



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:04 PM UTC

PDB ID : 2R4E / pdb_00002r4e
Title : Crystal structure of Escherichia coli Glycerol-3-phosphate Dehydrogenase in complex with DHAP
Authors : Yeh, J.I.; Du, S.; Chinte, U.
Deposited on : 2007-08-31
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

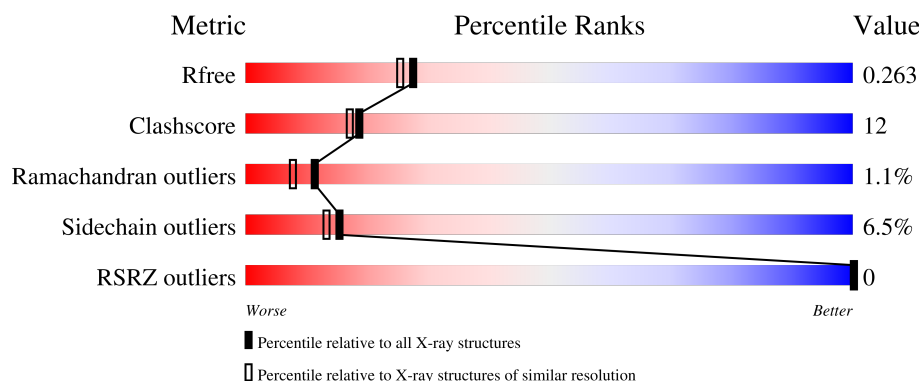
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	501	 77% 18% . .
1	B	501	 74% 19% . .

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
4	FAD	A	600	X	-	-	-
5	13P	A	1955	-	X	-	-
5	13P	B	7067	-	X	X	-

2 Entry composition [i](#)

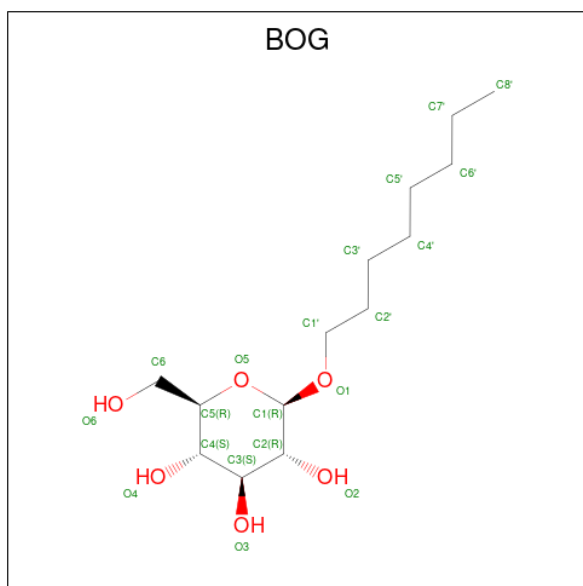
There are 9 unique types of molecules in this entry. The entry contains 8532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	494	Total	C	N	O	S	0	0	0
			3953	2510	703	727	13			
1	B	494	Total	C	N	O	S	0	0	0
			3953	2510	703	727	13			

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



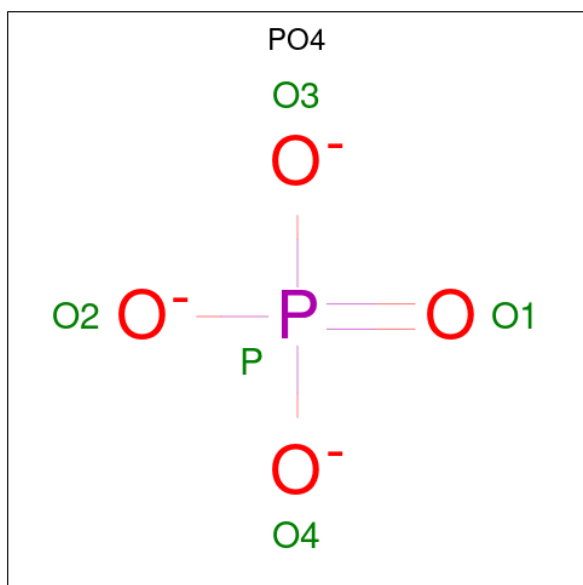
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

Continued on next page...

Continued from previous page...

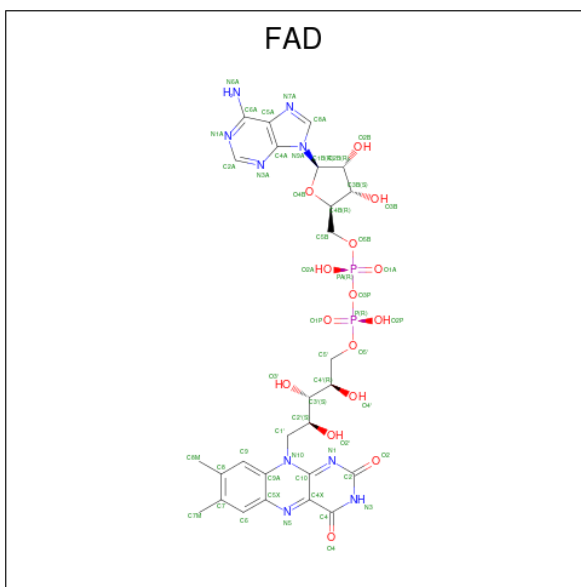
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



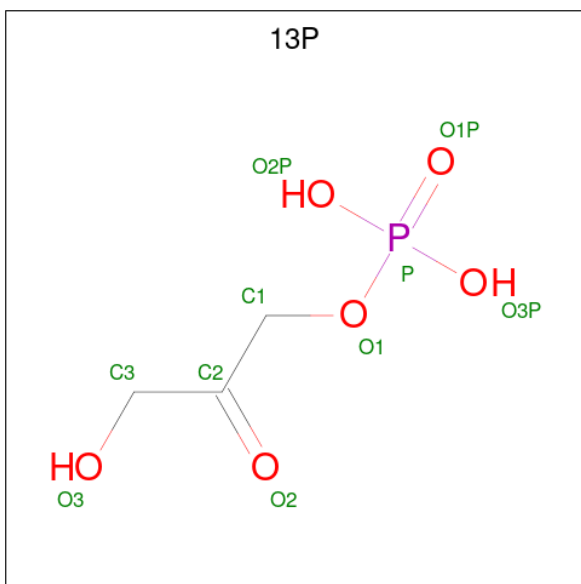
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

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



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

- Molecule 5 is 1,3-DIHYDROXYACETONEPHOSPHATE (CCD ID: 13P) (formula: $\text{C}_3\text{H}_7\text{O}_6\text{P}$).



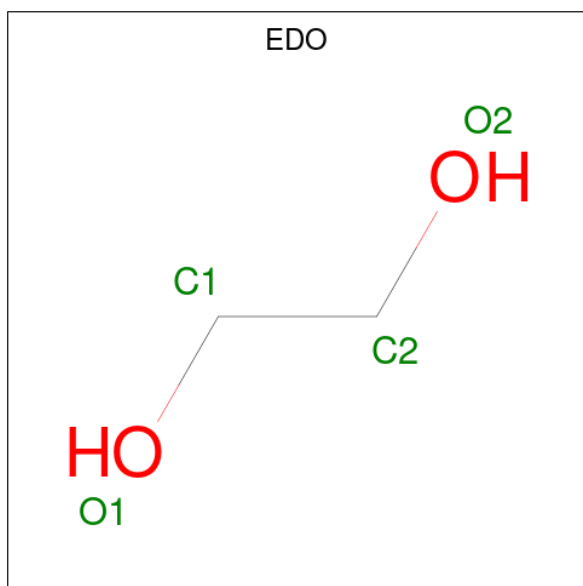
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			10	3	6	1		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



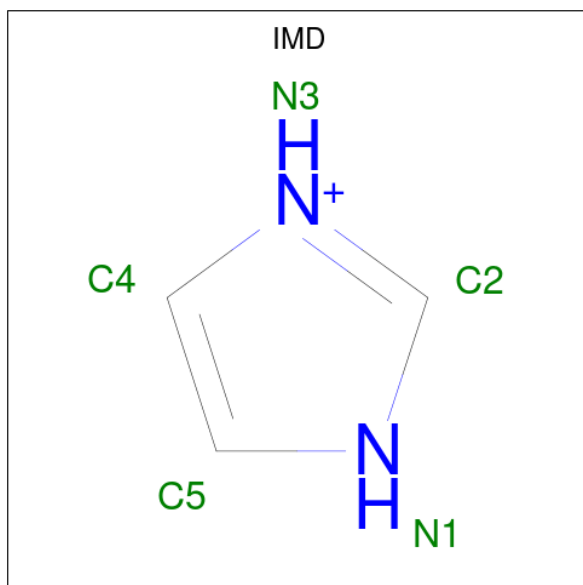
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total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

Continued on next page...

Continued from previous page...

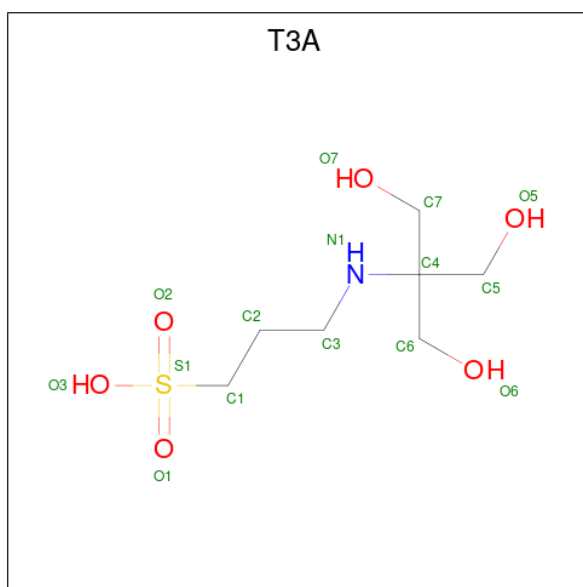
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



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

- Molecule 8 is N-(TRIS(HYDROXYMETHYL)METHYL)-3-AMINOPROPANESULFONIC ACID (CCD ID: T3A) (formula: $C_7H_{17}NO_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	7	1	6	1		
8	B	1	Total	C	N	O	S	0	0
			15	7	1	6	1		

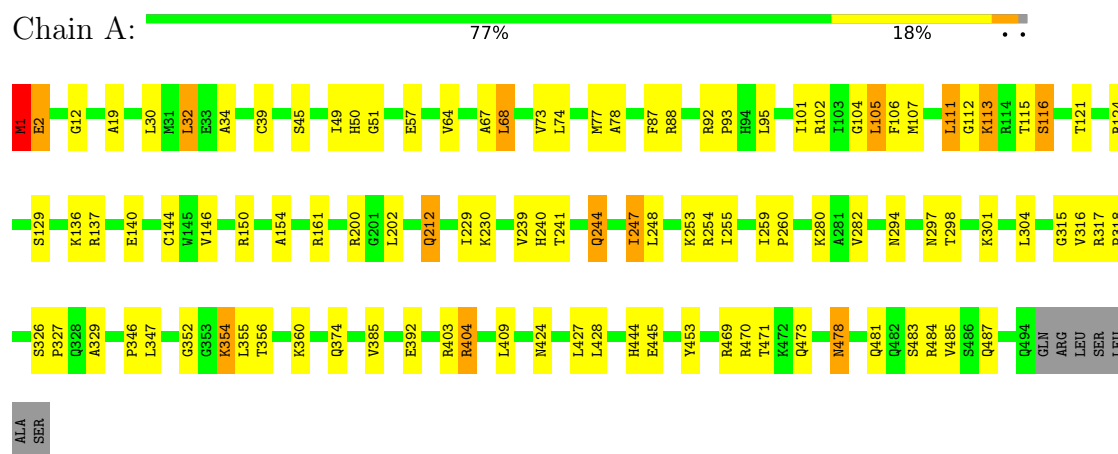
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	131	Total	O	0	0
			131	131		
9	B	132	Total	O	0	0
			132	132		

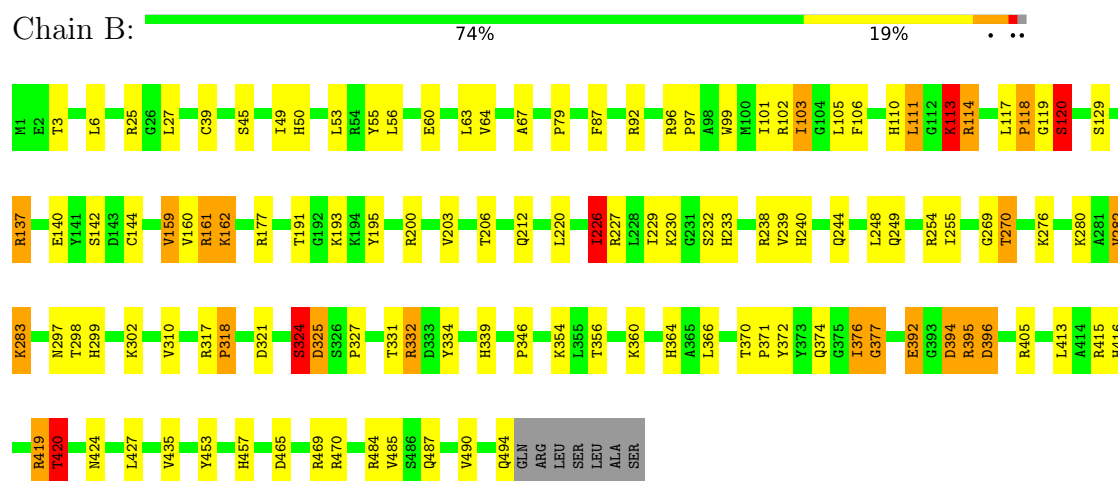
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase



- Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.85Å 113.82Å 193.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-2.10) 99.8 (10.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.256 0.205 , 0.263	Depositor DCC
R_{free} test set	3882 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.470 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 13P, T3A, IMD, PO4, EDO, FAD, BOG

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	1.31	8/4048 (0.2%)	1.15	4/5482 (0.1%)
1	B	1.31	7/4048 (0.2%)	1.21	16/5482 (0.3%)
All	All	1.31	15/8096 (0.2%)	1.18	20/10964 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	VAL	CA-CB	6.85	1.63	1.54
1	A	316	VAL	CA-CB	6.38	1.62	1.54
1	A	329	ALA	CA-CB	5.92	1.64	1.53
1	B	282	VAL	CA-CB	5.87	1.60	1.54
1	B	120	SER	CA-C	-5.83	1.45	1.52
1	A	19	ALA	CA-CB	5.67	1.62	1.53
1	B	318	PRO	CA-C	5.44	1.60	1.52
1	A	471	THR	CA-CB	5.36	1.61	1.53
1	A	154	ALA	CA-CB	-5.24	1.45	1.53
1	B	485	VAL	CA-CB	5.24	1.60	1.54
1	A	78	ALA	CA-CB	5.20	1.59	1.53
1	B	435	VAL	CA-CB	5.16	1.60	1.54
1	A	315	GLY	C-O	-5.05	1.18	1.23
1	B	310	VAL	N-CA	5.04	1.52	1.46
1	B	113	LYS	CA-C	5.00	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	SER	N-CA-C	9.86	121.62	111.07
1	B	226	ILE	N-CA-C	6.67	123.21	109.34
1	B	113	LYS	N-CA-C	6.65	124.97	110.80
1	B	420	THR	CB-CA-C	6.48	121.06	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ILE	CB-CA-C	-6.44	103.61	112.24
1	B	392	GLU	N-CA-C	6.40	119.01	111.02
1	B	159	VAL	CA-C-N	6.00	128.99	120.53
1	B	159	VAL	C-N-CA	6.00	128.99	120.53
1	A	116	SER	N-CA-C	5.67	122.88	110.80
1	B	111	LEU	N-CA-C	5.66	118.99	111.75
1	B	220	LEU	CA-C-N	-5.64	114.12	119.76
1	B	220	LEU	C-N-CA	-5.64	114.12	119.76
1	A	385	VAL	N-CA-C	-5.46	99.64	107.78
1	B	377	GLY	N-CA-C	-5.26	101.61	112.34
1	B	297	ASN	CA-C-N	5.14	128.13	120.31
1	B	297	ASN	C-N-CA	5.14	128.13	120.31
1	B	191	THR	N-CA-C	5.12	119.53	113.28
1	B	3	THR	N-CA-C	5.03	116.47	108.67
1	A	1	MET	CA-C-N	5.00	130.71	121.70
1	A	1	MET	C-N-CA	5.00	130.71	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3953	0	3903	81	0
1	B	3953	0	3903	109	0
2	A	80	0	112	13	0
2	B	40	0	56	3	0
3	A	10	0	0	1	0
3	B	15	0	0	2	0
4	A	53	0	29	8	0
4	B	53	0	30	7	0
5	A	10	0	5	3	0
5	B	10	0	5	4	0
6	A	24	0	36	4	0
6	B	28	0	42	4	0
7	A	5	0	5	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	5	0	5	0	0
8	A	15	0	17	1	0
8	B	15	0	17	1	0
9	A	131	0	0	5	0
9	B	132	0	0	7	0
All	All	8532	0	8165	195	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 12.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA3	1:A:68:LEU:HD13	1.30	1.10
1:B:395:ARG:O	1:B:396:ASP:HB2	1.54	1.05
1:B:484:ARG:NH1	1:B:487:GLN:HE21	1.54	1.04
1:B:50:HIS:HE1	1:B:354:LYS:NZ	1.58	1.01
1:B:50:HIS:CE1	1:B:354:LYS:NZ	2.30	1.00
1:A:57:GLU:HG3	2:A:1950:BOG:O2	1.64	0.97
1:A:50:HIS:HE1	1:A:354:LYS:HZ1	1.05	0.97
1:B:50:HIS:HE1	1:B:354:LYS:HZ1	1.10	0.96
1:B:484:ARG:HH11	1:B:487:GLN:NE2	1.65	0.93
1:A:297:ASN:HD21	1:A:304:LEU:H	1.19	0.89
1:A:137:ARG:HH22	2:A:1949:BOG:H5	1.37	0.89
1:A:50:HIS:CE1	1:A:354:LYS:HZ1	1.92	0.85
1:B:324:SER:O	1:B:325:ASP:HB2	1.74	0.84
1:A:57:GLU:CG	2:A:1950:BOG:O2	2.26	0.82
1:A:51:GLY:CA	1:A:68:LEU:HD13	2.09	0.82
1:B:117:LEU:O	1:B:118:PRO:O	1.96	0.81
1:B:113:LYS:HB3	1:B:114:ARG:HA	1.62	0.81
1:B:416:HIS:O	1:B:420:THR:HG23	1.79	0.81
1:A:50:HIS:HE1	1:A:354:LYS:NZ	1.78	0.80
1:A:101:ILE:HA	2:A:1950:BOG:H61	1.63	0.80
1:A:50:HIS:CE1	1:A:354:LYS:NZ	2.50	0.80
1:A:73:VAL:O	1:A:77:MET:HG3	1.81	0.80
1:A:12:GLY:HA3	4:A:600:FAD:O2A	1.82	0.79
1:B:395:ARG:O	1:B:396:ASP:CB	2.28	0.79
1:B:376:ILE:HG12	1:B:377:GLY:N	1.98	0.77
1:B:376:ILE:HG12	1:B:377:GLY:H	1.48	0.76
1:A:107:MET:HE1	2:A:1950:BOG:H3'1	1.67	0.76
1:A:107:MET:O	1:A:111:LEU:HB2	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HH11	1:B:137:ARG:HG2	1.51	0.75
1:B:394:ASP:OD1	1:B:395:ARG:O	2.05	0.75
1:B:25:ARG:HD3	1:B:377:GLY:HA2	1.67	0.74
1:B:394:ASP:OD1	1:B:394:ASP:C	2.30	0.73
1:B:118:PRO:CB	1:B:119:GLY:HA3	2.18	0.73
1:B:113:LYS:CB	1:B:114:ARG:HA	2.19	0.72
1:A:254:ARG:HH11	5:A:1955:13P:H12	1.55	0.72
1:B:484:ARG:HH11	1:B:487:GLN:HE21	0.80	0.71
1:B:50:HIS:CE1	1:B:354:LYS:HZ3	2.06	0.71
1:B:117:LEU:C	1:B:118:PRO:O	2.33	0.71
1:B:324:SER:O	1:B:325:ASP:CB	2.39	0.70
1:B:484:ARG:NH1	1:B:487:GLN:NE2	2.29	0.70
1:A:93:PRO:CB	2:A:1952:BOG:H5	2.21	0.70
9:A:7185:HOH:O	1:B:457:HIS:HE1	1.73	0.70
1:A:161:ARG:HB2	6:A:1962:EDO:O1	1.92	0.70
1:B:137:ARG:HH11	1:B:137:ARG:CG	2.06	0.69
1:A:102:ARG:NH1	2:A:1949:BOG:O5	2.25	0.69
1:B:161:ARG:HB2	6:B:1961:EDO:O2	1.93	0.68
1:B:50:HIS:CE1	1:B:354:LYS:CE	2.77	0.68
1:B:212:GLN:HB2	3:B:1952:PO4:O1	1.94	0.67
1:A:294:ASN:O	1:A:298:THR:HG23	1.95	0.66
1:B:96:ARG:HH11	1:B:249:GLN:HE21	1.41	0.65
1:A:51:GLY:HA3	1:A:68:LEU:CD1	2.18	0.65
6:A:1962:EDO:H12	8:A:7066:T3A:O3	1.97	0.64
1:A:93:PRO:HB2	2:A:1952:BOG:H5	1.80	0.64
6:B:1961:EDO:H21	8:B:7066:T3A:O3	1.98	0.64
1:A:478:ASN:ND2	1:A:481:GLN:H	1.95	0.63
1:B:50:HIS:CE1	1:B:354:LYS:HZ1	2.00	0.62
1:A:487:GLN:HG2	9:A:7137:HOH:O	1.98	0.62
1:A:317:ARG:HG3	4:A:600:FAD:HM81	1.80	0.62
1:B:114:ARG:O	1:B:114:ARG:HG2	1.98	0.61
1:A:200:ARG:O	1:A:346:PRO:HD2	2.00	0.61
6:B:1959:EDO:H12	9:B:7168:HOH:O	2.00	0.60
1:B:79:PRO:O	1:B:395:ARG:HD2	2.02	0.60
1:B:27:LEU:HD21	1:B:376:ILE:HG13	1.83	0.60
1:A:102:ARG:NH1	2:A:1949:BOG:H62	2.17	0.60
1:B:118:PRO:HB3	1:B:119:GLY:HA3	1.84	0.60
1:A:254:ARG:HH11	5:A:1955:13P:C1	2.14	0.60
1:B:193:LYS:HE2	1:B:195:TYR:CE1	2.37	0.59
1:B:254:ARG:HH21	5:B:7067:13P:H12	1.67	0.59
1:B:55:TYR:CZ	1:B:332:ARG:HD2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLY:O	1:B:120:SER:HB3	2.01	0.59
1:B:339:HIS:HD2	9:B:7089:HOH:O	1.86	0.58
1:B:55:TYR:CE1	1:B:332:ARG:HD2	2.37	0.58
1:A:150:ARG:HD2	1:A:470:ARG:O	2.04	0.57
1:A:49:ILE:HB	1:A:144:CYS:HB2	1.87	0.56
1:B:161:ARG:CB	6:B:1961:EDO:O2	2.53	0.56
1:B:317:ARG:HG3	4:B:600:FAD:HM81	1.87	0.56
1:B:113:LYS:HB3	1:B:114:ARG:CA	2.36	0.55
1:B:415:ARG:HG2	1:B:419:ARG:HD2	1.89	0.55
1:A:445:GLU:HB2	7:A:1957:IMD:H5	1.89	0.55
1:B:118:PRO:CB	1:B:119:GLY:CA	2.84	0.55
1:A:317:ARG:CG	4:A:600:FAD:HM81	2.37	0.54
1:B:49:ILE:HB	1:B:144:CYS:HB2	1.89	0.54
1:B:161:ARG:HG3	1:B:162:LYS:HD3	1.89	0.54
1:A:105:LEU:HD13	2:A:1950:BOG:O6	2.07	0.54
1:A:241:THR:HG22	1:A:241:THR:O	2.06	0.54
1:A:239:VAL:HG23	1:A:240:HIS:CD2	2.42	0.54
1:B:370:THR:O	1:B:371:PRO:C	2.51	0.53
1:A:317:ARG:HG3	4:A:600:FAD:C8M	2.38	0.53
1:B:299:HIS:HE1	9:B:7078:HOH:O	1.92	0.53
1:B:102:ARG:NH1	2:B:1949:BOG:O2	2.42	0.52
1:B:427:LEU:HD12	9:B:7159:HOH:O	2.08	0.52
1:B:87:PHE:O	1:B:140:GLU:HA	2.09	0.52
1:B:405:ARG:HD3	3:B:1951:PO4:O3	2.10	0.52
1:A:241:THR:O	1:A:241:THR:CG2	2.58	0.52
1:A:424:ASN:HB3	1:A:453:TYR:OH	2.09	0.52
1:B:96:ARG:HB2	1:B:249:GLN:HE22	1.76	0.51
1:A:478:ASN:C	1:A:478:ASN:HD22	2.18	0.51
1:A:230:LYS:HD3	1:A:282:VAL:HG23	1.93	0.51
1:B:229:ILE:HD12	1:B:327:PRO:HB3	1.91	0.51
1:B:137:ARG:HG2	1:B:137:ARG:NH1	2.24	0.51
1:B:465:ASP:O	1:B:470:ARG:HG2	2.12	0.51
1:A:137:ARG:NH2	2:A:1949:BOG:H5	2.18	0.50
1:A:88:ARG:NE	1:A:244:GLN:HG3	2.26	0.50
1:B:317:ARG:HG3	4:B:600:FAD:C8M	2.41	0.50
4:A:600:FAD:O2A	4:A:600:FAD:H4B	2.11	0.49
1:A:1:MET:HA	1:A:2:GLU:HG3	1.93	0.49
1:B:67:ALA:HB1	1:B:356:THR:HG21	1.94	0.49
1:A:50:HIS:HD2	9:A:7189:HOH:O	1.95	0.49
1:A:50:HIS:O	1:A:356:THR:HG21	2.13	0.49
1:A:112:GLY:O	1:A:113:LYS:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ASP:OD1	1:B:394:ASP:O	2.31	0.48
1:B:118:PRO:HB2	1:B:119:GLY:HA3	1.96	0.48
1:A:39:CYS:HA	1:A:469:ARG:HD3	1.96	0.48
1:A:67:ALA:HB1	1:A:356:THR:HG21	1.96	0.48
1:B:101:ILE:HD12	2:B:1950:BOG:H61	1.96	0.48
1:A:478:ASN:HD22	1:A:481:GLN:H	1.61	0.48
1:B:45:SER:HA	4:B:600:FAD:C6	2.44	0.48
1:A:34:ALA:HB3	6:A:1956:EDO:H11	1.96	0.47
1:A:202:LEU:HD23	1:A:347:LEU:HD13	1.95	0.47
1:B:254:ARG:HH21	5:B:7067:13P:C1	2.27	0.47
1:B:25:ARG:HB3	1:B:377:GLY:H	1.80	0.47
1:B:114:ARG:NH1	1:B:118:PRO:O	2.48	0.47
1:A:212:GLN:HB2	3:A:1954:PO4:O4	2.15	0.46
1:A:301:LYS:CE	9:A:7091:HOH:O	2.62	0.46
1:B:101:ILE:CD1	2:B:1950:BOG:H61	2.44	0.46
1:B:490:VAL:O	1:B:494:GLN:HB2	2.15	0.46
1:B:200:ARG:O	1:B:346:PRO:HD2	2.16	0.46
1:A:229:ILE:HD12	1:A:327:PRO:HB3	1.97	0.46
1:B:45:SER:HB2	4:B:600:FAD:C4X	2.46	0.46
1:B:317:ARG:CG	4:B:600:FAD:HM81	2.46	0.46
1:B:60:GLU:O	1:B:64:VAL:HG23	2.16	0.46
1:B:50:HIS:CE1	1:B:354:LYS:HE2	2.51	0.45
1:B:50:HIS:O	1:B:356:THR:HG21	2.15	0.45
1:B:92:ARG:HD2	1:B:299:HIS:CE1	2.51	0.45
1:A:93:PRO:HB3	2:A:1952:BOG:H3	1.98	0.45
1:B:360:LYS:HA	1:B:360:LYS:HD2	1.71	0.45
1:B:424:ASN:HB3	1:B:453:TYR:OH	2.15	0.45
1:A:30:LEU:HG	1:A:32:LEU:HD13	1.98	0.45
1:B:226:ILE:HD11	1:B:318:PRO:CB	2.46	0.45
1:A:404:ARG:NH2	1:B:162:LYS:O	2.50	0.45
1:B:395:ARG:CZ	1:B:419:ARG:HG2	2.47	0.45
1:B:332:ARG:HH11	5:B:7067:13P:P	2.40	0.45
5:B:7067:13P:H31	5:B:7067:13P:O3P	2.15	0.45
1:B:226:ILE:HD11	1:B:318:PRO:HB2	1.99	0.44
1:B:283:LYS:HB2	1:B:283:LYS:HE2	1.55	0.44
1:A:50:HIS:CE1	1:A:354:LYS:HZ3	2.34	0.44
1:B:60:GLU:OE1	1:B:331:THR:OG1	2.24	0.44
1:B:230:LYS:HD3	1:B:282:VAL:HG23	2.00	0.44
1:B:39:CYS:HA	1:B:469:ARG:HD3	2.00	0.44
1:B:120:SER:HA	1:B:140:GLU:O	2.16	0.44
1:B:193:LYS:HE2	1:B:195:TYR:CZ	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LYS:HA	1:B:162:LYS:HD2	1.71	0.43
1:B:370:THR:O	1:B:372:TYR:N	2.51	0.43
1:A:49:ILE:HD11	1:A:146:VAL:HB	2.00	0.43
1:A:360:LYS:HD2	1:A:360:LYS:HA	1.72	0.43
1:A:297:ASN:HD22	1:A:297:ASN:HA	1.67	0.43
4:A:600:FAD:HM83	4:A:600:FAD:HM71	1.83	0.43
1:A:161:ARG:HB2	6:A:1962:EDO:HO1	1.82	0.43
1:A:248:LEU:O	1:A:255:ILE:HA	2.17	0.43
1:B:334:TYR:OH	1:B:364:HIS:CD2	2.72	0.43
1:B:419:ARG:HH11	1:B:419:ARG:CG	2.31	0.43
1:A:444:HIS:HD2	1:A:473:GLN:OE1	2.02	0.43
1:A:64:VAL:O	1:A:68:LEU:HB2	2.19	0.43
1:B:233:HIS:CD2	1:B:269:GLY:HA3	2.53	0.43
1:A:318:PRO:O	1:A:352:GLY:HA2	2.19	0.43
1:A:129:SER:HB2	9:A:7108:HOH:O	2.19	0.42
1:A:106:PHE:CD2	1:A:106:PHE:C	2.97	0.42
1:B:6:LEU:HD11	1:B:203:VAL:HG23	2.01	0.42
1:A:403:ARG:NH1	1:A:409:LEU:O	2.45	0.42
1:B:129:SER:HB2	9:B:7094:HOH:O	2.19	0.42
1:A:57:GLU:CD	2:A:1950:BOG:O2	2.63	0.41
1:A:87:PHE:O	1:A:140:GLU:HA	2.19	0.41
1:B:232:SER:O	1:B:270:THR:CG2	2.68	0.41
1:B:248:LEU:O	1:B:255:ILE:HA	2.19	0.41
1:B:97:PRO:HB2	1:B:99:TRP:CD1	2.55	0.41
1:B:239:VAL:HG23	1:B:240:HIS:CD2	2.55	0.41
1:B:346:PRO:HG3	1:B:372:TYR:CG	2.55	0.41
1:A:92:ARG:HD3	1:A:95:LEU:HD12	2.03	0.41
1:A:484:ARG:HH11	1:A:487:GLN:CD	2.28	0.41
1:B:117:LEU:HD22	1:B:142:SER:HB3	2.03	0.41
1:A:12:GLY:CA	4:A:600:FAD:O2A	2.62	0.41
1:B:106:PHE:O	1:B:110:HIS:HD2	2.04	0.41
1:B:177:ARG:HD2	9:B:7105:HOH:O	2.20	0.41
1:B:45:SER:HA	4:B:600:FAD:C5X	2.51	0.41
1:A:45:SER:HA	4:A:600:FAD:C6	2.50	0.41
1:A:254:ARG:NH1	5:A:1955:13P:H12	2.31	0.41
1:A:247:ILE:HD13	1:A:247:ILE:HG21	1.87	0.41
1:A:428:LEU:C	1:A:428:LEU:HD23	2.45	0.41
1:B:114:ARG:O	1:B:114:ARG:CG	2.68	0.41
1:B:206:THR:HA	4:B:600:FAD:H52A	2.03	0.41
1:B:299:HIS:CE1	9:B:7078:HOH:O	2.70	0.41
1:A:259:ILE:HA	1:A:260:PRO:HD3	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ARG:HG2	1:B:321:ASP:CB	2.51	0.40
1:A:354:LYS:HB3	1:A:354:LYS:HE3	1.68	0.40
1:A:104:GLY:HA2	1:A:107:MET:HE3	2.02	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%)	471 (96%)	18 (4%)	3 (1%)	21	18
1	B	492/501 (98%)	462 (94%)	22 (4%)	8 (2%)	7	4
All	All	984/1002 (98%)	933 (95%)	40 (4%)	11 (1%)	11	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	A	374	GLN
1	B	113	LYS
1	B	118	PRO
1	B	325	ASP
1	B	374	GLN
1	B	396	ASP
1	B	226	ILE
1	B	120	SER
1	A	113	LYS
1	B	159	VAL

5.3.2 Protein sidechains ⓘ

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	413/419 (99%)	389 (94%)	24 (6%)	18	16
1	B	413/419 (99%)	383 (93%)	30 (7%)	13	10
All	All	826/838 (99%)	772 (94%)	54 (6%)	15	13

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	32	LEU
1	A	68	LEU
1	A	74	LEU
1	A	105	LEU
1	A	111	LEU
1	A	116	SER
1	A	121	THR
1	A	124	ARG
1	A	136	LYS
1	A	212	GLN
1	A	244	GLN
1	A	247	ILE
1	A	253	LYS
1	A	280	LYS
1	A	326	SER
1	A	354	LYS
1	A	355	LEU
1	A	392	GLU
1	A	404	ARG
1	A	427	LEU
1	A	478	ASN
1	A	483	SER
1	B	53	LEU
1	B	56	LEU
1	B	63	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	103	ILE
1	B	105	LEU
1	B	111	LEU
1	B	114	ARG
1	B	137	ARG
1	B	160	VAL
1	B	161	ARG
1	B	162	LYS
1	B	226	ILE
1	B	238	ARG
1	B	244	GLN
1	B	270	THR
1	B	276	LYS
1	B	280	LYS
1	B	283	LYS
1	B	298	THR
1	B	302	LYS
1	B	324	SER
1	B	332	ARG
1	B	366	LEU
1	B	376	ILE
1	B	392	GLU
1	B	394	ASP
1	B	395	ARG
1	B	413	LEU
1	B	419	ARG
1	B	420	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	50	HIS
1	A	110	HIS
1	A	128	ASN
1	A	198	GLN
1	A	212	GLN
1	A	242	GLN
1	A	250	ASN
1	A	297	ASN
1	A	444	HIS
1	A	478	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	482	GLN
1	B	50	HIS
1	B	110	HIS
1	B	155	ASN
1	B	212	GLN
1	B	244	GLN
1	B	249	GLN
1	B	290	ASN
1	B	299	HIS
1	B	364	HIS
1	B	424	ASN
1	B	457	HIS
1	B	473	GLN
1	B	487	GLN
1	B	494	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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
6	EDO	B	1954	-	3,3,3	0.73	0	2,2,2	1.47	1 (50%)
6	EDO	B	1956	-	3,3,3	0.46	0	2,2,2	0.25	0
6	EDO	B	1958	-	3,3,3	0.84	0	2,2,2	0.49	0
2	BOG	A	1952	-	20,20,20	0.85	1 (5%)	25,25,25	1.23	3 (12%)
2	BOG	B	1949	-	20,20,20	0.92	1 (5%)	25,25,25	1.27	2 (8%)
2	BOG	A	1950	-	20,20,20	0.47	0	25,25,25	0.59	0
6	EDO	A	1962	-	3,3,3	0.84	0	2,2,2	0.70	0
3	PO4	B	1952	-	4,4,4	0.76	0	6,6,6	1.17	1 (16%)
8	T3A	A	7066	-	14,14,14	2.42	1 (7%)	19,19,19	2.12	7 (36%)
3	PO4	A	1953	-	4,4,4	0.85	0	6,6,6	0.49	0
6	EDO	B	1959	-	3,3,3	0.45	0	2,2,2	0.43	0
5	13P	B	7067	-	9,9,9	4.33	6 (66%)	10,12,12	3.70	4 (40%)
2	BOG	B	1950	-	20,20,20	0.61	0	25,25,25	1.30	3 (12%)
6	EDO	A	1956	-	3,3,3	0.68	0	2,2,2	0.41	0
6	EDO	B	1957	-	3,3,3	0.96	0	2,2,2	0.73	0
7	IMD	B	1960	-	5,5,5	0.79	0	5,5,5	0.16	0
2	BOG	A	1949	-	20,20,20	0.99	1 (5%)	25,25,25	1.74	6 (24%)
6	EDO	B	1955	-	3,3,3	0.82	0	2,2,2	1.41	0
6	EDO	A	1961	-	3,3,3	0.62	0	2,2,2	0.58	0
6	EDO	A	1959	-	3,3,3	0.52	0	2,2,2	0.54	0
4	FAD	B	600	-	58,58,58	1.11	5 (8%)	85,89,89	1.86	16 (18%)
6	EDO	A	1960	-	3,3,3	0.50	0	2,2,2	0.09	0
2	BOG	A	1951	-	20,20,20	0.99	1 (5%)	25,25,25	0.92	1 (4%)
7	IMD	A	1957	-	5,5,5	0.77	0	5,5,5	0.44	0
3	PO4	B	1953	-	4,4,4	0.87	0	6,6,6	0.55	0
3	PO4	B	1951	-	4,4,4	1.10	0	6,6,6	0.54	0
5	13P	A	1955	-	9,9,9	4.46	6 (66%)	10,12,12	4.00	4 (40%)
6	EDO	A	1958	-	3,3,3	1.09	0	2,2,2	0.48	0
3	PO4	A	1954	-	4,4,4	0.92	0	6,6,6	0.82	0
6	EDO	B	1961	-	3,3,3	0.70	0	2,2,2	0.74	0
4	FAD	A	600	-	58,58,58	1.45	6 (10%)	85,89,89	1.71	17 (20%)
8	T3A	B	7066	-	14,14,14	2.35	1 (7%)	19,19,19	2.21	9 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	1954	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	1956	-	-	0/1/1/1	-
6	EDO	B	1958	-	-	0/1/1/1	-
2	BOG	A	1952	-	-	7/11/31/31	0/1/1/1
2	BOG	B	1949	-	-	3/11/31/31	0/1/1/1
2	BOG	A	1950	-	-	7/11/31/31	0/1/1/1
6	EDO	A	1962	-	-	1/1/1/1	-
8	T3A	A	7066	-	-	2/18/18/18	-
6	EDO	B	1959	-	-	1/1/1/1	-
5	13P	B	7067	-	-	7/8/8/8	-
2	BOG	B	1950	-	-	6/11/31/31	0/1/1/1
6	EDO	A	1956	-	-	1/1/1/1	-
6	EDO	B	1957	-	-	1/1/1/1	-
7	IMD	B	1960	-	-	-	0/1/1/1
2	BOG	A	1949	-	-	5/11/31/31	0/1/1/1
6	EDO	B	1955	-	-	1/1/1/1	-
6	EDO	A	1961	-	-	1/1/1/1	-
6	EDO	A	1959	-	-	1/1/1/1	-
4	FAD	B	600	-	-	7/34/50/50	0/6/6/6
6	EDO	A	1960	-	-	1/1/1/1	-
2	BOG	A	1951	-	-	6/11/31/31	0/1/1/1
7	IMD	A	1957	-	-	-	0/1/1/1
5	13P	A	1955	-	-	7/8/8/8	-
6	EDO	A	1958	-	-	1/1/1/1	-
6	EDO	B	1961	-	-	1/1/1/1	-
4	FAD	A	600	-	1/1/9/9	4/34/50/50	0/6/6/6
8	T3A	B	7066	-	-	6/18/18/18	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	7066	T3A	C1-S1	-8.38	1.65	1.77
5	B	7067	13P	O1-C1	8.37	1.51	1.43
8	B	7066	T3A	C1-S1	-8.34	1.65	1.77
5	A	1955	13P	O1-C1	8.01	1.51	1.43
4	A	600	FAD	O2B-C2B	-7.20	1.25	1.43
5	A	1955	13P	O2-C2	6.43	1.33	1.21
5	B	7067	13P	C1-C2	5.91	1.61	1.50
5	B	7067	13P	O2-C2	5.66	1.31	1.21
5	A	1955	13P	C1-C2	5.62	1.61	1.50
5	A	1955	13P	C3-C2	4.17	1.61	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	7067	13P	C3-C2	3.70	1.59	1.50
4	A	600	FAD	C4X-N5	3.58	1.38	1.30
4	B	600	FAD	C4X-N5	3.57	1.38	1.30
5	A	1955	13P	O3-C3	3.51	1.53	1.41
2	B	1949	BOG	O1-C1	3.29	1.45	1.40
2	A	1951	BOG	O1-C1	3.18	1.45	1.40
5	B	7067	13P	O3-C3	2.95	1.51	1.41
2	A	1949	BOG	O1-C1	2.73	1.44	1.40
5	B	7067	13P	P-O1	2.69	1.68	1.60
4	A	600	FAD	C10-N1	2.63	1.38	1.33
2	A	1952	BOG	O1-C1	2.61	1.44	1.40
4	B	600	FAD	C10-N1	2.60	1.38	1.33
4	B	600	FAD	C2A-N3A	2.58	1.38	1.33
4	A	600	FAD	C2A-N3A	2.56	1.38	1.33
4	B	600	FAD	C2A-N1A	2.56	1.38	1.33
4	A	600	FAD	C2A-N1A	2.55	1.38	1.33
5	A	1955	13P	P-O1	2.47	1.68	1.60
4	B	600	FAD	C8A-N7A	2.10	1.35	1.31
4	A	600	FAD	C8A-N7A	2.07	1.35	1.31

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	FAD	O2B-C2B-C3B	9.23	141.40	111.82
5	A	1955	13P	O3P-P-O1	-8.89	83.49	106.67
5	B	7067	13P	O3P-P-O1	-8.02	85.75	106.67
5	B	7067	13P	O2P-P-O1	6.44	123.47	106.67
5	A	1955	13P	O2P-P-O1	6.28	123.04	106.67
4	A	600	FAD	N3A-C2A-N1A	-5.51	120.24	128.58
4	B	600	FAD	N3A-C2A-N1A	-5.51	120.24	128.58
4	A	600	FAD	O2B-C2B-C3B	5.20	128.47	111.82
8	A	7066	T3A	C3-N1-C4	5.13	123.67	116.17
4	A	600	FAD	C5A-C4A-N3A	-4.65	120.31	126.72
4	B	600	FAD	C5A-C4A-N3A	-4.64	120.33	126.72
5	A	1955	13P	O1-P-O1P	-4.55	94.16	106.44
5	B	7067	13P	O3P-P-O1P	4.46	128.20	110.83
8	B	7066	T3A	C3-N1-C4	4.40	122.61	116.17
2	B	1949	BOG	O1-C1-C2	4.21	114.66	108.27
5	A	1955	13P	O3P-P-O1P	4.20	127.20	110.83
2	A	1949	BOG	C1'-O1-C1	4.12	120.72	113.68
4	B	600	FAD	N9A-C8A-N7A	-3.81	108.53	113.94
4	A	600	FAD	N9A-C8A-N7A	-3.77	108.58	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	7066	T3A	O1-S1-C1	3.77	112.43	106.73
4	A	600	FAD	O2B-C2B-C1B	3.72	122.91	110.10
2	A	1949	BOG	C1-O5-C5	3.62	120.78	113.72
8	A	7066	T3A	C2-C1-S1	-3.55	107.81	113.25
2	A	1952	BOG	O5-C5-C4	3.54	116.08	109.70
4	B	600	FAD	C2A-N3A-C4A	3.45	120.26	111.83
4	A	600	FAD	C2A-N3A-C4A	3.45	120.25	111.83
4	A	600	FAD	C5A-N7A-C8A	3.36	108.73	103.45
4	B	600	FAD	C5A-N7A-C8A	3.34	108.71	103.45
8	B	7066	T3A	O3-S1-C1	3.30	112.46	106.00
2	B	1950	BOG	C1-C2-C3	3.18	116.71	110.01
4	B	600	FAD	C4-N3-C2	-3.13	120.09	125.64
4	A	600	FAD	N3A-C4A-N9A	3.13	132.48	127.17
4	B	600	FAD	N3A-C4A-N9A	3.12	132.47	127.17
4	A	600	FAD	C4-N3-C2	-3.10	120.14	125.64
8	B	7066	T3A	C2-C1-S1	-2.93	108.76	113.25
8	A	7066	T3A	C5-C4-N1	-2.84	100.55	109.02
8	A	7066	T3A	C6-C4-C5	2.77	116.09	110.02
2	A	1952	BOG	C4-C3-C2	-2.76	105.98	110.83
4	A	600	FAD	C4X-C4-N3	2.62	119.92	113.25
4	B	600	FAD	C4X-C4-N3	2.60	119.88	113.25
2	A	1949	BOG	O1-C1-C2	-2.60	104.32	108.27
8	B	7066	T3A	O3-S1-O2	-2.58	104.94	111.40
5	B	7067	13P	O1-P-O1P	-2.52	99.63	106.44
4	A	600	FAD	C4X-C10-N10	2.52	120.08	116.48
8	A	7066	T3A	O1-S1-C1	2.48	110.47	106.73
8	A	7066	T3A	C7-C4-N1	2.48	116.41	109.02
4	B	600	FAD	C4X-C10-N10	2.47	120.02	116.48
4	A	600	FAD	O4-C4-C4X	-2.47	120.02	126.53
2	B	1950	BOG	C3-C4-C5	-2.45	105.79	110.23
4	B	600	FAD	O4-C4-C4X	-2.44	120.09	126.53
2	A	1949	BOG	C1-C2-C3	2.39	115.04	110.01
2	A	1951	BOG	O1-C1-C2	2.36	111.86	108.27
4	A	600	FAD	C10-C4X-N5	-2.35	120.01	124.81
8	A	7066	T3A	O3-S1-C1	2.33	110.57	106.00
4	A	600	FAD	C9A-C5X-N5	-2.33	119.98	122.45
4	A	600	FAD	C3B-C2B-C1B	2.32	105.86	101.46
4	B	600	FAD	C3B-C2B-C1B	2.32	105.85	101.46
4	A	600	FAD	C4A-C5A-N7A	-2.32	107.93	110.58
4	B	600	FAD	C10-C4X-N5	-2.31	120.08	124.81
4	A	600	FAD	C5X-C9A-N10	2.31	120.06	117.97
2	B	1950	BOG	O4-C4-C5	2.31	115.01	109.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	FAD	C4A-C5A-N7A	-2.28	107.97	110.58
4	B	600	FAD	C5X-C9A-N10	2.27	120.02	117.97
4	B	600	FAD	C9A-C5X-N5	-2.27	120.05	122.45
2	A	1949	BOG	O6-C6-C5	2.23	118.94	111.33
2	A	1949	BOG	C3-C4-C5	2.19	114.21	110.23
8	B	7066	T3A	O2-S1-C1	2.16	110.00	106.73
3	B	1952	PO4	O3-P-O2	2.13	114.55	107.91
2	B	1949	BOG	O5-C5-C6	2.13	111.71	106.44
8	B	7066	T3A	C3-C2-C1	-2.13	105.93	112.72
8	B	7066	T3A	C7-C4-C6	-2.10	105.41	110.02
2	A	1952	BOG	C1-O5-C5	2.10	117.81	113.72
6	B	1954	EDO	O1-C1-C2	-2.06	96.68	112.39
8	B	7066	T3A	C6-C4-C5	2.02	114.45	110.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	600	FAD	C2B

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	FAD	C5B-O5B-PA-O2A
4	A	600	FAD	C5B-O5B-PA-O3P
4	A	600	FAD	C4B-C5B-O5B-PA
4	B	600	FAD	C5B-O5B-PA-O1A
4	B	600	FAD	C5B-O5B-PA-O2A
4	B	600	FAD	C5B-O5B-PA-O3P
4	B	600	FAD	O4B-C4B-C5B-O5B
5	A	1955	13P	C1-O1-P-O2P
5	A	1955	13P	C1-O1-P-O3P
5	A	1955	13P	C2-C1-O1-P
5	A	1955	13P	O1-C1-C2-O2
5	A	1955	13P	C1-C2-C3-O3
5	A	1955	13P	O2-C2-C3-O3
5	B	7067	13P	C1-O1-P-O1P
5	B	7067	13P	C1-O1-P-O2P
5	B	7067	13P	C1-O1-P-O3P
5	B	7067	13P	C2-C1-O1-P
5	B	7067	13P	O1-C1-C2-O2
5	B	7067	13P	C1-C2-C3-O3
5	B	7067	13P	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	B	7066	T3A	N1-C4-C5-O5
8	B	7066	T3A	C6-C4-C5-O5
8	B	7066	T3A	C7-C4-C5-O5
8	B	7066	T3A	N1-C4-C6-O6
8	B	7066	T3A	C5-C4-C6-O6
4	B	600	FAD	C3B-C4B-C5B-O5B
2	B	1949	BOG	C3'-C4'-C5'-C6'
2	A	1952	BOG	C2'-C1'-O1-C1
2	A	1951	BOG	C3'-C4'-C5'-C6'
2	B	1949	BOG	C4'-C5'-C6'-C7'
2	A	1949	BOG	C1'-C2'-C3'-C4'
2	A	1951	BOG	C2'-C3'-C4'-C5'
2	B	1950	BOG	C3'-C4'-C5'-C6'
6	A	1956	EDO	O1-C1-C2-O2
6	A	1962	EDO	O1-C1-C2-O2
6	B	1954	EDO	O1-C1-C2-O2
6	B	1959	EDO	O1-C1-C2-O2
2	A	1952	BOG	C3'-C4'-C5'-C6'
2	A	1950	BOG	O5-C1-O1-C1'
2	A	1950	BOG	C3'-C4'-C5'-C6'
2	A	1950	BOG	C4-C5-C6-O6
2	A	1951	BOG	C1'-C2'-C3'-C4'
2	A	1952	BOG	O1-C1'-C2'-C3'
2	A	1952	BOG	C4'-C5'-C6'-C7'
2	A	1952	BOG	C2'-C3'-C4'-C5'
2	A	1949	BOG	O1-C1'-C2'-C3'
2	A	1949	BOG	C3'-C4'-C5'-C6'
2	B	1949	BOG	C2'-C3'-C4'-C5'
2	A	1951	BOG	O1-C1'-C2'-C3'
2	A	1950	BOG	C2-C1-O1-C1'
6	B	1955	EDO	O1-C1-C2-O2
6	B	1961	EDO	O1-C1-C2-O2
5	A	1955	13P	C1-O1-P-O1P
2	A	1951	BOG	C5'-C6'-C7'-C8'
2	B	1950	BOG	C2'-C1'-O1-C1
2	A	1949	BOG	O5-C5-C6-O6
2	A	1950	BOG	O5-C5-C6-O6
6	A	1959	EDO	O1-C1-C2-O2
2	A	1949	BOG	C5'-C6'-C7'-C8'
2	B	1950	BOG	C2'-C3'-C4'-C5'
4	B	600	FAD	C4B-C5B-O5B-PA
4	B	600	FAD	PA-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	600	FAD	C5B-O5B-PA-O1A
2	B	1950	BOG	C2-C1-O1-C1'
8	A	7066	T3A	C5-C4-C7-O7
6	A	1960	EDO	O1-C1-C2-O2
2	A	1951	BOG	C2'-C1'-O1-C1
2	A	1950	BOG	C5'-C6'-C7'-C8'
2	A	1950	BOG	C1'-C2'-C3'-C4'
8	B	7066	T3A	C7-C4-C6-O6
6	A	1958	EDO	O1-C1-C2-O2
6	A	1961	EDO	O1-C1-C2-O2
2	A	1952	BOG	C1'-C2'-C3'-C4'
8	A	7066	T3A	N1-C4-C7-O7
2	A	1952	BOG	C5'-C6'-C7'-C8'
2	B	1950	BOG	O5-C1-O1-C1'
2	B	1950	BOG	O1-C1'-C2'-C3'
6	B	1957	EDO	O1-C1-C2-O2

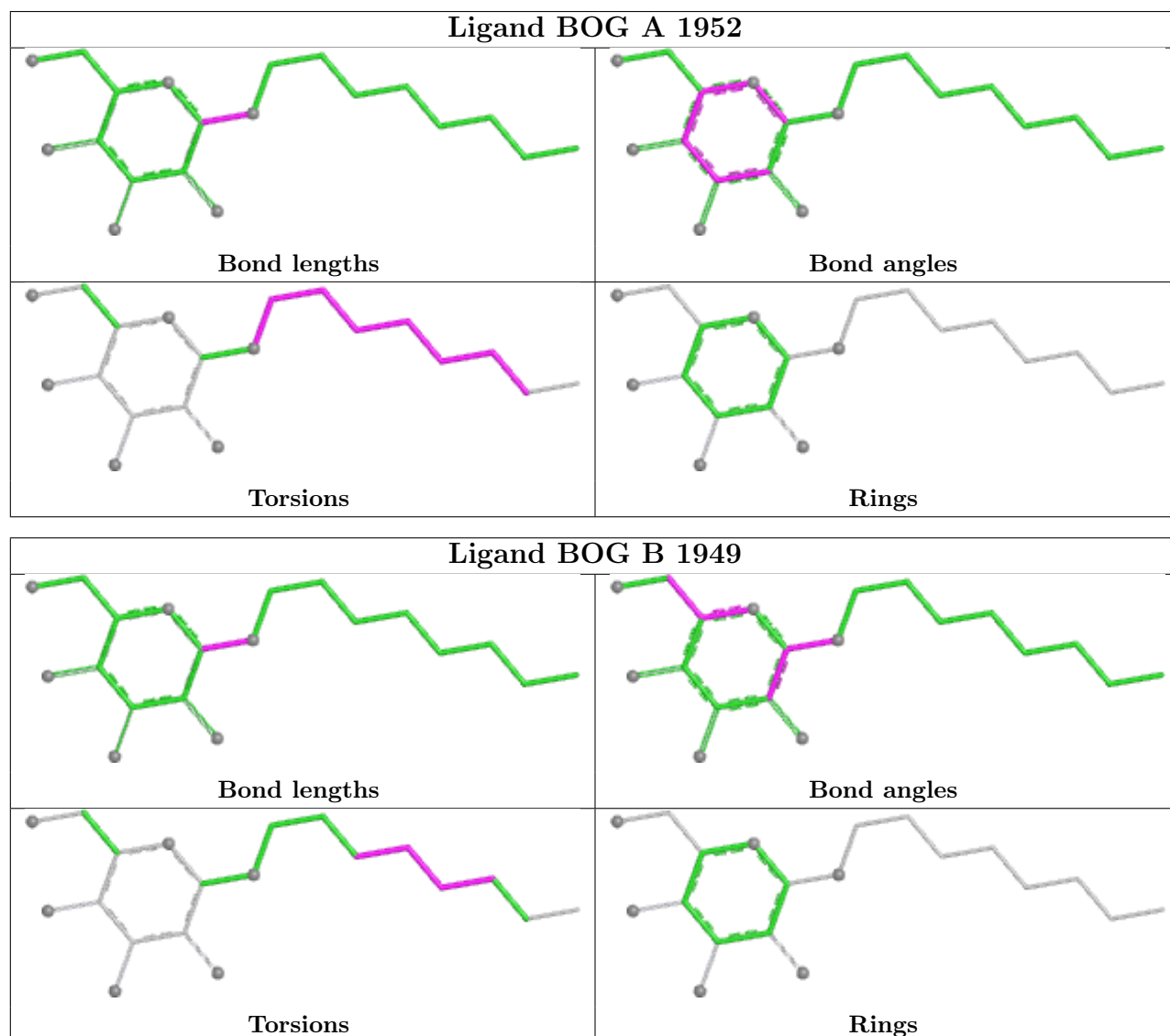
There are no ring outliers.

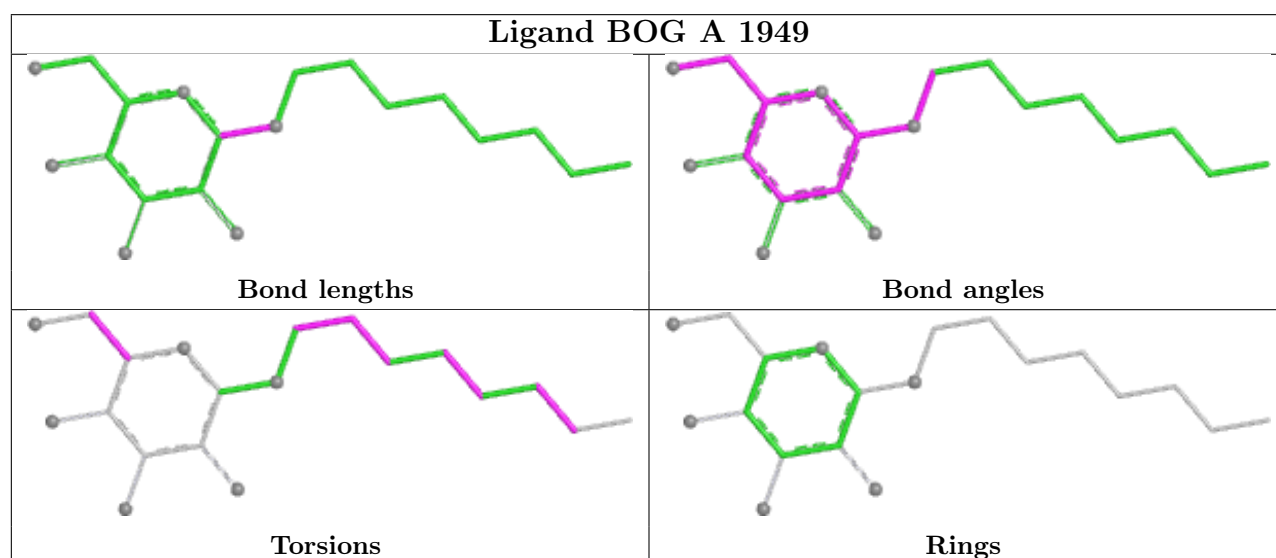
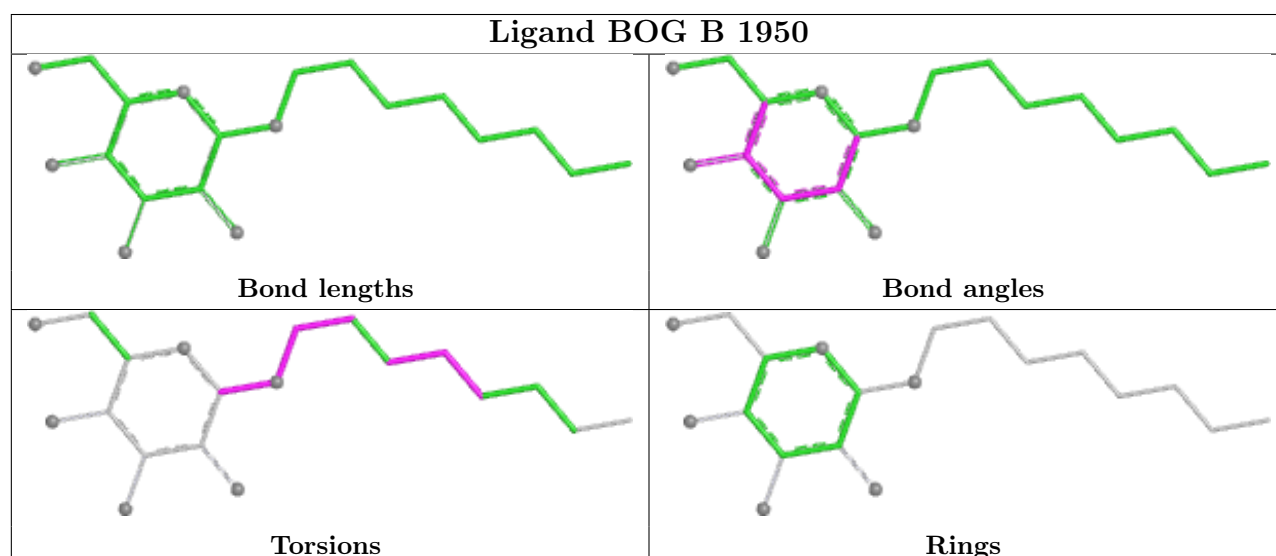
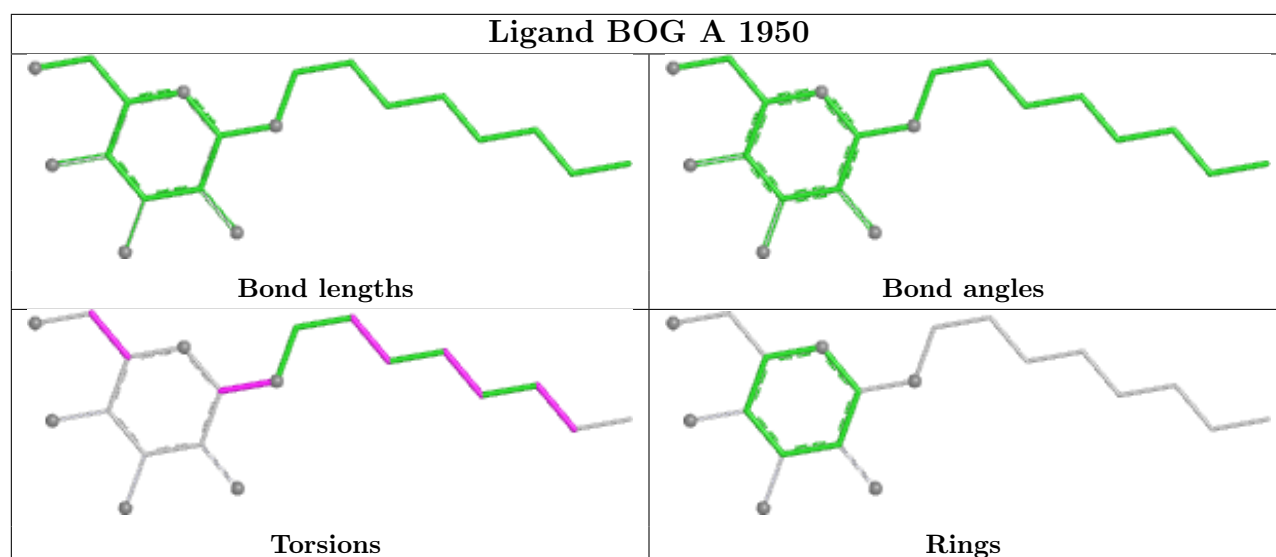
19 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1952	BOG	3	0
2	B	1949	BOG	1	0
2	A	1950	BOG	6	0
6	A	1962	EDO	3	0
3	B	1952	PO4	1	0
8	A	7066	T3A	1	0
6	B	1959	EDO	1	0
5	B	7067	13P	4	0
2	B	1950	BOG	2	0
6	A	1956	EDO	1	0
2	A	1949	BOG	4	0
4	B	600	FAD	7	0
7	A	1957	IMD	1	0
3	B	1951	PO4	1	0
5	A	1955	13P	3	0
3	A	1954	PO4	1	0
6	B	1961	EDO	3	0
4	A	600	FAD	8	0
8	B	7066	T3A	1	0

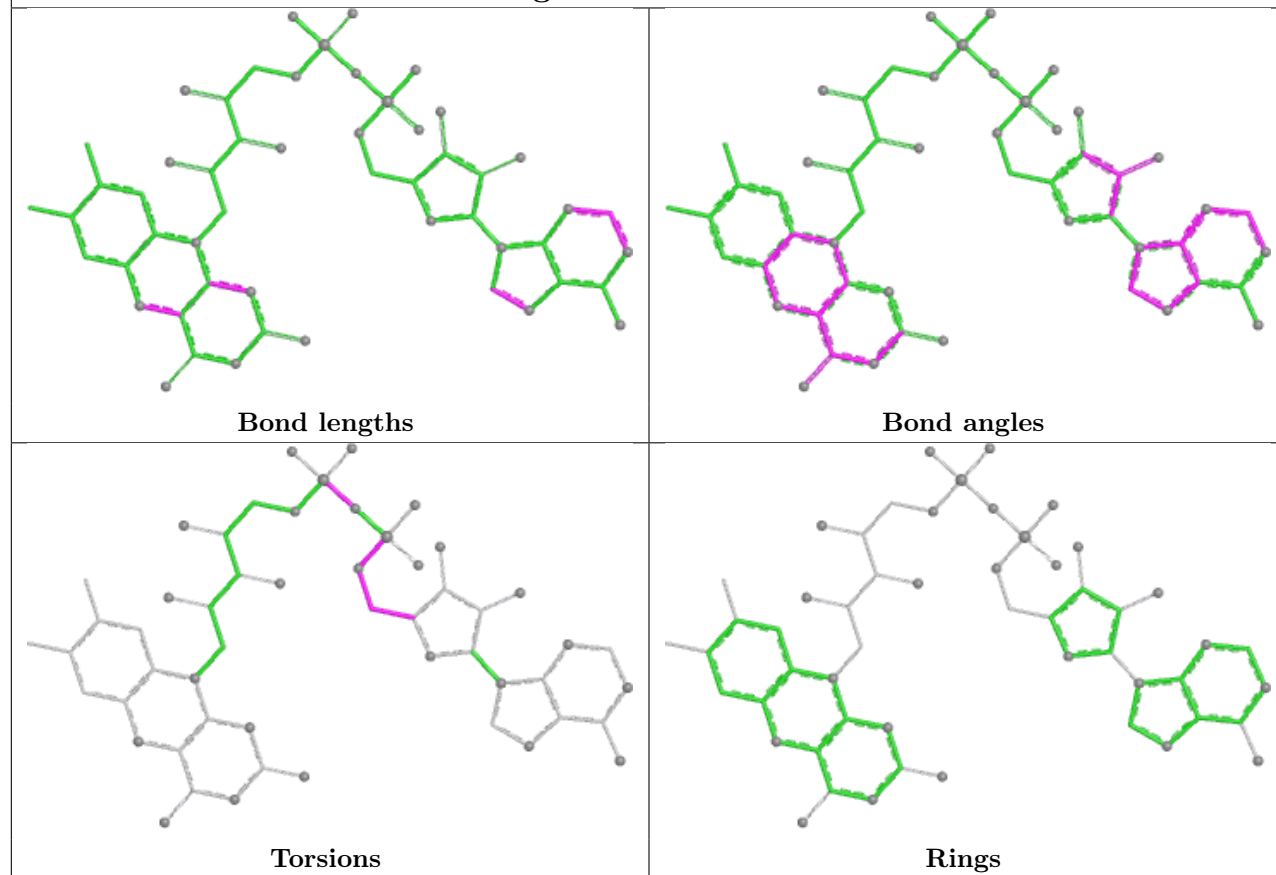
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

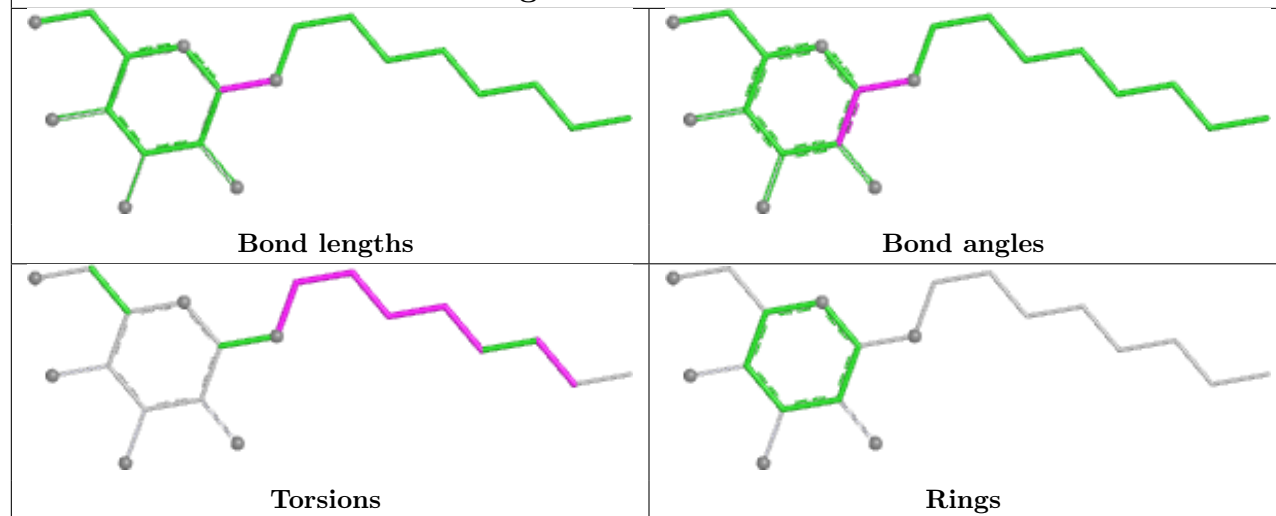


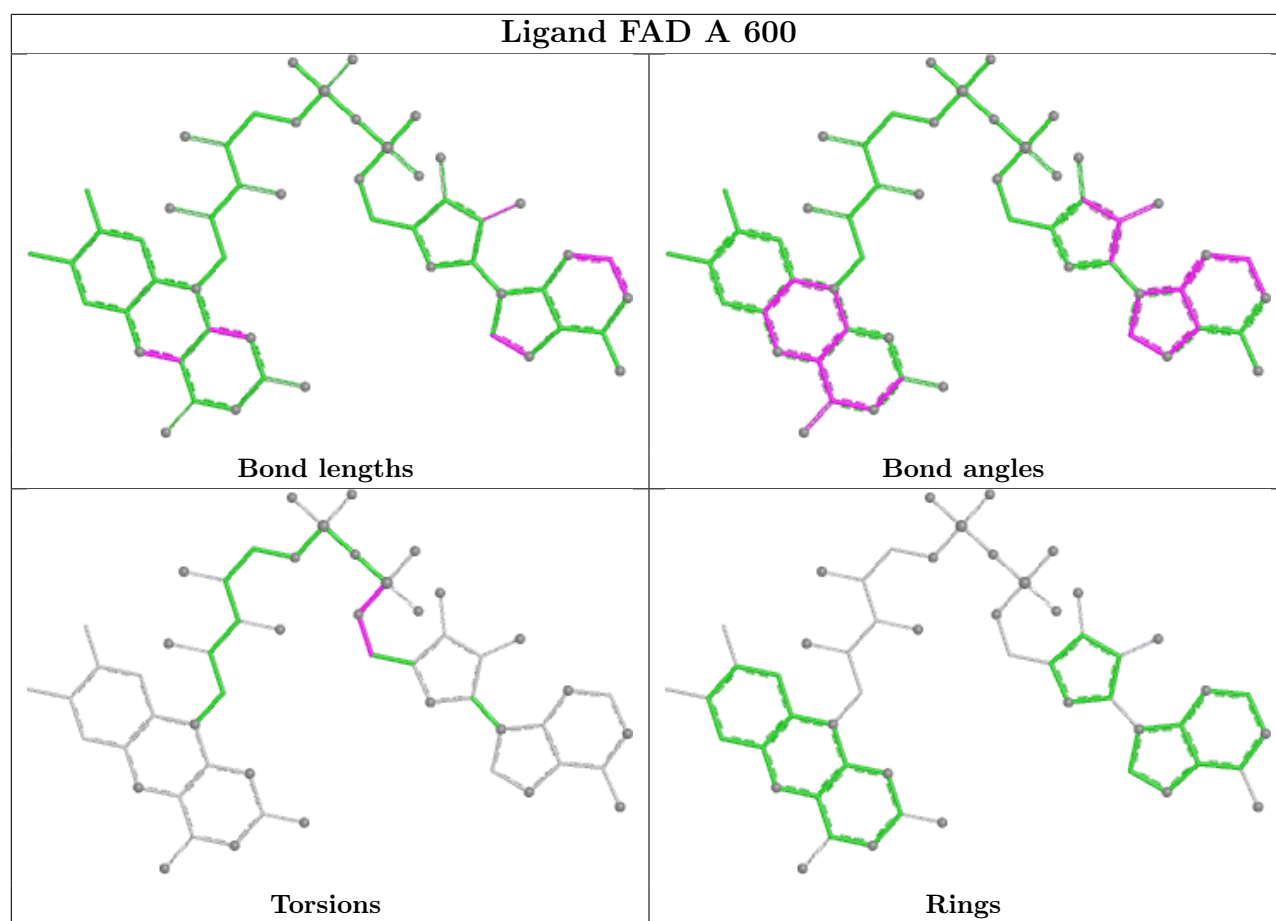


Ligand FAD B 600



Ligand BOG A 1951





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	494/501 (98%)	-1.52	0 100 100	16, 33, 53, 78	0
1	B	494/501 (98%)	-1.53	0 100 100	16, 33, 53, 75	0
All	All	988/1002 (98%)	-1.52	0 100 100	16, 33, 53, 78	0

There are no RSRZ outliers to report.

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 oligosaccharides 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	1950	20/20	0.97	0.09	110,112,114,114	0
2	BOG	A	1952	20/20	0.97	0.06	103,105,106,106	0
3	PO4	B	1953	5/5	0.97	0.05	109,109,109,110	0
6	EDO	B	1959	4/4	0.97	0.04	55,57,57,58	0
2	BOG	B	1949	20/20	0.98	0.03	60,66,69,70	0
2	BOG	B	1950	20/20	0.98	0.06	116,117,119,119	0
3	PO4	A	1953	5/5	0.98	0.06	92,92,93,93	0

Continued on next page...

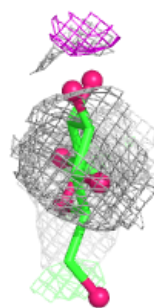
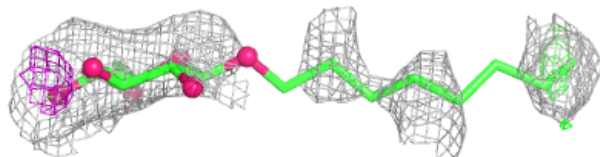
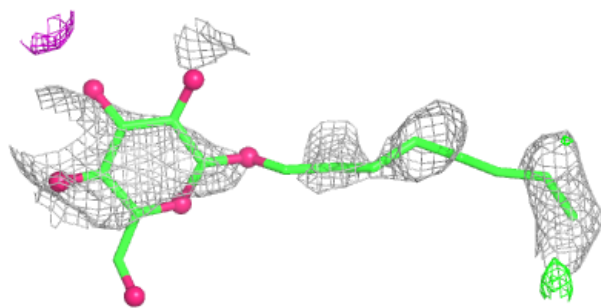
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BOG	A	1951	20/20	0.98	0.04	92,95,97,97	0
6	EDO	A	1956	4/4	0.98	0.04	50,50,52,53	0
6	EDO	A	1961	4/4	0.98	0.05	52,57,57,59	0
6	EDO	A	1962	4/4	0.98	0.04	43,44,45,50	0
6	EDO	B	1956	4/4	0.98	0.03	42,44,44,49	0
6	EDO	B	1957	4/4	0.98	0.04	25,35,38,40	0
6	EDO	B	1958	4/4	0.98	0.04	48,50,51,53	0
2	BOG	A	1949	20/20	0.98	0.04	58,64,73,74	0
3	PO4	B	1951	5/5	0.99	0.06	75,76,77,78	0
6	EDO	A	1958	4/4	0.99	0.03	24,33,36,38	0
6	EDO	A	1959	4/4	0.99	0.03	38,44,44,47	0
6	EDO	A	1960	4/4	0.99	0.04	35,41,44,49	0
3	PO4	B	1952	5/5	0.99	0.04	70,71,75,75	0
3	PO4	A	1954	5/5	0.99	0.04	70,71,74,76	0
6	EDO	B	1954	4/4	0.99	0.03	35,39,40,44	0
6	EDO	B	1955	4/4	0.99	0.04	57,58,60,61	0
4	FAD	A	600	53/53	0.99	0.03	17,20,24,35	0
4	FAD	B	600	53/53	0.99	0.03	15,19,22,25	0
5	13P	A	1955	10/10	0.99	0.04	28,38,43,44	0
5	13P	B	7067	10/10	0.99	0.04	28,40,45,45	0
6	EDO	B	1961	4/4	0.99	0.04	46,47,47,50	0
7	IMD	A	1957	5/5	0.99	0.04	59,60,61,62	0
7	IMD	B	1960	5/5	0.99	0.03	59,59,62,62	0
8	T3A	A	7066	15/15	0.99	0.03	23,37,44,49	0
8	T3A	B	7066	15/15	0.99	0.04	24,39,45,47	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.

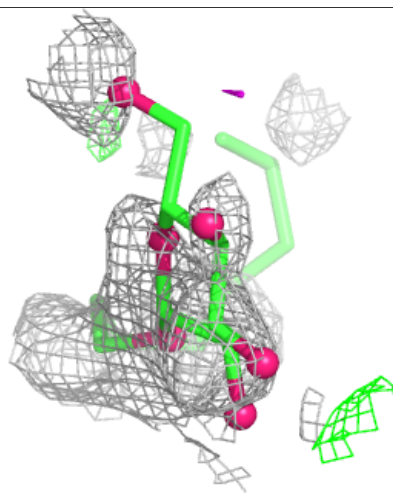
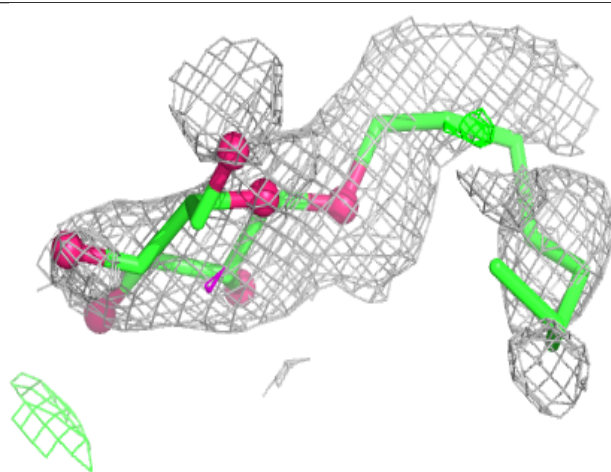
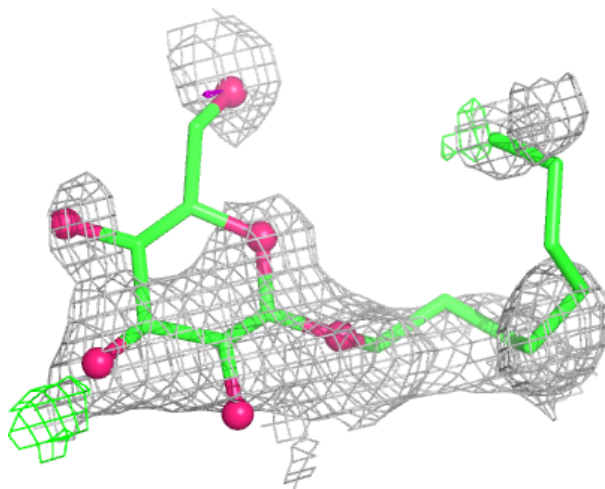
Electron density around BOG A 1950:

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



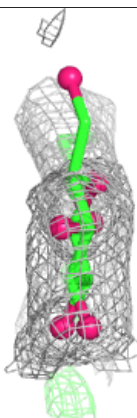
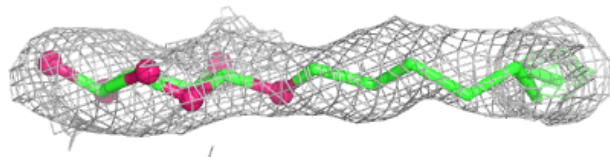
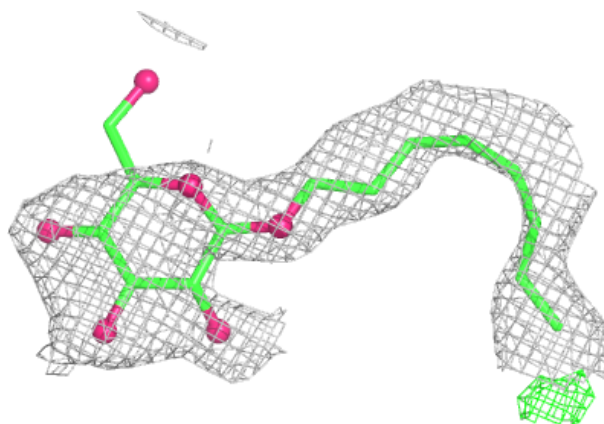
Electron density around BOG A 1952:

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

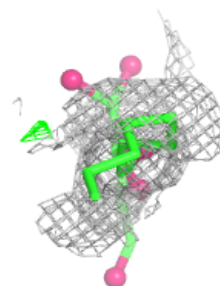
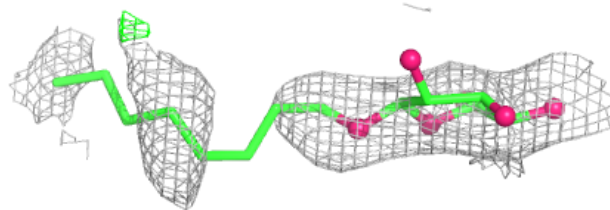
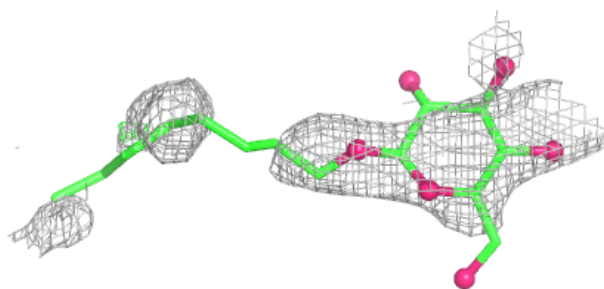


Electron density around BOG B 1949:

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

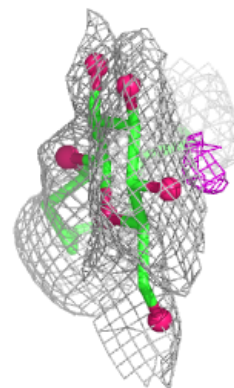
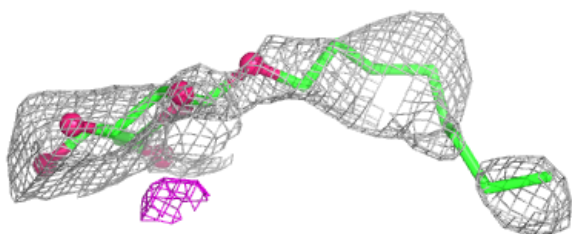
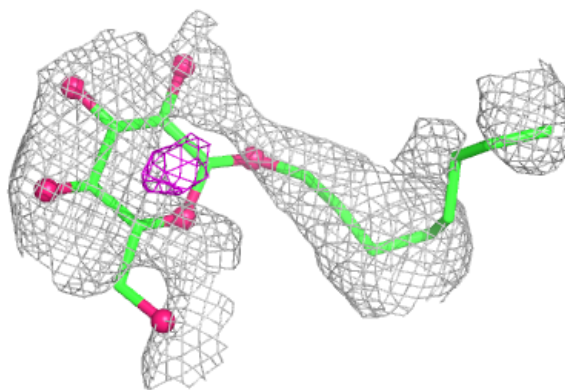
**Electron density around BOG B 1950:**

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

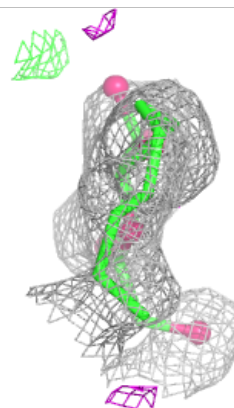
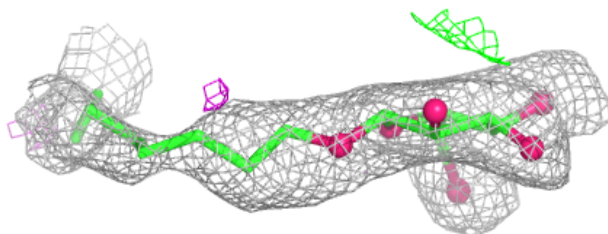
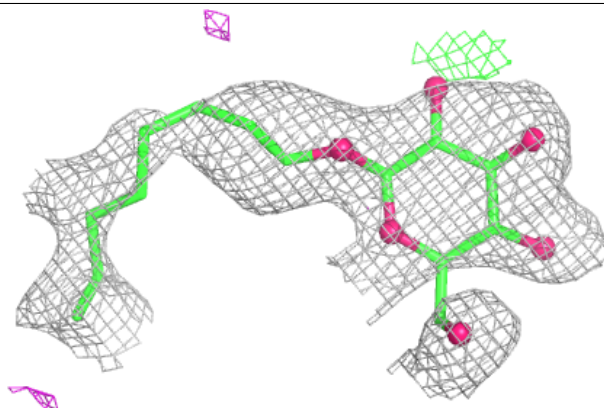


Electron density around BOG A 1951:

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

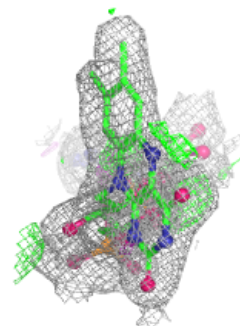
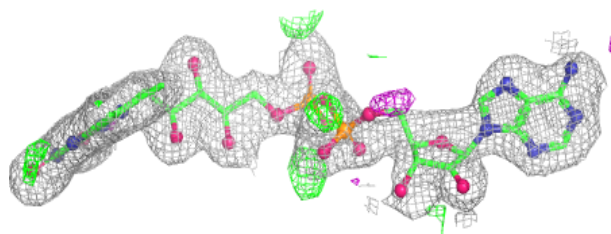
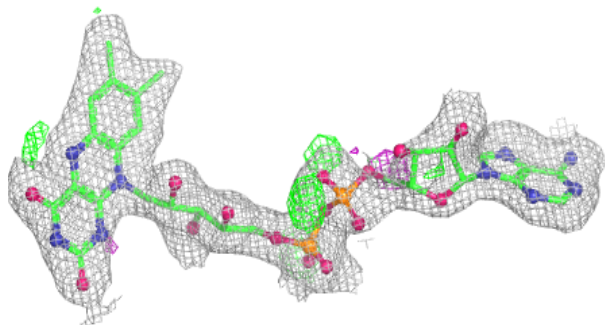
**Electron density around BOG A 1949:**

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

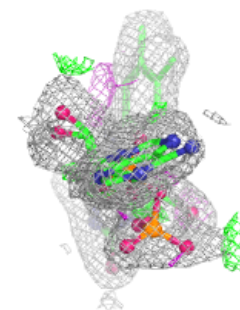
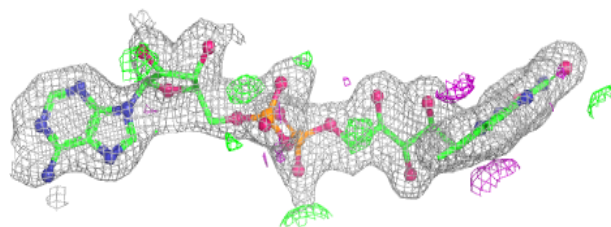
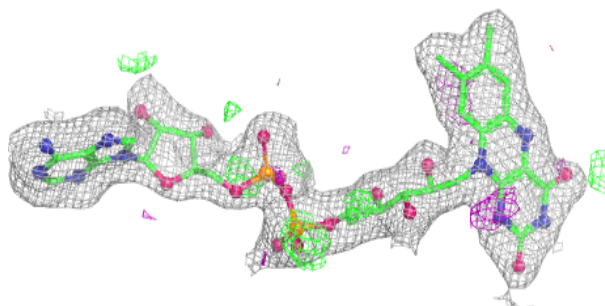


Electron density around FAD A 600:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.