Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:57 AM EDT

PDB ID	:	4G73
Title	:	Crystal structure of NDH with NADH and Quinone
Authors	:	Li, W.; Feng, Y.; Ge, J.; Yang, M.
Deposited on	:	2012-07-19
Resolution	:	2.52 Å(reported)

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

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

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

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

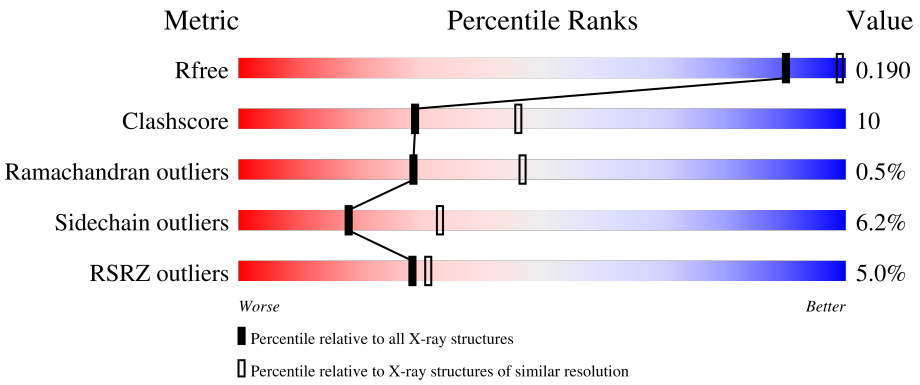
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	502	4% 77% 15% • 6%
1	B	502	6% 77% 16% • 6%

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	601	-	X	-	-
2	UQ5	A	602	-	X	-	-
2	UQ5	A	604	-	-	X	X
2	UQ5	B	604	-	X	-	-
2	UQ5	B	605	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8170 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.

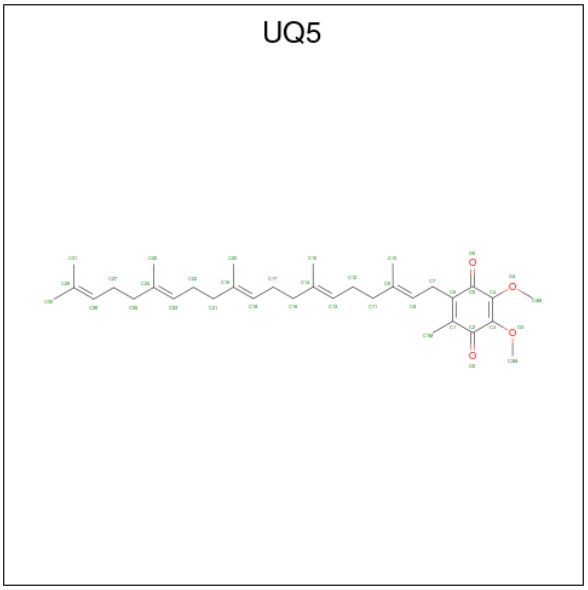
- Molecule 1 is a protein called Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3738	2415	635	683	5	0	0	0
1	B	472	3738	2415	635	683	5	0	0	0

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 (three-letter code: UQ5) (formula: $C_{34}H_{50}O_4$).



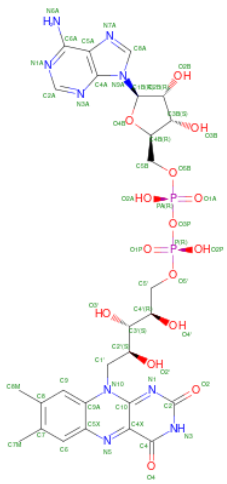
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 24 20 4	0	0
2	B	1	Total C 20 20	0	0
2	B	1	Total C O 28 24 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

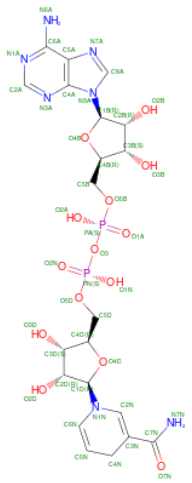
FAD



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

- Molecule 5 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

NAI



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	44	21	7	14	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	44	21	7	14	2	0	0

- Molecule 6 is water.

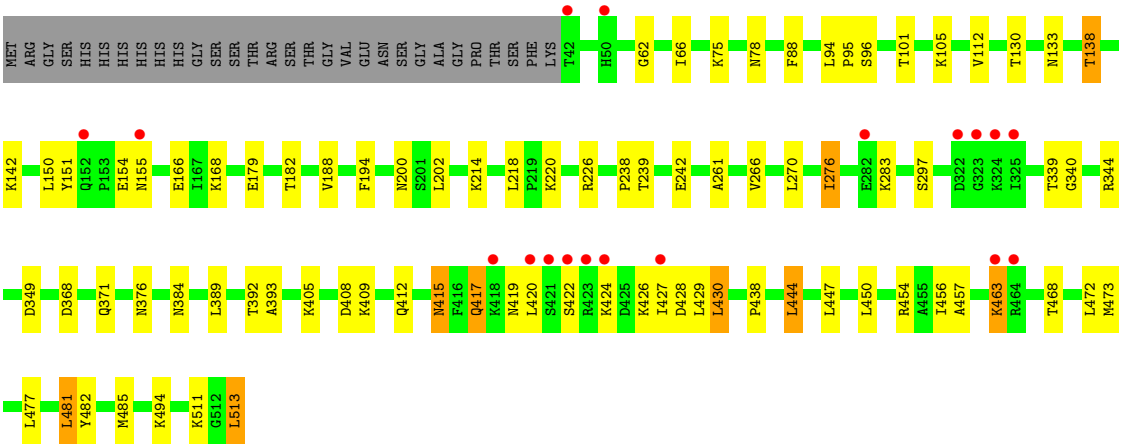
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	198	198	198	0	0
			Total	O		
6	B	189	189	189	0	0

3 Residue-property plots (i)

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

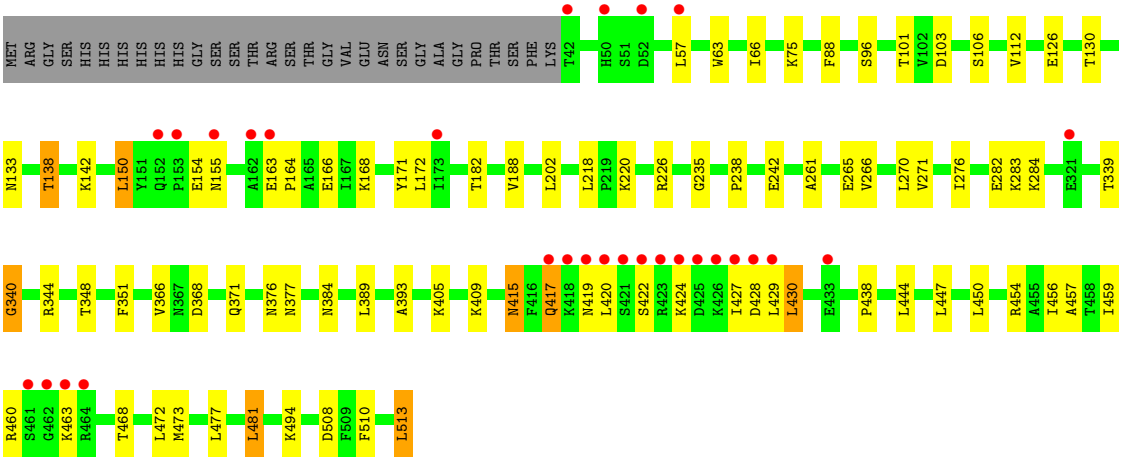
• Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	127.41Å 230.19Å 112.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.36 – 2.52 29.62 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.36-2.52) 99.7 (29.62-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.189 , 0.217 0.189 , 0.190	Depositor DCC
R_{free} test set	3094 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 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	8170	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.55	0/3824	0.73	9/5177 (0.2%)
1	B	0.56	0/3824	0.80	9/5177 (0.2%)
All	All	0.56	0/7648	0.76	18/10354 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	454	ARG	NE-CZ-NH2	-17.13	111.73	120.30
1	B	454	ARG	NE-CZ-NH1	15.86	128.23	120.30
1	B	344	ARG	NE-CZ-NH2	-14.22	113.19	120.30
1	B	344	ARG	NE-CZ-NH1	13.07	126.83	120.30
1	A	226	ARG	NE-CZ-NH2	11.74	126.17	120.30
1	A	226	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	B	226	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	A	454	ARG	NE-CZ-NH1	-11.45	114.58	120.30
1	B	226	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	A	344	ARG	NE-CZ-NH1	-11.14	114.73	120.30
1	A	454	ARG	NE-CZ-NH2	11.01	125.80	120.30
1	A	344	ARG	NE-CZ-NH2	10.32	125.46	120.30
1	B	454	ARG	CD-NE-CZ	7.53	134.14	123.60
1	B	344	ARG	CD-NE-CZ	6.47	132.66	123.60
1	B	226	ARG	CD-NE-CZ	6.18	132.26	123.60
1	A	226	ARG	CD-NE-CZ	6.04	132.05	123.60
1	A	454	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	344	ARG	CD-NE-CZ	5.27	130.98	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3738	0	3803	64	0
1	B	3738	0	3803	61	0
2	A	54	0	62	27	0
2	B	48	0	56	23	0
3	A	5	0	0	0	0
3	B	6	0	0	0	0
4	A	53	0	31	5	0
4	B	53	0	31	4	0
5	A	44	0	27	4	0
5	B	44	0	27	6	0
6	A	198	0	0	9	0
6	B	189	0	0	15	0
All	All	8170	0	7840	150	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 10.

All (150) 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:605:UQ5:C1M	2:B:605:UQ5:H112	1.41	1.47
2:B:605:UQ5:C11	2:B:605:UQ5:H1M1	1.52	1.37
1:A:393:ALA:CB	2:A:604:UQ5:H4M1	1.65	1.25
1:A:393:ALA:CB	2:A:604:UQ5:C4M	2.24	1.15
1:A:393:ALA:HB1	2:A:604:UQ5:H4M1	1.25	1.11
1:A:393:ALA:HB3	2:A:604:UQ5:C4M	1.84	1.07
2:A:604:UQ5:C1M	2:A:604:UQ5:H121	1.87	1.04
1:A:393:ALA:HB1	2:A:604:UQ5:C4M	1.91	0.97
2:A:604:UQ5:H121	2:A:604:UQ5:H1M1	1.46	0.97
1:A:214:LYS:NZ	6:A:795:HOH:O	2.01	0.92
1:B:368:ASP:HB3	1:B:438:PRO:HB3	1.57	0.87
1:A:368:ASP:HB3	1:A:438:PRO:HB3	1.57	0.86
2:B:605:UQ5:H1M1	2:B:605:UQ5:C8	2.05	0.84
2:B:605:UQ5:C1M	2:B:605:UQ5:C11	2.30	0.84
1:B:238:PRO:HB2	5:B:603:NAI:H42N	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:UQ5:H1M1	2:B:605:UQ5:C9	2.09	0.83
1:A:393:ALA:HB3	2:A:604:UQ5:H4M2	1.60	0.83
2:A:604:UQ5:H1M1	2:A:604:UQ5:C8	2.09	0.82
2:B:605:UQ5:H112	2:B:605:UQ5:H1M1	0.84	0.82
1:A:238:PRO:HB2	5:A:610:NAI:H42N	1.60	0.81
1:A:393:ALA:CB	2:A:604:UQ5:H4M2	2.09	0.81
1:B:459:ILE:HD12	2:B:605:UQ5:H101	1.64	0.80
1:A:78:ASN:ND2	6:A:845:HOH:O	2.07	0.79
1:A:349:ASP:OD2	6:A:805:HOH:O	1.99	0.79
2:A:604:UQ5:H1M1	2:A:604:UQ5:C12	2.15	0.77
1:A:463:LYS:NZ	6:A:893:HOH:O	2.18	0.76
1:B:393:ALA:CB	2:B:605:UQ5:H4M1	2.16	0.75
2:B:605:UQ5:H112	2:B:605:UQ5:H1M2	1.65	0.75
1:B:377:ASN:OD1	6:B:702:HOH:O	2.05	0.75
5:B:603:NAI:H4N	6:B:889:HOH:O	1.87	0.75
1:B:138:THR:HG21	1:B:166:GLU:OE1	1.87	0.74
1:A:485:MET:HE1	2:A:604:UQ5:H72	1.69	0.74
1:B:510:PHE:O	6:B:859:HOH:O	2.05	0.74
1:B:366:VAL:O	6:B:810:HOH:O	2.07	0.73
1:B:271:VAL:HG12	5:B:603:NAI:H2A	1.71	0.72
1:B:282:GLU:OE1	6:B:718:HOH:O	2.07	0.72
2:B:605:UQ5:H3M2	2:B:605:UQ5:O2	1.89	0.71
1:A:138:THR:HG21	1:A:166:GLU:OE1	1.90	0.71
2:B:605:UQ5:C4M	2:B:605:UQ5:O3	2.38	0.71
1:B:513:LEU:O	6:B:859:HOH:O	2.08	0.70
1:B:265:GLU:OE2	6:B:767:HOH:O	2.09	0.70
2:A:604:UQ5:H3M2	2:A:604:UQ5:O2	1.92	0.69
1:A:393:ALA:HB3	2:A:604:UQ5:H4M1	1.47	0.67
1:A:151:TYR:OH	6:A:825:HOH:O	2.12	0.66
1:B:126:GLU:OE1	6:B:728:HOH:O	2.13	0.66
1:A:485:MET:CE	2:A:604:UQ5:H72	2.26	0.65
2:A:604:UQ5:H1M1	2:A:604:UQ5:C11	2.26	0.65
1:B:282:GLU:OE2	6:B:779:HOH:O	2.14	0.64
1:A:485:MET:SD	2:A:604:UQ5:C6	2.85	0.64
1:B:133:ASN:HB2	1:B:138:THR:HG22	1.78	0.64
1:B:238:PRO:HB2	5:B:603:NAI:C4N	2.28	0.63
1:B:393:ALA:HB1	2:B:605:UQ5:H4M1	1.80	0.63
1:A:133:ASN:HB2	1:A:138:THR:HG22	1.82	0.61
1:A:371:GLN:HE21	1:A:376:ASN:HA	1.65	0.61
1:A:238:PRO:HB2	5:A:610:NAI:C4N	2.30	0.61
1:B:393:ALA:HB3	2:B:605:UQ5:H4M1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:UQ5:O2	2:B:605:UQ5:C3M	2.50	0.60
1:A:447:LEU:CD1	2:A:604:UQ5:H103	2.31	0.59
1:B:130:THR:HG21	1:B:142:LYS:HG3	1.83	0.59
1:B:371:GLN:HE21	1:B:376:ASN:HA	1.68	0.58
1:A:405:LYS:HE2	1:A:409:LYS:HE3	1.85	0.58
1:B:282:GLU:CD	6:B:779:HOH:O	2.42	0.58
1:A:130:THR:HG21	1:A:142:LYS:HG3	1.85	0.57
1:B:419:ASN:ND2	1:B:424:LYS:O	2.28	0.57
1:A:419:ASN:ND2	1:A:424:LYS:O	2.28	0.57
1:B:508:ASP:OD1	6:B:788:HOH:O	2.16	0.57
1:B:63:TRP:HB2	4:B:606:FAD:H5'2	1.85	0.56
1:B:393:ALA:CB	2:B:605:UQ5:C4M	2.84	0.56
1:B:393:ALA:HB3	2:B:605:UQ5:C4M	2.36	0.55
1:A:482:TYR:OH	5:A:610:NAI:N7N	2.39	0.55
1:A:393:ALA:C	2:A:604:UQ5:H4M2	2.27	0.55
2:B:605:UQ5:O3	2:B:605:UQ5:H4M2	2.06	0.54
1:A:349:ASP:OD1	6:A:863:HOH:O	2.19	0.53
1:A:485:MET:SD	2:A:604:UQ5:C5	2.97	0.53
1:B:405:LYS:HE2	1:B:409:LYS:HE3	1.91	0.53
1:A:447:LEU:HD12	2:A:604:UQ5:H103	1.91	0.52
2:A:604:UQ5:C1M	2:A:604:UQ5:C8	2.86	0.52
1:B:508:ASP:OD2	6:B:821:HOH:O	2.19	0.52
4:B:606:FAD:O4'	4:B:606:FAD:PA	2.68	0.52
2:A:604:UQ5:O2	2:A:604:UQ5:C3M	2.57	0.51
1:A:415:ASN:OD1	1:A:415:ASN:N	2.43	0.51
1:A:392:THR:HB	4:A:605:FAD:O2	2.10	0.50
1:B:182:THR:HG22	1:B:188:VAL:HG22	1.93	0.50
1:B:419:ASN:HA	1:B:422:SER:HB3	1.93	0.50
1:A:412:GLN:NE2	6:A:775:HOH:O	2.44	0.50
1:B:284:LYS:NZ	6:B:779:HOH:O	2.25	0.50
1:B:415:ASN:N	1:B:415:ASN:OD1	2.44	0.50
2:B:605:UQ5:O3	2:B:605:UQ5:H4M3	2.12	0.50
1:B:477:LEU:HG	1:B:481:LEU:HD22	1.95	0.49
4:B:606:FAD:O4'	4:B:606:FAD:O2A	2.30	0.49
1:A:220:LYS:HE3	1:A:261:ALA:HB1	1.95	0.49
1:B:150:LEU:O	6:B:861:HOH:O	2.19	0.49
1:B:457:ALA:O	1:B:468:THR:HA	2.12	0.49
2:A:604:UQ5:O3	2:A:604:UQ5:H4M3	2.12	0.48
1:B:419:ASN:OD1	1:B:427:ILE:HG13	2.13	0.48
1:B:66:ILE:HG13	1:B:88:PHE:HB2	1.95	0.48
1:A:447:LEU:HD11	2:A:604:UQ5:H103	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.95	0.48
1:A:419:ASN:OD1	1:A:427:ILE:HG13	2.14	0.48
2:A:604:UQ5:H121	2:A:604:UQ5:H1M2	1.87	0.48
1:A:96:SER:HB3	1:A:101:THR:HB	1.96	0.47
1:A:419:ASN:HA	1:A:422:SER:HB3	1.95	0.47
1:A:62:GLY:HA3	4:A:605:FAD:O5B	2.15	0.47
1:A:426:LYS:HB3	1:A:426:LYS:HE2	1.77	0.47
2:B:605:UQ5:C1M	2:B:605:UQ5:C8	2.83	0.47
1:B:63:TRP:CH2	2:B:605:UQ5:H4M3	2.50	0.47
1:B:447:LEU:HD11	2:B:605:UQ5:H103	1.97	0.46
1:B:459:ILE:CD1	2:B:605:UQ5:H101	2.41	0.46
1:B:96:SER:HB3	1:B:101:THR:HB	1.97	0.46
1:A:75:LYS:HE3	1:A:75:LYS:HB2	1.79	0.45
1:A:450:LEU:HD11	1:A:456:ILE:HG23	1.99	0.45
1:B:417:GLN:HA	1:B:420:LEU:HD22	1.99	0.45
1:B:220:LYS:HE3	1:B:261:ALA:HB1	1.98	0.45
1:B:63:TRP:CD1	4:B:606:FAD:H4'	2.52	0.45
1:B:450:LEU:HD11	1:B:456:ILE:HG23	1.99	0.45
1:B:348:THR:O	1:B:351:PHE:HB2	2.17	0.44
1:B:460:ARG:HD3	6:B:840:HOH:O	2.16	0.44
1:A:95:PRO:HD3	4:A:605:FAD:HM72	2.00	0.44
1:B:57:LEU:O	1:B:172:LEU:HD12	2.17	0.44
1:A:444:LEU:HB3	2:A:604:UQ5:H122	1.99	0.44
1:B:171:TYR:CZ	1:B:420:LEU:HD11	2.53	0.43
1:A:179:GLU:OE1	6:A:771:HOH:O	2.21	0.43
1:B:238:PRO:O	1:B:242:GLU:HG3	2.18	0.43
1:A:66:ILE:HG13	1:A:88:PHE:HB2	2.00	0.43
1:B:481:LEU:HD12	1:B:481:LEU:HA	1.85	0.43
1:B:513:LEU:HD13	1:B:513:LEU:HA	1.71	0.43
1:A:405:LYS:O	1:A:408:ASP:HB2	2.19	0.42
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.80	0.42
1:A:239:THR:OG1	5:A:610:NAI:H5N	2.19	0.42
1:A:276:ILE:H	1:A:276:ILE:HD13	1.83	0.42
1:A:194:PHE:O	1:A:200:ASN:HB3	2.19	0.42
1:A:417:GLN:HA	1:A:420:LEU:HD22	2.02	0.42
1:A:511:LYS:NZ	6:A:866:HOH:O	1.96	0.42
1:A:105:LYS:NZ	1:B:103:ASP:OD1	2.44	0.41
1:A:238:PRO:O	1:A:242:GLU:HG3	2.21	0.41
1:A:133:ASN:OD1	1:A:138:THR:HG22	2.21	0.41
1:A:94:LEU:HB3	4:A:605:FAD:HM72	2.02	0.41
1:B:163:GLU:HA	1:B:164:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLY:HA2	5:B:603:NAI:O2N	2.20	0.41
1:A:513:LEU:HD13	1:A:513:LEU:HA	1.71	0.41
4:A:605:FAD:H9	4:A:605:FAD:H1'1	1.84	0.41
1:B:75:LYS:HE3	1:B:75:LYS:HB2	1.78	0.41
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.91	0.40
1:A:182:THR:HG22	1:A:188:VAL:HG22	2.02	0.40
1:B:235:GLY:HA2	5:B:603:NAI:O4B	2.20	0.40
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.92	0.40
1:B:106:SER:HA	1:B:494:LYS:HD3	2.02	0.40
1:B:393:ALA:HB1	2:B:605:UQ5:C4M	2.46	0.40
1:A:457:ALA:O	1:A:468:THR:HA	2.22	0.40
1:A:494:LYS:HE3	1:B:508:ASP:OD1	2.21	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	470/502 (94%)	453 (96%)	14 (3%)	3 (1%)	25 41
1	B	470/502 (94%)	454 (97%)	14 (3%)	2 (0%)	34 53
All	All	940/1004 (94%)	907 (96%)	28 (3%)	5 (0%)	29 47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	GLY
1	B	340	GLY
1	A	154	GLU
1	A	297	SER
1	B	154	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	403/427 (94%)	378 (94%)	25 (6%)	18	33
1	B	403/427 (94%)	378 (94%)	25 (6%)	18	33
All	All	806/854 (94%)	756 (94%)	50 (6%)	18	33

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	138	THR
1	A	150	LEU
1	A	155	ASN
1	A	168	LYS
1	A	202	LEU
1	A	218	LEU
1	A	266	VAL
1	A	270	LEU
1	A	276	ILE
1	A	283	LYS
1	A	339	THR
1	A	384	ASN
1	A	389	LEU
1	A	415	ASN
1	A	417	GLN
1	A	428	ASP
1	A	429	LEU
1	A	430	LEU
1	A	444	LEU
1	A	463	LYS
1	A	472	LEU
1	A	473	MET
1	A	481	LEU
1	A	513	LEU
1	B	112	VAL
1	B	138	THR

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Mol	Chain	Res	Type
1	B	150	LEU
1	B	155	ASN
1	B	168	LYS
1	B	202	LEU
1	B	218	LEU
1	B	266	VAL
1	B	270	LEU
1	B	276	ILE
1	B	283	LYS
1	B	339	THR
1	B	384	ASN
1	B	389	LEU
1	B	415	ASN
1	B	417	GLN
1	B	428	ASP
1	B	429	LEU
1	B	430	LEU
1	B	444	LEU
1	B	463	LYS
1	B	472	LEU
1	B	473	MET
1	B	481	LEU
1	B	513	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	377	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 11 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
4	FAD	B	606	3	54,58,58	1.27	4 (7%)	71,89,89	1.24	7 (9%)
2	UQ5	A	602	-	9,9,38	3.44	2 (22%)	9,10,49	2.72	8 (88%)
2	UQ5	A	601	-	19,19,38	4.37	5 (26%)	18,22,49	3.24	13 (72%)
5	NAI	B	603	-	43,48,48	2.36	10 (23%)	50,73,73	1.85	11 (22%)
2	UQ5	B	605	-	28,28,38	3.54	11 (39%)	36,37,49	2.41	14 (38%)
4	FAD	A	605	3	54,58,58	1.27	4 (7%)	71,89,89	1.23	7 (9%)
2	UQ5	B	604	-	19,19,38	4.30	4 (21%)	18,22,49	3.18	12 (66%)
5	NAI	A	610	-	43,48,48	2.24	11 (25%)	50,73,73	1.64	7 (14%)
2	UQ5	A	604	-	24,24,38	3.47	10 (41%)	30,32,49	2.53	10 (33%)

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	FAD	B	606	3	-	14/30/50/50	0/6/6/6
2	UQ5	A	602	-	-	6/8/8/57	-
2	UQ5	A	601	-	-	12/20/20/57	-
5	NAI	B	603	-	-	7/25/72/72	0/5/5/5
2	UQ5	B	605	-	-	13/21/45/57	0/1/1/1
4	FAD	A	605	3	-	1/30/50/50	0/6/6/6
2	UQ5	B	604	-	-	13/20/20/57	-
5	NAI	A	610	-	-	7/25/72/72	0/5/5/5
2	UQ5	A	604	-	-	11/17/41/57	0/1/1/1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	UQ5	C13-C14	10.10	1.56	1.33
5	B	603	NAI	PA-O3	-9.99	1.48	1.59
2	B	604	UQ5	C13-C14	9.74	1.55	1.33
2	A	601	UQ5	C6-C1	9.63	1.55	1.33
2	B	604	UQ5	C8-C9	9.52	1.55	1.33
2	B	604	UQ5	C6-C1	9.50	1.54	1.33
5	A	610	NAI	PA-O3	-9.45	1.49	1.59
2	A	601	UQ5	C8-C9	9.34	1.54	1.33
2	B	605	UQ5	C13-C14	8.93	1.53	1.33
2	A	604	UQ5	C13-C14	8.90	1.53	1.33
2	A	604	UQ5	C8-C9	8.28	1.52	1.33
2	B	605	UQ5	C8-C9	8.26	1.52	1.33
2	A	602	UQ5	C13-C14	7.51	1.54	1.32
2	A	601	UQ5	C18-C19	7.51	1.54	1.32
2	B	605	UQ5	C18-C19	7.47	1.54	1.32
2	B	604	UQ5	C18-C19	7.36	1.54	1.32
2	A	604	UQ5	O5-C5	6.52	1.38	1.23
2	B	605	UQ5	O5-C5	6.47	1.37	1.23
2	B	605	UQ5	O2-C2	6.46	1.37	1.23
2	A	602	UQ5	C8-C9	6.44	1.53	1.33
2	A	604	UQ5	O2-C2	6.41	1.37	1.23
4	B	606	FAD	C9A-C5X	5.09	1.49	1.41
4	A	605	FAD	C9A-C5X	5.03	1.49	1.41
5	B	603	NAI	C7N-N7N	4.89	1.47	1.33
5	A	610	NAI	C7N-N7N	4.62	1.46	1.33
5	A	610	NAI	C4N-C3N	-3.92	1.42	1.50
5	B	603	NAI	C4N-C3N	-3.90	1.42	1.50
5	A	610	NAI	C2A-N3A	3.72	1.37	1.32
2	B	605	UQ5	C6-C1	3.59	1.41	1.35
2	A	604	UQ5	C6-C1	3.55	1.41	1.35
4	B	606	FAD	C8-C7	3.34	1.49	1.40
4	A	605	FAD	C8-C7	3.32	1.48	1.40
5	B	603	NAI	C2A-N3A	3.02	1.36	1.32
5	B	603	NAI	C2A-N1A	2.97	1.39	1.33
5	B	603	NAI	C6A-N6A	2.92	1.44	1.34
2	B	605	UQ5	C3-C2	-2.92	1.40	1.48
2	A	604	UQ5	C3-C2	-2.89	1.40	1.48
2	B	605	UQ5	O4-C4M	-2.84	1.39	1.45
4	B	606	FAD	C5X-N5	-2.84	1.34	1.39
5	A	610	NAI	C6A-N6A	2.84	1.44	1.34
2	A	604	UQ5	O4-C4M	-2.82	1.39	1.45
5	B	603	NAI	PA-O5B	-2.81	1.48	1.59
5	B	603	NAI	C4N-C5N	-2.78	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	FAD	C5X-N5	-2.78	1.34	1.39
5	A	610	NAI	C4N-C5N	-2.69	1.42	1.49
5	B	603	NAI	C6N-C5N	2.67	1.41	1.33
2	B	605	UQ5	C4-C5	-2.66	1.41	1.48
2	A	604	UQ5	C4-C5	-2.62	1.41	1.48
4	A	605	FAD	C4-N3	-2.58	1.34	1.38
4	B	606	FAD	C4-N3	-2.58	1.34	1.38
5	B	603	NAI	C2N-C3N	2.53	1.42	1.35
5	A	610	NAI	C2N-C3N	2.44	1.41	1.35
5	A	610	NAI	C6N-C5N	2.42	1.40	1.33
5	A	610	NAI	PA-O5B	-2.39	1.50	1.59
5	A	610	NAI	C2A-N1A	2.31	1.38	1.33
5	A	610	NAI	C6N-N1N	2.26	1.42	1.37
2	B	605	UQ5	C6-C5	-2.24	1.40	1.46
2	A	601	UQ5	C16-C14	2.23	1.55	1.51
2	A	604	UQ5	C6-C5	-2.18	1.40	1.46
2	B	605	UQ5	O3-C3M	-2.11	1.40	1.45
2	A	604	UQ5	O3-C3M	-2.08	1.40	1.45

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	603	NAI	N3A-C2A-N1A	-6.79	119.45	128.67
2	A	604	UQ5	C15-C14-C16	-6.00	109.06	116.13
5	A	610	NAI	N3A-C2A-N1A	-5.89	120.67	128.67
2	A	604	UQ5	C10-C9-C8	-5.54	109.41	123.63
2	B	605	UQ5	C10-C9-C8	-5.52	109.45	123.63
2	A	601	UQ5	C1M-C1-C2	-5.48	109.68	116.13
2	B	604	UQ5	C1M-C1-C6	-5.34	109.92	123.63
2	A	604	UQ5	C7-C8-C9	-5.27	117.75	126.83
2	B	605	UQ5	C7-C8-C9	-5.25	117.78	126.83
2	A	601	UQ5	C10-C9-C8	-5.25	110.14	123.63
2	A	601	UQ5	C1M-C1-C6	-4.90	111.05	123.63
2	A	604	UQ5	C15-C14-C13	-4.84	111.19	123.63
2	B	605	UQ5	C15-C14-C13	-4.82	111.26	123.63
5	B	603	NAI	O2A-PA-O3	-4.49	95.12	107.27
2	B	604	UQ5	C10-C9-C8	-4.36	112.43	123.63
2	B	605	UQ5	C12-C13-C14	-4.33	117.71	127.62
2	A	604	UQ5	C12-C13-C14	-4.32	117.73	127.62
2	B	604	UQ5	C1M-C1-C2	-4.29	111.07	116.13
2	A	601	UQ5	C15-C14-C13	-4.28	112.65	123.63
2	B	604	UQ5	C10-C9-C11	-4.10	108.11	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	604	UQ5	C15-C14-C13	-3.84	113.76	123.63
2	A	601	UQ5	C10-C9-C11	-3.81	108.61	115.23
4	A	605	FAD	N3A-C2A-N1A	-3.80	123.51	128.67
4	B	606	FAD	N3A-C2A-N1A	-3.76	123.57	128.67
2	B	605	UQ5	C16-C14-C13	-3.74	112.77	121.17
2	B	604	UQ5	C20-C19-C18	-3.71	111.54	122.66
5	A	610	NAI	O2A-PA-O3	-3.64	97.43	107.27
2	B	604	UQ5	C11-C9-C8	-3.61	113.06	121.17
2	B	605	UQ5	C15-C14-C16	-3.59	109.00	115.23
2	A	601	UQ5	C20-C19-C18	-3.56	111.96	122.66
2	A	604	UQ5	C11-C9-C8	-3.55	113.20	121.17
2	B	605	UQ5	C11-C9-C8	-3.38	113.59	121.17
2	B	604	UQ5	C16-C14-C13	-3.33	113.69	121.17
5	B	603	NAI	O4D-C1D-N1N	3.31	114.40	108.08
5	A	610	NAI	O3-PA-O1A	3.31	120.66	110.70
2	A	602	UQ5	C15-C14-C13	-3.27	112.84	122.66
2	B	604	UQ5	C21-C19-C18	-3.21	113.03	122.66
5	A	610	NAI	C3N-C2N-N1N	-3.20	118.50	123.20
2	A	601	UQ5	C11-C9-C8	-3.19	114.01	121.17
5	B	603	NAI	O3-PA-O1A	3.19	120.29	110.70
2	A	602	UQ5	C10-C9-C11	-3.18	109.71	115.23
2	B	604	UQ5	C12-C13-C14	-3.16	120.39	127.62
2	A	602	UQ5	C11-C9-C8	-3.13	113.42	120.36
2	B	604	UQ5	C17-C18-C19	-3.10	117.30	127.64
2	A	602	UQ5	C16-C14-C13	-3.09	113.38	122.66
2	A	601	UQ5	C21-C19-C18	-2.99	113.69	122.66
2	B	605	UQ5	C17-C18-C19	-2.97	117.75	127.64
2	B	605	UQ5	C20-C19-C18	-2.95	113.82	122.66
5	B	603	NAI	O4B-C1B-N9A	2.94	112.65	108.75
4	A	605	FAD	C4-C4X-N5	2.94	122.27	118.21
2	B	605	UQ5	C21-C19-C18	-2.94	113.83	122.66
2	A	604	UQ5	C10-C9-C11	-2.94	110.13	115.23
2	B	605	UQ5	C10-C9-C11	-2.92	110.16	115.23
2	A	602	UQ5	C12-C13-C14	-2.86	118.11	127.64
2	A	601	UQ5	C12-C13-C14	-2.84	121.11	127.62
2	B	605	UQ5	C7-C6-C1	-2.78	120.13	124.89
2	A	604	UQ5	C7-C6-C1	-2.73	120.20	124.89
4	A	605	FAD	C4A-C5A-N7A	-2.70	106.48	109.34
2	A	604	UQ5	C1M-C1-C6	-2.68	120.05	124.45
4	B	606	FAD	C4-C4X-N5	2.68	121.91	118.21
4	B	606	FAD	C4A-C5A-N7A	-2.68	106.51	109.34
2	A	601	UQ5	C16-C14-C13	-2.60	115.34	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	605	UQ5	C1M-C1-C6	-2.59	120.19	124.45
5	A	610	NAI	C4B-O4B-C1B	-2.58	107.57	109.92
5	B	603	NAI	O2A-PA-O5B	-2.57	95.92	107.57
2	A	602	UQ5	C7-C8-C9	-2.53	120.68	126.44
5	B	603	NAI	O5B-PA-O1A	2.48	118.76	108.94
4	B	606	FAD	C4X-C10-N1	-2.39	118.72	124.59
2	B	604	UQ5	C12-C11-C9	2.37	121.03	113.19
4	A	605	FAD	C4X-C10-N1	-2.32	118.90	124.59
2	A	604	UQ5	C8-C7-C6	2.32	117.80	112.08
2	A	601	UQ5	C12-C11-C9	2.26	120.69	113.19
4	B	606	FAD	C4'-C3'-C2'	-2.26	109.81	113.57
2	B	605	UQ5	C8-C7-C6	2.25	117.63	112.08
5	B	603	NAI	C3N-C2N-N1N	-2.22	119.94	123.20
5	A	610	NAI	O4B-C4B-C3B	2.22	109.56	105.15
2	A	602	UQ5	C16-C14-C15	-2.22	109.48	114.59
2	A	601	UQ5	C21-C19-C20	-2.19	109.56	114.59
5	B	603	NAI	O4D-C4D-C5D	2.18	116.32	109.33
4	B	606	FAD	C10-N1-C2	2.17	121.55	116.85
4	A	605	FAD	C10-N1-C2	2.16	121.53	116.85
4	A	605	FAD	O4-C4-C4X	-2.13	120.90	126.53
4	B	606	FAD	O4-C4-C4X	-2.12	120.95	126.53
5	B	603	NAI	C4D-O4D-C1D	-2.11	104.80	109.47
4	A	605	FAD	C4'-C3'-C2'	-2.11	110.05	113.57
2	A	601	UQ5	C17-C18-C19	-2.10	120.64	127.64
5	A	610	NAI	C4A-C5A-N7A	-2.09	107.13	109.34
5	B	603	NAI	O4B-C4B-C3B	2.07	109.26	105.15
2	A	602	UQ5	C12-C11-C9	2.03	119.92	113.19

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	UQ5	C6-C1-C2-C3
2	A	601	UQ5	C1M-C1-C6-C7
2	A	601	UQ5	C7-C8-C9-C10
2	A	601	UQ5	C12-C13-C14-C15
2	A	601	UQ5	C12-C13-C14-C16
2	A	601	UQ5	C17-C18-C19-C21
2	A	602	UQ5	C7-C8-C9-C10
2	A	602	UQ5	C7-C8-C9-C11
2	A	604	UQ5	C7-C8-C9-C11
2	A	604	UQ5	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
2	A	604	UQ5	C13-C14-C16-C17
2	A	604	UQ5	C15-C14-C16-C17
2	B	604	UQ5	C1M-C1-C2-C3
2	B	604	UQ5	C1M-C1-C6-C7
2	B	604	UQ5	C7-C8-C9-C10
2	B	604	UQ5	C7-C8-C9-C11
2	B	604	UQ5	C12-C13-C14-C15
2	B	604	UQ5	C12-C13-C14-C16
2	B	605	UQ5	C7-C8-C9-C11
2	B	605	UQ5	C12-C13-C14-C16
4	B	606	FAD	C5B-O5B-PA-O1A
4	B	606	FAD	C2'-C3'-C4'-O4'
4	B	606	FAD	O3'-C3'-C4'-O4'
4	B	606	FAD	O3'-C3'-C4'-C5'
4	B	606	FAD	C3'-C4'-C5'-O5'
4	B	606	FAD	O4'-C4'-C5'-O5'
4	B	606	FAD	C5'-O5'-P-O1P
4	B	606	FAD	C5'-O5'-P-O2P
4	B	606	FAD	C5'-O5'-P-O3P
5	A	610	NAI	O4D-C4D-C5D-O5D
5	A	610	NAI	O4D-C1D-N1N-C2N
5	B	603	NAI	C5B-O5B-PA-O2A
2	A	602	UQ5	C12-C13-C14-C15
2	A	602	UQ5	C12-C13-C14-C16
2	B	604	UQ5	C17-C18-C19-C20
2	B	605	UQ5	C17-C18-C19-C20
2	B	605	UQ5	C13-C14-C16-C17
2	A	604	UQ5	C7-C8-C9-C10
2	B	605	UQ5	C7-C8-C9-C10
2	B	605	UQ5	C12-C13-C14-C15
2	A	601	UQ5	C17-C18-C19-C20
5	B	603	NAI	O4D-C1D-N1N-C2N
5	A	610	NAI	C3D-C4D-C5D-O5D
2	A	602	UQ5	C12-C11-C9-C8
2	B	605	UQ5	C12-C11-C9-C8
2	A	601	UQ5	C14-C16-C17-C18
2	A	602	UQ5	C9-C11-C12-C13
2	B	605	UQ5	C14-C16-C17-C18
4	B	606	FAD	C2'-C3'-C4'-C5'
2	B	605	UQ5	C4-C3-O3-C3M
5	B	603	NAI	O4B-C4B-C5B-O5B
2	B	605	UQ5	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	604	UQ5	C5-C6-C7-C8
2	B	605	UQ5	C5-C6-C7-C8
5	B	603	NAI	O4D-C4D-C5D-O5D
2	A	604	UQ5	C4-C3-O3-C3M
2	A	604	UQ5	C12-C13-C14-C15
5	B	603	NAI	C3B-C4B-C5B-O5B
2	A	604	UQ5	C1-C6-C7-C8
5	A	610	NAI	PN-O3-PA-O1A
2	B	604	UQ5	C9-C11-C12-C13
2	A	601	UQ5	C7-C8-C9-C11
4	B	606	FAD	C5B-O5B-PA-O2A
4	B	606	FAD	C5B-O5B-PA-O3P
5	A	610	NAI	C5D-O5D-PN-O3
2	A	601	UQ5	C15-C14-C16-C17
2	B	604	UQ5	C13-C14-C16-C17
2	A	604	UQ5	C12-C11-C9-C10
2	A	601	UQ5	C9-C11-C12-C13
4	B	606	FAD	P-O3P-PA-O2A
2	B	604	UQ5	C12-C11-C9-C10
4	B	606	FAD	C4'-C5'-O5'-P
2	A	604	UQ5	C5-C4-O4-C4M
2	A	601	UQ5	C1M-C1-C2-C3
5	A	610	NAI	O4B-C4B-C5B-O5B
2	B	605	UQ5	C5-C4-O4-C4M
2	B	605	UQ5	C2-C3-O3-C3M
4	A	605	FAD	O4B-C4B-C5B-O5B
2	B	604	UQ5	C2-C1-C6-C7
2	B	604	UQ5	C14-C16-C17-C18
5	A	610	NAI	PN-O3-PA-O2A
2	B	604	UQ5	C11-C12-C13-C14
5	B	603	NAI	C3D-C4D-C5D-O5D
5	B	603	NAI	PA-O3-PN-O1N

There are no ring outliers.

6 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	606	FAD	4	0
5	B	603	NAI	6	0
2	B	605	UQ5	23	0
4	A	605	FAD	5	0
5	A	610	NAI	4	0

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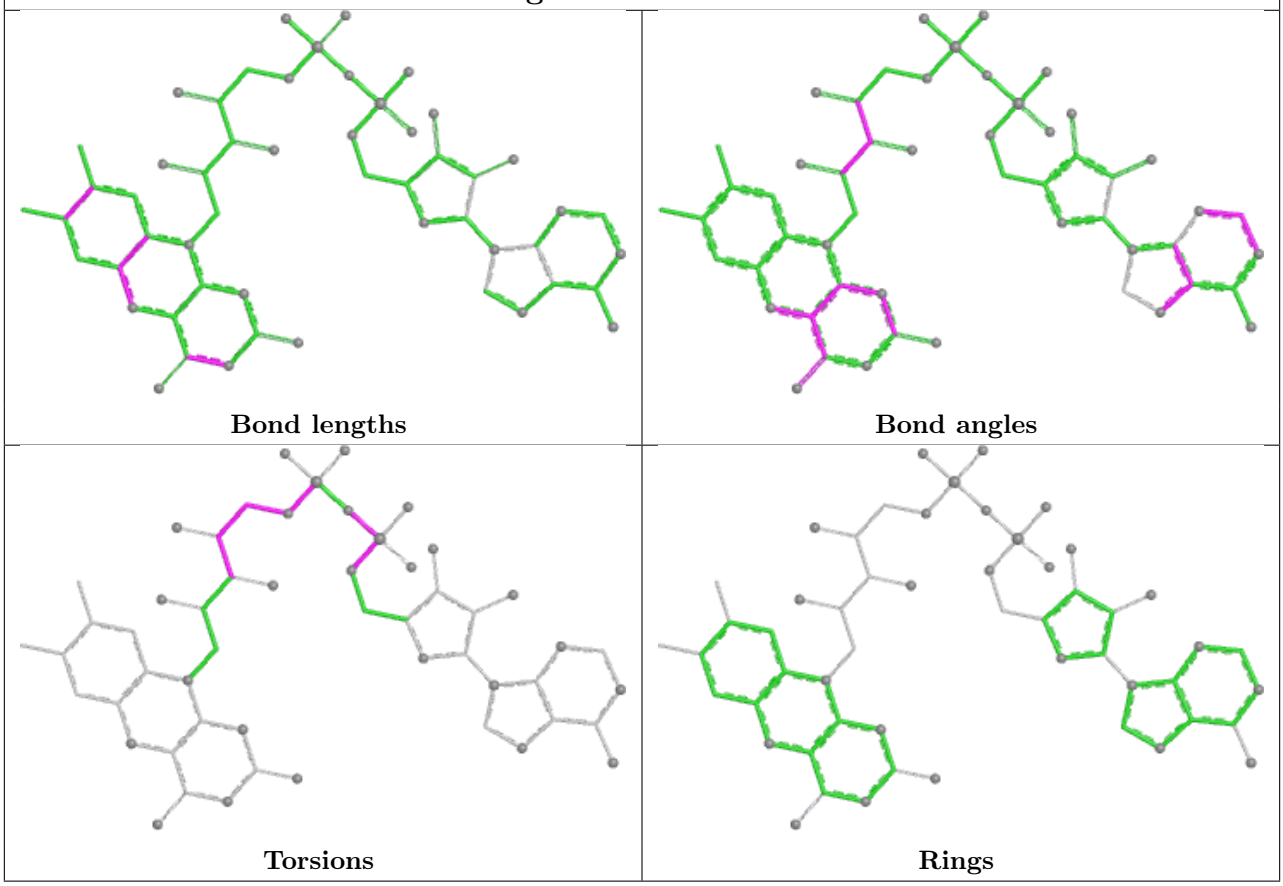
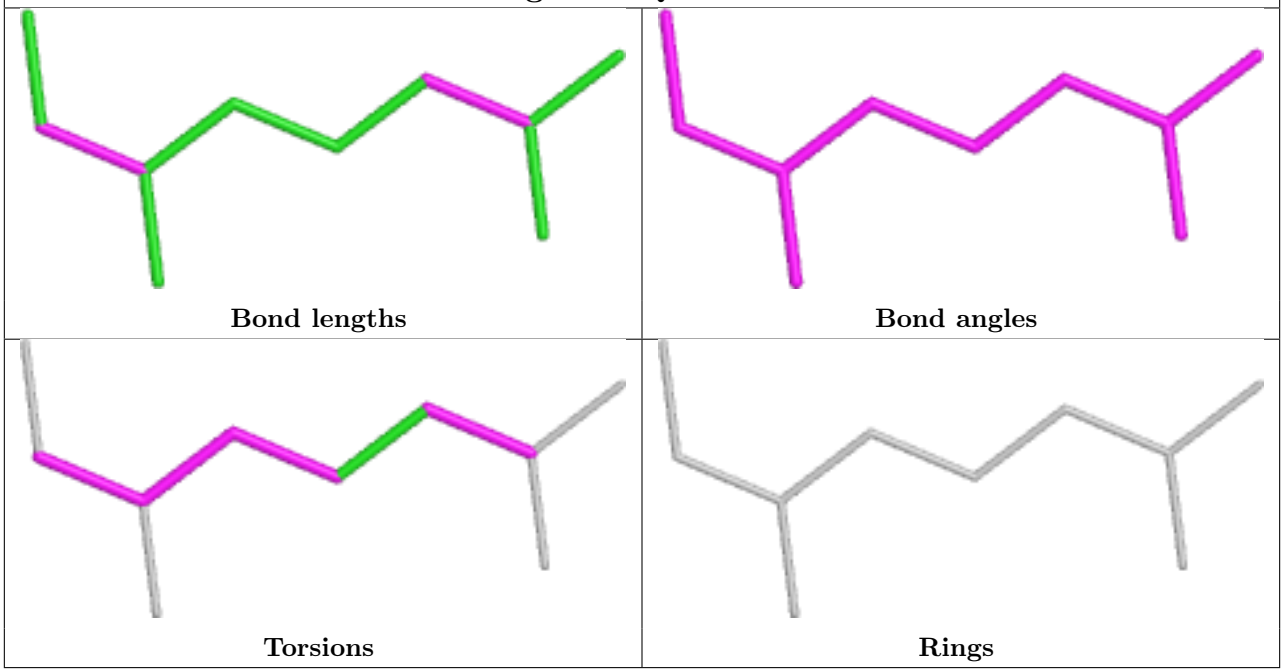
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	UQ5	27	0

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

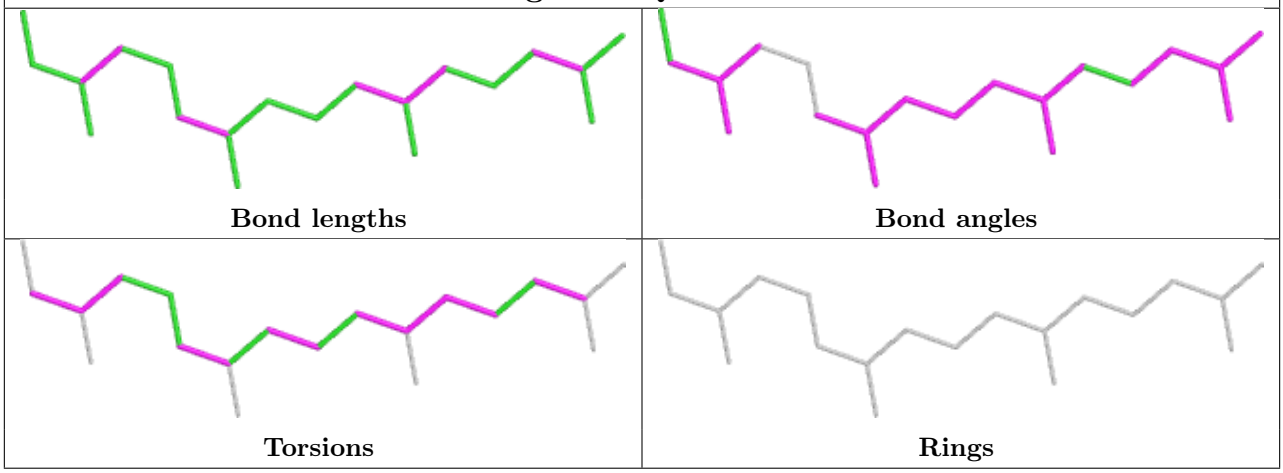
Ligand FAD B 606



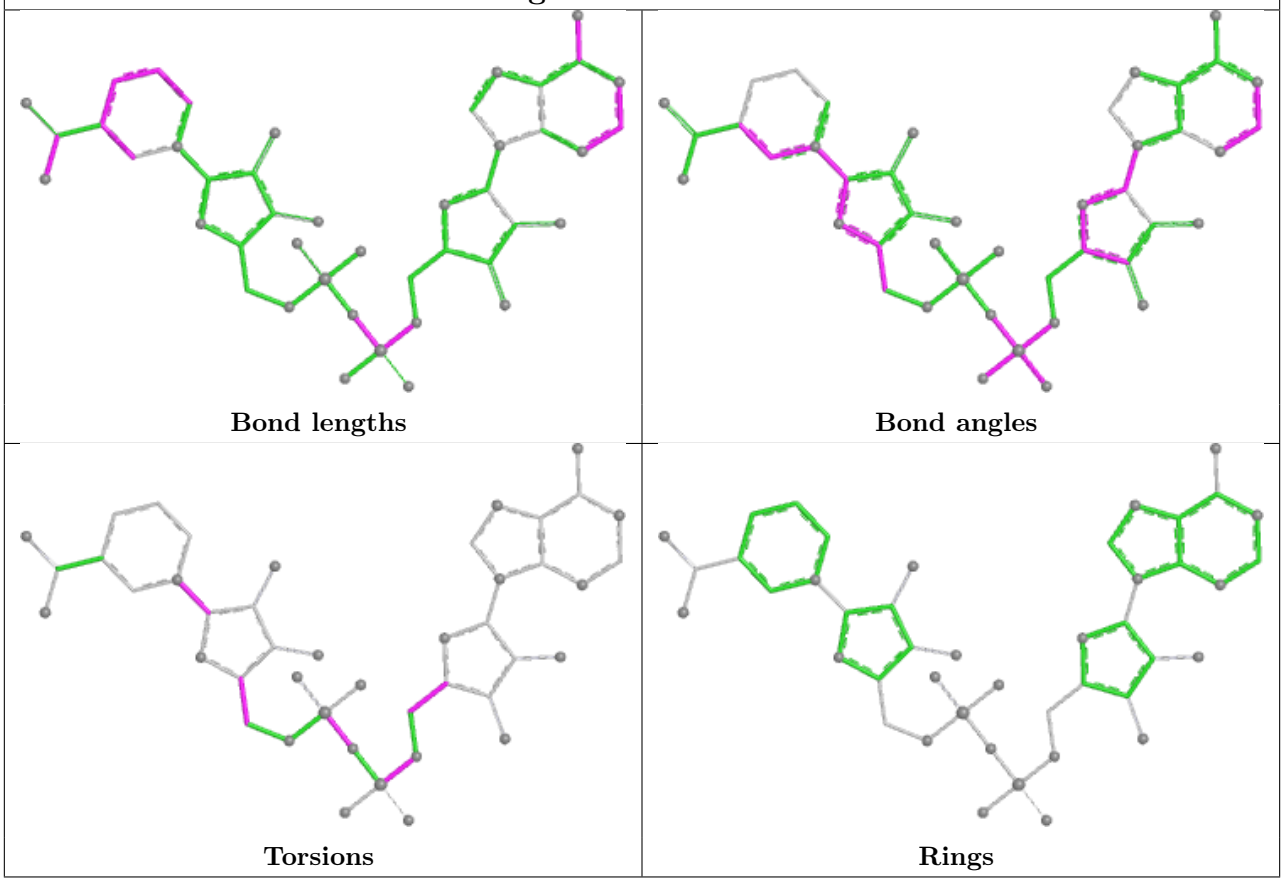
Ligand UQ5 A 602



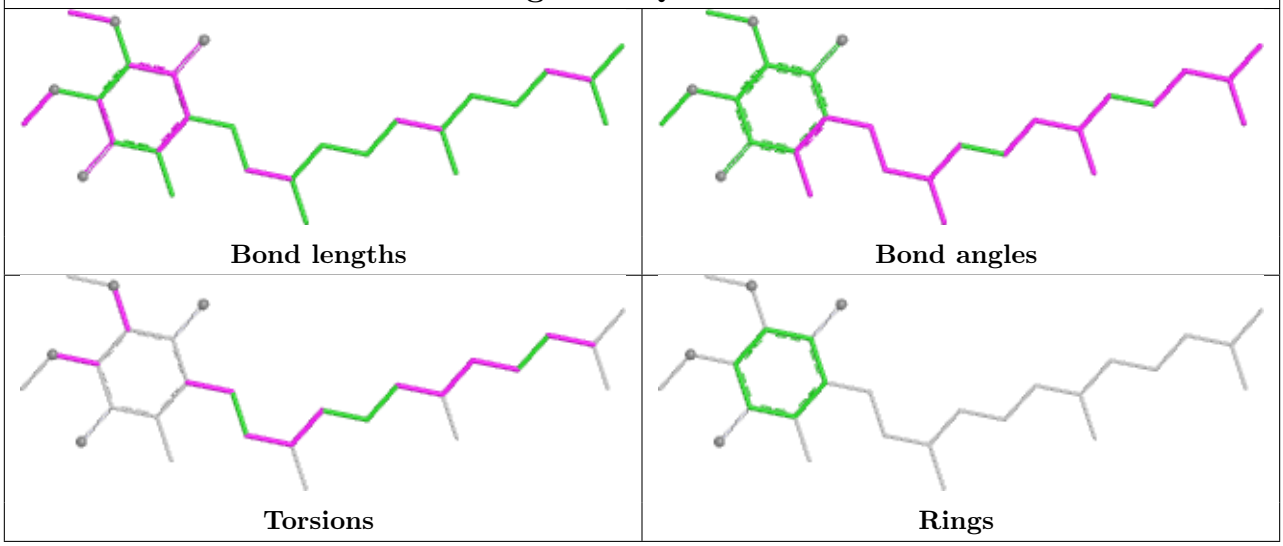
Ligand UQ5 A 601



Ligand NAI B 603



Ligand UQ5 B 605



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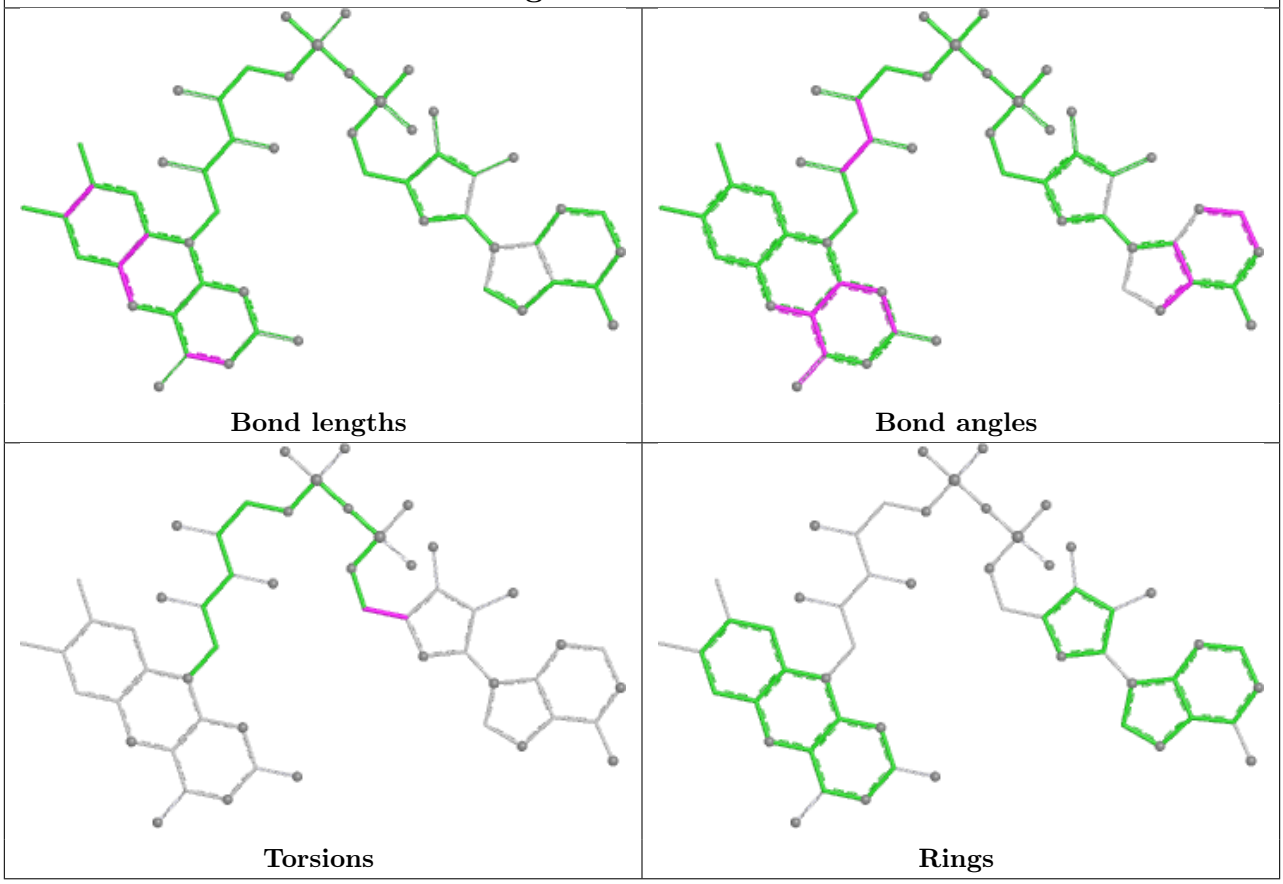

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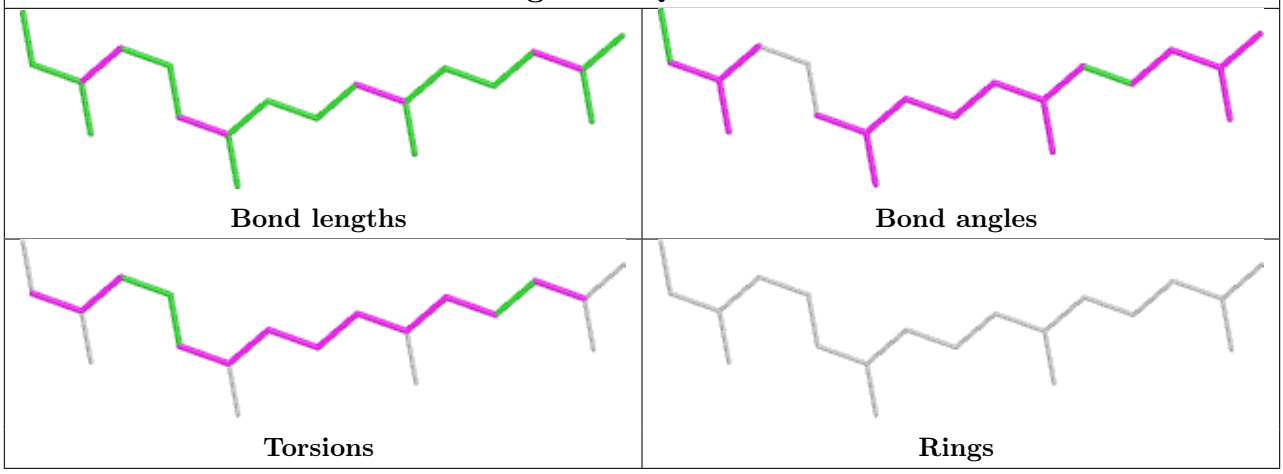

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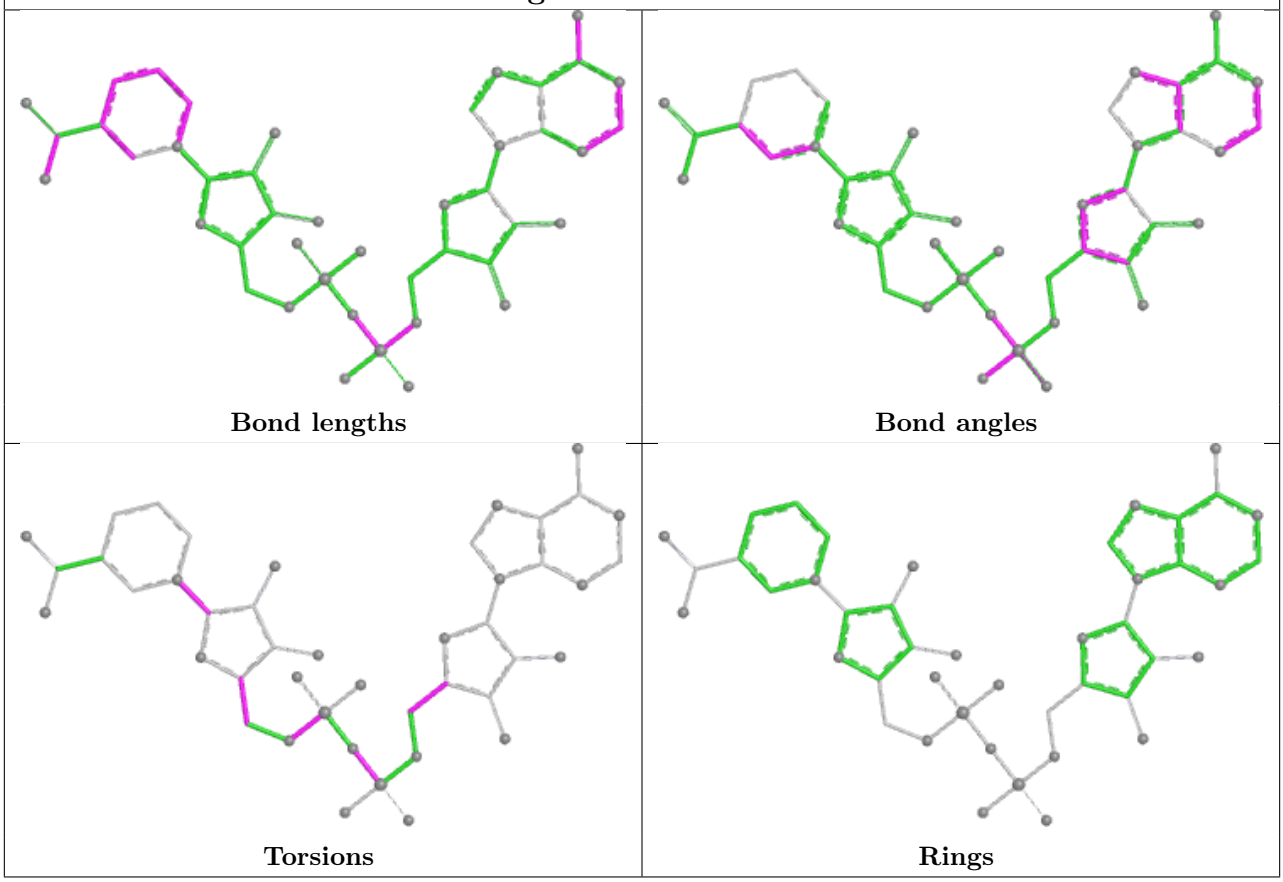
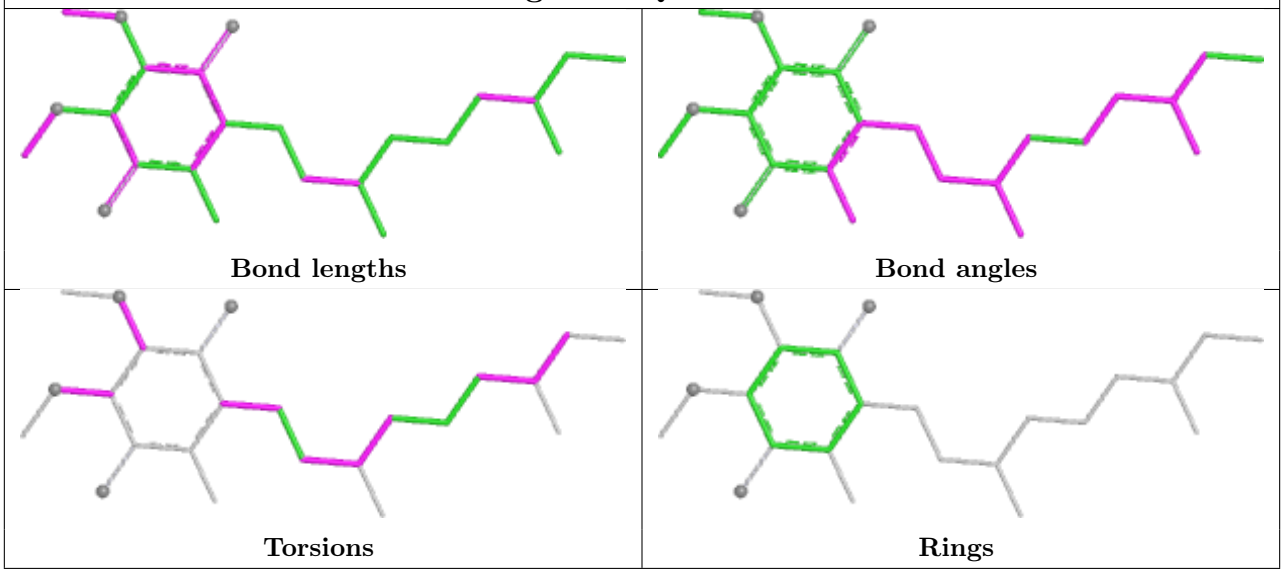


Ligand UQ5 A 604



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	472/502 (94%)	-0.15	18 (3%)	40	44	23, 37, 80, 117	0
1	B	472/502 (94%)	-0.06	29 (6%)	21	22	23, 38, 81, 119	0
All	All	944/1004 (94%)	-0.10	47 (4%)	28	31	23, 37, 81, 119	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	422	SER	6.6
1	A	152	GLN	6.6
1	B	423	ARG	6.4
1	B	152	GLN	6.0
1	A	421	SER	6.0
1	B	421	SER	5.3
1	A	50	HIS	4.9
1	B	427	ILE	4.8
1	B	425	ASP	4.7
1	B	420	LEU	4.4
1	B	424	LYS	4.1
1	B	429	LEU	4.1
1	A	423	ARG	4.0
1	A	324	LYS	3.9
1	A	422	SER	3.7
1	B	50	HIS	3.7
1	B	418	LYS	3.3
1	B	426	LYS	3.3
1	A	325	ILE	3.1
1	A	463	LYS	3.1
1	B	321	GLU	3.0
1	B	52	ASP	3.0
1	A	322	ASP	2.9
1	B	42	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	42	THR	2.8
1	A	323	GLY	2.7
1	B	155	ASN	2.7
1	B	153	PRO	2.7
1	B	428	ASP	2.6
1	B	463	LYS	2.6
1	B	163	GLU	2.6
1	B	162	ALA	2.5
1	A	424	LYS	2.5
1	B	417	GLN	2.5
1	A	155	ASN	2.5
1	A	420	LEU	2.5
1	A	464	ARG	2.5
1	A	282	GLU	2.4
1	B	461	SER	2.4
1	B	173	ILE	2.3
1	B	464	ARG	2.2
1	A	418	LYS	2.2
1	B	462	GLY	2.2
1	A	427	ILE	2.2
1	B	57	LEU	2.1
1	B	419	ASN	2.0
1	B	433	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

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

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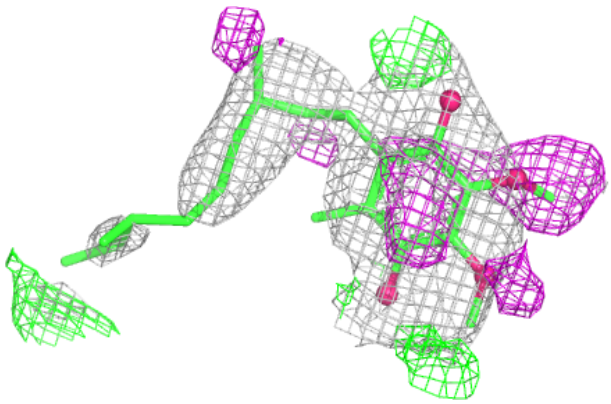
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

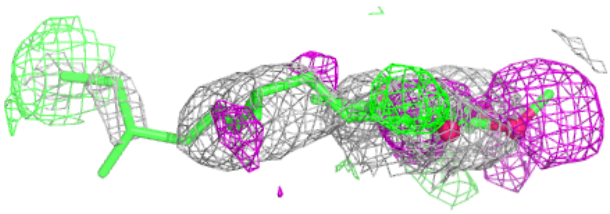
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UQ5	A	604	24/38	0.69	0.43	49,67,84,87	0
3	MG	A	603	1/1	0.75	0.24	70,70,70,70	0
2	UQ5	B	605	28/38	0.77	0.39	51,62,84,88	0
2	UQ5	A	602	10/38	0.79	0.19	44,65,75,82	0
2	UQ5	B	604	20/38	0.80	0.37	48,73,86,93	0
2	UQ5	A	601	20/38	0.84	0.34	51,65,79,81	0
5	NAI	B	603	44/44	0.84	0.25	30,63,102,126	0
5	NAI	A	610	44/44	0.86	0.17	21,65,85,102	0
3	MG	B	602	1/1	0.88	0.09	60,60,60,60	0
3	MG	B	610	1/1	0.88	0.22	51,51,51,51	0
3	MG	A	609	1/1	0.92	0.18	51,51,51,51	0
3	MG	B	607	1/1	0.93	0.12	42,42,42,42	0
3	MG	B	608	1/1	0.94	0.27	45,45,45,45	0
4	FAD	B	606	53/53	0.96	0.17	20,30,37,40	0
3	MG	B	609	1/1	0.96	0.15	46,46,46,46	0
3	MG	A	608	1/1	0.96	0.09	41,41,41,41	0
4	FAD	A	605	53/53	0.97	0.14	15,28,34,37	0
3	MG	B	601	1/1	0.97	0.09	23,23,23,23	0
3	MG	A	606	1/1	0.98	0.09	38,38,38,38	0
3	MG	A	607	1/1	0.98	0.12	42,42,42,42	0

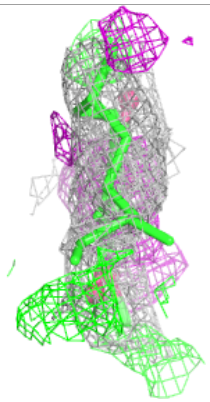
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ5 A 604:

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

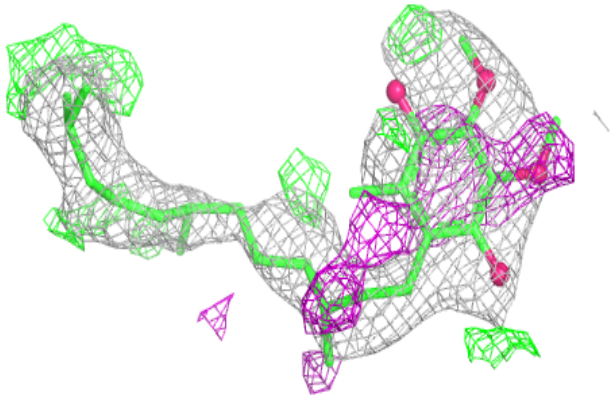


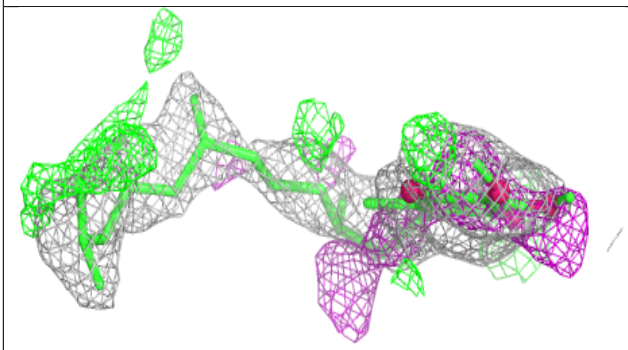


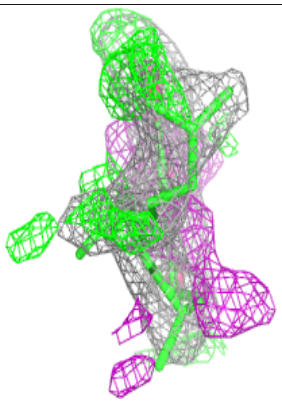


Electron density around UQ5 B 605:

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

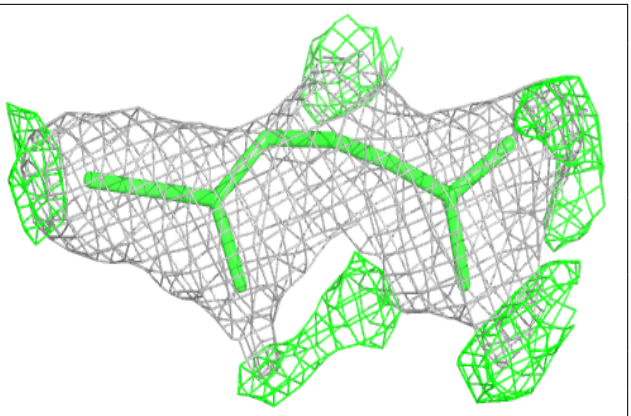


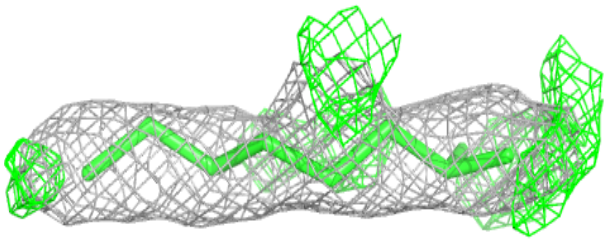


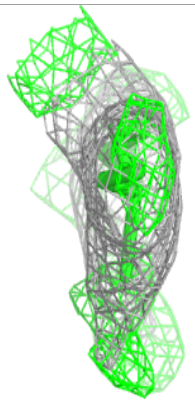


Electron density around UQ5 A 602:

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

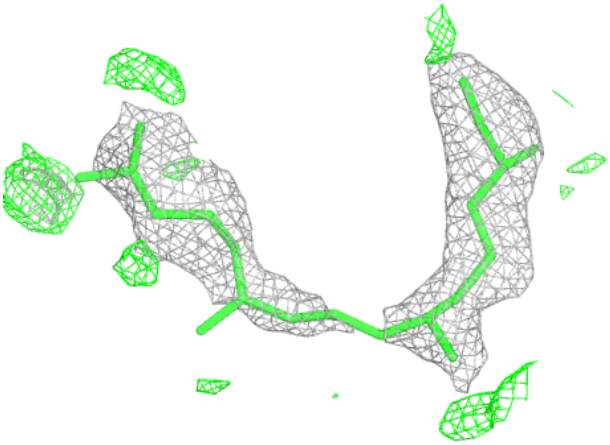


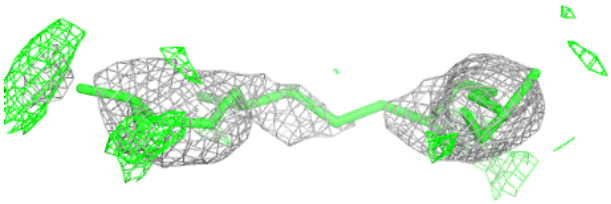


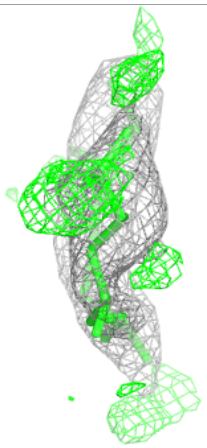


Electron density around UQ5 B 604:

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

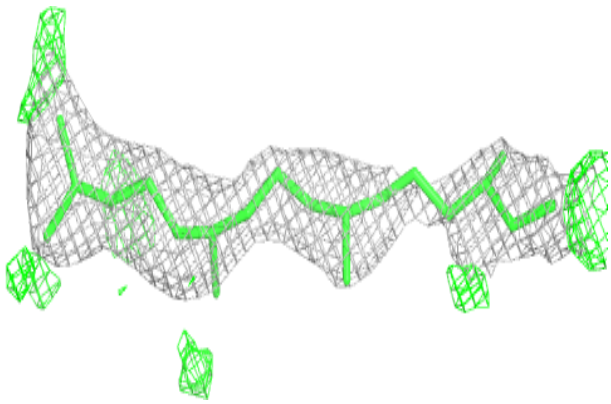


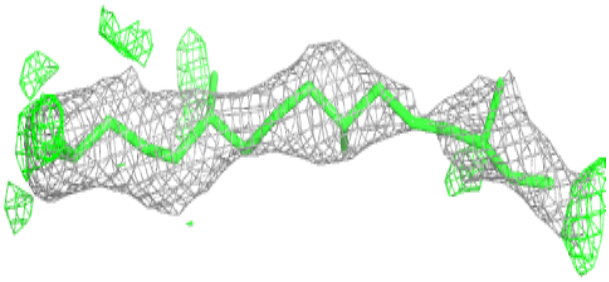


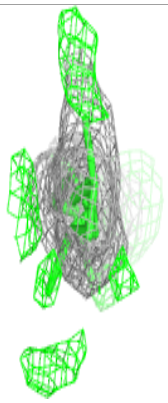


Electron density around UQ5 A 601:

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

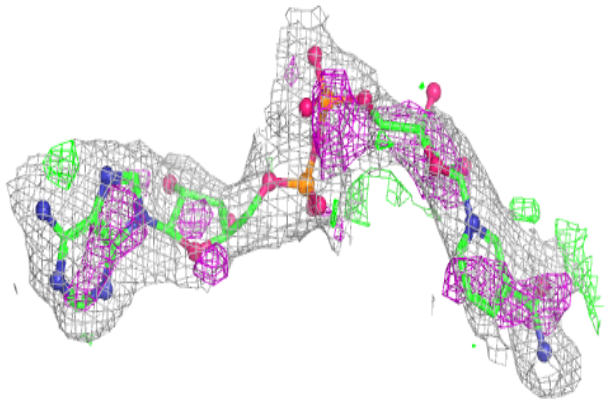


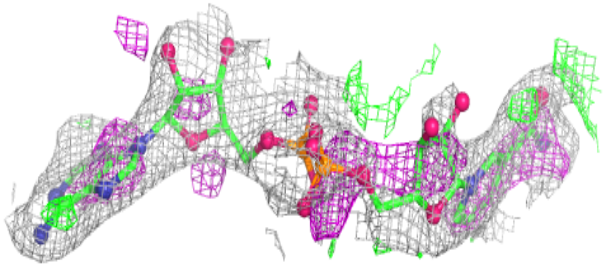


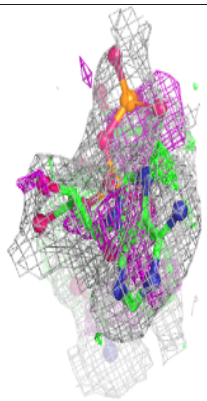


Electron density around NAI B 603:

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

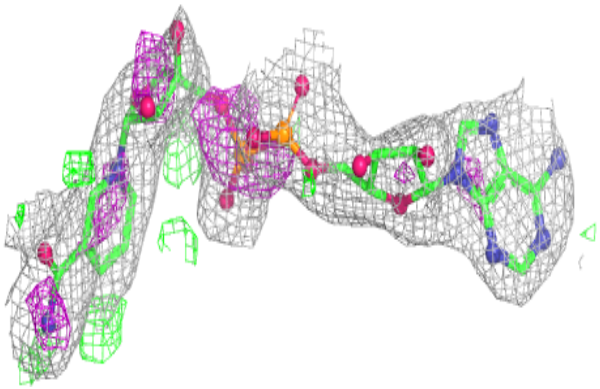


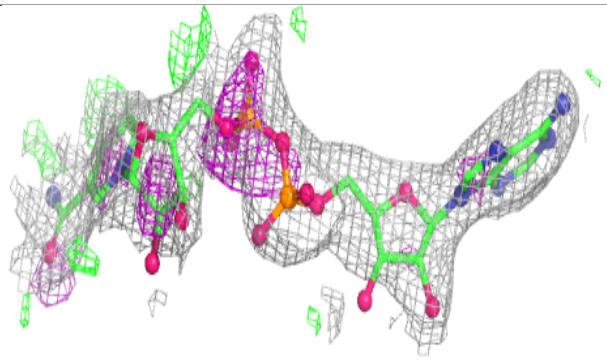


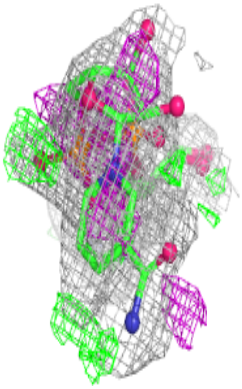


Electron density around NAI A 610:

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

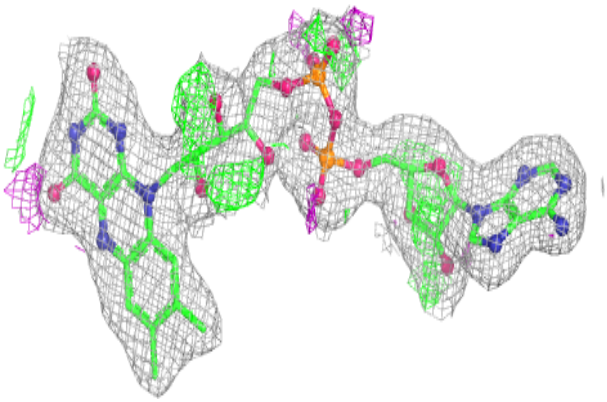


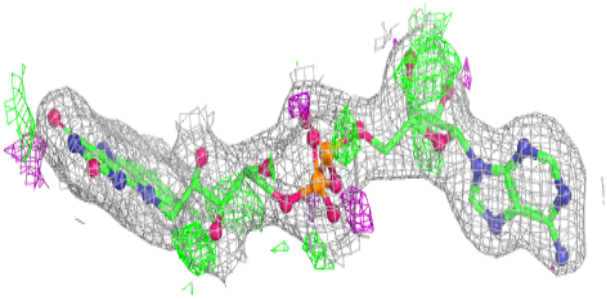


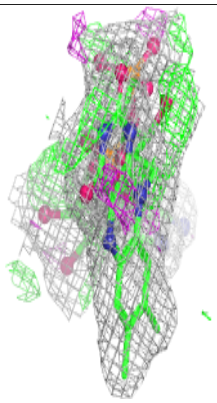


Electron density around FAD B 606:

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

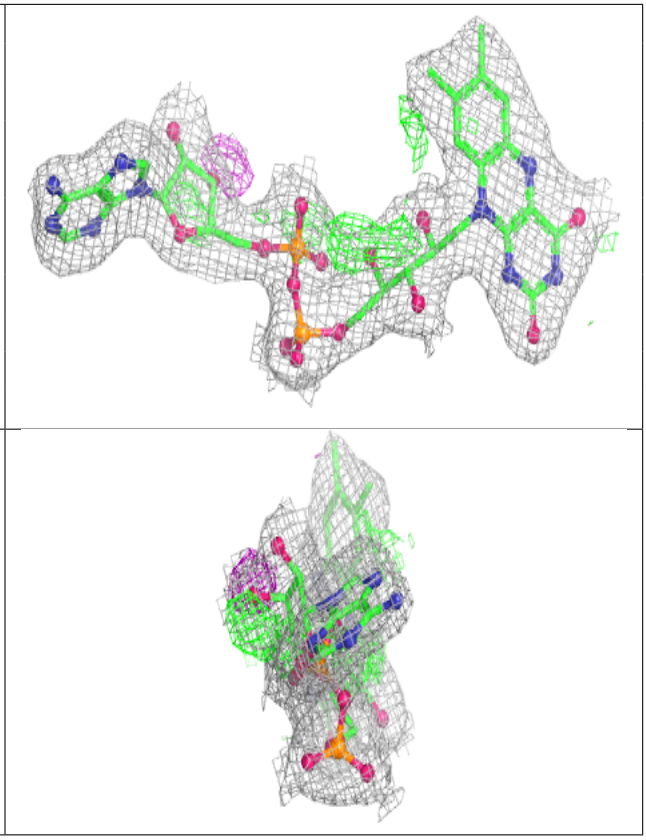






Electron density around FAD A 605:

$2mF_o$-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.