Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 02:32 PM EST

PDB ID	:	2R45
Title	:	Crystal structure of Escherichia coli Glycerol-3-phosphate Dehydrogenase in complex with 2-phospho-d-glyceric acid
Authors	:	Yeh, J.I.; Du, S.; Chinte, U.
Deposited on	:	2007-08-30
Resolution	:	2.30 Å(reported)

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

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

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

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

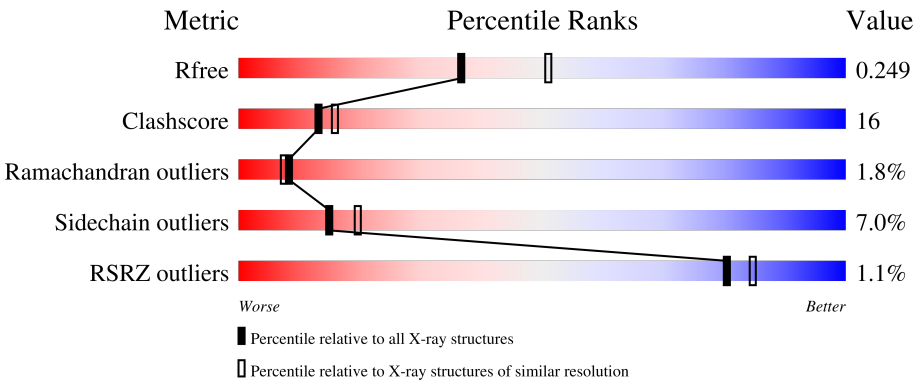
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	% 71% 24% • ••
1	B	501	% 72% 22% 5% •

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	800	-	-	-	X
8	2PG	A	700	X	X	X	-
8	2PG	B	700	X	-	X	-

2 Entry composition (i)

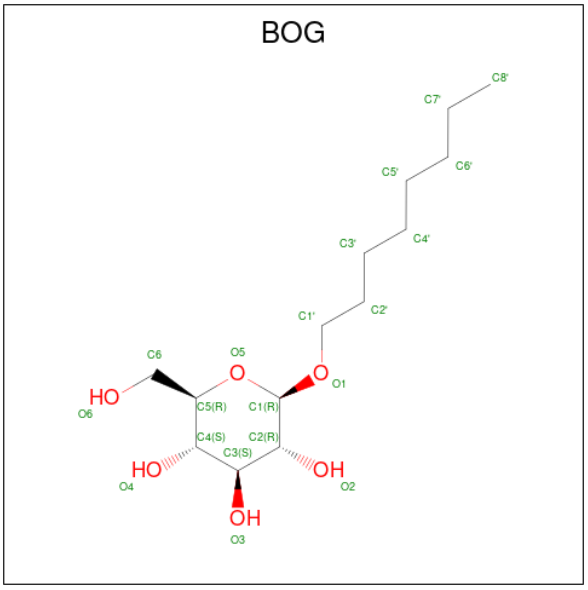
There are 9 unique types of molecules in this entry. The entry contains 8627 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			
1	A	495	3962	2515	705	729	13	0	0	0
1	B	495	3962	2515	705	729	13	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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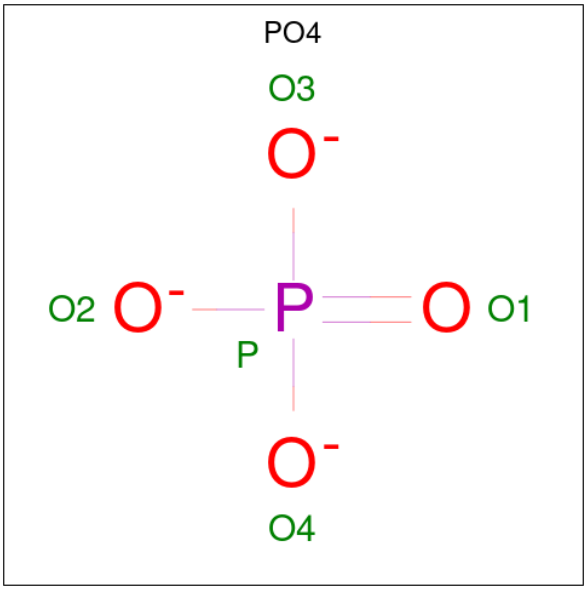
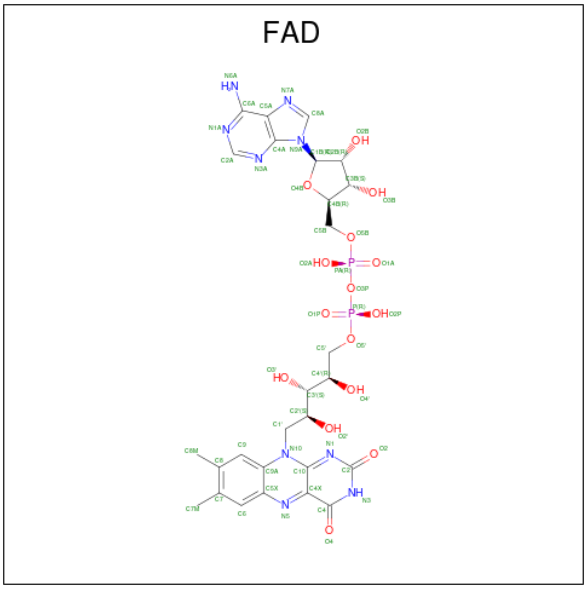
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	20	14	6	0	0
			Total	C	O		
2	B	1	20	14	6	0	0

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



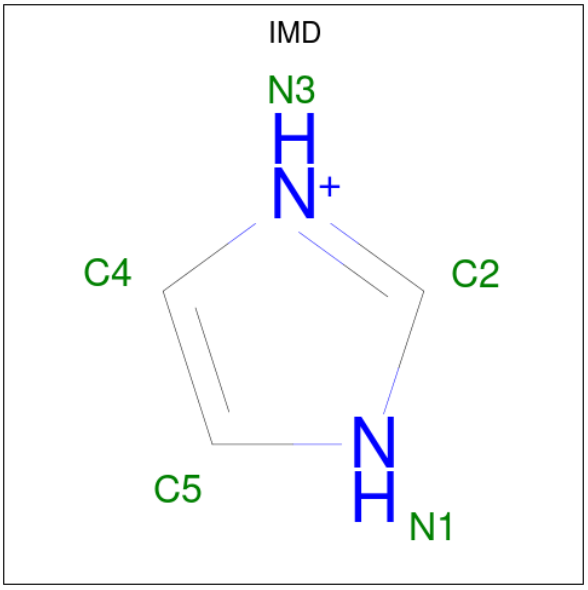
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O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

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



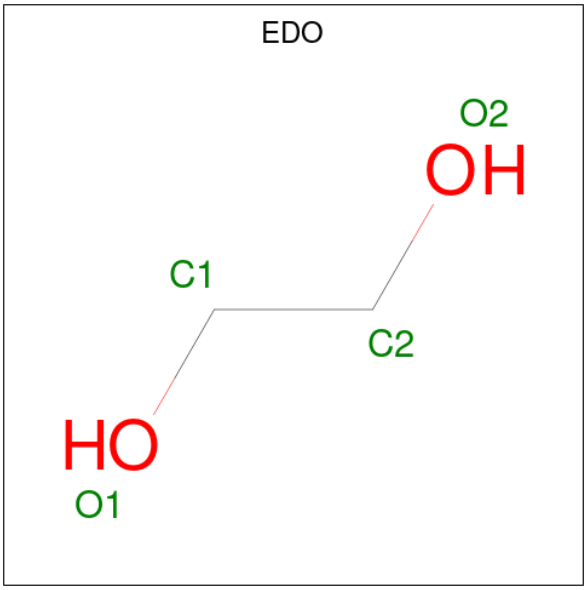
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
4	B	1	53	27	9	15	2	0	0

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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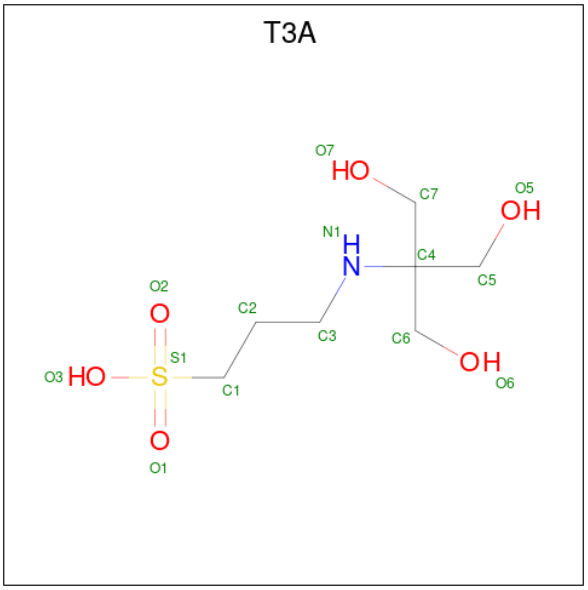
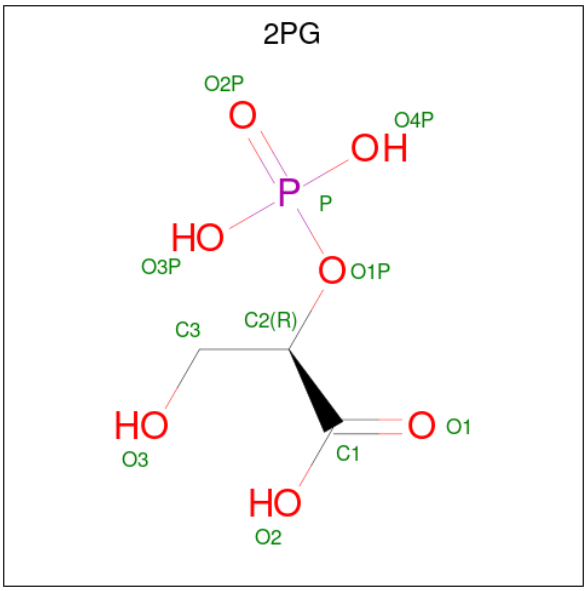
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0

- Molecule 7 is N-(TRIS(HYDROXYMETHYL)METHYL)-3-AMINOPROPANESULFONIC ACID (three-letter code: T3A) (formula: $C_7H_{17}NO_6S$).



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

- Molecule 8 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
8	A	1	11	3	7	1	0	0
			Total	C	O	P		
8	B	1	11	3	7	1	0	0

- Molecule 9 is water.

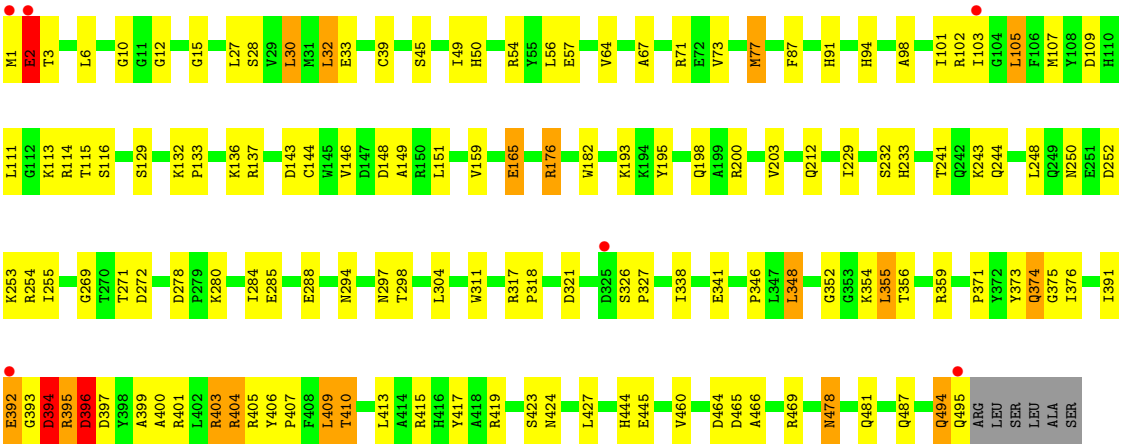
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	152	152	152	0	0
			Total	O		
9	B	153	153	153	0	0

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.

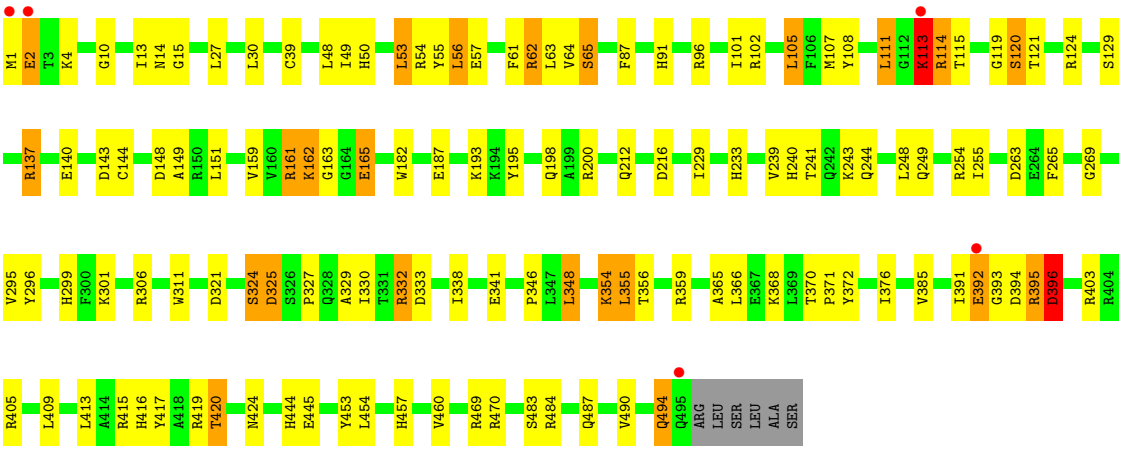
• Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase

Chain A:



• Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	113.74Å 113.91Å 193.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 9.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (10.00-2.30) 98.1 (9.99-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.270 0.186 , 0.249	Depositor DCC
R_{free} test set	2754 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 26.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.478 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8627	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, PO4, EDO, T3A, IMD, 2PG, 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	1.20	1/4057 (0.0%)	1.03	9/5494 (0.2%)
1	B	1.20	3/4057 (0.1%)	1.06	7/5494 (0.1%)
All	All	1.20	4/8114 (0.0%)	1.04	16/10988 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	417	TYR	CE1-CZ	5.89	1.46	1.38
1	B	265	PHE	CD1-CE1	5.75	1.50	1.39
1	A	417	TYR	CD2-CE2	5.51	1.47	1.39
1	B	329	ALA	CA-CB	5.28	1.63	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	464	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	470	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	216	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	30	LEU	CB-CG-CD2	-5.63	101.44	111.00
1	A	464	ASP	CB-CG-OD2	-5.55	113.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	LEU	CA-CB-CG	-5.50	102.66	115.30
1	A	465	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	77	MET	CG-SD-CE	5.39	108.82	100.20
1	B	113	LYS	N-CA-C	5.33	125.40	111.00
1	B	354	LYS	CD-CE-NZ	5.28	123.84	111.70
1	B	306	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	A	278	ASP	CB-CG-OD2	5.22	122.99	118.30
1	B	393	GLY	N-CA-C	5.17	126.02	113.10
1	A	396	ASP	N-CA-C	-5.10	97.22	111.00
1	B	359	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	393	GLY	N-CA-C	5.02	125.65	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	TYR	Peptide
1	A	391	ILE	Peptide
1	A	394	ASP	Peptide
1	B	391	ILE	Peptide

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	3962	0	3911	129	0
1	B	3962	0	3911	135	0
2	A	80	0	112	13	0
2	B	40	0	56	7	0
3	A	25	0	0	2	0
3	B	20	0	0	1	0
4	A	53	0	29	5	0
4	B	53	0	31	2	0
5	A	10	0	10	2	0
5	B	5	0	5	0	0
6	A	28	0	42	10	0
6	B	32	0	48	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	15	0	16	0	0
7	B	15	0	16	1	0
8	A	11	0	4	4	0
8	B	11	0	4	4	0
9	A	152	0	0	11	0
9	B	153	0	0	7	0
All	All	8627	0	8195	269	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 16.

All (269) 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:494:GLN:CB	1:A:495:GLN:HB2	1.55	1.34
1:B:13:ILE:HG12	1:B:355:LEU:HD12	1.22	1.14
1:A:1:MET:HA	1:A:3:THR:H	1.08	1.13
1:B:119:GLY:O	1:B:120:SER:HB3	1.44	1.08
1:A:54:ARG:HA	2:A:900:BOG:H61	1.36	1.07
1:B:13:ILE:HG21	1:B:355:LEU:HD13	1.37	1.07
1:A:374:GLN:CB	1:A:375:GLY:HA3	1.84	1.05
1:A:50:HIS:CE1	1:A:354:LYS:HZ1	1.75	1.03
1:B:324:SER:O	1:B:325:ASP:HB2	1.54	1.02
1:B:13:ILE:HG21	1:B:355:LEU:CD1	1.91	1.01
1:A:395:ARG:HD3	1:A:419:ARG:HH21	1.22	0.99
1:A:494:GLN:HB3	1:A:495:GLN:HB2	0.99	0.99
1:B:416:HIS:O	1:B:420:THR:HG23	1.63	0.99
1:B:50:HIS:HE1	1:B:354:LYS:NZ	1.61	0.98
1:B:50:HIS:HE1	1:B:354:LYS:HZ1	1.02	0.98
6:A:1957:EDO:H22	9:A:7209:HOH:O	1.61	0.98
1:B:355:LEU:HD22	4:B:600:FAD:H2'	1.46	0.96
1:A:494:GLN:HB3	1:A:495:GLN:CB	1.95	0.95
1:A:54:ARG:HA	2:A:900:BOG:C6	1.96	0.95
1:A:50:HIS:HE1	1:A:354:LYS:NZ	1.63	0.95
1:B:50:HIS:CE1	1:B:354:LYS:NZ	2.35	0.94
1:B:13:ILE:CG1	1:B:355:LEU:HD12	1.96	0.94
1:A:494:GLN:CB	1:A:495:GLN:CB	2.46	0.92
1:B:62:ARG:HD3	1:B:333:ASP:OD2	1.70	0.92
1:B:50:HIS:CE1	1:B:354:LYS:HZ1	1.88	0.91
1:B:484:ARG:NH1	1:B:487:GLN:HE21	1.69	0.91
1:B:13:ILE:HB	1:B:355:LEU:HD11	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLY:HA3	4:A:600:FAD:O2A	1.72	0.90
1:A:410:THR:HG22	1:A:413:LEU:H	1.36	0.90
1:A:494:GLN:HB2	1:A:495:GLN:HB2	1.53	0.89
1:B:395:ARG:HG2	1:B:395:ARG:HH11	1.36	0.89
1:A:374:GLN:HB2	1:A:375:GLY:HA3	1.54	0.88
1:A:374:GLN:HB3	1:A:375:GLY:HA3	1.55	0.87
1:A:1:MET:HA	1:A:3:THR:N	1.88	0.87
1:B:324:SER:O	1:B:325:ASP:CB	2.23	0.87
1:B:484:ARG:HH11	1:B:487:GLN:HE21	0.88	0.86
1:B:13:ILE:CB	1:B:355:LEU:CD1	2.53	0.85
1:B:484:ARG:HH11	1:B:487:GLN:NE2	1.73	0.85
1:B:13:ILE:CG2	1:B:355:LEU:CD1	2.54	0.84
1:A:50:HIS:CE1	1:A:354:LYS:NZ	2.40	0.84
1:B:137:ARG:HG2	1:B:137:ARG:HH11	1.43	0.84
1:A:50:HIS:HE1	1:A:354:LYS:HZ1	0.86	0.83
1:B:96:ARG:HH11	1:B:249:GLN:HE21	1.26	0.83
1:A:297:ASN:HD21	1:A:304:LEU:H	1.25	0.83
1:B:394:ASP:OD2	1:B:395:ARG:NH1	2.12	0.82
1:B:61:PHE:O	1:B:65:SER:HB2	1.80	0.80
1:A:410:THR:CG2	1:A:413:LEU:H	1.94	0.80
1:A:395:ARG:CD	1:A:419:ARG:HH21	1.95	0.80
1:B:119:GLY:O	1:B:120:SER:CB	2.22	0.79
1:B:57:GLU:HG3	2:B:900:BOG:H2	1.64	0.78
1:B:129:SER:O	1:B:301:LYS:HE2	1.84	0.78
1:A:280:LYS:HE2	1:A:280:LYS:HA	1.65	0.77
1:A:478:ASN:ND2	1:A:481:GLN:H	1.83	0.77
1:B:13:ILE:HB	1:B:355:LEU:CD1	2.15	0.77
1:B:348:LEU:HD21	1:B:365:ALA:HB1	1.67	0.76
1:A:50:HIS:HD2	9:A:7122:HOH:O	1.67	0.76
1:A:374:GLN:CB	1:A:375:GLY:CA	2.63	0.75
1:A:1:MET:H1	1:A:2:GLU:HG3	1.52	0.75
1:A:54:ARG:NE	8:A:700:2PG:H31	2.01	0.75
1:B:13:ILE:CB	1:B:355:LEU:HD11	2.15	0.74
1:B:27:LEU:HD21	1:B:376:ILE:HG13	1.69	0.74
1:B:57:GLU:HG3	2:B:900:BOG:C2	2.18	0.74
1:B:50:HIS:CE1	1:B:354:LYS:CE	2.71	0.74
1:B:355:LEU:HD22	4:B:600:FAD:C2'	2.17	0.74
1:A:374:GLN:OE1	1:A:374:GLN:HA	1.86	0.73
1:B:107:MET:HG2	1:B:111:LEU:CD2	2.20	0.71
1:B:129:SER:HB2	9:B:7182:HOH:O	1.89	0.71
1:A:424:ASN:HD21	6:A:7067:EDO:H21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD13	1:B:64:VAL:HG21	1.72	0.71
1:A:107:MET:HE3	1:A:111:LEU:HD11	1.72	0.71
1:A:487:GLN:HG2	9:A:7203:HOH:O	1.90	0.71
1:A:374:GLN:HB3	1:A:375:GLY:CA	2.20	0.71
1:A:444:HIS:HE1	9:A:7102:HOH:O	1.73	0.71
1:A:410:THR:HG21	1:A:445:GLU:OE2	1.90	0.70
1:A:1:MET:N	1:A:2:GLU:HG3	2.07	0.70
1:A:494:GLN:HB2	1:A:495:GLN:CB	2.17	0.69
1:A:73:VAL:O	1:A:77:MET:HG3	1.93	0.69
1:B:62:ARG:HG3	1:B:63:LEU:N	2.07	0.69
1:A:57:GLU:HG3	2:A:900:BOG:H62	1.72	0.69
1:A:151:LEU:HD23	1:A:355:LEU:HD21	1.75	0.69
1:B:1:MET:HE2	1:B:2:GLU:HG3	1.73	0.69
1:B:53:LEU:HD22	2:B:900:BOG:H5	1.75	0.68
1:A:396:ASP:HA	1:A:399:ALA:HB3	1.76	0.67
1:A:137:ARG:HG3	2:A:1949:BOG:H3'2	1.77	0.67
1:B:137:ARG:HH11	1:B:137:ARG:CG	2.08	0.67
1:A:57:GLU:HG3	2:A:900:BOG:C6	2.25	0.66
1:A:294:ASN:HD21	6:A:1961:EDO:H11	1.61	0.66
1:B:395:ARG:HA	1:B:419:ARG:HH12	1.61	0.66
1:B:1:MET:HG3	1:B:2:GLU:H	1.59	0.65
1:B:395:ARG:HA	1:B:419:ARG:NH1	2.11	0.65
1:B:62:ARG:CD	1:B:333:ASP:OD2	2.44	0.65
1:A:49:ILE:HD11	1:A:146:VAL:HB	1.77	0.65
1:B:403:ARG:NE	1:B:409:LEU:O	2.27	0.64
1:B:445:GLU:OE2	6:B:909:EDO:H11	1.98	0.63
1:B:30:LEU:HD13	1:B:165:GLU:HG2	1.79	0.63
1:A:311:TRP:HZ2	6:A:1960:EDO:H22	1.62	0.63
1:B:55:TYR:CZ	1:B:332:ARG:HD2	2.34	0.62
1:B:229:ILE:HD12	1:B:327:PRO:HB3	1.81	0.62
1:B:55:TYR:CE1	1:B:332:ARG:HD2	2.34	0.62
1:B:62:ARG:HG3	1:B:63:LEU:H	1.63	0.62
1:B:50:HIS:HE1	1:B:354:LYS:CE	2.11	0.62
1:A:107:MET:CE	1:A:111:LEU:HD11	2.29	0.62
1:A:54:ARG:CZ	8:A:700:2PG:H31	2.30	0.61
1:B:101:ILE:HG22	1:B:105:LEU:HD22	1.82	0.61
1:A:406:TYR:HB2	1:A:409:LEU:HD22	1.83	0.60
1:B:1:MET:CE	1:B:2:GLU:HG3	2.30	0.60
1:A:254:ARG:NH2	8:A:700:2PG:H2	2.16	0.60
1:A:410:THR:HG22	1:A:413:LEU:N	2.15	0.59
1:A:415:ARG:HG2	1:A:419:ARG:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:7161:HOH:O	1:B:457:HIS:HE1	1.84	0.58
1:B:107:MET:HG2	1:B:111:LEU:HD22	1.84	0.58
1:A:109:ASP:O	1:A:114:ARG:NH1	2.37	0.58
1:B:385:VAL:H	6:B:910:EDO:H21	1.69	0.57
1:A:395:ARG:HD3	1:A:419:ARG:NH2	2.05	0.57
1:A:254:ARG:HH21	8:A:700:2PG:H2	1.70	0.57
1:B:30:LEU:CD1	1:B:165:GLU:HG2	2.34	0.57
1:B:457:HIS:HD2	7:B:7066:T3A:O1	1.88	0.56
1:B:348:LEU:CD2	1:B:365:ALA:HB1	2.35	0.56
1:A:478:ASN:HD22	1:A:478:ASN:C	2.08	0.56
2:A:1949:BOG:H2'1	2:A:1949:BOG:H7'1	1.88	0.56
1:B:161:ARG:HB3	6:B:7067:EDO:O2	2.04	0.56
1:B:254:ARG:HH21	8:B:700:2PG:H32	1.70	0.56
1:A:49:ILE:HB	1:A:144:CYS:HB2	1.87	0.56
1:A:56:LEU:HD21	1:A:64:VAL:HG11	1.88	0.55
1:B:239:VAL:HG23	1:B:240:HIS:CD2	2.42	0.55
1:B:13:ILE:CB	1:B:355:LEU:HD12	2.26	0.55
1:A:30:LEU:HD13	1:A:165:GLU:HG3	1.89	0.55
1:B:62:ARG:HG3	9:B:7220:HOH:O	2.05	0.55
1:B:394:ASP:C	1:B:396:ASP:H	2.09	0.55
1:B:107:MET:HG2	1:B:111:LEU:HD21	1.88	0.54
1:B:49:ILE:HB	1:B:144:CYS:HB2	1.88	0.54
1:B:56:LEU:HB3	2:B:900:BOG:H1'2	1.89	0.54
1:B:102:ARG:NH1	2:B:800:BOG:O2	2.40	0.54
1:A:102:ARG:HD2	2:A:800:BOG:H1'2	1.88	0.54
1:B:114:ARG:O	1:B:114:ARG:HG2	2.08	0.54
1:B:48:LEU:HD22	1:B:87:PHE:HZ	1.72	0.53
1:B:338:ILE:HD11	1:B:346:PRO:HB2	1.89	0.53
1:A:478:ASN:HD22	1:A:481:GLN:H	1.55	0.53
1:A:30:LEU:HG	1:A:32:LEU:HD13	1.90	0.53
1:A:101:ILE:HG22	1:A:105:LEU:HD22	1.89	0.53
1:B:96:ARG:HB2	1:B:249:GLN:HE22	1.73	0.52
1:B:54:ARG:CZ	8:B:700:2PG:H31	2.38	0.52
1:B:13:ILE:CG2	1:B:355:LEU:HD11	2.38	0.52
1:A:396:ASP:O	1:A:397:ASP:C	2.48	0.52
1:A:487:GLN:CG	9:A:7203:HOH:O	2.54	0.52
1:A:87:PHE:CE1	1:A:143:ASP:HB2	2.45	0.52
1:B:395:ARG:HD3	1:B:419:ARG:NH2	2.25	0.51
1:B:370:THR:O	1:B:372:TYR:N	2.44	0.51
1:A:338:ILE:HD11	1:A:346:PRO:HB2	1.93	0.51
1:B:129:SER:O	1:B:301:LYS:CE	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TRP:O	1:A:198:GLN:HA	2.11	0.50
1:B:50:HIS:HD2	9:B:7123:HOH:O	1.94	0.50
1:A:107:MET:HE3	1:A:111:LEU:CD1	2.40	0.50
1:B:200:ARG:O	1:B:346:PRO:HD2	2.12	0.50
1:A:317:ARG:HG3	4:A:600:FAD:HM83	1.92	0.49
1:B:424:ASN:HB3	1:B:453:TYR:OH	2.12	0.49
1:A:233:HIS:CD2	1:A:269:GLY:HA3	2.47	0.49
1:A:374:GLN:OE1	1:A:374:GLN:CA	2.57	0.49
6:A:1957:EDO:C2	9:A:7209:HOH:O	2.38	0.49
1:B:50:HIS:O	1:B:356:THR:HG21	2.12	0.49
1:A:252:ASP:O	1:A:253:LYS:HB2	2.12	0.49
1:A:39:CYS:HA	1:A:469:ARG:HD3	1.94	0.49
1:B:1:MET:HG3	1:B:2:GLU:OE1	2.13	0.49
1:B:370:THR:HG23	1:B:376:ILE:HG21	1.94	0.49
1:B:233:HIS:CD2	1:B:269:GLY:HA3	2.48	0.48
1:B:87:PHE:CE1	1:B:143:ASP:HB2	2.48	0.48
1:A:98:ALA:O	1:A:102:ARG:HG3	2.14	0.48
1:A:137:ARG:HD3	2:A:1949:BOG:O1	2.13	0.48
2:A:800:BOG:O4	2:A:1949:BOG:H4	2.14	0.48
1:B:62:ARG:CG	9:B:7220:HOH:O	2.60	0.48
1:B:241:THR:O	1:B:241:THR:CG2	2.62	0.48
1:A:212:GLN:HG2	3:A:1955:PO4:O3	2.14	0.48
1:A:271:THR:HB	6:A:1962:EDO:H22	1.95	0.48
1:B:311:TRP:HZ2	6:B:907:EDO:H12	1.79	0.47
1:A:395:ARG:HD2	1:A:395:ARG:HA	1.70	0.47
1:B:415:ARG:HG2	1:B:419:ARG:HD2	1.96	0.47
1:A:45:SER:HA	4:A:600:FAD:C6	2.45	0.47
1:B:96:ARG:HD2	1:B:249:GLN:NE2	2.29	0.47
1:A:103:ILE:O	1:A:107:MET:HG3	2.15	0.47
1:A:176:ARG:HH11	1:A:176:ARG:HG3	1.80	0.47
1:A:394:ASP:OD2	5:A:1956:IMD:N1	2.48	0.47
1:A:395:ARG:O	1:A:396:ASP:HB2	2.15	0.47
1:A:115:THR:HG22	1:A:116:SER:N	2.30	0.46
1:A:241:THR:O	1:A:241:THR:CG2	2.62	0.46
1:A:354:LYS:HB3	1:A:354:LYS:HE3	1.75	0.46
1:A:394:ASP:OD2	5:A:1956:IMD:C2	2.63	0.46
1:B:161:ARG:CB	6:B:7067:EDO:O2	2.64	0.46
1:B:39:CYS:HA	1:B:469:ARG:HD3	1.97	0.46
1:B:416:HIS:CE1	1:B:420:THR:HG21	2.51	0.46
1:B:96:ARG:NH1	1:B:249:GLN:HE21	2.03	0.46
1:A:232:SER:CB	1:A:284:ILE:HG13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:O	1:A:298:THR:HG23	2.16	0.46
1:B:395:ARG:HG2	1:B:395:ARG:NH1	2.15	0.46
1:A:27:LEU:HD21	1:A:376:ILE:HG13	1.98	0.46
1:A:136:LYS:HD3	9:A:7174:HOH:O	2.16	0.46
1:A:200:ARG:O	1:A:346:PRO:HD2	2.15	0.46
1:B:296:TYR:CD2	1:B:296:TYR:C	2.90	0.46
1:A:102:ARG:HD2	2:A:800:BOG:C1'	2.46	0.46
1:A:50:HIS:O	1:A:356:THR:HG21	2.16	0.45
1:A:107:MET:O	1:A:111:LEU:HB2	2.16	0.45
1:A:129:SER:HB2	9:A:7108:HOH:O	2.17	0.45
1:B:148:ASP:OD1	1:B:149:ALA:N	2.49	0.45
1:A:229:ILE:HD12	1:A:327:PRO:HB3	1.98	0.45
1:B:444:HIS:NE2	9:B:7107:HOH:O	2.35	0.45
1:A:6:LEU:HD11	1:A:203:VAL:HG23	1.99	0.45
1:A:401:ARG:NH2	3:A:1954:PO4:O2	2.42	0.45
1:B:91:HIS:CD2	9:B:7077:HOH:O	2.69	0.45
1:A:248:LEU:O	1:A:255:ILE:HA	2.16	0.45
1:A:494:GLN:HA	1:A:494:GLN:OE1	2.16	0.45
1:B:327:PRO:HA	1:B:330:ILE:HD12	1.98	0.45
1:B:366:LEU:HD13	1:B:366:LEU:HA	1.77	0.45
1:B:454:LEU:HB3	1:B:460:VAL:HG21	1.99	0.45
1:A:294:ASN:HD21	6:A:1961:EDO:C1	2.27	0.45
1:A:49:ILE:HG22	1:A:71:ARG:HG2	1.99	0.45
1:B:248:LEU:O	1:B:255:ILE:HA	2.16	0.45
1:A:148:ASP:OD1	1:A:149:ALA:N	2.47	0.44
1:B:13:ILE:CG1	1:B:355:LEU:CD1	2.75	0.44
1:B:50:HIS:CE1	1:B:354:LYS:HE2	2.49	0.44
1:A:67:ALA:HB1	1:A:356:THR:HG21	1.98	0.44
1:A:396:ASP:O	1:A:400:ALA:N	2.39	0.44
1:B:193:LYS:HE3	1:B:195:TYR:CE1	2.52	0.44
1:B:394:ASP:CG	1:B:395:ARG:NH1	2.71	0.44
1:A:12:GLY:CA	4:A:600:FAD:O2A	2.55	0.44
1:A:77:MET:SD	1:A:359:ARG:HD3	2.58	0.44
6:A:1960:EDO:H21	9:A:7094:HOH:O	2.17	0.44
1:B:102:ARG:NH1	1:B:137:ARG:HH22	2.16	0.44
1:A:33:GLU:OE2	4:A:600:FAD:O2B	2.36	0.43
1:A:54:ARG:HA	2:A:900:BOG:O6	2.17	0.43
1:B:120:SER:C	1:B:121:THR:HG23	2.39	0.43
1:B:394:ASP:CG	1:B:395:ARG:N	2.72	0.43
1:A:285:GLU:HG2	1:A:288:GLU:OE1	2.18	0.43
1:B:87:PHE:O	1:B:140:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ILE:HG22	1:B:368:LYS:HE3	2.01	0.43
1:A:132:LYS:HA	1:A:133:PRO:HD3	1.91	0.43
1:B:1:MET:CG	1:B:2:GLU:H	2.25	0.43
1:B:54:ARG:NE	8:B:700:2PG:H31	2.33	0.43
1:B:162:LYS:HD2	1:B:162:LYS:HA	1.66	0.43
1:A:30:LEU:CD1	1:A:165:GLU:HG3	2.48	0.43
6:A:1959:EDO:H21	9:A:7127:HOH:O	2.17	0.43
1:A:193:LYS:HE3	1:A:195:TYR:CE1	2.54	0.43
1:A:374:GLN:CD	1:A:374:GLN:H	2.22	0.43
1:B:420:THR:HG21	9:B:7162:HOH:O	2.18	0.43
1:B:13:ILE:HG23	1:B:14:ASN:N	2.34	0.42
1:A:91:HIS:CD2	2:A:1949:BOG:H2	2.54	0.42
1:A:10:GLY:O	1:A:15:GLY:HA3	2.19	0.42
1:A:57:GLU:HG3	2:A:900:BOG:O6	2.20	0.42
1:A:318:PRO:O	1:A:352:GLY:HA2	2.19	0.42
1:B:1:MET:HE3	1:B:2:GLU:N	2.34	0.42
1:B:56:LEU:HD12	1:B:56:LEU:HA	1.92	0.42
1:A:405:ARG:O	1:A:407:PRO:HD3	2.19	0.42
1:B:57:GLU:HG3	2:B:900:BOG:O2	2.19	0.42
1:A:460:VAL:HG11	1:A:466:ALA:HB2	2.02	0.42
1:B:10:GLY:O	1:B:15:GLY:HA3	2.20	0.42
1:B:120:SER:C	1:B:121:THR:CG2	2.88	0.42
1:B:254:ARG:HH21	8:B:700:2PG:C3	2.32	0.41
1:A:272:ASP:H	6:A:1962:EDO:H22	1.85	0.41
1:B:113:LYS:NZ	1:B:113:LYS:HB2	2.36	0.41
1:A:403:ARG:NE	1:A:409:LEU:O	2.36	0.41
1:A:133:PRO:O	1:A:136:LYS:HE3	2.21	0.41
1:A:404:ARG:HG2	1:B:163:GLY:HA3	2.03	0.41
1:B:182:TRP:O	1:B:198:GLN:HA	2.21	0.41
1:A:102:ARG:HH21	1:A:137:ARG:NH2	2.19	0.40
1:B:295:VAL:O	1:B:299:HIS:HD2	2.03	0.40
1:B:405:ARG:HD3	3:B:901:PO4:O3	2.21	0.40
1:A:151:LEU:CD2	1:A:355:LEU:HD21	2.49	0.40
1:A:410:THR:HG22	1:A:413:LEU:CB	2.51	0.40
1:B:137:ARG:HG2	1:B:137:ARG:NH1	2.23	0.40
1:B:490:VAL:HG22	1:B:494:GLN:HE22	1.86	0.40
1:B:101:ILE:HG23	2:B:900:BOG:H61	2.03	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	493/501 (98%)	457 (93%)	26 (5%)	10 (2%)	7 6
1	B	493/501 (98%)	450 (91%)	35 (7%)	8 (2%)	9 9
All	All	986/1002 (98%)	907 (92%)	61 (6%)	18 (2%)	8 7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	392	GLU
1	B	325	ASP
1	A	321	ASP
1	A	374	GLN
1	A	396	ASP
1	A	494	GLN
1	B	120	SER
1	B	321	ASP
1	B	392	GLU
1	A	394	ASP
1	A	423	SER
1	B	396	ASP
1	A	159	VAL
1	A	371	PRO
1	B	159	VAL
1	B	263	ASP
1	B	371	PRO

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	414/419 (99%)	390 (94%)	24 (6%)	20	27
1	B	414/419 (99%)	380 (92%)	34 (8%)	11	14
All	All	828/838 (99%)	770 (93%)	58 (7%)	15	19

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	28	SER
1	A	32	LEU
1	A	94	HIS
1	A	105	LEU
1	A	113	LYS
1	A	165	GLU
1	A	176	ARG
1	A	243	LYS
1	A	244	GLN
1	A	250	ASN
1	A	326	SER
1	A	341	GLU
1	A	348	LEU
1	A	355	LEU
1	A	392	GLU
1	A	395	ARG
1	A	396	ASP
1	A	403	ARG
1	A	404	ARG
1	A	409	LEU
1	A	410	THR
1	A	427	LEU
1	A	478	ASN
1	B	2	GLU
1	B	4	LYS
1	B	53	LEU
1	B	56	LEU
1	B	62	ARG
1	B	65	SER
1	B	105	LEU
1	B	108	TYR
1	B	111	LEU

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Mol	Chain	Res	Type
1	B	113	LYS
1	B	114	ARG
1	B	115	THR
1	B	124	ARG
1	B	137	ARG
1	B	151	LEU
1	B	161	ARG
1	B	162	LYS
1	B	165	GLU
1	B	187	GLU
1	B	212	GLN
1	B	243	LYS
1	B	244	GLN
1	B	324	SER
1	B	332	ARG
1	B	341	GLU
1	B	348	LEU
1	B	355	LEU
1	B	392	GLU
1	B	395	ARG
1	B	396	ASP
1	B	413	LEU
1	B	420	THR
1	B	483	SER
1	B	494	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	212	GLN
1	A	242	GLN
1	A	250	ASN
1	A	290	ASN
1	A	294	ASN
1	A	297	ASN
1	A	424	ASN
1	A	444	HIS
1	A	473	GLN

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Mol	Chain	Res	Type
1	A	478	ASN
1	A	482	GLN
1	B	50	HIS
1	B	91	HIS
1	B	110	HIS
1	B	244	GLN
1	B	249	GLN
1	B	290	ASN
1	B	294	ASN
1	B	299	HIS
1	B	457	HIS
1	B	473	GLN
1	B	487	GLN
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)

39 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	910	-	3,3,3	1.11	0	2,2,2	0.39	0
3	PO4	B	901	-	4,4,4	0.91	0	6,6,6	0.56	0
6	EDO	B	907	-	3,3,3	0.58	0	2,2,2	0.35	0
7	T3A	A	7066	-	14,14,14	2.33	2 (14%)	18,19,19	2.33	8 (44%)
3	PO4	A	1954	-	4,4,4	0.89	0	6,6,6	0.85	0
6	EDO	A	1963	-	3,3,3	0.85	0	2,2,2	0.63	0
3	PO4	A	1951	-	4,4,4	0.82	0	6,6,6	0.66	0
5	IMD	B	912	-	3,5,5	0.58	0	4,5,5	0.33	0
2	BOG	A	1950	-	20,20,20	1.10	1 (5%)	25,25,25	1.53	5 (20%)
6	EDO	A	1957	-	3,3,3	0.43	0	2,2,2	0.69	0
2	BOG	A	1949	-	20,20,20	1.08	1 (5%)	25,25,25	2.36	9 (36%)
8	2PG	A	700	-	9,10,10	3.31	5 (55%)	11,14,14	3.61	4 (36%)
5	IMD	A	1958	-	3,5,5	0.38	0	4,5,5	0.67	0
3	PO4	B	903	-	4,4,4	1.18	1 (25%)	6,6,6	1.06	0
6	EDO	A	1959	-	3,3,3	1.10	0	2,2,2	0.76	0
6	EDO	B	908	-	3,3,3	0.95	0	2,2,2	0.64	0
4	FAD	A	600	-	53,58,58	1.22	5 (9%)	68,89,89	1.66	11 (16%)
2	BOG	A	800	-	20,20,20	0.47	0	25,25,25	0.59	0
6	EDO	B	911	-	3,3,3	0.70	0	2,2,2	0.20	0
2	BOG	B	800	-	20,20,20	0.46	0	25,25,25	0.59	0
3	PO4	A	1955	-	4,4,4	0.66	0	6,6,6	1.36	0
4	FAD	B	600	-	53,58,58	1.57	9 (16%)	68,89,89	1.88	19 (27%)
6	EDO	B	906	-	3,3,3	0.83	0	2,2,2	0.74	0
2	BOG	A	900	-	20,20,20	0.80	1 (5%)	25,25,25	1.73	7 (28%)
6	EDO	B	905	-	3,3,3	0.55	0	2,2,2	1.23	0
6	EDO	A	1960	-	3,3,3	0.65	0	2,2,2	0.22	0
6	EDO	A	7067	-	3,3,3	0.89	0	2,2,2	0.09	0
5	IMD	A	1956	-	3,5,5	0.40	0	4,5,5	0.81	0
3	PO4	B	904	-	4,4,4	0.81	0	6,6,6	0.44	0
7	T3A	B	7066	-	14,14,14	2.26	2 (14%)	18,19,19	2.89	11 (61%)
3	PO4	B	902	-	4,4,4	0.85	0	6,6,6	0.72	0
6	EDO	B	909	-	3,3,3	0.54	0	2,2,2	0.25	0
6	EDO	B	7067	-	3,3,3	0.74	0	2,2,2	0.71	0
2	BOG	B	900	-	20,20,20	0.76	1 (5%)	25,25,25	1.70	6 (24%)
3	PO4	A	1953	-	4,4,4	0.72	0	6,6,6	0.56	0
6	EDO	A	1961	-	3,3,3	0.40	0	2,2,2	0.80	0
3	PO4	A	1952	-	4,4,4	0.48	0	6,6,6	0.95	0
6	EDO	A	1962	-	3,3,3	0.76	0	2,2,2	0.06	0
8	2PG	B	700	-	9,10,10	3.13	4 (44%)	11,14,14	3.01	2 (18%)

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	910	-	-	1/1/1/1	-
6	EDO	B	907	-	-	1/1/1/1	-
7	T3A	A	7066	-	-	6/18/18/18	-
6	EDO	A	1963	-	-	1/1/1/1	-
5	IMD	B	912	-	-	-	0/1/1/1
2	BOG	A	1950	-	-	10/11/31/31	0/1/1/1
6	EDO	A	1957	-	-	1/1/1/1	-
8	2PG	A	700	-	1/1/3/3	5/11/11/11	-
2	BOG	A	1949	-	-	9/11/31/31	0/1/1/1
5	IMD	A	1958	-	-	-	0/1/1/1
6	EDO	A	1959	-	-	1/1/1/1	-
6	EDO	B	908	-	-	0/1/1/1	-
4	FAD	A	600	-	-	5/30/50/50	0/6/6/6
2	BOG	A	800	-	-	7/11/31/31	0/1/1/1
6	EDO	B	911	-	-	1/1/1/1	-
2	BOG	B	800	-	-	8/11/31/31	0/1/1/1
4	FAD	B	600	-	-	3/30/50/50	0/6/6/6
6	EDO	B	906	-	-	1/1/1/1	-
2	BOG	A	900	-	-	9/11/31/31	0/1/1/1
6	EDO	B	905	-	-	0/1/1/1	-
6	EDO	A	1960	-	-	1/1/1/1	-
6	EDO	A	7067	-	-	1/1/1/1	-
5	IMD	A	1956	-	-	-	0/1/1/1
7	T3A	B	7066	-	-	3/18/18/18	-
6	EDO	B	909	-	-	0/1/1/1	-
6	EDO	B	7067	-	-	0/1/1/1	-
2	BOG	B	900	-	-	5/11/31/31	0/1/1/1
6	EDO	A	1961	-	-	1/1/1/1	-
6	EDO	A	1962	-	-	0/1/1/1	-
8	2PG	B	700	-	1/1/3/3	5/11/11/11	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	7066	T3A	C1-S1	-7.79	1.66	1.77
7	B	7066	T3A	C1-S1	-7.62	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	700	2PG	C2-C1	6.73	1.58	1.52
8	B	700	2PG	C2-C1	6.31	1.58	1.52
8	B	700	2PG	O1-C1	5.06	1.37	1.22
8	A	700	2PG	O1-C1	4.74	1.36	1.22
4	B	600	FAD	C4X-N5	4.09	1.38	1.30
4	A	600	FAD	C2A-N3A	4.03	1.38	1.32
4	B	600	FAD	C6-C7	-3.97	1.33	1.39
4	A	600	FAD	C4X-N5	3.96	1.38	1.30
4	B	600	FAD	C9-C9A	-3.61	1.33	1.39
8	A	700	2PG	P-O1P	3.57	1.66	1.59
2	A	1950	BOG	O1-C1	3.41	1.46	1.40
4	A	600	FAD	O2B-C2B	-3.27	1.35	1.43
4	B	600	FAD	O4-C4	3.09	1.29	1.23
4	B	600	FAD	C10-N1	3.06	1.39	1.33
8	A	700	2PG	C3-C2	3.05	1.59	1.52
8	B	700	2PG	C3-C2	3.02	1.58	1.52
2	A	1949	BOG	O1-C1	2.79	1.45	1.40
2	A	900	BOG	O1-C1	2.70	1.44	1.40
4	B	600	FAD	C7M-C7	-2.59	1.45	1.51
4	A	600	FAD	C10-N1	2.55	1.38	1.33
4	A	600	FAD	C2A-N1A	2.46	1.38	1.33
4	B	600	FAD	C2A-N3A	2.40	1.36	1.32
8	A	700	2PG	O3-C3	2.37	1.52	1.42
7	A	7066	T3A	C5-C4	2.34	1.56	1.53
4	B	600	FAD	O2'-C2'	-2.33	1.38	1.43
2	B	900	BOG	O1-C1	2.30	1.44	1.40
8	B	700	2PG	O3-C3	2.28	1.52	1.42
7	B	7066	T3A	C5-C4	2.26	1.56	1.53
3	B	903	PO4	P-O1	2.22	1.56	1.50
4	B	600	FAD	O4B-C4B	-2.09	1.40	1.45

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	700	2PG	P-O1P-C2	9.67	145.22	123.04
8	B	700	2PG	P-O1P-C2	8.91	143.47	123.04
4	A	600	FAD	O2B-C2B-C3B	7.63	136.50	111.82
4	B	600	FAD	N3A-C2A-N1A	-7.51	116.94	128.68
7	B	7066	T3A	C6-C4-C5	5.68	122.06	110.04
4	B	600	FAD	O4-C4-N3	-5.41	109.75	120.12
4	A	600	FAD	N3A-C2A-N1A	-5.39	120.25	128.68
2	A	1949	BOG	C1-C2-C3	5.28	120.98	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	BOG	C1-O5-C5	5.12	123.73	113.69
2	A	1950	BOG	O1-C1-C2	4.81	115.82	108.30
8	A	700	2PG	O3-C3-C2	4.81	123.96	111.73
7	B	7066	T3A	O5-C5-C4	4.33	120.39	111.63
7	A	7066	T3A	O3-S1-C1	4.12	112.44	105.77
2	B	900	BOG	C3-C4-C5	-3.98	103.13	110.24
7	B	7066	T3A	O3-S1-C1	3.92	112.11	105.77
8	A	700	2PG	O4P-P-O2P	-3.90	95.40	110.68
7	A	7066	T3A	C2-C1-S1	-3.84	107.36	113.25
2	A	1949	BOG	O3-C3-C2	3.68	118.85	110.35
2	A	1949	BOG	O5-C5-C6	3.61	115.42	106.44
4	A	600	FAD	P-O3P-PA	-3.59	120.50	132.83
2	B	900	BOG	C1-C2-C3	3.57	117.44	110.00
7	B	7066	T3A	C3-N1-C4	3.56	121.13	116.08
7	A	7066	T3A	O1-S1-C1	3.55	111.19	106.92
2	A	1949	BOG	C6-C5-C4	3.49	121.18	113.00
2	A	1949	BOG	O4-C4-C5	3.38	117.70	109.30
2	A	1949	BOG	C1-O5-C5	-3.37	107.07	113.69
8	B	700	2PG	O4P-P-O2P	-3.35	97.55	110.68
7	B	7066	T3A	C7-C4-C6	-3.33	103.01	110.04
4	B	600	FAD	O5'-C5'-C4'	-3.31	100.53	109.36
4	A	600	FAD	C3B-C2B-C1B	3.25	105.87	100.98
2	A	1949	BOG	O1-C1-C2	3.23	113.35	108.30
4	B	600	FAD	C4X-C10-N10	3.20	121.16	116.48
7	B	7066	T3A	C7-C4-N1	3.18	118.59	109.03
4	B	600	FAD	C10-C4X-N5	-3.15	118.18	124.86
2	A	1949	BOG	C3-C4-C5	-3.10	104.71	110.24
7	B	7066	T3A	O2-S1-C1	3.06	110.61	106.92
7	B	7066	T3A	C2-C1-S1	-3.00	108.65	113.25
4	A	600	FAD	C4-N3-C2	-2.99	120.11	125.64
2	A	1949	BOG	O2-C2-C1	-2.99	102.77	110.05
7	B	7066	T3A	O1-S1-C1	2.99	110.51	106.92
4	B	600	FAD	C6-C5X-C9A	2.98	123.15	118.94
7	A	7066	T3A	O5-C5-C4	2.96	117.62	111.63
2	A	900	BOG	O5-C5-C4	2.85	114.86	109.69
4	B	600	FAD	C1'-N10-C9A	2.82	125.21	120.51
4	B	600	FAD	C2A-N1A-C6A	2.80	123.54	118.75
2	B	900	BOG	O4-C4-C5	2.79	116.21	109.30
7	A	7066	T3A	C6-C4-C5	2.78	115.93	110.04
7	A	7066	T3A	C7-C4-N1	2.77	117.37	109.03
2	B	900	BOG	C4-C3-C2	2.73	115.59	110.82
2	A	900	BOG	C3-C4-C5	-2.71	105.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	600	FAD	C9A-C5X-N5	-2.71	119.49	122.43
7	A	7066	T3A	C3-N1-C4	2.71	119.92	116.08
7	B	7066	T3A	C5-C4-N1	-2.70	100.91	109.03
4	B	600	FAD	O2-C2-N1	2.69	126.29	121.83
4	B	600	FAD	C5A-C6A-N6A	2.67	124.41	120.35
4	A	600	FAD	C4X-C4-N3	2.64	119.90	113.19
7	A	7066	T3A	O2-S1-O1	-2.64	104.81	113.95
2	B	900	BOG	O1-C1-C2	2.61	112.38	108.30
4	B	600	FAD	C5X-N5-C4X	2.58	122.37	118.07
2	A	1950	BOG	C1'-O1-C1	2.55	118.07	113.84
2	A	1950	BOG	O4-C4-C5	2.50	115.51	109.30
2	A	900	BOG	O4-C4-C3	2.47	116.07	110.35
4	A	600	FAD	O4-C4-C4X	-2.47	120.06	126.60
4	A	600	FAD	C4X-C10-N10	2.43	120.04	116.48
2	A	900	BOG	O1-C1-C2	2.41	112.07	108.30
4	B	600	FAD	O2-C2-N3	-2.39	114.00	118.65
4	B	600	FAD	O5B-PA-O1A	-2.37	99.82	109.07
2	B	900	BOG	O4-C4-C3	-2.31	105.00	110.35
4	B	600	FAD	C4-C4X-C10	2.31	120.67	116.79
4	A	600	FAD	C10-C4X-N5	-2.26	120.07	124.86
7	B	7066	T3A	O2-S1-O1	-2.24	106.20	113.95
2	A	1950	BOG	O3-C3-C2	2.17	115.37	110.35
4	A	600	FAD	C9A-C5X-N5	-2.17	120.08	122.43
4	B	600	FAD	C4X-C10-N1	-2.16	119.72	124.73
2	A	900	BOG	O5-C1-O1	2.13	115.02	109.97
4	A	600	FAD	C4X-C10-N1	-2.09	119.88	124.73
2	A	1950	BOG	O4-C4-C3	-2.06	105.59	110.35
4	B	600	FAD	O2A-PA-O5B	2.04	117.24	107.75
4	B	600	FAD	C4-C4X-N5	2.04	121.13	118.23
4	B	600	FAD	N6A-C6A-N1A	-2.04	114.35	118.57
8	A	700	2PG	O1P-P-O2P	2.03	117.21	109.39
2	A	900	BOG	O5-C5-C6	2.01	111.43	106.44

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	700	2PG	C2
8	B	700	2PG	C2

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BOG	C2-C1-O1-C1'
2	A	1949	BOG	C2-C1-O1-C1'
2	A	1949	BOG	O5-C1-O1-C1'
2	A	1950	BOG	C2-C1-O1-C1'
2	A	1950	BOG	O5-C1-O1-C1'
2	A	1950	BOG	C2'-C1'-O1-C1
2	B	800	BOG	C2'-C1'-O1-C1
4	A	600	FAD	C5B-O5B-PA-O2A
7	A	7066	T3A	C6-C4-C5-O5
7	A	7066	T3A	N1-C4-C7-O7
7	A	7066	T3A	C5-C4-C7-O7
7	A	7066	T3A	C6-C4-C7-O7
8	A	700	2PG	O2-C1-C2-O1P
8	A	700	2PG	C1-C2-C3-O3
8	A	700	2PG	C2-O1P-P-O4P
8	B	700	2PG	O2-C1-C2-O1P
8	B	700	2PG	C1-C2-C3-O3
8	B	700	2PG	O1P-C2-C3-O3
8	B	700	2PG	C2-O1P-P-O2P
2	A	1950	BOG	O5-C5-C6-O6
2	A	1949	BOG	C4-C5-C6-O6
4	A	600	FAD	C4B-C5B-O5B-PA
2	A	1950	BOG	C4-C5-C6-O6
2	A	1949	BOG	O5-C5-C6-O6
2	A	1949	BOG	C4'-C5'-C6'-C7'
2	A	800	BOG	O1-C1'-C2'-C3'
2	B	800	BOG	O5-C5-C6-O6
2	A	900	BOG	O5-C1-O1-C1'
2	B	900	BOG	O1-C1'-C2'-C3'
2	A	1950	BOG	O1-C1'-C2'-C3'
2	A	800	BOG	C2'-C3'-C4'-C5'
2	A	1950	BOG	C3'-C4'-C5'-C6'
2	A	1949	BOG	C2'-C3'-C4'-C5'
2	B	800	BOG	C2'-C3'-C4'-C5'
2	A	900	BOG	C4-C5-C6-O6
2	B	900	BOG	C2-C1-O1-C1'
8	B	700	2PG	C3-C2-O1P-P
2	A	1949	BOG	C3'-C4'-C5'-C6'
2	B	900	BOG	O5-C1-O1-C1'
2	A	1950	BOG	C2'-C3'-C4'-C5'
2	A	800	BOG	C4'-C5'-C6'-C7'
2	A	900	BOG	C3'-C4'-C5'-C6'
7	A	7066	T3A	N1-C4-C5-O5

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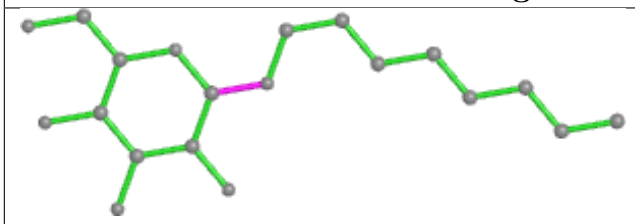
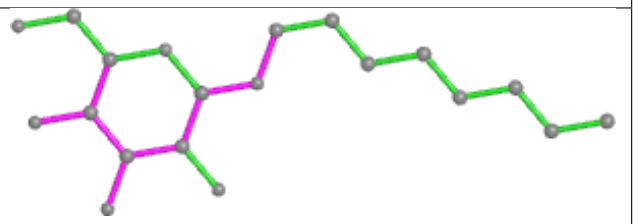
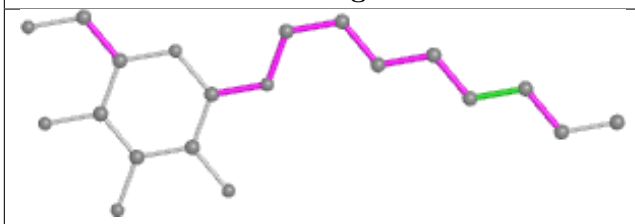
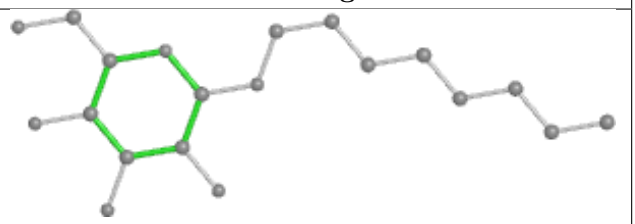
Mol	Chain	Res	Type	Atoms
2	A	1949	BOG	C1'-C2'-C3'-C4'
2	A	1950	BOG	C1'-C2'-C3'-C4'
2	A	800	BOG	C1'-C2'-C3'-C4'
6	B	906	EDO	O1-C1-C2-O2
2	B	800	BOG	O1-C1'-C2'-C3'
2	A	900	BOG	C1'-C2'-C3'-C4'
2	A	900	BOG	C5'-C6'-C7'-C8'
2	A	1950	BOG	C5'-C6'-C7'-C8'
2	B	800	BOG	C4'-C5'-C6'-C7'
2	A	1949	BOG	C2'-C1'-O1-C1
7	A	7066	T3A	C7-C4-C5-O5
2	B	800	BOG	C4-C5-C6-O6
2	B	900	BOG	C1'-C2'-C3'-C4'
6	B	911	EDO	O1-C1-C2-O2
2	B	800	BOG	C3'-C4'-C5'-C6'
2	A	800	BOG	O5-C1-O1-C1'
4	A	600	FAD	C5B-O5B-PA-O3P
4	B	600	FAD	O4B-C4B-C5B-O5B
4	A	600	FAD	C5B-O5B-PA-O1A
6	B	907	EDO	O1-C1-C2-O2
4	B	600	FAD	N10-C1'-C2'-O2'
2	A	900	BOG	O5-C5-C6-O6
7	B	7066	T3A	C6-C4-C5-O5
2	A	900	BOG	C4'-C5'-C6'-C7'
6	A	1963	EDO	O1-C1-C2-O2
6	B	910	EDO	O1-C1-C2-O2
2	B	800	BOG	C1'-C2'-C3'-C4'
6	A	1959	EDO	O1-C1-C2-O2
2	A	800	BOG	C5'-C6'-C7'-C8'
8	A	700	2PG	C3-C2-O1P-P
2	A	900	BOG	C2'-C3'-C4'-C5'
2	A	800	BOG	C3'-C4'-C5'-C6'
6	A	1961	EDO	O1-C1-C2-O2
4	A	600	FAD	O4B-C4B-C5B-O5B
6	A	1960	EDO	O1-C1-C2-O2
6	A	7067	EDO	O1-C1-C2-O2
7	B	7066	T3A	N1-C4-C5-O5
8	A	700	2PG	O1-C1-C2-O1P
4	B	600	FAD	C3B-C4B-C5B-O5B
6	A	1957	EDO	O1-C1-C2-O2
7	B	7066	T3A	C6-C4-N1-C3
2	B	900	BOG	C2'-C1'-O1-C1

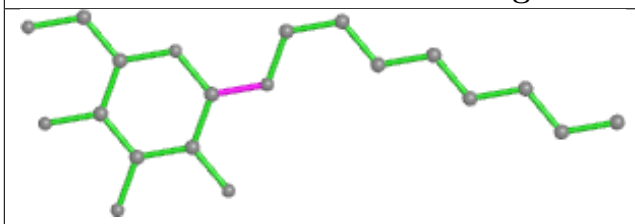
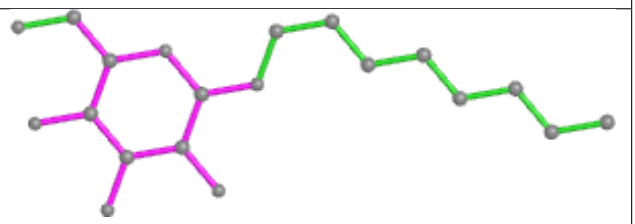
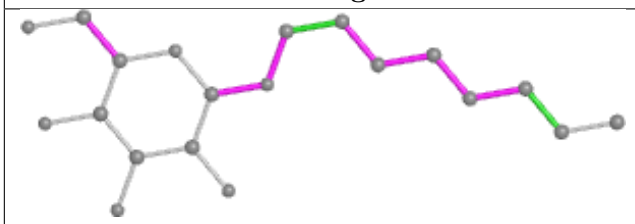
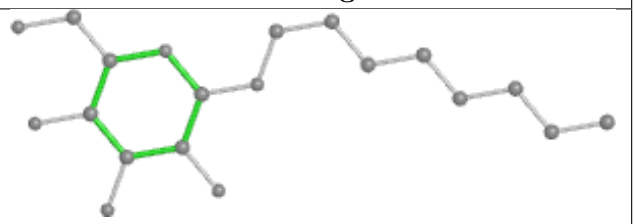
There are no ring outliers.

24 monomers are involved in 56 short contacts:

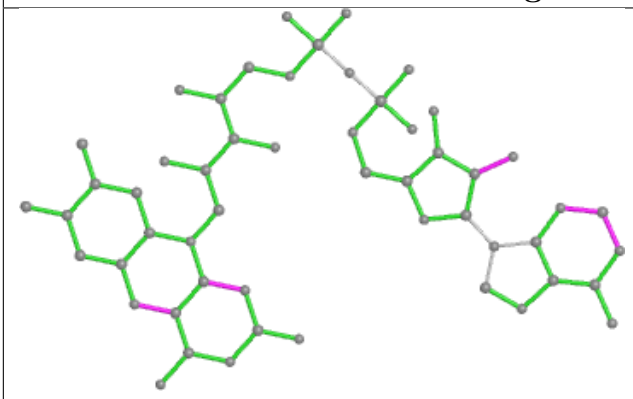
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	910	EDO	1	0
3	B	901	PO4	1	0
6	B	907	EDO	1	0
3	A	1954	PO4	1	0
6	A	1957	EDO	2	0
2	A	1949	BOG	5	0
8	A	700	2PG	4	0
6	A	1959	EDO	1	0
4	A	600	FAD	5	0
2	A	800	BOG	3	0
2	B	800	BOG	1	0
3	A	1955	PO4	1	0
4	B	600	FAD	2	0
2	A	900	BOG	6	0
6	A	1960	EDO	2	0
6	A	7067	EDO	1	0
5	A	1956	IMD	2	0
7	B	7066	T3A	1	0
6	B	909	EDO	1	0
6	B	7067	EDO	2	0
2	B	900	BOG	6	0
6	A	1961	EDO	2	0
6	A	1962	EDO	2	0
8	B	700	2PG	4	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.

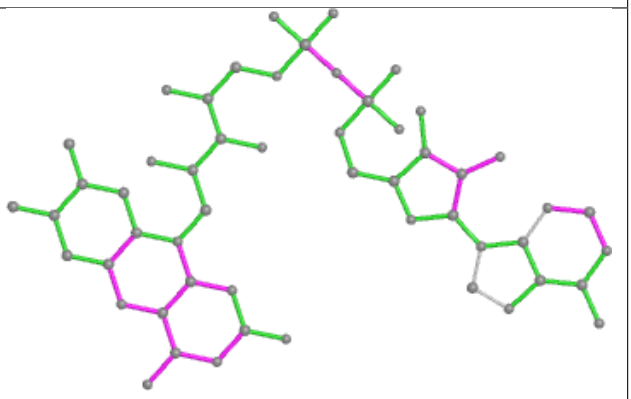
Ligand BOG A 1950	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BOG A 1949	
 Bond lengths	 Bond angles
 Torsions	 Rings

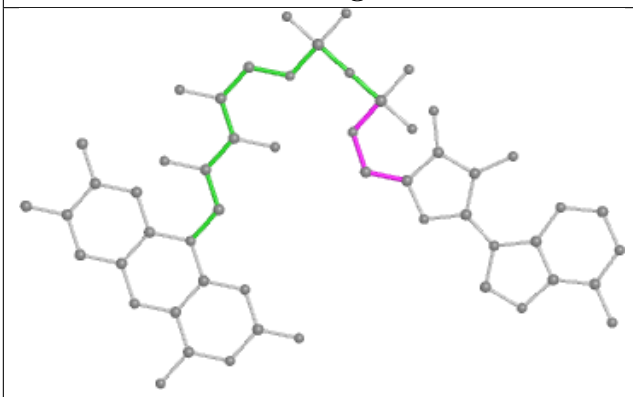
Ligand FAD A 600



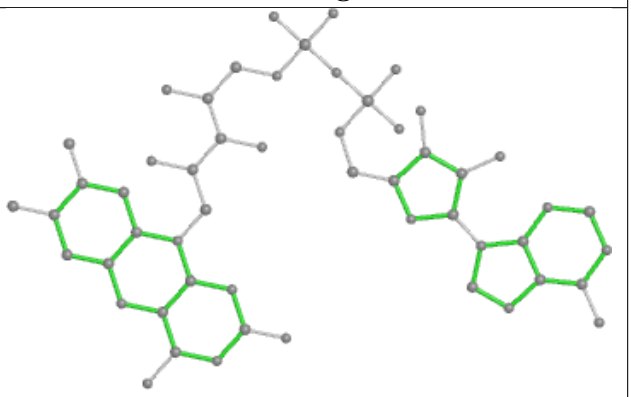
Bond lengths



Bond angles

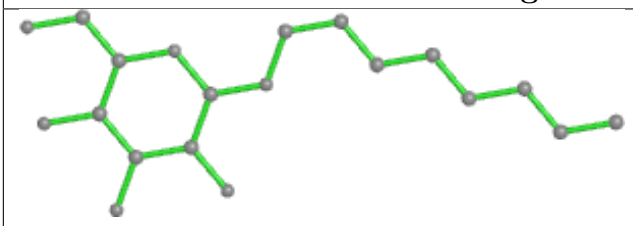


Torsions

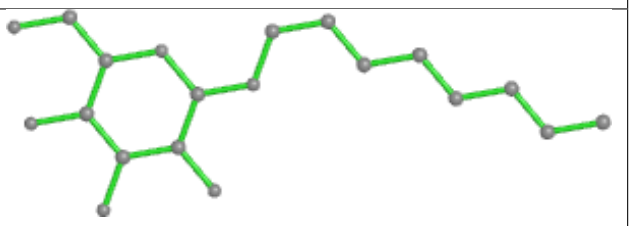


Rings

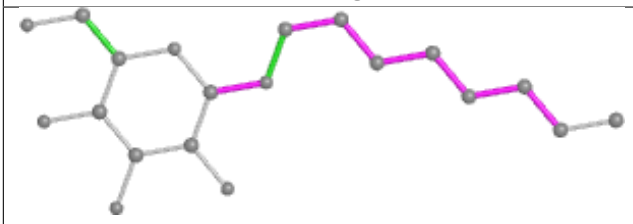
Ligand BOG A 800



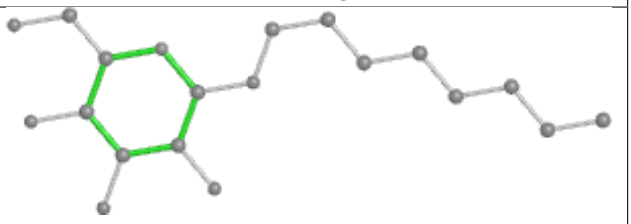
Bond lengths



Bond angles

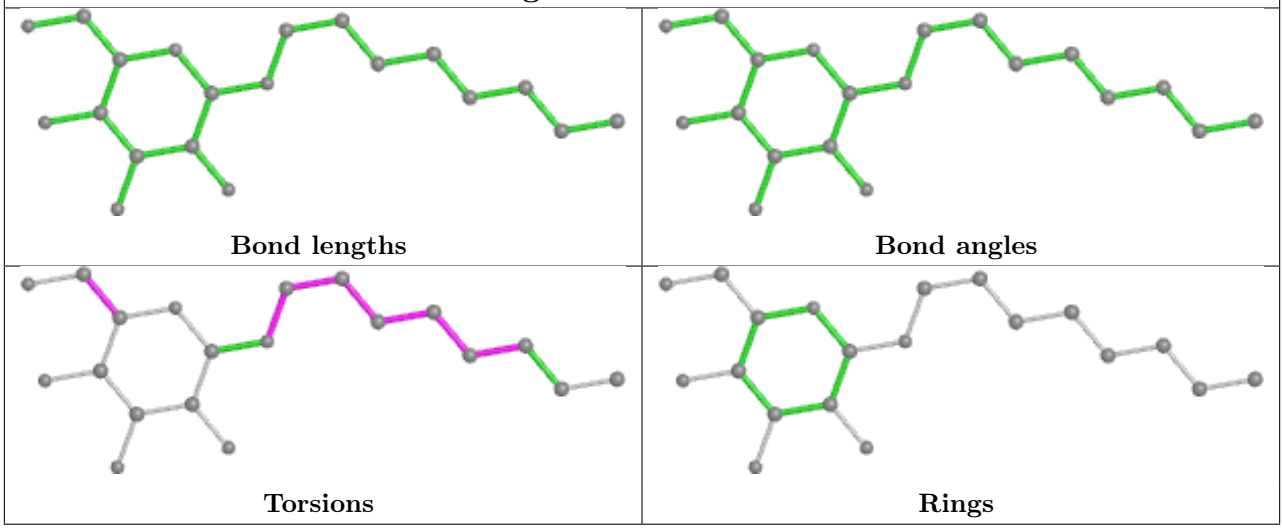


Torsions

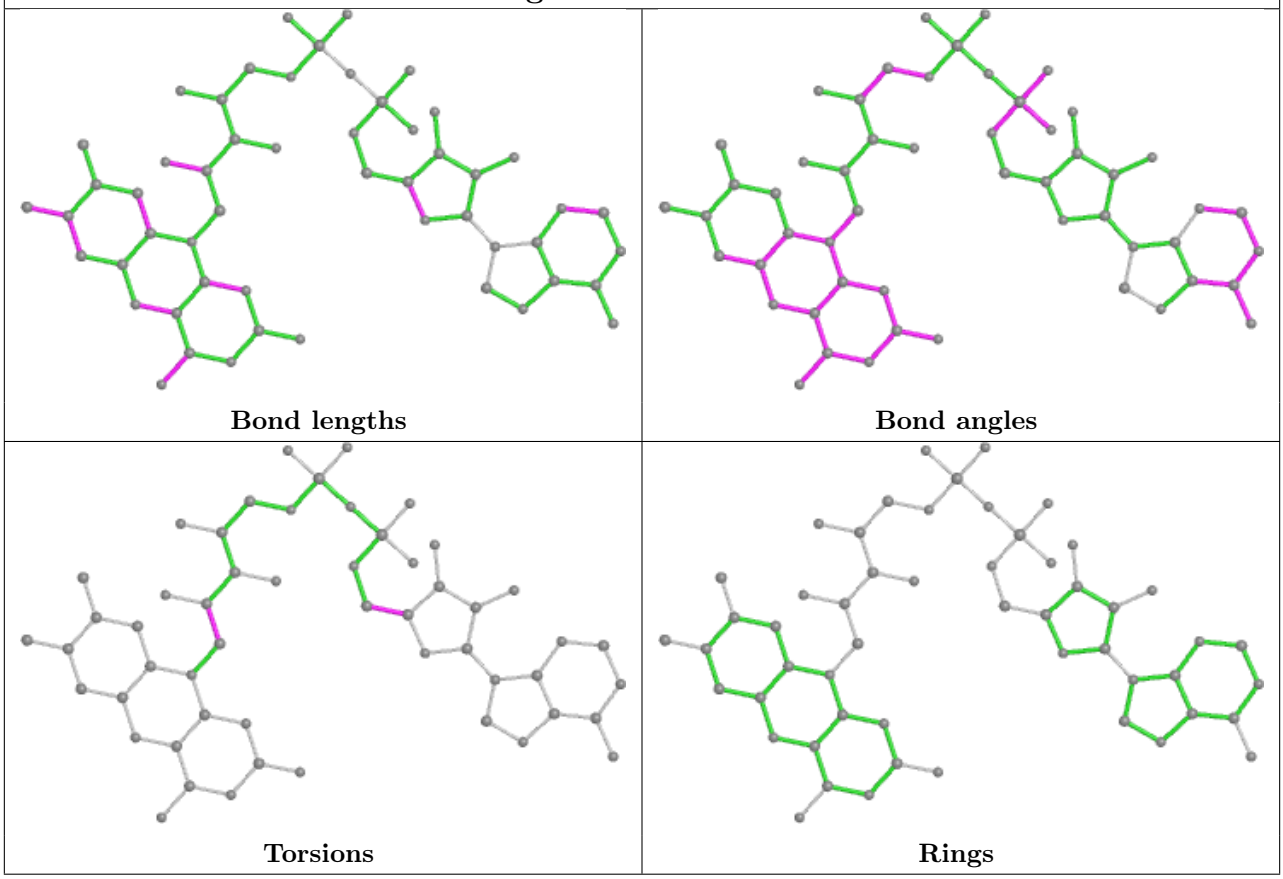


Rings

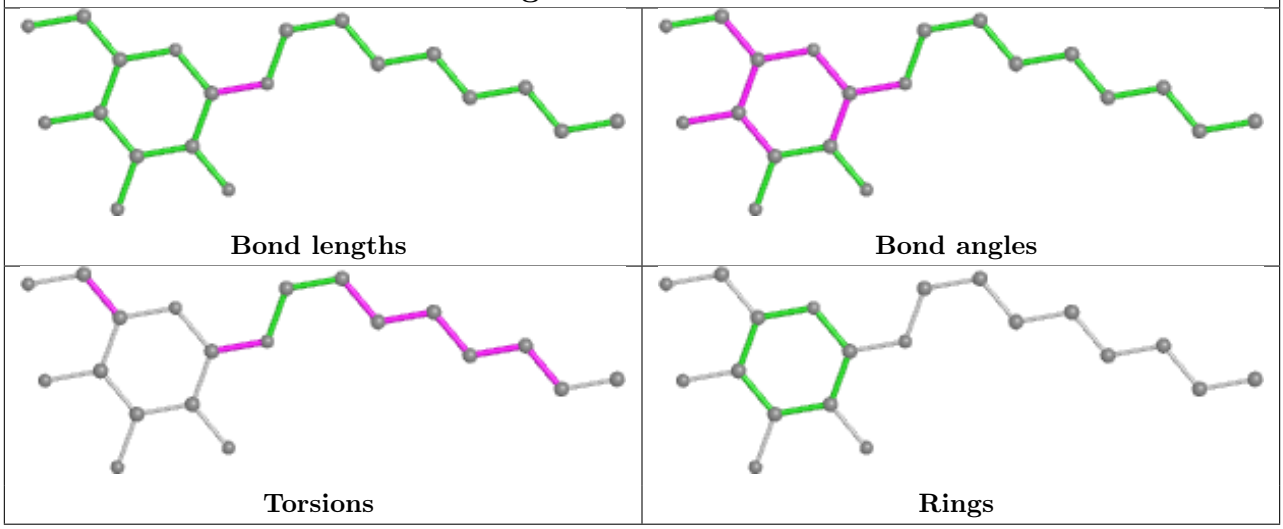
Ligand BOG B 800



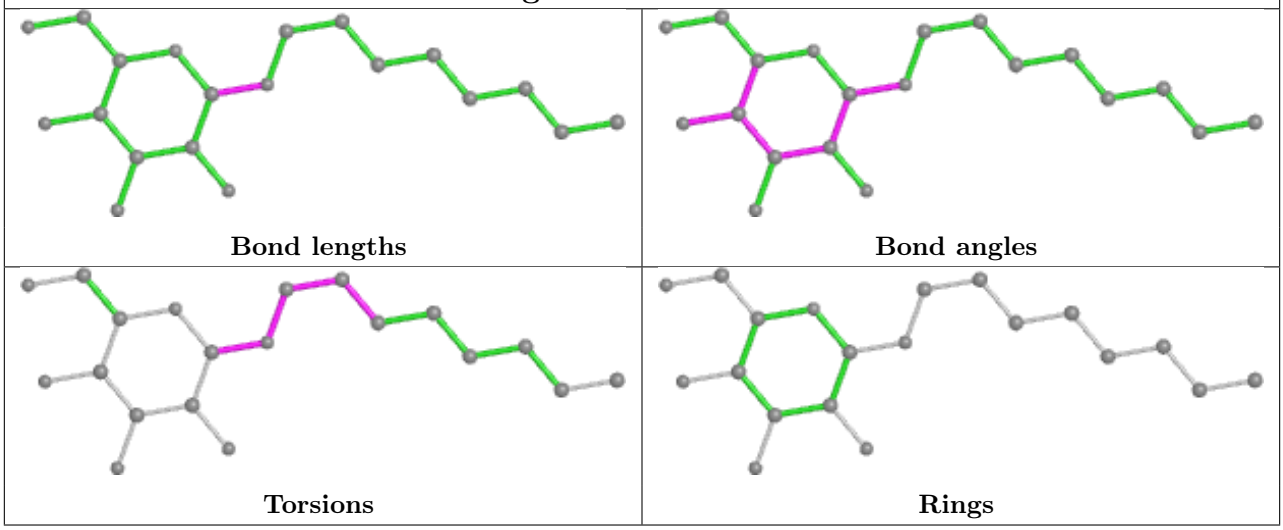
Ligand FAD B 600



Ligand BOG A 900



Ligand BOG B 900



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	495/501 (98%)	-0.35	6 (1%)	79	83	18, 36, 57, 89	0
1	B	495/501 (98%)	-0.35	5 (1%)	82	86	18, 36, 57, 87	0
All	All	990/1002 (98%)	-0.35	11 (1%)	80	85	18, 36, 57, 89	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.1
1	B	1	MET	4.4
1	B	495	GLN	2.7
1	A	495	GLN	2.7
1	A	103	ILE	2.5
1	B	392	GLU	2.4
1	A	2	GLU	2.3
1	B	2	GLU	2.3
1	B	113	LYS	2.3
1	A	325	ASP	2.1
1	A	392	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	910	4/4	0.57	0.27	54,55,55,55	0
2	BOG	A	1949	20/20	0.67	0.39	77,93,97,98	0
6	EDO	A	1963	4/4	0.74	0.22	57,58,58,59	0
2	BOG	B	800	20/20	0.75	0.40	101,105,108,108	0
2	BOG	A	900	20/20	0.76	0.38	89,96,99,100	0
6	EDO	B	7067	4/4	0.77	0.21	49,49,49,50	0
2	BOG	A	800	20/20	0.78	0.49	108,112,114,114	0
2	BOG	A	1950	20/20	0.78	0.29	88,91,94,94	0
2	BOG	B	900	20/20	0.82	0.51	100,105,106,107	0
6	EDO	B	911	4/4	0.89	0.17	53,55,59,59	0
6	EDO	A	7067	4/4	0.91	0.12	45,47,48,50	0
6	EDO	B	906	4/4	0.92	0.15	46,48,56,60	0
6	EDO	A	1959	4/4	0.92	0.14	31,39,39,44	0
3	PO4	A	1955	5/5	0.92	0.18	77,79,81,82	0
5	IMD	A	1958	5/5	0.92	0.21	79,80,81,81	0
8	2PG	A	700	11/11	0.92	0.19	34,39,48,49	0
3	PO4	B	902	5/5	0.93	0.19	79,81,82,83	0
5	IMD	A	1956	5/5	0.93	0.16	62,64,65,66	0
6	EDO	A	1960	4/4	0.93	0.12	44,46,47,49	0
6	EDO	B	909	4/4	0.93	0.18	55,57,60,64	0
6	EDO	A	1961	4/4	0.94	0.32	63,65,65,65	0
3	PO4	A	1952	5/5	0.94	0.16	49,55,56,58	0
3	PO4	B	904	5/5	0.94	0.13	73,74,78,80	0
3	PO4	A	1951	5/5	0.94	0.16	83,84,87,87	0
6	EDO	B	908	4/4	0.94	0.17	30,42,45,46	0
8	2PG	B	700	11/11	0.94	0.19	32,42,48,49	0
3	PO4	A	1953	5/5	0.95	0.12	75,75,76,77	0
5	IMD	B	912	5/5	0.95	0.17	64,65,68,68	0
6	EDO	A	1957	4/4	0.95	0.16	47,50,52,55	0
3	PO4	B	903	5/5	0.95	0.11	54,59,61,61	0
4	FAD	A	600	53/53	0.96	0.13	14,23,26,35	0
6	EDO	B	907	4/4	0.96	0.14	53,53,55,55	0
3	PO4	A	1954	5/5	0.96	0.20	89,90,90,90	0
7	T3A	A	7066	15/15	0.97	0.13	31,45,50,54	0
7	T3A	B	7066	15/15	0.97	0.13	30,42,52,53	0
3	PO4	B	901	5/5	0.97	0.27	98,98,98,99	0
4	FAD	B	600	53/53	0.97	0.12	16,22,26,29	0

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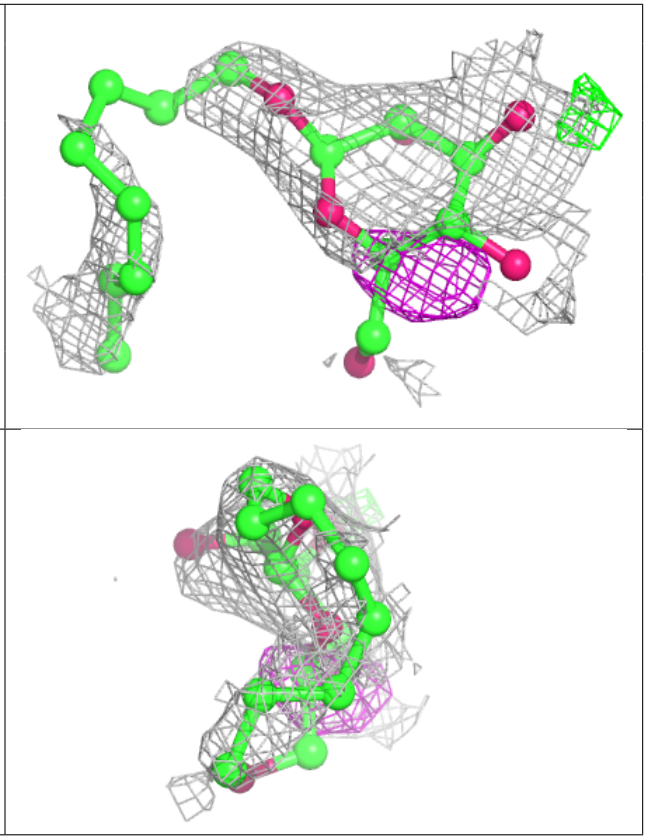
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	905	4/4	0.98	0.14	37,40,44,45	0
6	EDO	A	1962	4/4	0.98	0.11	40,41,46,47	0

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.

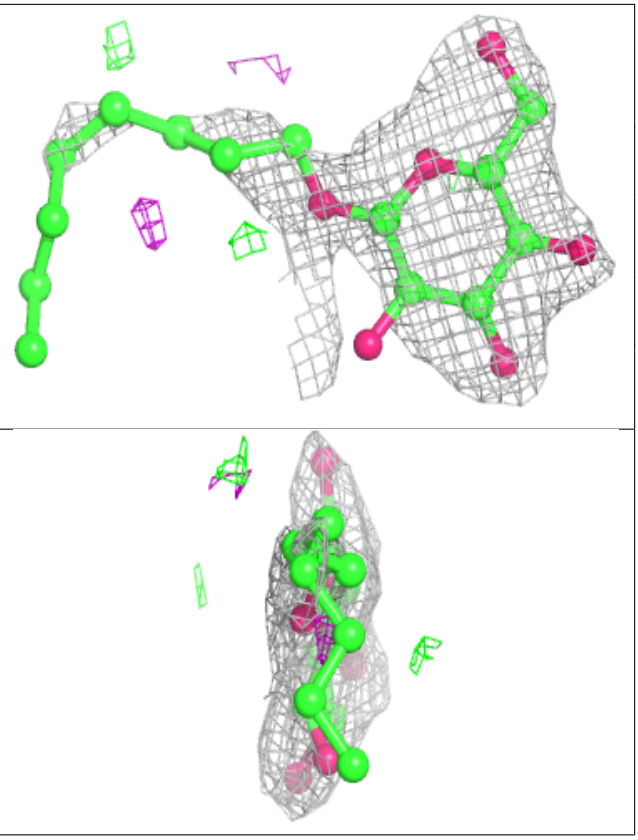
Electron density around BOG A 1949:

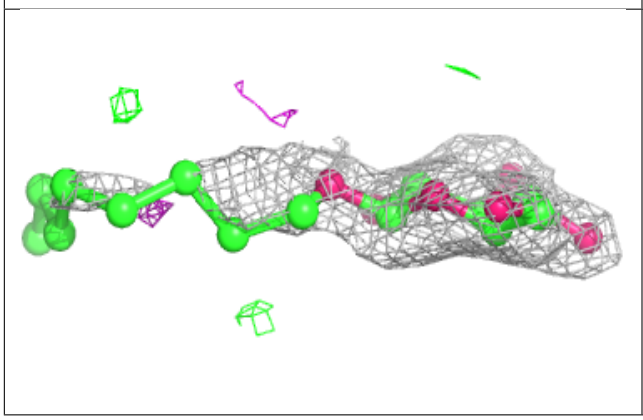
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BOG B 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 900:

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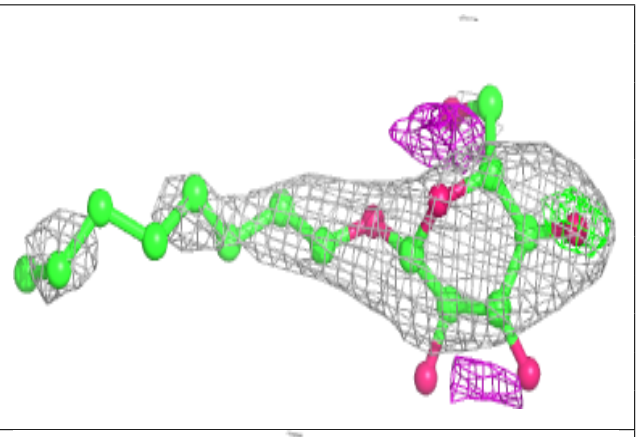
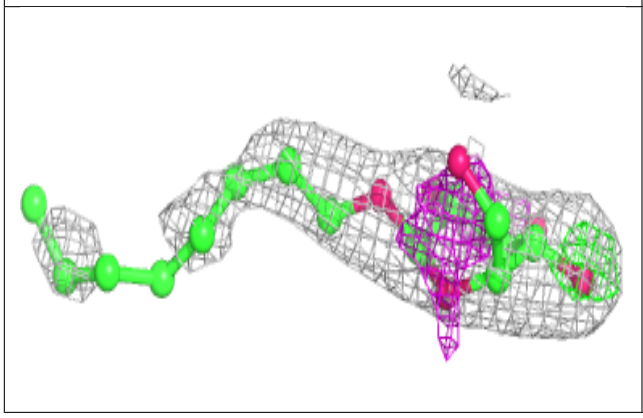
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around BOG A 800:

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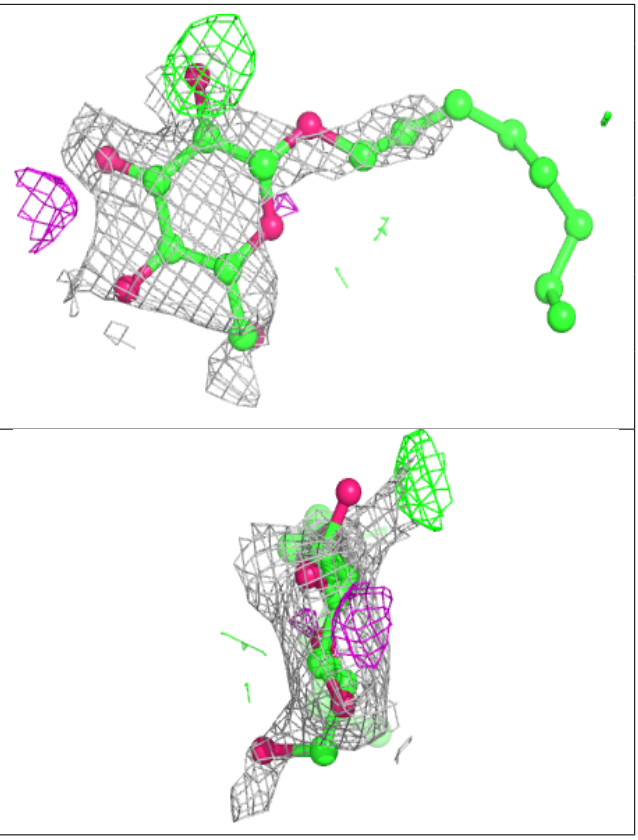
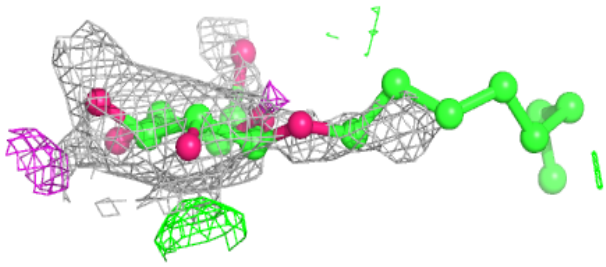
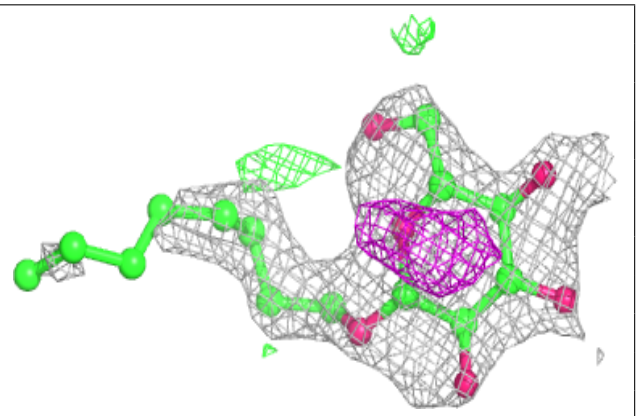
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

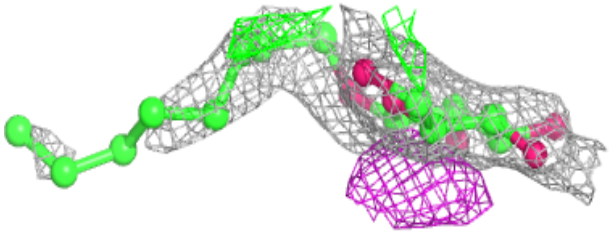


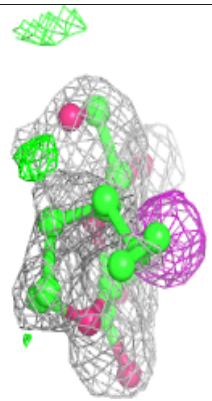


Electron density around BOG A 1950:

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

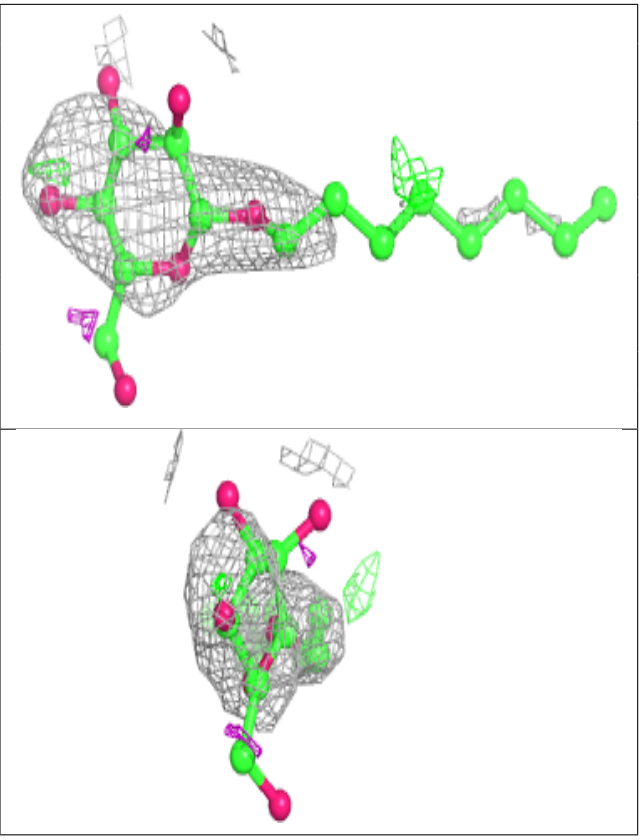


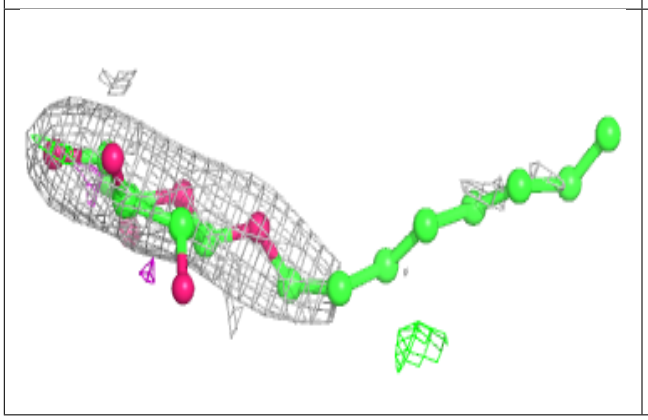




Electron density around BOG B 900:

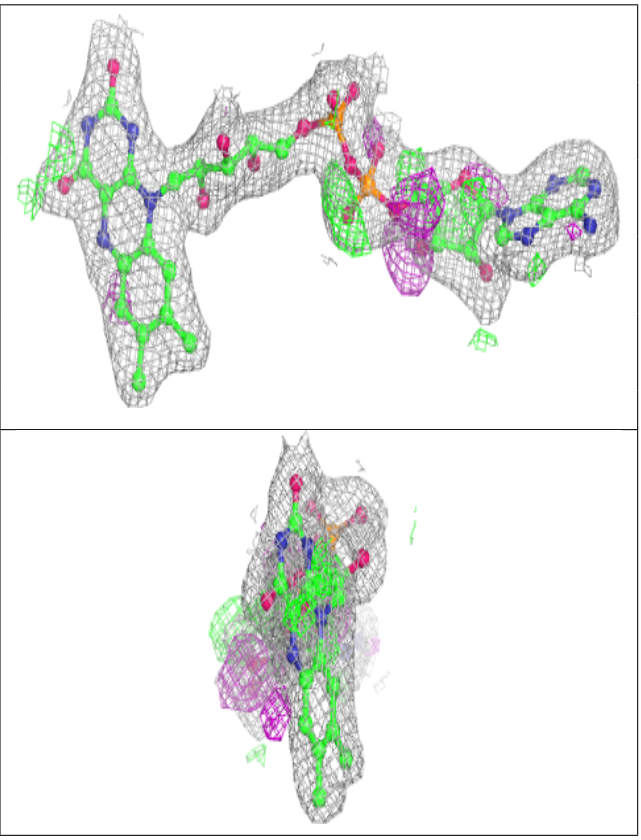
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

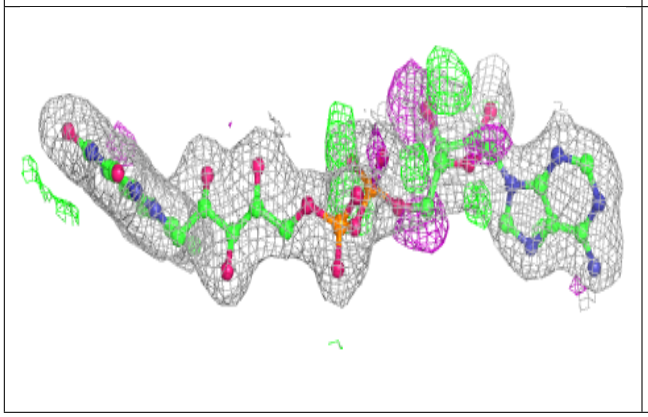




Electron density around FAD A 600:

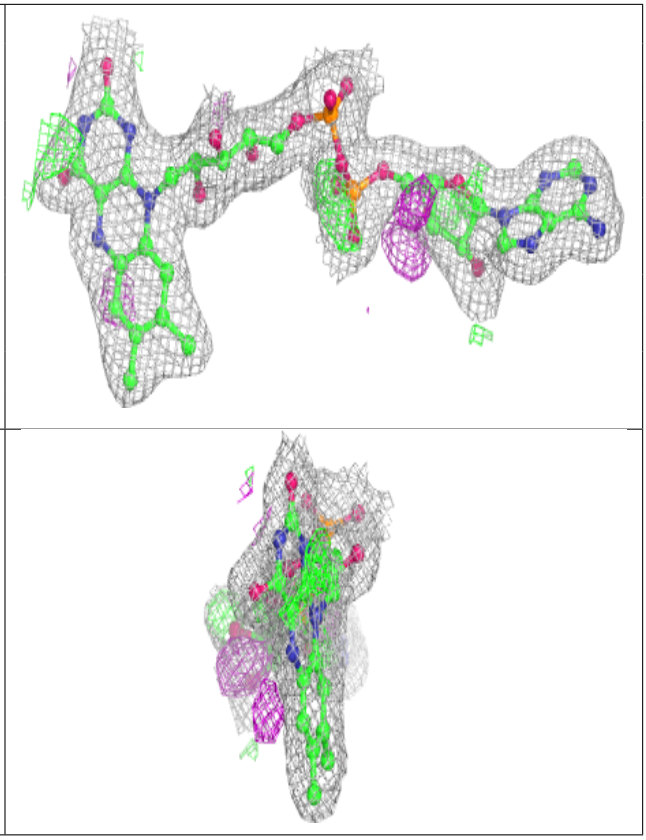
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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.