



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:56 PM UTC

PDB ID : 4G6G / pdb_00004g6g
Title : Crystal structure of NDH with TRT
Authors : Li, W.; Feng, Y.; Ge, J.; Yang, M.
Deposited on : 2012-07-19
Resolution : 2.39 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

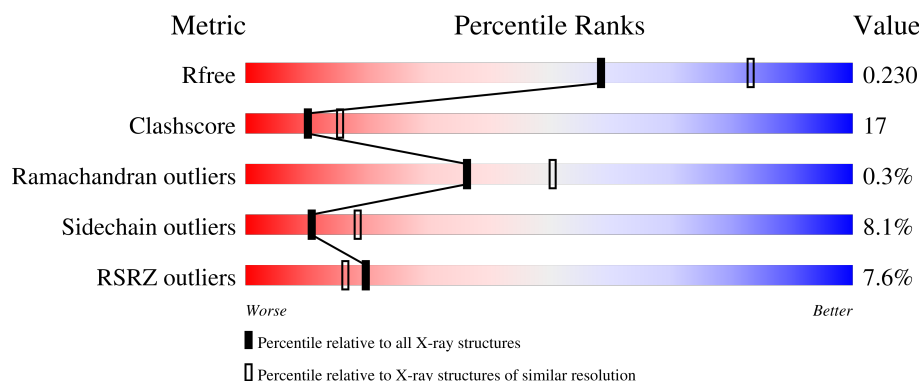
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	8% 71% 19% • 6%
1	B	502	6% 71% 18% • 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	TRT	A	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8067 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.

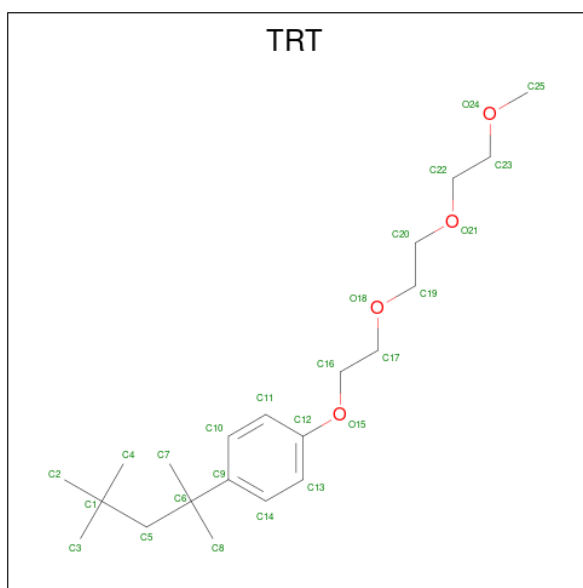
- Molecule 1 is a protein called Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3713	2403	627	678	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 FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula: $C_{21}H_{36}O_4$).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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

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

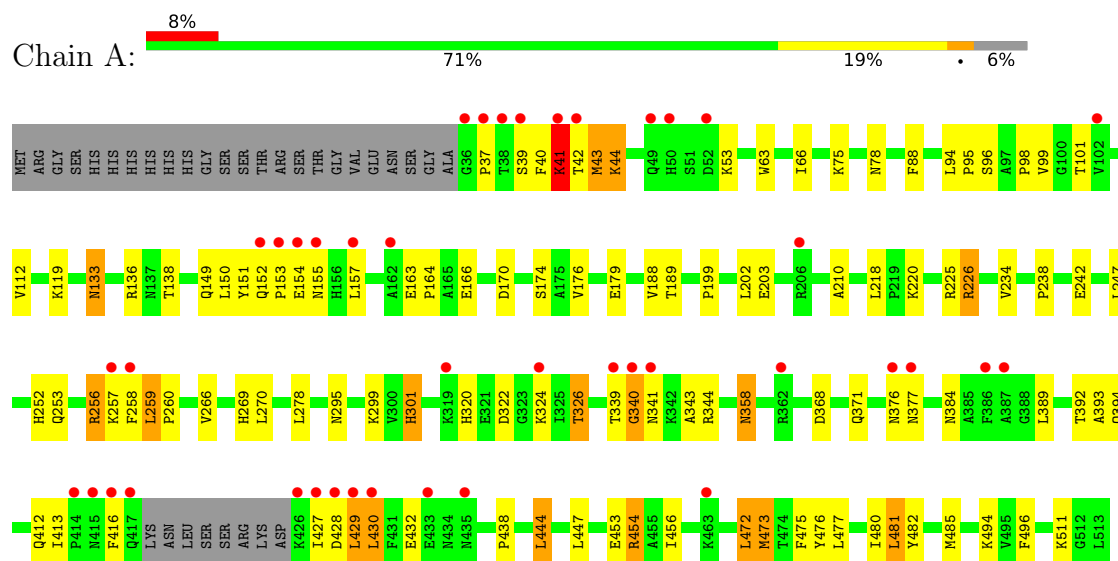
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total	O	0	0
			250	250		
5	B	214	Total	O	0	0
			214	214		

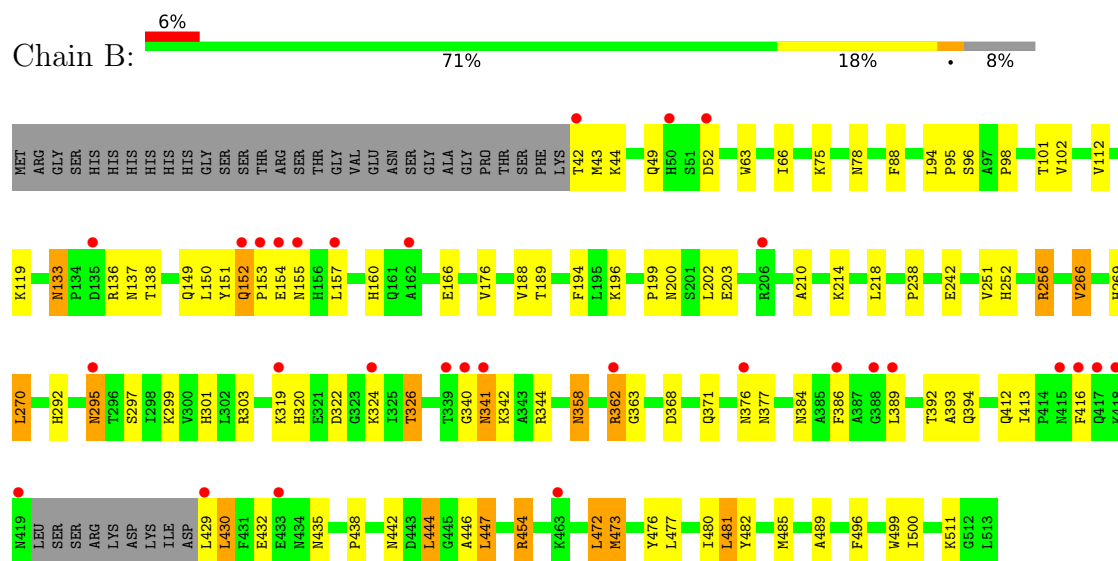
3 Residue-property plots

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

- Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.92Å 230.60Å 112.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.59 – 2.39 35.59 – 2.39	Depositor EDS
% Data completeness (in resolution range)	91.3 (35.59-2.39) 96.8 (35.59-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.193 , 0.234 0.191 , 0.230	Depositor DCC
R_{free} test set	3488 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.017 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8067	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: FAD, TRT, MG

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	0.50	0/3800	0.82	11/5147 (0.2%)
1	B	0.48	0/3743	0.82	10/5070 (0.2%)
All	All	0.49	0/7543	0.82	21/10217 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ARG	NE-CZ-NH2	-7.52	112.44	119.20
1	B	454	ARG	NE-CZ-NH2	-7.19	112.73	119.20
1	A	454	ARG	NE-CZ-NH2	7.13	125.62	119.20
1	A	226	ARG	NE-CZ-NH2	7.08	125.57	119.20
1	A	454	ARG	NE-CZ-NH1	-6.99	114.51	121.50
1	A	344	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	A	226	ARG	NE-CZ-NH1	-6.71	114.79	121.50
1	A	344	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	B	454	ARG	CD-NE-CZ	6.53	133.54	124.40
1	B	344	ARG	CD-NE-CZ	6.42	133.38	124.40
1	B	413	ILE	CA-C-N	6.15	126.33	119.32
1	B	413	ILE	C-N-CA	6.15	126.33	119.32
1	A	413	ILE	CA-C-N	6.14	126.31	119.32
1	A	413	ILE	C-N-CA	6.14	126.31	119.32
1	B	344	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	B	133	ASN	CA-C-N	5.81	125.50	119.05
1	B	133	ASN	C-N-CA	5.81	125.50	119.05
1	B	454	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	A	133	ASN	CA-C-N	5.15	124.94	119.28
1	A	133	ASN	C-N-CA	5.15	124.94	119.28
1	A	454	ARG	CD-NE-CZ	5.07	131.50	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3713	0	3765	95	1
1	B	3658	0	3708	95	1
2	A	36	0	48	44	0
2	B	80	0	108	60	0
3	A	53	0	31	2	0
3	B	53	0	31	1	0
4	A	4	0	0	0	0
4	B	6	0	0	0	0
5	A	250	0	0	7	0
5	B	214	0	0	7	0
All	All	8067	0	7691	262	1

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 17.

All (262) 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:604:TRT:C14	2:B:604:TRT:H2C2	1.40	1.49
2:B:603:TRT:C3	2:B:603:TRT:H14	1.43	1.49
2:A:602:TRT:H2C3	2:A:602:TRT:C7	1.52	1.38
2:B:604:TRT:H8C2	2:B:604:TRT:C2	1.52	1.33
2:B:604:TRT:C2	2:B:604:TRT:H14	1.57	1.32
2:B:604:TRT:H2C3	2:B:604:TRT:C8	1.53	1.32
2:A:601:TRT:C14	2:A:601:TRT:H4C3	1.60	1.31
2:B:602:TRT:C8	2:B:602:TRT:H2C2	1.59	1.26
2:B:602:TRT:H8C1	2:B:602:TRT:C2	1.54	1.25
2:A:601:TRT:H4C3	2:A:601:TRT:H14	1.17	1.17
2:B:603:TRT:H3C3	2:B:603:TRT:C14	1.73	1.16
2:A:602:TRT:H7C1	2:A:602:TRT:C2	1.74	1.14
2:B:601:TRT:C7	2:B:601:TRT:H3C2	1.79	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:TRT:C14	2:A:601:TRT:C4	2.30	1.10
2:B:603:TRT:C3	2:B:603:TRT:C14	2.30	1.08
2:B:601:TRT:H7C1	2:B:601:TRT:C2	1.84	1.07
2:B:601:TRT:H7C1	2:B:601:TRT:H2C3	1.16	1.07
2:A:601:TRT:H4C2	2:A:601:TRT:H7C3	1.31	1.07
2:A:602:TRT:H7C3	2:A:602:TRT:H4C2	1.37	1.07
2:B:603:TRT:C3	2:B:603:TRT:H7C3	1.80	1.07
2:B:603:TRT:H3C2	2:B:603:TRT:C7	1.83	1.04
2:B:604:TRT:H13	2:B:604:TRT:O18	1.59	1.02
2:A:602:TRT:C17	2:A:602:TRT:H11	1.88	1.02
2:B:603:TRT:H7C1	2:B:603:TRT:H4C3	1.37	1.02
1:B:500:ILE:HD13	2:B:601:TRT:C8	1.90	1.01
1:A:220:LYS:HG2	1:A:225:ARG:HH12	1.24	1.00
2:B:601:TRT:H2C2	2:B:601:TRT:H8C1	1.44	1.00
2:B:603:TRT:C7	2:B:603:TRT:H4C3	1.95	0.97
2:B:603:TRT:H7C3	2:B:603:TRT:H3C2	0.99	0.97
2:A:601:TRT:H14	2:A:601:TRT:C4	1.92	0.96
1:A:496:PHE:CE1	2:A:601:TRT:C8	2.50	0.95
2:A:602:TRT:H11	2:A:602:TRT:H171	1.48	0.94
2:A:601:TRT:H2C3	2:A:601:TRT:C7	1.99	0.92
2:B:604:TRT:C14	2:B:604:TRT:C2	2.30	0.91
2:B:601:TRT:H3C2	2:B:601:TRT:H7C3	1.54	0.89
1:A:371:GLN:HE21	1:A:376:ASN:HA	1.39	0.88
1:B:152:GLN:H	1:B:152:GLN:HE21	1.19	0.88
2:A:602:TRT:H2C3	2:A:602:TRT:H7C1	0.88	0.88
1:B:269:HIS:HD2	1:B:301:HIS:HE1	1.17	0.88
1:A:394:GLN:NE2	1:A:444:LEU:H	1.71	0.88
1:A:496:PHE:HE1	2:A:601:TRT:C8	1.85	0.87
1:B:269:HIS:CD2	1:B:301:HIS:HE1	1.91	0.87
1:B:394:GLN:NE2	1:B:444:LEU:H	1.72	0.87
2:B:603:TRT:H14	2:B:603:TRT:H3C2	1.53	0.87
1:B:136:ARG:HG3	1:B:138:THR:HG22	1.58	0.85
1:B:322:ASP:OD2	1:B:324:LYS:HG2	1.76	0.85
1:A:322:ASP:OD2	1:A:324:LYS:HG2	1.76	0.85
2:A:601:TRT:C4	2:A:601:TRT:H7C3	2.05	0.84
1:B:341:ASN:N	1:B:341:ASN:HD22	1.71	0.84
1:B:371:GLN:HE21	1:B:376:ASN:HA	1.39	0.84
1:A:220:LYS:HG2	1:A:225:ARG:NH1	1.93	0.83
2:A:602:TRT:C7	2:A:602:TRT:C2	2.30	0.82
1:A:136:ARG:HG3	1:A:138:THR:HG22	1.60	0.81
2:B:602:TRT:H2C2	2:B:602:TRT:H8C1	0.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:TRT:H14	2:B:603:TRT:H3C3	0.81	0.80
2:A:602:TRT:H2C3	2:A:602:TRT:H7C3	1.63	0.80
1:B:341:ASN:HD22	1:B:341:ASN:H	1.26	0.80
1:B:394:GLN:HE22	1:B:444:LEU:H	1.29	0.79
1:B:151:TYR:O	1:B:154:GLU:HG3	1.82	0.79
1:A:269:HIS:HD2	1:A:301:HIS:CE1	2.01	0.79
1:A:394:GLN:HE22	1:A:444:LEU:H	1.31	0.79
1:A:151:TYR:O	1:A:154:GLU:HG3	1.83	0.78
2:A:601:TRT:H2C3	2:A:601:TRT:H7C1	1.63	0.78
2:A:602:TRT:H4C3	2:A:602:TRT:H10	1.67	0.76
1:B:500:ILE:HD13	2:B:601:TRT:H8C1	1.68	0.75
1:A:138:THR:OG1	1:A:166:GLU:HB3	1.86	0.75
1:B:444:LEU:HB3	2:B:604:TRT:H2C3	1.68	0.75
1:B:269:HIS:CD2	1:B:301:HIS:CE1	2.76	0.74
1:B:341:ASN:N	1:B:341:ASN:ND2	2.30	0.73
2:B:601:TRT:H4C1	2:B:602:TRT:C20	2.17	0.73
1:B:447:LEU:HD11	2:B:604:TRT:H7C3	1.70	0.73
1:B:269:HIS:HD2	1:B:301:HIS:CE1	2.04	0.73
1:B:303:ARG:NH1	5:B:893:HOH:O	2.21	0.73
1:A:427:ILE:HA	1:A:430:LEU:HD23	1.71	0.72
2:A:602:TRT:H171	2:A:602:TRT:C11	2.18	0.72
2:A:602:TRT:H10	2:A:602:TRT:C4	2.20	0.72
2:A:601:TRT:H7C3	2:A:601:TRT:H2C3	1.71	0.71
1:B:152:GLN:HE21	1:B:152:GLN:N	1.89	0.70
1:B:444:LEU:HB3	2:B:604:TRT:H8C2	1.72	0.70
2:A:602:TRT:H11	2:A:602:TRT:O18	1.91	0.70
2:A:602:TRT:H7C3	2:A:602:TRT:C4	2.08	0.70
2:A:601:TRT:C4	2:A:601:TRT:C9	2.67	0.70
1:B:152:GLN:H	1:B:152:GLN:NE2	1.90	0.70
1:B:295:ASN:ND2	5:B:804:HOH:O	2.25	0.70
2:B:603:TRT:C3	2:B:603:TRT:C7	2.56	0.70
1:A:253:GLN:O	1:A:257:LYS:HE3	1.93	0.69
1:B:371:GLN:NE2	1:B:376:ASN:HA	2.08	0.68
2:B:604:TRT:H2C2	2:B:604:TRT:H14	0.72	0.68
2:A:602:TRT:C17	2:A:602:TRT:C11	2.62	0.68
1:A:496:PHE:CE1	2:A:601:TRT:H8C1	2.27	0.68
1:B:447:LEU:CD1	2:B:604:TRT:H7C3	2.23	0.67
1:B:138:THR:OG1	1:B:166:GLU:HB3	1.95	0.67
1:B:500:ILE:HG21	2:B:601:TRT:H8C2	1.76	0.67
1:A:258:PHE:O	1:A:259:LEU:HD13	1.94	0.67
1:A:269:HIS:HD2	1:A:301:HIS:HE1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASP:HB3	1:A:438:PRO:HB3	1.76	0.66
1:A:394:GLN:HG3	5:A:897:HOH:O	1.94	0.66
2:A:601:TRT:H4C2	2:A:601:TRT:C7	2.06	0.66
2:B:601:TRT:C2	2:B:601:TRT:H8C1	2.24	0.66
2:B:603:TRT:C7	2:B:603:TRT:C4	2.64	0.66
2:B:604:TRT:H14	2:B:604:TRT:C1	2.22	0.65
1:A:371:GLN:NE2	1:A:376:ASN:HA	2.10	0.64
1:B:496:PHE:CD1	2:B:603:TRT:H8C1	2.32	0.64
1:A:496:PHE:CE1	2:A:601:TRT:H8C3	2.31	0.64
2:B:603:TRT:C14	2:B:603:TRT:H3C2	2.14	0.64
1:A:269:HIS:HE1	5:A:928:HOH:O	1.81	0.64
1:B:368:ASP:HB3	1:B:438:PRO:HB3	1.80	0.64
1:A:40:PHE:O	1:A:41:LYS:C	2.40	0.63
2:B:601:TRT:H7C1	2:B:601:TRT:C3	2.29	0.62
2:A:602:TRT:C2	2:A:602:TRT:H7C3	2.26	0.62
2:A:601:TRT:H4C2	2:A:601:TRT:C9	2.30	0.61
1:A:299:LYS:HG2	1:A:301:HIS:CE1	2.35	0.61
1:B:489:ALA:CB	2:B:602:TRT:H8C2	2.31	0.61
2:B:601:TRT:H3C2	2:B:601:TRT:H7C1	1.58	0.61
1:B:152:GLN:HB2	1:B:153:PRO:HD3	1.81	0.61
1:B:152:GLN:HB2	1:B:153:PRO:CD	2.30	0.61
1:B:489:ALA:HB2	2:B:602:TRT:H8C2	1.83	0.60
1:A:496:PHE:HE1	2:A:601:TRT:H8C1	1.65	0.60
1:A:269:HIS:CD2	1:A:301:HIS:CE1	2.87	0.60
1:A:75:LYS:HE2	1:A:119:LYS:HD3	1.85	0.59
1:A:42:THR:HG22	5:A:804:HOH:O	2.02	0.59
1:A:473:MET:HE2	1:A:476:TYR:HD2	1.68	0.58
1:B:75:LYS:HE2	1:B:119:LYS:HD3	1.85	0.58
1:B:500:ILE:HD13	2:B:601:TRT:H8C3	1.85	0.58
1:A:138:THR:HG21	1:A:166:GLU:OE1	2.05	0.57
2:A:601:TRT:H7C3	2:A:601:TRT:C2	2.32	0.57
1:B:176:VAL:HG22	1:B:384:ASN:HD22	1.69	0.57
1:B:362:ARG:CZ	1:B:386:PHE:HD1	2.18	0.57
1:B:136:ARG:HG3	1:B:138:THR:CG2	2.34	0.57
1:B:500:ILE:HG21	2:B:601:TRT:C8	2.35	0.57
1:B:454:ARG:NH2	1:B:472:LEU:HG	2.20	0.57
1:A:496:PHE:CD1	2:A:601:TRT:C8	2.89	0.56
1:A:258:PHE:O	1:A:259:LEU:CD1	2.54	0.56
1:A:42:THR:HG23	1:A:42:THR:O	2.05	0.56
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.86	0.56
1:B:362:ARG:HG3	1:B:363:GLY:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:HIS:HD2	1:A:256:ARG:NH2	2.05	0.55
1:B:75:LYS:HE2	1:B:119:LYS:CD	2.37	0.55
1:A:53:LYS:HE3	1:A:75:LYS:O	2.07	0.55
1:A:149:GLN:NE2	1:A:157:LEU:HD11	2.23	0.54
1:A:176:VAL:HG22	1:A:384:ASN:HD22	1.72	0.54
1:A:75:LYS:HE2	1:A:119:LYS:CD	2.37	0.54
1:B:394:GLN:HE22	1:B:444:LEU:N	2.03	0.54
1:A:496:PHE:HE1	2:A:601:TRT:H8C2	1.70	0.54
1:A:444:LEU:HB3	2:A:602:TRT:H5C2	1.88	0.53
2:A:601:TRT:C4	2:A:601:TRT:C7	2.75	0.53
1:B:199:PRO:O	1:B:203:GLU:HG3	2.08	0.53
2:B:602:TRT:C8	2:B:602:TRT:C2	2.30	0.53
1:A:444:LEU:HB3	2:A:602:TRT:C5	2.38	0.53
1:A:176:VAL:H	1:A:384:ASN:ND2	2.07	0.53
1:A:428:ASP:OD2	1:A:429:LEU:HD13	2.08	0.53
1:B:473:MET:HE2	1:B:476:TYR:HD2	1.74	0.52
1:B:430:LEU:HD22	5:B:894:HOH:O	2.08	0.52
1:B:252:HIS:HD2	1:B:256:ARG:NH2	2.08	0.52
1:B:477:LEU:HG	1:B:481:LEU:HD22	1.91	0.52
1:B:149:GLN:NE2	1:B:157:LEU:HD11	2.23	0.52
1:A:152:GLN:HB2	1:A:153:PRO:CD	2.39	0.52
1:A:220:LYS:HA	1:A:225:ARG:HH11	1.75	0.52
2:A:601:TRT:C7	2:A:601:TRT:C2	2.70	0.52
1:B:444:LEU:HB3	2:B:604:TRT:C2	2.40	0.52
1:A:394:GLN:HE22	1:A:444:LEU:N	2.02	0.51
1:B:152:GLN:NE2	1:B:153:PRO:HD2	2.26	0.51
2:B:603:TRT:H7C1	2:B:603:TRT:C4	2.23	0.51
1:A:133:ASN:HD22	1:A:138:THR:HG23	1.75	0.51
1:B:447:LEU:HD21	1:B:481:LEU:HD23	1.92	0.51
1:B:446:ALA:C	1:B:447:LEU:HG	2.36	0.51
1:B:292:HIS:CE1	1:B:454:ARG:HG3	2.46	0.50
1:B:138:THR:HG21	1:B:166:GLU:OE1	2.11	0.50
2:B:604:TRT:H13	2:B:604:TRT:C17	2.41	0.50
1:A:234:VAL:HG12	1:A:339:THR:HG21	1.94	0.50
1:A:199:PRO:O	1:A:203:GLU:HG3	2.12	0.50
1:B:362:ARG:CZ	1:B:386:PHE:CD1	2.95	0.50
1:B:362:ARG:HG2	1:B:386:PHE:CD1	2.47	0.50
1:A:96:SER:HB2	1:A:101:THR:HB	1.92	0.49
1:A:301:HIS:ND1	1:A:301:HIS:N	2.60	0.49
1:A:447:LEU:HD11	2:A:602:TRT:H7C2	1.93	0.49
1:A:256:ARG:HD2	5:A:894:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:NE	1:B:386:PHE:HD1	2.10	0.49
1:A:482:TYR:HD1	1:A:485:MET:HE3	1.76	0.49
1:B:214:LYS:HD3	5:B:878:HOH:O	2.12	0.49
1:A:339:THR:O	1:A:340:GLY:O	2.30	0.48
1:A:152:GLN:O	1:A:153:PRO:C	2.56	0.48
2:B:603:TRT:H7C3	2:B:603:TRT:H4C3	1.90	0.48
1:A:252:HIS:HD2	1:A:256:ARG:HH21	1.61	0.48
1:B:269:HIS:HE1	5:B:900:HOH:O	1.95	0.48
1:A:496:PHE:CD1	2:A:601:TRT:H8C1	2.48	0.48
1:B:96:SER:HB2	1:B:101:THR:HB	1.94	0.48
2:B:602:TRT:H2C2	2:B:602:TRT:H8C2	1.80	0.48
1:A:238:PRO:O	1:A:242:GLU:HG3	2.14	0.47
1:A:392:THR:HB	3:A:603:FAD:O2	2.13	0.47
1:B:133:ASN:HD22	1:B:138:THR:HG23	1.79	0.47
1:B:392:THR:HB	3:B:607:FAD:O2	2.15	0.47
1:B:444:LEU:HB3	2:B:604:TRT:C8	2.42	0.47
1:B:49:GLN:OE1	1:B:49:GLN:HA	2.14	0.47
1:A:496:PHE:CD1	2:A:601:TRT:H8C3	2.49	0.47
1:A:136:ARG:HG3	1:A:138:THR:CG2	2.38	0.47
1:A:454:ARG:NH2	1:A:472:LEU:HG	2.30	0.47
1:A:66:ILE:HG13	1:A:88:PHE:HB2	1.97	0.47
2:B:601:TRT:H161	2:B:601:TRT:H191	1.34	0.47
1:A:42:THR:O	1:A:42:THR:CG2	2.63	0.46
1:B:362:ARG:NE	1:B:386:PHE:CD1	2.84	0.46
1:A:179:GLU:O	1:A:341:ASN:HB3	2.15	0.46
2:A:602:TRT:C4	2:A:602:TRT:C10	2.91	0.46
1:B:319:LYS:HG3	5:B:912:HOH:O	2.14	0.46
1:A:94:LEU:N	1:A:95:PRO:CD	2.79	0.46
1:A:473:MET:HE2	1:A:476:TYR:CD2	2.50	0.46
1:B:66:ILE:HG13	1:B:88:PHE:HB2	1.96	0.46
1:B:416:PHE:CZ	1:B:430:LEU:HB3	2.51	0.46
1:B:299:LYS:HG2	1:B:301:HIS:CE1	2.50	0.46
1:B:42:THR:O	1:B:42:THR:HG23	2.16	0.46
1:A:63:TRP:CD2	1:A:393:ALA:HB1	2.51	0.46
1:B:295:ASN:ND2	5:B:786:HOH:O	2.48	0.46
1:B:210:ALA:HB2	1:B:511:LYS:HE3	1.96	0.46
1:B:238:PRO:O	1:B:242:GLU:HG3	2.15	0.46
1:A:44:LYS:NZ	1:A:157:LEU:O	2.47	0.45
1:B:358:ASN:N	1:B:358:ASN:HD22	2.13	0.45
1:A:394:GLN:NE2	1:A:444:LEU:HB2	2.31	0.45
1:B:252:HIS:HD2	1:B:256:ARG:HH21	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:HIS:CD2	1:A:301:HIS:HE1	2.28	0.45
1:A:260:PRO:HG3	5:A:798:HOH:O	2.17	0.45
1:B:442:ASN:O	1:B:444:LEU:HD13	2.17	0.45
1:B:480:ILE:HG13	2:B:603:TRT:H4C1	1.99	0.45
1:B:94:LEU:N	1:B:95:PRO:CD	2.79	0.44
2:B:603:TRT:H7C3	2:B:603:TRT:C4	2.43	0.44
2:B:604:TRT:H14	2:B:604:TRT:C3	2.47	0.44
1:A:43:MET:HE2	1:A:43:MET:HB2	1.70	0.44
1:A:152:GLN:HB2	1:A:153:PRO:HD3	1.99	0.44
1:A:358:ASN:N	1:A:358:ASN:HD22	2.16	0.44
1:A:416:PHE:CZ	1:A:430:LEU:HB3	2.52	0.44
1:B:482:TYR:HD1	1:B:485:MET:HE3	1.82	0.44
1:A:210:ALA:HB2	1:A:511:LYS:HE3	1.99	0.44
1:A:343:ALA:HA	5:A:710:HOH:O	2.17	0.44
1:A:393:ALA:HB2	3:A:603:FAD:H2'	2.00	0.43
1:B:394:GLN:NE2	1:B:444:LEU:HB2	2.33	0.43
1:A:480:ILE:HG13	2:A:601:TRT:H2C2	2.01	0.43
1:B:499:TRP:CE3	2:B:603:TRT:H7C2	2.52	0.43
1:B:500:ILE:HD13	2:B:601:TRT:H8C2	1.94	0.43
1:A:494:LYS:NZ	5:A:899:HOH:O	2.52	0.43
1:A:163:GLU:HA	1:A:164:PRO:HD3	1.90	0.42
1:B:251:VAL:HG21	1:B:266:VAL:HG21	2.01	0.42
1:B:496:PHE:CZ	1:B:500:ILE:HD11	2.54	0.42
1:A:94:LEU:O	1:A:98:PRO:HD3	2.20	0.42
1:A:174:SER:C	1:A:384:ASN:HD21	2.28	0.42
1:A:376:ASN:O	1:A:427:ILE:HD12	2.19	0.42
1:A:453:GLU:HG3	1:A:475:PHE:CE2	2.54	0.42
1:A:447:LEU:HD21	1:A:481:LEU:HD23	2.02	0.42
1:A:278:LEU:HD13	1:A:456:ILE:HD11	2.02	0.42
1:A:170:ASP:O	1:A:377:ASN:OD1	2.39	0.41
1:A:320:HIS:NE2	1:A:326:THR:OG1	2.53	0.41
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.87	0.41
1:B:496:PHE:HD1	2:B:603:TRT:H8C1	1.81	0.41
1:A:252:HIS:CD2	1:A:256:ARG:HH21	2.39	0.41
1:B:444:LEU:HD23	2:B:604:TRT:H2C1	2.01	0.41
1:B:43:MET:HE2	1:B:43:MET:HB2	1.92	0.41
1:B:137:ASN:OD1	1:B:377:ASN:ND2	2.54	0.41
1:B:176:VAL:H	1:B:384:ASN:ND2	2.19	0.41
1:B:320:HIS:NE2	1:B:326:THR:OG1	2.52	0.41
1:B:194:PHE:O	1:B:200:ASN:HB3	2.21	0.40
1:A:99:VAL:CG1	1:A:247:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HD12	1:A:259:LEU:HA	1.85	0.40
1:B:63:TRP:CD2	1:B:393:ALA:HB1	2.57	0.40
1:B:94:LEU:O	1:B:98:PRO:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PRO:O	1:B:340:GLY:N[6_555]	1.92	0.28

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	466/502 (93%)	446 (96%)	18 (4%)	2 (0%)	30	43
1	B	459/502 (91%)	442 (96%)	16 (4%)	1 (0%)	43	58
All	All	925/1004 (92%)	888 (96%)	34 (4%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	GLY
1	A	41	LYS
1	B	297	SER

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%)	369 (92%)	30 (8%)	12	21
1	B	392/427 (92%)	358 (91%)	34 (9%)	9	16
All	All	791/854 (93%)	727 (92%)	64 (8%)	11	18

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	41	LYS
1	A	43	MET
1	A	44	LYS
1	A	78	ASN
1	A	112	VAL
1	A	150	LEU
1	A	155	ASN
1	A	188	VAL
1	A	189	THR
1	A	202	LEU
1	A	218	LEU
1	A	226	ARG
1	A	256	ARG
1	A	259	LEU
1	A	266	VAL
1	A	270	LEU
1	A	295	ASN
1	A	301	HIS
1	A	326	THR
1	A	358	ASN
1	A	389	LEU
1	A	412	GLN
1	A	429	LEU
1	A	430	LEU
1	A	432	GLU
1	A	444	LEU
1	A	472	LEU
1	A	473	MET
1	A	481	LEU
1	B	44	LYS
1	B	52	ASP
1	B	78	ASN

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Mol	Chain	Res	Type
1	B	102	VAL
1	B	112	VAL
1	B	150	LEU
1	B	152	GLN
1	B	155	ASN
1	B	160	HIS
1	B	188	VAL
1	B	189	THR
1	B	196	LYS
1	B	202	LEU
1	B	218	LEU
1	B	256	ARG
1	B	266	VAL
1	B	270	LEU
1	B	295	ASN
1	B	326	THR
1	B	341	ASN
1	B	342	LYS
1	B	358	ASN
1	B	362	ARG
1	B	389	LEU
1	B	412	GLN
1	B	429	LEU
1	B	430	LEU
1	B	432	GLU
1	B	435	ASN
1	B	444	LEU
1	B	447	LEU
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	50	HIS
1	A	149	GLN
1	A	155	ASN
1	A	156	HIS
1	A	161	GLN
1	A	252	HIS

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Mol	Chain	Res	Type
1	A	269	HIS
1	A	301	HIS
1	A	358	ASN
1	A	384	ASN
1	A	394	GLN
1	A	435	ASN
1	B	71	HIS
1	B	149	GLN
1	B	152	GLN
1	B	155	ASN
1	B	156	HIS
1	B	252	HIS
1	B	269	HIS
1	B	301	HIS
1	B	341	ASN
1	B	358	ASN
1	B	384	ASN
1	B	394	GLN
1	B	435	ASN

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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	$\# Z > 2$
2	TRT	A	601	-	16,16,25	0.65	1 (6%)	24,24,33	0.99	1 (4%)
3	FAD	A	603	4	58,58,58	1.15	5 (8%)	85,89,89	1.62	17 (20%)
2	TRT	B	602	-	20,20,25	0.61	1 (5%)	28,28,33	2.56	5 (17%)
3	FAD	B	607	4	58,58,58	1.13	5 (8%)	85,89,89	1.56	16 (18%)
2	TRT	B	604	-	20,20,25	0.62	1 (5%)	28,28,33	0.90	1 (3%)
2	TRT	A	602	-	20,20,25	0.61	1 (5%)	28,28,33	0.90	1 (3%)
2	TRT	B	603	-	20,20,25	0.63	1 (5%)	28,28,33	0.91	1 (3%)
2	TRT	B	601	-	20,20,25	0.61	1 (5%)	28,28,33	2.57	5 (17%)

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
2	TRT	A	601	-	-	5/14/14/23	0/1/1/1
3	FAD	A	603	4	-	6/34/50/50	0/6/6/6
2	TRT	B	602	-	-	16/18/18/23	0/1/1/1
3	FAD	B	607	4	-	7/34/50/50	0/6/6/6
2	TRT	B	604	-	-	7/18/18/23	0/1/1/1
2	TRT	A	602	-	-	14/18/18/23	0/1/1/1
2	TRT	B	603	-	-	7/18/18/23	0/1/1/1
2	TRT	B	601	-	-	8/18/18/23	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	FAD	C4X-N5	3.80	1.39	1.30
3	B	607	FAD	C4X-N5	3.44	1.38	1.30
3	A	603	FAD	PA-O3P	2.73	1.62	1.59
3	B	607	FAD	C2A-N1A	2.61	1.38	1.33
3	A	603	FAD	C2A-N1A	2.60	1.38	1.33
3	B	607	FAD	C10-N1	2.53	1.38	1.33
3	A	603	FAD	C10-N1	2.45	1.38	1.33
3	B	607	FAD	C8A-N7A	2.38	1.36	1.31
3	B	607	FAD	C2A-N3A	2.28	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	FAD	C8A-N7A	2.27	1.36	1.31
2	A	601	TRT	C6-C9	-2.24	1.50	1.53
2	B	603	TRT	C6-C9	-2.23	1.50	1.53
2	B	602	TRT	C6-C9	-2.18	1.50	1.53
2	B	601	TRT	C6-C9	-2.17	1.50	1.53
2	A	602	TRT	C6-C9	-2.14	1.50	1.53
2	B	604	TRT	C6-C9	-2.13	1.50	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	TRT	C3-C1-C2	-7.54	85.91	108.96
2	B	601	TRT	C3-C1-C4	-7.53	85.96	108.96
2	B	601	TRT	C3-C1-C2	-7.52	85.98	108.96
2	B	602	TRT	C3-C1-C4	-7.49	86.07	108.96
3	A	603	FAD	N3A-C2A-N1A	-5.91	119.63	128.58
3	B	607	FAD	N3A-C2A-N1A	-5.85	119.73	128.58
2	B	601	TRT	C3-C1-C5	-5.37	85.95	110.61
2	B	602	TRT	C3-C1-C5	-5.37	85.97	110.61
3	A	603	FAD	N9A-C8A-N7A	-4.47	107.59	113.94
3	B	607	FAD	N9A-C8A-N7A	-4.13	108.07	113.94
3	A	603	FAD	C5A-C4A-N3A	-4.02	121.17	126.72
3	B	607	FAD	C5A-C4A-N3A	-3.87	121.39	126.72
2	A	601	TRT	C1-C5-C6	-3.71	109.40	123.78
2	B	601	TRT	C1-C5-C6	-3.70	109.45	123.78
2	B	603	TRT	C1-C5-C6	-3.69	109.50	123.78
2	A	602	TRT	C1-C5-C6	-3.62	109.77	123.78
3	A	603	FAD	C5A-N7A-C8A	3.61	109.12	103.45
2	B	602	TRT	C1-C5-C6	-3.61	109.82	123.78
2	B	604	TRT	C1-C5-C6	-3.59	109.86	123.78
2	B	601	TRT	C4-C1-C2	3.45	119.52	108.96
2	B	602	TRT	C4-C1-C2	3.45	119.49	108.96
3	A	603	FAD	C2A-N3A-C4A	3.44	120.23	111.83
3	B	607	FAD	C2A-N3A-C4A	3.29	119.87	111.83
3	B	607	FAD	C5A-N7A-C8A	3.22	108.51	103.45
3	B	607	FAD	C4'-C3'-C2'	-3.19	108.26	113.57
3	A	603	FAD	C4'-C3'-C2'	-3.07	108.46	113.57
3	B	607	FAD	C4-N3-C2	-2.94	120.42	125.64
3	A	603	FAD	C4-N3-C2	-2.93	120.44	125.64
3	A	603	FAD	O4-C4-C4X	-2.85	119.00	126.53
3	A	603	FAD	C4X-C4-N3	2.83	120.44	113.25
3	B	607	FAD	C4X-C4-N3	2.62	119.92	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	FAD	N3A-C4A-N9A	2.60	131.59	127.17
3	A	603	FAD	C4A-C5A-N7A	-2.51	107.71	110.58
3	A	603	FAD	C4A-N9A-C8A	2.47	108.33	105.74
3	B	607	FAD	C4X-C10-N10	2.44	119.98	116.48
3	B	607	FAD	N3A-C4A-N9A	2.43	131.31	127.17
3	A	603	FAD	C4X-C10-N10	2.42	119.95	116.48
3	B	607	FAD	C4A-N9A-C8A	2.34	108.19	105.74
3	B	607	FAD	C4A-C5A-N7A	-2.32	107.92	110.58
3	B	607	FAD	O4-C4-C4X	-2.27	120.53	126.53
3	B	607	FAD	C10-C4X-N5	-2.26	120.19	124.81
3	B	607	FAD	C9A-C5X-N5	-2.20	120.11	122.45
3	B	607	FAD	O2A-PA-O3P	2.15	113.08	107.27
3	A	603	FAD	O2A-PA-O3P	2.10	112.94	107.27
3	A	603	FAD	O5'-C5'-C4'	-2.10	103.77	109.36
3	A	603	FAD	C5X-C9A-N10	2.09	119.86	117.97
3	A	603	FAD	C9A-C5X-N5	-2.02	120.31	122.45

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	TRT	C1-C5-C6-C9
2	B	602	TRT	C1-C5-C6-C8
2	B	601	TRT	C16-C17-O18-C19
2	A	601	TRT	C13-C12-O15-C16
2	A	601	TRT	C11-C12-O15-C16
2	A	602	TRT	C1-C5-C6-C7
2	B	603	TRT	C1-C5-C6-C7
2	B	603	TRT	O15-C16-C17-O18
2	B	601	TRT	C13-C12-O15-C16
2	B	601	TRT	C2-C1-C5-C6
2	B	601	TRT	C11-C12-O15-C16
2	A	602	TRT	C1-C5-C6-C8
2	B	602	TRT	C1-C5-C6-C9
2	B	603	TRT	C1-C5-C6-C9
2	B	602	TRT	C13-C12-O15-C16
2	B	602	TRT	C11-C12-O15-C16
2	B	602	TRT	C3-C1-C5-C6
2	B	604	TRT	C2-C1-C5-C6
2	B	604	TRT	C3-C1-C5-C6
2	A	602	TRT	O15-C16-C17-O18
2	B	604	TRT	C4-C1-C5-C6

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Mol	Chain	Res	Type	Atoms
2	B	602	TRT	O15-C16-C17-O18
2	B	601	TRT	O15-C16-C17-O18
2	B	602	TRT	C1-C5-C6-C7
2	B	602	TRT	C2-C1-C5-C6
2	B	603	TRT	C11-C12-O15-C16
2	B	603	TRT	C1-C5-C6-C8
2	B	603	TRT	C13-C12-O15-C16
2	B	601	TRT	C5-C6-C9-C10
2	B	601	TRT	C5-C6-C9-C14
2	B	602	TRT	C5-C6-C9-C10
2	A	602	TRT	C17-C16-O15-C12
3	B	607	FAD	O3'-C3'-C4'-O4'
2	A	601	TRT	C5-C6-C9-C14
2	B	602	TRT	C5-C6-C9-C14
2	A	601	TRT	C5-C6-C9-C10
2	A	602	TRT	C20-C19-O18-C17
2	B	603	TRT	C20-C19-O18-C17
2	B	604	TRT	C11-C12-O15-C16
2	A	602	TRT	C5-C6-C9-C10
3	B	607	FAD	C2'-C3'-C4'-O4'
2	B	604	TRT	C13-C12-O15-C16
2	A	601	TRT	C1-C5-C6-C7
3	A	603	FAD	C2'-C3'-C4'-O4'
2	A	602	TRT	C13-C12-O15-C16
2	B	602	TRT	C20-C19-O18-C17
3	A	603	FAD	O3'-C3'-C4'-O4'
3	A	603	FAD	C2B-C1B-N9A-C8A
3	B	607	FAD	C2B-C1B-N9A-C8A
3	B	607	FAD	O3'-C3'-C4'-C5'
2	B	604	TRT	C1-C5-C6-C8
2	A	602	TRT	C11-C12-O15-C16
2	A	602	TRT	C5-C6-C9-C14
2	A	602	TRT	C7-C6-C9-C14
2	B	601	TRT	C1-C5-C6-C9
2	A	602	TRT	C7-C6-C9-C10
3	A	603	FAD	O3'-C3'-C4'-C5'
2	B	602	TRT	C16-C17-O18-C19
3	B	607	FAD	P-O3P-PA-O1A
2	A	602	TRT	C8-C6-C9-C10
2	B	602	TRT	C7-C6-C9-C14
2	B	602	TRT	C8-C6-C9-C14
2	B	602	TRT	C7-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	602	TRT	C8-C6-C9-C14
3	B	607	FAD	C2'-C3'-C4'-C5'
3	A	603	FAD	C2B-C1B-N9A-C4A
2	B	604	TRT	C16-C17-O18-C19
3	B	607	FAD	O4B-C1B-N9A-C8A
2	B	602	TRT	C8-C6-C9-C10
3	A	603	FAD	C2'-C3'-C4'-C5'

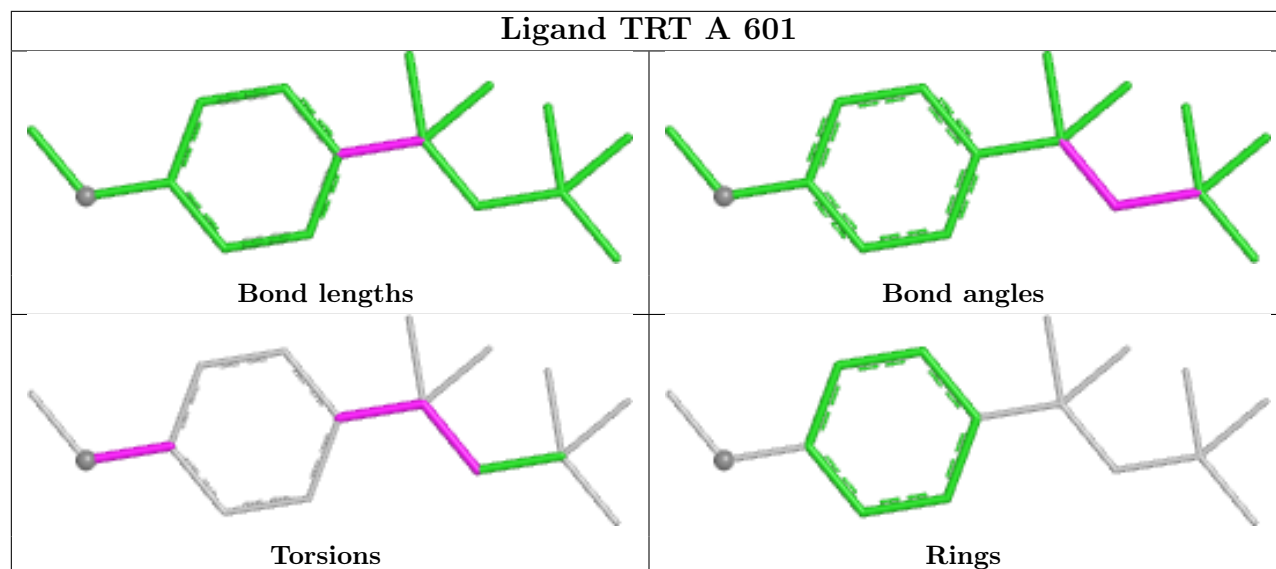
There are no ring outliers.

8 monomers are involved in 107 short contacts:

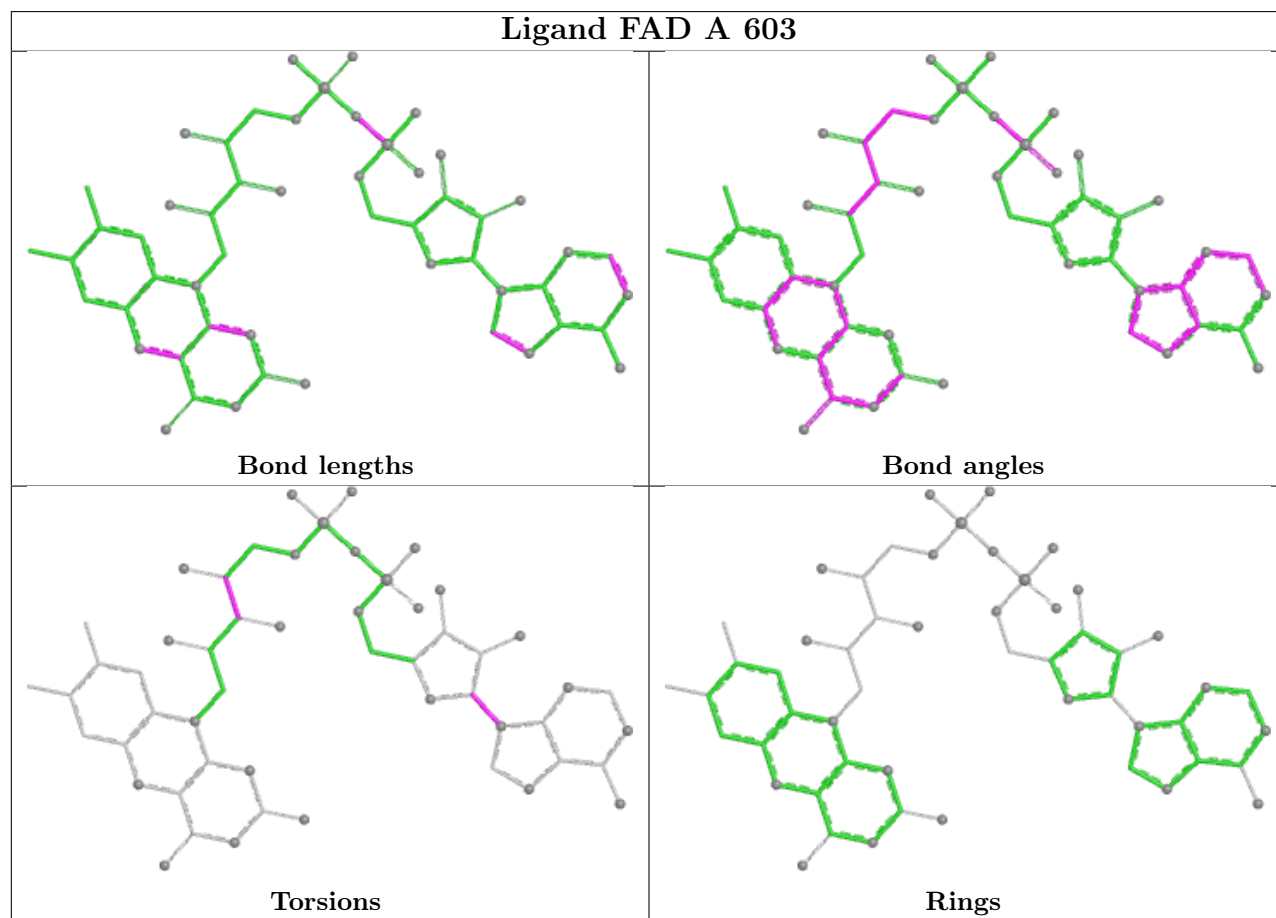
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TRT	25	0
3	A	603	FAD	2	0
2	B	602	TRT	8	0
3	B	607	FAD	1	0
2	B	604	TRT	17	0
2	A	602	TRT	19	0
2	B	603	TRT	20	0
2	B	601	TRT	16	0

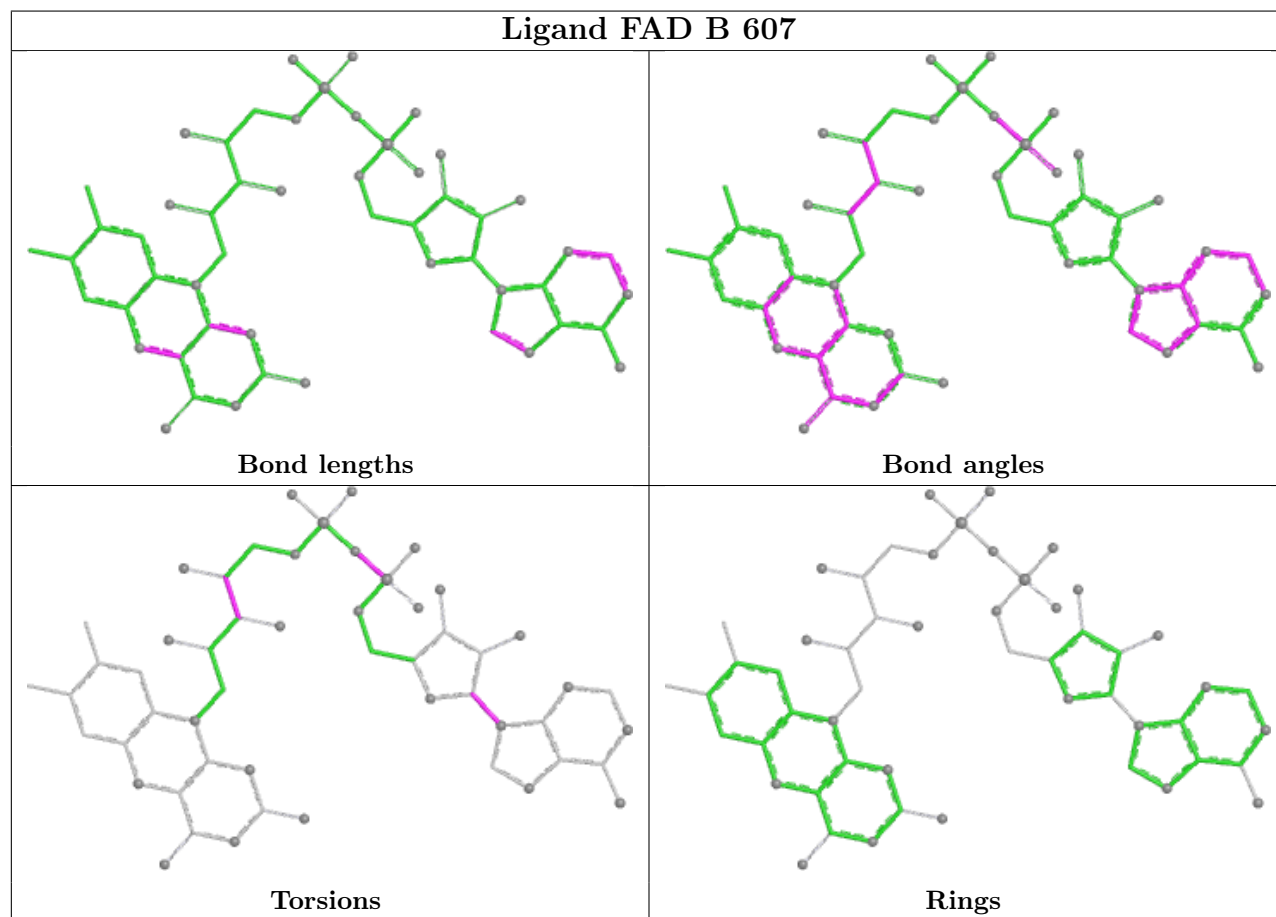
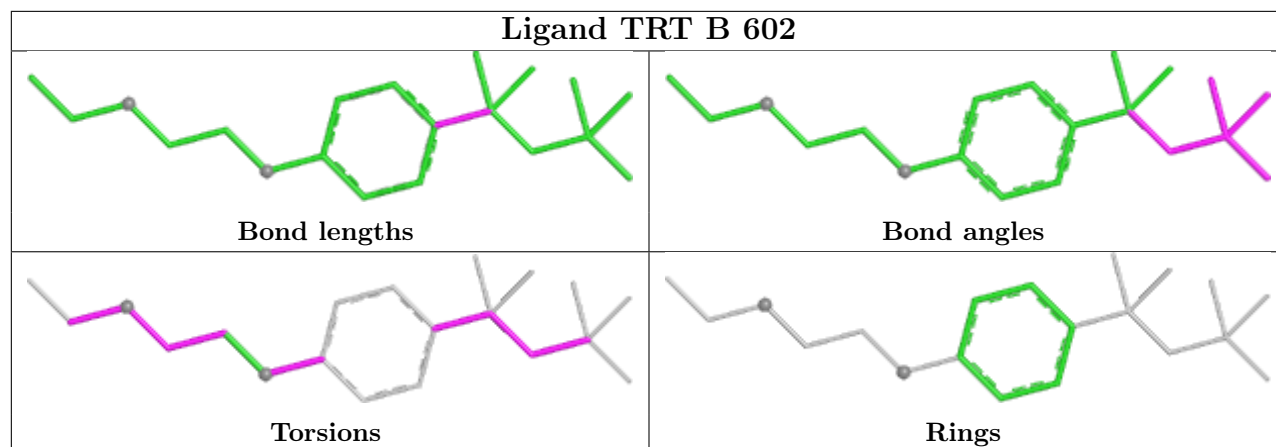
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

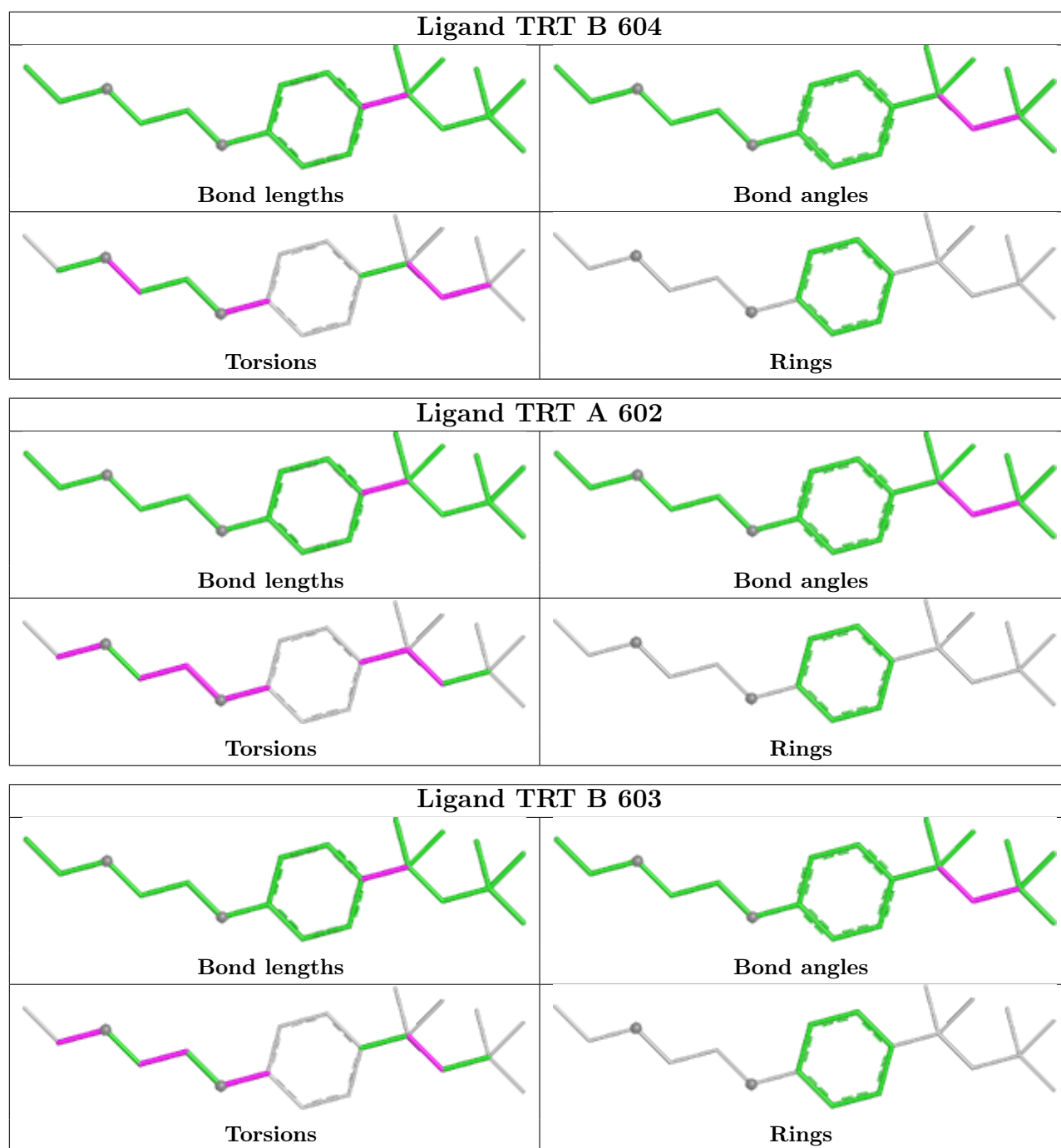
Ligand TRT A 601

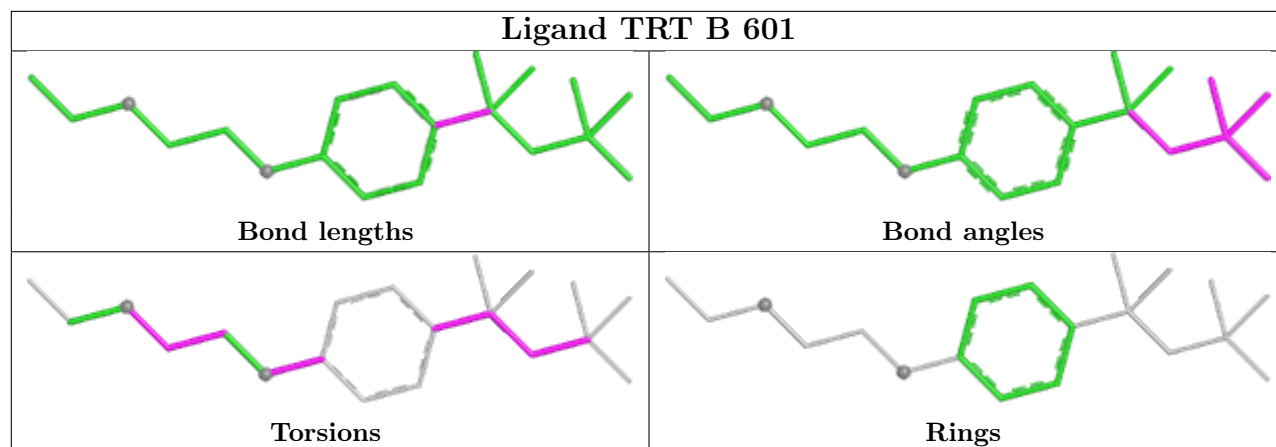


Ligand FAD A 603









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	470/502 (93%)	0.16	41 (8%)	16 13	20, 37, 86, 137	0
1	B	463/502 (92%)	0.13	30 (6%)	25 21	18, 41, 90, 138	0
All	All	933/1004 (92%)	0.14	71 (7%)	20 16	18, 39, 90, 138	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	GLN	6.7
1	B	419	ASN	6.7
1	B	429	LEU	6.4
1	A	153	PRO	5.7
1	A	417	GLN	5.4
1	A	50	HIS	5.4
1	A	376	ASN	5.1
1	A	386	PHE	4.7
1	A	41	LYS	4.6
1	B	362	ARG	4.5
1	B	50	HIS	4.3
1	A	429	LEU	4.1
1	A	426	LYS	4.0
1	B	42	THR	4.0
1	A	37	PRO	3.9
1	B	417	GLN	3.7
1	B	162	ALA	3.7
1	A	427	ILE	3.5
1	A	155	ASN	3.5
1	A	341	ASN	3.5
1	B	153	PRO	3.5
1	A	463	LYS	3.5
1	B	295	ASN	3.4
1	A	162	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	418	LYS	3.1
1	A	433	GLU	3.1
1	A	324	LYS	3.1
1	B	376	ASN	3.1
1	A	42	THR	3.0
1	A	339	THR	3.0
1	B	155	ASN	3.0
1	A	430	LEU	3.0
1	B	206	ARG	3.0
1	B	154	GLU	3.0
1	B	341	ASN	2.9
1	A	414	PRO	2.9
1	A	362	ARG	2.8
1	A	257	LYS	2.8
1	B	386	PHE	2.7
1	A	206	ARG	2.7
1	B	388	GLY	2.7
1	A	49	GLN	2.6
1	A	428	ASP	2.6
1	A	415	ASN	2.6
1	B	135	ASP	2.6
1	B	152	GLN	2.5
1	B	324	LYS	2.5
1	B	340	GLY	2.5
1	A	319	LYS	2.5
1	B	463	LYS	2.5
1	B	52	ASP	2.4
1	B	415	ASN	2.4
1	B	433	GLU	2.4
1	B	157	LEU	2.3
1	A	340	GLY	2.3
1	B	339	THR	2.3
1	A	39	SER	2.3
1	A	36	GLY	2.3
1	A	157	LEU	2.3
1	B	389	LEU	2.3
1	A	435	ASN	2.2
1	A	52	ASP	2.2
1	A	258	PHE	2.2
1	B	416	PHE	2.2
1	A	102	VAL	2.1
1	A	416	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	387	ALA	2.1
1	A	38	THR	2.0
1	A	154	GLU	2.0
1	B	319	LYS	2.0
1	A	377	ASN	2.0

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](#)

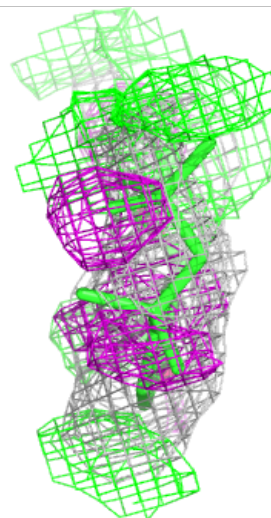
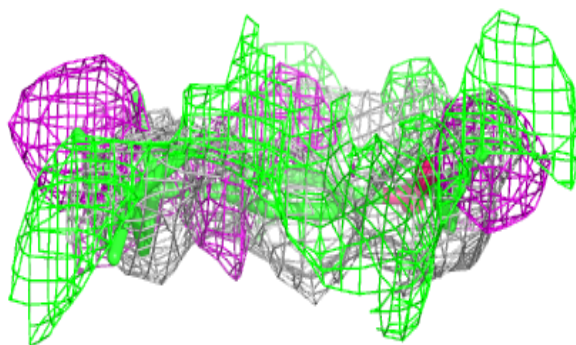
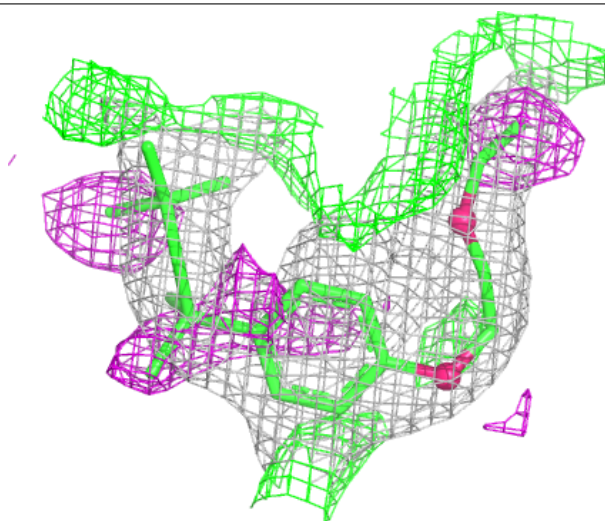
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TRT	A	602	20/25	0.67	0.29	2,63,97,104	0
2	TRT	B	602	20/25	0.72	0.34	73,102,149,157	0
2	TRT	B	603	20/25	0.75	0.28	32,70,107,121	0
2	TRT	B	604	20/25	0.77	0.30	56,81,106,124	0
4	MG	B	606	1/1	0.77	0.24	67,67,67,67	0
2	TRT	B	601	20/25	0.79	0.27	62,92,123,139	0
2	TRT	A	601	16/25	0.84	0.24	52,76,104,115	0
4	MG	B	611	1/1	0.84	0.18	62,62,62,62	0
4	MG	A	607	1/1	0.93	0.12	54,54,54,54	0
4	MG	A	606	1/1	0.97	0.06	36,36,36,36	0
4	MG	B	608	1/1	0.97	0.13	56,56,56,56	0
4	MG	B	609	1/1	0.97	0.08	54,54,54,54	0
3	FAD	B	607	53/53	0.97	0.07	14,30,42,44	0
4	MG	B	610	1/1	0.98	0.14	57,57,57,57	0
3	FAD	A	603	53/53	0.98	0.06	15,25,36,41	0
4	MG	B	605	1/1	0.99	0.04	15,15,15,15	0
4	MG	A	604	1/1	0.99	0.04	43,43,43,43	0
4	MG	A	605	1/1	0.99	0.05	40,40,40,40	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.

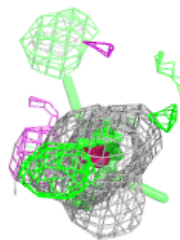
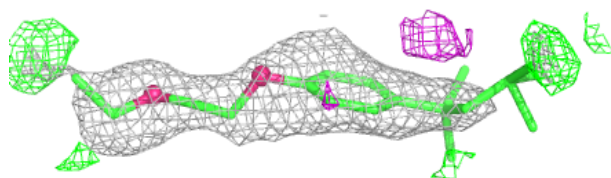
Electron density around TRT A 602:

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

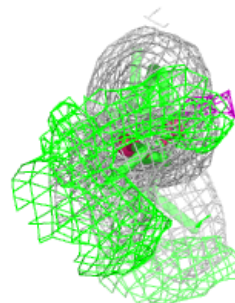
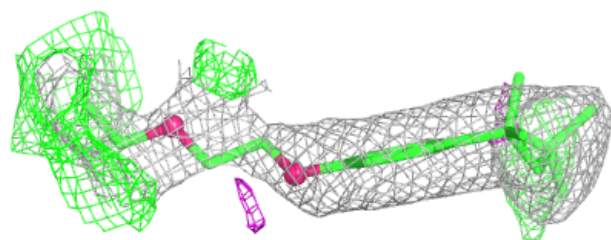
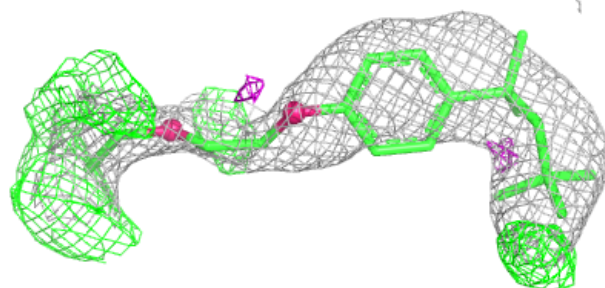


Electron density around TRT B 602:

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

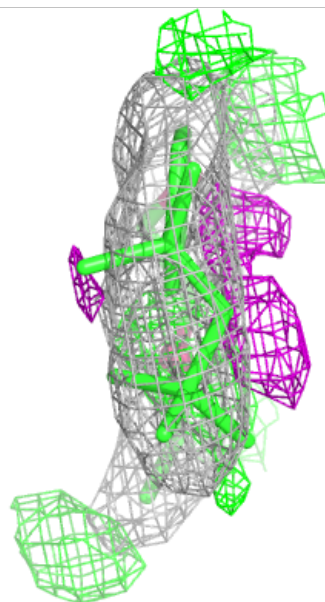
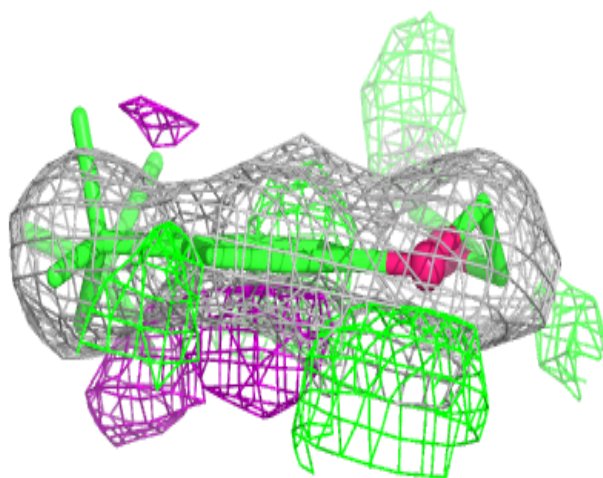
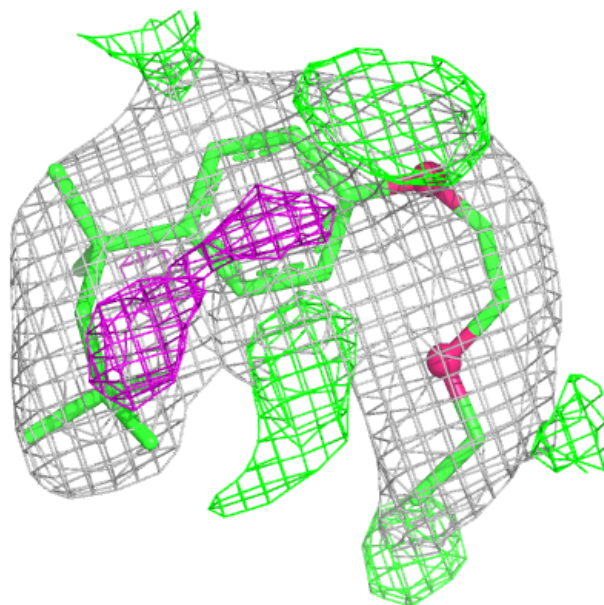
**Electron density around TRT B 603:**

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



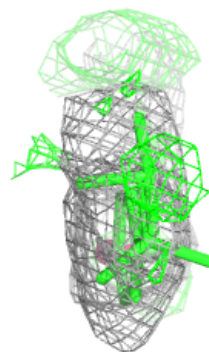
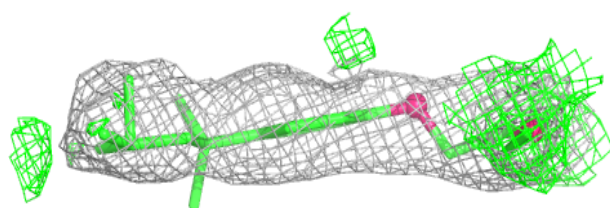
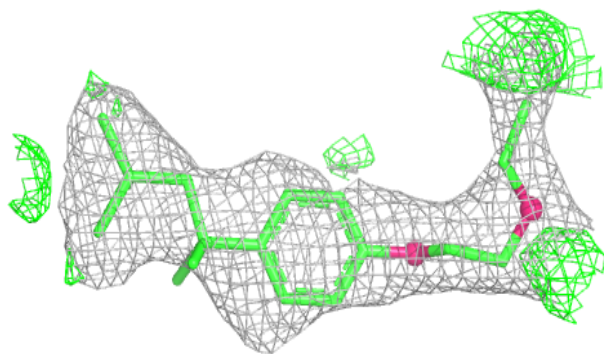
Electron density around TRT B 604:

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

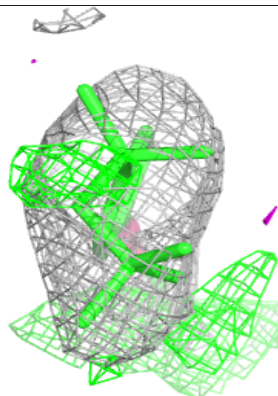
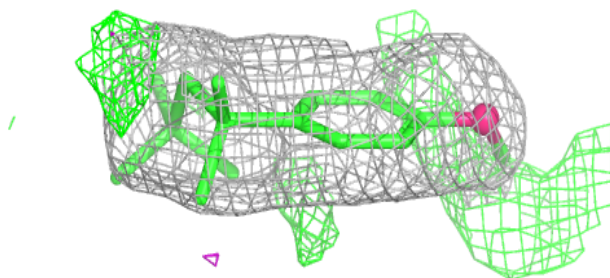
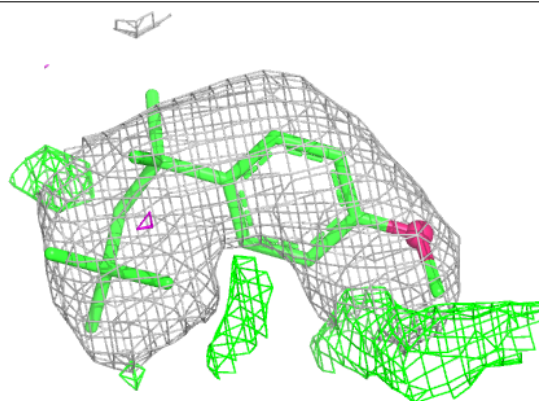


Electron density around TRT B 601:

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

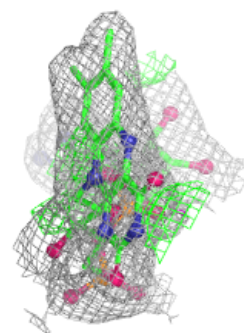
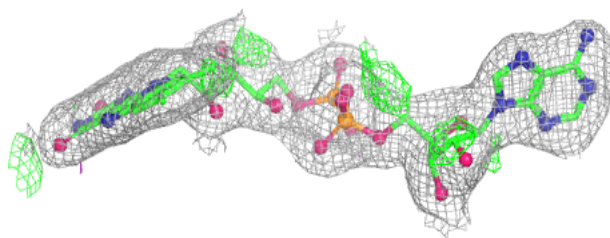
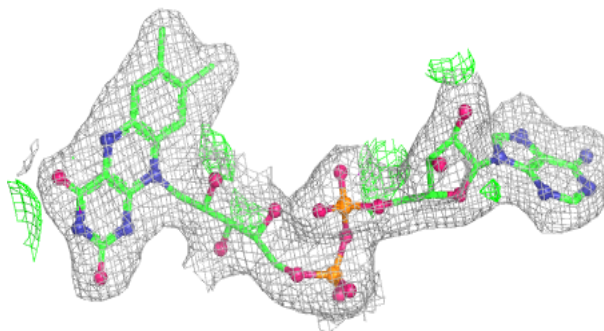
**Electron density around TRT A 601:**

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

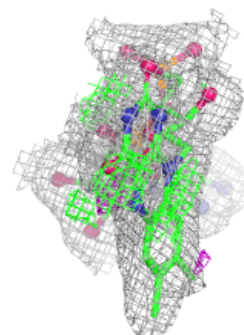
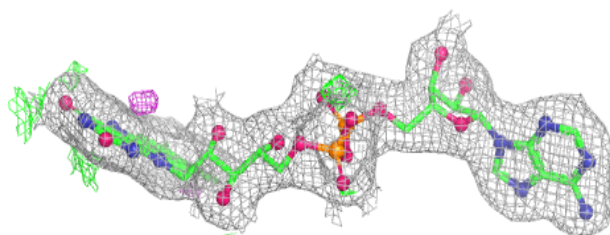
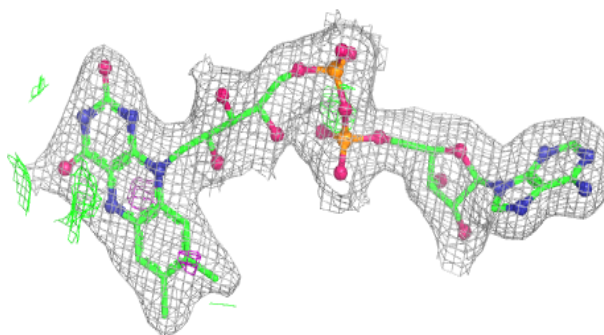


Electron density around FAD B 607:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.