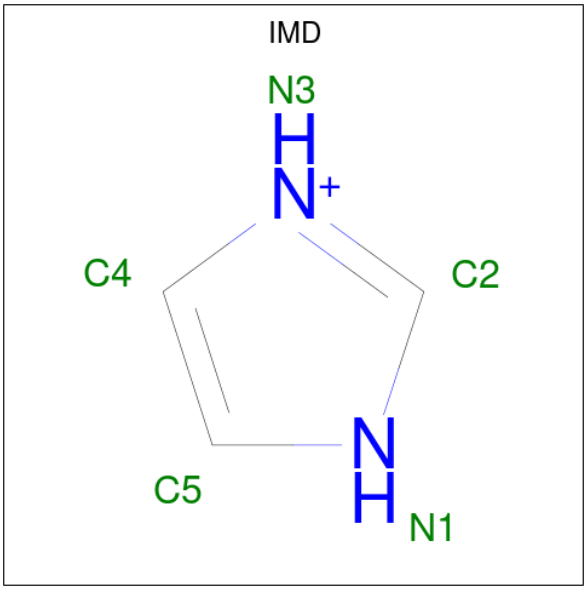
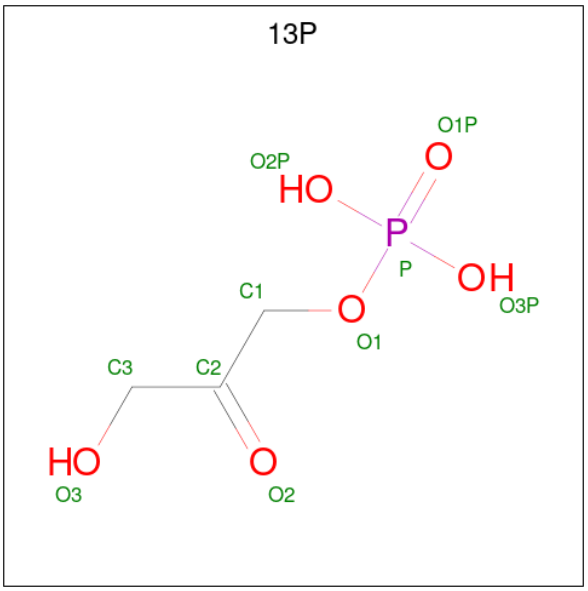
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0

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



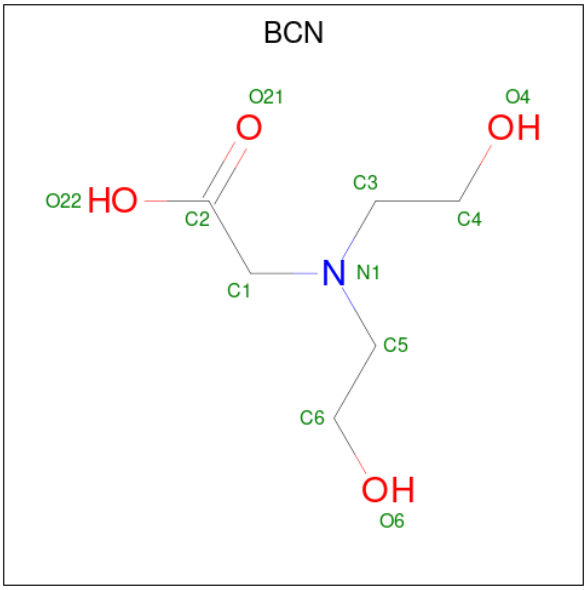
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	A	1	5	3	2	0	0
			Total	C	N		
6	B	1	5	3	2	0	0

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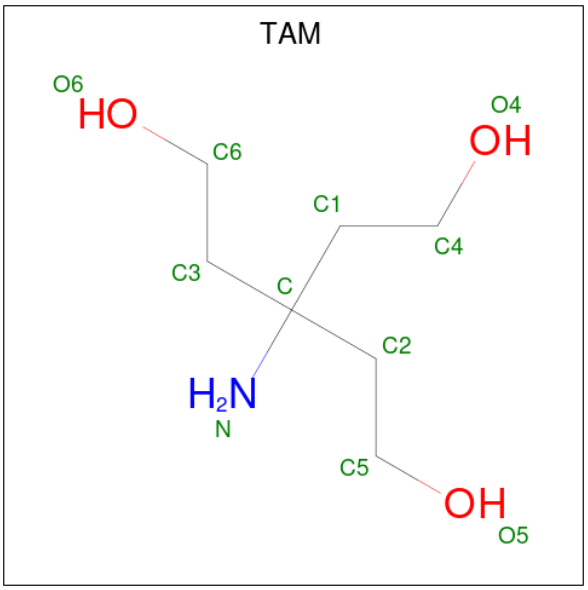
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	11	6	1	4	0	0

- 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.

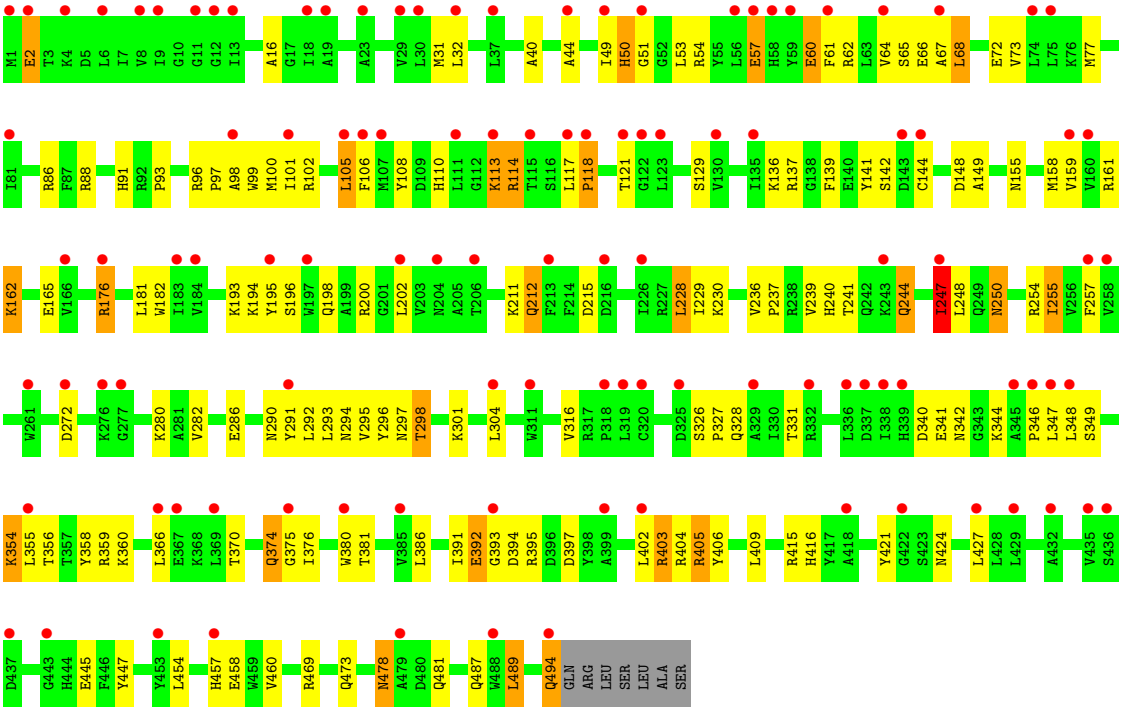
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	140	140	140	0	0
10	B	137	137	137	0	0

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.

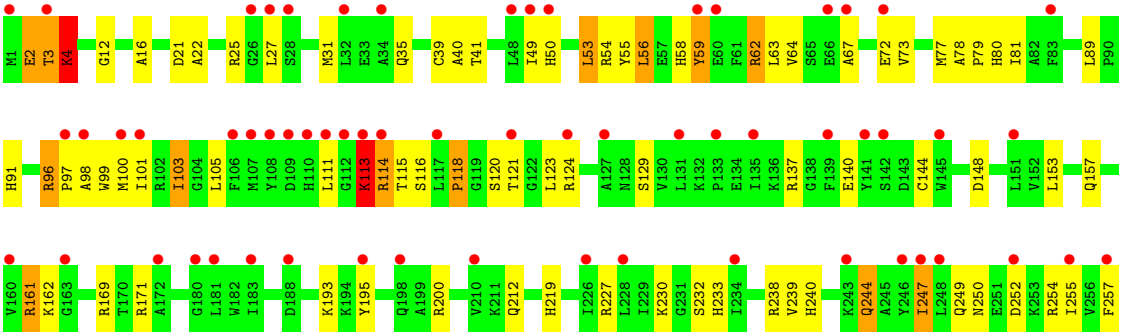
• Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase

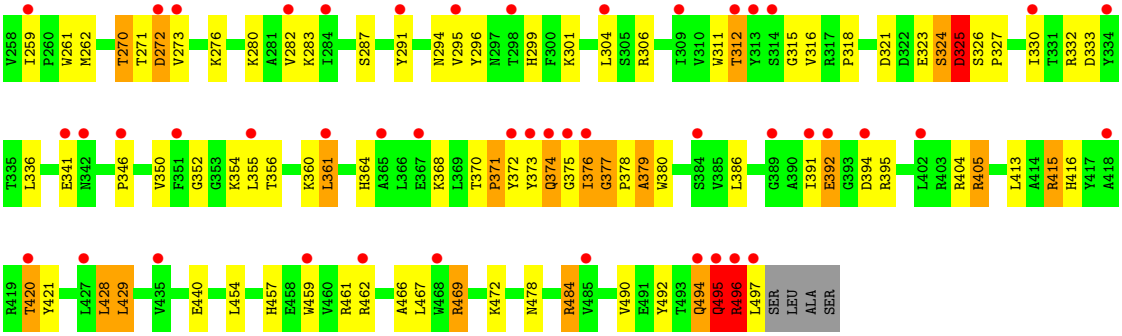
Chain A:



• 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%)

All (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
1	B	466	ALA	CA-CB	5.07	1.63	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	B	304	LEU	CB-CG-CD1	-5.58	101.52	111.00
1	B	429	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	86	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	B	153	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	113	LYS	N-CA-C	5.40	125.58	111.00
1	B	96	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	469	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	228	LEU	CA-CB-CG	-5.28	103.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	489	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	53	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	B	96	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	283	LYS	CB-CA-C	-5.13	100.15	110.40
1	B	462	ARG	NE-CZ-NH1	5.08	122.84	120.30

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.

All (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
5:A:1959:EDO:H21	6:A:1963:IMD:H5	1.22	1.17
1:A:237:PRO:HG3	6:A:1966:IMD:N3	1.60	1.16
1:B:361:LEU:HD12	1:B:361:LEU:O	1.44	1.14
1:A:51:GLY:HA3	1:A:68:LEU:HD13	1.29	1.12
1:A:374:GLN:CB	1:A:375:GLY:HA3	1.78	1.12
1:A:237:PRO:HG3	6:A:1966:IMD:HN3	1.02	1.11
1:A:341:GLU:CG	1:A:342:ASN:H	1.63	1.11
1:B:374:GLN:HB2	1:B:375:GLY:CA	1.79	1.10
1:A:374:GLN:HB2	1:A:375:GLY:HA3	1.28	1.10
5:A:1957:EDO:H11	6:A:1960:IMD:H5	1.29	1.10
1:A:237:PRO:CG	6:A:1966:IMD:HN3	1.66	1.07
5:B:807:EDO:H11	5:B:808:EDO:O1	1.55	1.06
1:B:50:HIS:CE1	1:B:354:LYS:NZ	2.24	1.06
1:A:341:GLU:HG3	1:A:342:ASN:N	1.65	1.05
1:B:27:LEU:HD21	1:B:376:ILE:HD12	1.13	1.05
1:B:361:LEU:HD12	1:B:361:LEU:C	1.77	1.04
5:A:1959:EDO:H21	6:A:1963:IMD:C5	1.86	1.04
1:B:50:HIS:CE1	1:B:354:LYS:HZ3	1.75	1.03
1:A:158:MSE:CE	1:A:161:ARG:HD2	1.87	1.03
1:B:113:LYS:HB3	1:B:114:ARG:HA	1.41	1.02
1:B:50:HIS:HE1	1:B:354:LYS:NZ	1.58	1.01
1:A:158:MSE:HE1	1:A:161:ARG:HD2	1.02	0.99
1:B:428:LEU:HD12	1:B:428:LEU:C	1.82	0.98
1:A:294:ASN:O	1:A:298:THR:HG23	1.62	0.97
5:A:1959:EDO:C2	6:A:1963:IMD:H5	1.95	0.97
1:A:176:ARG:HG2	1:A:176:ARG:HH11	1.29	0.96
1:A:341:GLU:HG3	1:A:342:ASN:H	0.81	0.95
1:B:62:ARG:HD3	1:B:333:ASP:OD2	1.66	0.95
1:A:158:MSE:HE1	1:A:161:ARG:CD	1.96	0.95
5:A:1957:EDO:C1	6:A:1960:IMD:H5	1.97	0.93
1:B:73:VAL:HG12	1:B:77:MSE:CE	1.96	0.93
1:A:297:ASN:HD21	1:A:304:LEU:H	1.05	0.93
1:A:457:HIS:C	6:A:1963:IMD:H4	1.89	0.93
1:B:467:LEU:HD23	10:B:938:HOH:O	1.68	0.92
1:B:50:HIS:CE1	1:B:354:LYS:CE	2.53	0.91
1:B:27:LEU:CD2	1:B:376:ILE:HD12	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TYR:OH	1:A:247:ILE:CD1	2.21	0.88
1:B:376:ILE:HG23	1:B:376:ILE:O	1.70	0.88
1:B:374:GLN:HB2	1:B:375:GLY:HA3	0.88	0.88
1:B:315:GLY:HA2	5:B:813:EDO:H11	1.56	0.88
1:B:73:VAL:HG12	1:B:77:MSE:HE1	1.55	0.87
1:B:27:LEU:CD2	1:B:376:ILE:CD1	2.49	0.85
1:A:51:GLY:HA3	1:A:68:LEU:CD1	2.06	0.84
1:A:176:ARG:HH11	1:A:176:ARG:CG	1.91	0.83
1:B:315:GLY:CA	5:B:813:EDO:H11	2.09	0.83
1:B:212:GLN:HG2	5:B:810:EDO:H22	1.59	0.82
1:A:158:MSE:HE3	1:A:158:MSE:HA	1.61	0.82
1:A:445:GLU:HB2	6:A:1960:IMD:H2	1.61	0.82
1:B:323:GLU:O	1:B:324:SER:HB3	1.80	0.82
1:B:27:LEU:HD11	1:B:376:ILE:HD11	1.60	0.82
1:B:374:GLN:CB	1:B:375:GLY:CA	2.43	0.82
1:A:478:ASN:ND2	1:A:481:GLN:H	1.78	0.80
1:A:487:GLN:HG2	10:A:2079:HOH:O	1.80	0.80
5:B:807:EDO:H11	5:B:808:EDO:HO1	1.47	0.80
1:A:374:GLN:CB	1:A:375:GLY:CA	2.59	0.80
1:B:161:ARG:HB2	9:B:812:TAM:O5	1.81	0.79
1:A:141:TYR:OH	1:A:247:ILE:HD11	1.82	0.79
1:B:50:HIS:HE1	1:B:354:LYS:CE	1.93	0.79
1:B:59:TYR:CE2	2:B:800:BOG:H5'2	2.17	0.79
1:A:392:GLU:CA	1:A:392:GLU:OE1	2.30	0.78
1:B:416:HIS:O	1:B:420:THR:HG23	1.83	0.78
1:A:280:LYS:HE2	1:A:280:LYS:HA	1.65	0.78
1:B:56:LEU:HD13	1:B:64:VAL:HG21	1.66	0.78
1:B:262:MSE:HE2	5:B:807:EDO:H12	1.67	0.77
1:B:361:LEU:C	1:B:361:LEU:CD1	2.52	0.77
1:A:392:GLU:OE1	1:A:392:GLU:HA	1.84	0.75
1:B:113:LYS:CB	1:B:114:ARG:HA	2.12	0.75
1:B:364:HIS:HB2	10:B:885:HOH:O	1.86	0.75
1:A:254:ARG:HD2	1:A:328:GLN:HB3	1.68	0.74
1:B:316:VAL:H	5:B:813:EDO:C1	2.00	0.74
1:B:361:LEU:O	1:B:361:LEU:CD1	2.30	0.74
1:B:157:GLN:HG2	9:B:812:TAM:N	2.01	0.74
1:B:27:LEU:HD21	1:B:376:ILE:HD11	1.67	0.74
1:A:96:ARG:NE	2:A:800:BOG:H5	2.02	0.73
1:B:114:ARG:O	1:B:114:ARG:HG2	1.88	0.73
1:A:374:GLN:HB3	1:A:375:GLY:HA3	1.71	0.72
1:B:324:SER:O	1:B:325:ASP:HB2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HD12	1:B:364:HIS:HD2	1.52	0.72
1:B:324:SER:OG	1:B:325:ASP:N	2.23	0.72
1:B:99:TRP:O	1:B:103:ILE:HG12	1.90	0.71
1:B:376:ILE:O	1:B:376:ILE:CG2	2.38	0.71
1:A:202:LEU:HD23	1:A:347:LEU:HD13	1.71	0.71
1:A:424:ASN:ND2	6:A:1961:IMD:H4	2.06	0.70
1:B:129:SER:O	1:B:301:LYS:HE2	1.91	0.69
1:A:176:ARG:HG2	1:A:176:ARG:NH1	2.06	0.69
1:B:299:HIS:HE1	10:B:882:HOH:O	1.75	0.68
1:B:50:HIS:CE1	1:B:354:LYS:HE2	2.28	0.68
1:B:113:LYS:HB3	1:B:114:ARG:CA	2.20	0.68
1:A:53:LEU:HG	2:A:800:BOG:H2	1.76	0.68
1:B:114:ARG:NH1	1:B:118:PRO:O	2.26	0.68
1:B:72:GLU:OE2	1:B:114:ARG:HB2	1.93	0.68
1:A:370:THR:HG23	1:A:376:ILE:HG21	1.76	0.68
1:B:378:PRO:O	1:B:379:ALA:O	2.12	0.67
1:A:406:TYR:HE1	10:A:2045:HOH:O	1.76	0.67
5:B:806:EDO:H21	10:B:958:HOH:O	1.95	0.67
1:B:250:ASN:ND2	1:B:291:TYR:CZ	2.63	0.67
1:B:405:ARG:HG3	10:B:894:HOH:O	1.93	0.67
1:B:461:ARG:NH1	10:B:942:HOH:O	2.29	0.66
5:A:1958:EDO:C2	10:A:2097:HOH:O	2.44	0.66
1:B:496:ARG:O	1:B:497:LEU:HG	1.96	0.66
1:B:336:LEU:HD12	1:B:364:HIS:CD2	2.30	0.66
1:A:254:ARG:NE	1:A:272:ASP:OD2	2.27	0.65
1:A:392:GLU:OE1	1:A:392:GLU:N	2.30	0.65
1:B:492:TYR:HB2	6:B:819:IMD:H4	1.79	0.65
1:A:51:GLY:CA	1:A:68:LEU:HD13	2.17	0.65
1:B:2:GLU:O	1:B:4:LYS:HB2	1.97	0.65
1:A:290:ASN:HA	5:A:1956:EDO:H12	1.79	0.64
1:B:301:LYS:NZ	10:B:933:HOH:O	2.29	0.64
1:A:181:LEU:HD23	10:A:2063:HOH:O	1.98	0.64
1:B:428:LEU:C	1:B:428:LEU:CD1	2.58	0.64
1:B:161:ARG:HB2	9:B:812:TAM:HO5	1.63	0.63
1:A:50:HIS:NE2	1:A:354:LYS:NZ	2.44	0.62
1:B:273:VAL:HG13	8:B:820:BCN:H32	1.80	0.62
1:A:403:ARG:NH1	1:A:409:LEU:O	2.28	0.62
1:B:428:LEU:O	1:B:428:LEU:CD1	2.30	0.62
1:A:117:LEU:O	1:A:118:PRO:O	2.17	0.62
1:A:93:PRO:HB3	2:A:1950:BOG:H2	1.82	0.61
1:A:54:ARG:HA	2:A:800:BOG:O6	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:TYR:HB2	1:B:376:ILE:HD13	1.82	0.61
1:B:287:SER:CB	8:B:821:BCN:H62	2.30	0.61
1:B:73:VAL:CG1	1:B:77:MSE:HE1	2.30	0.61
1:B:239:VAL:HG12	1:B:240:HIS:CD2	2.36	0.60
1:B:421:TYR:OH	1:B:454:LEU:HD21	2.00	0.60
1:B:440:GLU:OE2	1:B:484:ARG:NH1	2.34	0.60
1:B:16:ALA:HA	1:B:31:MSE:HE2	1.82	0.60
1:B:59:TYR:CE2	2:B:800:BOG:C5'	2.84	0.60
1:B:323:GLU:O	1:B:324:SER:CB	2.48	0.59
1:B:316:VAL:H	5:B:813:EDO:H11	1.66	0.59
1:A:297:ASN:ND2	1:A:304:LEU:H	1.89	0.59
1:B:370:THR:HG23	1:B:376:ILE:HG21	1.84	0.59
1:A:391:ILE:O	1:A:393:GLY:N	2.30	0.59
1:B:262:MSE:HE2	5:B:807:EDO:C1	2.33	0.59
1:A:239:VAL:HG23	1:A:240:HIS:CD2	2.38	0.59
1:A:394:ASP:HB3	1:A:397:ASP:HB2	1.84	0.58
1:A:148:ASP:OD1	1:A:149:ALA:N	2.35	0.58
1:A:478:ASN:HD22	1:A:478:ASN:C	2.06	0.58
1:A:250:ASN:OD1	1:A:291:TYR:CZ	2.56	0.58
1:A:290:ASN:CA	5:A:1956:EDO:H12	2.34	0.58
1:A:137:ARG:HH22	2:A:700:BOG:H5	1.68	0.57
1:A:406:TYR:CE1	10:A:2045:HOH:O	2.52	0.57
1:A:141:TYR:CZ	1:A:247:ILE:HD11	2.40	0.57
1:B:316:VAL:N	5:B:813:EDO:H11	2.20	0.57
1:A:341:GLU:CG	1:A:342:ASN:N	2.36	0.57
1:B:254:ARG:HH21	7:B:816:13P:H12	1.70	0.56
1:B:378:PRO:O	1:B:379:ALA:C	2.43	0.56
5:A:1958:EDO:H21	10:A:2097:HOH:O	2.04	0.56
1:B:73:VAL:CG1	1:B:77:MSE:CE	2.77	0.56
1:B:50:HIS:HE1	1:B:354:LYS:HZ1	1.52	0.56
1:B:62:ARG:HG3	1:B:63:LEU:N	2.20	0.56
1:B:405:ARG:NH2	10:B:947:HOH:O	2.37	0.56
1:A:211:LYS:NZ	1:A:215:ASP:OD2	2.37	0.56
1:A:370:THR:HG23	1:A:376:ILE:CG2	2.36	0.55
1:A:454:LEU:HB3	1:A:460:VAL:HG21	1.87	0.55
5:B:804:EDO:H21	10:B:924:HOH:O	2.04	0.55
1:B:262:MSE:HE1	5:B:807:EDO:O2	2.07	0.55
1:B:103:ILE:CD1	2:B:700:BOG:H6'2	2.37	0.55
1:A:101:ILE:HG22	1:A:105:LEU:HD22	1.88	0.55
1:A:473:GLN:NE2	5:A:1957:EDO:H21	2.22	0.55
1:B:262:MSE:CE	5:B:807:EDO:H12	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE2	1:A:114:ARG:HB2	2.07	0.54
5:B:811:EDO:H11	9:B:812:TAM:H62	1.88	0.54
1:A:57:GLU:HB2	2:A:800:BOG:O6	2.08	0.54
1:A:97:PRO:HG2	1:A:100:MET:HB2	1.90	0.54
1:A:469:ARG:NH1	5:A:1953:EDO:O2	2.40	0.54
1:B:373:TYR:CB	1:B:376:ILE:HD13	2.36	0.54
1:A:230:LYS:HD3	1:A:282:VAL:HG23	1.87	0.54
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.07	0.54
1:A:494:GLN:HA	1:A:494:GLN:OE1	2.06	0.54
1:B:25:ARG:HD3	1:B:377:GLY:O	2.08	0.54
1:B:157:GLN:HG2	9:B:812:TAM:HN2	1.70	0.54
1:A:193:LYS:HD2	1:A:195:TYR:CZ	2.43	0.53
1:A:155:ASN:O	1:A:159:VAL:HG23	2.09	0.53
1:A:374:GLN:HB2	1:A:375:GLY:CA	2.19	0.52
1:B:376:ILE:O	1:B:377:GLY:O	2.28	0.52
1:A:229:ILE:HD12	1:A:327:PRO:HB3	1.92	0.52
1:B:101:ILE:HG23	2:B:800:BOG:H61	1.92	0.52
1:B:97:PRO:HD2	1:B:100:MET:SD	2.50	0.52
1:B:232:SER:O	1:B:270:THR:HG22	2.10	0.52
1:B:120:SER:HA	1:B:140:GLU:O	2.10	0.52
1:A:97:PRO:HB2	1:A:99:TRP:CD1	2.45	0.51
1:A:50:HIS:NE2	1:A:354:LYS:CE	2.74	0.51
1:A:391:ILE:C	1:A:393:GLY:H	2.13	0.51
1:B:27:LEU:CD1	1:B:376:ILE:HD11	2.38	0.51
1:A:54:ARG:HG2	10:A:2109:HOH:O	2.11	0.51
1:A:64:VAL:HG12	1:A:68:LEU:HD22	1.91	0.51
1:B:58:HIS:O	1:B:59:TYR:O	2.27	0.51
1:A:340:ASP:HB2	1:A:344:LYS:O	2.11	0.50
1:A:129:SER:O	1:A:301:LYS:HE2	2.12	0.50
1:A:40:ALA:O	5:A:1965:EDO:O1	2.28	0.50
1:A:114:ARG:O	1:A:114:ARG:HG2	2.09	0.50
1:B:97:PRO:HG2	1:B:100:MET:HB2	1.92	0.50
5:A:1958:EDO:H22	10:A:2097:HOH:O	2.07	0.50
1:B:272:ASP:HB2	5:B:802:EDO:H21	1.94	0.50
5:A:1953:EDO:H12	5:A:1965:EDO:O2	2.12	0.50
1:B:490:VAL:O	1:B:494:GLN:HB2	2.10	0.50
1:B:324:SER:O	1:B:325:ASP:CB	2.58	0.50
1:A:478:ASN:HD21	1:A:481:GLN:H	1.55	0.49
1:A:478:ASN:HD22	1:A:481:GLN:H	1.57	0.49
1:B:27:LEU:HD21	1:B:376:ILE:HD13	1.77	0.49
1:B:227:ARG:HG2	1:B:321:ASP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:O	1:A:346:PRO:HD2	2.12	0.49
5:A:1959:EDO:H11	6:A:1961:IMD:H2	1.94	0.49
1:B:49:ILE:HB	1:B:144:CYS:HB2	1.94	0.49
1:B:376:ILE:O	1:B:377:GLY:C	2.49	0.49
1:B:252:ASP:OD1	1:B:254:ARG:HB2	2.12	0.49
1:A:193:LYS:HE3	1:A:195:TYR:OH	2.12	0.49
1:A:294:ASN:ND2	5:A:1955:EDO:O2	2.46	0.49
1:A:237:PRO:CG	6:A:1966:IMD:N3	2.43	0.49
1:A:424:ASN:HD21	6:A:1961:IMD:H4	1.75	0.49
1:B:212:GLN:CG	5:B:810:EDO:H22	2.37	0.49
1:B:391:ILE:C	1:B:392:GLU:HG2	2.32	0.49
1:A:96:ARG:HE	2:A:800:BOG:H5	1.78	0.49
1:A:316:VAL:HG22	5:A:1958:EDO:H11	1.95	0.49
1:B:39:CYS:HA	1:B:469:ARG:HD3	1.95	0.49
1:B:287:SER:HB3	8:B:821:BCN:H62	1.95	0.49
1:B:2:GLU:O	1:B:4:LYS:HD2	2.13	0.48
1:B:67:ALA:HB1	1:B:356:THR:HG21	1.94	0.48
1:B:311:TRP:O	1:B:312:THR:HG22	2.12	0.48
1:B:336:LEU:CD2	1:B:350:VAL:HG22	2.43	0.48
1:A:416:HIS:ND1	5:A:1957:EDO:H11	2.27	0.48
1:B:59:TYR:HE2	2:B:800:BOG:C5'	2.25	0.48
1:B:459:TRP:CE2	5:B:811:EDO:H12	2.49	0.48
1:A:457:HIS:CA	6:A:1963:IMD:H4	2.44	0.48
1:B:457:HIS:C	5:B:811:EDO:H21	2.34	0.48
1:A:16:ALA:HA	1:A:31:MSE:HE2	1.95	0.48
1:A:421:TYR:OH	1:A:454:LEU:HD21	2.14	0.47
1:A:469:ARG:NH1	1:A:469:ARG:HG3	2.28	0.47
1:B:54:ARG:HA	2:B:800:BOG:O2	2.14	0.47
1:B:336:LEU:HD22	1:B:350:VAL:HG22	1.95	0.47
1:A:106:PHE:HE2	5:A:1964:EDO:HO1	1.63	0.47
1:A:254:ARG:HB3	1:A:254:ARG:NH1	2.30	0.47
1:B:3:THR:HA	1:B:4:LYS:HB2	1.97	0.47
1:A:114:ARG:NH2	1:A:118:PRO:O	2.47	0.47
1:A:158:MSE:HE3	1:A:161:ARG:HB3	1.97	0.47
1:A:241:THR:O	1:A:241:THR:CG2	2.63	0.47
1:A:88:ARG:NE	1:A:244:GLN:HG3	2.30	0.47
1:B:193:LYS:HD3	1:B:195:TYR:CZ	2.49	0.47
1:B:478:ASN:OD1	1:B:478:ASN:C	2.52	0.47
7:B:816:13P:O3P	7:B:816:13P:H31	2.15	0.47
1:A:67:ALA:HB1	1:A:356:THR:HG21	1.95	0.46
1:A:255:ILE:H	1:A:255:ILE:HG13	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TYR:HE2	2:B:800:BOG:H5'2	1.73	0.46
1:B:457:HIS:HD2	9:B:812:TAM:O6	1.98	0.46
1:A:458:GLU:N	6:A:1963:IMD:H4	2.29	0.46
5:A:1957:EDO:H12	6:A:1960:IMD:H5	1.93	0.46
8:A:1969:BCN:H62	8:A:1969:BCN:H11	1.55	0.46
1:B:415:ARG:HH11	1:B:415:ARG:HG2	1.80	0.46
1:A:293:LEU:HB2	5:A:1956:EDO:H21	1.98	0.46
1:A:298:THR:HG22	5:A:1955:EDO:O1	2.15	0.46
1:B:311:TRP:C	1:B:312:THR:CG2	2.84	0.46
1:B:296:TYR:CD2	1:B:296:TYR:C	2.89	0.46
1:B:415:ARG:HG2	1:B:415:ARG:NH1	2.31	0.45
1:A:296:TYR:CD1	1:A:296:TYR:C	2.89	0.45
1:B:96:ARG:HH11	1:B:249:GLN:HE21	1.65	0.45
1:A:106:PHE:O	1:A:110:HIS:CD2	2.70	0.45
1:A:416:HIS:ND1	5:A:1957:EDO:C1	2.80	0.45
1:B:497:LEU:HD23	1:B:497:LEU:HA	1.85	0.45
4:A:600:FAD:H4B	4:A:600:FAD:O2A	2.17	0.45
1:B:200:ARG:O	1:B:346:PRO:HD2	2.16	0.45
1:A:469:ARG:HG3	1:A:469:ARG:HH11	1.82	0.45
8:B:821:BCN:O4	8:B:821:BCN:H12	2.17	0.45
1:A:106:PHE:O	1:A:110:HIS:HD2	2.00	0.45
5:A:1959:EDO:C1	6:A:1961:IMD:H2	2.47	0.45
1:B:73:VAL:O	1:B:77:MSE:HE3	2.16	0.45
1:B:244:GLN:HE21	1:B:244:GLN:HB2	1.61	0.45
1:B:364:HIS:NE2	1:B:368:LYS:NZ	2.65	0.45
1:B:370:THR:O	1:B:372:TYR:N	2.50	0.45
1:A:254:ARG:HD2	1:A:328:GLN:CB	2.42	0.44
1:B:21:ASP:O	1:B:22:ALA:C	2.56	0.44
1:B:113:LYS:HE3	1:B:113:LYS:H	1.82	0.44
1:B:232:SER:O	1:B:270:THR:CG2	2.66	0.44
1:A:359:ARG:NH1	1:A:381:THR:OG1	2.45	0.44
1:B:103:ILE:HD13	2:B:700:BOG:H6'2	1.99	0.44
1:B:336:LEU:HD21	1:B:361:LEU:CD1	2.47	0.44
1:B:77:MSE:HG2	1:B:386:LEU:HG	1.98	0.44
1:B:89:LEU:HD12	1:B:247:ILE:O	2.17	0.44
1:B:59:TYR:HE2	2:B:800:BOG:C6'	2.31	0.44
1:B:227:ARG:HG2	1:B:321:ASP:CB	2.48	0.44
1:B:262:MSE:CE	5:B:807:EDO:C1	2.93	0.44
1:B:250:ASN:ND2	1:B:291:TYR:CE1	2.86	0.44
1:B:261:TRP:CZ2	1:B:472:LYS:HD2	2.53	0.44
1:B:294:ASN:ND2	5:B:803:EDO:O1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:MSE:HE2	1:A:386:LEU:HG	2.00	0.43
1:B:254:ARG:HH21	7:B:816:13P:C1	2.30	0.43
1:B:233:HIS:CE1	1:B:270:THR:HG23	2.53	0.43
1:A:117:LEU:HD22	1:A:142:SER:HB3	2.00	0.43
1:B:3:THR:HA	1:B:4:LYS:CB	2.49	0.43
5:B:803:EDO:H21	5:B:817:EDO:H11	2.01	0.43
1:A:91:HIS:CE1	1:A:98:ALA:HB2	2.54	0.42
1:A:366:LEU:HD13	1:A:366:LEU:HA	1.92	0.42
1:B:323:GLU:CB	10:B:912:HOH:O	2.67	0.42
1:A:44:ALA:HB2	5:A:1965:EDO:C2	2.49	0.42
1:A:247:ILE:HG23	1:A:257:PHE:CE1	2.54	0.42
1:B:55:TYR:OH	7:B:816:13P:O1P	2.24	0.42
1:B:295:VAL:O	1:B:299:HIS:HD2	2.02	0.42
8:B:820:BCN:H31	8:B:820:BCN:H62	1.64	0.42
1:A:139:PHE:N	1:A:139:PHE:CD2	2.87	0.42
1:A:158:MSE:HE3	1:A:158:MSE:CA	2.41	0.42
1:A:248:LEU:O	1:A:255:ILE:HA	2.19	0.42
1:B:232:SER:N	1:B:270:THR:HG22	2.34	0.42
1:B:259:ILE:HG21	1:B:259:ILE:HD13	1.83	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.79	0.42
1:B:370:THR:O	1:B:371:PRO:C	2.57	0.42
1:A:374:GLN:HB3	1:A:375:GLY:CA	2.39	0.42
1:A:415:ARG:HD3	10:A:2077:HOH:O	2.18	0.42
1:A:457:HIS:HA	6:A:1963:IMD:C4	2.50	0.42
1:A:358:TYR:CD2	1:A:358:TYR:C	2.93	0.42
1:A:61:PHE:O	1:A:62:ARG:C	2.57	0.42
1:A:212:GLN:HE21	1:A:212:GLN:HB3	1.71	0.42
5:A:1959:EDO:O1	6:A:1961:IMD:N1	2.53	0.42
1:B:80:HIS:CD2	1:B:81:ILE:HG23	2.54	0.42
1:B:440:GLU:CD	1:B:484:ARG:NH1	2.73	0.42
1:B:91:HIS:NE2	1:B:98:ALA:HB2	2.35	0.42
1:B:157:GLN:NE2	9:B:812:TAM:H41	2.35	0.42
1:A:241:THR:O	1:A:241:THR:HG22	2.20	0.42
1:A:68:LEU:HD11	1:A:108:TYR:CE2	2.55	0.41
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.77	0.41
1:B:270:THR:HB	1:B:271:THR:H	1.40	0.41
1:B:495:GLN:C	1:B:497:LEU:H	2.22	0.41
1:A:66:GLU:HG3	1:A:360:LYS:HD2	2.02	0.41
5:A:1959:EDO:H21	6:A:1963:IMD:C4	2.46	0.41
1:B:77:MSE:HE3	1:B:77:MSE:HB2	1.96	0.41
1:B:257:PHE:HB3	1:B:259:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:HD3	5:A:1962:EDO:O2	2.20	0.41
1:A:254:ARG:HB3	1:A:254:ARG:CZ	2.51	0.41
1:A:158:MSE:O	1:A:162:LYS:HG3	2.20	0.41
1:B:171:ARG:HD2	5:B:815:EDO:O2	2.21	0.41
1:B:40:ALA:O	1:B:41:THR:C	2.58	0.41
1:B:58:HIS:O	1:B:59:TYR:C	2.59	0.41
1:B:326:SER:HA	1:B:327:PRO:HD3	1.89	0.41
1:B:378:PRO:C	1:B:379:ALA:O	2.59	0.41
1:A:73:VAL:O	1:A:77:MSE:HG3	2.21	0.41
1:B:230:LYS:HD3	1:B:282:VAL:HG23	2.03	0.41
1:B:299:HIS:CE1	10:B:882:HOH:O	2.61	0.41
1:B:416:HIS:CE1	1:B:420:THR:HG21	2.56	0.41
1:B:318:PRO:O	1:B:352:GLY:HA2	2.21	0.41
1:B:327:PRO:HA	1:B:330:ILE:HD12	2.02	0.41
1:A:49:ILE:HB	1:A:144:CYS:HB2	2.03	0.40
1:A:60:GLU:OE1	1:A:331:THR:OG1	2.31	0.40
1:A:176:ARG:CG	1:A:176:ARG:NH1	2.61	0.40
1:B:78:ALA:N	1:B:79:PRO:CD	2.85	0.40
1:A:182:TRP:O	1:A:198:GLN:HA	2.21	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	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

All (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
1	B	325	ASP
1	B	379	ALA
1	B	59	TYR
1	B	495	GLN
1	B	496	ARG
1	A	374	GLN
1	B	380	TRP
1	A	2	GLU
1	A	380	TRP
1	B	4	LYS
1	B	115	THR
1	B	374	GLN
1	A	354	LYS
1	B	371	PRO
1	B	377	GLY
1	B	376	ILE

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

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	32	LEU
1	A	50	HIS

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	60	GLU
1	A	65	SER
1	A	68	LEU
1	A	102	ARG
1	A	105	LEU
1	A	113	LYS
1	A	114	ARG
1	A	121	THR
1	A	136	LYS
1	A	162	LYS
1	A	176	ARG
1	A	194	LYS
1	A	196	SER
1	A	212	GLN
1	A	244	GLN
1	A	247	ILE
1	A	250	ASN
1	A	255	ILE
1	A	298	THR
1	A	326	SER
1	A	348	LEU
1	A	349	SER
1	A	392	GLU
1	A	395	ARG
1	A	402	LEU
1	A	403	ARG
1	A	404	ARG
1	A	405	ARG
1	A	427	LEU
1	A	478	ASN
1	A	489	LEU
1	A	494	GLN
1	B	2	GLU
1	B	3	THR
1	B	4	LYS
1	B	35	GLN
1	B	53	LEU
1	B	56	LEU
1	B	62	ARG
1	B	103	ILE
1	B	105	LEU

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Mol	Chain	Res	Type
1	B	111	LEU
1	B	113	LYS
1	B	114	ARG
1	B	116	SER
1	B	121	THR
1	B	123	LEU
1	B	124	ARG
1	B	137	ARG
1	B	161	ARG
1	B	162	LYS
1	B	219	HIS
1	B	238	ARG
1	B	244	GLN
1	B	247	ILE
1	B	255	ILE
1	B	270	THR
1	B	272	ASP
1	B	276	LYS
1	B	280	LYS
1	B	306	ARG
1	B	312	THR
1	B	325	ASP
1	B	332	ARG
1	B	341	GLU
1	B	355	LEU
1	B	360	LYS
1	B	361	LEU
1	B	392	GLU
1	B	394	ASP
1	B	395	ARG
1	B	404	ARG
1	B	405	ARG
1	B	413	LEU
1	B	415	ARG
1	B	420	THR
1	B	428	LEU
1	B	429	LEU
1	B	484	ARG
1	B	494	GLN
1	B	495	GLN
1	B	496	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	110	HIS
1	A	128	ASN
1	A	212	GLN
1	A	242	GLN
1	A	244	GLN
1	A	250	ASN
1	A	290	ASN
1	A	297	ASN
1	A	364	HIS
1	A	424	ASN
1	A	444	HIS
1	A	473	GLN
1	A	478	ASN
1	A	482	GLN
1	B	50	HIS
1	B	244	GLN
1	B	249	GLN
1	B	294	ASN
1	B	299	HIS
1	B	424	ASN
1	B	457	HIS
1	B	494	GLN
1	B	495	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

All (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
7	A	1968	13P	C1-C2	5.63	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	FAD	C6-C7	-5.34	1.32	1.39
4	B	600	FAD	C4X-N5	4.59	1.40	1.30
4	B	600	FAD	C10-N1	4.48	1.42	1.33
4	B	600	FAD	C4'-C3'	-4.20	1.46	1.53
7	A	1968	13P	C3-C2	4.17	1.61	1.50
4	A	600	FAD	PA-O3P	-3.94	1.55	1.59
7	B	816	13P	C3-C2	3.70	1.59	1.50
7	A	1968	13P	O3-C3	3.53	1.53	1.41
4	B	600	FAD	C1'-N10	3.29	1.55	1.47
2	A	1949	BOG	O1-C1	3.13	1.45	1.40
2	A	1950	BOG	O1-C1	3.10	1.45	1.40
4	A	600	FAD	PA-O2A	-3.03	1.41	1.55
7	B	816	13P	O3-C3	2.96	1.51	1.41
4	A	600	FAD	O4'-C4'	-2.96	1.37	1.43
4	B	600	FAD	C4-N3	-2.91	1.33	1.38
2	B	700	BOG	O1-C1	2.88	1.45	1.40
4	B	600	FAD	O4B-C4B	-2.81	1.38	1.45
4	A	600	FAD	P-O2P	-2.79	1.42	1.55
4	B	600	FAD	PA-O5B	-2.78	1.48	1.59
4	A	600	FAD	P-O1P	-2.76	1.41	1.50
4	A	600	FAD	O2'-C2'	-2.75	1.37	1.43
4	A	600	FAD	C9A-C5X	-2.73	1.36	1.41
4	A	600	FAD	O2-C2	-2.72	1.19	1.24
7	B	816	13P	P-O1	2.70	1.68	1.60
4	A	600	FAD	C6-C7	-2.58	1.36	1.39
4	B	600	FAD	C9A-C5X	-2.49	1.37	1.41
7	A	1968	13P	P-O1	2.49	1.68	1.60
4	A	600	FAD	C9A-N10	-2.47	1.36	1.41
4	A	600	FAD	O4B-C4B	-2.47	1.39	1.45
4	B	600	FAD	C2A-N3A	2.43	1.35	1.32
4	A	600	FAD	C5X-N5	-2.39	1.35	1.39
4	A	600	FAD	PA-O5B	-2.39	1.50	1.59
4	A	600	FAD	C6-C5X	-2.37	1.36	1.40
4	A	600	FAD	C4X-C10	-2.37	1.37	1.44
4	A	600	FAD	O3'-C3'	-2.36	1.37	1.43
2	A	700	BOG	O1-C1	2.36	1.44	1.40
4	B	600	FAD	PA-O1A	2.33	1.58	1.50
4	A	600	FAD	C5A-N7A	-2.31	1.31	1.39
4	A	600	FAD	C4-N3	-2.25	1.34	1.38
4	A	600	FAD	C4X-N5	2.23	1.35	1.30
4	B	600	FAD	C9-C9A	-2.22	1.36	1.39
4	A	600	FAD	C8M-C8	-2.19	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	FAD	C5'-C4'	2.16	1.54	1.51
4	B	600	FAD	P-O2P	-2.16	1.45	1.55
8	B	821	BCN	C1-C2	2.15	1.55	1.51
2	A	800	BOG	O1-C1	2.15	1.43	1.40
4	B	600	FAD	C4X-C10	-2.09	1.38	1.44
4	B	600	FAD	C8M-C8	-2.08	1.47	1.51
4	B	600	FAD	C7M-C7	-2.06	1.47	1.51
4	A	600	FAD	C9-C8	-2.06	1.36	1.39
4	A	600	FAD	O3B-C3B	-2.02	1.37	1.43
4	B	600	FAD	PA-O2A	-2.01	1.46	1.55

All (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
2	A	1950	BOG	C3-C4-C5	5.08	119.44	110.23
8	B	821	BCN	C1-N1-C5	4.95	123.85	111.91
4	A	600	FAD	N3A-C2A-N1A	-4.95	121.96	128.67
8	B	820	BCN	C1-N1-C3	4.86	123.63	111.91
8	A	1969	BCN	C5-N1-C3	4.74	122.72	111.44
7	A	1968	13P	O1-P-O1P	-4.54	94.16	106.44
4	A	600	FAD	O2A-PA-O5B	-4.53	87.04	107.57
7	B	816	13P	O3P-P-O1P	4.47	128.24	110.83
9	B	812	TAM	C3-C-C2	-4.24	103.02	110.50
4	B	600	FAD	C9A-C5X-N5	-4.22	117.97	122.45
7	A	1968	13P	O3P-P-O1P	4.20	127.21	110.83
4	B	600	FAD	O2'-C2'-C3'	-4.16	99.51	109.25
4	B	600	FAD	C5X-N5-C4X	4.13	124.77	118.09
9	B	812	TAM	C3-C-N	-4.00	98.18	108.22
4	B	600	FAD	C10-C4X-N5	-3.94	116.75	124.81
4	B	600	FAD	C4-C4X-N5	3.92	123.62	118.21
4	B	600	FAD	O4-C4-N3	-3.70	113.15	120.11
9	B	812	TAM	C5-C2-C	3.50	120.10	115.97
8	B	820	BCN	C5-N1-C3	3.50	119.77	111.44
8	B	821	BCN	C2-C1-N1	3.46	124.73	113.77
2	B	800	BOG	C1-C2-C3	3.45	117.28	110.01
2	A	800	BOG	O5-C5-C4	3.36	115.76	109.70
2	A	800	BOG	C3-C4-C5	3.36	116.33	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	812	TAM	C2-C-N	3.33	116.59	108.22
4	A	600	FAD	C4B-O4B-C1B	3.30	112.95	109.92
2	A	1950	BOG	C4-C3-C2	3.13	116.33	110.83
2	A	800	BOG	C4-C3-C2	3.11	116.29	110.83
4	B	600	FAD	O3'-C3'-C2'	-3.09	101.91	108.93
8	B	821	BCN	C1-N1-C3	3.03	119.22	111.91
2	A	1950	BOG	O5-C5-C4	2.99	115.08	109.70
4	B	600	FAD	C4B-O4B-C1B	-2.96	107.21	109.92
2	B	700	BOG	O5-C5-C6	2.94	113.72	106.44
4	B	600	FAD	C9-C9A-N10	2.89	125.74	121.85
8	A	1969	BCN	C1-N1-C5	2.87	118.83	111.91
4	A	600	FAD	O5B-C5B-C4B	2.87	118.77	108.99
2	A	800	BOG	O3-C3-C4	-2.86	103.63	110.38
4	B	600	FAD	C1'-C2'-C3'	-2.76	102.16	109.66
8	A	1969	BCN	C1-N1-C3	2.71	118.44	111.91
4	B	600	FAD	C5A-C6A-N6A	2.65	124.34	120.31
4	B	600	FAD	C9A-N10-C10	2.61	124.72	120.75
2	A	1950	BOG	O1-C1-C2	2.56	112.16	108.27
4	A	600	FAD	C4X-C4-N3	2.54	119.73	113.25
7	B	816	13P	O1-P-O1P	-2.52	99.64	106.44
4	A	600	FAD	O4-C4-N3	-2.48	115.44	120.11
8	B	820	BCN	C2-C1-N1	2.44	121.52	113.77
4	A	600	FAD	O5B-PA-O1A	2.44	118.60	108.94
2	A	700	BOG	C1-O5-C5	2.42	118.44	113.72
4	B	600	FAD	O5'-P-O1P	-2.41	99.38	108.94
9	B	812	TAM	C2-C-C1	2.41	114.75	110.50
9	B	812	TAM	C6-C3-C	-2.39	113.15	115.97
4	B	600	FAD	C4X-C10-N1	-2.39	118.72	124.59
2	A	1949	BOG	O1-C1-C2	2.38	111.88	108.27
4	A	600	FAD	C10-C4X-N5	-2.35	120.02	124.81
2	A	800	BOG	O5-C1-C2	-2.35	105.55	110.37
2	B	800	BOG	C4-C3-C2	2.33	114.92	110.83
2	A	1950	BOG	O4-C4-C3	-2.31	104.93	110.38
4	B	600	FAD	C4X-C4-N3	2.31	119.12	113.25
4	A	600	FAD	O4-C4-C4X	-2.30	120.47	126.53
8	B	821	BCN	C5-N1-C3	2.29	116.90	111.44
2	A	700	BOG	O2-C2-C1	2.24	115.42	110.08
4	A	600	FAD	C4X-C10-N10	2.20	119.64	116.48
4	B	600	FAD	C2B-C3B-C4B	2.19	106.84	102.61
4	B	600	FAD	C4'-C3'-C2'	-2.19	109.93	113.57
9	B	812	TAM	C3-C-C1	2.18	114.36	110.50
4	A	600	FAD	C9A-C5X-N5	-2.17	120.15	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	600	FAD	O4'-C4'-C3'	2.16	114.31	109.25
4	B	600	FAD	O4B-C1B-N9A	-2.12	105.93	108.75
4	A	600	FAD	C8M-C8-C7	-2.12	116.44	120.76
8	A	1969	BCN	C6-C5-N1	-2.11	106.03	113.44
4	A	600	FAD	C4-C4X-N5	2.07	121.07	118.21
2	B	700	BOG	O5-C1-O1	2.07	114.93	110.04
4	A	600	FAD	C4-N3-C2	-2.06	121.99	125.64

There are no chirality outliers.

All (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
7	A	1968	13P	C1-O1-P-O3P
7	A	1968	13P	C2-C1-O1-P
7	A	1968	13P	O1-C1-C2-O2
7	A	1968	13P	C1-C2-C3-O3
7	A	1968	13P	O2-C2-C3-O3
7	B	816	13P	C1-O1-P-O1P
7	B	816	13P	C1-O1-P-O2P
7	B	816	13P	C1-O1-P-O3P
7	B	816	13P	C2-C1-O1-P
7	B	816	13P	O1-C1-C2-O2
7	B	816	13P	C1-C2-C3-O3
7	B	816	13P	O2-C2-C3-O3
8	B	820	BCN	C6-C5-N1-C3
8	B	820	BCN	N1-C1-C2-O21
8	B	820	BCN	N1-C1-C2-O22
8	B	821	BCN	N1-C1-C2-O21
8	B	821	BCN	N1-C1-C2-O22
9	B	812	TAM	N-C-C2-C5
8	B	820	BCN	N1-C3-C4-O4
2	A	800	BOG	O5-C5-C6-O6
2	B	700	BOG	O5-C5-C6-O6
8	B	820	BCN	C4-C3-N1-C1
2	A	1950	BOG	O5-C5-C6-O6
2	B	700	BOG	C4-C5-C6-O6
8	A	1969	BCN	N1-C1-C2-O22

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Mol	Chain	Res	Type	Atoms
2	A	800	BOG	C4-C5-C6-O6
2	A	800	BOG	C2-C1-O1-C1'
2	A	1950	BOG	C4-C5-C6-O6
2	A	700	BOG	C4-C5-C6-O6
8	A	1969	BCN	N1-C1-C2-O21
2	A	700	BOG	O1-C1'-C2'-C3'
2	A	700	BOG	O5-C5-C6-O6
8	A	1969	BCN	C6-C5-N1-C1
2	B	800	BOG	C2-C1-O1-C1'
2	B	800	BOG	O5-C1-O1-C1'
2	A	700	BOG	C3'-C4'-C5'-C6'
2	A	1949	BOG	C3'-C4'-C5'-C6'
2	A	700	BOG	C2'-C3'-C4'-C5'
8	B	820	BCN	N1-C5-C6-O6
2	A	1949	BOG	C2'-C3'-C4'-C5'
5	B	802	EDO	O1-C1-C2-O2
5	B	809	EDO	O1-C1-C2-O2
5	B	811	EDO	O1-C1-C2-O2
8	B	821	BCN	C2-C1-N1-C5
2	A	1949	BOG	C1'-C2'-C3'-C4'
2	B	700	BOG	C3'-C4'-C5'-C6'
2	B	800	BOG	C3'-C4'-C5'-C6'
2	A	1949	BOG	O1-C1'-C2'-C3'
9	B	812	TAM	C1-C-C2-C5
9	B	812	TAM	C3-C-C2-C5
5	A	1956	EDO	O1-C1-C2-O2
5	A	1962	EDO	O1-C1-C2-O2
5	B	815	EDO	O1-C1-C2-O2
2	A	800	BOG	C3'-C4'-C5'-C6'
2	B	700	BOG	C1'-C2'-C3'-C4'
7	A	1968	13P	C1-O1-P-O1P
2	A	700	BOG	C5'-C6'-C7'-C8'
2	A	1949	BOG	C5'-C6'-C7'-C8'
2	A	800	BOG	C1'-C2'-C3'-C4'
2	A	700	BOG	O5-C1-O1-C1'
2	B	700	BOG	C5'-C6'-C7'-C8'
5	B	810	EDO	O1-C1-C2-O2
5	B	813	EDO	O1-C1-C2-O2
8	B	820	BCN	C2-C1-N1-C5
8	A	1969	BCN	N1-C3-C4-O4
2	B	800	BOG	C5'-C6'-C7'-C8'
2	B	800	BOG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
9	B	812	TAM	C-C3-C6-O6
2	B	800	BOG	O1-C1'-C2'-C3'
2	A	1950	BOG	C4'-C5'-C6'-C7'
2	A	1950	BOG	C2'-C1'-O1-C1
8	B	821	BCN	N1-C5-C6-O6
4	A	600	FAD	C4B-C5B-O5B-PA
2	A	800	BOG	C5'-C6'-C7'-C8'
9	B	812	TAM	C2-C-C1-C4
5	A	1964	EDO	O1-C1-C2-O2
4	A	600	FAD	C5B-O5B-PA-O1A
8	B	821	BCN	C6-C5-N1-C1
5	B	804	EDO	O1-C1-C2-O2
5	B	818	EDO	O1-C1-C2-O2
2	A	1949	BOG	C2'-C1'-O1-C1
5	A	1957	EDO	O1-C1-C2-O2
5	A	1965	EDO	O1-C1-C2-O2
5	B	806	EDO	O1-C1-C2-O2
5	A	1955	EDO	O1-C1-C2-O2
5	B	808	EDO	O1-C1-C2-O2
5	B	817	EDO	O1-C1-C2-O2
2	A	1950	BOG	O1-C1'-C2'-C3'
8	A	1969	BCN	C4-C3-N1-C5
5	A	1958	EDO	O1-C1-C2-O2
5	B	803	EDO	O1-C1-C2-O2
8	B	821	BCN	C4-C3-N1-C5
8	B	821	BCN	C2-C1-N1-C3
4	A	600	FAD	O4B-C4B-C5B-O5B
5	B	805	EDO	O1-C1-C2-O2
5	B	807	EDO	O1-C1-C2-O2

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

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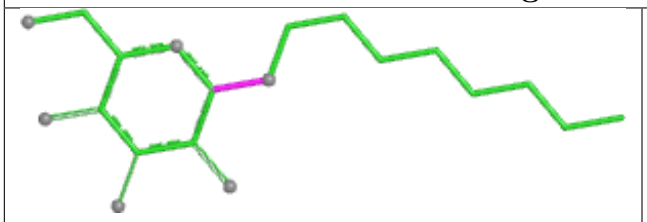
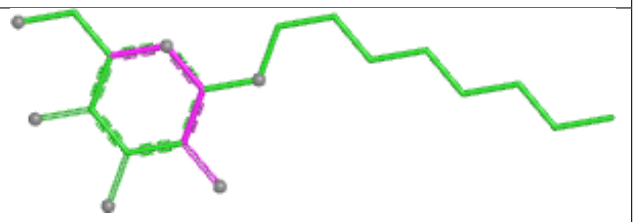
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1950	BOG	1	0
5	B	803	EDO	2	0
5	A	1964	EDO	1	0
5	A	1959	EDO	7	0
5	A	1965	EDO	3	0
5	B	810	EDO	2	0
4	A	600	FAD	1	0
2	B	700	BOG	2	0
8	B	821	BCN	3	0
5	B	817	EDO	1	0
5	B	804	EDO	1	0
5	A	1958	EDO	4	0
5	B	813	EDO	6	0
7	B	816	13P	4	0
5	B	808	EDO	2	0
5	B	811	EDO	3	0
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
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.

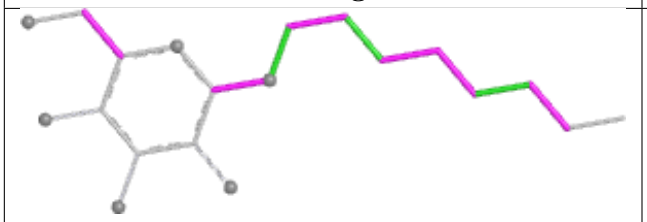
Ligand BOG A 700



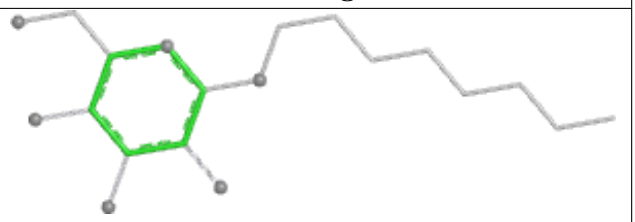
Bond lengths



Bond angles

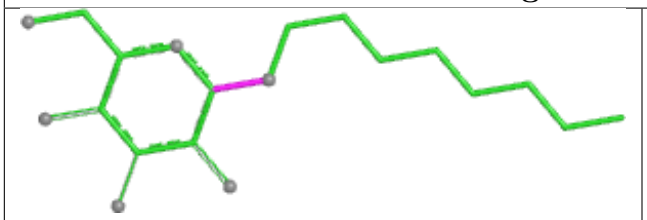


Torsions

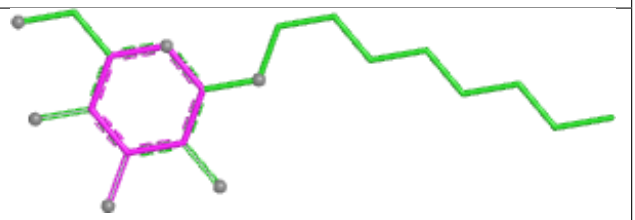


Rings

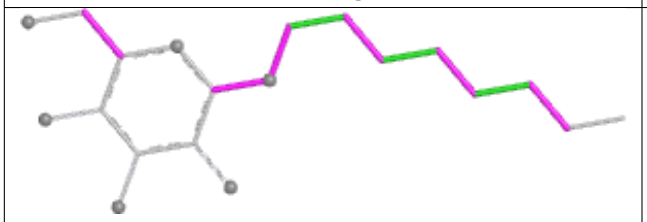
Ligand BOG A 800



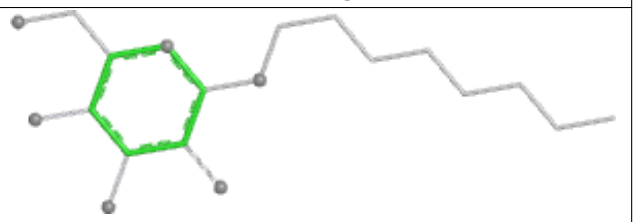
Bond lengths



Bond angles

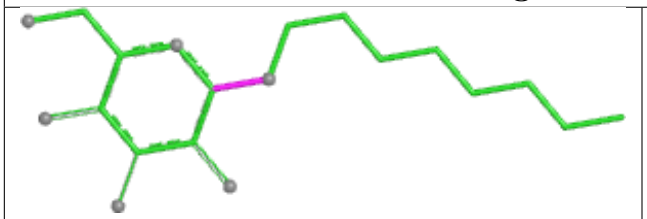


Torsions

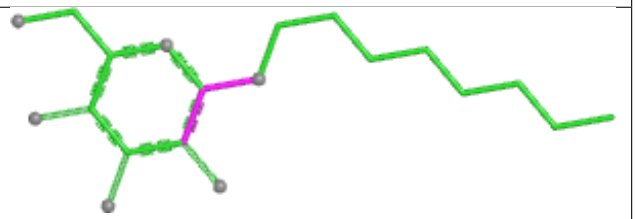


Rings

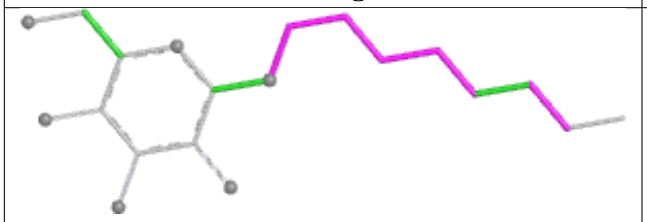
Ligand BOG A 1949



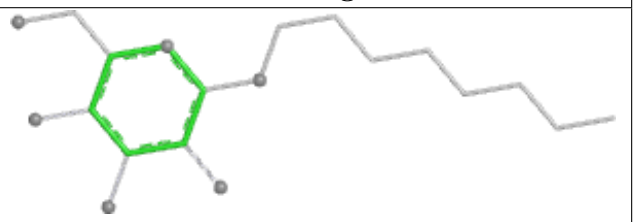
Bond lengths



Bond angles

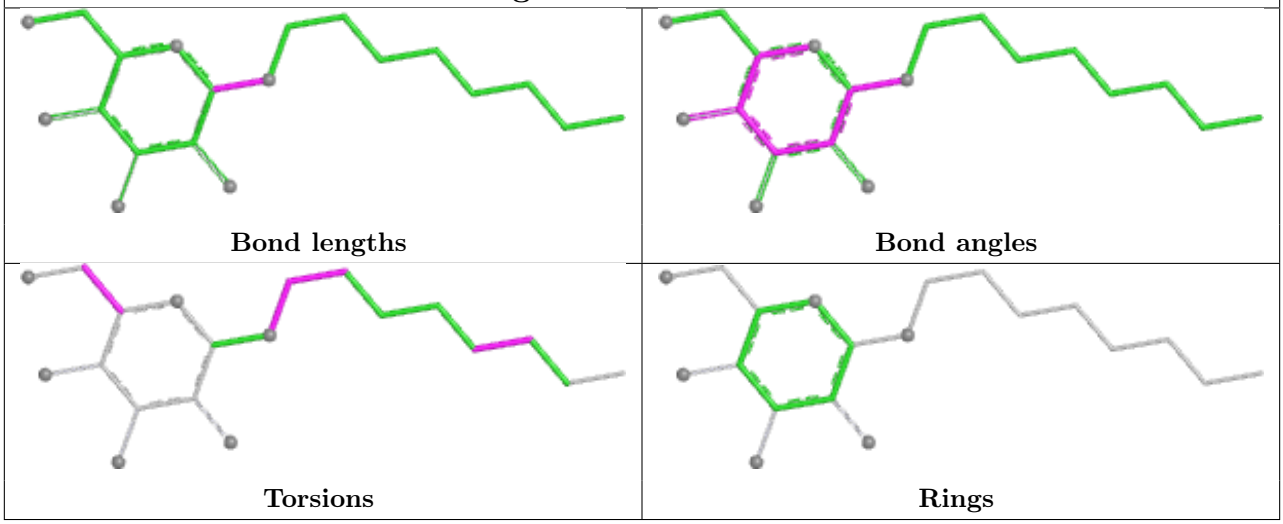


Torsions

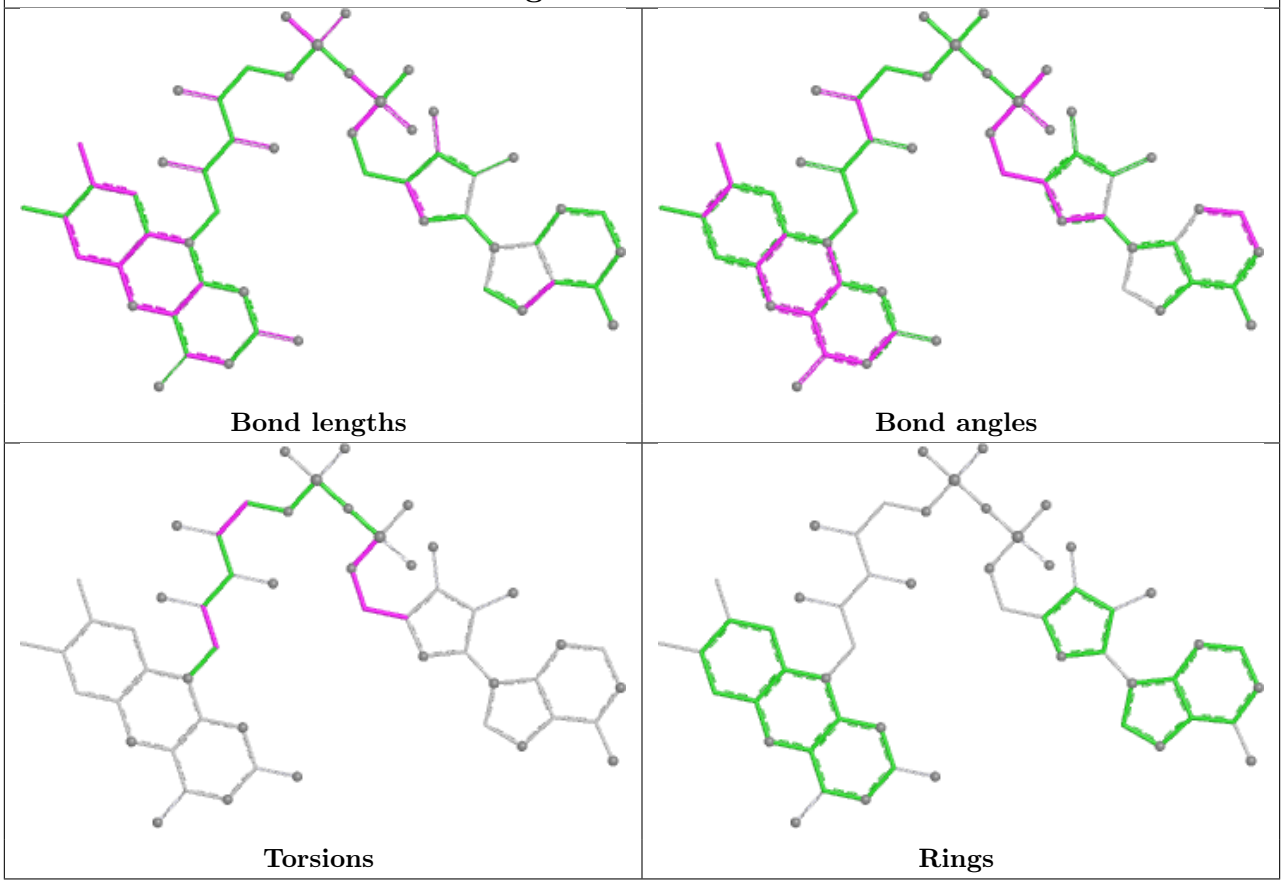


Rings

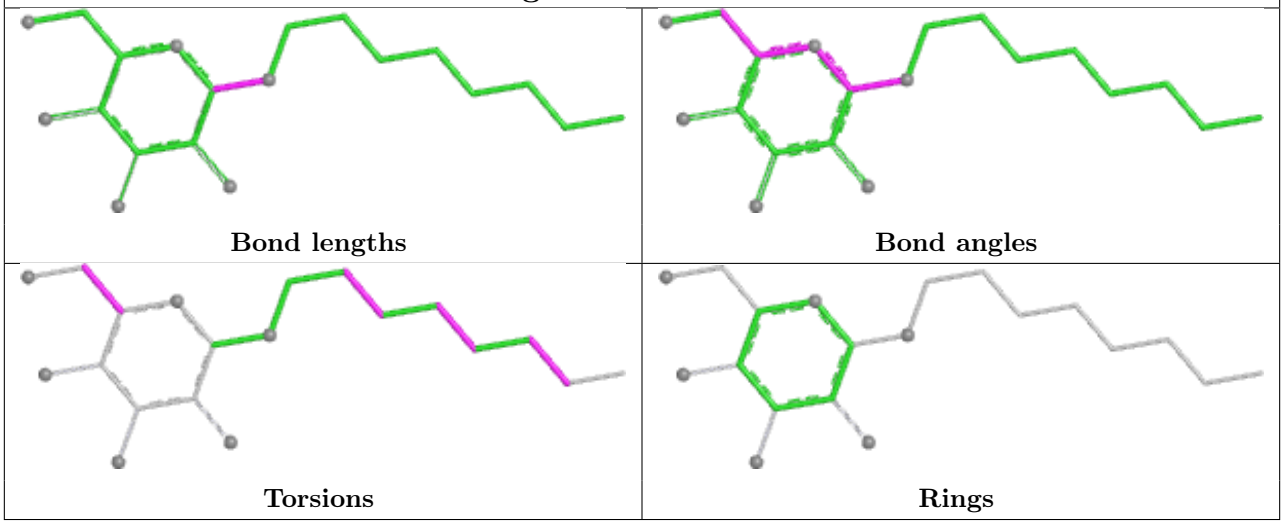
Ligand BOG A 1950



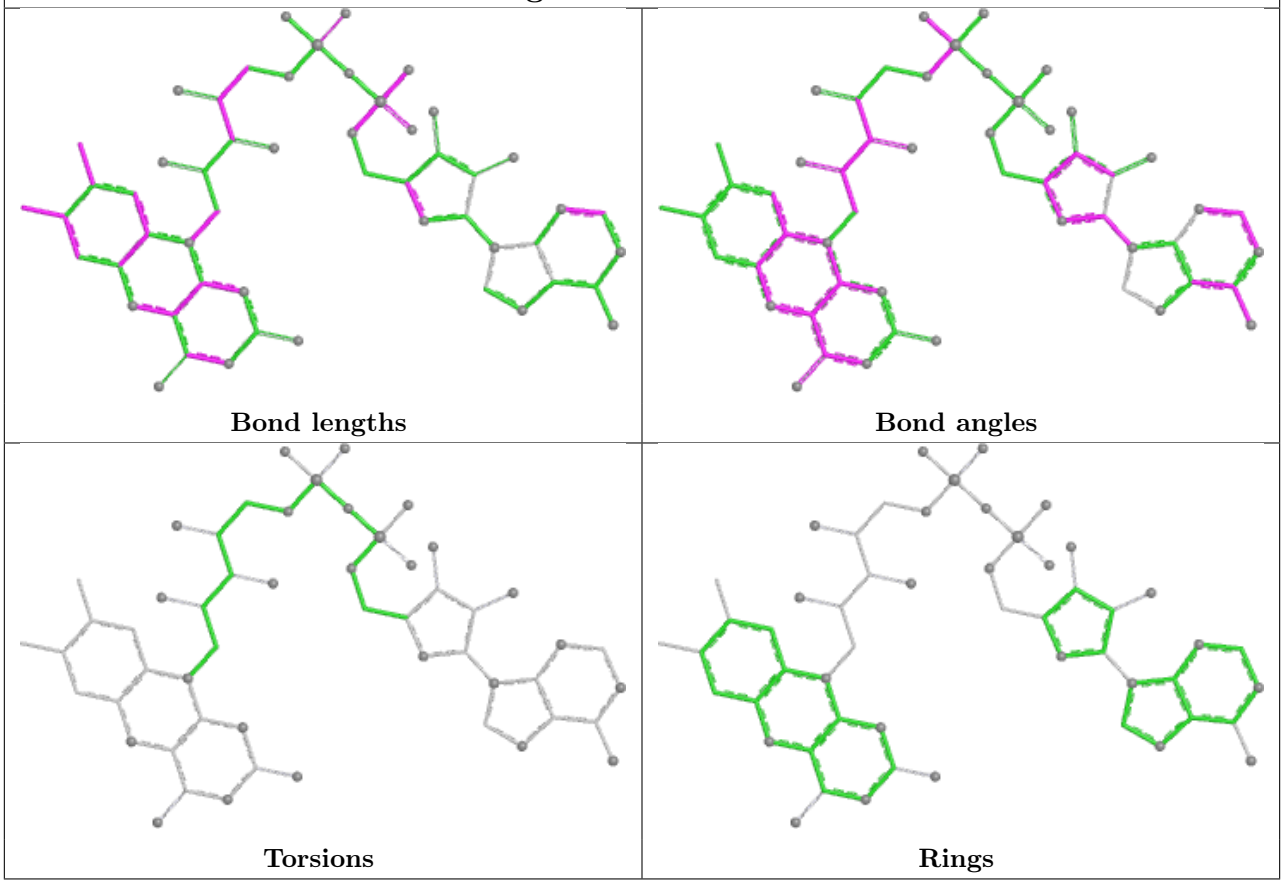
Ligand FAD A 600

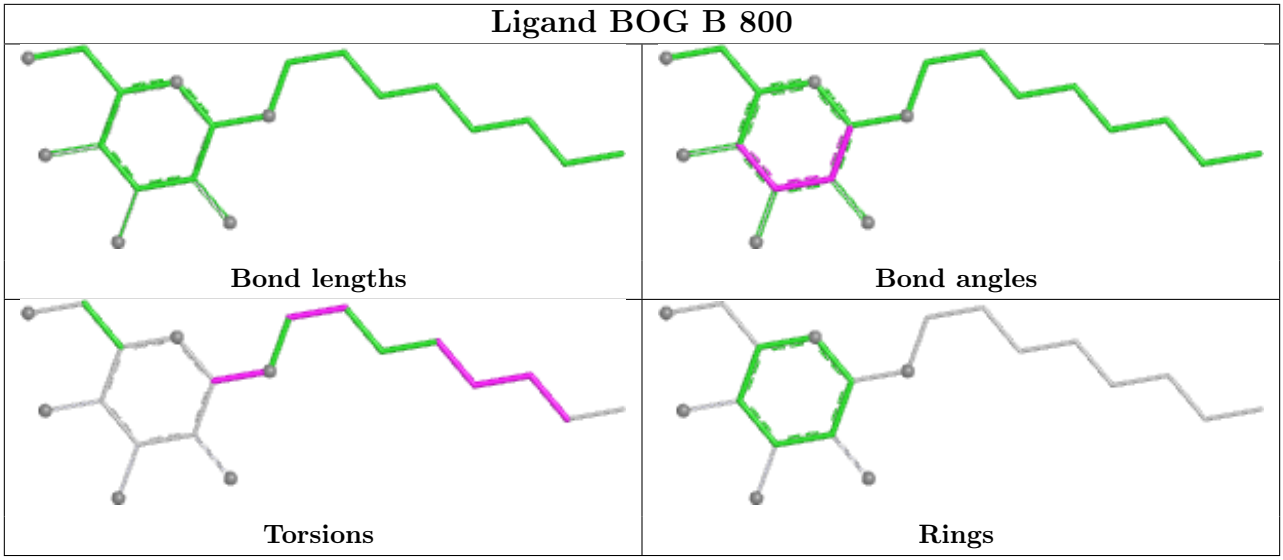


Ligand BOG B 700



Ligand FAD B 600





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

All (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
1	B	1	MET	6.6
1	A	115	THR	6.1
1	A	325	ASP	5.7
1	B	376	ILE	5.4
1	B	141	TYR	4.7
1	A	197	TRP	4.6
1	B	135	ILE	4.6
1	A	23	ALA	4.5
1	B	497	LEU	4.4
1	B	111	LEU	4.4
1	A	369	LEU	4.2
1	A	320	CYS	4.2
1	A	58	HIS	4.1
1	B	391	ILE	4.0
1	B	110	HIS	4.0
1	B	100	MET	4.0
1	B	374	GLN	4.0
1	B	26	GLY	3.9
1	B	49	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	163	GLY	3.8
1	B	389	GLY	3.7
1	A	318	PRO	3.7
1	A	98	ALA	3.7
1	A	113	LYS	3.6
1	A	111	LEU	3.6
1	B	402	LEU	3.6
1	A	345	ALA	3.5
1	A	453	TYR	3.5
1	A	117	LEU	3.4
1	B	117	LEU	3.4
1	B	435	VAL	3.4
1	A	19	ALA	3.4
1	A	319	LEU	3.4
1	B	139	PHE	3.3
1	A	81	ILE	3.3
1	B	72	GLU	3.3
1	B	375	GLY	3.2
1	A	106	PHE	3.2
1	B	181	LEU	3.1
1	B	247	ILE	3.1
1	A	122	GLY	3.1
1	A	59	TYR	3.1
1	A	64	VAL	3.1
1	A	121	THR	3.1
1	B	124	ARG	3.1
1	B	346	PRO	3.0
1	A	8	VAL	3.0
1	A	272	ASP	3.0
1	A	380	TRP	3.0
1	A	107	MET	3.0
1	B	131	LEU	2.9
1	B	133	PRO	2.9
1	B	367	GLU	2.9
1	A	427	LEU	2.9
1	A	437	ASP	2.9
1	A	367	GLU	2.9
1	B	66	GLU	2.9
1	B	273	VAL	2.9
1	A	123	LEU	2.9
1	B	83	PHE	2.9
1	B	142	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	291	TYR	2.8
1	B	365	ALA	2.8
1	B	330	ILE	2.8
1	A	243	LYS	2.8
1	A	355	LEU	2.8
1	A	402	LEU	2.8
1	A	195	TYR	2.8
1	A	337	ASP	2.8
1	A	304	LEU	2.8
1	B	361	LEU	2.8
1	A	12	GLY	2.8
1	A	160	VAL	2.8
1	A	51	GLY	2.7
1	B	309	ILE	2.7
1	A	6	LEU	2.7
1	B	198	GLN	2.7
1	A	393	GLY	2.7
1	A	329	ALA	2.7
1	A	204	ASN	2.7
1	A	29	VAL	2.7
1	B	108	TYR	2.7
1	A	74	LEU	2.7
1	B	355	LEU	2.7
1	B	210	VAL	2.6
1	A	37	LEU	2.6
1	B	312	THR	2.6
1	A	144	CYS	2.6
1	A	432	ALA	2.6
1	B	98	ALA	2.6
1	B	183	ILE	2.6
1	A	11	GLY	2.6
1	A	443	GLY	2.6
1	A	61	PHE	2.6
1	B	228	LEU	2.6
1	B	67	ALA	2.6
1	A	429	LEU	2.6
1	A	488	TRP	2.6
1	B	145	TRP	2.6
1	B	107	MET	2.6
1	B	259	ILE	2.6
1	A	436	SER	2.6
1	B	27	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	143	ASP	2.5
1	A	184	VAL	2.5
1	B	282	VAL	2.5
1	A	399	ALA	2.5
1	B	127	ALA	2.5
1	B	252	ASP	2.5
1	B	226	ILE	2.5
1	B	341	GLU	2.5
1	A	291	TYR	2.5
1	B	180	GLY	2.5
1	A	159	VAL	2.5
1	A	247	ILE	2.4
1	B	342	ASN	2.4
1	B	392	GLU	2.4
1	A	418	ALA	2.4
1	A	13	ILE	2.4
1	B	255	ILE	2.4
1	A	347	LEU	2.4
1	B	257	PHE	2.4
1	A	375	GLY	2.4
1	B	60	GLU	2.4
1	A	118	PRO	2.4
1	B	195	TYR	2.4
1	A	44	ALA	2.4
1	A	277	GLY	2.4
1	A	9	ILE	2.4
1	B	314	SER	2.3
1	B	462	ARG	2.3
1	B	459	TRP	2.3
1	A	49	ILE	2.3
1	B	101	ILE	2.3
1	A	32	LEU	2.3
1	A	261	TRP	2.3
1	B	246	TYR	2.3
1	B	373	TYR	2.3
1	A	166	VAL	2.3
1	A	226	ILE	2.3
1	B	384	SER	2.3
1	B	496	ARG	2.3
1	A	135	ILE	2.3
1	B	34	ALA	2.3
1	A	276	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	339	HIS	2.3
1	A	18	ILE	2.2
1	B	272	ASP	2.2
1	A	336	LEU	2.2
1	A	67	ALA	2.2
1	A	338	ILE	2.2
1	A	105	LEU	2.2
1	B	248	LEU	2.2
1	B	334	TYR	2.2
1	B	48	LEU	2.2
1	B	114	ARG	2.2
1	B	468	TRP	2.2
1	B	188	ASP	2.2
1	A	346	PRO	2.2
1	A	213	PHE	2.2
1	A	101	ILE	2.2
1	A	183	ILE	2.2
1	A	348	LEU	2.2
1	B	427	LEU	2.2
1	B	121	THR	2.2
1	B	420	THR	2.2
1	B	372	TYR	2.2
1	B	295	VAL	2.2
1	B	284	ILE	2.1
1	A	176	ARG	2.1
1	A	206	THR	2.1
1	B	304	LEU	2.1
1	A	479	ALA	2.1
1	A	258	VAL	2.1
1	A	385	VAL	2.1
1	B	3	THR	2.1
1	A	57	GLU	2.1
1	A	257	PHE	2.1
1	B	109	ASP	2.1
1	B	495	GLN	2.1
1	A	4	LYS	2.1
1	A	422	GLY	2.1
1	B	112	GLY	2.1
1	A	435	VAL	2.1
1	A	332	ARG	2.1
1	A	56	LEU	2.1
1	A	202	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	394	ASP	2.1
1	B	313	TYR	2.1
1	B	160	VAL	2.1
1	B	351	PHE	2.1
1	A	457	HIS	2.1
1	B	172	ALA	2.1
1	A	366	LEU	2.1
1	B	243	LYS	2.1
1	B	298	THR	2.0
1	A	216	ASP	2.0
1	A	130	VAL	2.0
1	B	485	VAL	2.0
1	B	418	ALA	2.0
1	B	97	PRO	2.0
1	A	75	LEU	2.0
1	B	234	ILE	2.0
1	A	2	GLU	2.0
1	B	28	SER	2.0
1	B	50	HIS	2.0
1	A	311	TRP	2.0
1	A	494	GLN	2.0
1	A	30	LEU	2.0
1	B	32	LEU	2.0
1	B	151	LEU	2.0

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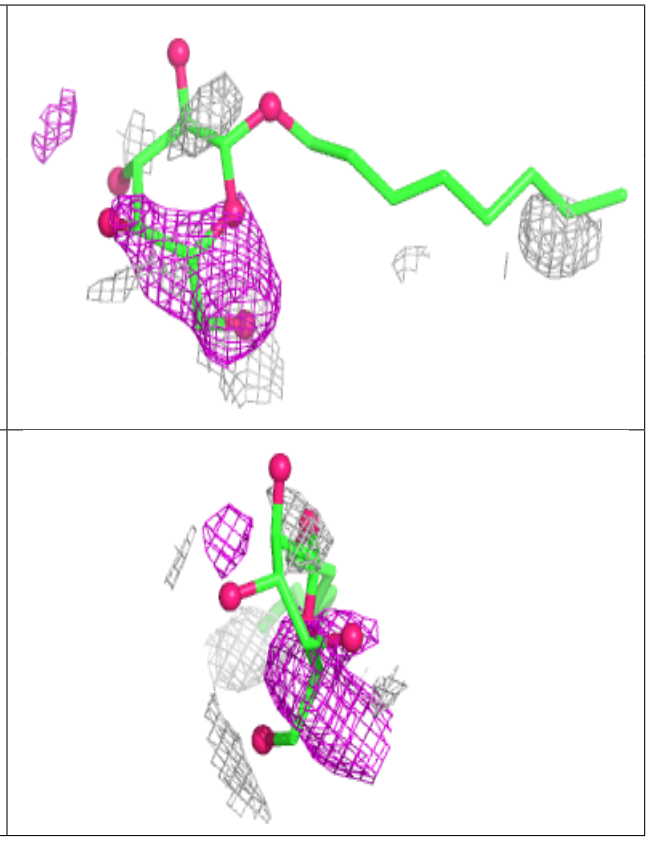
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1959	4/4	0.90	0.14	43,48,49,52	0
4	FAD	B	600	53/53	0.90	0.15	19,25,29,32	0
5	EDO	B	811	4/4	0.91	0.28	36,43,44,49	0
5	EDO	A	1958	4/4	0.92	0.36	32,34,40,46	0
4	FAD	A	600	53/53	0.92	0.16	18,26,29,36	0

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.

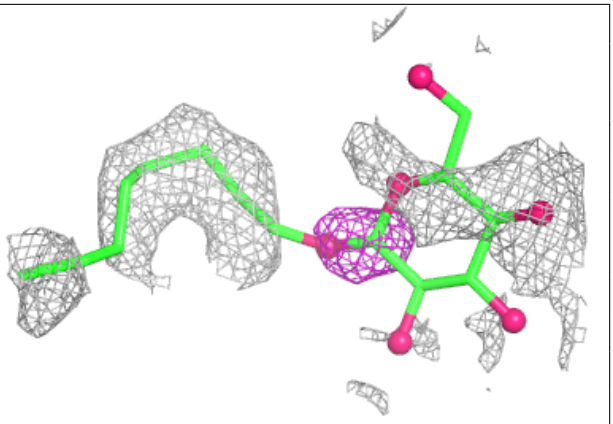
Electron density around BOG A 800:

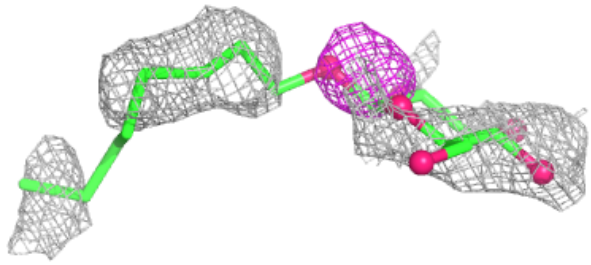
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

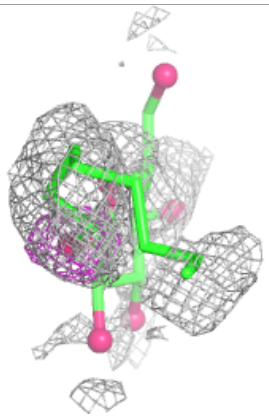


Electron density around BOG A 1949:

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

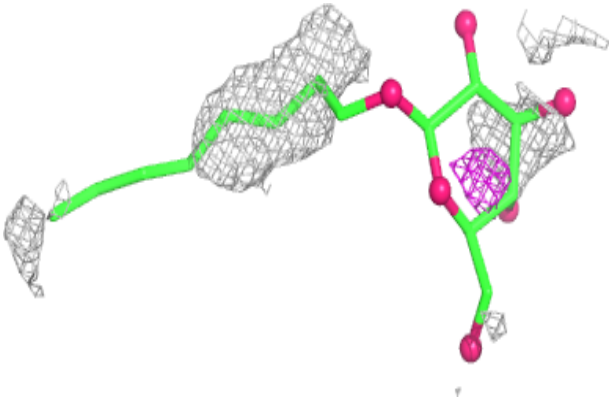


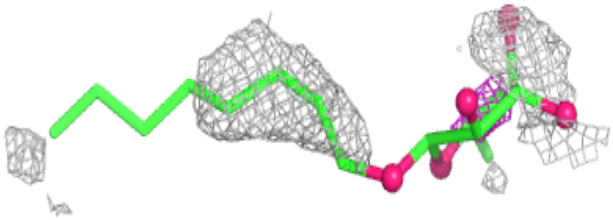




Electron density around BOG A 1950:

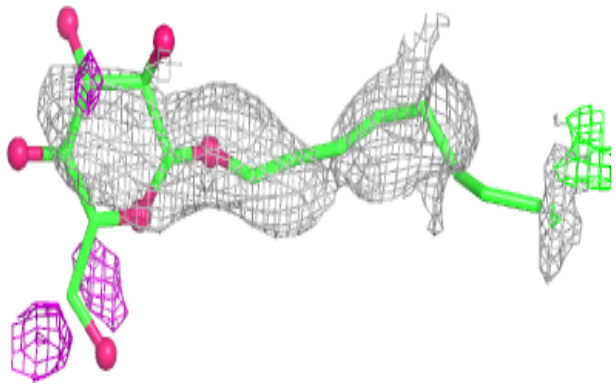
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

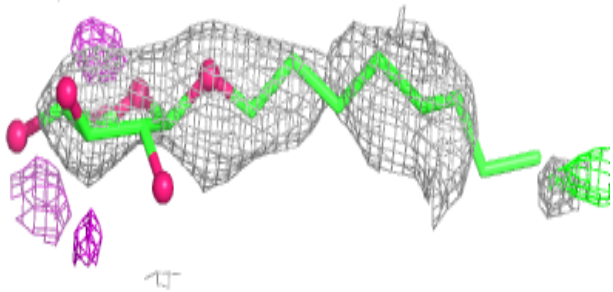


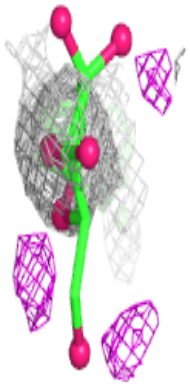


Electron density around BOG B 800:

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

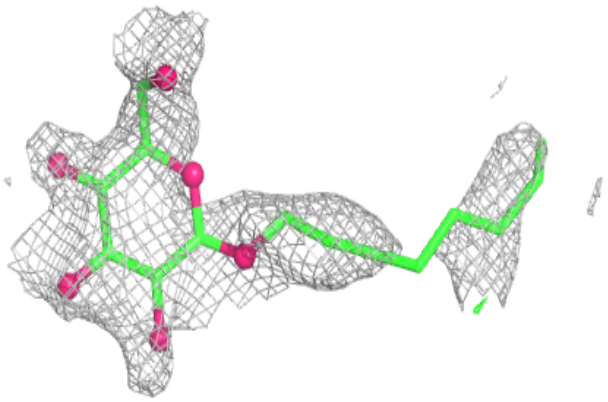


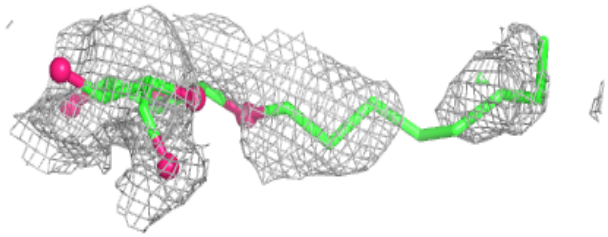


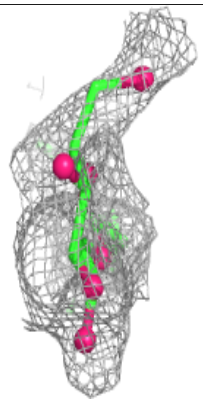


Electron density around BOG A 700:

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

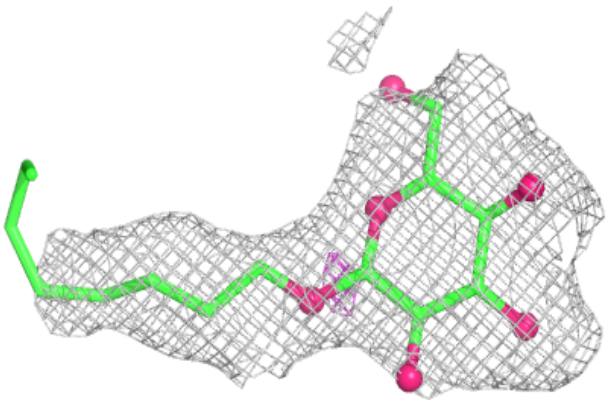


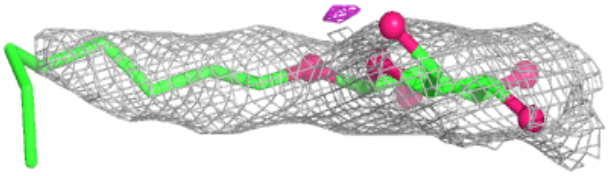


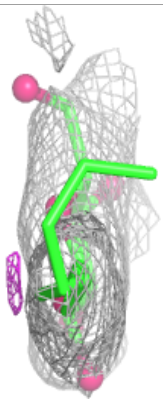


Electron density around BOG B 700:

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

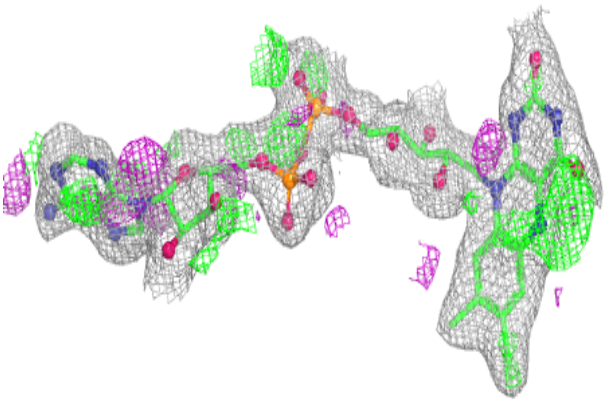


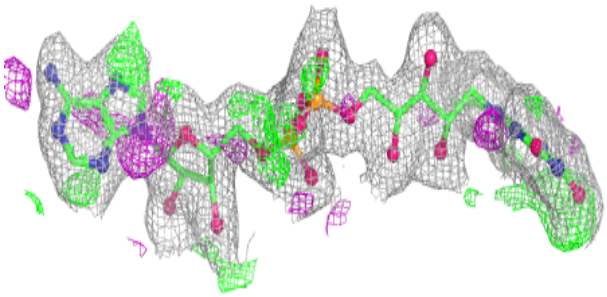


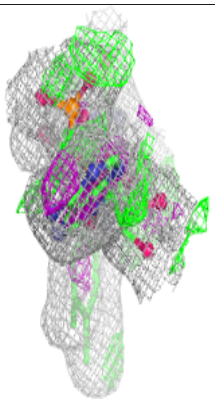


Electron density around FAD B 600:

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

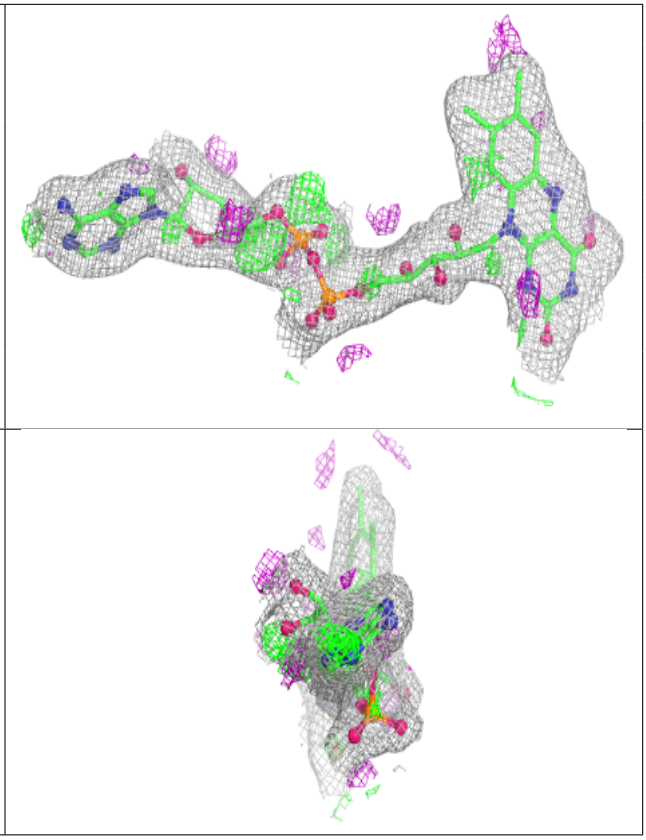






Electron density around FAD A 600:

$2mF_o$-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.