Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:36 PM EDT

PDB ID	:	6GQI
Title	:	Thermocrispum municipale cyclohexanone monooxygenase bound to hexanoic acid
Authors	:	Mattevi, A.; Gomez Castellanos, J.R.
Deposited on	:	2018-06-07
Resolution	:	2.00 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:

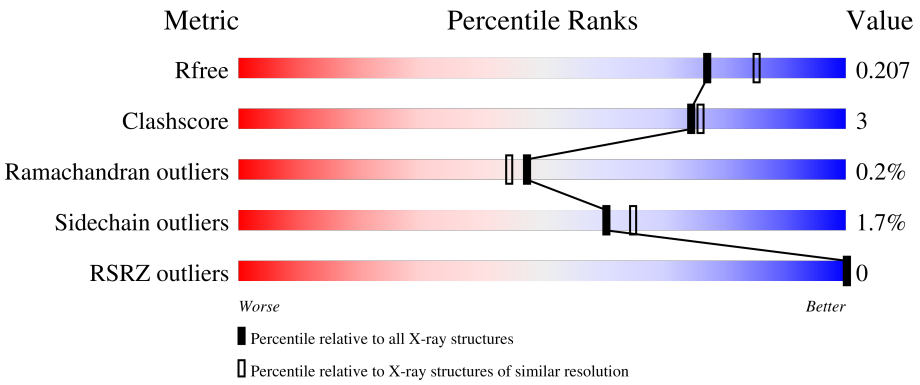
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	541	84% 13% • •
1	B	541	87% 11% • •

2 Entry composition (i)

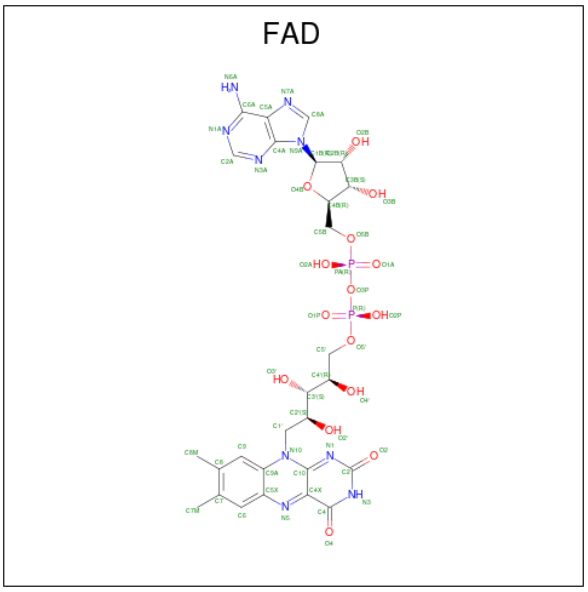
There are 6 unique types of molecules in this entry. The entry contains 9383 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cyclohexanone Monooxygenase from Thermocrispum municipale.

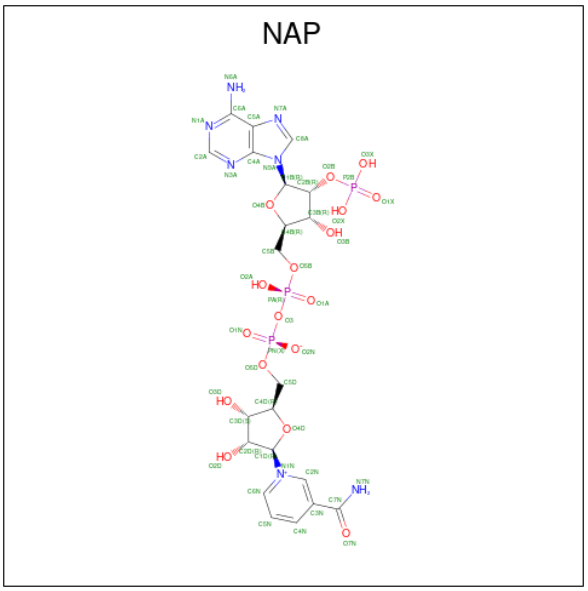
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	529	4184	2644	721	805	14	0	5	0
1	B	529	4169	2638	715	802	14	0	4	0

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



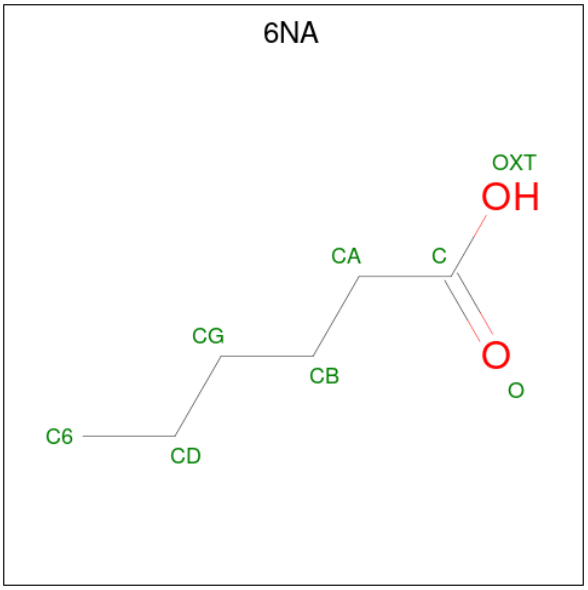
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is HEXANOIC ACID (three-letter code: 6NA) (formula: $C_6H_{12}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	8	6	2	0	0
			Total	C	O		
4	B	1	8	6	2	0	0

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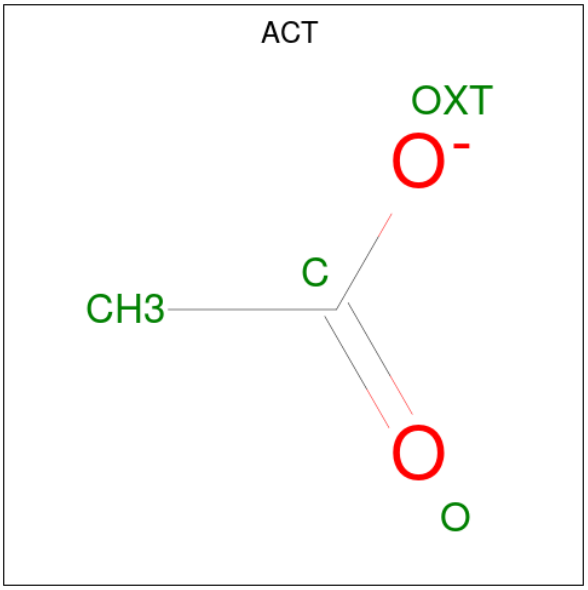
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	8	6	2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0

- Molecule 6 is water.

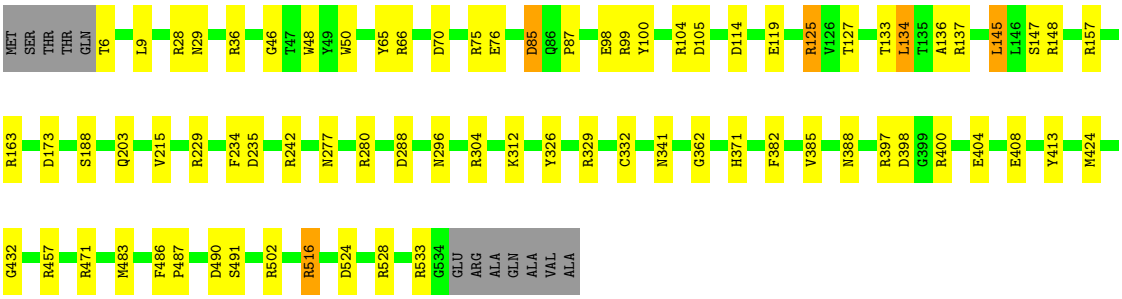
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	409	409	409	0	0
			Total	O		
6	B	391	391	391	0	0

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.

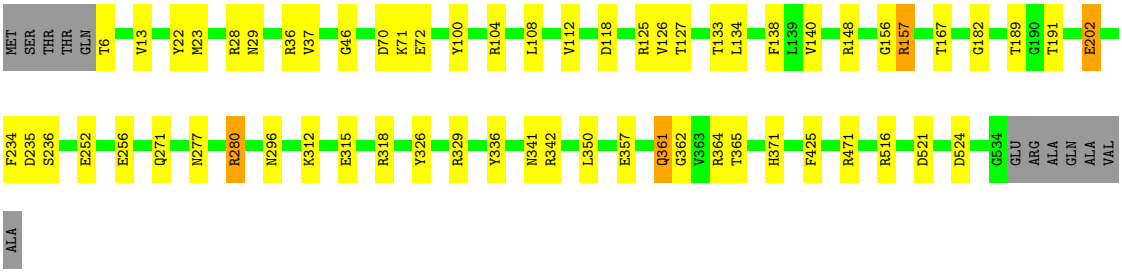
• Molecule 1: Cyclohexanone Monooxygenase from Thermocrispum municipale

Chain A:



• Molecule 1: Cyclohexanone Monooxygenase from Thermocrispum municipale

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.07Å 93.69Å 159.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 2.00 44.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.40-2.00) 98.8 (44.41-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.139 , 0.199 0.151 , 0.207	Depositor DCC
R_{free} test set	3307 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9383	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0025e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, NAP, 6NA, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	1.27	8/4286 (0.2%)	1.18	37/5824 (0.6%)
1	B	1.24	5/4271 (0.1%)	1.16	26/5805 (0.4%)
All	All	1.25	13/8557 (0.2%)	1.17	63/11629 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	ASP	CB-CG	8.38	1.69	1.51
1	A	119	GLU	CD-OE2	-8.35	1.16	1.25
1	B	72	GLU	CD-OE2	7.40	1.33	1.25
1	A	65	TYR	CE1-CZ	7.36	1.48	1.38
1	B	138	PHE	C-O	-6.16	1.11	1.23
1	B	236	SER	CB-OG	-5.95	1.34	1.42
1	B	22	TYR	CB-CG	5.94	1.60	1.51
1	A	413	TYR	CB-CG	5.87	1.60	1.51
1	A	280	ARG	CZ-NH1	-5.73	1.25	1.33
1	A	404	GLU	CD-OE2	5.45	1.31	1.25
1	A	50	TRP	CE3-CZ3	5.37	1.47	1.38
1	B	100	TYR	CB-CG	5.08	1.59	1.51
1	A	48	TRP	CD1-NE1	5.04	1.46	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	516	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	424	MET	CG-SD-CE	-8.47	86.65	100.20
1	A	75	ARG	NE-CZ-NH2	8.40	124.50	120.30
1	B	342	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	280[A]	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	B	280[B]	ARG	NE-CZ-NH1	-7.74	116.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	235	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	85	ASP	CB-CG-OD1	7.66	125.19	118.30
1	B	342	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	137	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	A	157	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	516[A]	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	516[B]	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	125	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	157	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	36	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	72	GLU	OE1-CD-OE2	6.92	131.61	123.30
1	A	36	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	148	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	521	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	533	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	A	471	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	173	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	288	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	70	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	157	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	521	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	490	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	145	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	A	99	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	280	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	242	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	163	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	36	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	105	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	75	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	104	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	202	GLU	OE1-CD-OE2	5.67	130.11	123.30
1	B	235	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	118	ASP	CB-CG-OD2	-5.58	113.27	118.30
1	B	471	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	364	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	114	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	A	288	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	329	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	A	125	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	66	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	502	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	108	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	A	524[A]	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	524[B]	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	280[A]	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	B	280[B]	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	134	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	229	ARG	CG-CD-NE	5.30	122.92	111.80
1	A	397	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	A	114	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	182	GLY	N-CA-C	-5.16	100.19	113.10
1	A	304	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	457	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	148	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	104	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	4184	0	4030	23	0
1	B	4169	0	4012	28	1
2	A	53	0	31	2	0
2	B	53	0	31	2	0
3	A	48	0	25	2	0
3	B	48	0	25	2	0
4	A	8	0	11	2	0
4	B	16	0	22	1	0
5	A	4	0	3	0	0
6	A	409	0	0	4	1
6	B	391	0	0	6	1
All	All	9383	0	8190	54	2

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 3.

All (54) 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)
1:B:361:GLN:HE21	1:B:361:GLN:H	1.26	0.82
1:A:398:ASP:OD2	1:A:400:ARG:NH1	2.15	0.79
1:B:312:LYS:H	1:B:341:ASN:HD21	1.34	0.76
1:B:280[A]:ARG:HH11	1:B:280[A]:ARG:HG3	1.52	0.75
1:B:296:ASN:HD21	1:B:326:TYR:H	1.36	0.73
1:B:28:ARG:HH21	1:B:29:ASN:HD21	1.37	0.71
1:B:71:LYS:HD2	6:B:1037:HOH:O	1.90	0.70
2:B:601:FAD:HM73	3:B:602:NAP:C5N	2.21	0.70
1:A:28:ARG:HH21	1:A:29:ASN:HD21	1.40	0.67
1:A:70:ASP:OD2	1:A:100:TYR:OH	2.13	0.64
1:A:296:ASN:HD21	1:A:326:TYR:H	1.45	0.64
1:B:365:THR:OG1	1:B:371:HIS:HE1	1.81	0.64
1:B:280[A]:ARG:HG3	1:B:280[A]:ARG:NH1	2.13	0.63
1:A:125:ARG:HD3	6:A:822:HOH:O	1.98	0.62
1:A:85:ASP:HB3	1:A:87:PRO:HD2	1.83	0.61
1:A:147[A]:SER:OG	1:A:388:ASN:ND2	2.35	0.59
1:B:271:GLN:NE2	6:B:703:HOH:O	2.36	0.59
2:A:601:FAD:HM73	3:A:602:NAP:C5N	2.34	0.58
1:A:329:ARG:NE	4:A:603:6NA:O	2.28	0.57
1:A:312:LYS:H	1:A:341:ASN:HD21	1.55	0.55
4:B:603:6NA:O	4:B:603:6NA:CG	2.51	0.55
1:B:46:GLY:HA2	2:B:601:FAD:O3B	2.07	0.54
1:A:329:ARG:HH11	4:A:603:6NA:C	2.22	0.53
1:A:98:GLU:CB	6:B:1086:HOH:O	2.58	0.51
1:B:127:THR:OG1	1:B:133:THR:HG22	2.11	0.50
1:A:432:GLY:HA3	6:A:919:HOH:O	2.14	0.48
1:A:215:VAL:O	1:A:332:CYS:HA	2.14	0.47
1:B:167:THR:HG21	1:B:189:THR:CG2	2.45	0.47
1:A:188[A]:SER:OG	3:A:602:NAP:C3N	2.64	0.46
1:A:486:PHE:N	1:A:487:PRO:CD	2.78	0.46
1:B:140:VAL:HA	1:B:425:PHE:O	2.16	0.45
1:B:312:LYS:H	1:B:341:ASN:ND2	2.08	0.45
1:B:191:THR:HG22	1:B:336:TYR:CZ	2.51	0.45
1:B:13:VAL:O	1:B:37:VAL:HA	2.18	0.45
1:B:133:THR:HG21	6:B:976:HOH:O	2.16	0.44
1:B:156:GLY:O	1:B:157:ARG:C	2.54	0.44
1:A:46:GLY:HA2	2:A:601:FAD:O3B	2.17	0.44
1:A:145:LEU:HD22	1:A:385:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLU:HA	1:B:315:GLU:OE1	2.18	0.43
1:B:362:GLY:HA3	1:B:371:HIS:O	2.18	0.43
1:B:71:LYS:CD	6:B:1037:HOH:O	2.59	0.42
1:B:252:GLU:HB3	6:B:773:HOH:O	2.20	0.42
1:A:362:GLY:HA3	1:A:371:HIS:O	2.20	0.42
1:A:127:THR:OG1	1:A:133:THR:HG22	2.20	0.42
1:B:112:VAL:HG13	1:B:126:VAL:HG13	2.01	0.42
1:B:315:GLU:OE2	1:B:318:ARG:NH2	2.42	0.42
1:B:361:GLN:HE21	1:B:361:GLN:N	2.05	0.42
1:B:350:LEU:HD12	3:B:602:NAP:H2A	2.03	0.41
1:A:516[B]:ARG:NH2	6:A:723:HOH:O	2.49	0.41
1:B:280[A]:ARG:NH1	1:B:280[A]:ARG:CG	2.75	0.41
1:A:203:GLN:HG2	6:A:954:HOH:O	2.19	0.41
1:A:382:PHE:CD1	1:A:382:PHE:N	2.88	0.41
1:A:9:LEU:O	1:A:136:ALA:HA	2.21	0.40
1:B:23:MET:HG2	1:B:140:VAL:HG11	2.03	0.40

All (2) 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)
6:A:1099:HOH:O	6:B:1049:HOH:O[4_455]	1.93	0.27
1:B:280[A]:ARG:NH1	1:B:524:ASP:OD1[4_565]	2.00	0.20

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	532/541 (98%)	519 (98%)	12 (2%)	1 (0%)	47	44
1	B	531/541 (98%)	516 (97%)	14 (3%)	1 (0%)	47	44
All	All	1063/1082 (98%)	1035 (97%)	26 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	277	ASN
1	A	277	ASN

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	439/444 (99%)	430 (98%)	9 (2%)	53	57
1	B	436/444 (98%)	429 (98%)	7 (2%)	62	67
All	All	875/888 (98%)	859 (98%)	16 (2%)	60	63

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	76	GLU
1	A	134	LEU
1	A	234	PHE
1	A	408	GLU
1	A	483	MET
1	A	491[A]	SER
1	A	491[B]	SER
1	A	528	ARG
1	B	6	THR
1	B	134	LEU
1	B	202	GLU
1	B	234	PHE
1	B	256	GLU
1	B	357	GLU
1	B	361	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	296	ASN
1	A	341	ASN
1	A	371	HIS
1	A	388	ASN
1	A	482	ASN
1	A	514	ASN
1	B	29	ASN
1	B	271	GLN
1	B	296	ASN
1	B	341	ASN
1	B	361	GLN
1	B	371	HIS
1	B	482	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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAP	B	602	-	46,52,52	1.44	5 (10%)	61,80,80	1.63	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	6NA	B	603	-	7,7,7	1.07	1 (14%)	7,7,7	2.54	3 (42%)
3	NAP	A	602	-	46,52,52	1.34	4 (8%)	61,80,80	1.65	16 (26%)
4	6NA	B	604	-	7,7,7	0.73	0	7,7,7	1.08	0
5	ACT	A	604	-	3,3,3	1.06	0	3,3,3	0.76	0
4	6NA	A	603	-	7,7,7	1.11	1 (14%)	7,7,7	1.72	1 (14%)
2	FAD	B	601	-	54,58,58	2.02	15 (27%)	71,89,89	1.67	12 (16%)
2	FAD	A	601	-	54,58,58	1.81	12 (22%)	71,89,89	1.63	14 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	B	602	-	-	6/31/67/67	0/5/5/5
4	6NA	B	603	-	-	1/5/5/5	-
3	NAP	A	602	-	-	4/31/67/67	0/5/5/5
4	6NA	B	604	-	-	2/5/5/5	-
4	6NA	A	603	-	-	1/5/5/5	-
2	FAD	B	601	-	-	6/30/50/50	0/6/6/6
2	FAD	A	601	-	-	5/30/50/50	0/6/6/6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	P-O3P	6.51	1.66	1.59
2	A	601	FAD	C9A-C5X	5.70	1.50	1.41
3	B	602	NAP	C4A-N3A	5.48	1.43	1.35
2	B	601	FAD	PA-O3P	5.04	1.64	1.59
3	A	602	NAP	P2B-O2B	5.03	1.68	1.59
3	B	602	NAP	O4D-C1D	4.21	1.46	1.40
2	B	601	FAD	C9A-C5X	4.10	1.47	1.41
2	B	601	FAD	C4-N3	-3.98	1.31	1.38
2	A	601	FAD	C4-N3	-3.88	1.31	1.38
2	A	601	FAD	C8-C7	3.51	1.49	1.40
2	A	601	FAD	C10-N10	3.26	1.44	1.37
2	A	601	FAD	P-O3P	3.23	1.63	1.59
2	B	601	FAD	C4X-N5	3.12	1.37	1.30
2	B	601	FAD	C2-N3	-3.09	1.32	1.39
2	A	601	FAD	C2-N3	-3.03	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O4B-C1B	3.02	1.44	1.40
2	B	601	FAD	C2A-N3A	2.91	1.36	1.32
2	B	601	FAD	C9-C8	-2.86	1.35	1.39
2	A	601	FAD	C4X-N5	2.74	1.36	1.30
2	A	601	FAD	C4A-N3A	2.73	1.39	1.35
3	A	602	NAP	C7N-N7N	2.67	1.37	1.33
3	B	602	NAP	PN-O3	-2.65	1.56	1.59
2	B	601	FAD	O4B-C1B	2.54	1.44	1.40
4	B	603	6NA	OXT-C	-2.47	1.22	1.30
3	A	602	NAP	C2A-N3A	2.47	1.35	1.32
2	B	601	FAD	C8M-C8	2.42	1.55	1.51
2	A	601	FAD	O4'-C4'	2.39	1.48	1.43
3	B	602	NAP	P2B-O3X	-2.38	1.45	1.54
3	A	602	NAP	C3N-C7N	-2.37	1.47	1.50
2	A	601	FAD	C2A-N3A	2.29	1.35	1.32
2	A	601	FAD	O4-C4	2.25	1.27	1.23
3	B	602	NAP	C3N-C7N	-2.23	1.47	1.50
2	B	601	FAD	C4X-C10	2.22	1.50	1.44
2	B	601	FAD	C5A-N7A	-2.21	1.31	1.39
2	B	601	FAD	C2A-N1A	2.16	1.37	1.33
2	B	601	FAD	C7M-C7	-2.11	1.47	1.51
2	B	601	FAD	C6-C5X	-2.09	1.36	1.40
4	A	603	6NA	O-C	2.07	1.28	1.22

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	NAP	N3A-C2A-N1A	-7.49	118.51	128.67
4	B	603	6NA	CB-CA-C	-5.10	101.19	114.51
2	B	601	FAD	C4-C4X-N5	4.71	124.72	118.21
2	A	601	FAD	O2-C2-N1	-4.20	114.83	121.80
2	A	601	FAD	C4B-O4B-C1B	-4.01	106.25	109.92
4	A	603	6NA	CB-CA-C	-4.00	104.06	114.51
3	A	602	NAP	O7N-C7N-N7N	3.87	128.21	122.62
3	B	602	NAP	C2N-C3N-C4N	3.81	122.69	118.26
3	A	602	NAP	C5A-C6A-N6A	-3.76	114.59	120.31
2	B	601	FAD	C4A-C5A-N7A	-3.71	105.42	109.34
2	B	601	FAD	N6A-C6A-N1A	3.70	126.23	118.33
3	A	602	NAP	N3A-C2A-N1A	-3.58	123.82	128.67
2	A	601	FAD	O2P-P-O3P	-3.55	97.67	107.27
3	A	602	NAP	O3-PA-O1A	-3.51	100.14	110.70
2	B	601	FAD	N3A-C2A-N1A	-3.44	124.01	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C4B-O4B-C1B	-3.40	106.81	109.92
2	A	601	FAD	N3A-C2A-N1A	-3.33	124.15	128.67
3	A	602	NAP	C5N-C4N-C3N	-3.29	117.13	120.36
3	A	602	NAP	N6A-C6A-N1A	3.19	125.15	118.33
4	B	603	6NA	OXT-C-CA	3.08	123.74	114.00
2	A	601	FAD	C4X-C10-N10	3.07	120.87	116.48
2	B	601	FAD	O2-C2-N1	-2.99	116.84	121.80
2	A	601	FAD	C4-C4X-N5	2.91	122.23	118.21
3	A	602	NAP	C6N-N1N-C2N	2.89	124.34	121.88
3	B	602	NAP	C3N-C7N-N7N	-2.87	114.20	117.74
2	A	601	FAD	O3B-C3B-C4B	-2.82	102.98	111.08
3	B	602	NAP	C5N-C4N-C3N	-2.80	117.61	120.36
3	A	602	NAP	C1B-N9A-C4A	-2.65	121.99	126.64
2	A	601	FAD	O3P-PA-O1A	-2.64	102.75	110.70
3	B	602	NAP	O7N-C7N-C3N	2.61	122.79	119.60
4	B	603	6NA	O-C-CA	-2.60	114.84	123.09
2	B	601	FAD	O2P-P-O3P	-2.59	100.27	107.27
2	B	601	FAD	C5A-C6A-N1A	-2.57	114.09	120.23
2	A	601	FAD	O4-C4-C4X	-2.56	119.78	126.53
2	A	601	FAD	O2A-PA-O1A	2.55	124.30	112.44
2	B	601	FAD	O4'-C4'-C5'	-2.53	104.41	109.99
3	A	602	NAP	C3N-C7N-N7N	-2.47	114.69	117.74
2	A	601	FAD	C4X-C10-N1	-2.40	118.72	124.59
2	A	601	FAD	C1'-C2'-C3'	2.37	116.08	109.66
3	B	602	NAP	C6A-C5A-C4A	-2.36	113.30	117.90
2	B	601	FAD	C4X-C4-N3	2.36	119.25	113.25
3	A	602	NAP	C5N-C6N-N1N	-2.27	117.29	120.38
3	A	602	NAP	C2N-C3N-C4N	2.24	120.86	118.26
2	A	601	FAD	N6A-C6A-N1A	2.17	122.97	118.33
2	A	601	FAD	C9A-N10-C10	-2.17	117.45	120.75
3	A	602	NAP	O5D-C5D-C4D	-2.14	101.70	108.99
3	B	602	NAP	O2N-PN-O1N	2.13	122.35	112.44
3	A	602	NAP	C4B-O4B-C1B	-2.11	108.00	109.92
2	B	601	FAD	C8M-C8-C7	2.08	125.00	120.76
2	B	601	FAD	C6-C5X-C9A	-2.08	116.20	119.05
3	A	602	NAP	C2D-C3D-C4D	-2.05	98.64	102.61
3	A	602	NAP	O7N-C7N-C3N	-2.05	117.09	119.60
3	A	602	NAP	O2A-PA-O3	2.01	112.69	107.27
3	B	602	NAP	O4B-C4B-C5B	-2.00	102.93	109.33

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
3	A	602	NAP	C5D-O5D-PN-O3
3	A	602	NAP	O4D-C1D-N1N-C2N
3	A	602	NAP	O4D-C1D-N1N-C6N
3	B	602	NAP	C5D-O5D-PN-O3
3	B	602	NAP	O4D-C1D-N1N-C2N
4	B	603	6NA	CA-CB-CG-CD
4	A	603	6NA	C-CA-CB-CG
2	B	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O3'-C3'-C4'-O4'
4	B	604	6NA	OXT-C-CA-CB
3	B	602	NAP	C2N-C3N-C7N-N7N
4	B	604	6NA	O-C-CA-CB
3	B	602	NAP	C4N-C3N-C7N-N7N
2	A	601	FAD	O4B-C4B-C5B-O5B
3	B	602	NAP	C2N-C3N-C7N-O7N
3	B	602	NAP	C4N-C3N-C7N-O7N
3	A	602	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

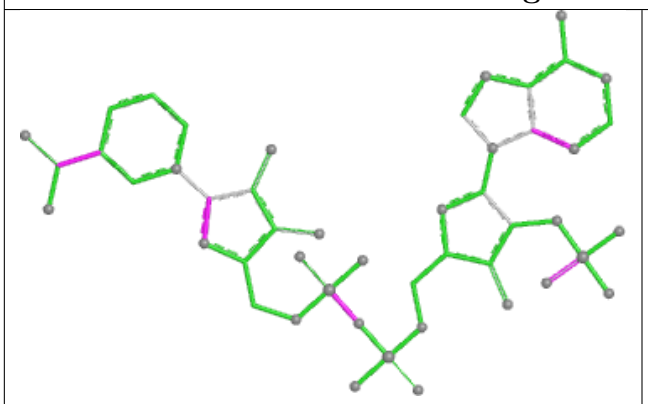
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	NAP	2	0
4	B	603	6NA	1	0
3	A	602	NAP	2	0
4	A	603	6NA	2	0
2	B	601	FAD	2	0
2	A	601	FAD	2	0

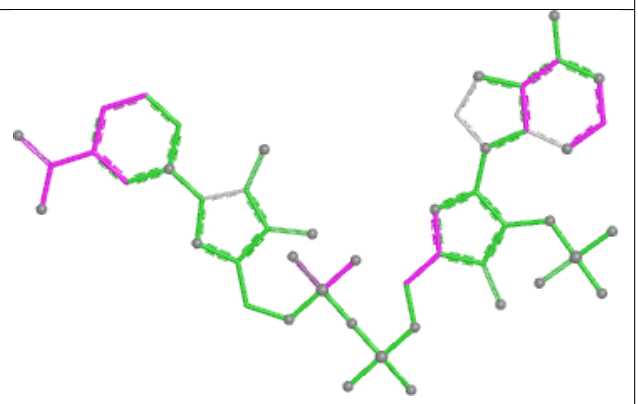
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

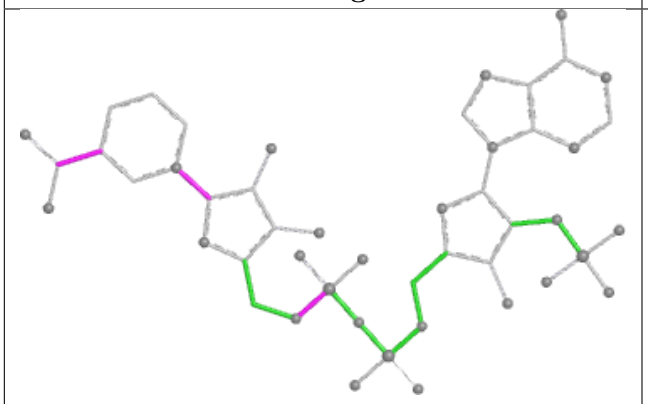
Ligand NAP B 602



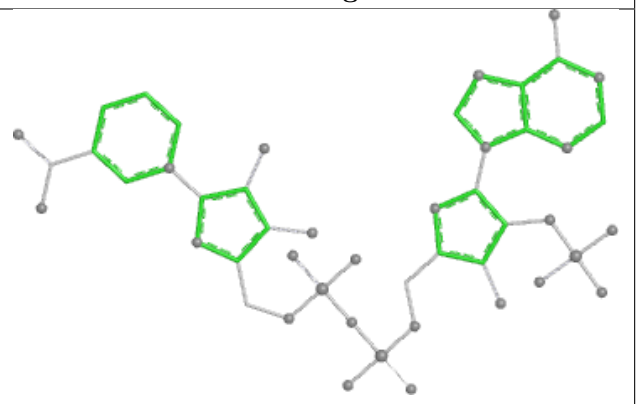
Bond lengths



Bond angles

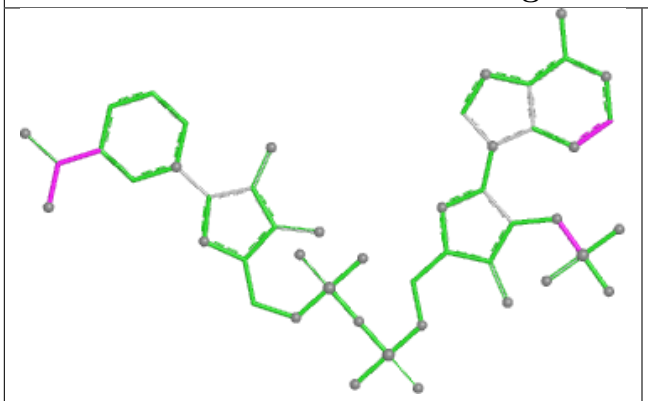


Torsions



Rings

Ligand NAP A 602



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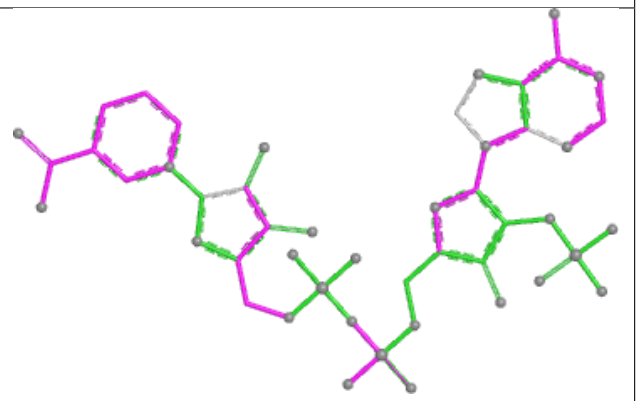

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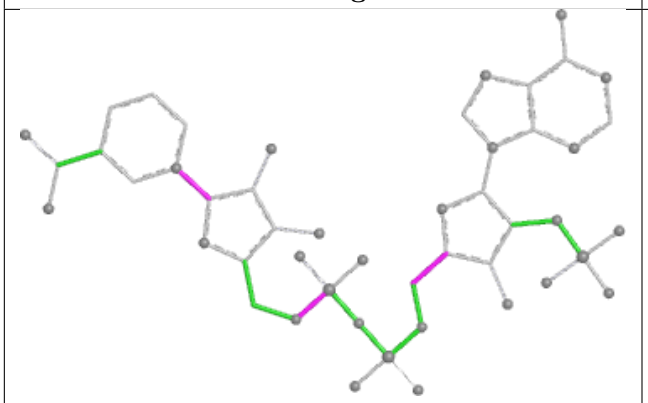
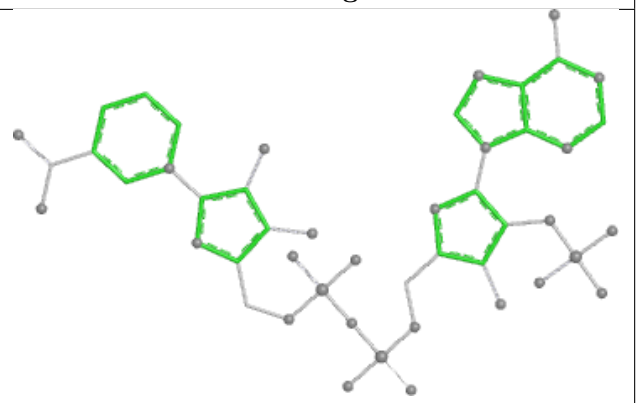
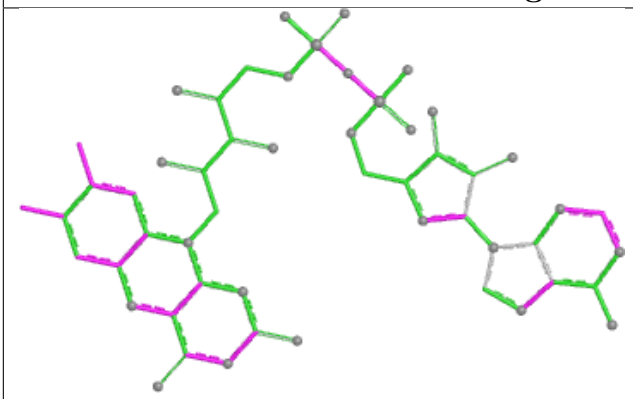


Torsions

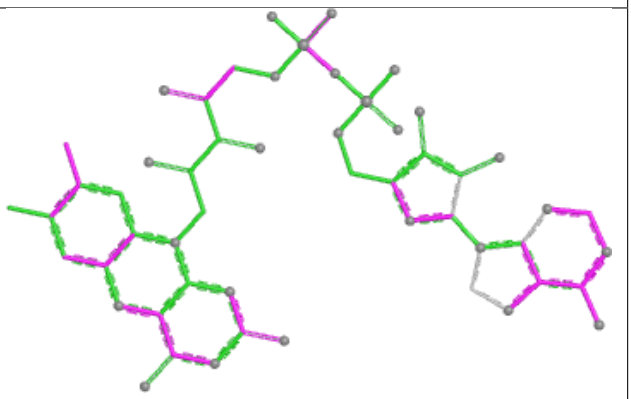


Rings

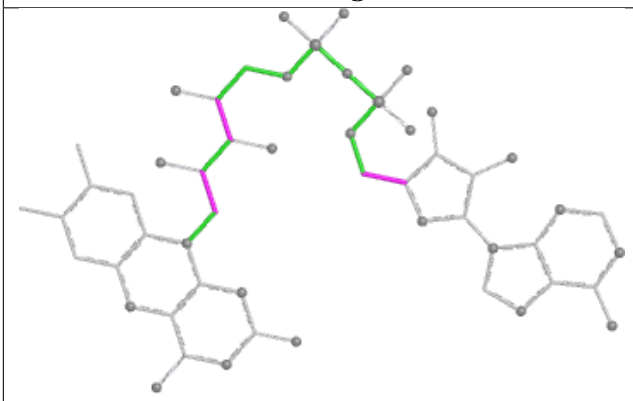
Ligand FAD B 601



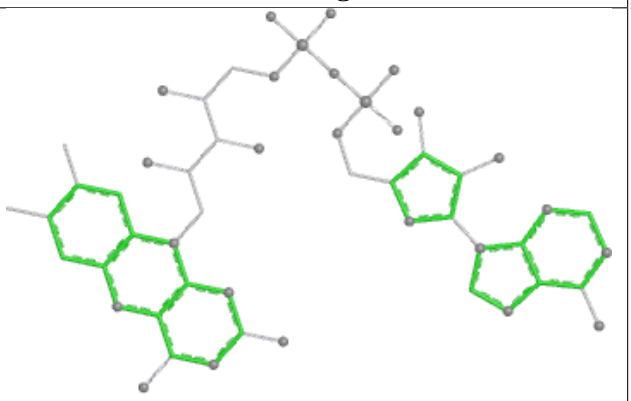
Bond lengths



Bond angles

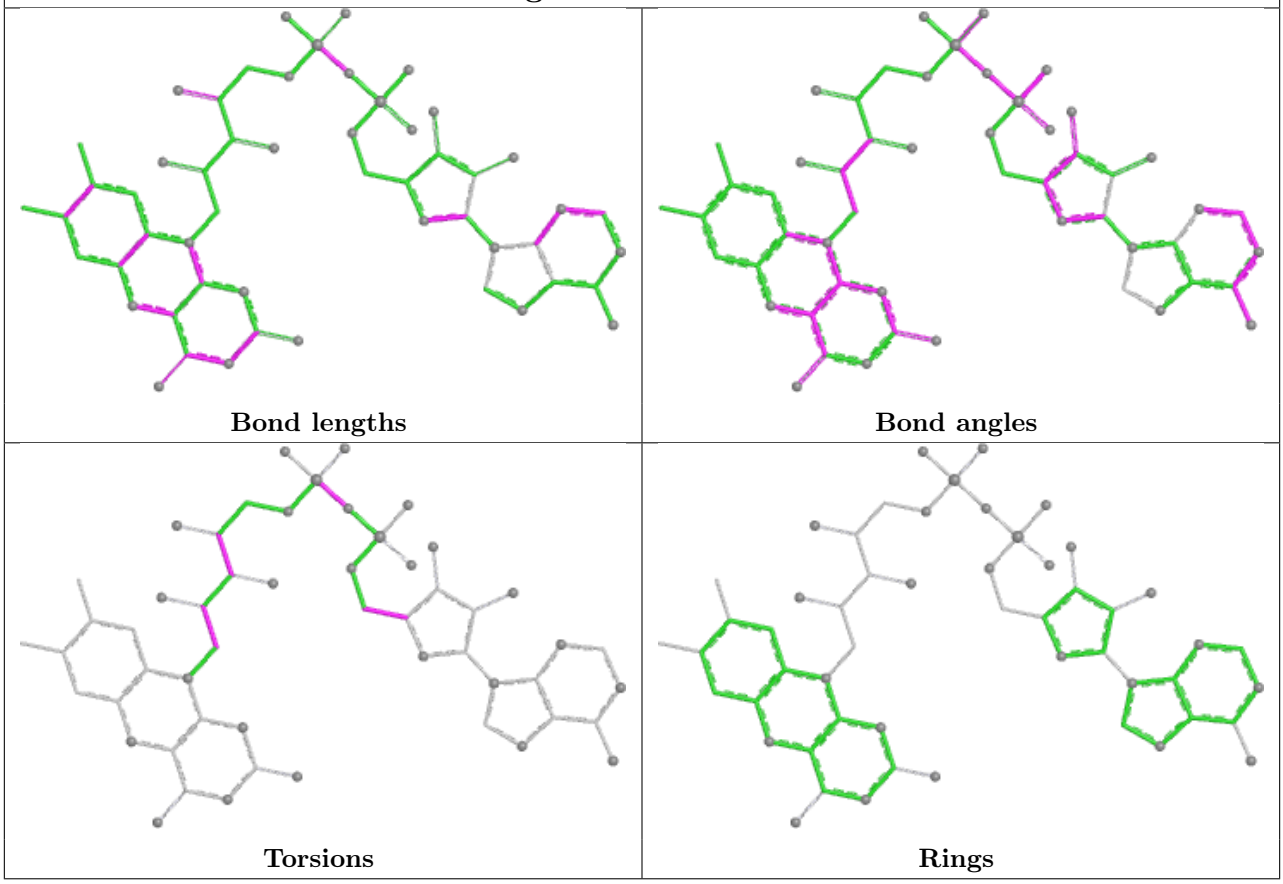


Torsions



Rings

Ligand FAD A 601



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	529/541 (97%)	-0.73	0	100	100	13, 21, 36, 49	0
1	B	529/541 (97%)	-0.67	0	100	100	12, 22, 45, 63	0
All	All	1058/1082 (97%)	-0.70	0	100	100	12, 21, 42, 63	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	6NA	B	603	8/8	0.93	0.13	23,29,44,54	0
4	6NA	A	603	8/8	0.94	0.15	28,32,38,44	0
3	NAP	A	602	48/48	0.97	0.08	14,21,27,30	0
4	6NA	B	604	8/8	0.97	0.10	21,28,32,33	0
2	FAD	B	601	53/53	0.98	0.07	11,16,25,28	0
2	FAD	A	601	53/53	0.98	0.09	11,16,28,37	0
3	NAP	B	602	48/48	0.98	0.08	15,20,27,28	0

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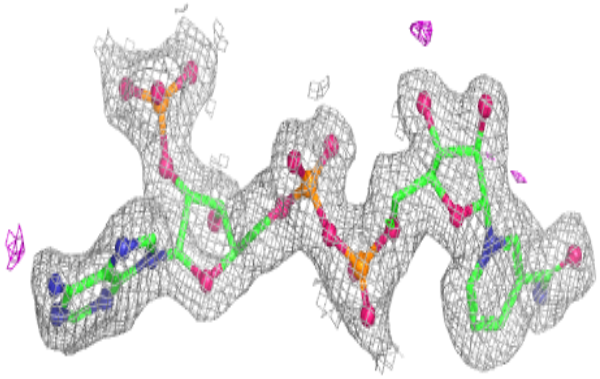
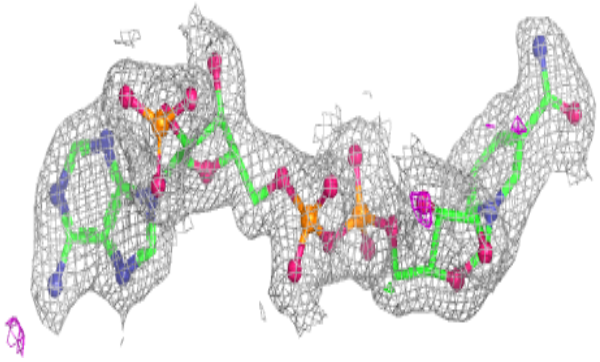
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	A	604	4/4	0.98	0.09	19,22,23,23	0

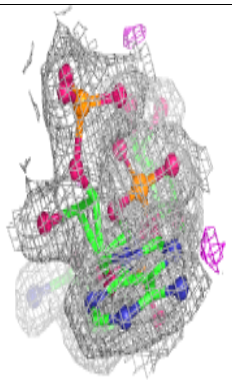
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

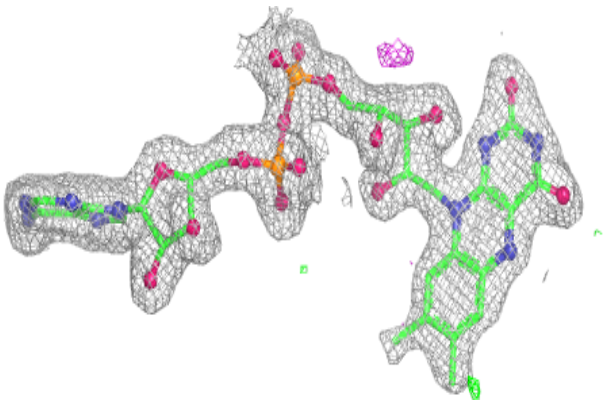


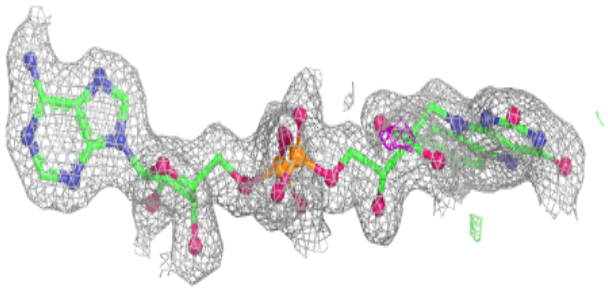


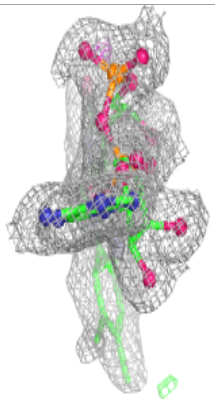


Electron density around FAD B 601:

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

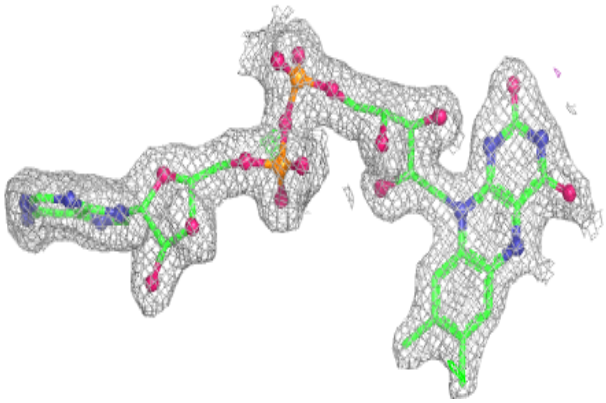


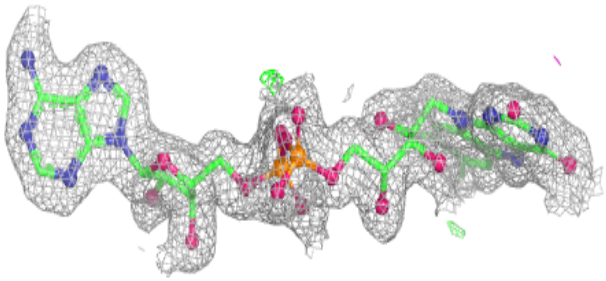


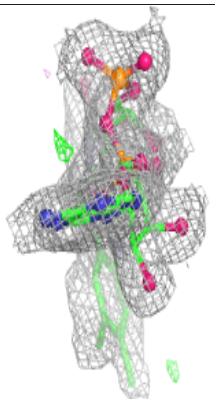


Electron density around FAD A 601:

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

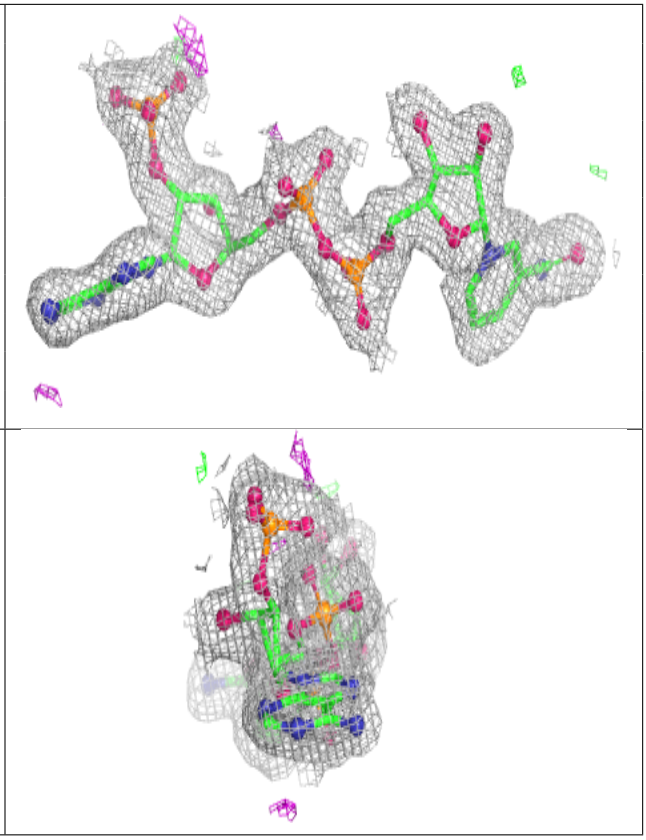






Electron density around NAP B 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.