Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 09:29 AM EDT

PDB ID	:	1BZL
Title	:	CRYSTAL STRUCTURE OF TRYPANOSOMA CRUZI TRYPANOTHIONE REDUCTASE IN COMPLEX WITH TRYPANOTHIONE, AND THE STRUCTURE-BASED DISCOVERY OF NEW NATURAL PRODUCT INHIBITORS
Authors	:	Bond, C.S.; Zhang, Y.; Berriman, M.; Cunningham, M.; Fairlamb, A.H.; Hunter, W.N.
Deposited on	:	1998-11-02
Resolution	:	2.40 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:

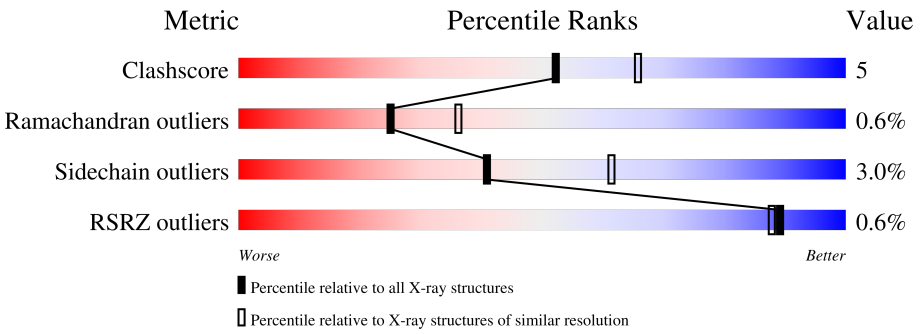
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

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

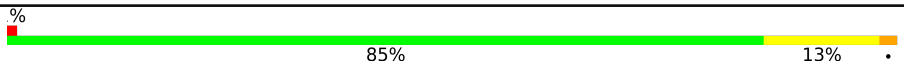
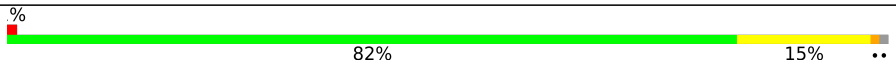
The reported resolution of this entry is 2.40 Å.

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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	486	
1	B	486	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8070 atoms, of which 0 are hydrogens and 0 are deuteriums.

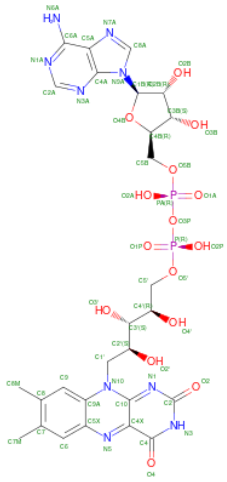
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE (OXIDIZED FORM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	486	3741	2378	636	705	22	0	0	0
1	B	483	3718	2364	632	701	21	0	0	0

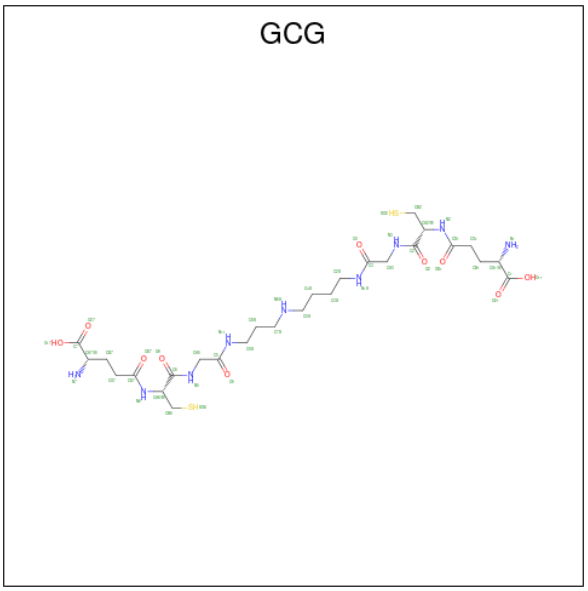
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD



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

- Molecule 3 is BIS(GAMMA-GLUTAMYL-CYSTEINYL-GLYCINYL)SPERMIDINE (three-letter code: GCG) (formula: $C_{27}H_{49}N_9O_{10}S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	48	27	9	10	2	0	0
			Total	C	N	O	S		
3	A	1	48	27	9	10	2	0	0

- Molecule 4 is water.

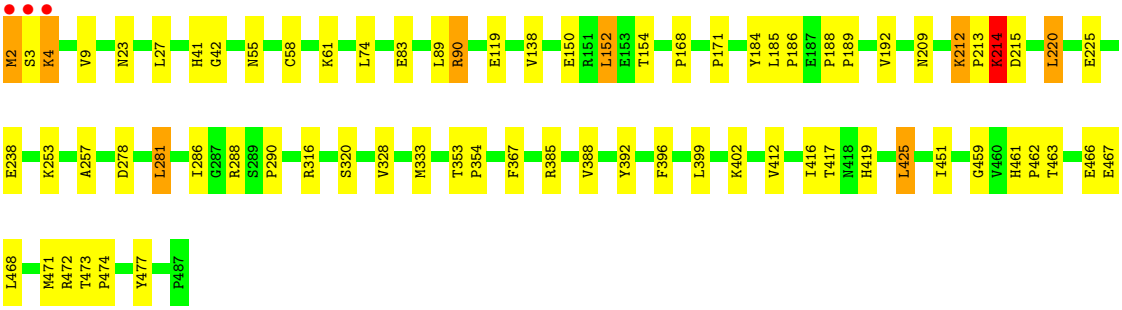
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	220	220	220	0	0
			Total	O		
4	B	189	189	189	0	0

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.

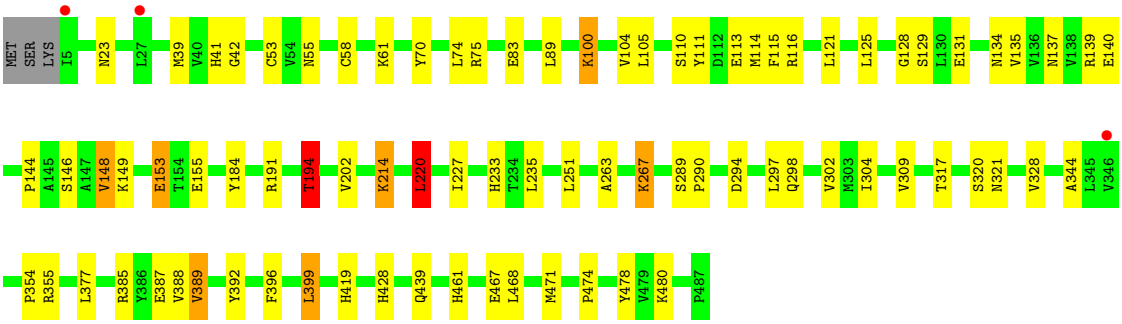
• Molecule 1: TRYPANOTHIONE REDUCTASE (OXIDIZED FORM)

Chain A:



• Molecule 1: TRYPANOTHIONE REDUCTASE (OXIDIZED FORM)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	93.33Å 93.33Å 157.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.4 (8.00-2.40) 94.8 (19.98-2.40)	Depositor EDS
R_{merge}	0.75	Depositor
R_{sym}	0.75	Depositor
$< I/\sigma(I) >$ [1]	6.06 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.209 , (Not available) 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.1	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 97.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.216 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	8070	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, GCG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.61	0/3818	0.87	9/5170 (0.2%)
1	B	0.59	0/3795	0.89	15/5141 (0.3%)
All	All	0.60	0/7613	0.88	24/10311 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	191	ARG	CB-CG-CD	-10.43	84.48	111.60
1	A	281	LEU	CA-CB-CG	9.35	136.80	115.30
1	B	220	LEU	CA-CB-CG	8.81	135.56	115.30
1	A	220	LEU	CA-CB-CG	8.45	134.74	115.30
1	A	152	LEU	CA-CB-CG	7.28	132.04	115.30
1	B	23	ASN	CA-CB-CG	6.43	127.55	113.40
1	B	399	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	316	ARG	CB-CG-CD	-6.09	95.77	111.60
1	B	194	THR	N-CA-CB	-5.83	99.22	110.30
1	B	105	LEU	CA-CB-CG	5.83	128.70	115.30
1	B	214	LYS	CB-CG-CD	-5.77	96.59	111.60
1	B	75	ARG	CB-CG-CD	-5.66	96.89	111.60
1	B	148	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	B	194	THR	CB-CA-C	5.48	126.39	111.60
1	A	385	ARG	CB-CG-CD	-5.37	97.63	111.60
1	B	389	VAL	CG1-CB-CG2	-5.34	102.35	110.90
1	B	191	ARG	CG-CD-NE	5.29	122.90	111.80
1	B	354	PRO	N-CA-C	-5.28	98.38	112.10
1	A	9	VAL	CG1-CB-CG2	-5.27	102.46	110.90
1	A	3	SER	C-N-CA	5.20	134.71	121.70
1	A	425	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	472	ARG	CB-CG-CD	5.06	124.76	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	385	ARG	CB-CG-CD	-5.03	98.52	111.60
1	B	202	VAL	CG1-CB-CG2	-5.00	102.90	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3741	0	3752	37	0
1	B	3718	0	3725	46	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	96	0	90	8	0
4	A	220	0	0	3	0
4	B	189	0	0	8	0
All	All	8070	0	7629	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (84) 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)
3:A:603:GCG:H5	3:A:603:GCG:HB22	1.53	0.73
1:B:233:HIS:HB2	4:B:631:HOH:O	1.93	0.68
1:A:225:GLU:HG2	1:A:253:LYS:HE3	1.77	0.66
3:A:603:GCG:SG6	1:B:461:HIS:CE1	2.91	0.63
1:B:317:THR:HB	4:B:686:HOH:O	1.98	0.62
3:A:604:GCG:HG11	4:A:766:HOH:O	2.00	0.61
1:B:113:GLU:HG3	1:B:116:ARG:HH21	1.66	0.61
1:A:214:LYS:HD2	1:A:215:ASP:H	1.65	0.61
1:B:290:PRO:HB3	1:B:328:VAL:HA	1.81	0.60
1:B:155:GLU:O	1:B:321:ASN:HB2	2.02	0.59
1:B:387:GLU:HG3	1:B:480:LYS:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HA	1:A:471:MET:HE3	1.86	0.57
1:B:113:GLU:HG3	1:B:116:ARG:NH2	2.20	0.56
1:B:139:ARG:NH1	1:B:148:VAL:HG23	2.21	0.56
1:A:90:ARG:HG3	1:B:83:GLU:HG3	1.89	0.53
1:B:70:TYR:O	1:B:74:LEU:HG	2.08	0.53
1:B:131:GLU:HB3	1:B:135:VAL:HB	1.91	0.53
3:A:604:GCG:HA6	3:A:604:GCG:HB22	1.91	0.52
1:B:294:ASP:HB2	4:B:764:HOH:O	2.10	0.52
1:A:4:LYS:HG2	4:A:691:HOH:O	2.10	0.52
1:A:41:HIS:HB3	1:A:55:ASN:OD1	2.11	0.51
1:B:396:PHE:CZ	1:B:467:GLU:HG3	2.46	0.51
1:B:53:CYS:HB3	4:B:625:HOH:O	2.10	0.50
1:B:131:GLU:HB2	1:B:137:ASN:OD1	2.12	0.50
1:A:367:PHE:HE2	4:B:690:HOH:O	1.94	0.50
1:B:297:LEU:HB3	1:B:302:VAL:HG22	1.93	0.50
1:A:290:PRO:HB3	1:A:328:VAL:HA	1.94	0.49
1:B:389:VAL:HB	1:B:478:TYR:HB2	1.94	0.49
1:A:388:VAL:HG12	1:A:419:HIS:HB3	1.93	0.49
1:B:388:VAL:HG12	1:B:419:HIS:HB3	1.95	0.48
1:A:320:SER:HA	4:A:689:HOH:O	2.14	0.48
1:B:115:PHE:CD1	1:B:121:LEU:HG	2.49	0.47
1:B:304:ILE:HD13	1:B:309:VAL:HA	1.96	0.47
1:A:392:TYR:CZ	1:A:474:PRO:HG3	2.49	0.47
1:A:2:MET:HA	1:A:2:MET:CE	2.44	0.46
1:A:463:THR:O	1:A:466:GLU:HG2	2.15	0.46
1:A:396:PHE:CE1	1:A:467:GLU:HG3	2.50	0.46
1:B:392:TYR:CZ	1:B:474:PRO:HG3	2.51	0.46
1:A:4:LYS:HD3	1:A:154:THR:O	2.16	0.46
1:B:39:MET:HG3	1:B:125:LEU:HD13	1.98	0.46
1:B:74:LEU:HD13	1:B:89:LEU:HD11	1.98	0.46
1:B:41:HIS:HB3	1:B:55:ASN:OD1	2.17	0.45
1:B:468:LEU:HA	1:B:471:MET:HE3	1.98	0.45
1:B:297:LEU:HD22	1:B:302:VAL:HG21	1.97	0.45
1:B:134:ASN:O	1:B:153:GLU:HA	2.15	0.45
1:A:459:GLY:HA2	1:B:439:GLN:OE1	2.16	0.45
1:A:288:ARG:HB2	1:A:333:MET:HE1	1.99	0.45
1:B:146:SER:HB2	4:B:776:HOH:O	2.17	0.45
1:A:473:THR:HA	1:A:474:PRO:HD3	1.89	0.45
1:A:461:HIS:HA	1:A:462:PRO:HA	1.82	0.44
1:A:189:PRO:HB2	1:A:192:VAL:HB	1.99	0.44
1:B:42:GLY:HA2	1:B:184:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:HA	1:A:402:LYS:HD2	1.99	0.44
1:B:194:THR:HG22	1:B:220:LEU:HA	1.99	0.44
1:B:227:ILE:HG23	4:B:719:HOH:O	2.17	0.43
1:B:140:GLU:HG2	1:B:149:LYS:HD2	1.99	0.43
1:A:209:ASN:O	1:A:212:LYS:HD2	2.18	0.43
3:A:603:GCG:OD7	1:B:461:HIS:CE1	2.71	0.43
1:A:83:GLU:O	1:B:89:LEU:HA	2.18	0.43
1:B:399:LEU:HD12	4:B:679:HOH:O	2.18	0.43
3:A:603:GCG:SG6	1:B:461:HIS:HE1	2.40	0.43
1:A:23:ASN:O	1:A:27:LEU:HB2	2.19	0.42
1:A:214:LYS:CD	1:A:215:ASP:H	2.31	0.42
1:A:353:THR:HA	1:A:354:PRO:HD3	1.89	0.42
3:A:603:GCG:SG6	1:B:461:HIS:NE2	2.93	0.42
1:B:267:LYS:N	1:B:267:LYS:HD2	2.35	0.42
1:A:171:PRO:HD2	1:A:257:ALA:O	2.18	0.42
1:A:168:PRO:HD3	1:A:286:ILE:HD11	2.01	0.42
3:A:604:GCG:H9S1	1:B:110:SER:OG	2.20	0.42
1:B:128:GLY:HA2	1:B:137:ASN:O	2.20	0.42
1:A:238:GLU:HG3	1:A:412:VAL:HG21	2.01	0.42
1:B:344:ALA:HB1	1:B:355:ARG:O	2.20	0.41
1:A:74:LEU:HD13	1:A:89:LEU:HD11	2.02	0.41
1:A:188:PRO:HG2	1:A:213:PRO:HD3	2.03	0.41
1:B:235:LEU:HD11	1:B:428:HIS:HB3	2.02	0.41
1:B:111:TYR:O	1:B:114:MET:HB3	2.21	0.41
1:A:417:THR:HG21	1:A:451:ILE:HB	2.03	0.40
1:A:477:TYR:CD1	1:A:477:TYR:N	2.89	0.40
2:B:602:FAD:H1'1	2:B:602:FAD:H9	1.86	0.40
1:A:185:LEU:HA	1:A:186:PRO:HD3	1.87	0.40
1:A:42:GLY:HA2	1:A:184:TYR:CZ	2.56	0.40
1:A:192:VAL:HG23	1:A:281:LEU:HD12	2.03	0.40
1:B:100:LYS:O	1:B:104:VAL:HG23	2.22	0.40
1:A:138:VAL:HB	1:A:150:GLU:HB2	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	484/486 (100%)	468 (97%)	14 (3%)	2 (0%)	34	48
1	B	481/486 (99%)	460 (96%)	17 (4%)	4 (1%)	19	29
All	All	965/972 (99%)	928 (96%)	31 (3%)	6 (1%)	25	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	ALA
1	B	320	SER
1	A	4	LYS
1	A	214	LYS
1	B	214	LYS
1	B	144	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	407/407 (100%)	395 (97%)	12 (3%)	42	62
1	B	404/407 (99%)	392 (97%)	12 (3%)	41	61
All	All	811/814 (100%)	787 (97%)	24 (3%)	41	61

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	58	CYS
1	A	61	LYS
1	A	90	ARG
1	A	119	GLU
1	A	152	LEU

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Mol	Chain	Res	Type
1	A	212	LYS
1	A	214	LYS
1	A	220	LEU
1	A	278	ASP
1	A	416	ILE
1	A	425	LEU
1	B	58	CYS
1	B	61	LYS
1	B	100	LYS
1	B	129	SER
1	B	153	GLU
1	B	194	THR
1	B	220	LEU
1	B	251	LEU
1	B	267	LYS
1	B	289	SER
1	B	298	GLN
1	B	377	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	106	ASN
1	A	137	ASN
1	A	156	HIS
1	A	180	ASN
1	A	209	ASN
1	A	217	GLN
1	A	306	ASN
1	A	433	ASN
1	B	106	ASN
1	B	134	ASN
1	B	180	ASN
1	B	249	GLN
1	B	298	GLN
1	B	299	ASN
1	B	433	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
3	GCG	A	604	-	45,47,47	0.93	3 (6%)	56,58,58	1.14	5 (8%)
2	FAD	B	602	-	53,58,58	1.26	6 (11%)	68,89,89	1.20	6 (8%)
2	FAD	A	601	-	53,58,58	1.34	7 (13%)	68,89,89	1.29	8 (11%)
3	GCG	A	603	-	45,47,47	0.74	0	56,58,58	0.96	4 (7%)

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
3	GCG	A	604	-	-	14/61/61/61	-
2	FAD	B	602	-	-	2/30/50/50	0/6/6/6
2	FAD	A	601	-	-	4/30/50/50	0/6/6/6
3	GCG	A	603	-	-	12/61/61/61	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C5X-N5	-3.69	1.32	1.39
2	B	602	FAD	C5X-N5	-3.41	1.32	1.39
2	A	601	FAD	C1'-C2'	-3.24	1.48	1.52
2	B	602	FAD	C6-C7	-3.16	1.34	1.39
3	A	604	GCG	CB6-CA6	-3.04	1.49	1.53
2	B	602	FAD	C9-C8	-3.00	1.35	1.39
2	A	601	FAD	C9-C8	-2.70	1.35	1.39
2	A	601	FAD	C8A-N7A	-2.44	1.30	1.34
2	B	602	FAD	C8A-N7A	-2.32	1.30	1.34
2	B	602	FAD	C9A-N10	-2.29	1.37	1.41
3	A	604	GCG	CB1-CA1	2.29	1.58	1.53
3	A	604	GCG	O17-C7	-2.25	1.23	1.30
2	B	602	FAD	C1'-N10	2.25	1.53	1.48
2	A	601	FAD	C2'-C3'	-2.19	1.49	1.53
2	A	601	FAD	C2-N1	2.09	1.41	1.36
2	A	601	FAD	C6-C7	-2.02	1.36	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	O4B-C1B-C2B	-5.52	98.87	106.93
2	B	602	FAD	C10-N1-C2	3.50	123.89	116.90
3	A	604	GCG	C8S-C9S-N11	3.28	121.60	112.21
3	A	604	GCG	C5-CA5-N5	-3.23	104.10	113.17
2	B	602	FAD	O4B-C1B-C2B	-3.21	102.24	106.93
2	A	601	FAD	C10-N1-C2	3.18	123.25	116.90
3	A	603	GCG	CA6-N6-CD7	2.86	129.01	121.65
3	A	604	GCG	C3S-C2S-N1S	2.82	120.26	112.21
2	B	602	FAD	C4X-C10-N1	-2.57	118.76	124.73
3	A	603	GCG	CA2-CB2-SG2	2.56	117.08	114.19
3	A	604	GCG	C4S-C3S-C2S	2.47	125.27	113.56
2	A	601	FAD	O2'-C2'-C1'	-2.38	104.04	109.80
2	B	602	FAD	O4'-C4'-C5'	-2.33	104.68	109.92
2	A	601	FAD	C5X-N5-C4X	2.28	121.86	118.07
2	B	602	FAD	C10-C4X-N5	-2.27	120.04	124.86
2	A	601	FAD	C4X-C10-N1	-2.20	119.63	124.73
2	A	601	FAD	O4'-C4'-C5'	-2.17	105.03	109.92
3	A	603	GCG	C2-CA2-N2	-2.17	105.26	111.16
3	A	604	GCG	CA6-CB6-SG6	-2.16	111.77	114.19
2	A	601	FAD	C10-C4X-N5	-2.14	120.32	124.86
2	B	602	FAD	C4X-C10-N10	2.14	119.60	116.48
3	A	603	GCG	C8S-C9S-N11	2.06	118.08	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	C9A-C5X-N5	-2.00	120.26	122.43

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	PA-O3P-P-O5'
3	A	603	GCG	N2-CA2-CB2-SG2
3	A	603	GCG	C2-CA2-CB2-SG2
3	A	603	GCG	C4S-C5S-N6S-C7S
3	A	603	GCG	C6-CA6-CB6-SG6
3	A	603	GCG	N6-CA6-CB6-SG6
3	A	604	GCG	O21-C1-CA1-N1
3	A	604	GCG	N2-CA2-CB2-SG2
3	A	604	GCG	C2-CA2-CB2-SG2
3	A	604	GCG	C6-CA6-CB6-SG6
3	A	604	GCG	N6-CA6-CB6-SG6
3	A	603	GCG	CA7-CB7-CG7-CD7
3	A	603	GCG	C3S-C4S-C5S-N6S
3	A	603	GCG	C7S-C8S-C9S-N11
3	A	603	GCG	CB6-CA6-N6-CD7
3	A	603	GCG	N1S-C2S-C3S-C4S
3	A	604	GCG	O11-C1-CA1-N1
2	B	602	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	P-O3P-PA-O1A
2	B	602	FAD	C3B-C4B-C5B-O5B
3	A	603	GCG	C6-CA6-N6-CD7
3	A	604	GCG	O17-C7-CA7-CB7
2	A	601	FAD	P-O3P-PA-O2A
3	A	604	GCG	C4S-C5S-N6S-C7S
3	A	603	GCG	C3-CA3-N3-C2
2	A	601	FAD	O4B-C4B-C5B-O5B
3	A	604	GCG	C2S-C3S-C4S-C5S
3	A	604	GCG	O27-C7-CA7-CB7
3	A	604	GCG	O21-C1-CA1-CB1
3	A	604	GCG	O11-C1-CA1-CB1
3	A	604	GCG	OD7-CD7-CG7-CB7
3	A	604	GCG	N6-CD7-CG7-CB7

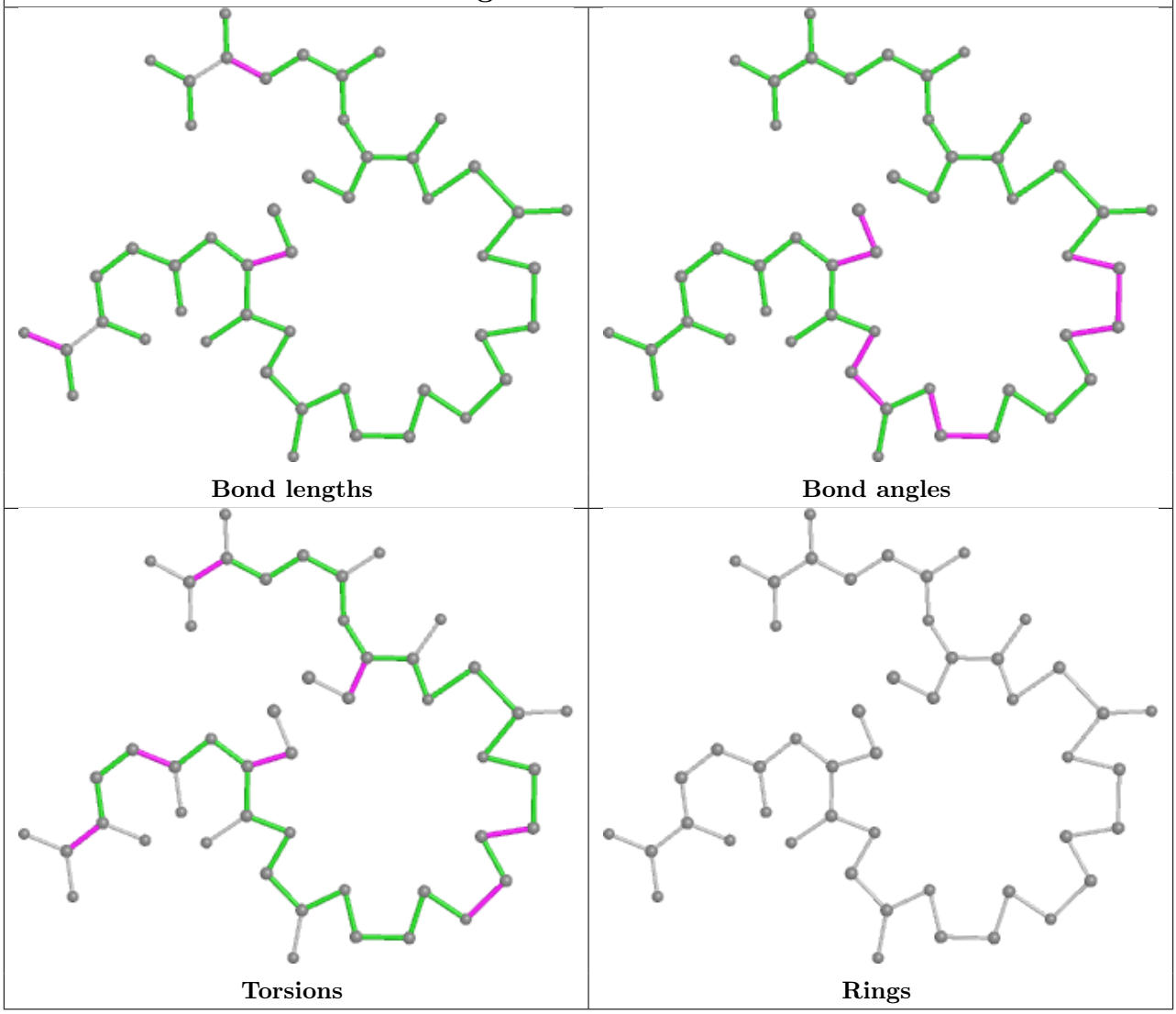
There are no ring outliers.

3 monomers are involved in 9 short contacts:

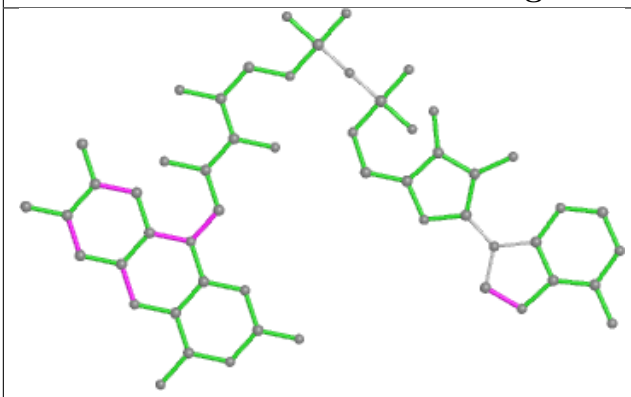
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	GCG	3	0
2	B	602	FAD	1	0
3	A	603	GCG	5	0

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.

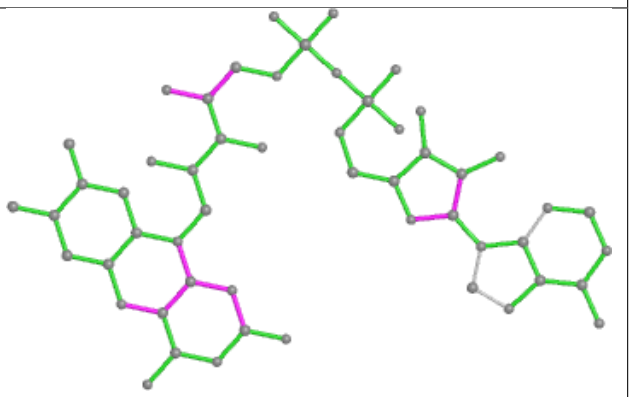
Ligand GCG A 604



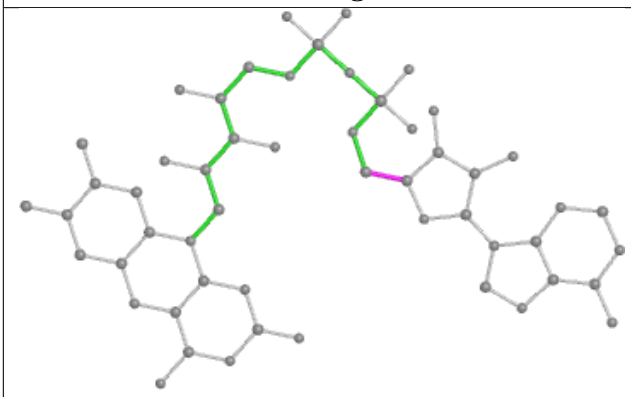
Ligand FAD B 602



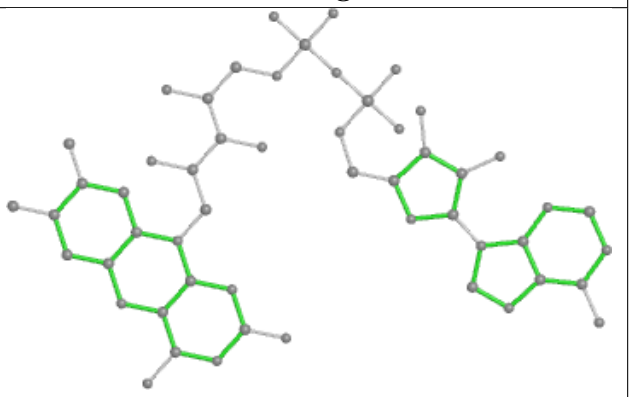
Bond lengths



Bond angles

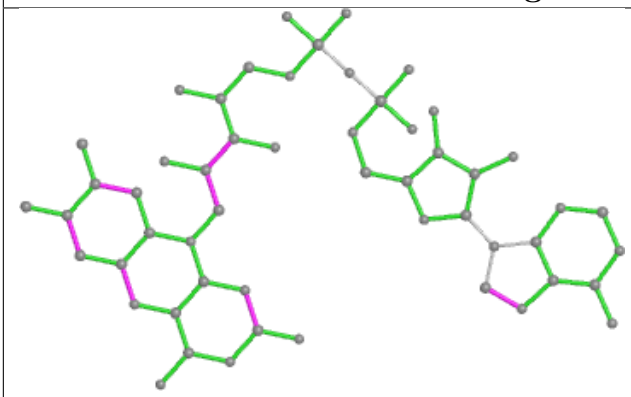


Torsions

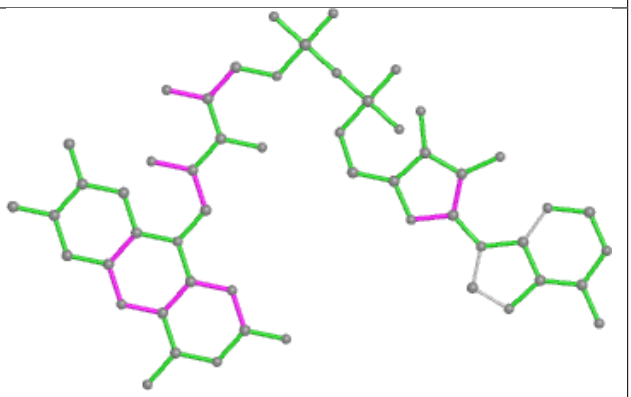


Rings

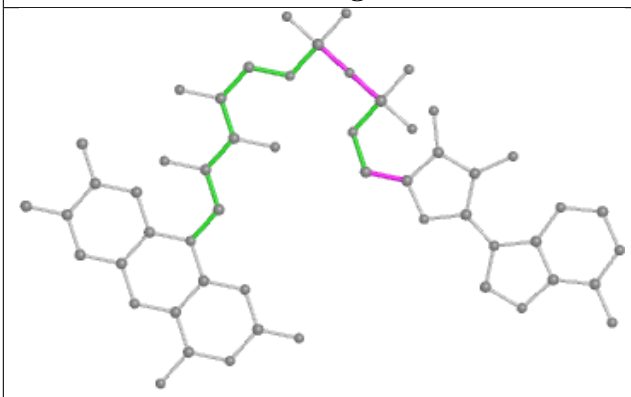
Ligand FAD A 601



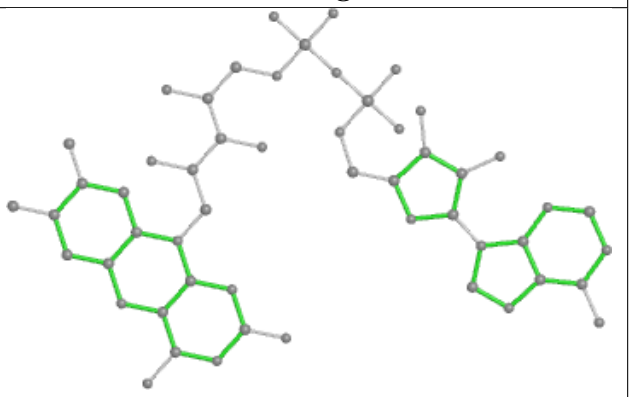
Bond lengths



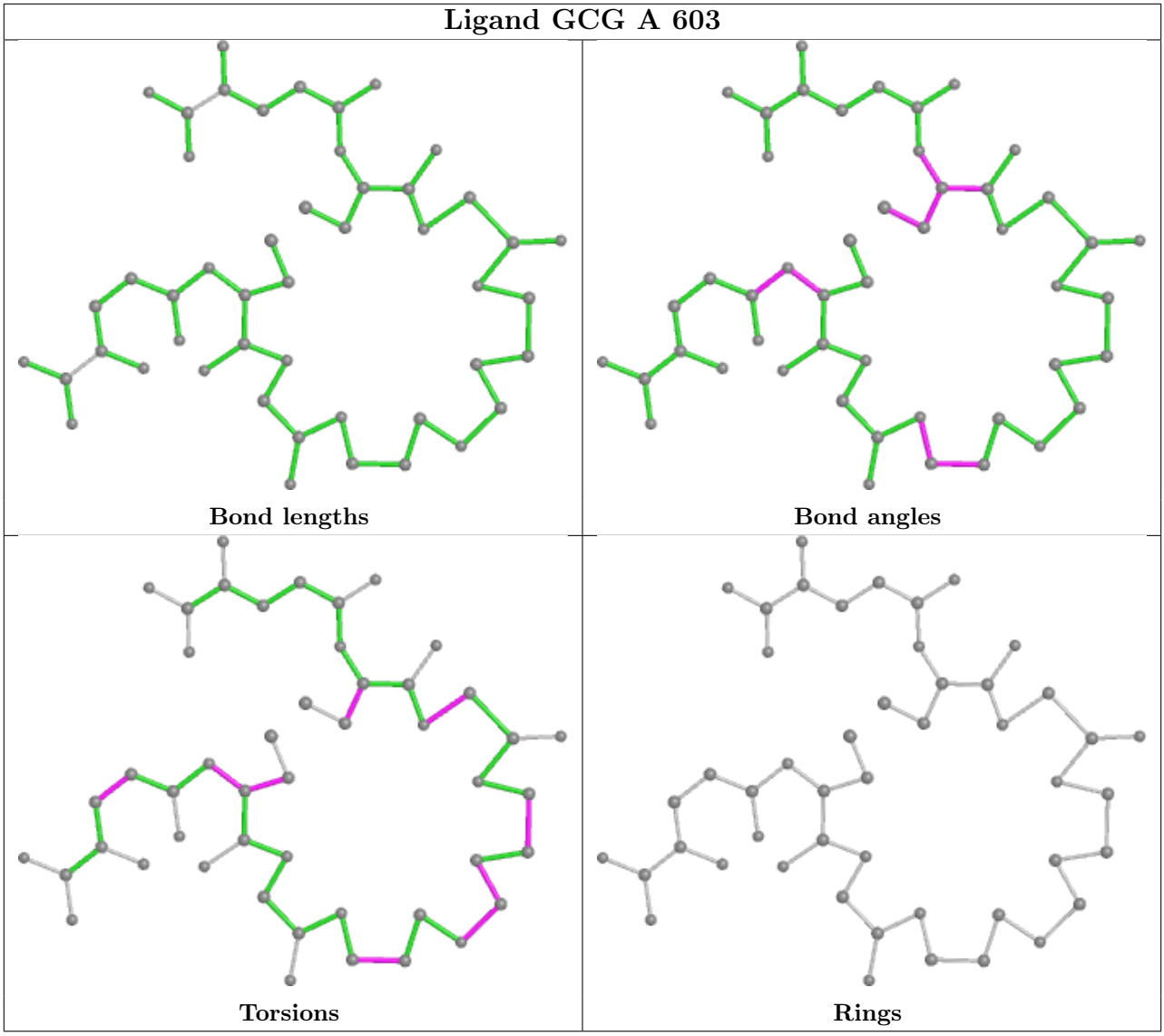
Bond angles



Torsions



Rings



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	486/486 (100%)	-0.69	3 (0%)	89	88	10, 25, 51, 87	0
1	B	483/486 (99%)	-0.47	3 (0%)	89	88	12, 33, 61, 72	0
All	All	969/972 (99%)	-0.58	6 (0%)	89	88	10, 28, 57, 87	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	MET	3.9
1	A	3	SER	3.4
1	B	346	VAL	3.2
1	A	4	LYS	3.1
1	B	27	LEU	2.2
1	B	5	ILE	2.2

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)

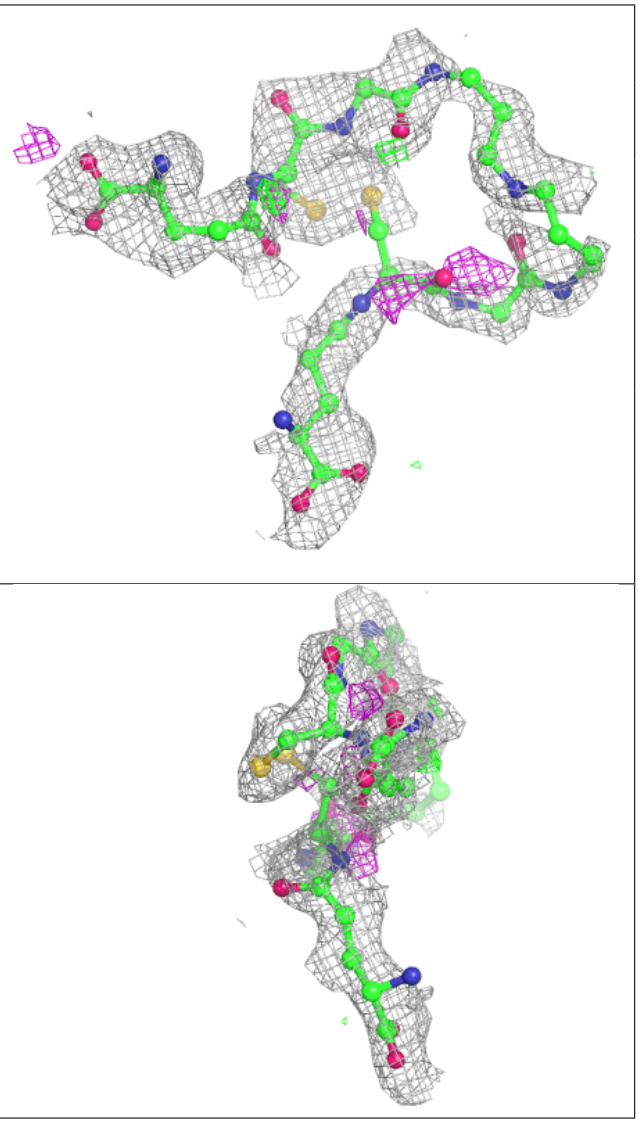
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GCG	A	604	48/48	0.72	0.30	62,69,75,77	0
3	GCG	A	603	48/48	0.74	0.31	53,71,78,84	0
2	FAD	B	602	53/53	0.96	0.10	13,21,39,44	0
2	FAD	A	601	53/53	0.97	0.09	3,15,23,29	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 GCG A 604:

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 GCG A 603:

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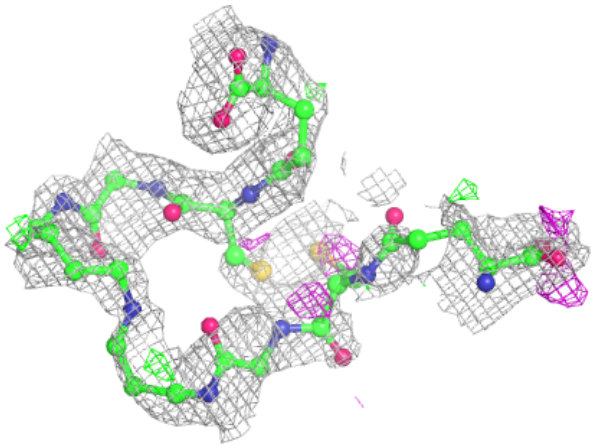
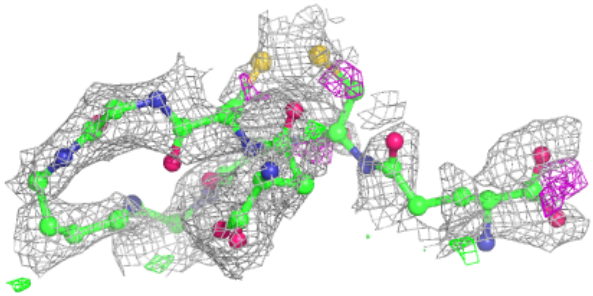
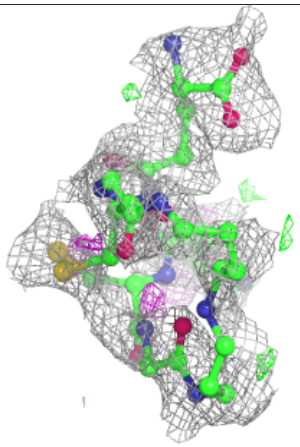
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FAD B 602:

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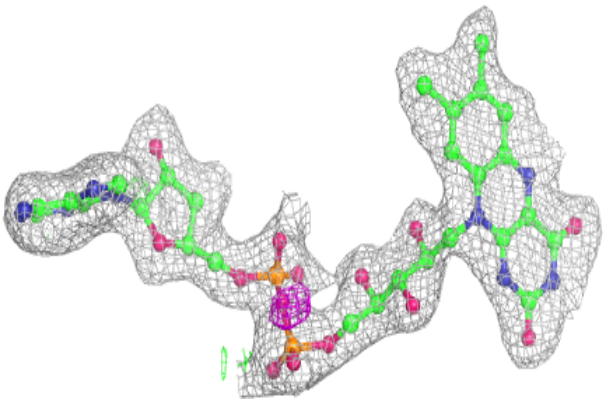
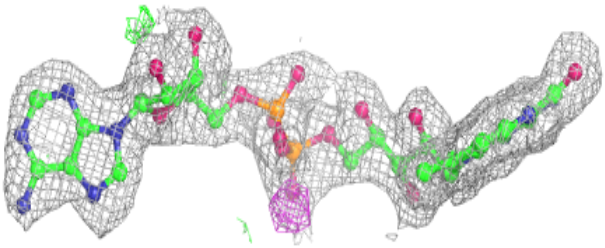
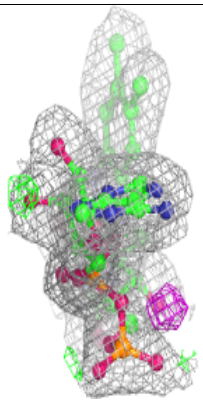
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

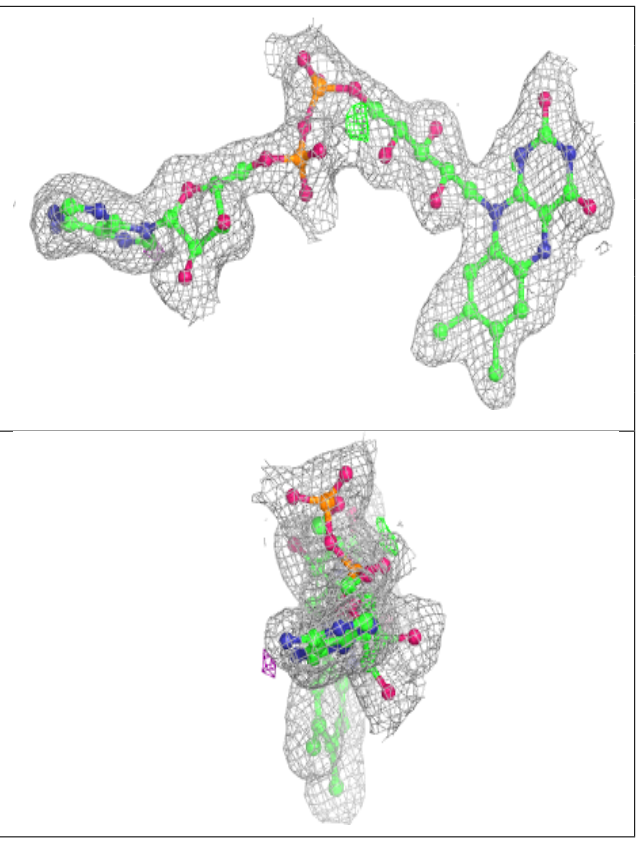






Electron density around FAD A 601:

$2mF_o$-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.