



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:17 PM UTC

PDB ID : 4G74 / pdb_00004g74
Title : Crystal structure of NDH with Quinone
Authors : Li, W.; Feng, Y.; Ge, J.; Yang, M.
Deposited on : 2012-07-19
Resolution : 2.48 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

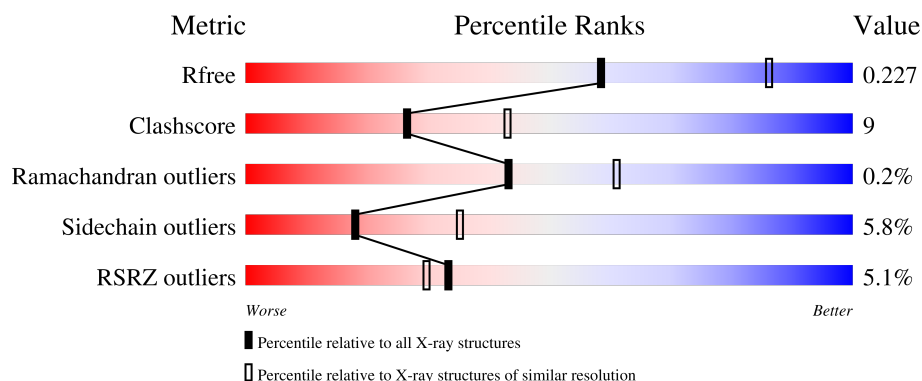
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	502	 4% 81% 12% • 6%
1	B	502	 5% 79% 11% • 8%

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	UQ5	A	602	-	-	X	-
2	UQ5	B	602	-	-	X	-
2	UQ5	B	603	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8024 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.

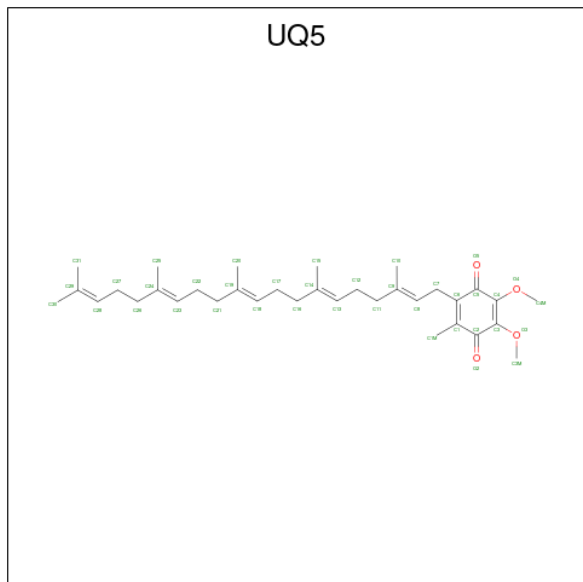
- Molecule 1 is a protein called Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3718	2406	628	679	5			
1	B	463	Total	C	N	O	S	0	0	0
			3658	2367	619	667	5			

There are 24 discrepancies between the modelled and reference sequences:

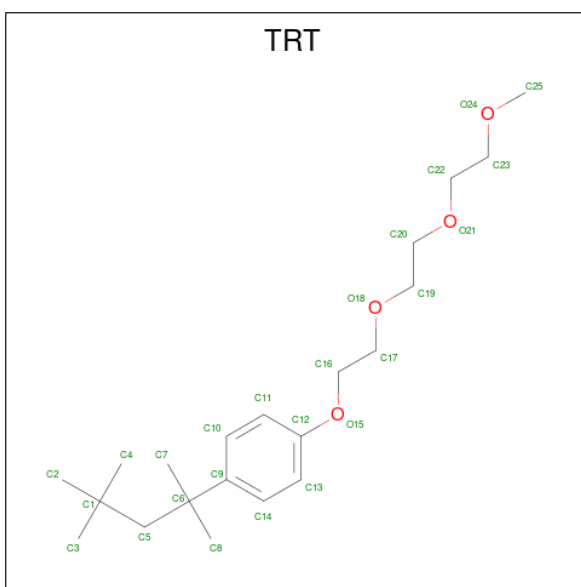
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP P32340
A	13	ARG	-	expression tag	UNP P32340
A	14	GLY	-	expression tag	UNP P32340
A	15	SER	-	expression tag	UNP P32340
A	16	HIS	-	expression tag	UNP P32340
A	17	HIS	-	expression tag	UNP P32340
A	18	HIS	-	expression tag	UNP P32340
A	19	HIS	-	expression tag	UNP P32340
A	20	HIS	-	expression tag	UNP P32340
A	21	HIS	-	expression tag	UNP P32340
A	22	GLY	-	expression tag	UNP P32340
A	23	SER	-	expression tag	UNP P32340
B	12	MET	-	expression tag	UNP P32340
B	13	ARG	-	expression tag	UNP P32340
B	14	GLY	-	expression tag	UNP P32340
B	15	SER	-	expression tag	UNP P32340
B	16	HIS	-	expression tag	UNP P32340
B	17	HIS	-	expression tag	UNP P32340
B	18	HIS	-	expression tag	UNP P32340
B	19	HIS	-	expression tag	UNP P32340
B	20	HIS	-	expression tag	UNP P32340
B	21	HIS	-	expression tag	UNP P32340
B	22	GLY	-	expression tag	UNP P32340
B	23	SER	-	expression tag	UNP P32340

- Molecule 2 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: $C_{34}H_{50}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	19	4		
2	A	1	Total	C	O	0	0
			27	23	4		
2	B	1	Total	C	O	0	0
			23	19	4		
2	B	1	Total	C	O	0	0
			23	19	4		

- Molecule 3 is FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula: $C_{21}H_{36}O_4$).

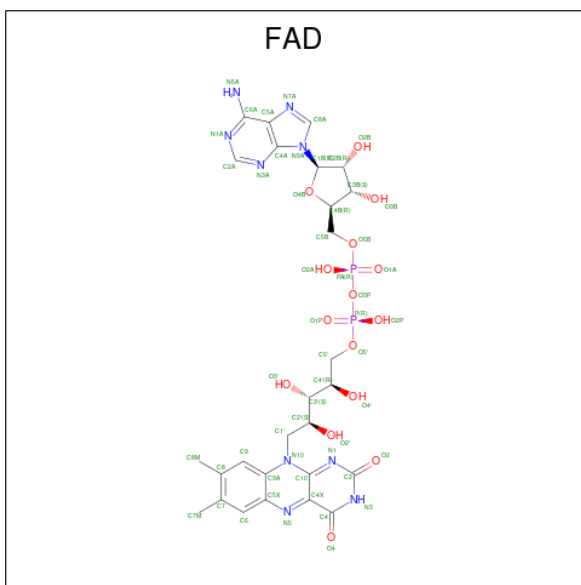


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			16	15	1		
3	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	B	6	Total	Mg	0	0
			6	6		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	191	Total O 191 191	0	0
6	B	168	Total O 168 168	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.91Å 230.84Å 112.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.61 – 2.48 43.61 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.61-2.48) 97.1 (43.61-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.195 , 0.233 0.191 , 0.227	Depositor DCC
R_{free} test set	3031 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.016 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8024	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UQ5, FAD, TRT

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	0.52	0/3805	0.85	3/5154 (0.1%)
1	B	0.50	0/3743	0.84	6/5070 (0.1%)
All	All	0.51	0/7548	0.84	9/10224 (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	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ASN	N-CA-C	-5.87	105.97	114.12
1	B	163	GLU	CA-C-N	5.66	125.67	119.90
1	B	163	GLU	C-N-CA	5.66	125.67	119.90
1	B	378	ILE	N-CA-C	5.30	115.73	107.99
1	A	413	ILE	CA-C-N	5.18	124.85	119.56
1	A	413	ILE	C-N-CA	5.18	124.85	119.56
1	A	427	ILE	N-CA-C	5.16	115.88	110.62
1	B	133	ASN	CA-C-N	5.07	124.56	119.19
1	B	133	ASN	C-N-CA	5.07	124.56	119.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	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	3718	0	3767	35	0
1	B	3658	0	3708	50	0
2	A	50	0	54	32	0
2	B	46	0	46	46	0
3	A	56	0	75	5	0
3	B	20	0	27	3	0
4	A	5	0	0	0	0
4	B	6	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	1	0
6	A	191	0	0	1	0
6	B	168	0	0	1	0
All	All	8024	0	7739	143	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 9.

All (143) 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)
2:B:602:UQ5:C3M	2:B:603:UQ5:H4M2	1.29	1.62
2:B:602:UQ5:C3M	2:B:603:UQ5:C4M	1.79	1.57
2:B:602:UQ5:H3M2	2:B:603:UQ5:C4M	1.35	1.48
2:A:602:UQ5:C11	2:A:602:UQ5:H1M2	1.45	1.44
2:B:603:UQ5:H122	2:B:603:UQ5:C1M	1.55	1.36
2:B:603:UQ5:C9	2:B:603:UQ5:H1M1	1.56	1.35
2:A:602:UQ5:H112	2:A:602:UQ5:C1M	1.72	1.17
2:A:601:UQ5:H8	2:A:601:UQ5:H1M3	1.26	1.12
2:A:601:UQ5:H8	2:A:601:UQ5:C1M	1.80	1.11
1:A:459:ILE:HD12	2:A:602:UQ5:H103	1.19	1.10
2:B:603:UQ5:H122	2:B:603:UQ5:H1M3	1.28	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:602:UQ5:C1M	2:A:602:UQ5:C9	2.30	1.10
2:B:602:UQ5:H3M3	2:B:603:UQ5:H4M2	1.27	1.08
2:B:602:UQ5:C9	2:B:602:UQ5:C1M	2.30	1.08
2:B:602:UQ5:H3M1	2:B:603:UQ5:C4M	1.81	1.08
2:B:603:UQ5:C1M	2:B:603:UQ5:C12	2.30	1.08
2:B:603:UQ5:C1M	2:B:603:UQ5:C9	2.30	1.08
2:A:602:UQ5:C11	2:A:602:UQ5:C1M	2.30	1.07
2:B:602:UQ5:C3M	2:B:603:UQ5:H4M1	1.65	1.06
2:B:602:UQ5:H3M1	2:B:603:UQ5:H4M1	1.30	1.06
2:A:602:UQ5:C9	2:A:602:UQ5:H1M1	1.84	1.05
2:A:601:UQ5:H1M3	2:A:601:UQ5:C8	1.83	1.02
2:B:603:UQ5:C12	2:B:603:UQ5:H1M2	1.89	1.02
2:B:602:UQ5:C9	2:B:602:UQ5:H1M1	1.94	0.97
2:B:602:UQ5:C9	2:B:602:UQ5:H1M2	1.93	0.96
2:B:603:UQ5:H1M2	2:B:603:UQ5:C11	1.95	0.96
2:A:601:UQ5:C3M	2:A:602:UQ5:O2	2.16	0.93
2:B:603:UQ5:C1M	2:B:603:UQ5:C11	2.47	0.93
2:B:603:UQ5:H122	2:B:603:UQ5:H1M2	1.43	0.93
1:A:459:ILE:CD1	2:A:602:UQ5:H103	2.00	0.92
1:A:459:ILE:HD12	2:A:602:UQ5:C10	2.02	0.88
1:B:368:ASP:HB3	1:B:438:PRO:HB3	1.55	0.87
2:A:602:UQ5:H1M2	2:A:602:UQ5:C9	2.01	0.85
1:A:447:LEU:HD11	2:A:602:UQ5:H8	1.57	0.83
2:A:602:UQ5:H1M2	2:A:602:UQ5:H112	0.84	0.83
2:A:601:UQ5:H3M1	2:A:602:UQ5:O2	1.81	0.80
3:A:603:TRT:H2C1	3:A:604:TRT:H4C1	1.66	0.78
1:B:137:ASN:OD1	1:B:377:ASN:ND2	2.18	0.77
1:A:447:LEU:CD1	2:A:602:UQ5:H8	2.15	0.76
2:B:602:UQ5:H1M2	2:B:602:UQ5:C11	2.17	0.75
2:B:602:UQ5:C4M	2:B:602:UQ5:O3	2.35	0.73
2:A:601:UQ5:C1M	2:A:601:UQ5:C8	2.50	0.72
1:B:155:ASN:OD1	1:B:155:ASN:N	2.23	0.72
1:A:484:SER:O	2:A:601:UQ5:H71	1.89	0.71
1:B:226:ARG:NH2	6:B:845:HOH:O	2.23	0.70
2:B:603:UQ5:C4M	2:B:603:UQ5:O3	2.40	0.70
1:B:355:PRO:O	1:B:358:ASN:ND2	2.24	0.70
2:B:602:UQ5:H3M2	2:B:603:UQ5:H4M2	0.98	0.70
2:A:601:UQ5:O5	2:A:601:UQ5:H4M2	1.92	0.69
2:A:601:UQ5:H3M2	2:A:602:UQ5:O2	1.92	0.68
2:A:601:UQ5:H8	2:A:601:UQ5:H1M2	1.75	0.68
2:A:602:UQ5:O2	2:A:602:UQ5:H3M2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:UQ5:H3M3	2:A:601:UQ5:O2	1.95	0.66
2:B:603:UQ5:O2	2:B:603:UQ5:H3M3	1.95	0.66
1:B:397:HIS:CD2	2:B:603:UQ5:C4M	2.78	0.66
2:B:603:UQ5:O3	2:B:603:UQ5:H4M3	1.95	0.65
2:A:601:UQ5:C3M	2:A:601:UQ5:O2	2.45	0.65
3:A:603:TRT:H4C1	3:A:604:TRT:H3C1	1.77	0.65
1:B:397:HIS:CD2	2:B:603:UQ5:H4M1	2.30	0.65
2:A:602:UQ5:H4M2	2:A:602:UQ5:O3	1.94	0.65
1:B:393:ALA:HB3	2:B:602:UQ5:C4M	2.27	0.65
2:B:602:UQ5:H3M2	2:B:603:UQ5:H4M1	1.40	0.64
2:A:602:UQ5:O2	2:A:602:UQ5:C3M	2.46	0.63
1:A:210:ALA:HB2	1:A:511:LYS:HE3	1.79	0.63
2:B:603:UQ5:O2	2:B:603:UQ5:C3M	2.47	0.62
1:B:415:ASN:O	1:B:419:ASN:N	2.33	0.61
2:B:603:UQ5:C1M	2:B:603:UQ5:C8	2.75	0.61
1:A:138:THR:HG21	1:A:166:GLU:OE1	2.01	0.61
1:A:368:ASP:HB3	1:A:438:PRO:HB3	1.82	0.61
1:B:432:GLU:OE1	1:B:432:GLU:N	2.27	0.59
2:B:602:UQ5:O3	2:B:602:UQ5:H4M2	2.03	0.59
1:B:480:ILE:HG13	3:B:604:TRT:H3C1	1.84	0.58
2:B:602:UQ5:H3M2	2:B:602:UQ5:O2	2.05	0.57
1:B:371:GLN:NE2	1:B:375:SER:O	2.39	0.56
1:A:482:TYR:HD1	1:A:485:MET:HE3	1.70	0.55
1:B:503:ALA:HB2	3:B:604:TRT:H11	1.89	0.55
1:B:178:ALA:O	1:B:196:LYS:HE2	2.07	0.54
1:B:180:PRO:HD3	1:B:196:LYS:HD2	1.90	0.54
1:B:376:ASN:OD1	1:B:376:ASN:N	2.39	0.53
1:B:444:LEU:O	2:B:602:UQ5:C10	2.58	0.52
1:A:106:SER:HA	1:A:494:LYS:HD3	1.92	0.51
2:A:601:UQ5:O5	2:A:601:UQ5:C4M	2.58	0.51
1:B:133:ASN:HB2	1:B:138:THR:HG22	1.92	0.51
3:A:605:TRT:H3C3	3:A:605:TRT:H7C1	1.93	0.50
1:A:278:LEU:HD13	1:A:456:ILE:HD11	1.93	0.50
1:B:393:ALA:CB	2:B:602:UQ5:C4M	2.90	0.50
1:B:393:ALA:HB3	2:B:602:UQ5:H4M1	1.93	0.50
1:B:53:LYS:HE2	1:B:75:LYS:O	2.11	0.50
1:B:444:LEU:O	2:B:602:UQ5:H101	2.11	0.50
1:B:138:THR:HG21	1:B:166:GLU:OE1	2.12	0.50
2:B:603:UQ5:H1M2	2:B:603:UQ5:H112	1.88	0.50
1:A:317:LYS:HG2	1:A:327:GLU:HG2	1.94	0.49
1:A:392:THR:HB	5:A:607:FAD:O2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:HB3	1:B:378:ILE:HG13	1.94	0.49
1:B:137:ASN:CG	1:B:377:ASN:HD21	2.18	0.49
1:B:367:ASN:HD21	1:B:371:GLN:HB3	1.77	0.49
1:A:494:LYS:HE2	1:B:501:LYS:HZ2	1.77	0.49
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.96	0.48
1:A:459:ILE:CD1	2:A:602:UQ5:C10	2.79	0.48
1:B:392:THR:HB	5:B:606:FAD:O2	2.14	0.48
1:B:484:SER:O	2:B:603:UQ5:H1M1	2.14	0.48
2:A:602:UQ5:O3	2:A:602:UQ5:C4M	2.62	0.48
2:B:602:UQ5:O3	2:B:602:UQ5:H4M3	2.10	0.48
1:A:66:ILE:HG13	1:A:88:PHE:HB2	1.94	0.47
1:A:251:VAL:HG21	1:A:266:VAL:HG21	1.97	0.47
1:B:152:GLN:CD	1:B:152:GLN:H	2.22	0.47
1:B:393:ALA:CB	2:B:602:UQ5:H4M1	2.45	0.47
1:A:94:LEU:O	1:A:98:PRO:HD3	2.15	0.46
1:A:494:LYS:HE2	1:B:501:LYS:NZ	2.31	0.46
2:A:602:UQ5:C1M	2:A:602:UQ5:C8	2.92	0.45
3:B:604:TRT:H5C2	3:B:604:TRT:H14	1.46	0.45
1:B:397:HIS:CG	2:B:603:UQ5:H4M1	2.51	0.45
1:A:137:ASN:OD1	1:A:377:ASN:ND2	2.50	0.45
1:B:66:ILE:HG13	1:B:88:PHE:HB2	1.98	0.45
1:B:450:LEU:HD11	1:B:456:ILE:HG23	1.98	0.45
1:B:496:PHE:CE2	1:B:500:ILE:HD11	2.52	0.45
1:A:383:ASP:OD2	6:A:732:HOH:O	2.20	0.45
1:B:345:PRO:HA	1:B:348:THR:HB	1.99	0.45
1:B:214:LYS:HE2	1:B:214:LYS:HB3	1.62	0.44
1:B:137:ASN:HB2	1:B:168:LYS:HZ2	1.81	0.44
3:A:603:TRT:H10	3:A:603:TRT:H5C2	1.76	0.44
1:A:487:LEU:HD21	2:A:601:UQ5:H4M1	2.00	0.43
1:B:393:ALA:HB3	2:B:602:UQ5:H4M2	2.00	0.43
1:A:105:LYS:NZ	1:B:103:ASP:OD1	2.29	0.43
1:B:163:GLU:HA	1:B:164:PRO:HD3	1.82	0.43
1:A:413:ILE:HA	1:A:414:PRO:HD3	1.84	0.43
1:A:41:LYS:HE2	1:A:41:LYS:HB2	1.84	0.43
1:B:444:LEU:C	2:B:602:UQ5:H102	2.44	0.42
1:B:501:LYS:HE2	1:B:501:LYS:HB3	1.92	0.42
1:B:444:LEU:HA	1:B:460:ARG:O	2.19	0.42
1:B:354:ILE:HA	1:B:355:PRO:HD2	1.73	0.42
2:B:602:UQ5:H1M2	2:B:602:UQ5:H112	1.97	0.42
1:A:322:ASP:OD2	1:A:324:LYS:NZ	2.52	0.42
1:A:355:PRO:C	1:A:357:GLN:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:HE2	1:A:214:LYS:HB3	1.88	0.41
1:A:405:LYS:O	1:A:408:ASP:HB2	2.20	0.41
1:A:227:ARG:O	1:A:230:SER:HB3	2.21	0.41
1:A:504:PHE:CD1	3:A:604:TRT:H13	2.56	0.41
1:B:152:GLN:HB2	1:B:153:PRO:HD3	2.03	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.89	0.40
1:B:481:LEU:HD12	1:B:481:LEU:HA	1.91	0.40
1:A:258:PHE:HB3	1:B:116:LEU:HD11	2.03	0.40
1:B:393:ALA:CB	2:B:602:UQ5:H4M2	2.52	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	467/502 (93%)	447 (96%)	19 (4%)	1 (0%)	43	61
1	B	459/502 (91%)	437 (95%)	21 (5%)	1 (0%)	43	61
All	All	926/1004 (92%)	884 (96%)	40 (4%)	2 (0%)	43	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	356	GLU

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	399/427 (93%)	377 (94%)	22 (6%)	19	37
1	B	392/427 (92%)	368 (94%)	24 (6%)	17	33
All	All	791/854 (93%)	745 (94%)	46 (6%)	18	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	138	THR
1	A	150	LEU
1	A	155	ASN
1	A	157	LEU
1	A	188	VAL
1	A	218	LEU
1	A	226	ARG
1	A	259	LEU
1	A	266	VAL
1	A	270	LEU
1	A	287	SER
1	A	322	ASP
1	A	324	LYS
1	A	384	ASN
1	A	389	LEU
1	A	429	LEU
1	A	430	LEU
1	A	444	LEU
1	A	472	LEU
1	A	481	LEU
1	A	501	LYS
1	B	50	HIS
1	B	138	THR
1	B	155	ASN
1	B	188	VAL
1	B	196	LYS
1	B	206	ARG
1	B	218	LEU
1	B	266	VAL
1	B	270	LEU
1	B	283	LYS
1	B	348	THR

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Mol	Chain	Res	Type
1	B	352	LYS
1	B	357	GLN
1	B	362	ARG
1	B	375	SER
1	B	376	ASN
1	B	384	ASN
1	B	389	LEU
1	B	417	GLN
1	B	444	LEU
1	B	464	ARG
1	B	472	LEU
1	B	473	MET
1	B	481	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	155	ASN
1	A	156	HIS
1	A	377	ASN
1	B	149	GLN
1	B	156	HIS
1	B	216	ASN
1	B	248	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	A	607	4	58,58,58	1.14	5 (8%)	85,89,89	1.70	17 (20%)
3	TRT	A	603	-	20,20,25	0.57	0	28,28,33	2.66	7 (25%)
2	UQ5	B	602	-	23,23,38	3.37	10 (43%)	30,31,49	2.30	11 (36%)
2	UQ5	B	603	-	23,23,38	3.38	10 (43%)	30,31,49	2.26	11 (36%)
3	TRT	B	604	-	20,20,25	0.71	1 (5%)	28,28,33	1.11	1 (3%)
2	UQ5	A	601	-	23,23,38	3.38	10 (43%)	30,31,49	2.29	11 (36%)
2	UQ5	A	602	-	27,27,38	3.34	11 (40%)	34,35,49	2.42	11 (32%)
3	TRT	A	604	-	20,20,25	0.57	0	28,28,33	2.54	6 (21%)
5	FAD	B	606	4	58,58,58	1.11	5 (8%)	85,89,89	1.63	15 (17%)
3	TRT	A	605	-	16,16,25	0.61	1 (6%)	24,24,33	1.03	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	A	607	4	-	7/34/50/50	0/6/6/6
3	TRT	A	603	-	-	6/18/18/23	0/1/1/1
2	UQ5	B	602	-	-	11/15/39/57	0/1/1/1
2	UQ5	B	603	-	-	10/15/39/57	0/1/1/1
3	TRT	B	604	-	-	9/18/18/23	0/1/1/1
2	UQ5	A	601	-	-	10/15/39/57	0/1/1/1
2	UQ5	A	602	-	-	14/20/44/57	0/1/1/1
3	TRT	A	604	-	-	5/18/18/23	0/1/1/1
5	FAD	B	606	4	-	8/34/50/50	0/6/6/6
3	TRT	A	605	-	-	5/14/14/23	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	UQ5	C13-C14	8.89	1.53	1.33
2	B	603	UQ5	C8-C9	8.34	1.52	1.33
2	A	601	UQ5	C8-C9	8.34	1.52	1.33
2	A	602	UQ5	C8-C9	8.31	1.52	1.33
2	B	602	UQ5	C8-C9	8.31	1.52	1.33
2	B	603	UQ5	C13-C14	7.06	1.53	1.32
2	B	602	UQ5	C13-C14	7.05	1.53	1.32
2	A	601	UQ5	C13-C14	7.04	1.53	1.32
2	A	601	UQ5	O5-C5	6.56	1.38	1.23
2	B	603	UQ5	O5-C5	6.50	1.37	1.23
2	B	602	UQ5	O5-C5	6.50	1.37	1.23
2	A	601	UQ5	O2-C2	6.46	1.37	1.23
2	A	602	UQ5	O5-C5	6.46	1.37	1.23
2	B	602	UQ5	O2-C2	6.45	1.37	1.23
2	B	603	UQ5	O2-C2	6.44	1.37	1.23
2	A	602	UQ5	O2-C2	6.43	1.37	1.23
5	A	607	FAD	C4X-N5	3.99	1.39	1.30
5	B	606	FAD	C4X-N5	3.75	1.38	1.30
2	B	603	UQ5	C6-C1	3.64	1.41	1.35
2	A	601	UQ5	C6-C1	3.52	1.41	1.35
2	B	602	UQ5	C6-C1	3.52	1.41	1.35
2	A	602	UQ5	C18-C19	3.46	1.54	1.29
2	A	602	UQ5	C6-C1	3.45	1.41	1.35
5	A	607	FAD	C8A-N7A	3.07	1.37	1.31
2	A	601	UQ5	C3-C2	-2.89	1.40	1.48
2	A	602	UQ5	C3-C2	-2.87	1.40	1.48
2	B	602	UQ5	C3-C2	-2.86	1.40	1.48
2	B	603	UQ5	C3-C2	-2.85	1.40	1.48
2	A	601	UQ5	O4-C4M	-2.82	1.39	1.45
2	B	602	UQ5	O4-C4M	-2.82	1.39	1.45
2	B	603	UQ5	O4-C4M	-2.81	1.39	1.45
2	A	602	UQ5	O4-C4M	-2.80	1.39	1.45
5	A	607	FAD	C2A-N1A	2.70	1.38	1.33
5	B	606	FAD	C10-N1	2.70	1.38	1.33
2	B	602	UQ5	C4-C5	-2.66	1.41	1.48
2	A	602	UQ5	C4-C5	-2.65	1.41	1.48
2	A	601	UQ5	C4-C5	-2.64	1.41	1.48
2	B	603	UQ5	C4-C5	-2.64	1.41	1.48
5	A	607	FAD	C10-N1	2.58	1.38	1.33
5	B	606	FAD	C2A-N1A	2.53	1.38	1.33
5	B	606	FAD	C8A-N7A	2.50	1.36	1.31
5	A	607	FAD	C2A-N3A	2.44	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C2A-N3A	2.29	1.38	1.33
3	B	604	TRT	C6-C9	-2.27	1.50	1.53
2	A	602	UQ5	C6-C5	-2.25	1.40	1.46
2	B	603	UQ5	C6-C5	-2.21	1.40	1.46
2	B	602	UQ5	C6-C5	-2.21	1.40	1.46
2	A	601	UQ5	C6-C5	-2.19	1.40	1.46
2	B	602	UQ5	O3-C3M	-2.10	1.40	1.45
2	B	603	UQ5	O3-C3M	-2.10	1.40	1.45
3	A	605	TRT	C6-C9	-2.09	1.50	1.53
2	A	602	UQ5	O3-C3M	-2.09	1.40	1.45
2	A	601	UQ5	O3-C3M	-2.08	1.40	1.45

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	TRT	C3-C1-C4	-7.74	85.29	108.96
3	A	603	TRT	C3-C1-C4	-7.66	85.54	108.96
3	A	603	TRT	C3-C1-C2	-7.63	85.65	108.96
3	A	604	TRT	C3-C1-C2	-7.38	86.39	108.96
5	A	607	FAD	N3A-C2A-N1A	-6.33	118.99	128.58
5	B	606	FAD	N3A-C2A-N1A	-5.95	119.57	128.58
2	A	602	UQ5	C10-C9-C8	-5.61	109.23	123.63
3	A	604	TRT	C3-C1-C5	-5.60	84.89	110.61
2	B	602	UQ5	C10-C9-C8	-5.59	109.28	123.63
2	A	601	UQ5	C10-C9-C8	-5.58	109.31	123.63
3	A	603	TRT	C3-C1-C5	-5.49	85.43	110.61
2	B	603	UQ5	C10-C9-C8	-5.44	109.65	123.63
2	A	601	UQ5	C7-C8-C9	-5.28	117.74	126.83
2	A	602	UQ5	C7-C8-C9	-5.24	117.80	126.83
2	B	602	UQ5	C7-C8-C9	-5.22	117.83	126.83
2	B	603	UQ5	C7-C8-C9	-5.18	117.90	126.83
2	A	602	UQ5	C15-C14-C13	-4.84	111.20	123.63
5	A	607	FAD	N9A-C8A-N7A	-4.69	107.28	113.94
5	B	606	FAD	N9A-C8A-N7A	-4.42	107.67	113.94
5	A	607	FAD	C5A-C4A-N3A	-4.29	120.82	126.72
2	A	602	UQ5	C12-C13-C14	-4.28	117.82	127.62
5	B	606	FAD	C4'-C3'-C2'	-4.10	106.75	113.57
5	B	606	FAD	C5A-C4A-N3A	-4.09	121.08	126.72
2	B	603	UQ5	C15-C14-C13	-3.88	111.00	122.66
5	A	607	FAD	C5A-N7A-C8A	3.83	109.46	103.45
2	A	601	UQ5	C15-C14-C13	-3.81	111.24	122.66
2	B	602	UQ5	C15-C14-C13	-3.78	111.30	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	UQ5	C16-C14-C13	-3.76	112.72	121.17
5	B	606	FAD	C5A-N7A-C8A	3.69	109.25	103.45
5	A	607	FAD	C2A-N3A-C4A	3.69	120.83	111.83
2	B	603	UQ5	C11-C9-C8	-3.61	113.06	121.17
2	A	602	UQ5	C15-C14-C16	-3.54	109.09	115.23
2	A	602	UQ5	C11-C9-C8	-3.50	113.32	121.17
2	B	602	UQ5	C11-C9-C8	-3.49	113.33	121.17
2	A	601	UQ5	C11-C9-C8	-3.46	113.40	121.17
5	A	607	FAD	C4'-C3'-C2'	-3.46	107.82	113.57
3	A	603	TRT	C4-C1-C2	3.38	119.30	108.96
5	B	606	FAD	C2A-N3A-C4A	3.38	120.08	111.83
2	B	603	UQ5	C16-C14-C13	-3.37	112.53	122.66
2	A	601	UQ5	C16-C14-C13	-3.34	112.62	122.66
2	B	602	UQ5	C16-C14-C13	-3.34	112.65	122.66
5	B	606	FAD	C4-N3-C2	-3.28	119.81	125.64
3	B	604	TRT	C5-C6-C9	-3.26	104.37	112.00
2	A	602	UQ5	C10-C9-C11	-3.18	109.70	115.23
3	A	604	TRT	C4-C1-C2	3.18	118.67	108.96
2	B	602	UQ5	C10-C9-C11	-3.17	109.73	115.23
5	A	607	FAD	C4X-C10-N10	3.10	120.92	116.48
2	A	601	UQ5	C10-C9-C11	-3.07	109.91	115.23
2	A	602	UQ5	C7-C6-C1	-3.04	119.67	124.89
2	B	603	UQ5	C10-C9-C11	-3.01	110.00	115.23
2	B	603	UQ5	C12-C13-C14	-2.98	117.71	127.64
3	A	603	TRT	C16-O15-C12	2.96	125.62	117.93
3	A	603	TRT	C5-C6-C9	-2.95	105.11	112.00
2	B	602	UQ5	C12-C13-C14	-2.93	117.87	127.64
2	A	601	UQ5	C7-C6-C1	-2.92	119.88	124.89
2	B	602	UQ5	C7-C6-C1	-2.92	119.88	124.89
2	A	601	UQ5	C12-C13-C14	-2.90	117.98	127.64
5	A	607	FAD	C4-N3-C2	-2.88	120.52	125.64
5	B	606	FAD	C4X-C4-N3	2.85	120.52	113.25
2	B	602	UQ5	C1M-C1-C6	-2.80	119.85	124.45
2	A	602	UQ5	C1M-C1-C6	-2.76	119.91	124.45
5	A	607	FAD	C4A-C5A-N7A	-2.75	107.43	110.58
5	A	607	FAD	O2A-PA-O3P	2.73	114.66	107.27
2	A	601	UQ5	C1M-C1-C6	-2.72	119.98	124.45
5	B	606	FAD	C9A-C5X-N5	-2.72	119.57	122.45
5	B	606	FAD	C4A-C5A-N7A	-2.72	107.48	110.58
5	A	607	FAD	N3A-C4A-N9A	2.70	131.75	127.17
5	B	606	FAD	N3A-C4A-N9A	2.67	131.71	127.17
2	B	603	UQ5	C7-C6-C1	-2.66	120.33	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	O4-C4-C4X	-2.65	119.54	126.53
3	A	604	TRT	C1-C5-C6	-2.63	113.60	123.78
2	A	601	UQ5	C16-C14-C15	-2.58	108.64	114.59
5	A	607	FAD	C5X-C9A-N10	2.55	120.28	117.97
5	A	607	FAD	O4-C4-C4X	-2.55	119.80	126.53
5	A	607	FAD	C4A-N9A-C8A	2.53	108.39	105.74
5	B	606	FAD	C4A-N9A-C8A	2.52	108.39	105.74
5	A	607	FAD	C4X-C4-N3	2.52	119.66	113.25
2	B	602	UQ5	C16-C14-C15	-2.50	108.83	114.59
2	B	603	UQ5	C1M-C1-C6	-2.46	120.40	124.45
2	B	603	UQ5	C8-C7-C6	2.45	118.12	112.08
2	A	602	UQ5	C16-C17-C18	2.43	117.84	112.57
2	B	603	UQ5	C16-C14-C15	-2.39	109.09	114.59
2	A	601	UQ5	C8-C7-C6	2.38	117.95	112.08
3	A	603	TRT	C1-C5-C6	-2.37	114.59	123.78
5	B	606	FAD	C10-C4X-N5	-2.31	120.10	124.81
5	B	606	FAD	C4X-C10-N10	2.26	119.72	116.48
5	A	607	FAD	C10-C4X-N5	-2.23	120.25	124.81
2	B	602	UQ5	C8-C7-C6	2.20	117.50	112.08
3	A	605	TRT	C3-C1-C4	-2.08	102.61	108.96
3	A	605	TRT	C16-O15-C12	2.03	121.86	117.50
3	A	604	TRT	C2-C1-C5	2.03	119.94	110.61
5	A	607	FAD	C9A-C5X-N5	-2.01	120.32	122.45

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	UQ5	C1-C6-C7-C8
2	A	601	UQ5	C5-C6-C7-C8
2	A	601	UQ5	C7-C8-C9-C10
2	A	601	UQ5	C7-C8-C9-C11
2	A	602	UQ5	C7-C8-C9-C10
2	A	602	UQ5	C12-C13-C14-C15
2	B	602	UQ5	C7-C8-C9-C10
2	B	602	UQ5	C7-C8-C9-C11
2	B	602	UQ5	C12-C13-C14-C15
2	B	603	UQ5	C1-C6-C7-C8
2	B	603	UQ5	C5-C6-C7-C8
2	B	603	UQ5	C7-C8-C9-C10
2	B	603	UQ5	C7-C8-C9-C11
2	A	601	UQ5	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	A	601	UQ5	C12-C13-C14-C16
2	B	603	UQ5	C12-C13-C14-C15
2	B	603	UQ5	C12-C13-C14-C16
3	A	605	TRT	C1-C5-C6-C8
3	A	605	TRT	C1-C5-C6-C7
2	A	602	UQ5	C7-C8-C9-C11
2	A	602	UQ5	C12-C13-C14-C16
2	B	602	UQ5	C12-C13-C14-C16
2	A	602	UQ5	C12-C11-C9-C10
2	B	602	UQ5	C12-C11-C9-C8
2	A	602	UQ5	C9-C11-C12-C13
2	A	602	UQ5	C14-C16-C17-C18
2	B	602	UQ5	C9-C11-C12-C13
3	A	603	TRT	C13-C12-O15-C16
3	A	603	TRT	C11-C12-O15-C16
3	A	605	TRT	C1-C5-C6-C9
3	A	605	TRT	C11-C12-O15-C16
2	A	602	UQ5	C15-C14-C16-C17
3	B	604	TRT	C11-C12-O15-C16
3	B	604	TRT	C13-C12-O15-C16
3	A	605	TRT	C13-C12-O15-C16
2	A	601	UQ5	C4-C3-O3-C3M
2	A	602	UQ5	C4-C3-O3-C3M
2	B	603	UQ5	C4-C3-O3-C3M
3	A	604	TRT	C11-C12-O15-C16
5	B	606	FAD	C2'-C3'-C4'-C5'
3	A	604	TRT	C13-C12-O15-C16
3	A	603	TRT	O15-C16-C17-O18
3	A	603	TRT	C4-C1-C5-C6
3	B	604	TRT	C5-C6-C9-C14
3	A	604	TRT	C4-C1-C5-C6
2	A	601	UQ5	C3-C4-O4-C4M
3	A	604	TRT	C2-C1-C5-C6
5	B	606	FAD	O4B-C4B-C5B-O5B
5	B	606	FAD	C2'-C3'-C4'-O4'
5	B	606	FAD	O3'-C3'-C4'-C5'
3	B	604	TRT	C5-C6-C9-C10
5	B	606	FAD	C3B-C4B-C5B-O5B
2	A	602	UQ5	C17-C18-C19-C20
2	A	602	UQ5	C1-C6-C7-C8
5	B	606	FAD	O3'-C3'-C4'-O4'
3	A	604	TRT	C1-C5-C6-C9

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Mol	Chain	Res	Type	Atoms
2	A	602	UQ5	C5-C6-C7-C8
2	B	602	UQ5	C5-C6-C7-C8
5	A	607	FAD	C2B-C1B-N9A-C8A
5	B	606	FAD	C2B-C1B-N9A-C8A
3	A	603	TRT	C2-C1-C5-C6
2	A	602	UQ5	C2-C3-O3-C3M
3	B	604	TRT	C1-C5-C6-C9
2	A	601	UQ5	C2-C3-O3-C3M
2	B	603	UQ5	C2-C3-O3-C3M
2	B	602	UQ5	C6-C7-C8-C9
2	B	602	UQ5	C1-C6-C7-C8
2	B	603	UQ5	C12-C11-C9-C10
2	A	602	UQ5	C5-C4-O4-C4M
2	B	602	UQ5	C4-C3-O3-C3M
5	A	607	FAD	O3'-C3'-C4'-C5'
2	B	602	UQ5	C5-C4-O4-C4M
2	A	601	UQ5	C12-C11-C9-C10
5	A	607	FAD	O3'-C3'-C4'-O4'
3	A	603	TRT	C1-C5-C6-C9
3	B	604	TRT	C1-C5-C6-C7
5	A	607	FAD	O4B-C1B-N9A-C8A
5	B	606	FAD	O4B-C1B-N9A-C8A
2	B	603	UQ5	C9-C11-C12-C13
5	A	607	FAD	O4B-C4B-C5B-O5B
5	A	607	FAD	C2B-C1B-N9A-C4A
5	A	607	FAD	C2'-C3'-C4'-O4'
3	B	604	TRT	C1-C5-C6-C8
3	B	604	TRT	C7-C6-C9-C10
3	B	604	TRT	C7-C6-C9-C14

There are no ring outliers.

10 monomers are involved in 88 short contacts:

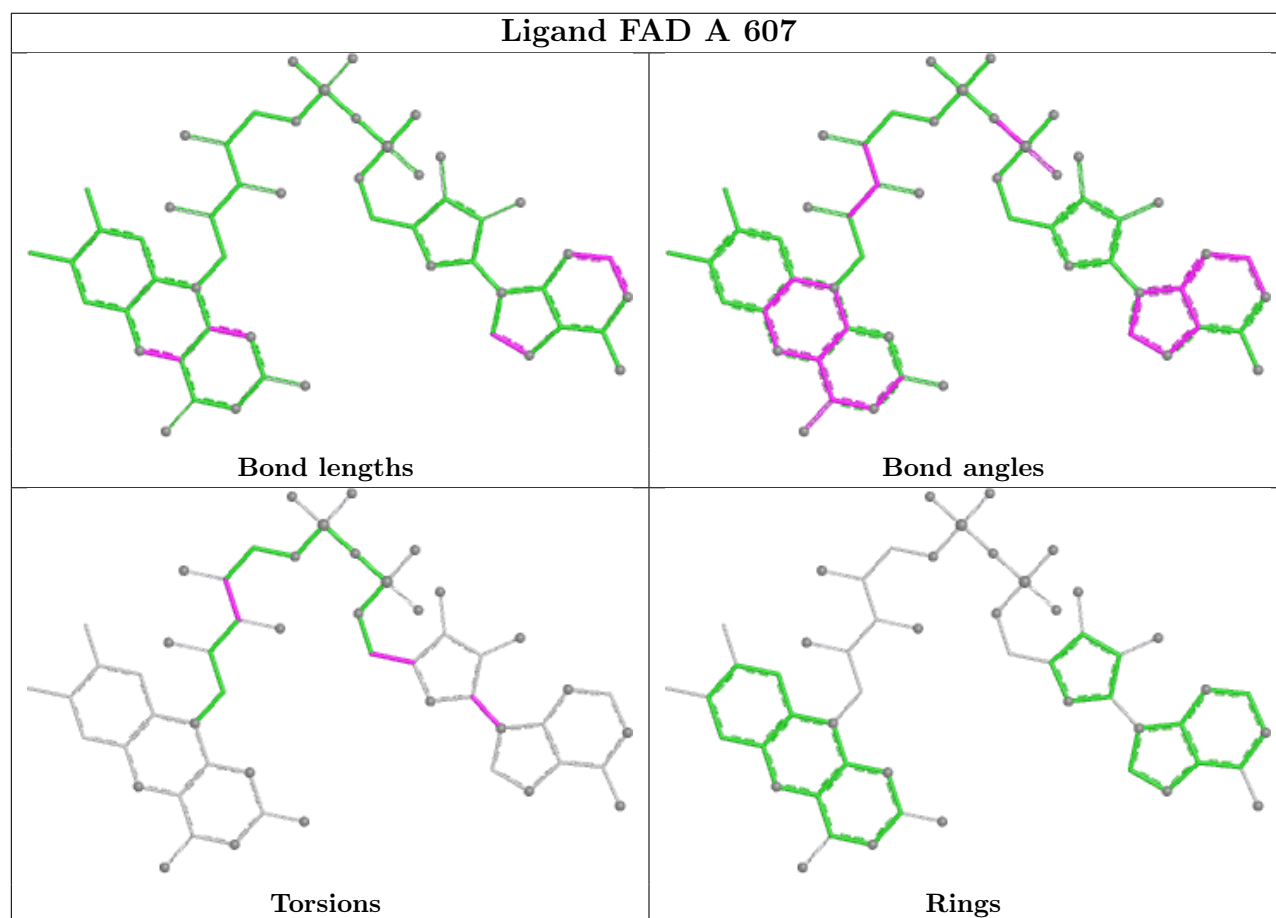
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	607	FAD	1	0
3	A	603	TRT	3	0
2	B	602	UQ5	27	0
2	B	603	UQ5	28	0
3	B	604	TRT	3	0
2	A	601	UQ5	14	0
2	A	602	UQ5	21	0
3	A	604	TRT	3	0

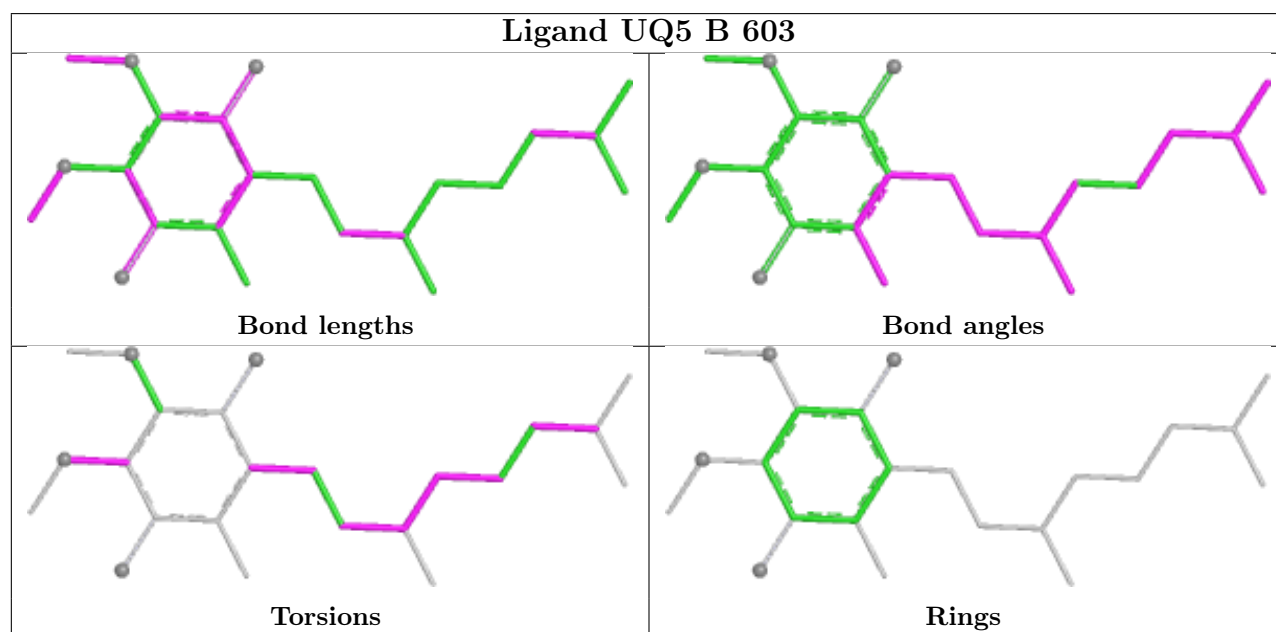
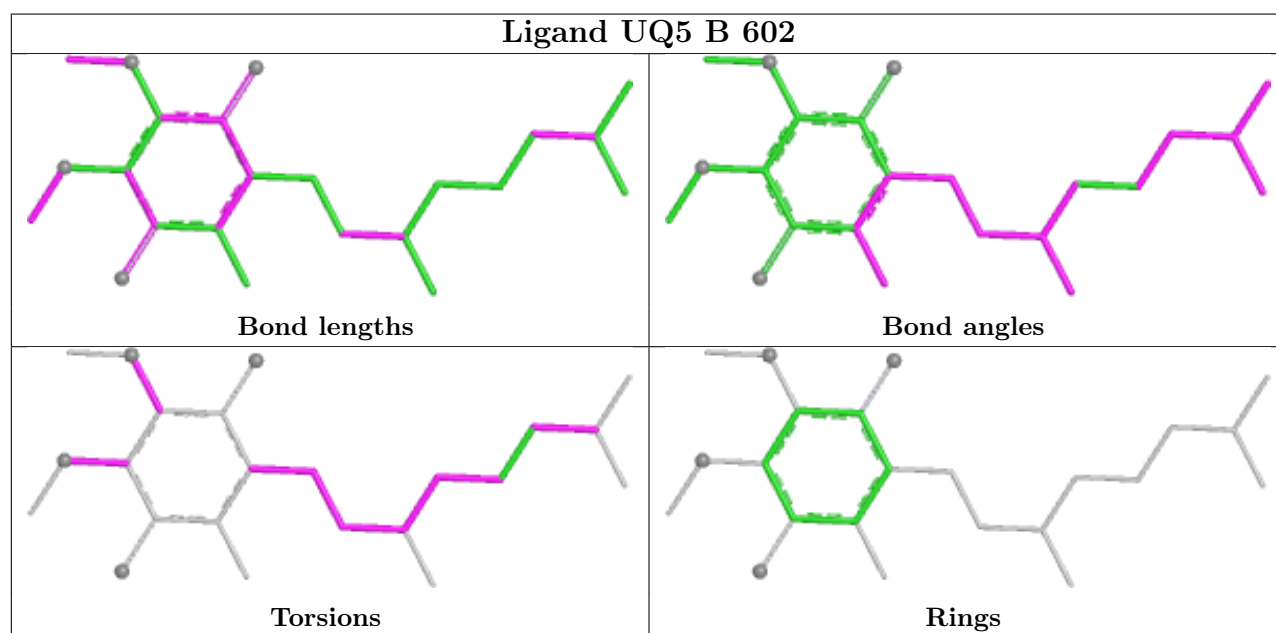
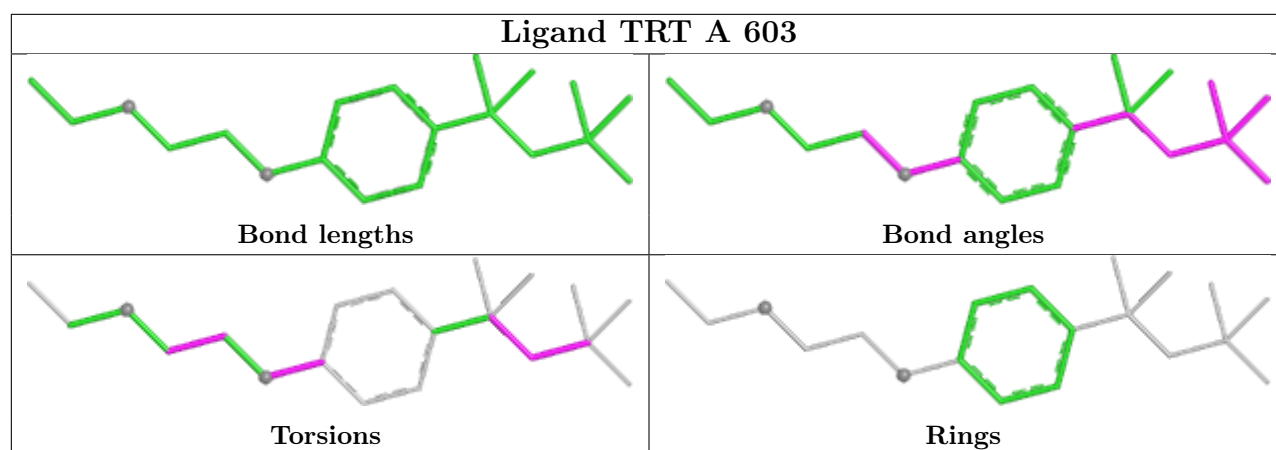
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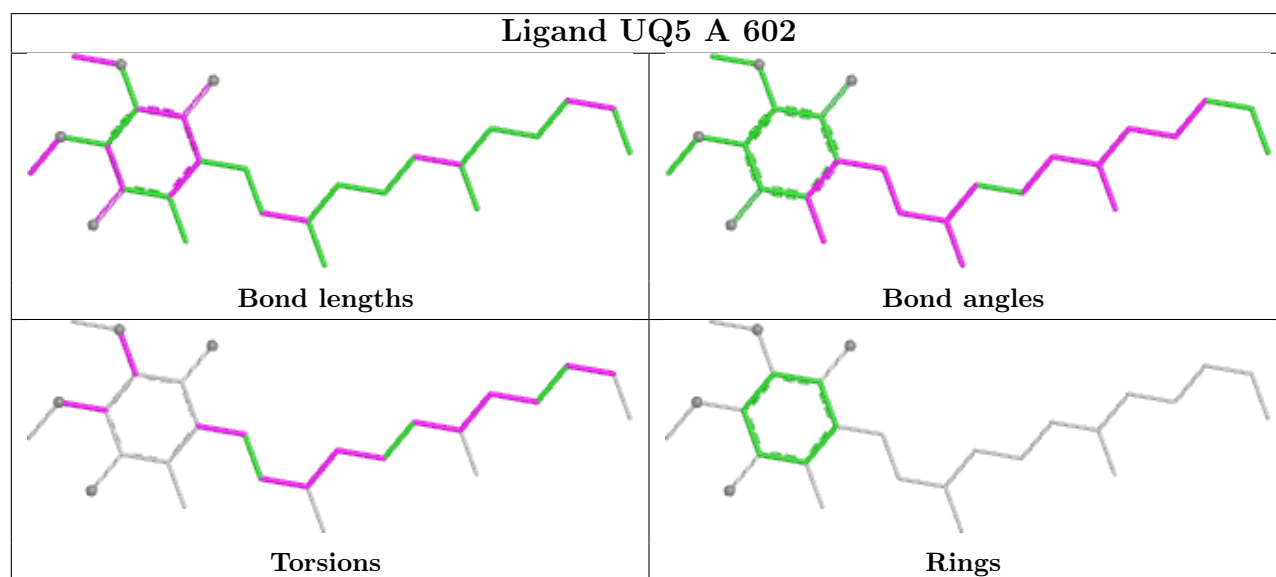
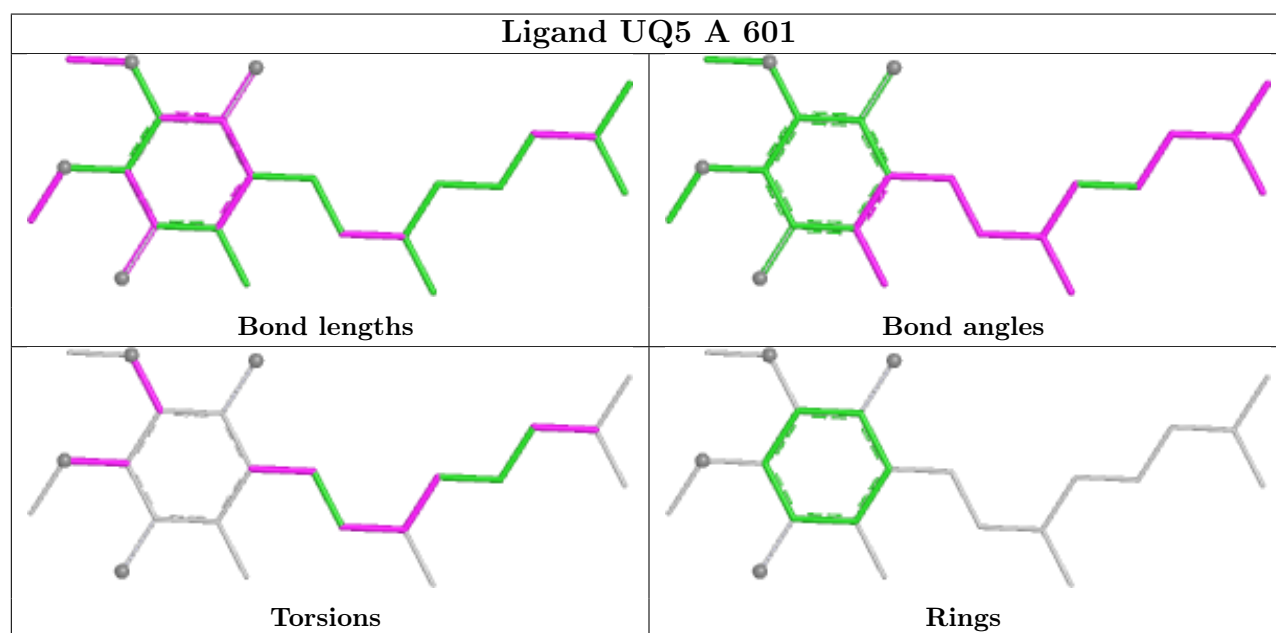
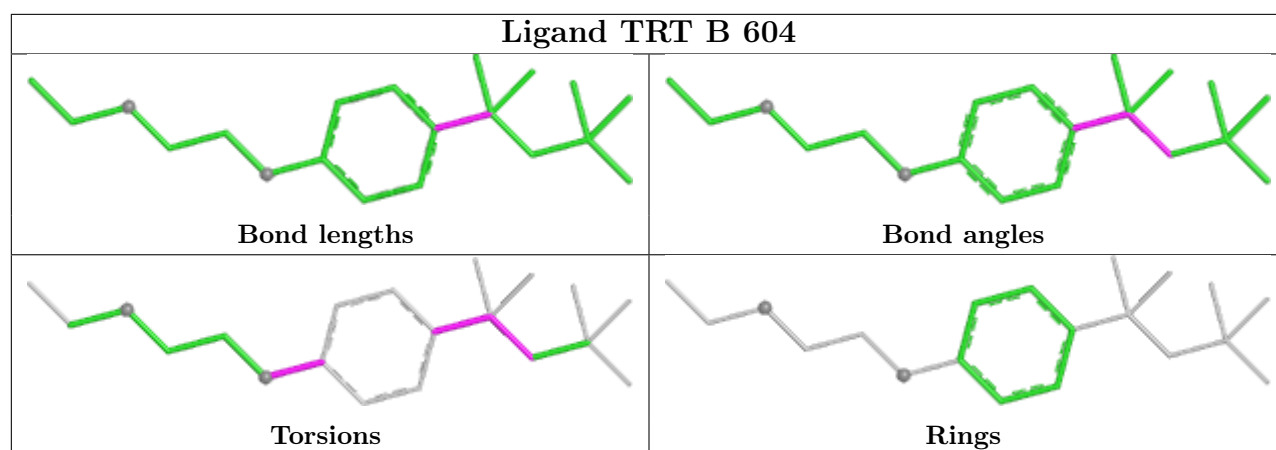
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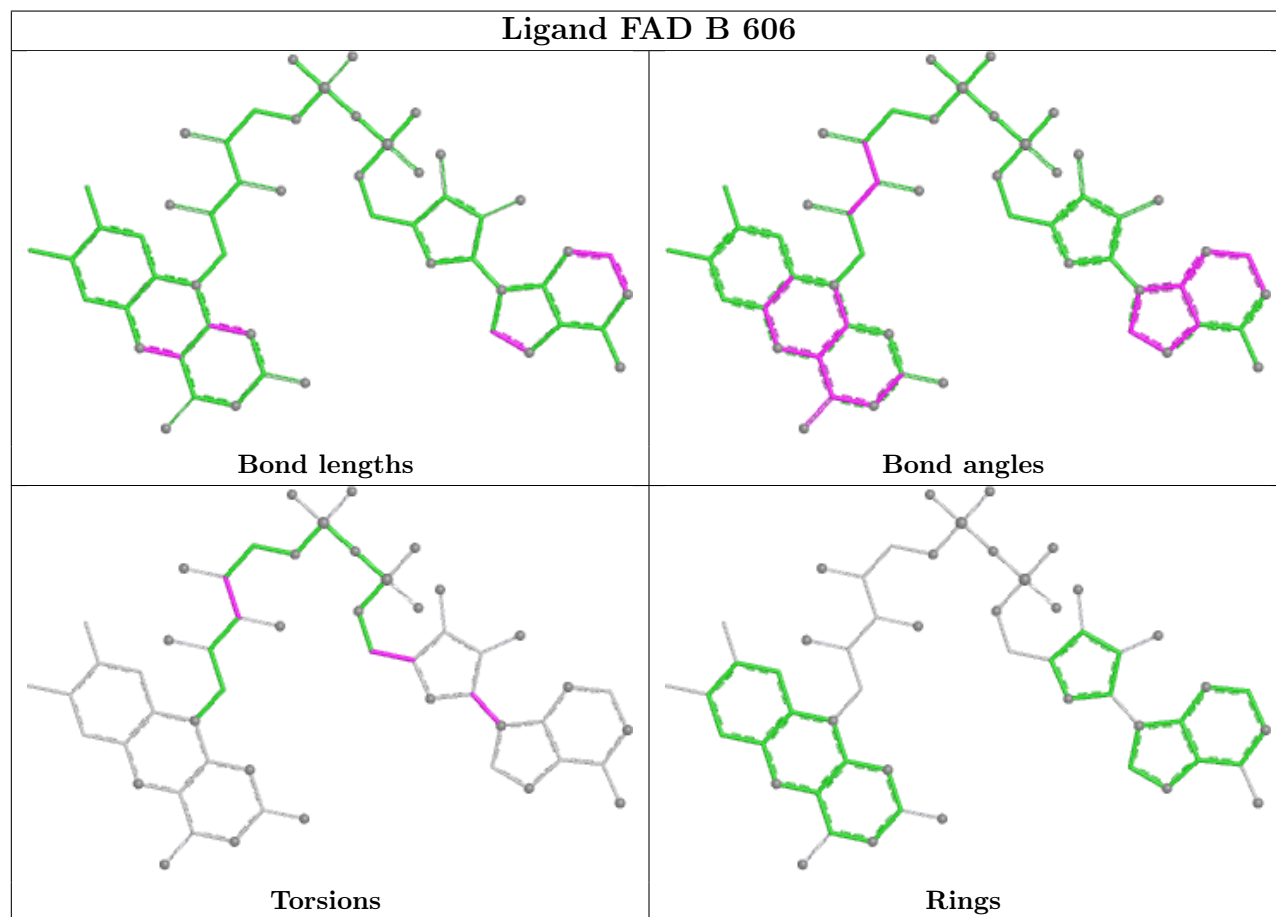
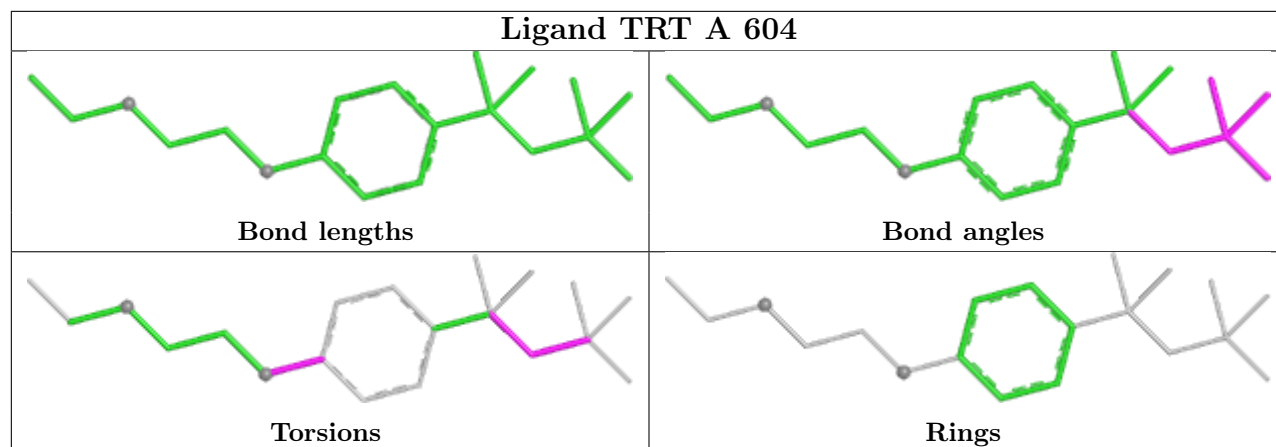
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	FAD	1	0
3	A	605	TRT	1	0

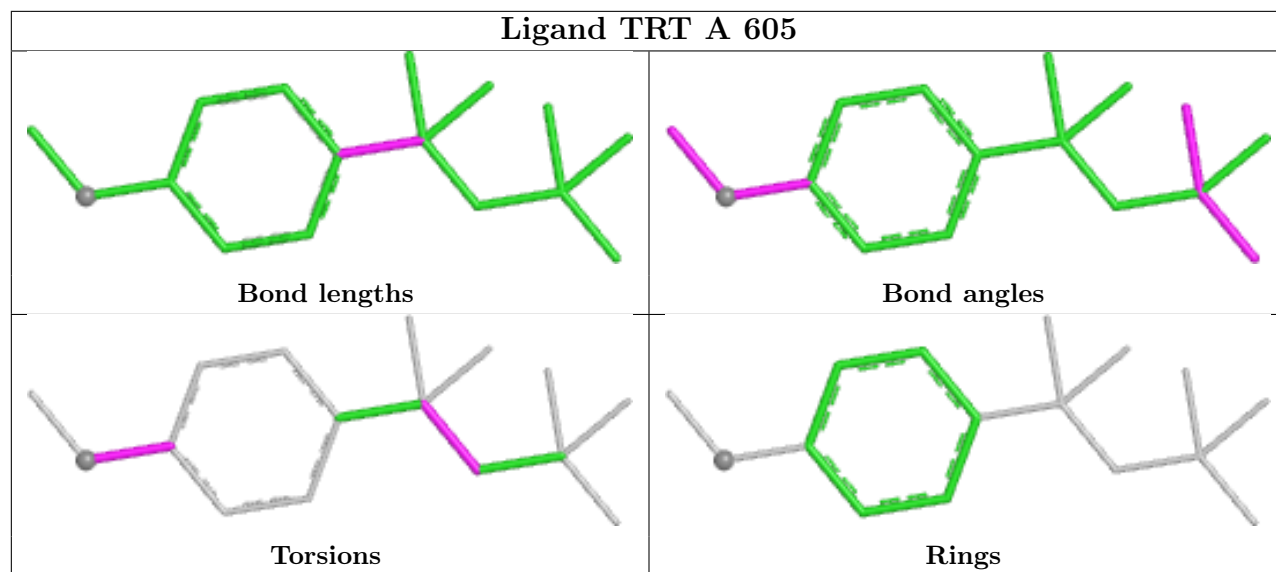
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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

6.1 Protein, DNA and RNA chains

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	471/502 (93%)	-0.08	21 (4%) 38 34	22, 36, 63, 91	0
1	B	463/502 (92%)	0.19	27 (5%) 29 25	22, 40, 78, 104	0
All	All	934/1004 (93%)	0.06	48 (5%) 33 30	22, 37, 72, 104	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	429	LEU	7.2
1	A	152	GLN	7.0
1	B	430	LEU	5.7
1	B	419	ASN	5.5
1	B	417	GLN	4.5
1	A	417	GLN	4.5
1	B	42	THR	4.4
1	A	38	THR	4.3
1	A	425	ASP	4.0
1	A	426	LYS	3.7
1	B	418	LYS	3.4
1	B	414	PRO	3.4
1	B	376	ASN	3.3
1	A	50	HIS	3.3
1	A	427	ILE	3.3
1	A	153	PRO	3.3
1	B	386	PHE	3.2
1	B	50	HIS	3.1
1	A	155	ASN	2.9
1	B	152	GLN	2.9
1	A	37	PRO	2.9
1	B	416	PHE	2.8
1	B	155	ASN	2.7
1	A	319	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	463	LYS	2.7
1	A	41	LYS	2.7
1	B	348	THR	2.7
1	B	355	PRO	2.6
1	B	388	GLY	2.6
1	B	172	LEU	2.6
1	A	154	GLU	2.6
1	B	160	HIS	2.6
1	A	428	ASP	2.6
1	B	377	ASN	2.6
1	B	463	LYS	2.5
1	B	154	GLU	2.4
1	A	376	ASN	2.4
1	B	162	ALA	2.4
1	B	415	ASN	2.4
1	A	323	GLY	2.3
1	B	413	ILE	2.3
1	B	464	ARG	2.3
1	A	414	PRO	2.2
1	A	51	SER	2.1
1	A	206	ARG	2.1
1	A	429	LEU	2.1
1	B	47	ASP	2.1
1	B	433	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

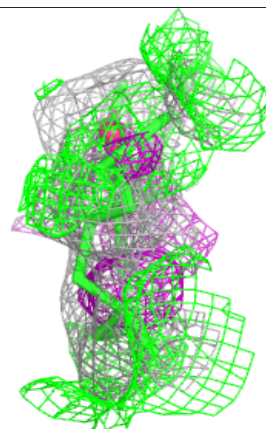
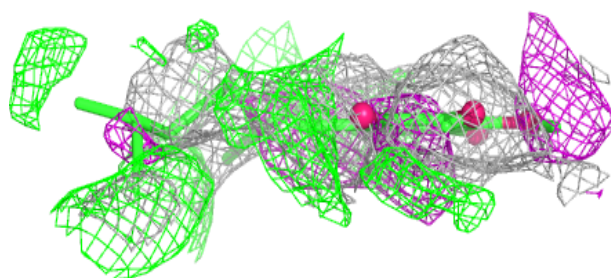
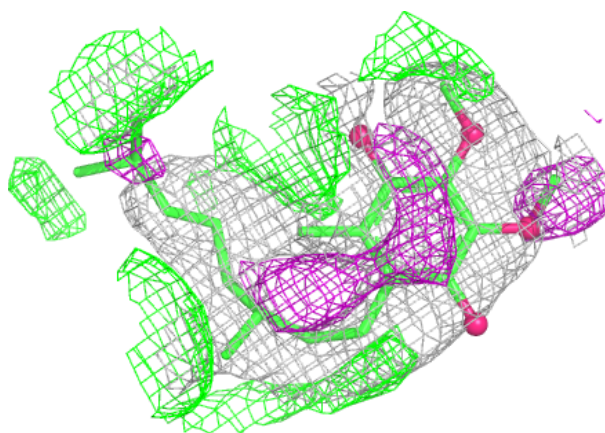
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UQ5	B	603	23/38	0.38	0.34	56,65,73,77	0
2	UQ5	A	601	23/38	0.59	0.31	45,62,70,78	0
3	TRT	B	604	20/25	0.66	0.28	46,60,71,71	0
3	TRT	A	605	16/25	0.68	0.27	50,60,72,79	0
3	TRT	A	604	20/25	0.69	0.32	53,72,83,83	0
2	UQ5	A	602	27/38	0.71	0.28	46,58,67,76	0
2	UQ5	B	602	23/38	0.76	0.22	51,58,65,69	0
3	TRT	A	603	20/25	0.79	0.25	44,69,81,83	0
4	MG	A	606	1/1	0.84	0.22	60,60,60,60	0
4	MG	B	605	1/1	0.87	0.13	52,52,52,52	0
4	MG	B	607	1/1	0.93	0.27	47,47,47,47	0
4	MG	A	611	1/1	0.94	0.12	40,40,40,40	0
4	MG	B	608	1/1	0.95	0.16	45,45,45,45	0
4	MG	B	610	1/1	0.95	0.08	48,48,48,48	0
4	MG	B	609	1/1	0.96	0.07	40,40,40,40	0
4	MG	A	610	1/1	0.96	0.14	33,33,33,33	0
4	MG	A	608	1/1	0.97	0.14	31,31,31,31	0
4	MG	B	601	1/1	0.98	0.08	20,20,20,20	0
4	MG	A	609	1/1	0.98	0.14	32,32,32,32	0
5	FAD	A	607	53/53	0.98	0.05	19,25,32,36	0
5	FAD	B	606	53/53	0.98	0.06	26,34,38,42	0

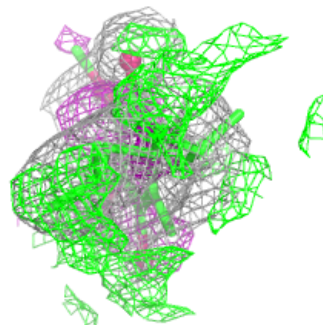
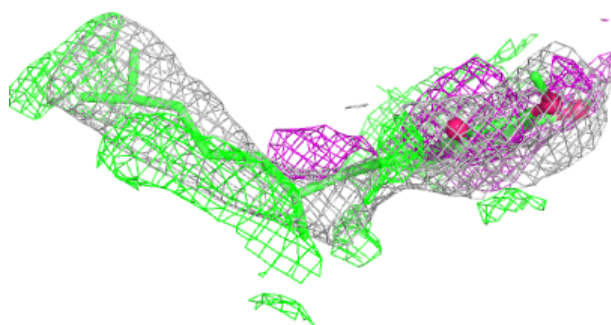
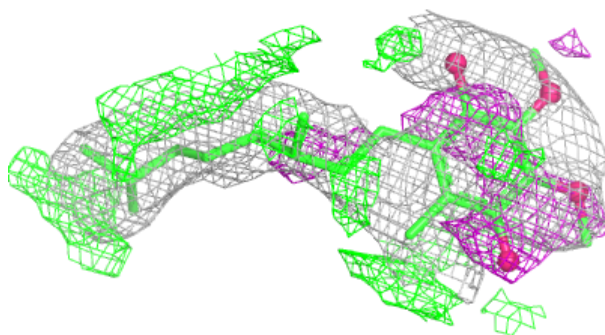
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UQ5 B 603:

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

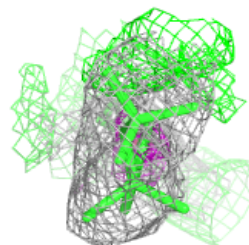
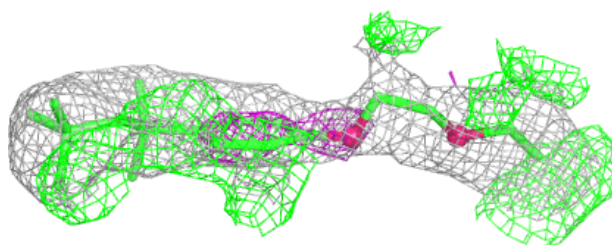
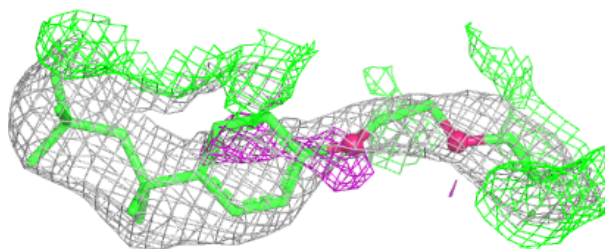
**Electron density around UQ5 A 601:**

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

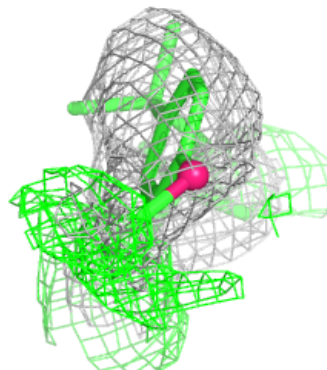
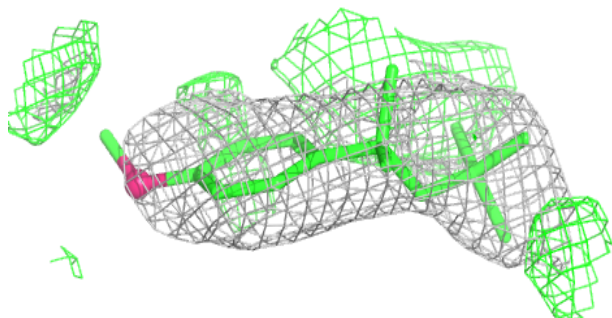
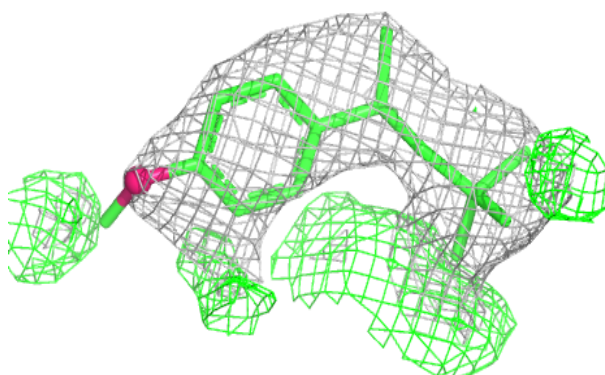


Electron density around TRT B 604:

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and green (positive)

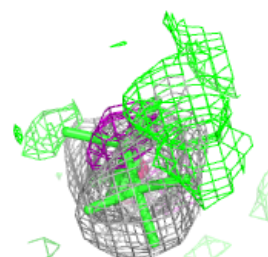
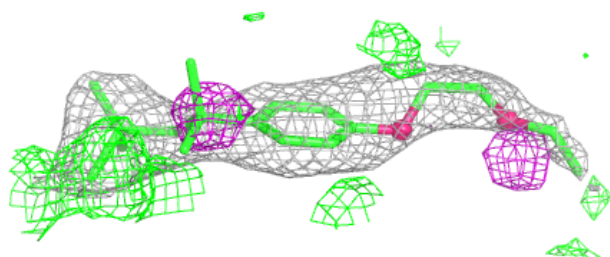
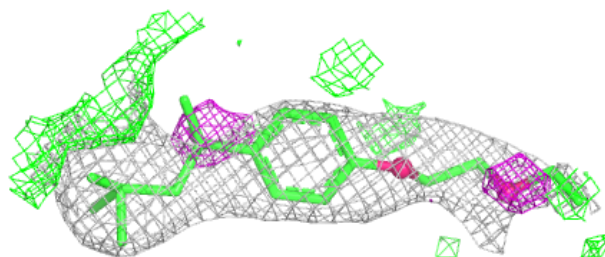
**Electron density around TRT A 605:**

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and green (positive)

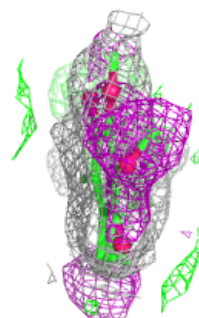
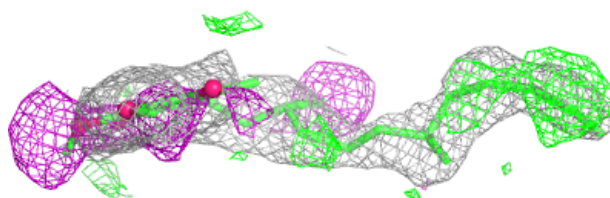
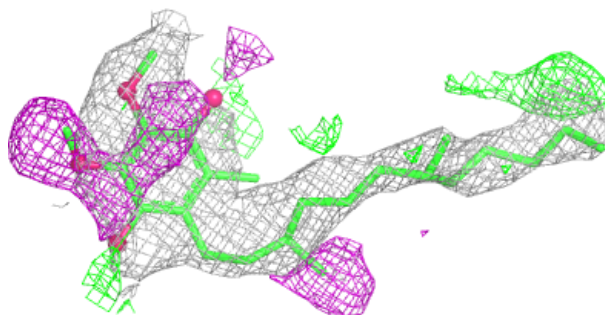


Electron density around TRT A 604:

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and green (positive)

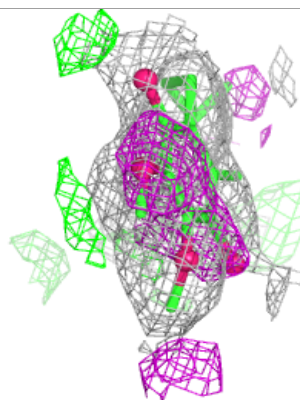
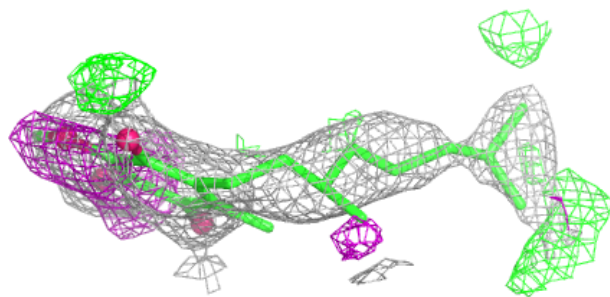
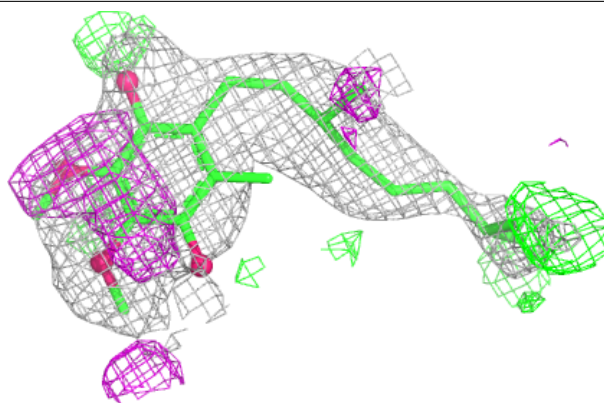
**Electron density around UQ5 A 602:**

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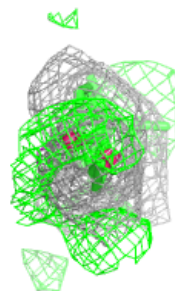
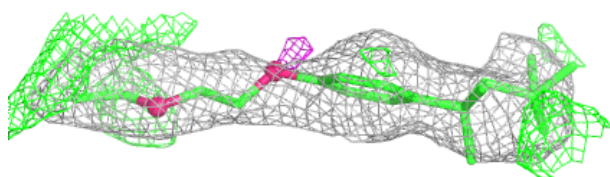
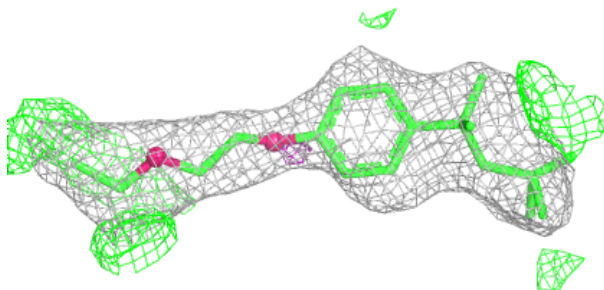


Electron density around UQ5 B 602:

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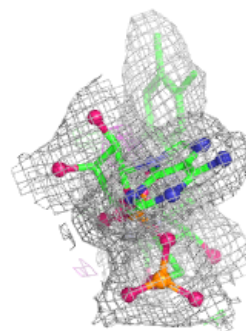
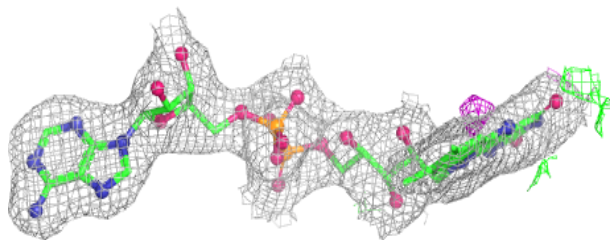
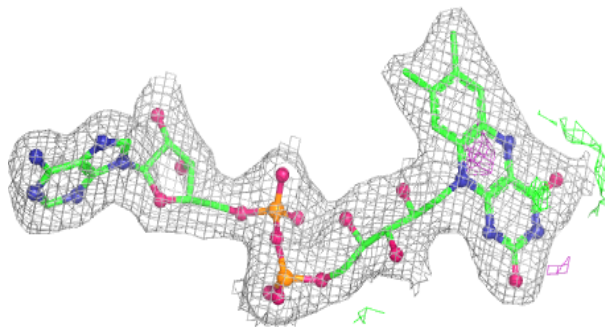
**Electron density around TRT A 603:**

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

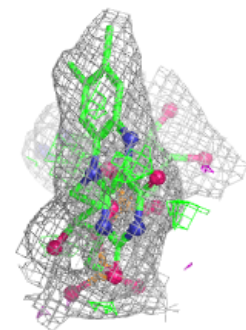
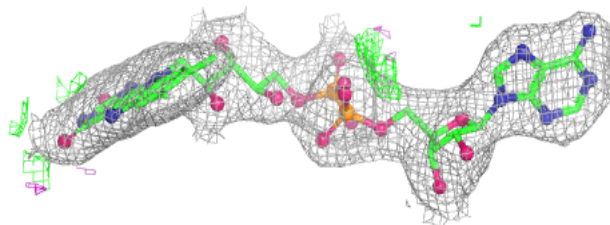
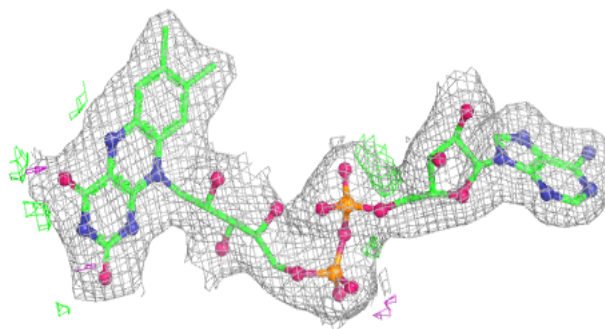


Electron density around FAD A 607:

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

**Electron density around FAD B 606:**

$2mF_o-DF_c$ (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.