



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:38 PM UTC

PDB ID : 2WOW / pdb_00002wow
Title : Trypanosoma brucei trypanothione reductase with NADP and trypanothione bound
Authors : Alphey, M.S.; Fairlamb, A.H.
Deposited on : 2009-07-30
Resolution : 2.20 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

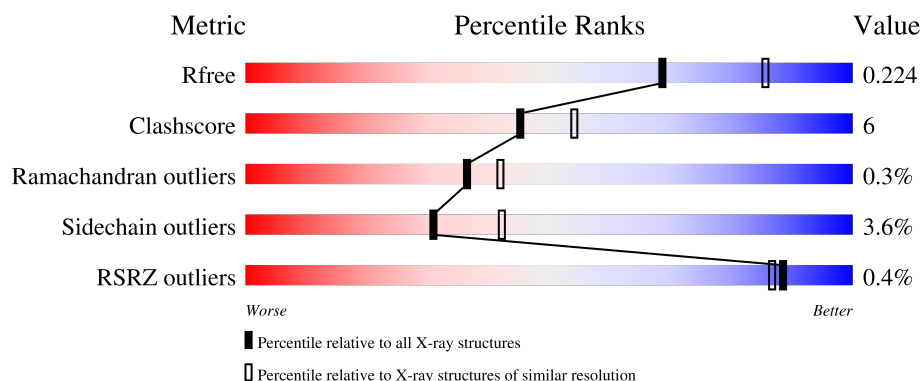
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	495	 82% 15% ..
1	B	495	 80% 17% ..
1	C	495	 87% 11% ..
1	D	495	 86% 13% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16222 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	2	0
			3733	2374	635	704	20			
1	B	488	Total	C	N	O	S	0	1	0
			3714	2363	630	702	19			
1	C	491	Total	C	N	O	S	0	1	0
			3736	2378	634	704	20			
1	D	490	Total	C	N	O	S	0	0	0
			3717	2363	631	704	19			

There are 12 discrepancies between the modelled and reference sequences:

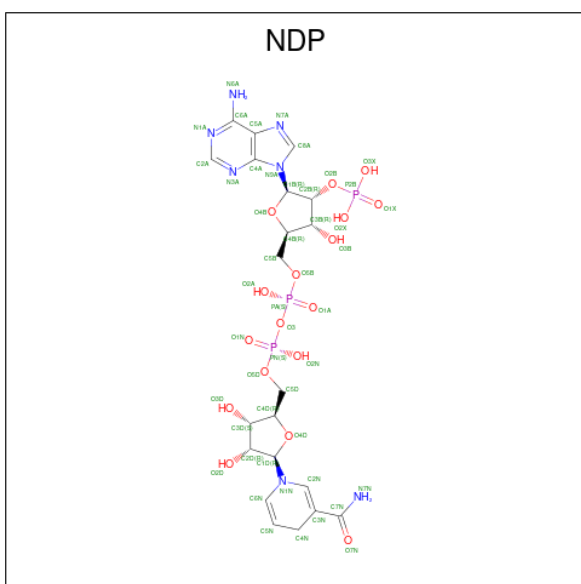
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
C	-1	SER	-	expression tag	UNP Q389T8
C	0	HIS	-	expression tag	UNP Q389T8
D	-2	GLY	-	expression tag	UNP Q389T8
D	-1	SER	-	expression tag	UNP Q389T8
D	0	HIS	-	expression tag	UNP Q389T8

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



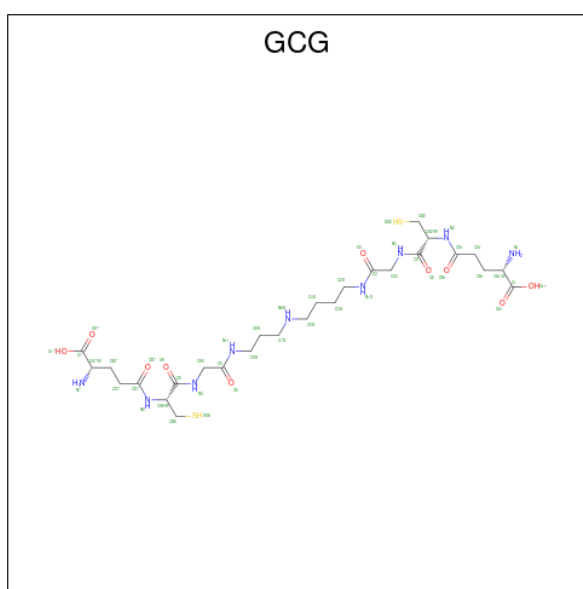
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is BIS(GAMMA-GLUTAMYL-CYSTEINYL-GLYCINYL)SPERMIDINE (CCD ID: GCG) (formula: $C_{27}H_{49}N_9O_{10}S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			71	40	13	15	3		
4	B	1	Total	C	N	O	S	0	1
			71	40	13	15	3		
4	C	1	Total	C	N	O	S	0	1
			71	40	13	15	3		
4	D	1	Total	C	N	O	S	0	1
			71	40	13	15	3		

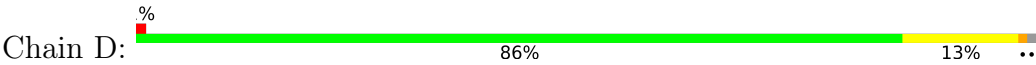
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	149	Total 149	O 149	0	0
5	C	171	Total 171	O 171	0	0
5	D	140	Total 140	O 140	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.70Å 63.70Å 169.60Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	19.87 – 2.20 19.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.87-2.20) 99.5 (19.87-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.172 , 0.226 0.172 , 0.224	Depositor DCC
R_{free} test set	5466 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16222	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.16% 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: GCG, FAD, NDP

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	1.33	10/3818 (0.3%)	1.18	8/5179 (0.2%)
1	B	1.25	4/3792 (0.1%)	1.18	12/5145 (0.2%)
1	C	1.31	6/3819 (0.2%)	1.18	7/5181 (0.1%)
1	D	1.27	3/3795 (0.1%)	1.15	3/5149 (0.1%)
All	All	1.29	23/15224 (0.2%)	1.17	30/20654 (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	B	0	1
1	C	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	ILE	CA-CB	6.85	1.62	1.54
1	C	378	ILE	CA-CB	6.43	1.61	1.54
1	A	335	THR	C-O	-6.24	1.19	1.24
1	C	191	VAL	CA-CB	6.21	1.62	1.54
1	B	278	VAL	CA-CB	6.08	1.65	1.55
1	B	199	ILE	CA-CB	6.07	1.61	1.54
1	B	441	VAL	CA-CB	6.05	1.62	1.54
1	D	204	ALA	CA-CB	-5.78	1.44	1.53
1	C	58	VAL	CA-C	5.69	1.58	1.52
1	C	0	HIS	N-CA	5.66	1.53	1.45
1	C	366	VAL	N-CA	5.65	1.53	1.46
1	D	331	ARG	C-O	-5.58	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	ALA	CA-CB	5.57	1.61	1.53
1	A	159	ALA	CA-CB	5.55	1.58	1.53
1	A	243	THR	CA-CB	5.52	1.62	1.53
1	C	42	PRO	C-O	-5.51	1.18	1.24
1	A	24	ALA	CA-CB	5.47	1.61	1.53
1	B	135	VAL	CA-CB	5.34	1.60	1.54
1	A	47	ALA	C-O	-5.27	1.20	1.24
1	A	169	ILE	CA-CB	5.16	1.60	1.54
1	A	52	CYS	C-O	-5.08	1.18	1.24
1	A	55	VAL	CA-CB	5.05	1.61	1.54
1	A	256	ALA	CA-CB	5.02	1.61	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	ASN	N-CA-C	7.61	120.47	111.71
1	A	116	ASP	N-CA-C	7.57	121.00	111.69
1	B	397	THR	CA-C-N	7.26	128.08	119.94
1	B	397	THR	C-N-CA	7.26	128.08	119.94
1	B	403	ILE	N-CA-C	7.16	117.95	110.72
1	A	369	ILE	N-CA-C	-6.91	101.31	108.15
1	A	292	ASN	N-CA-C	6.70	119.42	111.71
1	C	292	ASN	N-CA-C	6.62	119.32	111.71
1	B	398	PRO	O-C-N	-6.18	115.34	123.01
1	A	215	GLY	N-CA-C	6.11	121.25	112.82
1	C	187	PRO	CA-C-N	-5.97	113.79	119.76
1	C	187	PRO	C-N-CA	-5.97	113.79	119.76
1	B	319	VAL	N-CA-C	5.93	112.96	107.56
1	B	187	PRO	CA-C-N	-5.75	114.04	119.85
1	B	187	PRO	C-N-CA	-5.75	114.04	119.85
1	D	232	GLU	N-CA-C	5.62	117.09	111.07
1	C	234	ILE	N-CA-C	5.47	116.20	110.62
1	B	42	PRO	O-C-N	5.46	123.82	121.31
1	D	340	ASN	N-CA-C	-5.42	105.46	111.36
1	B	215	GLY	N-CA-C	5.36	118.23	112.33
1	B	198	PHE	CB-CA-C	-5.28	102.58	110.88
1	A	13	GLY	N-CA-C	-5.20	106.55	112.79
1	A	434	ALA	CA-C-N	-5.15	113.33	119.05
1	A	434	ALA	C-N-CA	-5.15	113.33	119.05
1	C	0	HIS	N-CA-C	5.15	117.21	109.23
1	B	111	GLU	N-CA-C	-5.14	105.13	111.40
1	A	403	ILE	CB-CA-C	5.12	115.45	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	SER	N-CA-C	5.09	116.03	108.60
1	C	361	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	232	GLU	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	353	LYS	Peptide
1	C	352	ASN	Peptide

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	3733	0	3748	45	0
1	B	3714	0	3723	60	0
1	C	3736	0	3744	39	0
1	D	3717	0	3721	32	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	48	0	26	0	0
3	B	48	0	26	0	0
3	C	48	0	26	1	0
3	D	48	0	26	0	0
4	A	71	0	46	3	0
4	B	71	0	46	4	0
4	C	71	0	46	4	0
4	D	71	0	46	6	0
5	A	174	0	0	0	0
5	B	149	0	0	4	0
5	C	171	0	0	5	0
5	D	140	0	0	2	0
All	All	16222	0	15348	184	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 6.

All (184) 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)
4:C:1001[A]:GCG:HG72	4:C:1001[A]:GCG:O27	1.53	1.08
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.17	1.06
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.40	1.02
1:B:399[B]:LEU:O	1:B:400:MET:HB3	1.68	0.91
1:A:446:ARG:HH11	1:A:446:ARG:CG	1.86	0.89
1:B:347:ASP:HB3	1:B:353:LYS:HG3	1.54	0.89
1:C:318:ASN:H	1:C:318:ASN:HD22	1.22	0.88
1:C:446:ARG:HH21	1:C:446:ARG:HG2	1.39	0.87
1:B:224:ASN:HD22	1:B:252:ASN:HD21	1.22	0.84
1:A:394:SER:HA	4:B:1001[A]:GCG:HA7	1.57	0.84
1:B:130:GLU:CD	1:B:150:ARG:HH12	1.87	0.82
1:C:455[A]:TYR:CZ	1:C:472:ARG:HD2	2.16	0.81
1:B:396:PHE:CE1	1:B:467:GLU:HG3	2.19	0.78
1:B:130:GLU:OE2	1:B:150:ARG:NH1	2.14	0.78
4:D:1001[B]:GCG:H8S2	4:D:1001[B]:GCG:O5	1.83	0.78
1:A:396:PHE:CE1	1:A:467:GLU:HG3	2.18	0.78
1:C:216:LYS:HE2	5:C:2065:HOH:O	1.89	0.73
1:C:403:ILE:HD11	1:D:102:ALA:HB2	1.70	0.73
1:D:224:ASN:HD22	1:D:252:ASN:HD21	1.35	0.72
1:A:157:LEU:HD11	1:A:325:ILE:HG12	1.72	0.72
1:A:318:ASN:HD22	1:A:318:ASN:H	1.38	0.72
1:B:130:GLU:HB2	1:B:136:VAL:CG2	2.20	0.71
4:B:1001[A]:GCG:HG72	4:B:1001[A]:GCG:O17	1.83	0.71
1:D:396:PHE:CE1	1:D:467:GLU:HG3	2.27	0.69
1:C:129:LEU:HD23	1:C:299:VAL:HG21	1.73	0.69
1:D:130:GLU:HB2	1:D:136:VAL:CG2	2.23	0.69
1:B:356:LYS:HE3	5:B:2109:HOH:O	1.92	0.69
1:C:396:PHE:CE1	1:C:467:GLU:HG2	2.30	0.67
1:C:446:ARG:HH21	1:C:446:ARG:CG	2.08	0.66
1:B:399[A]:LEU:CD1	1:B:402:ASN:HD22	2.08	0.66
1:A:455:TYR:CZ	1:A:472:ARG:HD2	2.31	0.65
1:D:130:GLU:HB2	1:D:136:VAL:HG23	1.79	0.64
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.78	0.63
4:C:1001[A]:GCG:O27	4:C:1001[A]:GCG:CG7	2.31	0.63
1:A:353:LYS:HE3	1:A:355:ARG:HE	1.64	0.63
1:B:370:PRO:HG2	1:B:430:LEU:HD11	1.79	0.63
1:D:117:THR:O	5:D:2018:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ASN:HB2	5:D:2021:HOH:O	1.99	0.62
1:C:318:ASN:HD22	1:C:318:ASN:N	1.95	0.62
1:C:250:MET:HE2	1:C:253:GLU:HG3	1.81	0.61
1:A:60:LYS:HD2	1:A:60:LYS:C	2.26	0.61
1:C:157:LEU:HD13	1:C:345:LEU:HD22	1.83	0.61
1:B:399[B]:LEU:O	1:B:400:MET:CB	2.47	0.60
1:C:455[A]:TYR:OH	1:C:472:ARG:HD2	2.02	0.59
1:D:129:LEU:HD22	1:D:296:LEU:HD23	1.84	0.59
1:B:347:ASP:HB3	1:B:353:LYS:CG	2.29	0.59
1:B:131:SER:O	1:B:133:ASN:N	2.36	0.59
1:A:446:ARG:HG2	1:A:446:ARG:NH1	1.98	0.59
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.83	0.58
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.69	0.58
1:C:224:ASN:HD22	1:C:252:ASN:HD21	1.52	0.57
1:A:142:ASP:OD1	1:A:144:LYS:HE3	2.05	0.57
1:C:369:ILE:HG23	5:C:2142:HOH:O	2.05	0.57
1:A:302:LYS:H	1:A:318:ASN:ND2	2.03	0.57
1:B:479:VAL:HB	1:B:484:MET:HE3	1.87	0.56
1:A:289:PRO:HG3	1:A:330:ASP:HB2	1.85	0.56
1:B:250:MET:CE	1:B:253:GLU:HG3	2.25	0.56
4:A:1001[A]:GCG:O27	4:A:1001[A]:GCG:HG72	2.06	0.55
1:B:155:HIS:HB3	1:B:323:TYR:HE2	1.71	0.55
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.72	0.55
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.55	0.55
1:A:401:HIS:HD2	1:A:404:SER:OG	1.90	0.54
4:A:1001[A]:GCG:OD7	4:A:1001[A]:GCG:O6	2.25	0.54
4:B:1001[A]:GCG:O17	4:B:1001[A]:GCG:CG7	2.53	0.54
1:C:302:LYS:H	1:C:318:ASN:ND2	2.05	0.54
1:B:320:PRO:O	1:B:321:ASN:ND2	2.41	0.54
1:A:84:ASP:OD1	1:A:86:SER:HB2	2.07	0.54
1:B:348:THR:HA	1:B:354:PRO:HA	1.89	0.54
1:A:370:PRO:HG2	1:A:430:LEU:HD11	1.90	0.53
1:A:394:SER:OG	4:B:1001[A]:GCG:HB72	2.09	0.53
1:B:131:SER:HA	1:B:299:VAL:CG1	2.39	0.52
1:C:199:ILE:HG13	3:C:800:NDP:H5N	1.91	0.52
1:B:4:ALA:HA	1:B:152:GLN:HB3	1.91	0.52
1:B:482:GLU:HG2	1:B:484:MET:HE2	1.90	0.52
1:C:302:LYS:H	1:C:318:ASN:HD21	1.56	0.52
1:C:293:ASP:HB2	5:C:2098:HOH:O	2.09	0.51
1:C:304:THR:HB	1:C:305:PRO:CD	2.41	0.51
1:D:157:LEU:HD11	1:D:325:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLU:HB3	1:D:404:SER:HB2	1.92	0.51
1:A:250:MET:HE3	1:A:253:GLU:HG3	1.93	0.50
1:B:250:MET:HE2	1:B:253:GLU:CG	2.27	0.50
4:D:1001[A]:GCG:O5	4:D:1001[A]:GCG:C7S	2.59	0.50
1:A:13:GLY:HA2	1:A:50:GLY:HA3	1.93	0.50
1:C:152:GLN:NE2	5:C:2048:HOH:O	2.45	0.50
1:C:396:PHE:HB2	4:D:1001[A]:GCG:HB62	1.94	0.50
1:B:19:ALA:O	1:B:346:VAL:HG21	2.11	0.49
1:B:224:ASN:ND2	1:B:252:ASN:HD21	2.00	0.49
4:C:1001[B]:GCG:N7	4:C:1001[B]:GCG:OD7	2.45	0.49
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.47	0.49
1:C:216:LYS:HE3	1:C:248:GLU:HB3	1.93	0.49
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.94	0.48
1:B:68:GLN:NE2	5:B:2012:HOH:O	2.42	0.48
1:D:397:THR:HG22	1:D:398:PRO:O	2.13	0.48
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.43	0.48
1:D:266:LYS:N	1:D:266:LYS:HD2	2.28	0.48
1:B:424:VAL:HG12	1:B:445:LEU:HD11	1.95	0.48
1:D:241:GLN:OE1	1:D:370:PRO:HG3	2.13	0.48
1:B:130:GLU:HB2	1:B:136:VAL:HG23	1.95	0.48
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.96	0.47
1:A:224:ASN:HD22	1:A:252:ASN:HD21	1.61	0.47
1:C:40:HIS:ND1	1:C:183:TYR:OH	2.40	0.47
4:D:1001[B]:GCG:O5	4:D:1001[B]:GCG:C8S	2.60	0.47
1:B:131:SER:HA	1:B:299:VAL:HG12	1.97	0.47
1:C:403:ILE:CD1	1:D:102:ALA:HB2	2.42	0.47
4:C:1001[A]:GCG:HN71	1:D:395:SER:H	1.59	0.47
1:D:92:TRP:HB3	1:D:187:PRO:HD3	1.97	0.47
1:A:302:LYS:H	1:A:318:ASN:HD21	1.62	0.47
1:B:399[A]:LEU:HD12	1:B:399[A]:LEU:HA	1.54	0.46
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.98	0.46
1:B:34:VAL:HG22	1:B:123:PHE:HB2	1.97	0.46
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.98	0.46
1:C:475:SER:OG	5:C:2157:HOH:O	2.05	0.46
1:D:176:ILE:HB	1:D:180:GLU:HB2	1.97	0.46
1:B:34:VAL:HG12	2:B:700:FAD:H2A	1.96	0.46
1:C:446:ARG:CG	1:C:446:ARG:NH2	2.71	0.46
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.99	0.45
1:B:331:ARG:HG3	5:B:2031:HOH:O	2.16	0.45
1:A:438:ILE:HG13	1:A:438:ILE:O	2.16	0.45
1:B:34:VAL:HA	1:B:123:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:THR:HG23	1:B:354:PRO:HB3	1.99	0.45
4:D:1001[A]:GCG:HA6	4:D:1001[A]:GCG:HA51	1.61	0.45
1:A:406:SER:HB3	1:A:409:LYS:HG3	1.97	0.45
1:B:130:GLU:HB3	1:B:134:VAL:HB	1.99	0.45
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.98	0.45
1:C:318:ASN:H	1:C:318:ASN:ND2	2.02	0.45
1:D:60:LYS:HD2	1:D:60:LYS:C	2.42	0.45
1:D:335:THR:HB	1:D:336:PRO:HD3	1.99	0.44
1:B:399[A]:LEU:HD11	1:B:402:ASN:HD22	1.80	0.44
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.82	0.44
4:A:1001[A]:GCG:O27	4:A:1001[A]:GCG:CG7	2.65	0.44
1:B:353:LYS:HB2	1:B:354:PRO:HA	1.98	0.44
1:A:314:PHE:O	1:A:315:SER:HB2	2.17	0.44
1:A:160:THR:OG1	1:A:328:ILE:HD12	2.17	0.44
2:B:700:FAD:H9	2:B:700:FAD:H1'1	1.75	0.44
1:A:445:LEU:HD12	1:A:445:LEU:N	2.32	0.43
1:C:56:GLY:HA2	2:C:700:FAD:C7	2.49	0.43
1:C:435:PRO:O	1:C:438:ILE:HG22	2.18	0.43
1:D:398:PRO:HD2	1:D:409:LYS:O	2.18	0.43
1:C:234:ILE:HG12	1:C:430:LEU:HB2	2.00	0.43
1:B:131:SER:O	1:B:132:LYS:C	2.62	0.43
1:D:234:ILE:HG12	1:D:430:LEU:HB2	2.01	0.43
1:A:287:ARG:HD2	2:A:700:FAD:HM82	2.01	0.43
1:A:64:VAL:O	1:A:68[A]:GLN:HG3	2.19	0.43
1:A:73:LEU:CD2	1:B:73:LEU:HD23	2.48	0.42
1:B:60:LYS:HE2	1:B:60:LYS:HB3	1.81	0.42
1:C:318:ASN:N	1:C:318:ASN:ND2	2.63	0.42
1:B:157:LEU:HD11	1:B:325:ILE:HG12	2.01	0.42
1:D:218:THR:HG23	1:D:248:GLU:HG2	2.00	0.42
1:A:461:HIS:HA	1:A:462:PRO:HA	1.82	0.42
1:B:223:ASN:HB3	5:B:2063:HOH:O	2.18	0.42
1:B:461:HIS:HA	1:B:462:PRO:HA	1.89	0.42
1:A:104:LEU:HG	1:A:108:LYS:HE3	2.01	0.42
1:D:304:THR:HB	1:D:305:PRO:CD	2.49	0.42
1:B:299:VAL:HG23	1:B:301:VAL:HG23	2.01	0.42
1:B:392:TYR:N	1:B:392:TYR:CD2	2.88	0.42
1:D:201:VAL:HG12	1:D:368:SER:HB3	2.01	0.42
1:B:397:THR:HA	1:B:398:PRO:HD3	1.90	0.42
1:B:17:LEU:HD13	1:B:110:TYR:CE1	2.54	0.41
1:A:8:VAL:HG23	1:A:153:ALA:HB2	2.01	0.41
1:B:399[A]:LEU:CD1	1:B:402:ASN:ND2	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASN:ND2	1:D:252:ASN:HD21	2.11	0.41
1:A:389:VAL:HB	1:A:478:TYR:HB2	2.01	0.41
1:C:394:SER:OG	4:D:1001[A]:GCG:HG71	2.20	0.41
1:D:104:LEU:HA	1:D:107:ASN:HD22	1.85	0.41
1:D:353:LYS:HG3	1:D:354:PRO:HD2	2.02	0.41
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.89	0.41
1:A:478:TYR:HA	1:A:482:GLU:O	2.21	0.41
1:B:219:LEU:C	1:B:219:LEU:HD23	2.46	0.41
1:B:260:LEU:H	1:C:152:GLN:NE2	2.18	0.41
1:B:189:ARG:HB3	1:B:279:ASP:OD2	2.21	0.41
1:C:219:LEU:C	1:C:219:LEU:HD23	2.46	0.41
1:D:268:VAL:O	1:D:275:THR:HA	2.21	0.41
1:D:304:THR:HB	1:D:305:PRO:HD2	2.03	0.40
1:A:355:ARG:HG2	1:A:355:ARG:HH21	1.86	0.40
1:B:104:LEU:HA	1:B:107:ASN:HD22	1.87	0.40
1:B:75:GLU:HB3	1:B:404:SER:HB2	2.02	0.40
1:D:129:LEU:N	1:D:129:LEU:CD1	2.83	0.40
1:A:353:LYS:HE3	1:A:355:ARG:NE	2.34	0.40
1:D:183:TYR:O	1:D:184:LEU:C	2.60	0.40
1:B:216:LYS:HE3	1:B:248:GLU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	490/495 (99%)	475 (97%)	14 (3%)	1 (0%)	43	51
1	B	487/495 (98%)	465 (96%)	19 (4%)	3 (1%)	21	23
1	C	490/495 (99%)	473 (96%)	17 (4%)	0	100	100
1	D	488/495 (99%)	471 (96%)	15 (3%)	2 (0%)	30	34
All	All	1955/1980 (99%)	1884 (96%)	65 (3%)	6 (0%)	36	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	LYS
1	A	480	LYS
1	B	400	MET
1	D	132	LYS
1	D	352	ASN
1	B	488	PRO

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	405/407 (100%)	390 (96%)	15 (4%)	30	41
1	B	402/407 (99%)	387 (96%)	15 (4%)	30	41
1	C	404/407 (99%)	390 (96%)	14 (4%)	32	43
1	D	402/407 (99%)	388 (96%)	14 (4%)	32	43
All	All	1613/1628 (99%)	1555 (96%)	58 (4%)	31	42

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

Mol	Chain	Res	Type
1	A	-1	SER
1	A	48	LEU
1	A	55	VAL
1	A	94	LYS
1	A	129	LEU
1	A	191	VAL
1	A	213	PRO
1	A	274	LYS
1	A	292	ASN
1	A	318	ASN
1	A	335	THR
1	A	353	LYS
1	A	370	PRO
1	A	446	ARG

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Mol	Chain	Res	Type
1	A	480	LYS
1	B	109	SER
1	B	128	SER
1	B	129	LEU
1	B	140	THR
1	B	144	LYS
1	B	149	GLU
1	B	154	ASP
1	B	260	LEU
1	B	302	LYS
1	B	321	ASN
1	B	322	ILE
1	B	323	TYR
1	B	335	THR
1	B	483	LYS
1	B	486	LYS
1	C	-1	SER
1	C	1	MET
1	C	37	GLN
1	C	248	GLU
1	C	318	ASN
1	C	328	ILE
1	C	335	THR
1	C	361	ARG
1	C	388	LYS
1	C	399	LEU
1	C	403	ILE
1	C	420	SER
1	C	446	ARG
1	C	487	LEU
1	D	2	SER
1	D	3	LYS
1	D	144	LYS
1	D	156	ILE
1	D	189	ARG
1	D	222	ARG
1	D	248	GLU
1	D	260	LEU
1	D	262	THR
1	D	274	LYS
1	D	306	LYS
1	D	335	THR

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Mol	Chain	Res	Type
1	D	353	LYS
1	D	489	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	223	ASN
1	A	252	ASN
1	A	318	ASN
1	A	359	HIS
1	A	401	HIS
1	B	68	GLN
1	B	107	ASN
1	B	133	ASN
1	B	223	ASN
1	B	224	ASN
1	B	252	ASN
1	B	402	ASN
1	C	0	HIS
1	C	115	ASN
1	C	152	GLN
1	C	223	ASN
1	C	252	ASN
1	C	318	ASN
1	C	321	ASN
1	C	419	HIS
1	D	68	GLN
1	D	107	ASN
1	D	133	ASN
1	D	208	ASN
1	D	252	ASN
1	D	321	ASN

5.3.3 RNA ⓘ

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](#)

16 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$
4	GCG	A	1001[B]	-	45,47,47	0.97	1 (2%)	52,58,58	1.71	14 (26%)
4	GCG	C	1001[A]	-	45,47,47	0.89	3 (6%)	52,58,58	1.34	8 (15%)
4	GCG	D	1001[A]	-	45,47,47	0.75	0	52,58,58	1.17	1 (1%)
3	NDP	A	800	-	51,52,52	1.92	13 (25%)	71,80,80	1.85	16 (22%)
3	NDP	B	800	-	51,52,52	2.11	15 (29%)	71,80,80	1.79	16 (22%)
2	FAD	C	700	-	58,58,58	1.32	6 (10%)	85,89,89	1.94	20 (23%)
4	GCG	B	1001[B]	-	45,47,47	1.02	2 (4%)	52,58,58	1.65	5 (9%)
4	GCG	A	1001[A]	-	45,47,47	0.88	1 (2%)	52,58,58	1.95	11 (21%)
4	GCG	B	1001[A]	-	45,47,47	0.79	0	52,58,58	1.51	7 (13%)
3	NDP	C	800	-	51,52,52	1.97	14 (27%)	71,80,80	1.61	14 (19%)
4	GCG	C	1001[B]	-	45,47,47	1.02	5 (11%)	52,58,58	1.38	6 (11%)
2	FAD	D	700	-	58,58,58	1.30	6 (10%)	85,89,89	1.74	18 (21%)
4	GCG	D	1001[B]	-	45,47,47	0.95	2 (4%)	52,58,58	1.31	2 (3%)
3	NDP	D	800	-	51,52,52	1.54	9 (17%)	71,80,80	1.91	14 (19%)
2	FAD	A	700	-	58,58,58	1.13	6 (10%)	85,89,89	1.77	18 (21%)
2	FAD	B	700	-	58,58,58	1.14	5 (8%)	85,89,89	1.70	17 (20%)

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
4	GCG	A	1001[B]	-	-	19/61/61/61	-
4	GCG	C	1001[A]	-	-	12/61/61/61	-
4	GCG	D	1001[A]	-	-	24/61/61/61	-
3	NDP	A	800	-	-	6/34/77/77	0/5/5/5
3	NDP	B	800	-	-	4/34/77/77	0/5/5/5
2	FAD	C	700	-	-	5/34/50/50	0/6/6/6
4	GCG	B	1001[B]	-	-	7/61/61/61	-
4	GCG	A	1001[A]	-	-	22/61/61/61	-
4	GCG	B	1001[A]	-	-	18/61/61/61	-
3	NDP	C	800	-	-	6/34/77/77	0/5/5/5
4	GCG	C	1001[B]	-	-	15/61/61/61	-
2	FAD	D	700	-	-	3/34/50/50	0/6/6/6
4	GCG	D	1001[B]	-	-	13/61/61/61	-
3	NDP	D	800	-	-	7/34/77/77	0/5/5/5
2	FAD	A	700	-	-	3/34/50/50	0/6/6/6
2	FAD	B	700	-	-	2/34/50/50	0/6/6/6

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	NDP	PN-O3	9.81	1.70	1.59
3	C	800	NDP	PA-O3	6.19	1.66	1.59
3	A	800	NDP	PA-O3	6.16	1.66	1.59
3	D	800	NDP	PN-O3	5.42	1.65	1.59
3	C	800	NDP	PN-O3	5.26	1.65	1.59
3	A	800	NDP	PN-O1N	4.89	1.67	1.50
2	C	700	FAD	C4X-N5	4.80	1.41	1.30
3	A	800	NDP	O4D-C1D	4.30	1.51	1.42
2	D	700	FAD	C4X-N5	4.09	1.39	1.30
3	B	800	NDP	PN-O1N	3.99	1.64	1.50
2	A	700	FAD	C4X-N5	3.92	1.39	1.30
3	C	800	NDP	PN-O1N	3.91	1.64	1.50
3	D	800	NDP	C4N-C5N	-3.77	1.39	1.49
2	C	700	FAD	C9-C8	3.57	1.44	1.39
3	C	800	NDP	C4A-N9A	-3.53	1.30	1.37
3	D	800	NDP	PA-O1A	3.43	1.62	1.50
3	A	800	NDP	C4N-C5N	-3.41	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	NDP	P2B-O2B	3.39	1.65	1.59
2	B	700	FAD	C2A-N3A	3.37	1.39	1.33
3	B	800	NDP	PA-O1A	3.35	1.62	1.50
4	A	1001[A]	GCG	CB6-CA6	3.28	1.56	1.53
2	B	700	FAD	C4X-N5	3.22	1.37	1.30
2	B	700	FAD	C10-N1	3.19	1.39	1.33
3	A	800	NDP	P2B-O1X	3.19	1.60	1.50
3	C	800	NDP	C4N-C5N	-3.16	1.40	1.49
2	A	700	FAD	C6-C5X	3.15	1.44	1.40
2	D	700	FAD	C4X-C10	-3.06	1.35	1.44
3	A	800	NDP	O4D-C4D	2.99	1.51	1.45
2	D	700	FAD	C8A-N7A	2.98	1.37	1.31
3	A	800	NDP	PN-O3	2.97	1.62	1.59
4	A	1001[B]	GCG	CG7-CD7	2.96	1.57	1.51
4	D	1001[B]	GCG	CB6-CA6	-2.96	1.49	1.53
3	B	800	NDP	C4N-C5N	-2.94	1.41	1.49
2	B	700	FAD	C2A-N1A	2.85	1.39	1.33
3	C	800	NDP	P2B-O1X	2.84	1.59	1.50
3	C	800	NDP	O4B-C1B	2.81	1.48	1.42
3	A	800	NDP	C4N-C3N	2.80	1.55	1.50
3	B	800	NDP	P2B-O3X	-2.75	1.44	1.54
3	D	800	NDP	C6N-C5N	2.68	1.41	1.33
3	B	800	NDP	O4B-C4B	2.68	1.51	1.45
3	C	800	NDP	O4D-C1D	2.65	1.48	1.42
3	A	800	NDP	C6N-C5N	2.61	1.41	1.33
3	B	800	NDP	C4A-N9A	-2.59	1.32	1.37
3	A	800	NDP	C1D-N1N	2.57	1.53	1.46
3	C	800	NDP	P2B-O3X	-2.56	1.45	1.54
3	B	800	NDP	C5A-N7A	-2.52	1.34	1.39
4	C	1001[A]	GCG	CA3-N3	2.52	1.51	1.45
4	C	1001[B]	GCG	CA3-N3	2.52	1.51	1.45
3	A	800	NDP	P2B-O3X	-2.49	1.45	1.54
3	B	800	NDP	P2B-O1X	2.44	1.58	1.50
4	B	1001[B]	GCG	CG7-CD7	2.42	1.56	1.51
4	C	1001[B]	GCG	CG7-CD7	2.41	1.56	1.51
3	D	800	NDP	C8A-N7A	2.37	1.36	1.31
3	C	800	NDP	C7N-C3N	2.37	1.53	1.48
3	A	800	NDP	C1B-N9A	2.35	1.52	1.46
4	D	1001[B]	GCG	CG7-CD7	2.35	1.56	1.51
2	C	700	FAD	O4-C4	2.33	1.28	1.23
3	C	800	NDP	C2N-C3N	2.32	1.41	1.35
3	D	800	NDP	C2N-C3N	2.30	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	800	NDP	C5A-N7A	-2.29	1.34	1.39
3	A	800	NDP	C5A-N7A	-2.28	1.34	1.39
4	C	1001[A]	GCG	CB2-SG2	2.28	1.86	1.81
4	C	1001[B]	GCG	CB2-SG2	2.28	1.86	1.81
2	C	700	FAD	C2A-N3A	2.27	1.38	1.33
2	D	700	FAD	O2'-C2'	-2.24	1.38	1.43
3	B	800	NDP	C4N-C3N	2.19	1.54	1.50
2	C	700	FAD	O2-C2	-2.17	1.20	1.24
3	D	800	NDP	C7N-C3N	2.17	1.53	1.48
2	B	700	FAD	C8A-N7A	2.16	1.35	1.31
2	A	700	FAD	C10-N1	2.14	1.37	1.33
3	B	800	NDP	C6N-C5N	2.13	1.39	1.33
2	A	700	FAD	C9A-C5X	-2.13	1.37	1.41
4	B	1001[B]	GCG	CA6-N6	2.12	1.50	1.45
3	B	800	NDP	PA-O3	2.12	1.61	1.59
3	B	800	NDP	P2B-O2B	2.09	1.63	1.59
3	D	800	NDP	C1B-N9A	2.09	1.52	1.46
3	B	800	NDP	PN-O5D	2.07	1.67	1.59
4	C	1001[A]	GCG	O21-C1	2.07	1.28	1.22
4	C	1001[B]	GCG	O21-C1	2.07	1.28	1.22
3	C	800	NDP	C6N-N1N	2.06	1.42	1.37
2	D	700	FAD	C9-C8	2.06	1.42	1.39
2	C	700	FAD	C9-C9A	2.06	1.43	1.39
2	A	700	FAD	C2A-N1A	2.06	1.37	1.33
4	C	1001[B]	GCG	CB6-CA6	-2.04	1.50	1.53
3	C	800	NDP	PA-O5B	2.04	1.67	1.59
3	B	800	NDP	O5D-C5D	2.04	1.52	1.44
2	D	700	FAD	C8M-C8	2.01	1.54	1.51
2	A	700	FAD	C4X-C10	-2.01	1.38	1.44

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001[A]	GCG	CA6-CB6-SG6	8.39	123.62	114.16
4	B	1001[B]	GCG	CA6-CB6-SG6	-7.51	105.69	114.16
3	A	800	NDP	O4D-C1D-N1N	6.88	121.20	108.08
2	D	700	FAD	N3A-C2A-N1A	-6.22	119.17	128.58
3	D	800	NDP	C5A-C4A-N3A	-6.09	118.33	126.72
2	C	700	FAD	C5A-C4A-N3A	-5.86	118.65	126.72
2	B	700	FAD	N3A-C2A-N1A	-5.70	119.96	128.58
3	B	800	NDP	O4D-C1D-N1N	5.67	118.90	108.08
3	C	800	NDP	O4D-C1D-N1N	5.41	118.41	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	FAD	N3A-C2A-N1A	-5.41	120.39	128.58
4	B	1001[A]	GCG	CA2-CB2-SG2	-5.37	108.11	114.16
4	B	1001[B]	GCG	CA2-CB2-SG2	-5.37	108.11	114.16
3	D	800	NDP	C2D-C1D-N1N	-5.29	100.30	113.31
3	D	800	NDP	O4D-C1D-N1N	5.16	117.93	108.08
3	D	800	NDP	N3A-C2A-N1A	-5.14	120.81	128.58
4	C	1001[B]	GCG	CA6-CB6-SG6	-5.07	108.44	114.16
3	B	800	NDP	C2D-C1D-N1N	-4.94	101.15	113.31
4	D	1001[A]	GCG	CA2-CB2-SG2	-4.90	108.64	114.16
4	D	1001[B]	GCG	CA2-CB2-SG2	-4.90	108.64	114.16
4	D	1001[B]	GCG	CA6-CB6-SG6	-4.76	108.80	114.16
3	A	800	NDP	C2D-C1D-N1N	-4.65	101.88	113.31
4	A	1001[A]	GCG	CA2-CB2-SG2	-4.59	108.99	114.16
4	A	1001[B]	GCG	CA2-CB2-SG2	-4.59	108.99	114.16
2	C	700	FAD	C4X-C10-N10	4.58	123.04	116.48
2	D	700	FAD	C4-N3-C2	-4.52	117.62	125.64
2	C	700	FAD	C4-N3-C2	-4.49	117.66	125.64
3	D	800	NDP	C2A-N3A-C4A	4.49	122.80	111.83
2	A	700	FAD	C9A-C5X-N5	-4.44	117.74	122.45
2	C	700	FAD	C4-C4X-N5	4.43	124.33	118.21
3	A	800	NDP	C5A-C4A-N3A	-4.43	120.62	126.72
2	B	700	FAD	N9A-C8A-N7A	-4.42	107.67	113.94
2	B	700	FAD	C5A-C4A-N3A	-4.38	120.69	126.72
3	B	800	NDP	N3A-C2A-N1A	-4.37	121.97	128.58
2	C	700	FAD	C10-C4X-N5	-4.35	115.92	124.81
2	C	700	FAD	C5A-N7A-C8A	4.16	109.99	103.45
2	C	700	FAD	N9A-C8A-N7A	-4.09	108.13	113.94
2	A	700	FAD	C5A-C4A-N3A	-4.07	121.11	126.72
3	A	800	NDP	N3A-C2A-N1A	-4.03	122.48	128.58
3	A	800	NDP	N9A-C8A-N7A	-4.00	108.26	113.94
2	D	700	FAD	C5A-C4A-N3A	-3.99	121.22	126.72
4	B	1001[A]	GCG	C6-CA6-N6	-3.98	100.33	111.11
2	A	700	FAD	N9A-C8A-N7A	-3.96	108.32	113.94
4	C	1001[A]	GCG	CB6-CA6-N6	-3.94	105.67	111.28
4	C	1001[B]	GCG	CG7-CB7-CA7	-3.94	104.83	113.86
3	C	800	NDP	O2B-P2B-O1X	-3.86	95.59	109.33
2	D	700	FAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	A	700	FAD	C4-N3-C2	-3.76	118.96	125.64
3	C	800	NDP	N3A-C2A-N1A	-3.74	122.91	128.58
2	B	700	FAD	C5A-N7A-C8A	3.74	109.33	103.45
2	C	700	FAD	N3A-C4A-N9A	3.70	133.46	127.17
2	C	700	FAD	N3A-C2A-N1A	-3.70	122.98	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	FAD	C5A-N7A-C8A	3.68	109.23	103.45
3	D	800	NDP	N3A-C4A-N9A	3.64	133.36	127.17
2	D	700	FAD	C2A-N3A-C4A	3.57	120.55	111.83
3	B	800	NDP	C5A-C4A-N3A	-3.57	121.81	126.72
4	A	1001[A]	GCG	CB6-CA6-C6	3.55	117.23	109.50
3	D	800	NDP	N9A-C8A-N7A	-3.51	108.95	113.94
3	B	800	NDP	O3X-P2B-O2X	3.48	120.86	107.80
4	A	1001[B]	GCG	CB6-CA6-C6	3.48	117.06	109.50
2	D	700	FAD	C4X-C10-N10	3.48	121.46	116.48
4	A	1001[B]	GCG	CA5-N5-C6	3.47	130.13	121.38
2	B	700	FAD	C4X-C10-N10	3.46	121.43	116.48
2	C	700	FAD	C2A-N3A-C4A	3.42	120.19	111.83
3	A	800	NDP	N3A-C4A-N9A	3.41	132.96	127.17
4	C	1001[A]	GCG	CA6-CB6-SG6	-3.39	110.34	114.16
2	A	700	FAD	C5X-N5-C4X	3.38	123.56	118.09
3	C	800	NDP	C2D-C1D-N1N	-3.36	105.03	113.31
2	A	700	FAD	C4A-C5A-N7A	-3.35	106.75	110.58
3	A	800	NDP	C4A-N9A-C8A	3.31	109.21	105.74
3	B	800	NDP	C4A-N9A-C8A	3.29	109.19	105.74
4	B	1001[A]	GCG	CB6-CA6-C6	3.27	116.62	109.50
2	B	700	FAD	N3A-C4A-N9A	3.22	132.64	127.17
2	A	700	FAD	C2A-N3A-C4A	3.20	119.65	111.83
3	B	800	NDP	N3A-C4A-N9A	3.18	132.58	127.17
3	C	800	NDP	C4A-N9A-C8A	3.18	109.08	105.74
2	B	700	FAD	C2A-N3A-C4A	3.16	119.56	111.83
2	C	700	FAD	O2A-PA-O3P	3.11	115.68	107.27
3	B	800	NDP	N9A-C8A-N7A	-3.11	109.53	113.94
2	C	700	FAD	C4A-C5A-N7A	-3.09	107.05	110.58
3	C	800	NDP	C5A-C4A-N3A	-3.09	122.46	126.72
2	D	700	FAD	C10-C4X-N5	-3.06	118.56	124.81
4	A	1001[B]	GCG	C6-CA6-N6	-3.05	102.86	111.11
3	A	800	NDP	C5A-N7A-C8A	3.04	108.23	103.45
2	C	700	FAD	O2-C2-N1	-3.02	116.78	121.80
2	C	700	FAD	C10-N1-C2	3.01	123.36	116.85
2	D	700	FAD	C4X-C4-N3	2.99	120.86	113.25
2	A	700	FAD	O3P-PA-O1A	-2.98	101.75	110.70
3	D	800	NDP	C5D-C4D-C3D	-2.95	104.58	115.21
3	B	800	NDP	C5D-C4D-C3D	-2.90	104.75	115.21
2	A	700	FAD	C10-C4X-N5	-2.88	118.94	124.81
3	D	800	NDP	O2B-P2B-O1X	-2.86	99.13	109.33
3	B	800	NDP	C3N-C2N-N1N	-2.85	119.01	123.20
2	B	700	FAD	C10-C4X-N5	-2.85	118.99	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	FAD	O4-C4-C4X	-2.85	119.02	126.53
2	B	700	FAD	O4B-C1B-N9A	-2.82	102.67	108.09
3	C	800	NDP	C6N-N1N-C2N	-2.81	116.31	119.32
4	C	1001[B]	GCG	CB6-CA6-N6	-2.78	107.32	111.28
4	A	1001[B]	GCG	CA6-C6-N5	-2.77	110.59	116.54
4	B	1001[A]	GCG	CG7-CB7-CA7	-2.75	107.55	113.86
2	D	700	FAD	C5A-N7A-C8A	2.74	107.76	103.45
4	A	1001[A]	GCG	CG1-CB1-CA1	-2.74	107.58	113.86
4	A	1001[B]	GCG	CG1-CB1-CA1	-2.74	107.58	113.86
4	B	1001[A]	GCG	CA6-N6-CD7	-2.71	114.88	121.68
4	A	1001[B]	GCG	C9S-N11-C5	2.66	127.77	122.82
3	B	800	NDP	C2A-N3A-C4A	2.66	118.32	111.83
2	A	700	FAD	O4-C4-C4X	-2.65	119.52	126.53
4	B	1001[A]	GCG	CG1-CB1-CA1	-2.65	107.78	113.86
4	B	1001[B]	GCG	CG1-CB1-CA1	-2.65	107.78	113.86
2	B	700	FAD	C2B-C1B-N9A	2.64	119.86	113.30
2	B	700	FAD	O3P-PA-O1A	2.62	118.58	110.70
2	A	700	FAD	C5X-C9A-N10	2.61	120.33	117.97
2	D	700	FAD	C4-C4X-N5	2.56	121.74	118.21
2	D	700	FAD	O2-C2-N1	-2.54	117.57	121.80
2	B	700	FAD	C4A-N9A-C8A	2.54	108.41	105.74
4	A	1001[B]	GCG	CG7-CB7-CA7	-2.53	108.05	113.86
2	C	700	FAD	C4X-C10-N1	-2.53	118.39	124.59
3	D	800	NDP	C5A-N7A-C8A	2.51	107.40	103.45
4	A	1001[A]	GCG	CA6-N6-CD7	2.51	127.98	121.68
2	D	700	FAD	C5A-C4A-N9A	2.50	108.53	105.81
4	A	1001[A]	GCG	OD1-CD1-CG1	-2.48	117.53	122.02
4	A	1001[B]	GCG	OD1-CD1-CG1	-2.48	117.53	122.02
2	C	700	FAD	C4X-C4-N3	2.46	119.51	113.25
4	C	1001[A]	GCG	CB1-CG1-CD1	-2.45	107.61	113.06
4	C	1001[B]	GCG	CB1-CG1-CD1	-2.45	107.61	113.06
2	D	700	FAD	C10-N1-C2	2.44	122.14	116.85
2	B	700	FAD	C9A-C5X-N5	-2.39	119.92	122.45
4	B	1001[B]	GCG	C6-CA6-N6	2.38	117.55	111.11
3	C	800	NDP	N3A-C4A-N9A	2.38	131.22	127.17
3	A	800	NDP	C4A-C5A-N7A	-2.38	107.86	110.58
4	A	1001[A]	GCG	C2-CA2-N2	2.37	117.53	111.11
4	A	1001[B]	GCG	C2-CA2-N2	2.37	117.53	111.11
2	B	700	FAD	C4A-C5A-N7A	-2.36	107.89	110.58
4	A	1001[B]	GCG	CA6-N6-CD7	-2.33	115.83	121.68
2	C	700	FAD	O3P-PA-O1A	-2.32	103.72	110.70
3	B	800	NDP	C1D-N1N-C2N	-2.31	117.33	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001[A]	GCG	OD7-CD7-N6	2.31	126.86	122.95
3	A	800	NDP	C3N-C2N-N1N	-2.30	119.83	123.20
2	B	700	FAD	C8M-C8-C9	-2.30	115.52	119.57
3	C	800	NDP	O7N-C7N-C3N	-2.29	116.58	120.90
3	D	800	NDP	C5A-C4A-N9A	2.28	108.30	105.81
3	C	800	NDP	O5D-PN-O1N	-2.28	99.91	108.94
3	D	800	NDP	C4A-C5A-N7A	-2.28	107.98	110.58
4	C	1001[A]	GCG	OD1-CD1-CG1	-2.27	117.90	122.02
4	C	1001[B]	GCG	OD1-CD1-CG1	-2.27	117.90	122.02
4	A	1001[B]	GCG	O6-C6-N5	2.27	127.79	122.98
3	A	800	NDP	C2A-N3A-C4A	2.27	117.38	111.83
3	A	800	NDP	O3B-C3B-C4B	-2.27	104.56	111.08
2	A	700	FAD	C4X-C4-N3	2.26	119.01	113.25
4	C	1001[A]	GCG	CB6-CA6-C6	2.24	114.37	109.50
3	A	800	NDP	C2B-C1B-N9A	2.23	117.43	113.75
2	A	700	FAD	C4-C4X-C10	2.23	120.76	116.93
2	D	700	FAD	O2A-PA-O1A	2.21	122.74	112.44
3	C	800	NDP	O2B-C2B-C1B	-2.21	102.28	110.05
3	C	800	NDP	N9A-C8A-N7A	-2.21	110.80	113.94
3	C	800	NDP	C2A-N3A-C4A	2.20	117.21	111.83
3	A	800	NDP	O3X-P2B-O2X	2.20	116.06	107.80
4	A	1001[A]	GCG	C2S-N1S-C3	-2.19	118.75	122.82
4	A	1001[B]	GCG	C2S-N1S-C3	-2.19	118.75	122.82
4	A	1001[A]	GCG	CB7-CG7-CD7	-2.18	108.19	113.06
2	C	700	FAD	C5X-N5-C4X	2.16	121.57	118.09
4	B	1001[A]	GCG	CA6-CB6-SG6	2.15	116.59	114.16
2	B	700	FAD	C6A-C5A-C4A	2.15	120.12	117.18
3	B	800	NDP	O5D-PN-O1N	-2.15	100.43	108.94
2	D	700	FAD	O3'-C3'-C4'	2.14	113.80	108.93
2	A	700	FAD	O2-C2-N1	-2.14	118.25	121.80
3	A	800	NDP	C2A-N1A-C6A	2.13	122.23	118.73
3	A	800	NDP	O7N-C7N-C3N	-2.12	116.90	120.90
4	C	1001[A]	GCG	CA6-N6-CD7	-2.12	116.36	121.68
4	C	1001[A]	GCG	C8S-C9S-N11	-2.11	106.28	112.20
3	B	800	NDP	C5A-C6A-N6A	-2.10	118.08	123.29
3	C	800	NDP	C2A-N1A-C6A	2.10	122.18	118.73
2	A	700	FAD	N3A-C4A-N9A	2.10	130.74	127.17
2	B	700	FAD	O2A-PA-O3P	-2.10	101.61	107.27
2	D	700	FAD	C4X-C10-N1	-2.09	119.48	124.59
2	C	700	FAD	C6A-C5A-C4A	2.07	120.01	117.18
3	D	800	NDP	O3X-P2B-O2X	2.07	115.55	107.80
2	C	700	FAD	O2P-P-O3P	-2.06	101.70	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	FAD	C4A-C5A-N7A	-2.06	108.22	110.58
3	B	800	NDP	O2N-PN-O3	2.04	112.79	107.27
3	B	800	NDP	C3N-C7N-N7N	-2.04	114.05	117.67
3	D	800	NDP	O3X-P2B-O1X	2.04	118.78	110.83
4	A	1001[A]	GCG	C4S-C5S-N6S	-2.04	106.60	112.07
4	A	1001[B]	GCG	C4S-C5S-N6S	-2.04	106.60	112.07
4	C	1001[A]	GCG	CA2-CB2-SG2	-2.03	111.87	114.16
4	C	1001[B]	GCG	CA2-CB2-SG2	-2.03	111.87	114.16
4	B	1001[B]	GCG	OD7-CD7-CG7	-2.02	118.36	122.02
2	A	700	FAD	C6A-C5A-C4A	2.01	119.92	117.18

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	FAD	PA-O3P-P-O5'
2	B	700	FAD	PA-O3P-P-O5'
2	C	700	FAD	PA-O3P-P-O5'
3	A	800	NDP	C5D-O5D-PN-O3
4	A	1001[A]	GCG	C2-CA2-CB2-SG2
4	A	1001[A]	GCG	C6-CA6-CB6-SG6
4	A	1001[A]	GCG	N6-CA6-CB6-SG6
4	A	1001[B]	GCG	C2-CA2-CB2-SG2
4	A	1001[B]	GCG	C7-CA7-CB7-CG7
4	B	1001[A]	GCG	C2-CA2-CB2-SG2
4	B	1001[A]	GCG	C6-CA6-CB6-SG6
4	B	1001[A]	GCG	C7-CA7-CB7-CG7
4	B	1001[A]	GCG	N7-CA7-CB7-CG7
4	B	1001[B]	GCG	C2-CA2-CB2-SG2
4	D	1001[A]	GCG	O21-C1-CA1-N1
4	D	1001[A]	GCG	C1-CA1-CB1-CG1
4	D	1001[A]	GCG	N1-CA1-CB1-CG1
4	D	1001[A]	GCG	C2-CA2-CB2-SG2
4	D	1001[A]	GCG	C6-CA6-CB6-SG6
4	D	1001[A]	GCG	N6-CA6-CB6-SG6
4	D	1001[A]	GCG	O27-C7-CA7-N7
4	D	1001[A]	GCG	C7-CA7-CB7-CG7
4	D	1001[A]	GCG	N7-CA7-CB7-CG7
4	D	1001[B]	GCG	O21-C1-CA1-N1
4	D	1001[B]	GCG	C1-CA1-CB1-CG1
4	D	1001[B]	GCG	N1-CA1-CB1-CG1
4	D	1001[B]	GCG	C2-CA2-CB2-SG2

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Mol	Chain	Res	Type	Atoms
4	D	1001[B]	GCG	C8S-C9S-N11-C5
4	D	1001[A]	GCG	C8S-C9S-N11-C5
4	A	1001[A]	GCG	N6S-C7S-C8S-C9S
3	A	800	NDP	O4D-C1D-N1N-C2N
3	B	800	NDP	O4D-C1D-N1N-C2N
3	C	800	NDP	O4D-C1D-N1N-C2N
3	D	800	NDP	O4D-C1D-N1N-C2N
4	A	1001[A]	GCG	O6-C6-N5-CA5
4	D	1001[A]	GCG	O6-C6-N5-CA5
4	A	1001[A]	GCG	CA6-C6-N5-CA5
4	D	1001[A]	GCG	CA6-C6-N5-CA5
4	A	1001[A]	GCG	C6-CA6-N6-CD7
4	A	1001[A]	GCG	O5-C5-N11-C9S
4	A	1001[B]	GCG	O5-C5-N11-C9S
4	B	1001[A]	GCG	N6S-C7S-C8S-C9S
4	C	1001[B]	GCG	N6S-C7S-C8S-C9S
4	D	1001[A]	GCG	N6S-C7S-C8S-C9S
4	C	1001[A]	GCG	C8S-C7S-N6S-C5S
4	D	1001[B]	GCG	C4S-C5S-N6S-C7S
4	C	1001[A]	GCG	C3S-C4S-C5S-N6S
4	C	1001[B]	GCG	C3S-C4S-C5S-N6S
4	B	1001[B]	GCG	C7S-C8S-C9S-N11
4	C	1001[A]	GCG	C7S-C8S-C9S-N11
4	B	1001[A]	GCG	CA7-CB7-CG7-CD7
4	D	1001[A]	GCG	CA1-CB1-CG1-CD1
4	D	1001[B]	GCG	CA1-CB1-CG1-CD1
4	A	1001[A]	GCG	CA5-C5-N11-C9S
4	D	1001[A]	GCG	O11-C1-CA1-N1
4	D	1001[A]	GCG	O17-C7-CA7-N7
4	D	1001[B]	GCG	O11-C1-CA1-N1
4	A	1001[B]	GCG	N6S-C7S-C8S-C9S
4	A	1001[B]	GCG	C7S-C8S-C9S-N11
4	A	1001[B]	GCG	CA5-C5-N11-C9S
4	D	1001[A]	GCG	O5-C5-CA5-N5
4	A	1001[A]	GCG	CA1-CB1-CG1-CD1
4	A	1001[A]	GCG	CA7-CB7-CG7-CD7
4	A	1001[B]	GCG	CA1-CB1-CG1-CD1
4	B	1001[A]	GCG	O17-C7-CA7-N7
4	C	1001[A]	GCG	O17-C7-CA7-N7
4	A	1001[A]	GCG	N11-C5-CA5-N5
4	D	1001[A]	GCG	N11-C5-CA5-N5
4	A	1001[A]	GCG	O5-C5-CA5-N5

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Mol	Chain	Res	Type	Atoms
4	A	1001[A]	GCG	C8S-C7S-N6S-C5S
4	C	1001[A]	GCG	C4S-C5S-N6S-C7S
4	D	1001[A]	GCG	CA7-CB7-CG7-CD7
4	A	1001[A]	GCG	C3S-C4S-C5S-N6S
4	A	1001[B]	GCG	C3S-C4S-C5S-N6S
4	C	1001[A]	GCG	C2S-C3S-C4S-C5S
4	C	1001[B]	GCG	C2S-C3S-C4S-C5S
4	C	1001[A]	GCG	N1S-C2S-C3S-C4S
4	C	1001[B]	GCG	N1S-C2S-C3S-C4S
2	A	700	FAD	P-O3P-PA-O1A
4	B	1001[B]	GCG	CA7-CB7-CG7-CD7
4	C	1001[B]	GCG	O6-C6-CA6-N6
4	C	1001[A]	GCG	O6-C6-CA6-N6
4	B	1001[A]	GCG	N6-CA6-CB6-SG6
2	D	700	FAD	PA-O3P-P-O5'
4	C	1001[B]	GCG	N5-C6-CA6-N6
4	C	1001[A]	GCG	N5-C6-CA6-N6
4	C	1001[B]	GCG	N11-C5-CA5-N5
4	A	1001[B]	GCG	CA7-CB7-CG7-CD7
4	D	1001[B]	GCG	CA7-CB7-CG7-CD7
4	D	1001[A]	GCG	C3S-C4S-C5S-N6S
4	D	1001[B]	GCG	C3S-C4S-C5S-N6S
4	C	1001[A]	GCG	C7-CA7-CB7-CG7
4	C	1001[B]	GCG	C7-CA7-CB7-CG7
4	A	1001[A]	GCG	OD7-CD7-CG7-CB7
4	A	1001[A]	GCG	N6-CD7-CG7-CB7
3	C	800	NDP	C2B-C1B-N9A-C8A
4	A	1001[B]	GCG	O6-C6-CA6-N6
4	C	1001[B]	GCG	O5-C5-CA5-N5
4	D	1001[A]	GCG	C7S-C8S-C9S-N11
4	A	1001[B]	GCG	N6-CA6-CB6-SG6
4	C	1001[B]	GCG	N6-CA6-CB6-SG6
4	C	1001[B]	GCG	CA7-CB7-CG7-CD7
3	D	800	NDP	C5D-O5D-PN-O3
4	B	1001[A]	GCG	O6-C6-CA6-N6
4	D	1001[A]	GCG	O21-C1-CA1-CB1
4	D	1001[B]	GCG	O21-C1-CA1-CB1
4	C	1001[B]	GCG	C7S-C8S-C9S-N11
4	A	1001[A]	GCG	O27-C7-CA7-CB7
4	D	1001[A]	GCG	O11-C1-CA1-CB1
4	D	1001[B]	GCG	O11-C1-CA1-CB1
2	C	700	FAD	P-O3P-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	700	FAD	P-O3P-PA-O2A
2	D	700	FAD	P-O3P-PA-O1A
2	C	700	FAD	C3B-C4B-C5B-O5B
3	B	800	NDP	C2B-C1B-N9A-C8A
4	A	1001[B]	GCG	C4S-C5S-N6S-C7S
4	C	1001[B]	GCG	C8S-C7S-N6S-C5S
3	D	800	NDP	C2B-O2B-P2B-O3X
4	A	1001[A]	GCG	O17-C7-CA7-CB7
4	A	1001[B]	GCG	N5-C6-CA6-N6
3	D	800	NDP	C2B-C1B-N9A-C8A
4	B	1001[B]	GCG	C6-CA6-CB6-SG6
4	B	1001[A]	GCG	C4S-C5S-N6S-C7S
3	B	800	NDP	C2B-O2B-P2B-O1X
3	D	800	NDP	C2B-O2B-P2B-O1X
4	C	1001[A]	GCG	O17-C7-CA7-CB7
2	A	700	FAD	P-O3P-PA-O2A
4	B	1001[A]	GCG	OD7-CD7-CG7-CB7
4	A	1001[B]	GCG	C8S-C7S-N6S-C5S
4	A	1001[A]	GCG	C7S-C8S-C9S-N11
4	B	1001[A]	GCG	O11-C1-CA1-N1
4	B	1001[B]	GCG	O11-C1-CA1-N1
4	B	1001[A]	GCG	N6-CD7-CG7-CB7
4	C	1001[A]	GCG	O27-C7-CA7-CB7
4	A	1001[A]	GCG	O11-C1-CA1-N1
4	A	1001[B]	GCG	O11-C1-CA1-N1
2	C	700	FAD	O4B-C4B-C5B-O5B
3	C	800	NDP	O4B-C4B-C5B-O5B
4	B	1001[A]	GCG	C8S-C7S-N6S-C5S
4	C	1001[B]	GCG	C4S-C5S-N6S-C7S
4	B	1001[A]	GCG	O6-C6-CA6-CB6
4	A	1001[B]	GCG	C5-CA5-N5-C6
3	A	800	NDP	O4B-C4B-C5B-O5B
3	B	800	NDP	C2B-O2B-P2B-O3X
4	C	1001[B]	GCG	C5-CA5-N5-C6
4	A	1001[B]	GCG	O5-C5-CA5-N5
4	D	1001[B]	GCG	O5-C5-CA5-N5
3	A	800	NDP	O4B-C1B-N9A-C8A
3	C	800	NDP	O4B-C1B-N9A-C8A
3	A	800	NDP	C2B-O2B-P2B-O1X
3	C	800	NDP	C2B-O2B-P2B-O1X
4	A	1001[B]	GCG	N11-C5-CA5-N5
3	A	800	NDP	C2B-C1B-N9A-C8A

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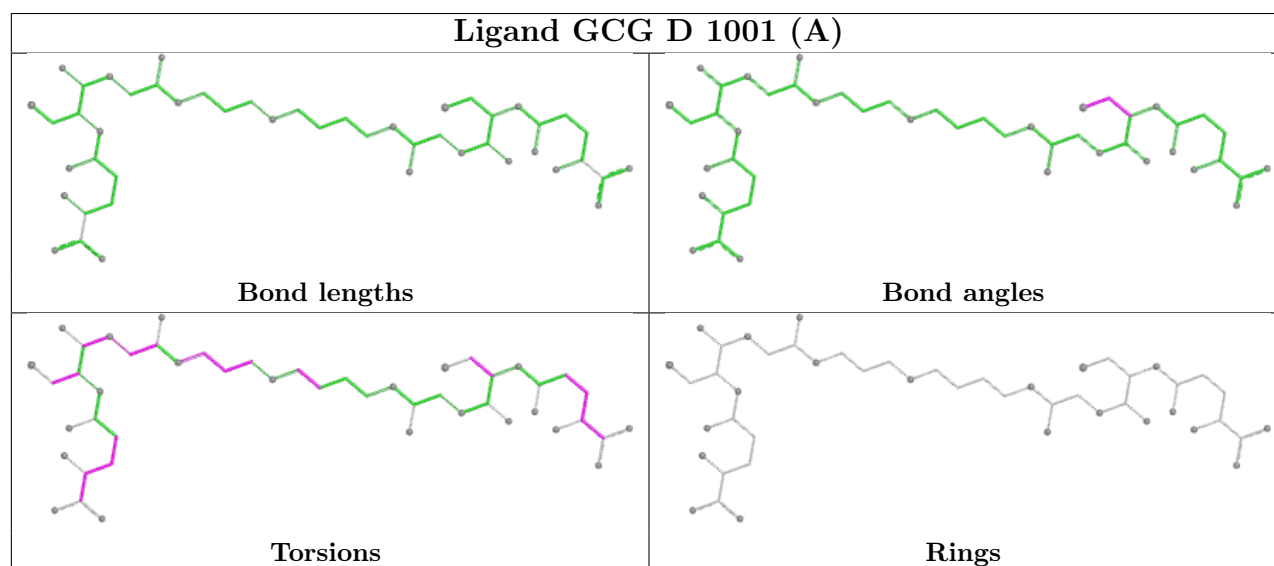
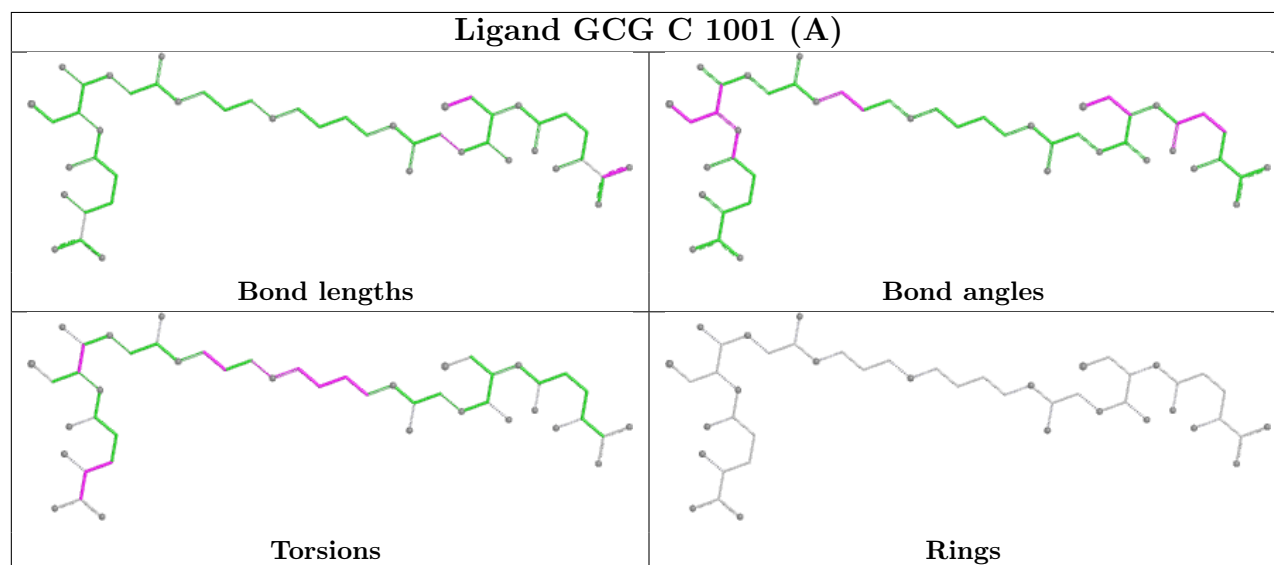
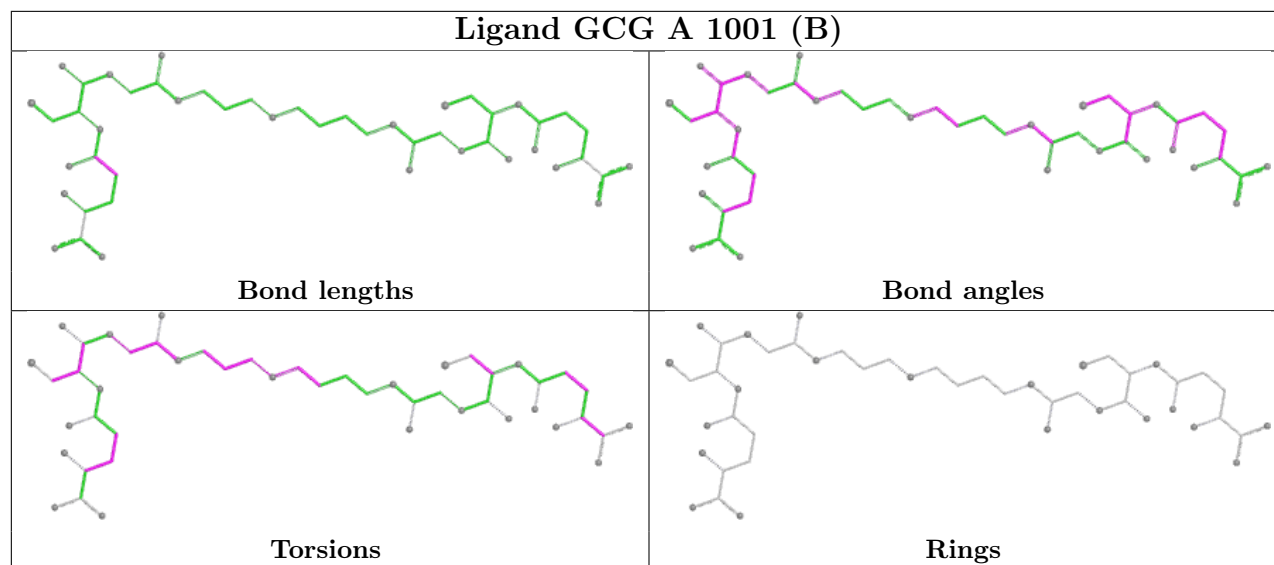
Mol	Chain	Res	Type	Atoms
4	D	1001[A]	GCG	C5-CA5-N5-C6
4	B	1001[A]	GCG	C3S-C4S-C5S-N6S
4	B	1001[B]	GCG	C3S-C4S-C5S-N6S
4	A	1001[A]	GCG	O21-C1-CA1-N1
4	A	1001[B]	GCG	O21-C1-CA1-N1
4	B	1001[A]	GCG	O21-C1-CA1-N1
4	B	1001[A]	GCG	O27-C7-CA7-N7
4	B	1001[B]	GCG	O21-C1-CA1-N1
2	B	700	FAD	P-O3P-PA-O2A
2	D	700	FAD	P-O3P-PA-O2A
3	C	800	NDP	PA-O3-PN-O2N
3	D	800	NDP	PA-O3-PN-O2N
3	D	800	NDP	O4B-C4B-C5B-O5B

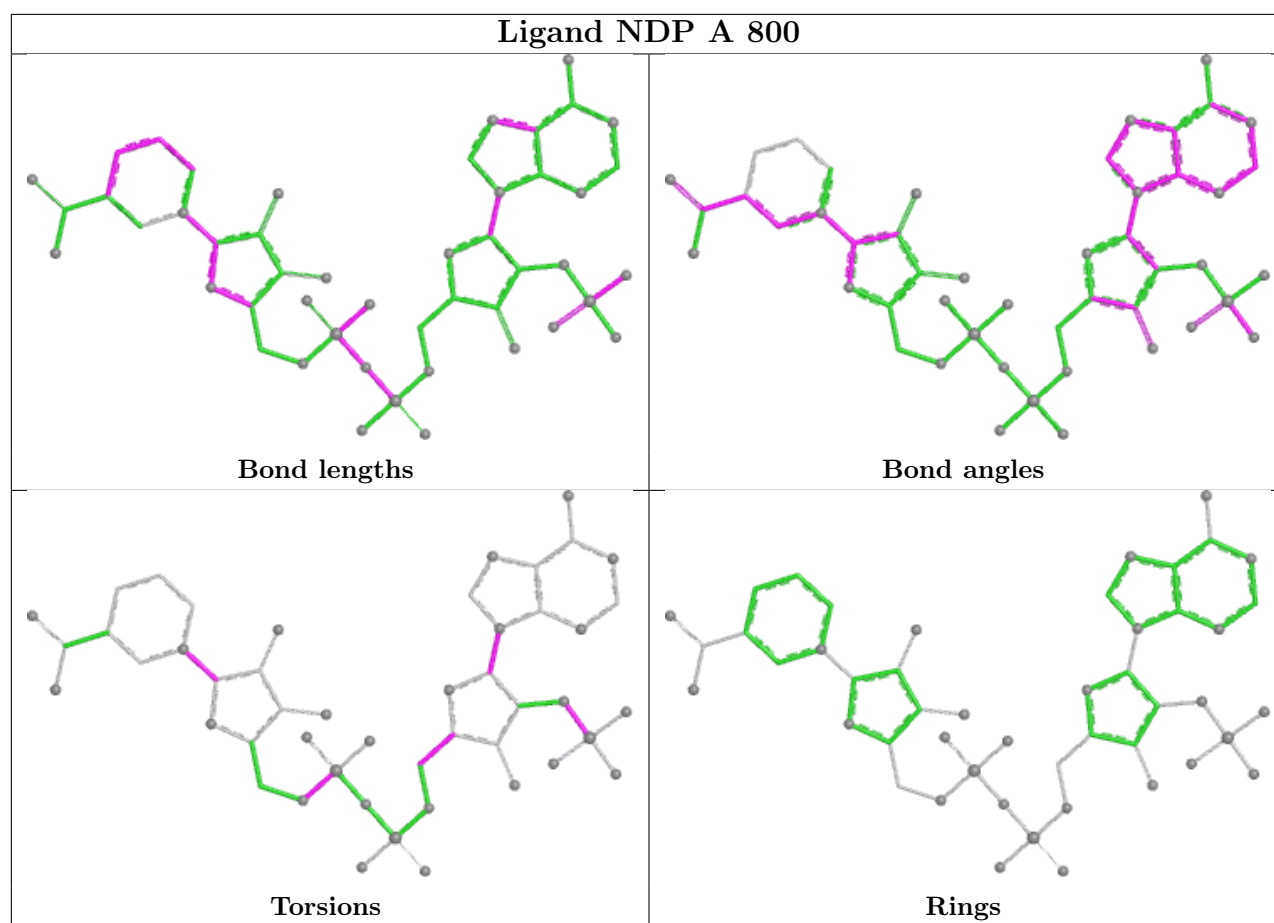
There are no ring outliers.

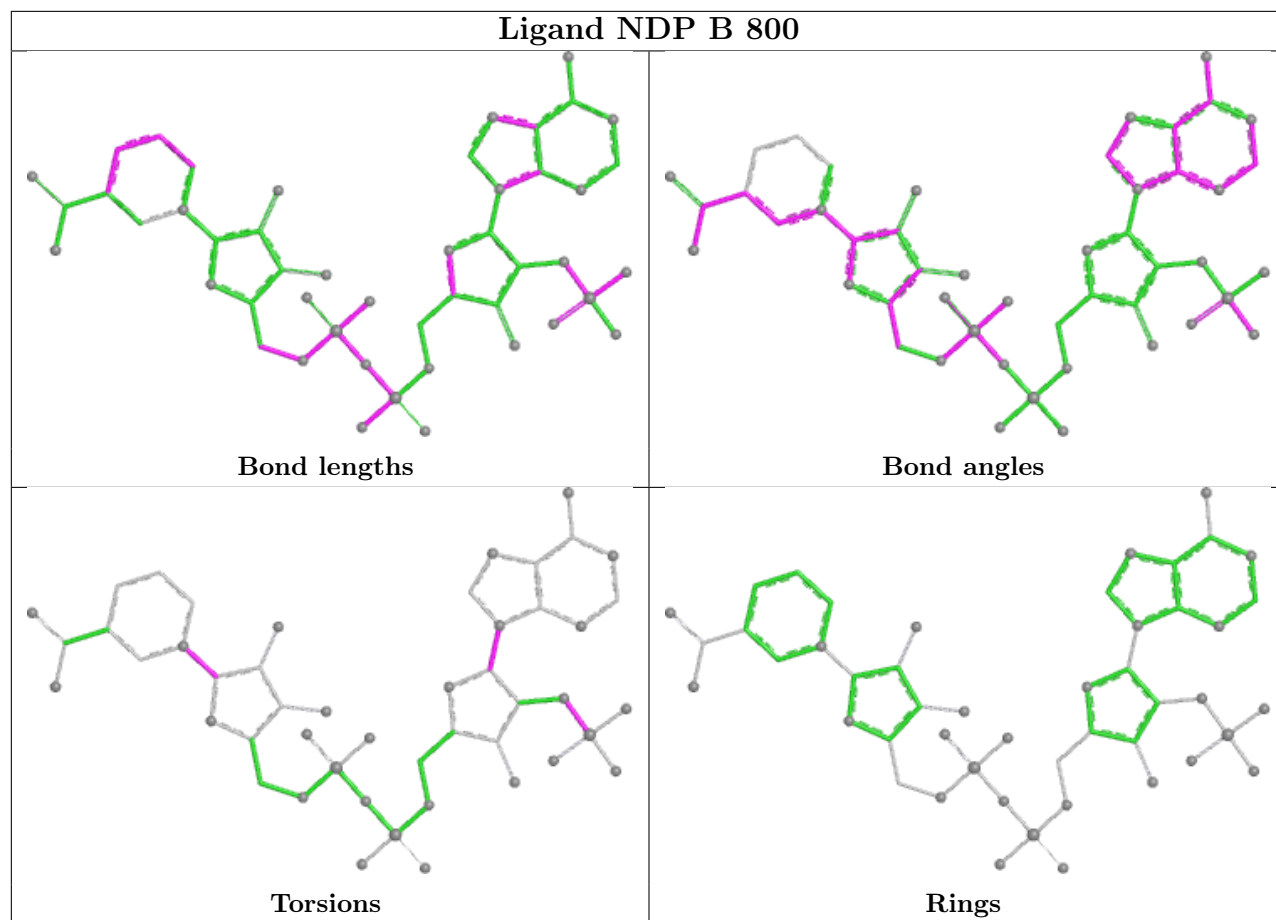
10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1001[A]	GCG	3	0
4	D	1001[A]	GCG	4	0
2	C	700	FAD	1	0
4	A	1001[A]	GCG	3	0
4	B	1001[A]	GCG	4	0
3	C	800	NDP	1	0
4	C	1001[B]	GCG	1	0
4	D	1001[B]	GCG	2	0
2	A	700	FAD	1	0
2	B	700	FAD	2	0

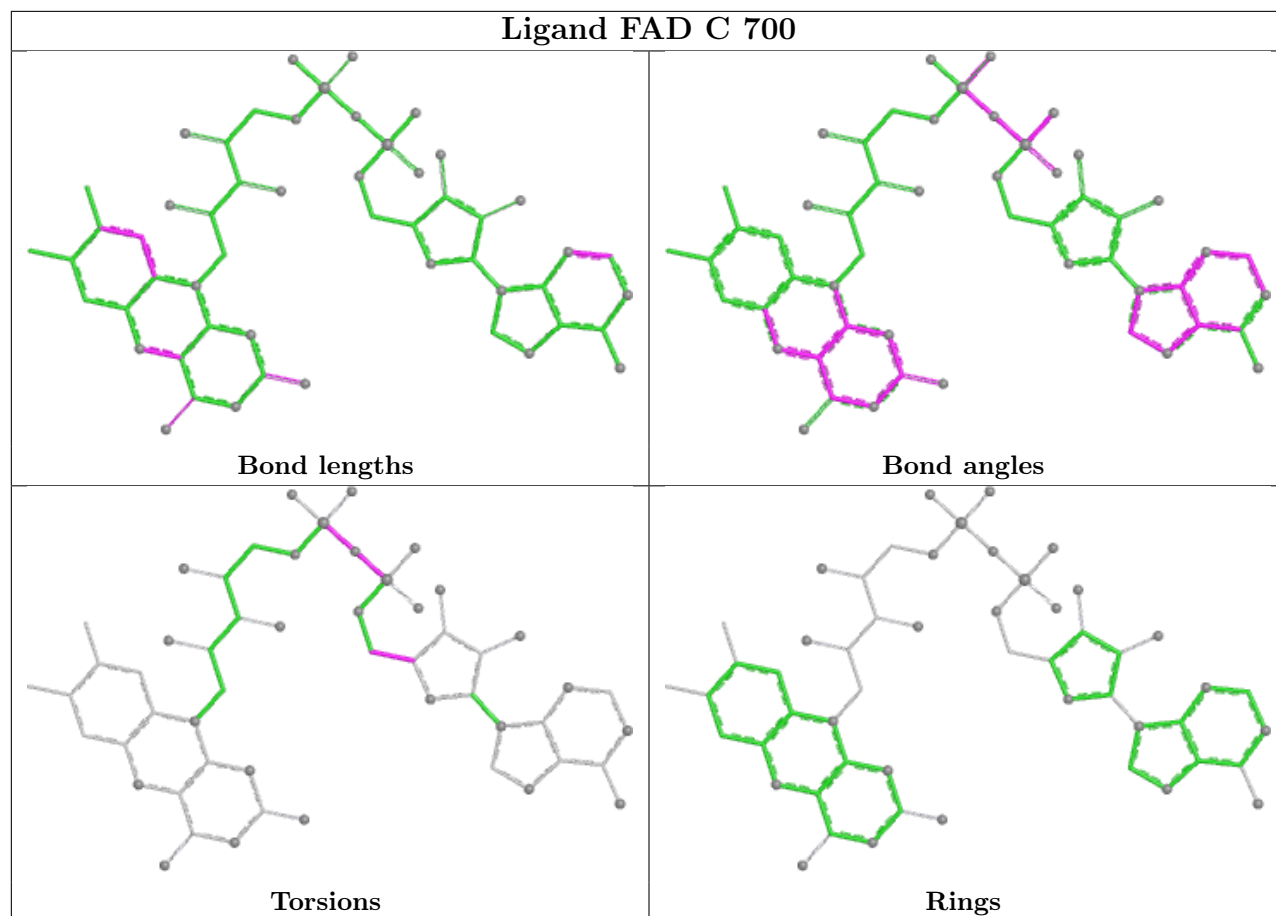
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



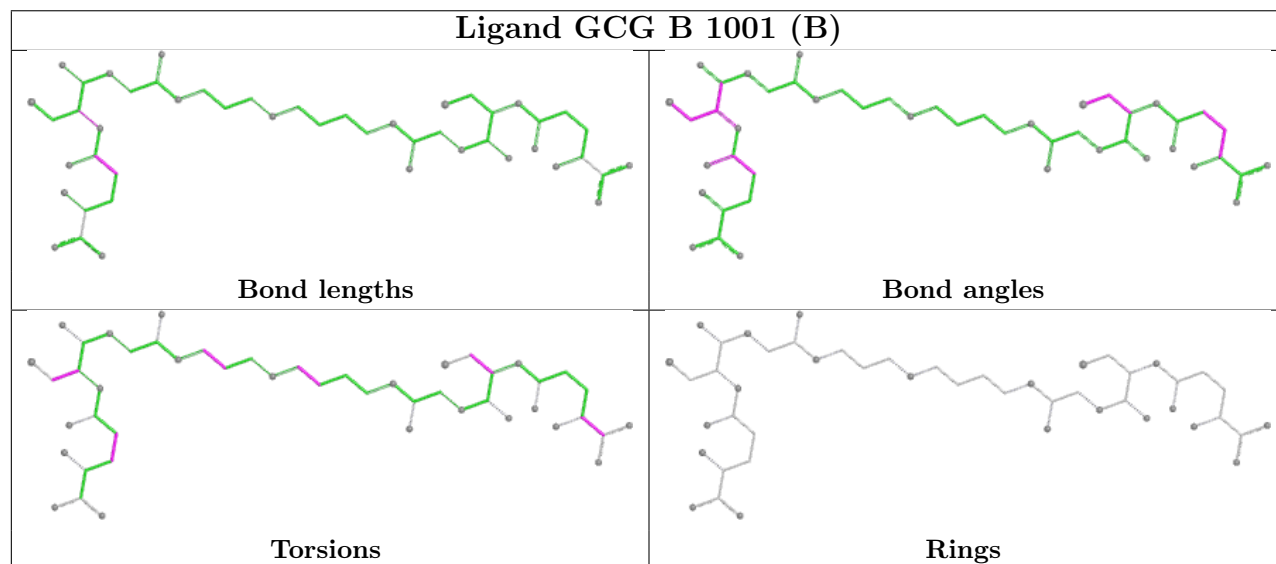


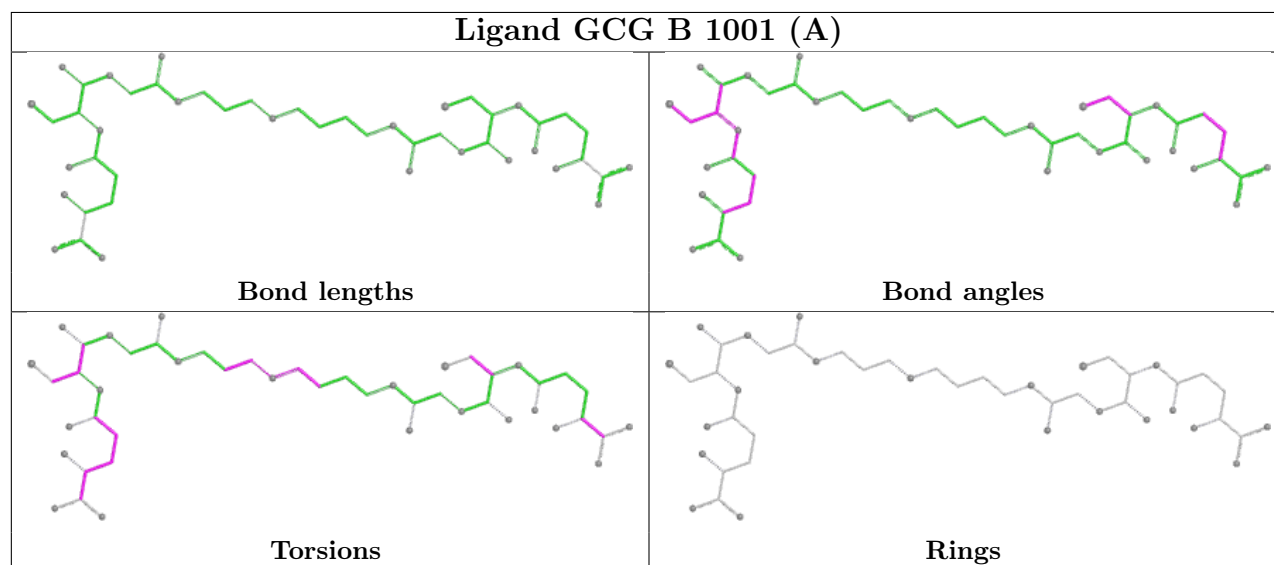
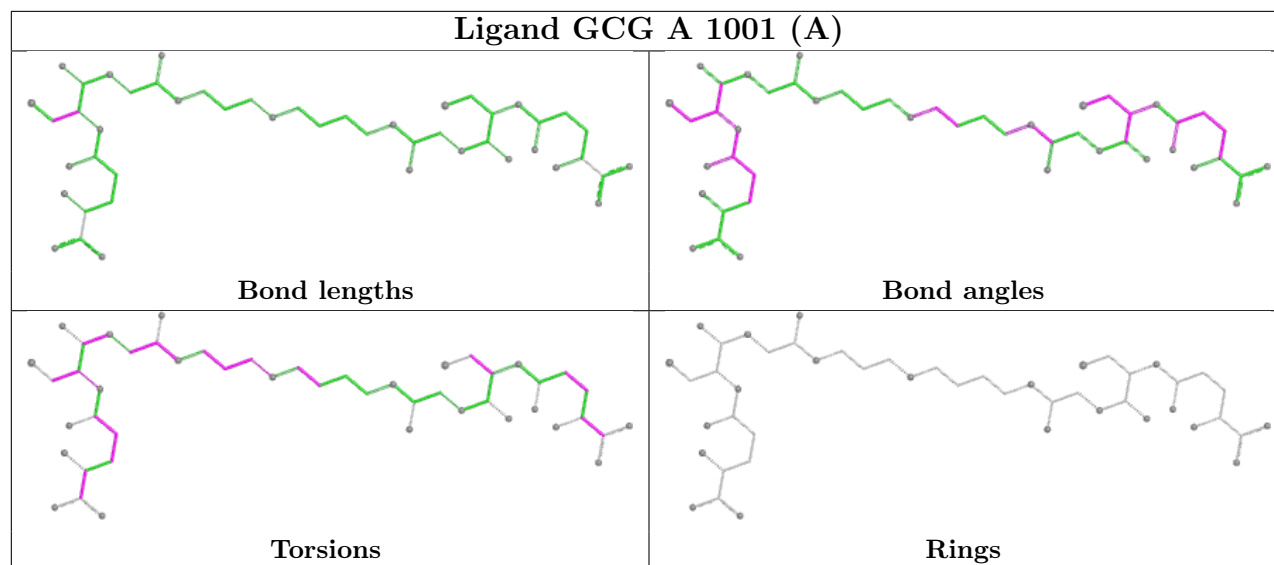


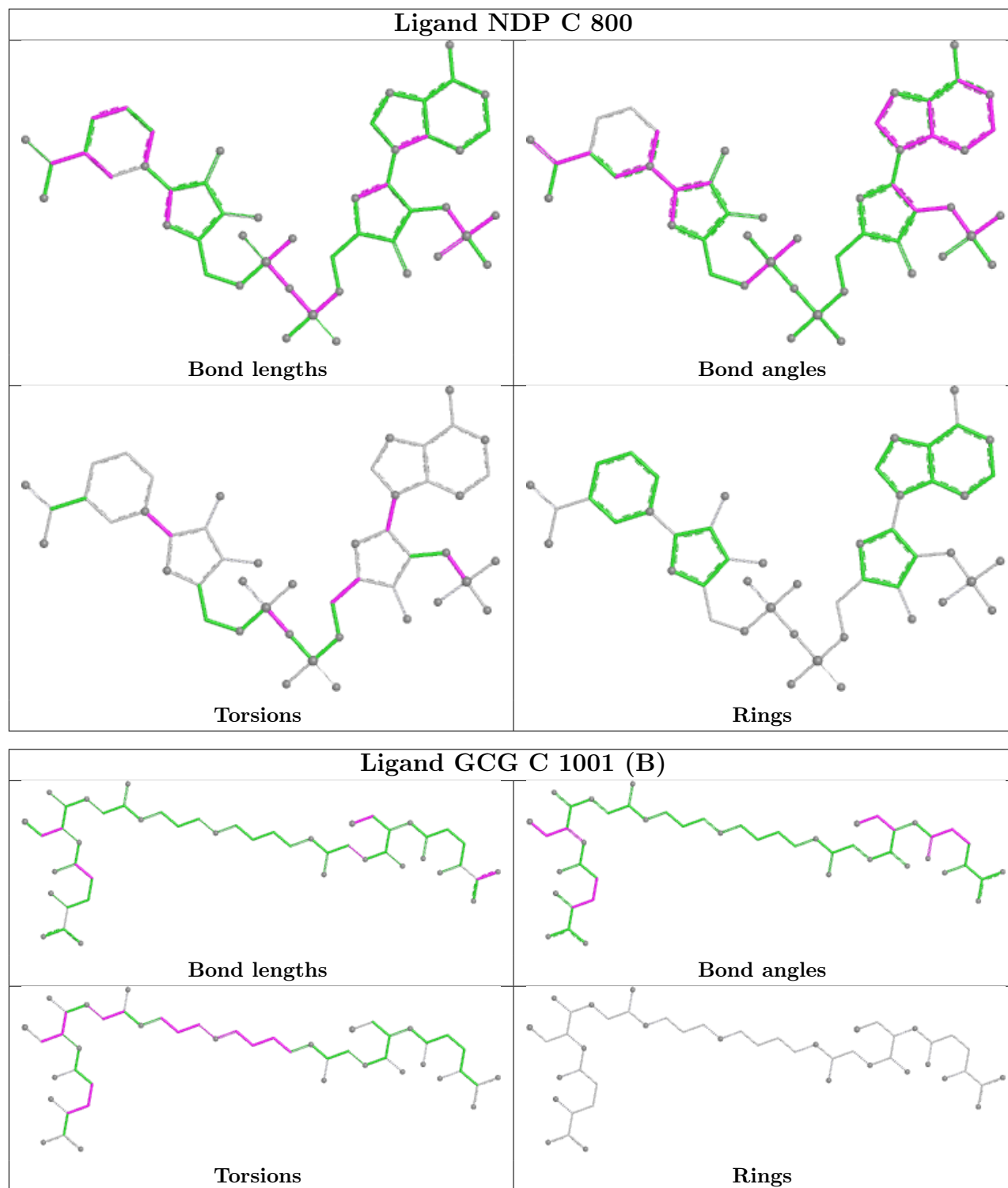
Ligand FAD C 700

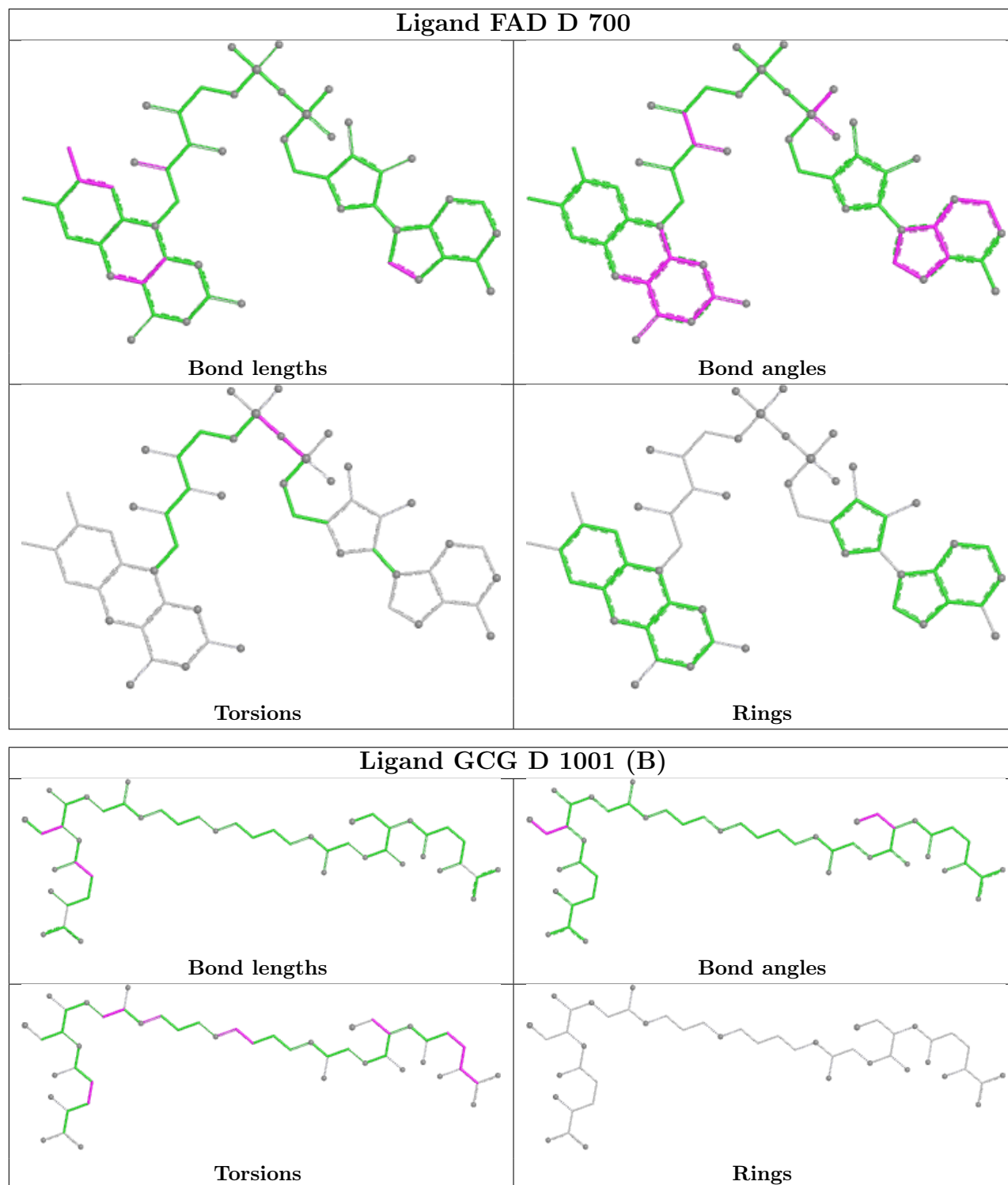


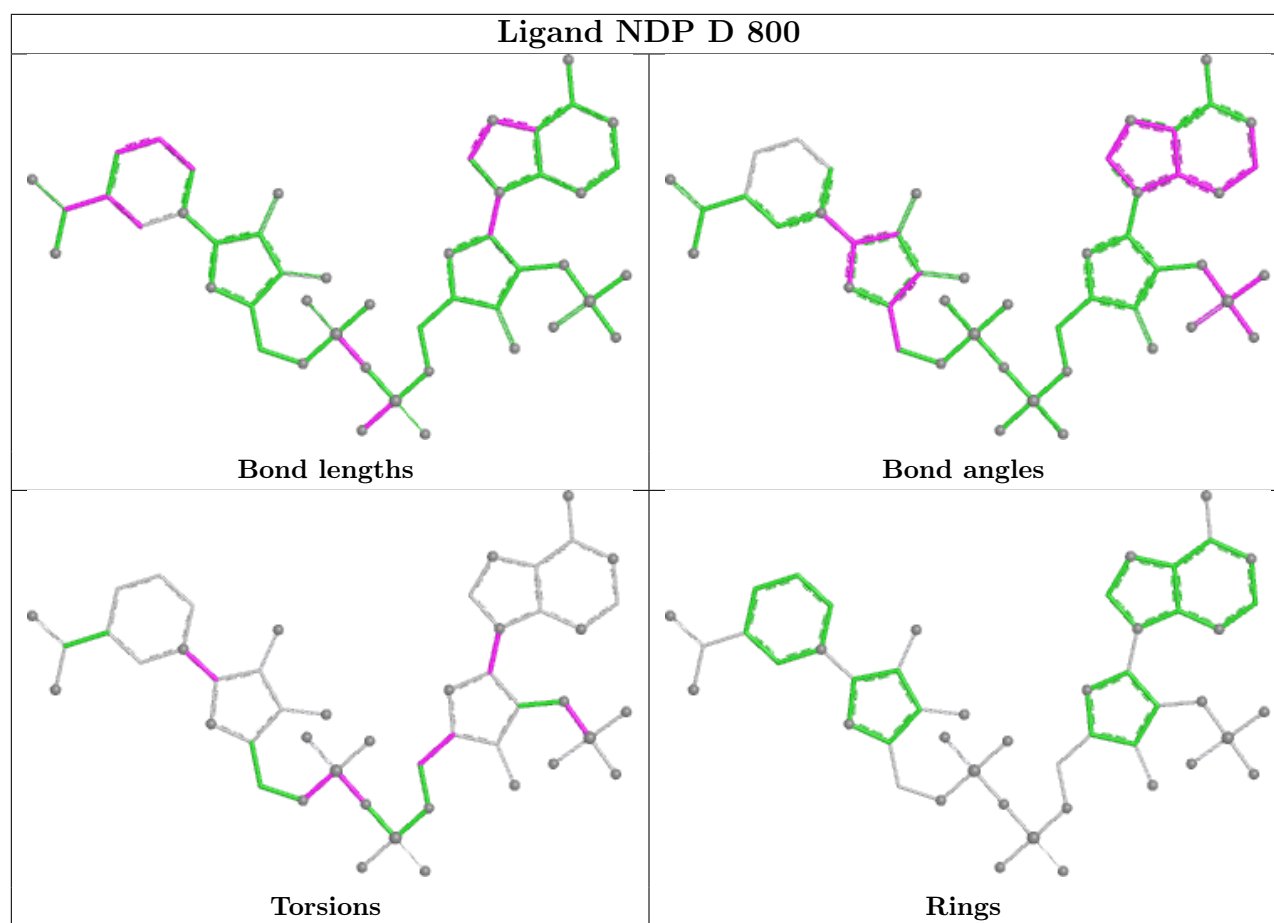
Ligand GCG B 1001 (B)

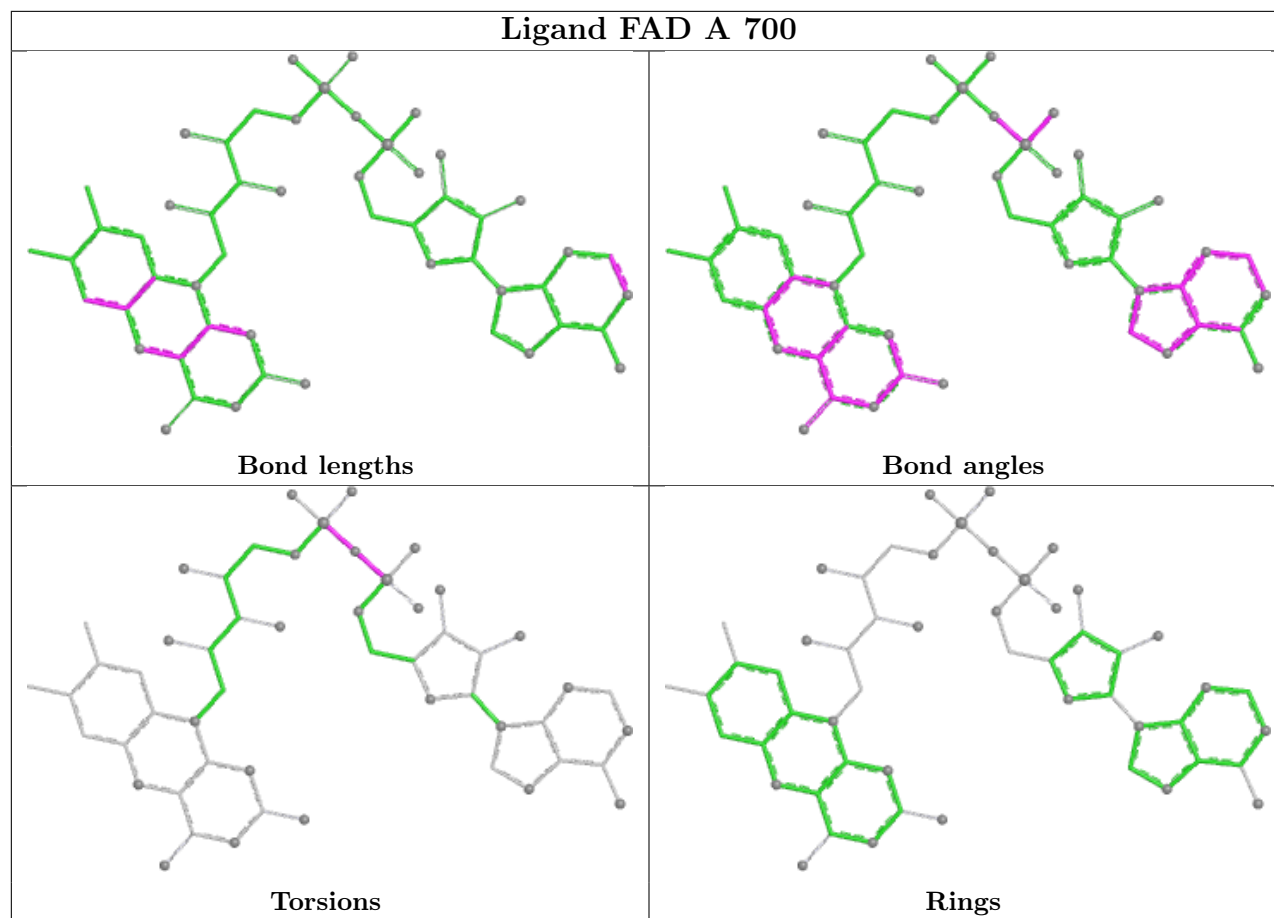


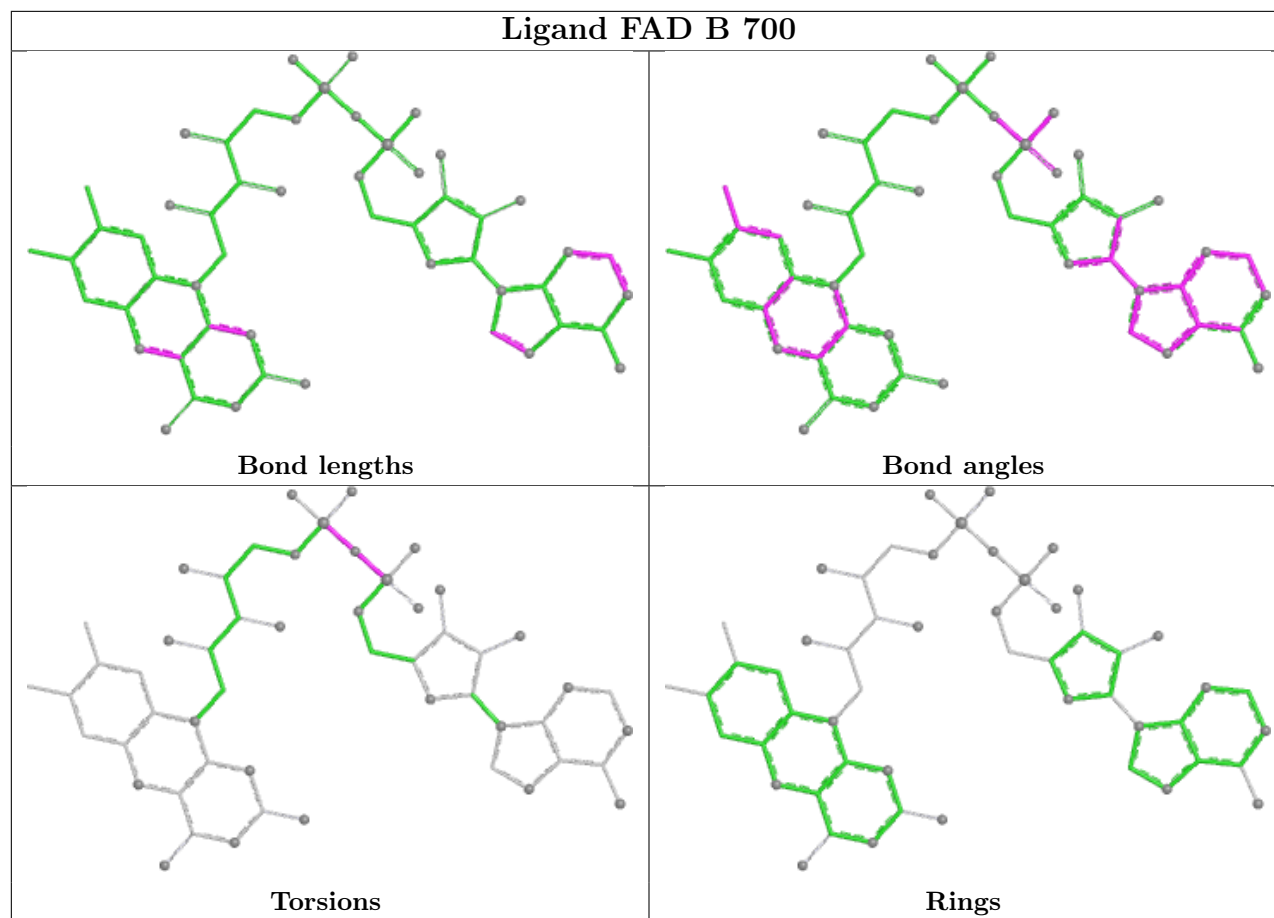












5.7 Other polymers [i](#)

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	490/495 (98%)	-0.73	0 100 100	11, 22, 36, 55	2 (0%)
1	B	488/495 (98%)	-0.43	3 (0%) 85 83	13, 26, 52, 74	2 (0%)
1	C	491/495 (99%)	-0.76	0 100 100	13, 21, 35, 56	1 (0%)
1	D	490/495 (98%)	-0.64	4 (0%) 82 80	13, 23, 42, 60	1 (0%)
All	All	1959/1980 (98%)	-0.64	7 (0%) 88 87	11, 23, 45, 74	6 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399[A]	LEU	3.9
1	D	491	ASN	3.3
1	D	489	ASP	2.6
1	B	4	ALA	2.3
1	D	2	SER	2.2
1	B	349	VAL	2.2
1	D	490	SER	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 oligosaccharides in this entry.

6.4 Ligands

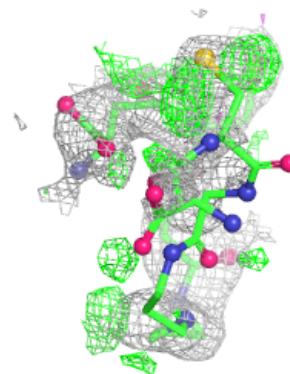
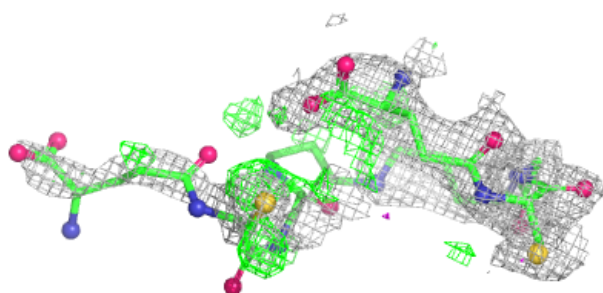
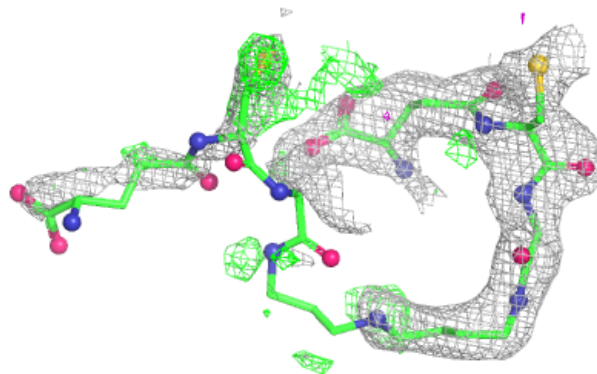
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GCG	D	1001[A]	48/48	0.82	0.18	27,42,51,51	48
4	GCG	D	1001[B]	48/48	0.82	0.18	17,37,50,51	48
4	GCG	C	1001[A]	48/48	0.83	0.15	15,28,41,43	48
4	GCG	C	1001[B]	48/48	0.83	0.15	7,32,47,49	48
4	GCG	B	1001[A]	48/48	0.88	0.11	19,34,40,42	48
4	GCG	B	1001[B]	48/48	0.88	0.11	16,34,40,42	48
4	GCG	A	1001[A]	48/48	0.89	0.14	14,29,37,40	48
4	GCG	A	1001[B]	48/48	0.89	0.14	13,27,41,43	48
3	NDP	A	800	48/48	0.97	0.05	19,24,29,32	0
3	NDP	B	800	48/48	0.97	0.05	18,25,30,33	0
3	NDP	C	800	48/48	0.98	0.05	17,22,26,28	0
3	NDP	D	800	48/48	0.98	0.05	15,25,31,33	0
2	FAD	D	700	53/53	0.98	0.04	12,19,24,26	0
2	FAD	B	700	53/53	0.98	0.05	10,20,30,33	0
2	FAD	C	700	53/53	0.98	0.04	12,16,18,21	0
2	FAD	A	700	53/53	0.99	0.03	10,14,18,21	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.

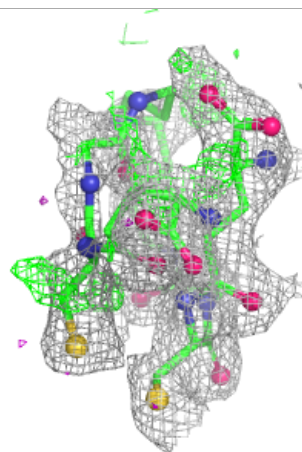
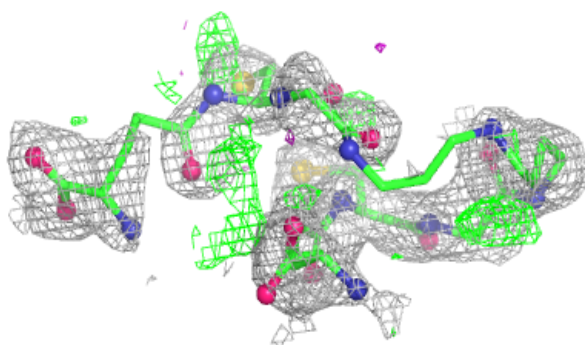
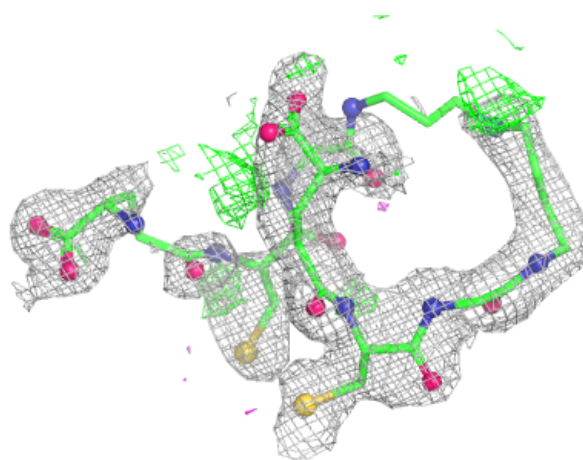
Electron density around GCG D 1001 (A):

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



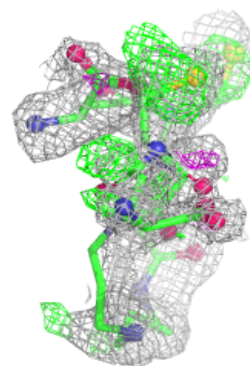
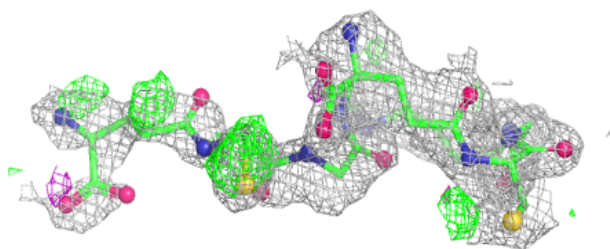
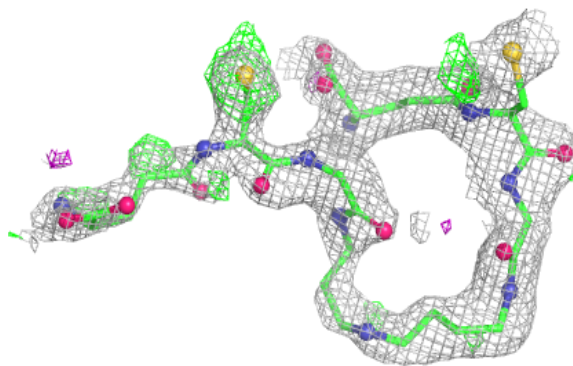
Electron density around GCG D 1001 (B):

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

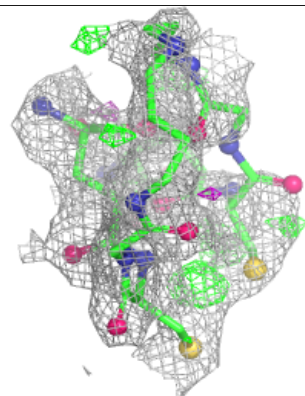
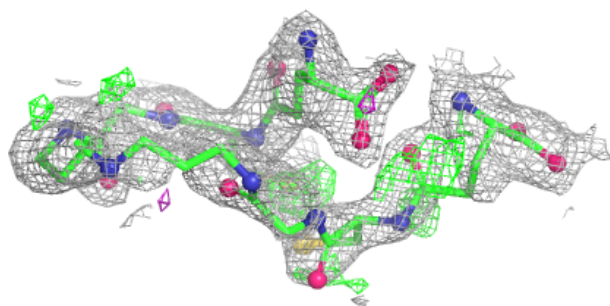
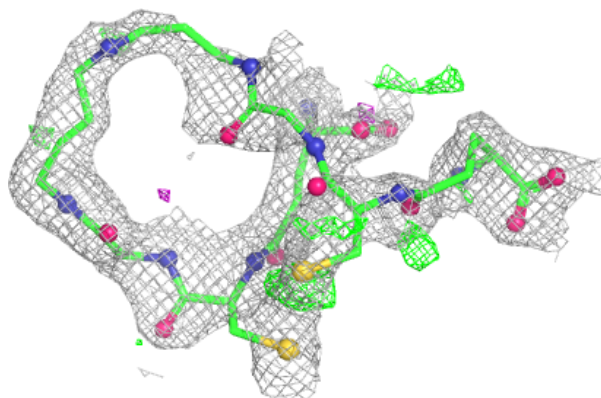


Electron density around GCG C 1001 (A):

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

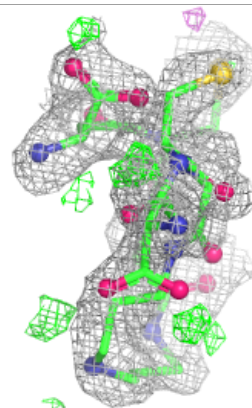
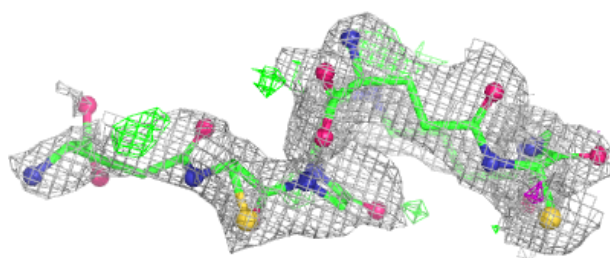
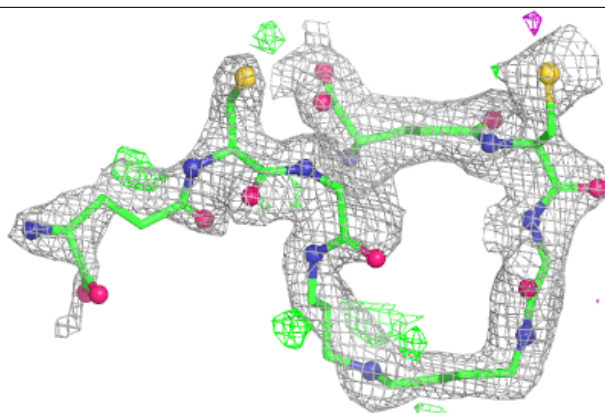
**Electron density around GCG C 1001 (B):**

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

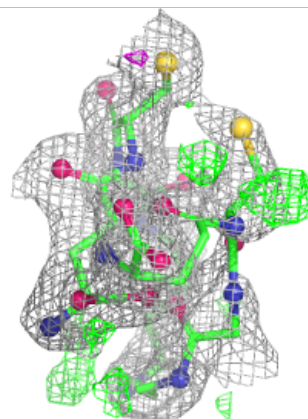
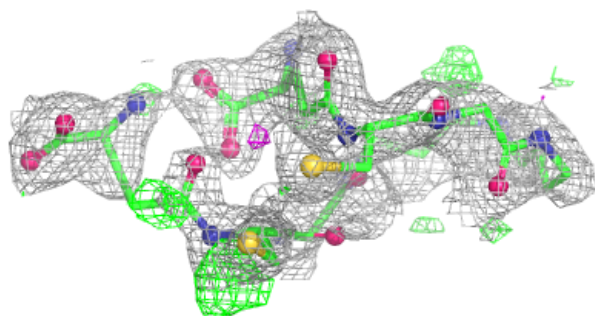
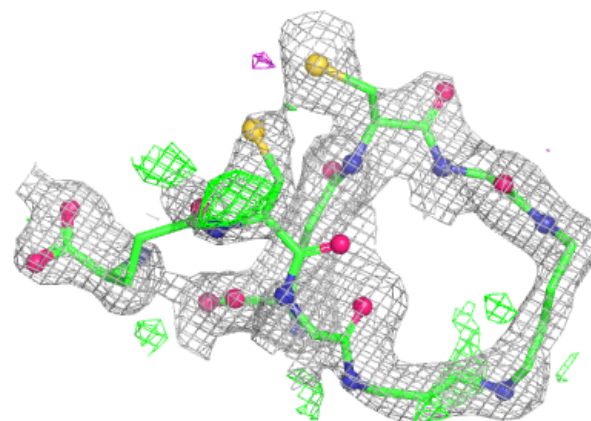


Electron density around GCG B 1001 (A):

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

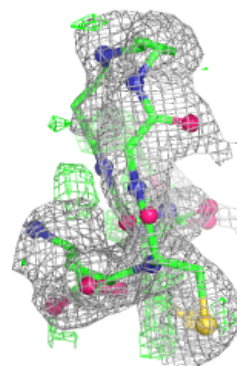
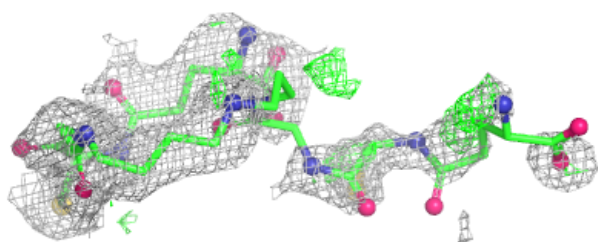
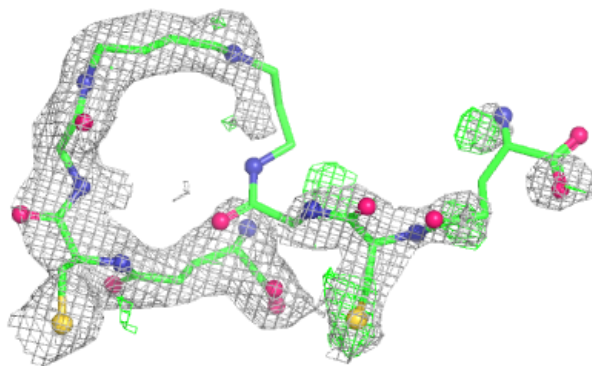
**Electron density around GCG B 1001 (B):**

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

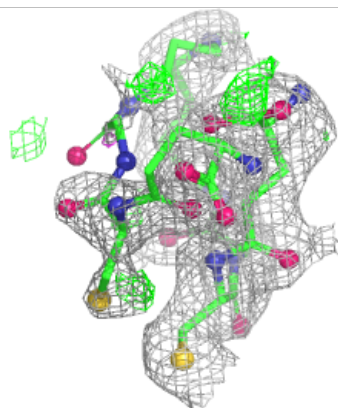
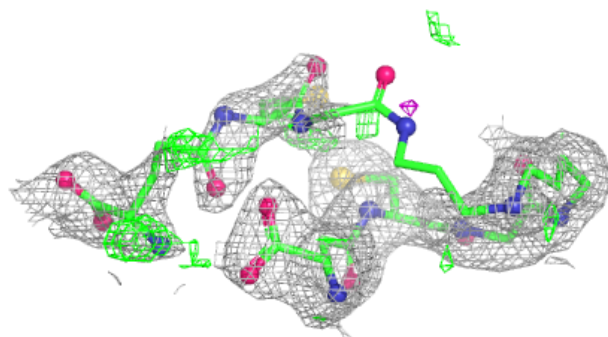
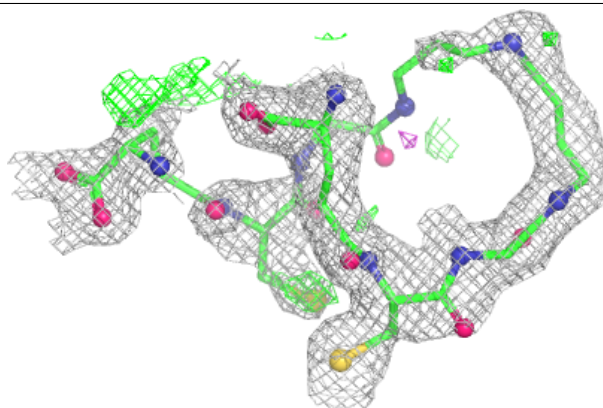


Electron density around GCG A 1001 (A):

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

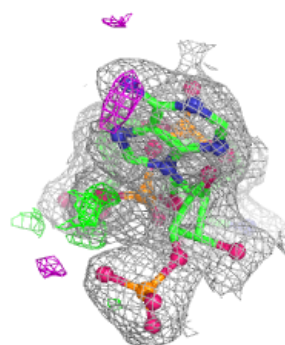
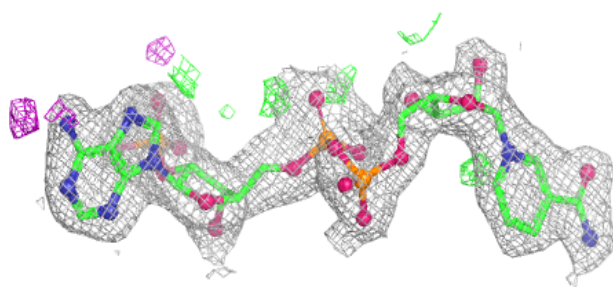
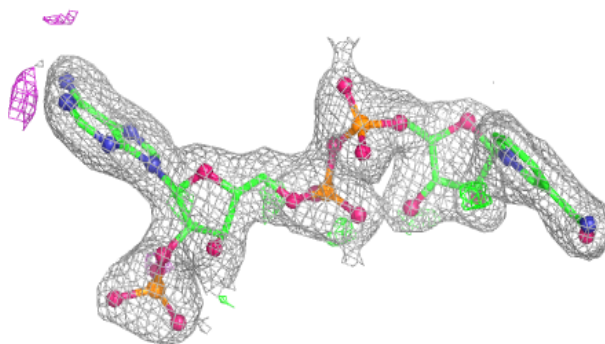
**Electron density around GCG A 1001 (B):**

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

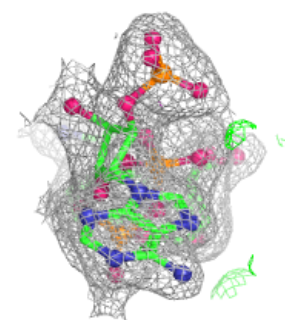
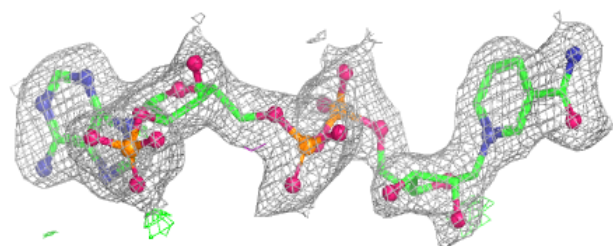
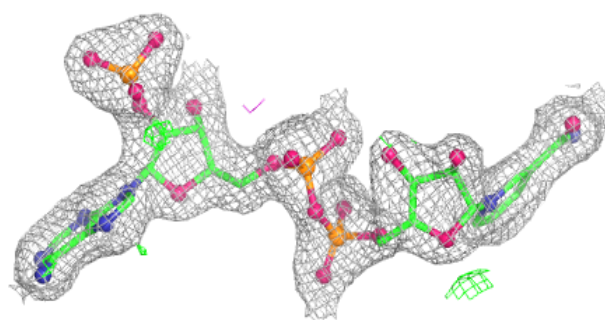


Electron density around NDP A 800:

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

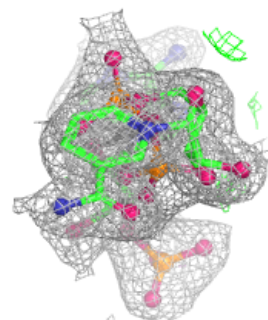
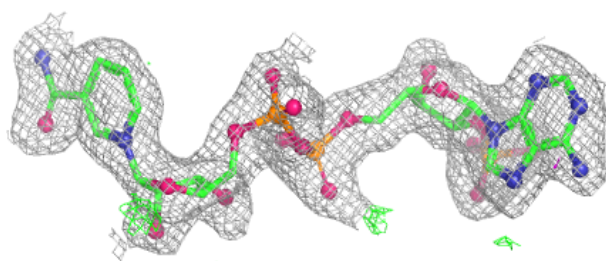
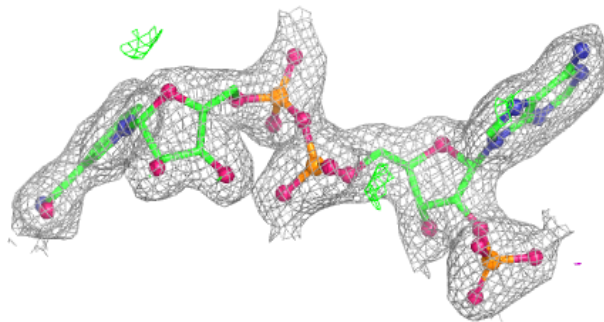
**Electron density around NDP B 800:**

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

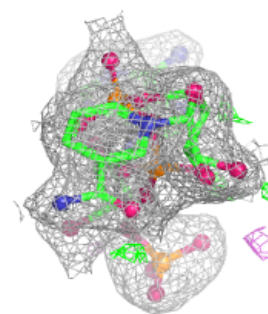
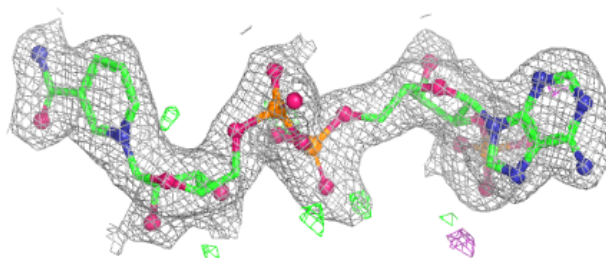
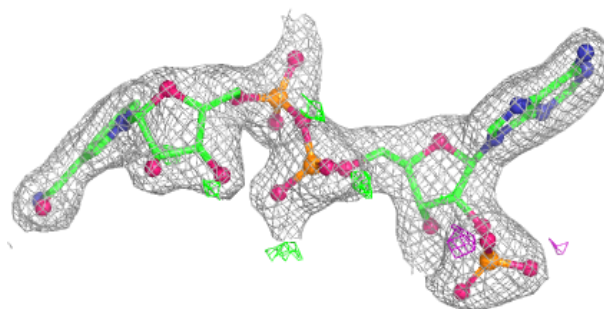


Electron density around NDP C 800:

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

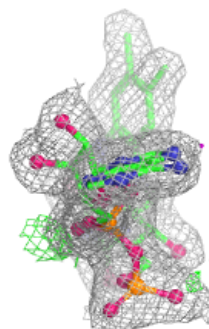
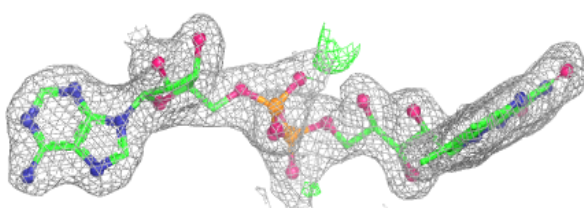
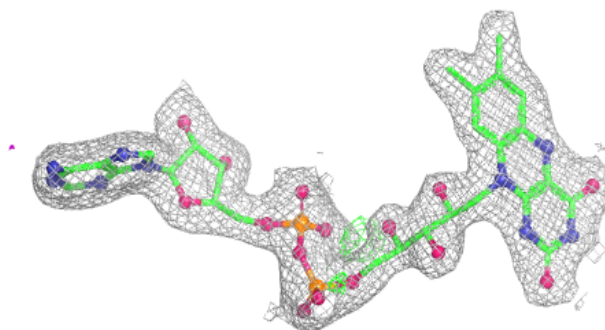
**Electron density around NDP D 800:**

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

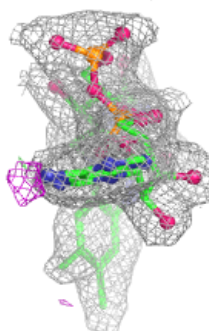
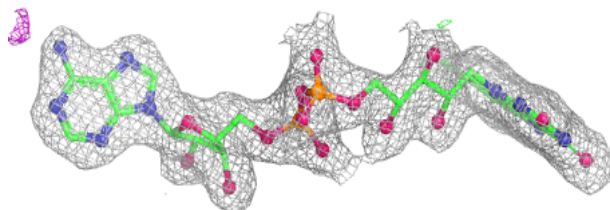
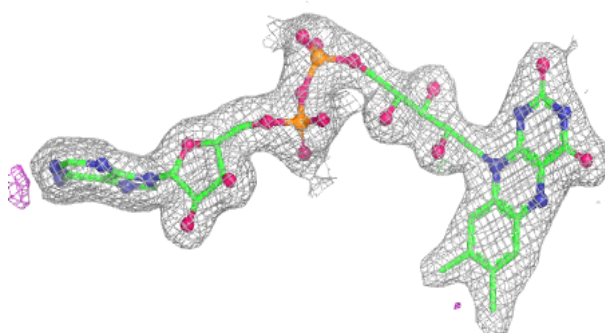


Electron density around FAD D 700:

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

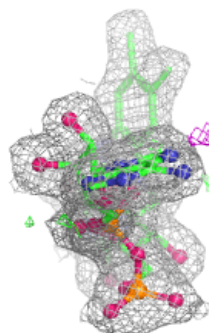
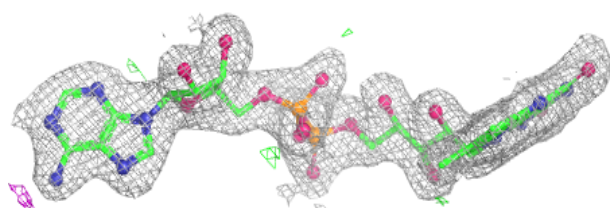
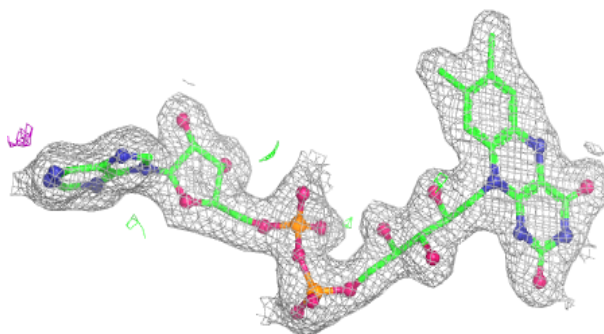
**Electron density around FAD B 700:**

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

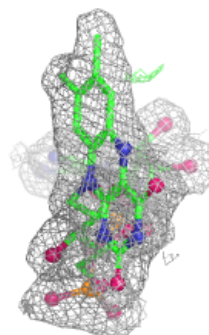
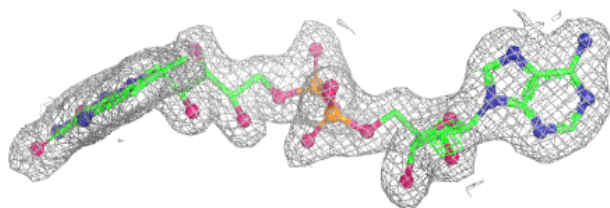
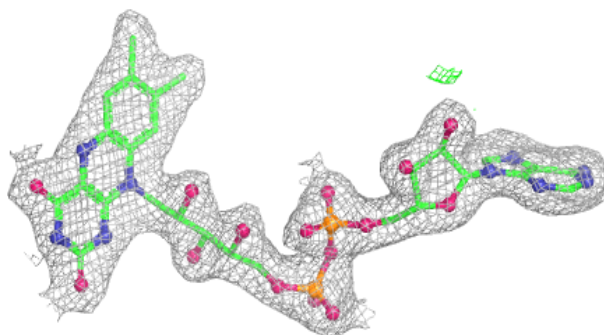


Electron density around FAD C 700:

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

**Electron density around FAD A 700:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.