



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 06:49 PM EDT

PDB ID : 6SF0
Title : Crystal Structure of Ancestral Flavin-containing monooxygenase (FMO) 2 in the presence of NADP+
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Deposited on : 2019-07-30
Resolution : 3.01 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	:	4.02b-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

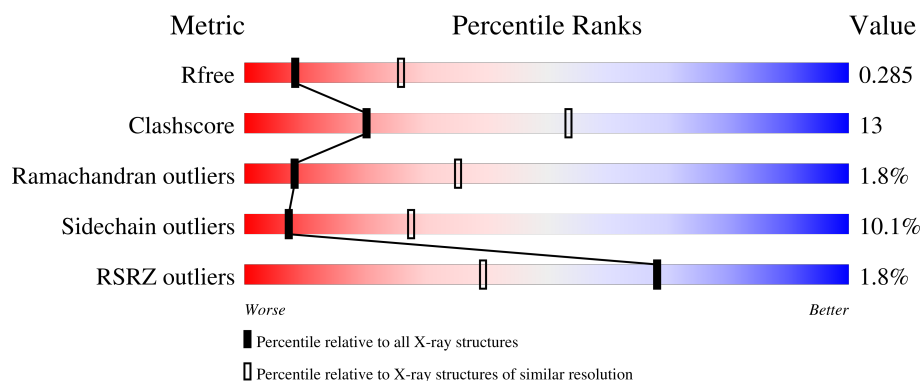
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 $\leq 5\%$. 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	535	
1	B	535	
1	C	535	
1	D	535	

2 Entry composition ⓘ

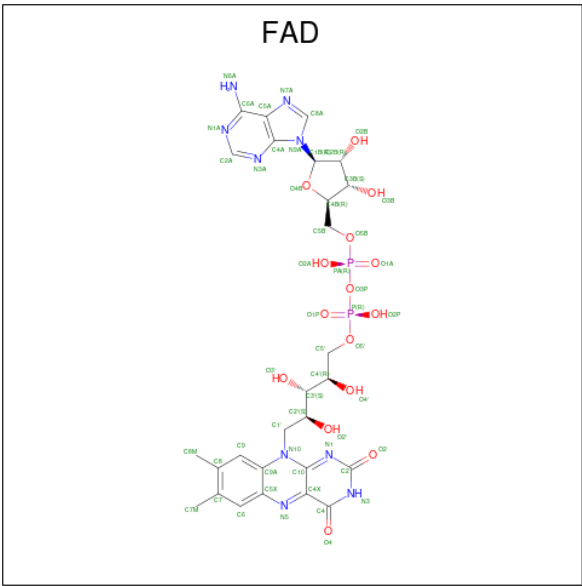
There are 5 unique types of molecules in this entry. The entry contains 17541 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ancestral Flavin-containing monooxygenase (FMO) 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	530	Total	C	N	O	S	0	0	0
			4268	2767	710	767	24			
1	A	530	Total	C	N	O	S	0	0	0
			4268	2767	710	767	24			
1	C	530	Total	C	N	O	S	0	0	0
			4268	2767	710	767	24			
1	D	530	Total	C	N	O	S	0	0	0
			4268	2767	710	767	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



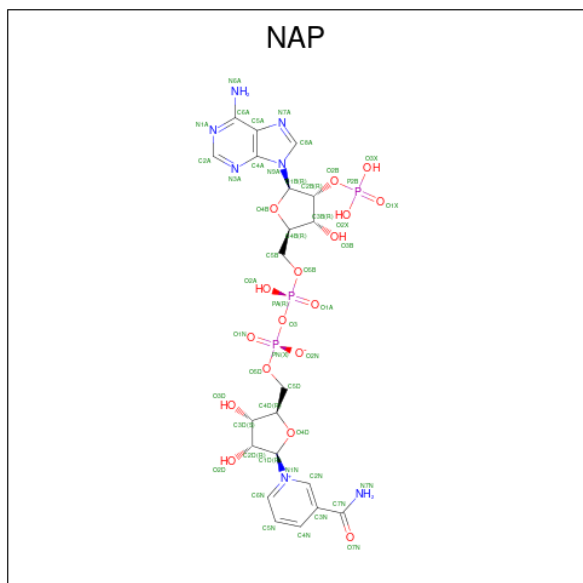
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0
			53	27	9	15	2	
2	A	1	Total	C	N	O	P	0
			53	27	9	15	2	

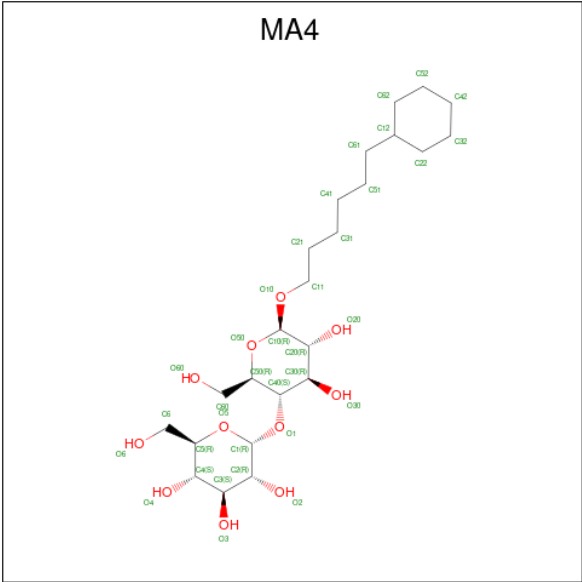
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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
4	D	1	Total	C	O	0	0
			24	13	11		

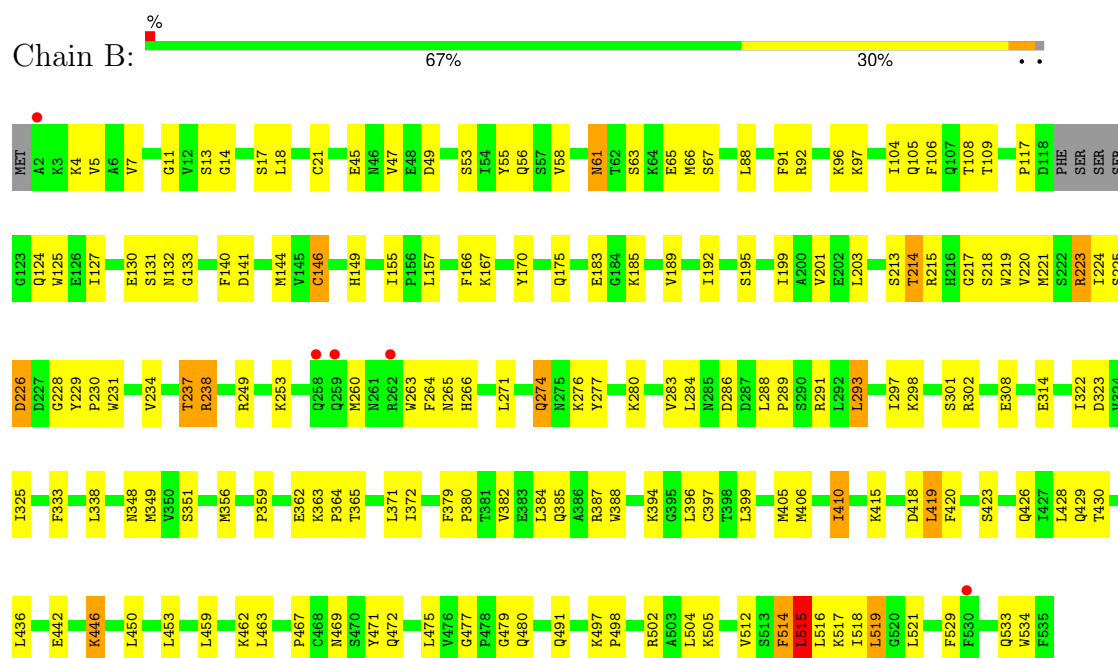
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	12	Total	O	0	0
			12	12		
5	A	10	Total	O	0	0
			10	10		
5	C	8	Total	O	0	0
			8	8		
5	D	11	Total	O	0	0
			11	11		

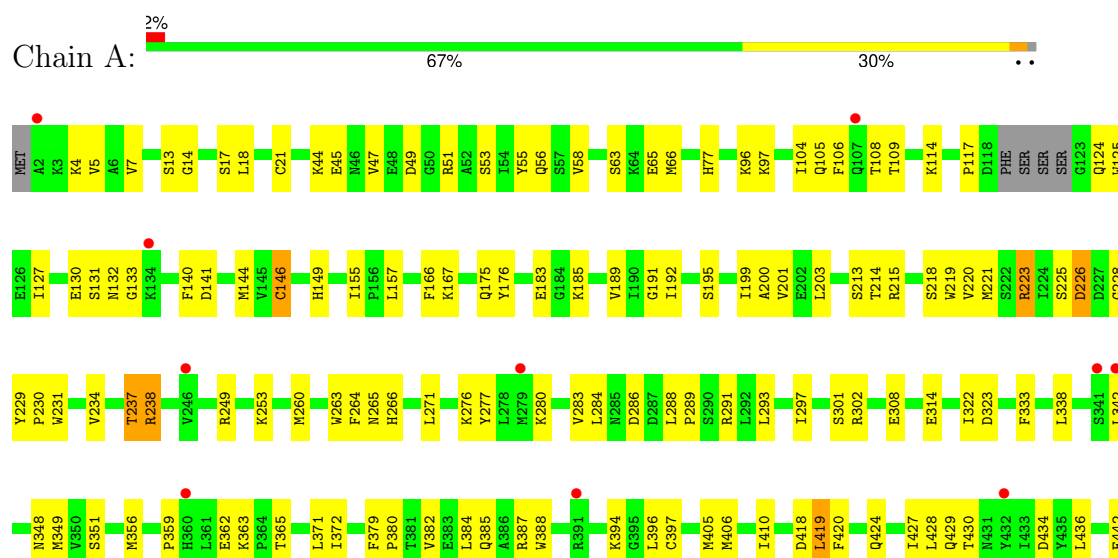
3 Residue-property plots

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: Ancestral Flavin-containing monooxygenase (FMO) 2



• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.75Å 148.68Å 139.12Å 90.00° 97.08° 90.00°	Depositor
Resolution (Å)	138.00 – 3.01 138.06 – 3.01	Depositor EDS
% Data completeness (in resolution range)	51.6 (138.00-3.01) 51.7 (138.06-3.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.211 , 0.285 0.215 , 0.285	Depositor DCC
R_{free} test set	1573 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17541	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MA4, FAD, NAP

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	0.44	0/4375	0.66	0/5914
1	B	0.45	0/4375	0.66	0/5914
1	C	0.45	0/4375	0.67	0/5914
1	D	0.44	0/4375	0.66	0/5914
All	All	0.44	0/17500	0.66	0/23656

There are no bond length outliers.

There are no bond angle outliers.

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	4268	0	4287	100	0
1	B	4268	0	4287	114	0
1	C	4268	0	4287	106	0
1	D	4268	0	4287	111	0
2	A	53	0	31	3	0
2	B	53	0	31	8	0
2	C	53	0	31	3	0
2	D	53	0	31	4	0
3	A	48	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	7	0
3	C	48	0	25	4	0
3	D	48	0	25	5	0
4	D	24	0	21	0	0
5	A	10	0	0	1	0
5	B	12	0	0	1	0
5	C	8	0	0	0	0
5	D	11	0	0	0	0
All	All	17541	0	17393	437	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 13.

All (437) 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:D:47:VAL:HG21	1:D:175:GLN:NE2	1.84	0.92
1:A:47:VAL:HG21	1:A:175:GLN:NE2	1.85	0.91
1:C:47:VAL:HG21	1:C:175:GLN:NE2	1.85	0.91
1:B:47:VAL:HG21	1:B:175:GLN:NE2	1.88	0.87
1:B:47:VAL:HG21	1:B:175:GLN:HE22	1.36	0.85
1:A:47:VAL:HG21	1:A:175:GLN:HE22	1.40	0.85
1:C:215:ARG:HH21	1:C:302:ARG:HD3	1.42	0.84
2:C:601:FAD:HM73	3:C:602:NAP:C5N	2.07	0.84
1:A:215:ARG:HH21	1:A:302:ARG:HD3	1.43	0.84
1:B:215:ARG:HH21	1:B:302:ARG:HD3	1.44	0.83
1:D:47:VAL:HG21	1:D:175:GLN:HE22	1.42	0.82
1:D:215:ARG:HH21	1:D:302:ARG:HD3	1.45	0.81
1:C:47:VAL:HG21	1:C:175:GLN:HE22	1.45	0.79
1:D:192:ILE:HG22	1:D:192:ILE:O	1.81	0.78
1:A:192:ILE:O	1:A:192:ILE:HG22	1.83	0.78
1:C:192:ILE:O	1:C:192:ILE:HG22	1.85	0.75
1:B:192:ILE:HG22	1:B:192:ILE:O	1.84	0.75
1:A:215:ARG:NH2	1:A:302:ARG:HD3	2.04	0.73
1:C:193:GLY:HA3	3:C:602:NAP:O1N	1.88	0.73
1:B:215:ARG:NH2	1:B:302:ARG:HD3	2.05	0.72
1:C:215:ARG:NH2	1:C:302:ARG:HD3	2.05	0.72
1:D:388:TRP:CZ3	1:D:442:GLU:HB3	2.25	0.71
1:A:388:TRP:CZ3	1:A:442:GLU:HB3	2.26	0.70
1:D:215:ARG:NH2	1:D:302:ARG:HD3	2.05	0.70
1:C:388:TRP:CZ3	1:C:442:GLU:HB3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ARG:NH1	1:D:472:GLN:OE1	2.24	0.70
1:B:388:TRP:CZ3	1:B:442:GLU:HB3	2.25	0.70
2:B:601:FAD:HM73	3:B:602:NAP:C5N	2.22	0.69
1:B:238:ARG:NH1	1:B:472:GLN:OE1	2.25	0.68
1:A:238:ARG:NH1	1:A:472:GLN:OE1	2.24	0.68
1:C:238:ARG:NH1	1:C:472:GLN:OE1	2.25	0.67
1:B:217:GLY:HA3	1:D:502:ARG:HH22	1.60	0.66
2:D:601:FAD:HM73	3:D:602:NAP:C4N	2.28	0.64
1:B:293:LEU:HD12	1:D:224:ILE:HD13	1.79	0.63
1:B:55:TYR:CE2	1:B:58:VAL:HG22	2.33	0.63
1:D:223:ARG:HG3	1:D:286:ASP:OD2	1.99	0.63
1:B:4:LYS:N	1:B:141:ASP:OD2	2.32	0.62
1:D:7:VAL:HG21	1:D:18:LEU:HD13	1.82	0.62
1:A:55:TYR:CE2	1:A:58:VAL:HG22	2.35	0.62
1:C:55:TYR:CE2	1:C:58:VAL:HG22	2.35	0.61
1:B:7:VAL:HG21	1:B:18:LEU:HD13	1.82	0.61
1:B:195:SER:O	1:B:199:ILE:HG12	2.00	0.61
1:A:424:GLN:HG3	1:A:427:ILE:HD11	1.83	0.61
1:B:388:TRP:CE3	1:B:442:GLU:HB3	2.37	0.60
1:A:388:TRP:CE3	1:A:442:GLU:HB3	2.36	0.60
1:D:4:LYS:N	1:D:141:ASP:OD2	2.35	0.60
1:C:388:TRP:CE3	1:C:442:GLU:HB3	2.37	0.60
1:D:223:ARG:HD2	1:D:286:ASP:OD1	2.01	0.60
1:B:502:ARG:NH2	1:D:271:LEU:HA	2.17	0.60
1:B:55:TYR:O	1:B:58:VAL:HG23	2.02	0.59
1:A:4:LYS:N	1:A:141:ASP:OD2	2.34	0.59
2:D:601:FAD:HM73	3:D:602:NAP:C5N	2.32	0.59
1:D:55:TYR:CE2	1:D:58:VAL:HG22	2.38	0.59
2:B:601:FAD:C6	3:B:602:NAP:C2N	2.80	0.59
1:D:388:TRP:CE3	1:D:442:GLU:HB3	2.37	0.59
1:B:223:ARG:HG3	1:B:286:ASP:OD2	2.02	0.59
1:C:4:LYS:N	1:C:141:ASP:OD2	2.34	0.59
1:A:7:VAL:HG21	1:A:18:LEU:HD13	1.84	0.59
2:A:601:FAD:HM73	3:A:602:NAP:C5N	2.33	0.59
1:C:220:VAL:HA	1:C:283:VAL:HG22	1.85	0.59
1:C:7:VAL:HG21	1:C:18:LEU:HD13	1.83	0.59
1:B:298:LYS:HG3	1:D:501:THR:HG21	1.85	0.59
1:B:423:SER:OG	1:B:426:GLN:OE1	2.20	0.59
1:D:55:TYR:O	1:D:58:VAL:HG23	2.03	0.59
1:C:362:GLU:HB3	1:D:165:ARG:CZ	2.33	0.58
1:A:512:VAL:O	1:A:512:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:HG3	1:A:286:ASP:OD2	2.02	0.58
1:A:55:TYR:O	1:A:58:VAL:HG23	2.04	0.58
1:A:504:LEU:O	1:A:505:LYS:HG2	2.03	0.58
1:A:125:TRP:HE1	1:A:365:THR:HG23	1.69	0.58
1:C:55:TYR:O	1:C:58:VAL:HG23	2.03	0.58
1:B:45:GLU:OE1	1:B:45:GLU:N	2.36	0.57
1:B:469:ASN:HD21	1:B:491:GLN:HE22	1.52	0.57
1:B:512:VAL:HG12	1:B:512:VAL:O	2.04	0.57
1:C:195:SER:O	1:C:199:ILE:HG12	2.03	0.57
1:B:223:ARG:HD2	1:B:286:ASP:OD1	2.04	0.57
1:B:504:LEU:O	1:B:505:LYS:HG2	2.04	0.57
1:A:195:SER:O	1:A:199:ILE:HG12	2.05	0.56
2:C:601:FAD:HM73	3:C:602:NAP:C4N	2.34	0.56
1:B:288:LEU:HB3	1:B:289:PRO:HD3	1.87	0.56
1:D:195:SER:O	1:D:199:ILE:HG12	2.06	0.56
1:C:504:LEU:O	1:C:505:LYS:HG2	2.05	0.56
1:C:406:MET:O	1:C:410:ILE:HD13	2.06	0.56
1:D:125:TRP:HE1	1:D:365:THR:HG23	1.71	0.56
1:A:469:ASN:HD21	1:A:491:GLN:HE22	1.54	0.56
1:B:125:TRP:HE1	1:B:365:THR:HG23	1.71	0.56
1:C:125:TRP:HE1	1:C:365:THR:HG23	1.71	0.56
1:C:225:SER:OG	1:C:234:VAL:HG21	2.06	0.55
1:A:45:GLU:N	1:A:45:GLU:OE1	2.35	0.55
1:C:223:ARG:NH1	1:C:284:LEU:O	2.34	0.55
1:B:65:GLU:OE1	1:B:471:TYR:OH	2.22	0.55
1:B:225:SER:OG	1:B:234:VAL:HG21	2.07	0.55
1:C:249:ARG:NH2	1:C:419:LEU:HA	2.22	0.55
1:D:505:LYS:CG	1:D:505:LYS:O	2.55	0.55
1:A:127:ILE:HD12	1:A:140:PHE:CD1	2.42	0.55
1:D:406:MET:O	1:D:410:ILE:HD13	2.07	0.55
1:C:127:ILE:HD12	1:C:140:PHE:CD1	2.42	0.55
1:D:505:LYS:O	1:D:505:LYS:HG2	2.05	0.54
1:A:505:LYS:CG	1:A:505:LYS:O	2.55	0.54
1:D:127:ILE:HD12	1:D:140:PHE:CD1	2.43	0.54
1:B:406:MET:O	1:B:410:ILE:HD12	2.07	0.54
1:B:446:LYS:O	1:B:446:LYS:HG3	2.08	0.54
1:A:249:ARG:NH2	1:A:419:LEU:HA	2.22	0.54
1:C:65:GLU:OE1	1:C:471:TYR:OH	2.22	0.54
1:D:249:ARG:NH2	1:D:419:LEU:HA	2.22	0.54
1:C:11:GLY:HA3	2:C:601:FAD:O1P	2.07	0.54
1:A:220:VAL:HA	1:A:283:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:MET:O	1:A:410:ILE:HD13	2.07	0.54
1:C:288:LEU:HB3	1:C:289:PRO:HD3	1.90	0.54
1:D:220:VAL:HA	1:D:283:VAL:HG22	1.89	0.54
1:B:249:ARG:NH2	1:B:419:LEU:HA	2.23	0.54
1:C:349:MET:CE	1:C:410:ILE:HA	2.37	0.54
1:B:127:ILE:HD12	1:B:140:PHE:CD1	2.43	0.54
1:A:225:SER:OG	1:A:234:VAL:HG21	2.08	0.54
1:A:363:LYS:O	1:A:365:THR:HG22	2.08	0.53
1:C:363:LYS:O	1:C:365:THR:HG22	2.07	0.53
1:D:264:PHE:O	1:D:266:HIS:HD2	1.91	0.53
1:D:446:LYS:O	1:D:446:LYS:HG3	2.08	0.53
1:D:469:ASN:HD21	1:D:491:GLN:HE22	1.55	0.53
1:D:225:SER:OG	1:D:234:VAL:HG21	2.08	0.53
1:B:220:VAL:HA	1:B:283:VAL:HG22	1.89	0.53
1:B:505:LYS:CG	1:B:505:LYS:O	2.55	0.53
1:D:45:GLU:OE1	1:D:45:GLU:N	2.36	0.53
1:B:61:ASN:OD1	1:B:61:ASN:N	2.41	0.53
1:D:192:ILE:O	1:D:192:ILE:CG2	2.52	0.53
1:C:192:ILE:O	1:C:192:ILE:CG2	2.55	0.53
1:C:505:LYS:CG	1:C:505:LYS:O	2.56	0.53
1:D:193:GLY:HA3	3:D:602:NAP:O1N	2.09	0.53
1:A:264:PHE:O	1:A:266:HIS:HD2	1.92	0.53
1:C:469:ASN:HD21	1:C:491:GLN:HE22	1.55	0.53
1:B:349:MET:CE	1:B:410:ILE:HA	2.38	0.53
1:A:446:LYS:O	1:A:446:LYS:HG3	2.09	0.53
1:D:288:LEU:HB3	1:D:289:PRO:HD3	1.90	0.53
1:A:288:LEU:HB3	1:A:289:PRO:HD3	1.92	0.52
1:B:219:TRP:HB3	1:B:260:MET:HE2	1.91	0.52
1:D:349:MET:CE	1:D:410:ILE:HA	2.40	0.52
1:B:264:PHE:CE1	1:B:289:PRO:HG3	2.45	0.52
1:B:363:LYS:O	1:B:365:THR:HG22	2.09	0.52
1:A:192:ILE:O	1:A:192:ILE:CG2	2.54	0.52
1:D:363:LYS:O	1:D:365:THR:HG22	2.09	0.52
1:B:264:PHE:O	1:B:266:HIS:HD2	1.93	0.51
1:C:264:PHE:O	1:C:266:HIS:HD2	1.93	0.51
1:B:104:ILE:HG21	1:B:106:PHE:CE1	2.45	0.51
1:B:238:ARG:HG3	1:B:238:ARG:HH11	1.74	0.51
1:B:192:ILE:O	1:B:192:ILE:CG2	2.54	0.51
1:B:192:ILE:HG21	1:B:218:SER:HB3	1.92	0.51
1:C:104:ILE:HG21	1:C:106:PHE:CE1	2.45	0.51
1:C:238:ARG:HG3	1:C:238:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:HD23	1:B:387:ARG:HD3	1.93	0.51
1:A:104:ILE:HG21	1:A:106:PHE:CE1	2.46	0.51
1:B:394:LYS:CB	1:B:396:LEU:HD13	2.41	0.51
2:A:601:FAD:C10	2:A:601:FAD:O2'	2.59	0.51
1:C:131:SER:O	1:C:133:GLY:N	2.44	0.51
1:D:104:ILE:HG21	1:D:106:PHE:CE1	2.45	0.51
1:A:349:MET:CE	1:A:410:ILE:HA	2.40	0.51
1:D:65:GLU:OE1	1:D:471:TYR:OH	2.25	0.51
1:C:446:LYS:HG3	1:C:446:LYS:O	2.09	0.50
1:B:131:SER:O	1:B:133:GLY:N	2.45	0.50
1:B:394:LYS:HB3	1:B:396:LEU:HD13	1.93	0.50
1:C:264:PHE:CE1	1:C:289:PRO:HG3	2.47	0.50
2:B:601:FAD:H5'1	5:B:707:HOH:O	2.10	0.50
1:A:225:SER:O	1:A:226:ASP:C	2.50	0.50
1:D:519:LEU:HD13	1:D:519:LEU:H	1.77	0.50
1:B:217:GLY:CA	1:D:502:ARG:HH22	2.24	0.50
3:B:602:NAP:O5D	3:B:602:NAP:O2A	2.29	0.50
1:A:238:ARG:HG3	1:A:238:ARG:HH11	1.76	0.50
1:C:192:ILE:HG21	1:C:218:SER:HB3	1.94	0.50
1:C:225:SER:O	1:C:226:ASP:C	2.50	0.50
1:A:477:GLY:O	1:A:480:GLN:NE2	2.26	0.50
1:B:519:LEU:HD13	1:B:519:LEU:H	1.77	0.50
1:A:264:PHE:CE1	1:A:289:PRO:HG3	2.46	0.50
1:C:360:HIS:HA	1:C:402:GLU:OE2	2.11	0.49
1:C:519:LEU:HD13	1:C:519:LEU:H	1.77	0.49
1:D:155:ILE:HG22	1:D:157:LEU:HG	1.93	0.49
1:D:396:LEU:N	1:D:396:LEU:HD12	2.27	0.49
1:A:131:SER:O	1:A:133:GLY:N	2.45	0.49
1:D:382:VAL:HA	1:D:385:GLN:HB2	1.94	0.49
1:B:225:SER:O	1:B:226:ASP:C	2.50	0.49
1:D:301:SER:OG	1:D:314:GLU:HB3	2.12	0.49
1:B:224:ILE:HD13	1:D:293:LEU:HD12	1.93	0.49
1:D:192:ILE:HG21	1:D:218:SER:HB3	1.94	0.49
1:A:65:GLU:OE1	1:A:471:TYR:OH	2.25	0.49
1:B:63:SER:O	1:B:67:SER:OG	2.23	0.49
1:B:301:SER:OG	1:B:314:GLU:HB3	2.13	0.49
1:B:453:LEU:HD23	1:B:453:LEU:O	2.13	0.49
1:C:263:TRP:CH2	1:C:289:PRO:HG2	2.48	0.49
1:A:519:LEU:N	1:A:519:LEU:HD22	2.27	0.49
1:C:301:SER:OG	1:C:314:GLU:HB3	2.13	0.49
1:C:372:ILE:HA	1:C:428:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:TRP:CH2	1:B:289:PRO:HG2	2.47	0.49
1:D:225:SER:O	1:D:226:ASP:C	2.50	0.49
1:D:264:PHE:CE1	1:D:289:PRO:HG3	2.48	0.49
1:D:388:TRP:CZ3	1:D:397:CYS:HB3	2.48	0.49
1:D:519:LEU:N	1:D:519:LEU:HD22	2.28	0.49
1:A:459:LEU:O	1:A:462:LYS:N	2.46	0.48
1:C:459:LEU:O	1:C:462:LYS:N	2.46	0.48
1:D:13:SER:HB2	1:D:146:CYS:HB3	1.95	0.48
1:D:131:SER:O	1:D:133:GLY:N	2.45	0.48
1:B:459:LEU:O	1:B:462:LYS:N	2.46	0.48
1:D:329:THR:HA	3:D:602:NAP:O4B	2.14	0.48
1:C:344:LYS:HD2	1:D:318:VAL:HB	1.95	0.48
1:D:459:LEU:O	1:D:462:LYS:N	2.47	0.48
1:B:382:VAL:HA	1:B:385:GLN:HB2	1.95	0.48
1:A:505:LYS:O	1:A:505:LYS:HG3	2.14	0.48
1:B:519:LEU:N	1:B:519:LEU:HD22	2.28	0.48
1:A:519:LEU:HD13	1:A:519:LEU:H	1.78	0.48
1:C:497:LYS:N	1:C:498:PRO:HD2	2.28	0.48
1:D:238:ARG:HG3	1:D:238:ARG:HH11	1.78	0.48
1:B:155:ILE:HG22	1:B:157:LEU:HG	1.96	0.48
1:C:519:LEU:N	1:C:519:LEU:HD22	2.29	0.48
1:D:263:TRP:CH2	1:D:289:PRO:HG2	2.49	0.48
1:B:66:MET:CE	1:B:467:PRO:HB2	2.43	0.48
1:A:301:SER:OG	1:A:314:GLU:HB3	2.13	0.48
1:C:237:THR:O	1:C:238:ARG:C	2.52	0.48
1:C:394:LYS:CB	1:C:396:LEU:HD13	2.44	0.48
1:B:237:THR:O	1:B:238:ARG:C	2.52	0.48
1:A:263:TRP:CH2	1:A:289:PRO:HG2	2.48	0.48
1:B:61:ASN:OD1	2:B:601:FAD:O4	2.32	0.47
1:A:199:ILE:HG22	1:A:203:LEU:HD12	1.96	0.47
1:C:199:ILE:HG22	1:C:203:LEU:HD12	1.95	0.47
1:C:219:TRP:HB3	1:C:260:MET:HE2	1.95	0.47
1:A:66:MET:CE	1:A:467:PRO:HB2	2.44	0.47
1:A:237:THR:O	1:A:238:ARG:C	2.52	0.47
1:B:514:PHE:HB3	1:B:515:LEU:H	1.58	0.47
1:D:237:THR:O	1:D:238:ARG:C	2.52	0.47
1:B:199:ILE:HG22	1:B:203:LEU:HD12	1.96	0.47
1:A:394:LYS:CB	1:A:396:LEU:HD13	2.45	0.47
1:C:105:GLN:O	1:C:108:THR:OG1	2.33	0.47
1:C:13:SER:HB2	1:C:146:CYS:HB3	1.95	0.47
1:B:21:CYS:SG	1:B:144:MET:CE	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:O	1:C:185:LYS:HG3	2.15	0.47
1:B:14:GLY:O	1:B:18:LEU:HB2	2.15	0.47
1:D:66:MET:CE	1:D:467:PRO:HB2	2.45	0.47
1:B:388:TRP:CZ3	1:B:397:CYS:HB3	2.49	0.47
1:C:463:LEU:HA	1:C:472:GLN:NE2	2.30	0.47
1:B:13:SER:HB2	1:B:146:CYS:HB3	1.96	0.46
1:A:105:GLN:O	1:A:108:THR:OG1	2.33	0.46
1:A:382:VAL:HA	1:A:385:GLN:HB2	1.97	0.46
1:C:149:HIS:HB2	1:C:333:PHE:HB3	1.97	0.46
1:A:14:GLY:O	1:A:18:LEU:HB2	2.15	0.46
1:D:231:TRP:CE2	1:D:284:LEU:HD21	2.51	0.46
1:D:372:ILE:HA	1:D:428:LEU:HB3	1.97	0.46
1:B:514:PHE:HD2	1:B:514:PHE:HA	1.66	0.46
1:D:105:GLN:O	1:D:108:THR:OG1	2.33	0.46
1:B:105:GLN:O	1:B:108:THR:OG1	2.33	0.46
1:B:505:LYS:O	1:B:505:LYS:HG3	2.16	0.46
1:C:384:LEU:HD23	1:C:387:ARG:HD3	1.98	0.46
1:B:11:GLY:HA3	2:B:601:FAD:O1P	2.15	0.46
3:B:602:NAP:H52N	3:B:602:NAP:C6N	2.45	0.46
1:A:497:LYS:N	1:A:498:PRO:HD2	2.31	0.46
1:C:388:TRP:CZ3	1:C:397:CYS:HB3	2.51	0.46
1:D:463:LEU:HA	1:D:472:GLN:NE2	2.30	0.46
1:D:477:GLY:O	1:D:480:GLN:NE2	2.27	0.46
1:B:21:CYS:SG	1:B:144:MET:HE1	2.56	0.46
1:A:77:HIS:HB3	5:A:710:HOH:O	2.15	0.46
1:C:231:TRP:CE2	1:C:284:LEU:HD21	2.50	0.46
1:D:219:TRP:HB3	1:D:260:MET:HE2	1.96	0.46
1:C:477:GLY:O	1:C:480:GLN:NE2	2.28	0.46
1:A:183:GLU:O	1:A:185:LYS:HG3	2.16	0.46
1:A:424:GLN:HE21	1:A:427:ILE:CD1	2.29	0.46
1:D:21:CYS:SG	1:D:144:MET:CE	3.03	0.46
1:A:379:PHE:N	1:A:380:PRO:HD2	2.31	0.46
1:B:372:ILE:HA	1:B:428:LEU:HB3	1.97	0.45
1:A:463:LEU:HA	1:A:472:GLN:NE2	2.30	0.45
1:A:13:SER:HB2	1:A:146:CYS:HB3	1.97	0.45
1:A:372:ILE:HA	1:A:428:LEU:HB3	1.97	0.45
1:C:66:MET:CE	1:C:467:PRO:HB2	2.47	0.45
1:D:497:LYS:N	1:D:498:PRO:HD2	2.31	0.45
1:C:396:LEU:N	1:C:396:LEU:HD12	2.31	0.45
1:B:183:GLU:O	1:B:185:LYS:HG3	2.16	0.45
1:A:155:ILE:HG22	1:A:157:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:MET:HE1	1:B:410:ILE:HA	1.98	0.45
1:A:192:ILE:HG21	1:A:218:SER:HB3	1.98	0.45
1:C:384:LEU:HD12	1:C:436:LEU:HG	1.99	0.45
1:D:201:VAL:HA	1:D:297:ILE:HD11	1.99	0.45
1:A:384:LEU:HD23	1:A:387:ARG:HD3	1.98	0.45
1:C:201:VAL:HA	1:C:297:ILE:HD11	1.97	0.45
1:C:505:LYS:O	1:C:505:LYS:HG3	2.17	0.45
1:C:419:LEU:HD22	1:C:420:PHE:CZ	2.52	0.45
1:D:14:GLY:O	1:D:18:LEU:HB2	2.16	0.45
1:D:394:LYS:CB	1:D:396:LEU:HD13	2.47	0.45
1:A:419:LEU:HD22	1:A:420:PHE:CZ	2.52	0.45
1:D:183:GLU:O	1:D:185:LYS:HG3	2.17	0.45
1:C:360:HIS:HE1	1:D:320:GLU:OE2	1.99	0.45
1:C:379:PHE:N	1:C:380:PRO:HD2	2.31	0.45
1:D:349:MET:HE1	1:D:410:ILE:HA	1.99	0.45
1:C:45:GLU:OE1	1:C:45:GLU:N	2.33	0.44
1:D:384:LEU:HD12	1:D:436:LEU:HG	1.99	0.44
1:B:420:PHE:CD2	1:B:429:GLN:HG2	2.52	0.44
1:C:14:GLY:O	1:C:18:LEU:HB2	2.17	0.44
1:B:214:THR:HA	3:B:602:NAP:H2A	1.98	0.44
1:B:265:ASN:C	1:B:265:ASN:OD1	2.56	0.44
1:A:21:CYS:SG	1:A:144:MET:CE	3.05	0.44
1:C:21:CYS:SG	1:C:144:MET:CE	3.06	0.44
2:B:601:FAD:HM73	3:B:602:NAP:C4N	2.48	0.44
1:A:396:LEU:N	1:A:396:LEU:HD12	2.32	0.44
1:C:382:VAL:HA	1:C:385:GLN:HB2	1.98	0.44
2:D:601:FAD:C6	3:D:602:NAP:C2N	2.95	0.44
1:B:384:LEU:HD12	1:B:436:LEU:HG	1.98	0.44
1:B:497:LYS:N	1:B:498:PRO:HD2	2.33	0.44
1:A:349:MET:HE1	1:A:410:ILE:HA	1.99	0.44
1:A:394:LYS:HB3	1:A:396:LEU:HD13	1.99	0.44
1:D:265:ASN:OD1	1:D:265:ASN:C	2.56	0.44
1:D:384:LEU:HD23	1:D:387:ARG:HD3	1.99	0.44
1:B:477:GLY:O	1:B:480:GLN:NE2	2.26	0.44
1:D:219:TRP:HB3	1:D:260:MET:CE	2.47	0.44
1:B:201:VAL:HA	1:B:297:ILE:HD11	1.99	0.44
1:C:219:TRP:HB3	1:C:260:MET:CE	2.47	0.44
1:B:149:HIS:HB2	1:B:333:PHE:HB3	2.00	0.44
1:C:394:LYS:HB3	1:C:396:LEU:HD13	2.00	0.44
1:C:429:GLN:HE21	1:C:429:GLN:HA	1.83	0.44
1:D:379:PHE:N	1:D:380:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:HB3	1:C:216:HIS:CD2	2.53	0.43
1:C:420:PHE:CD2	1:C:429:GLN:HG2	2.53	0.43
1:D:199:ILE:HG22	1:D:203:LEU:HD12	1.99	0.43
1:B:364:PRO:HB3	1:B:399:LEU:HD11	2.00	0.43
1:B:419:LEU:HD22	1:B:420:PHE:CZ	2.52	0.43
1:A:420:PHE:CD2	1:A:429:GLN:HG2	2.52	0.43
1:C:274:GLN:HE21	1:C:274:GLN:HA	1.83	0.43
1:D:420:PHE:CD2	1:D:429:GLN:HG2	2.53	0.43
1:B:249:ARG:HH22	1:B:419:LEU:HA	1.82	0.43
1:A:201:VAL:HA	1:A:297:ILE:HD11	1.99	0.43
1:A:424:GLN:HE21	1:A:427:ILE:HD13	1.83	0.43
1:D:223:ARG:HG3	1:D:223:ARG:H	1.54	0.43
1:D:463:LEU:HD23	1:D:472:GLN:NE2	2.34	0.43
1:C:497:LYS:N	1:C:498:PRO:CD	2.82	0.43
1:B:274:GLN:HE21	1:B:274:GLN:HA	1.81	0.43
1:A:191:GLY:HA2	3:A:602:NAP:H1B	1.99	0.43
1:D:149:HIS:HB2	1:D:333:PHE:HB3	2.00	0.43
1:B:223:ARG:HG3	1:B:223:ARG:H	1.64	0.43
1:A:388:TRP:CZ3	1:A:397:CYS:HB3	2.53	0.43
1:C:21:CYS:SG	1:C:144:MET:HE1	2.59	0.43
1:B:66:MET:HE2	1:B:467:PRO:HB2	2.01	0.43
1:A:231:TRP:CE2	1:A:284:LEU:HD21	2.53	0.43
1:A:265:ASN:OD1	1:A:265:ASN:C	2.56	0.43
1:B:253:LYS:HE2	1:B:276:LYS:HB2	2.00	0.43
1:B:463:LEU:HA	1:B:472:GLN:NE2	2.34	0.43
1:A:166:PHE:HA	1:A:308:GLU:HA	2.01	0.43
1:A:499:LEU:O	1:A:501:THR:HG22	2.19	0.43
1:D:7:VAL:HG23	1:D:7:VAL:O	2.19	0.43
1:B:88:LEU:HD21	1:B:92:ARG:HH21	1.84	0.43
1:B:225:SER:HB3	1:B:229:TYR:O	2.19	0.43
1:C:265:ASN:OD1	1:C:265:ASN:C	2.57	0.43
1:B:231:TRP:CE2	1:B:284:LEU:HD21	2.54	0.42
1:D:221:MET:CE	1:D:284:LEU:HD11	2.49	0.42
1:B:221:MET:CE	1:B:284:LEU:HD11	2.50	0.42
2:B:601:FAD:HM73	3:B:602:NAP:C6N	2.48	0.42
1:C:225:SER:HB3	1:C:229:TYR:O	2.20	0.42
1:B:359:PRO:HA	1:B:405:MET:CE	2.49	0.42
1:A:384:LEU:HD12	1:A:436:LEU:HG	2.00	0.42
1:D:192:ILE:CG2	1:D:283:VAL:HG11	2.49	0.42
1:D:253:LYS:HE2	1:D:276:LYS:HB2	2.00	0.42
1:B:63:SER:HB2	1:B:230:PRO:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HD12	1:B:450:LEU:HA	1.94	0.42
1:C:225:SER:O	1:C:228:GLY:N	2.53	0.42
1:D:499:LEU:O	1:D:501:THR:HG22	2.19	0.42
1:B:379:PHE:N	1:B:380:PRO:HD2	2.34	0.42
1:A:225:SER:HB3	1:A:229:TYR:O	2.20	0.42
1:A:359:PRO:HA	1:A:405:MET:HE2	2.01	0.42
1:D:419:LEU:HD22	1:D:420:PHE:CZ	2.54	0.42
1:D:429:GLN:HE21	1:D:429:GLN:HA	1.84	0.42
1:B:219:TRP:HB3	1:B:260:MET:CE	2.49	0.42
1:A:7:VAL:HG23	1:A:7:VAL:O	2.20	0.42
1:A:497:LYS:N	1:A:498:PRO:CD	2.82	0.42
1:C:483:GLY:HA2	1:C:486:ASN:HB3	2.01	0.42
1:B:225:SER:O	1:B:228:GLY:N	2.53	0.42
1:B:396:LEU:HD12	1:B:396:LEU:N	2.35	0.42
1:C:359:PRO:HA	1:C:405:MET:CE	2.50	0.42
1:D:63:SER:HB2	1:D:230:PRO:CB	2.50	0.42
1:D:176:TYR:CD2	1:D:199:ILE:CD1	3.03	0.42
1:A:176:TYR:CD2	1:A:199:ILE:CD1	3.03	0.42
1:C:463:LEU:HD23	1:C:472:GLN:NE2	2.35	0.42
1:A:192:ILE:CG2	1:A:283:VAL:HG11	2.50	0.42
1:C:63:SER:HB2	1:C:230:PRO:CB	2.50	0.42
1:D:225:SER:O	1:D:228:GLY:N	2.53	0.42
1:B:61:ASN:OD1	2:B:601:FAD:C4	2.68	0.41
1:B:497:LYS:N	1:B:498:PRO:CD	2.83	0.41
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.90	0.41
1:C:7:VAL:O	1:C:7:VAL:HG23	2.20	0.41
1:C:8:ILE:HD12	1:C:110:VAL:HG11	2.02	0.41
1:C:364:PRO:HB3	1:C:399:LEU:HD11	2.02	0.41
1:C:176:TYR:CD2	1:C:199:ILE:CD1	3.04	0.41
1:B:192:ILE:CG2	1:B:283:VAL:HG11	2.49	0.41
1:A:225:SER:O	1:A:228:GLY:N	2.53	0.41
1:C:221:MET:CE	1:C:284:LEU:HD11	2.50	0.41
1:D:41:TRP:CD2	1:D:87:LEU:HD23	2.56	0.41
1:D:44:LYS:CG	1:D:51:ARG:HH22	2.34	0.41
1:D:225:SER:HB3	1:D:229:TYR:O	2.20	0.41
1:A:63:SER:HB2	1:A:230:PRO:CB	2.49	0.41
1:A:221:MET:CE	1:A:284:LEU:HD11	2.50	0.41
1:A:463:LEU:HD23	1:A:472:GLN:NE2	2.35	0.41
1:D:21:CYS:SG	1:D:144:MET:HE1	2.60	0.41
1:D:44:LYS:HG3	1:D:51:ARG:HH22	1.86	0.41
1:D:63:SER:O	1:D:67:SER:OG	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PRO:HA	1:A:405:MET:CE	2.51	0.41
1:D:497:LYS:N	1:D:498:PRO:CD	2.83	0.41
1:B:7:VAL:HG23	1:B:7:VAL:O	2.21	0.41
1:A:149:HIS:HB2	1:A:333:PHE:HB3	2.02	0.41
1:A:219:TRP:HB3	1:A:260:MET:CE	2.50	0.41
1:A:483:GLY:HA2	1:A:486:ASN:HB3	2.03	0.41
2:A:601:FAD:O2'	2:A:601:FAD:N1	2.52	0.41
1:C:41:TRP:CD2	1:C:87:LEU:HD23	2.55	0.41
1:C:253:LYS:HE2	1:C:276:LYS:HB2	2.02	0.41
1:C:499:LEU:O	1:C:501:THR:HG22	2.20	0.41
1:A:515:LEU:HD13	1:A:515:LEU:HA	1.88	0.41
1:C:155:ILE:HG22	1:C:157:LEU:HG	2.02	0.41
1:C:362:GLU:HB3	1:D:165:ARG:NH1	2.36	0.41
1:D:249:ARG:HH22	1:D:419:LEU:HA	1.84	0.41
1:A:429:GLN:HA	1:A:429:GLN:HE21	1.85	0.41
1:C:396:LEU:N	1:C:396:LEU:CD1	2.84	0.41
1:D:396:LEU:N	1:D:396:LEU:CD1	2.84	0.41
1:B:88:LEU:O	1:B:91:PHE:HB2	2.21	0.41
1:B:170:TYR:HA	1:B:325:ILE:O	2.21	0.41
1:B:359:PRO:HA	1:B:405:MET:HE2	2.02	0.41
1:A:44:LYS:HG3	1:A:51:ARG:HH22	1.86	0.41
1:B:396:LEU:N	1:B:396:LEU:CD1	2.84	0.40
1:C:199:ILE:O	1:C:200:ALA:C	2.60	0.40
1:C:515:LEU:HD13	1:C:515:LEU:HA	1.91	0.40
1:D:166:PHE:HA	1:D:308:GLU:HA	2.03	0.40
1:D:438:GLU:HA	1:D:441:LEU:HD12	2.03	0.40
1:D:453:LEU:HD23	1:D:453:LEU:O	2.21	0.40
1:C:170:TYR:HA	1:C:325:ILE:O	2.21	0.40
1:B:463:LEU:HD23	1:B:472:GLN:NE2	2.37	0.40
1:C:44:LYS:CG	1:C:51:ARG:HH22	2.33	0.40
1:D:332:THR:OG1	1:D:333:PHE:N	2.54	0.40
1:A:199:ILE:O	1:A:200:ALA:C	2.60	0.40
1:A:396:LEU:N	1:A:396:LEU:CD1	2.84	0.40
1:C:192:ILE:CG2	1:C:283:VAL:HG11	2.52	0.40
1:C:193:GLY:CA	3:C:602:NAP:O1N	2.64	0.40
1:D:449:LEU:O	1:D:452:LEU:N	2.55	0.40
1:D:504:LEU:O	1:D:505:LYS:HG2	2.21	0.40
2:D:601:FAD:O2'	2:D:601:FAD:C10	2.70	0.40
1:B:166:PHE:HA	1:B:308:GLU:HA	2.03	0.40
1:A:253:LYS:HE2	1:A:276:LYS:HB2	2.04	0.40
1:A:450:LEU:HD12	1:A:450:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:PHE:HA	1:C:308:GLU:HA	2.03	0.40
1:D:199:ILE:O	1:D:200:ALA:C	2.59	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	526/535 (98%)	452 (86%)	65 (12%)	9 (2%)	9	37
1	B	526/535 (98%)	454 (86%)	63 (12%)	9 (2%)	9	37
1	C	526/535 (98%)	454 (86%)	63 (12%)	9 (2%)	9	37
1	D	526/535 (98%)	451 (86%)	65 (12%)	10 (2%)	8	34
All	All	2104/2140 (98%)	1811 (86%)	256 (12%)	37 (2%)	8	35

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	LYS
1	B	132	ASN
1	B	280	LYS
1	A	132	ASN
1	A	280	LYS
1	C	132	ASN
1	C	479	GLY
1	D	132	ASN
1	D	280	LYS
1	D	479	GLY
1	D	533	GLN
1	B	117	PRO
1	B	167	LYS

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Mol	Chain	Res	Type
1	B	515	LEU
1	B	533	GLN
1	A	117	PRO
1	A	167	LYS
1	A	226	ASP
1	A	479	GLY
1	A	514	PHE
1	A	516	LEU
1	C	167	LYS
1	C	515	LEU
1	C	533	GLN
1	D	117	PRO
1	D	167	LYS
1	D	515	LEU
1	D	516	LEU
1	B	226	ASP
1	B	479	GLY
1	B	516	LEU
1	C	117	PRO
1	C	226	ASP
1	C	516	LEU
1	A	533	GLN
1	D	226	ASP
1	D	505	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	472/477 (99%)	426 (90%)	46 (10%)	8	29
1	B	472/477 (99%)	426 (90%)	46 (10%)	8	29
1	C	472/477 (99%)	422 (89%)	50 (11%)	6	25
1	D	472/477 (99%)	424 (90%)	48 (10%)	7	27
All	All	1888/1908 (99%)	1698 (90%)	190 (10%)	7	27

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	VAL
1	B	17	SER
1	B	49	ASP
1	B	53	SER
1	B	56	GLN
1	B	61	ASN
1	B	96	LYS
1	B	97	LYS
1	B	109	THR
1	B	124	GLN
1	B	130	GLU
1	B	146	CYS
1	B	189	VAL
1	B	213	SER
1	B	214	THR
1	B	223	ARG
1	B	237	THR
1	B	238	ARG
1	B	271	LEU
1	B	274	GLN
1	B	277	TYR
1	B	291	ARG
1	B	293	LEU
1	B	322	ILE
1	B	323	ASP
1	B	338	LEU
1	B	348	ASN
1	B	351	SER
1	B	356	MET
1	B	362	GLU
1	B	371	LEU
1	B	410	ILE
1	B	415	LYS
1	B	418	ASP
1	B	419	LEU
1	B	430	THR
1	B	446	LYS
1	B	475	LEU
1	B	514	PHE
1	B	515	LEU
1	B	517	LYS
1	B	518	ILE

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Mol	Chain	Res	Type
1	B	519	LEU
1	B	521	LEU
1	B	529	PHE
1	B	534	TRP
1	A	5	VAL
1	A	17	SER
1	A	49	ASP
1	A	53	SER
1	A	56	GLN
1	A	96	LYS
1	A	97	LYS
1	A	109	THR
1	A	114	LYS
1	A	124	GLN
1	A	130	GLU
1	A	146	CYS
1	A	189	VAL
1	A	213	SER
1	A	214	THR
1	A	223	ARG
1	A	237	THR
1	A	238	ARG
1	A	271	LEU
1	A	277	TYR
1	A	291	ARG
1	A	293	LEU
1	A	322	ILE
1	A	323	ASP
1	A	338	LEU
1	A	348	ASN
1	A	351	SER
1	A	356	MET
1	A	362	GLU
1	A	371	LEU
1	A	418	ASP
1	A	419	LEU
1	A	430	THR
1	A	434	ASP
1	A	446	LYS
1	A	450	LEU
1	A	453	LEU
1	A	475	LEU

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Mol	Chain	Res	Type
1	A	502	ARG
1	A	514	PHE
1	A	515	LEU
1	A	518	ILE
1	A	519	LEU
1	A	521	LEU
1	A	529	PHE
1	A	534	TRP
1	C	5	VAL
1	C	17	SER
1	C	45	GLU
1	C	49	ASP
1	C	53	SER
1	C	56	GLN
1	C	76	GLU
1	C	96	LYS
1	C	97	LYS
1	C	109	THR
1	C	114	LYS
1	C	130	GLU
1	C	146	CYS
1	C	189	VAL
1	C	213	SER
1	C	214	THR
1	C	237	THR
1	C	238	ARG
1	C	271	LEU
1	C	274	GLN
1	C	277	TYR
1	C	291	ARG
1	C	293	LEU
1	C	300	LYS
1	C	322	ILE
1	C	323	ASP
1	C	338	LEU
1	C	348	ASN
1	C	351	SER
1	C	356	MET
1	C	362	GLU
1	C	371	LEU
1	C	418	ASP
1	C	419	LEU

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Mol	Chain	Res	Type
1	C	427	ILE
1	C	430	THR
1	C	446	LYS
1	C	453	LEU
1	C	475	LEU
1	C	482	GLU
1	C	493	GLN
1	C	509	ASN
1	C	514	PHE
1	C	515	LEU
1	C	517	LYS
1	C	518	ILE
1	C	519	LEU
1	C	521	LEU
1	C	529	PHE
1	C	534	TRP
1	D	5	VAL
1	D	17	SER
1	D	49	ASP
1	D	53	SER
1	D	56	GLN
1	D	96	LYS
1	D	97	LYS
1	D	109	THR
1	D	130	GLU
1	D	146	CYS
1	D	189	VAL
1	D	213	SER
1	D	214	THR
1	D	223	ARG
1	D	227	ASP
1	D	237	THR
1	D	238	ARG
1	D	271	LEU
1	D	274	GLN
1	D	277	TYR
1	D	291	ARG
1	D	293	LEU
1	D	300	LYS
1	D	322	ILE
1	D	323	ASP
1	D	338	LEU

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Mol	Chain	Res	Type
1	D	348	ASN
1	D	351	SER
1	D	356	MET
1	D	362	GLU
1	D	371	LEU
1	D	411	LYS
1	D	418	ASP
1	D	419	LEU
1	D	427	ILE
1	D	430	THR
1	D	446	LYS
1	D	475	LEU
1	D	509	ASN
1	D	514	PHE
1	D	515	LEU
1	D	517	LYS
1	D	518	ILE
1	D	519	LEU
1	D	521	LEU
1	D	529	PHE
1	D	532	LEU
1	D	534	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	84	ASN
1	B	175	GLN
1	B	266	HIS
1	B	274	GLN
1	B	469	ASN
1	B	509	ASN
1	A	84	ASN
1	A	175	GLN
1	A	266	HIS
1	A	424	GLN
1	A	469	ASN
1	A	509	ASN
1	C	84	ASN
1	C	124	GLN
1	C	175	GLN
1	C	266	HIS

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Mol	Chain	Res	Type
1	C	274	GLN
1	C	469	ASN
1	C	509	ASN
1	D	84	ASN
1	D	175	GLN
1	D	258	GLN
1	D	266	HIS
1	D	274	GLN
1	D	469	ASN
1	D	509	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	D	602	-	46,52,52	1.13	5 (10%)	61,80,80	1.79	10 (16%)
2	FAD	C	601	-	54,58,58	1.73	10 (18%)	71,89,89	1.72	18 (25%)
3	NAP	C	602	-	46,52,52	1.18	5 (10%)	61,80,80	1.81	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	601	-	54,58,58	1.45	8 (14%)	71,89,89	1.80	17 (23%)
4	MA4	D	603	-	25,25,37	1.04	1 (4%)	36,36,50	1.63	3 (8%)
2	FAD	D	601	-	54,58,58	1.57	9 (16%)	71,89,89	1.64	17 (23%)
2	FAD	A	601	-	54,58,58	1.64	10 (18%)	71,89,89	1.69	18 (25%)
3	NAP	B	602	-	46,52,52	1.16	5 (10%)	61,80,80	1.80	15 (24%)
3	NAP	A	602	-	46,52,52	1.22	5 (10%)	61,80,80	1.71	8 (13%)

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	D	602	-	-	1/31/67/67	0/5/5/5
2	FAD	C	601	-	-	8/30/50/50	0/6/6/6
3	NAP	C	602	-	-	7/31/67/67	0/5/5/5
2	FAD	B	601	-	-	11/30/50/50	0/6/6/6
4	MA4	D	603	-	-	6/10/50/66	0/2/2/3
2	FAD	D	601	-	-	11/30/50/50	0/6/6/6
2	FAD	A	601	-	-	11/30/50/50	0/6/6/6
3	NAP	B	602	-	-	11/31/67/67	0/5/5/5
3	NAP	A	602	-	-	9/31/67/67	0/5/5/5

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C9A-C5X	6.43	1.51	1.41
2	C	601	FAD	C9A-C5X	6.42	1.51	1.41
2	D	601	FAD	C9A-C5X	5.73	1.50	1.41
2	B	601	FAD	C9A-C5X	5.07	1.49	1.41
2	D	601	FAD	PA-O3P	3.91	1.63	1.59
4	D	603	MA4	O10-C10	3.86	1.46	1.40
2	C	601	FAD	PA-O3P	3.67	1.63	1.59
2	A	601	FAD	C8-C7	3.55	1.49	1.40
2	D	601	FAD	C8-C7	3.54	1.49	1.40
2	C	601	FAD	C8-C7	3.42	1.49	1.40
2	C	601	FAD	P-O3P	3.40	1.63	1.59
3	C	602	NAP	PA-O3	3.36	1.63	1.59
3	A	602	NAP	PA-O3	3.35	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C10-N10	3.29	1.44	1.37
2	B	601	FAD	C8-C7	3.27	1.48	1.40
3	A	602	NAP	P2B-O2B	3.24	1.65	1.59
3	D	602	NAP	PA-O3	3.15	1.62	1.59
3	A	602	NAP	PN-O3	3.13	1.62	1.59
2	A	601	FAD	C4-N3	-3.03	1.33	1.38
3	C	602	NAP	P2B-O2B	3.00	1.64	1.59
2	B	601	FAD	C4-N3	-2.97	1.33	1.38
3	A	602	NAP	C4A-N3A	2.92	1.39	1.35
3	D	602	NAP	O4D-C1D	2.89	1.44	1.40
2	D	601	FAD	O4B-C1B	2.87	1.44	1.40
2	D	601	FAD	C1'-C2'	2.81	1.56	1.52
3	D	602	NAP	C2A-N3A	2.80	1.36	1.32
3	D	602	NAP	PN-O3	2.74	1.62	1.59
3	B	602	NAP	PA-O3	2.73	1.62	1.59
2	A	601	FAD	C10-N10	2.68	1.43	1.37
2	C	601	FAD	C4X-N5	2.66	1.36	1.30
3	C	602	NAP	C2A-N3A	2.66	1.36	1.32
3	B	602	NAP	O4D-C1D	2.64	1.44	1.40
3	B	602	NAP	C2N-C3N	2.61	1.43	1.39
2	C	601	FAD	C1'-C2'	2.60	1.56	1.52
3	C	602	NAP	PN-O3	2.60	1.62	1.59
2	D	601	FAD	P-O3P	2.57	1.62	1.59
2	B	601	FAD	C10-N10	2.56	1.42	1.37
2	B	601	FAD	P-O3P	2.49	1.62	1.59
3	B	602	NAP	C2N-N1N	2.45	1.37	1.35
2	C	601	FAD	C5'-C4'	2.45	1.55	1.51
2	D	601	FAD	C4X-N5	2.44	1.36	1.30
3	A	602	NAP	O4D-C1D	2.44	1.44	1.40
2	C	601	FAD	C9A-N10	2.43	1.45	1.41
2	A	601	FAD	C4X-N5	2.42	1.36	1.30
2	A	601	FAD	P-O3P	2.41	1.62	1.59
2	A	601	FAD	C2A-N3A	2.41	1.35	1.32
2	C	601	FAD	C5A-N7A	-2.39	1.31	1.39
2	B	601	FAD	C5X-N5	-2.39	1.35	1.39
3	C	602	NAP	O4D-C1D	2.25	1.43	1.40
3	B	602	NAP	P2B-O2B	2.25	1.63	1.59
2	B	601	FAD	PA-O3P	2.24	1.61	1.59
2	A	601	FAD	PA-O3P	2.21	1.61	1.59
2	B	601	FAD	C4X-N5	2.14	1.35	1.30
2	A	601	FAD	O4B-C1B	2.10	1.43	1.40
2	A	601	FAD	C9A-N10	2.10	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NAP	C4A-N3A	2.07	1.38	1.35
2	D	601	FAD	C4-N3	-2.07	1.35	1.38
2	D	601	FAD	C10-N10	2.02	1.41	1.37

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	NAP	O4B-C1B-N9A	7.64	118.88	108.75
3	A	602	NAP	N3A-C2A-N1A	-6.03	120.49	128.67
3	A	602	NAP	O4B-C1B-N9A	6.00	116.70	108.75
4	D	603	MA4	O10-C10-C20	5.98	115.04	108.14
2	D	601	FAD	N3A-C2A-N1A	-5.33	121.44	128.67
3	B	602	NAP	N3A-C2A-N1A	-5.27	121.52	128.67
2	C	601	FAD	N3A-C2A-N1A	-5.14	121.69	128.67
3	B	602	NAP	C4B-O4B-C1B	-5.01	105.34	109.92
3	D	602	NAP	N3A-C2A-N1A	-4.97	121.92	128.67
3	C	602	NAP	O4B-C1B-N9A	4.75	115.05	108.75
3	C	602	NAP	N3A-C2A-N1A	-4.72	122.27	128.67
2	A	601	FAD	N3A-C2A-N1A	-4.64	122.38	128.67
3	A	602	NAP	C2B-C1B-N9A	-4.53	102.50	112.56
2	C	601	FAD	C4'-C3'-C2'	-4.52	106.04	113.57
2	B	601	FAD	C4-C4X-N5	4.40	124.29	118.21
2	D	601	FAD	O4B-C1B-N9A	4.40	114.58	108.75
2	B	601	FAD	N3A-C2A-N1A	-4.40	122.70	128.67
3	C	602	NAP	C4B-O4B-C1B	-4.37	105.93	109.92
3	A	602	NAP	C1B-N9A-C4A	-4.03	119.57	126.64
3	C	602	NAP	C6N-N1N-C2N	-4.02	118.45	121.88
2	A	601	FAD	C4-C4X-N5	4.00	123.73	118.21
2	D	601	FAD	C4-C4X-N5	3.93	123.64	118.21
2	A	601	FAD	C4X-C10-N10	3.71	121.79	116.48
2	B	601	FAD	C4'-C3'-C2'	-3.69	107.43	113.57
2	C	601	FAD	C4-C4X-N5	3.68	123.29	118.21
2	B	601	FAD	O3'-C3'-C4'	3.65	117.22	108.93
4	D	603	MA4	C1-O5-C5	3.59	120.73	113.72
3	D	602	NAP	O4B-C1B-C2B	-3.59	100.48	106.61
2	B	601	FAD	C4X-C10-N1	-3.50	116.00	124.59
2	B	601	FAD	C10-N1-C2	3.46	124.35	116.85
3	C	602	NAP	C3B-C2B-C1B	-3.46	96.18	102.81
2	B	601	FAD	O4B-C1B-N9A	3.44	113.31	108.75
3	C	602	NAP	C1B-N9A-C4A	-3.41	120.64	126.64
3	D	602	NAP	C4B-O4B-C1B	-3.36	106.85	109.92
3	D	602	NAP	C3N-C7N-N7N	3.33	121.84	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4X-C10-N10	3.33	121.24	116.48
2	C	601	FAD	O3'-C3'-C4'	3.31	116.45	108.93
3	B	602	NAP	C1B-N9A-C4A	-3.27	120.89	126.64
3	B	602	NAP	C3N-C7N-N7N	3.27	121.77	117.74
2	A	601	FAD	O4'-C4'-C3'	3.19	116.72	109.25
2	C	601	FAD	O2'-C2'-C3'	-3.17	101.83	109.25
3	B	602	NAP	O7N-C7N-N7N	-3.07	118.17	122.62
3	B	602	NAP	C4D-O4D-C1D	-3.07	107.11	109.92
2	A	601	FAD	C4X-C10-N1	-3.06	117.08	124.59
3	C	602	NAP	C3N-C7N-N7N	3.04	121.48	117.74
3	A	602	NAP	C4B-O4B-C1B	-3.01	107.17	109.92
3	B	602	NAP	C5D-C4D-C3D	-2.96	104.55	115.21
2	D	601	FAD	C4A-C5A-N7A	-2.95	106.22	109.34
3	B	602	NAP	O3D-C3D-C2D	2.95	121.26	111.82
2	B	601	FAD	O2A-PA-O1A	2.93	126.08	112.44
2	D	601	FAD	C10-N1-C2	2.93	123.19	116.85
2	B	601	FAD	C10-C4X-N5	-2.92	118.85	124.81
2	B	601	FAD	C5X-N5-C4X	2.89	122.76	118.09
2	C	601	FAD	C10-N1-C2	2.89	123.10	116.85
2	A	601	FAD	C10-C4X-N5	-2.89	118.92	124.81
2	A	601	FAD	C5X-N5-C4X	2.83	122.66	118.09
2	C	601	FAD	N6A-C6A-N1A	2.82	124.35	118.33
2	C	601	FAD	O2A-PA-O1A	2.80	125.47	112.44
2	D	601	FAD	O3'-C3'-C4'	2.78	115.25	108.93
2	C	601	FAD	O2-C2-N1	-2.78	117.18	121.80
3	B	602	NAP	C2N-C3N-C7N	2.75	127.40	119.46
4	D	603	MA4	C11-O10-C10	2.74	117.42	113.26
3	B	602	NAP	O2N-PN-O1N	2.73	125.14	112.44
2	C	601	FAD	C4X-C10-N1	-2.71	117.95	124.59
2	C	601	FAD	C4X-C10-N10	2.71	120.36	116.48
2	D	601	FAD	O2A-PA-O1A	2.68	124.91	112.44
2	B	601	FAD	C4-N3-C2	-2.65	120.94	125.64
2	A	601	FAD	N6A-C6A-N1A	2.65	123.99	118.33
2	C	601	FAD	O4B-C1B-N9A	2.64	112.25	108.75
2	C	601	FAD	C1'-C2'-C3'	2.62	116.76	109.66
2	B	601	FAD	C4X-C4-N3	2.60	119.88	113.25
3	B	602	NAP	O3X-P2B-O2X	2.59	117.50	107.80
2	B	601	FAD	N6A-C6A-N1A	2.57	123.83	118.33
3	D	602	NAP	C4A-C5A-N7A	-2.53	106.67	109.34
2	D	601	FAD	C4X-C10-N1	-2.53	118.40	124.59
2	B	601	FAD	O2'-C2'-C3'	-2.52	103.35	109.25
2	D	601	FAD	C4X-C4-N3	2.48	119.58	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C4X-C10-N10	2.48	120.03	116.48
2	A	601	FAD	C4B-O4B-C1B	-2.44	107.69	109.92
3	C	602	NAP	O3X-P2B-O1X	2.43	120.29	110.83
2	A	601	FAD	O2-C2-N1	-2.43	117.77	121.80
2	A	601	FAD	O2A-PA-O1A	2.42	123.71	112.44
2	A	601	FAD	C10-N1-C2	2.41	122.07	116.85
3	A	602	NAP	O3X-P2B-O2X	2.39	116.75	107.80
3	A	602	NAP	C6A-C5A-C4A	-2.35	113.34	117.90
3	C	602	NAP	O2A-PA-O1A	2.34	123.31	112.44
3	B	602	NAP	O5D-PN-O1N	-2.30	99.81	108.94
3	D	602	NAP	O2X-P2B-O1X	2.30	119.78	110.83
3	D	602	NAP	O3X-P2B-O2X	2.29	116.39	107.80
2	C	601	FAD	O4-C4-C4X	-2.29	120.50	126.53
3	C	602	NAP	C5N-C4N-C3N	-2.28	118.12	120.36
2	D	601	FAD	O4-C4-C4X	-2.27	120.54	126.53
3	C	602	NAP	N6A-C6A-N1A	2.22	123.07	118.33
2	A	601	FAD	C9A-N10-C10	-2.22	117.37	120.75
2	A	601	FAD	C1'-N10-C9A	2.21	124.92	120.63
2	B	601	FAD	O4-C4-N3	-2.20	115.97	120.11
2	A	601	FAD	C4-N3-C2	-2.18	121.77	125.64
2	C	601	FAD	C5A-C6A-N1A	-2.18	115.03	120.23
3	B	602	NAP	C4N-C3N-C7N	-2.18	115.13	121.06
2	D	601	FAD	C4'-C3'-C2'	-2.17	109.96	113.57
2	D	601	FAD	C1B-N9A-C4A	-2.17	122.83	126.64
3	A	602	NAP	O5D-C5D-C4D	2.15	116.33	108.99
2	C	601	FAD	C4X-C4-N3	2.14	118.69	113.25
2	A	601	FAD	O2P-P-O3P	-2.13	101.51	107.27
3	B	602	NAP	C2B-C3B-C4B	2.13	106.58	101.99
2	D	601	FAD	O2'-C2'-C3'	-2.12	104.29	109.25
2	A	601	FAD	O2P-P-O1P	2.11	122.27	112.44
3	B	602	NAP	O3B-C3B-C2B	-2.11	105.28	111.19
2	A	601	FAD	O4'-C4'-C5'	-2.09	105.38	109.99
3	C	602	NAP	O4D-C4D-C5D	2.08	115.98	109.33
3	C	602	NAP	C2B-C1B-N9A	-2.06	107.98	112.56
3	C	602	NAP	C2N-C3N-C4N	2.06	120.65	118.26
3	D	602	NAP	N6A-C6A-N1A	2.04	122.70	118.33
2	D	601	FAD	C1'-N10-C9A	2.04	124.59	120.63
2	B	601	FAD	C4B-O4B-C1B	-2.04	108.06	109.92
3	C	602	NAP	O7N-C7N-C3N	-2.03	117.12	119.60
3	D	602	NAP	O2B-P2B-O1X	-2.02	102.13	109.33
2	C	601	FAD	C9A-N10-C10	-2.02	117.68	120.75
2	C	601	FAD	C5X-N5-C4X	2.01	121.34	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C5X-N5-C4X	2.01	121.34	118.09
3	C	602	NAP	C5N-C6N-N1N	2.01	123.12	120.38
2	D	601	FAD	C4-N3-C2	-2.00	122.08	125.64

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	N10-C1'-C2'-C3'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-C5'
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-C3'
2	D	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	O3'-C3'-C4'-C5'
3	B	602	NAP	C5D-O5D-PN-O3
3	B	602	NAP	C4D-C5D-O5D-PN
3	B	602	NAP	C3D-C4D-C5D-O5D
3	B	602	NAP	O4D-C1D-N1N-C2N
3	A	602	NAP	C5B-O5B-PA-O1A
3	A	602	NAP	C5B-O5B-PA-O3

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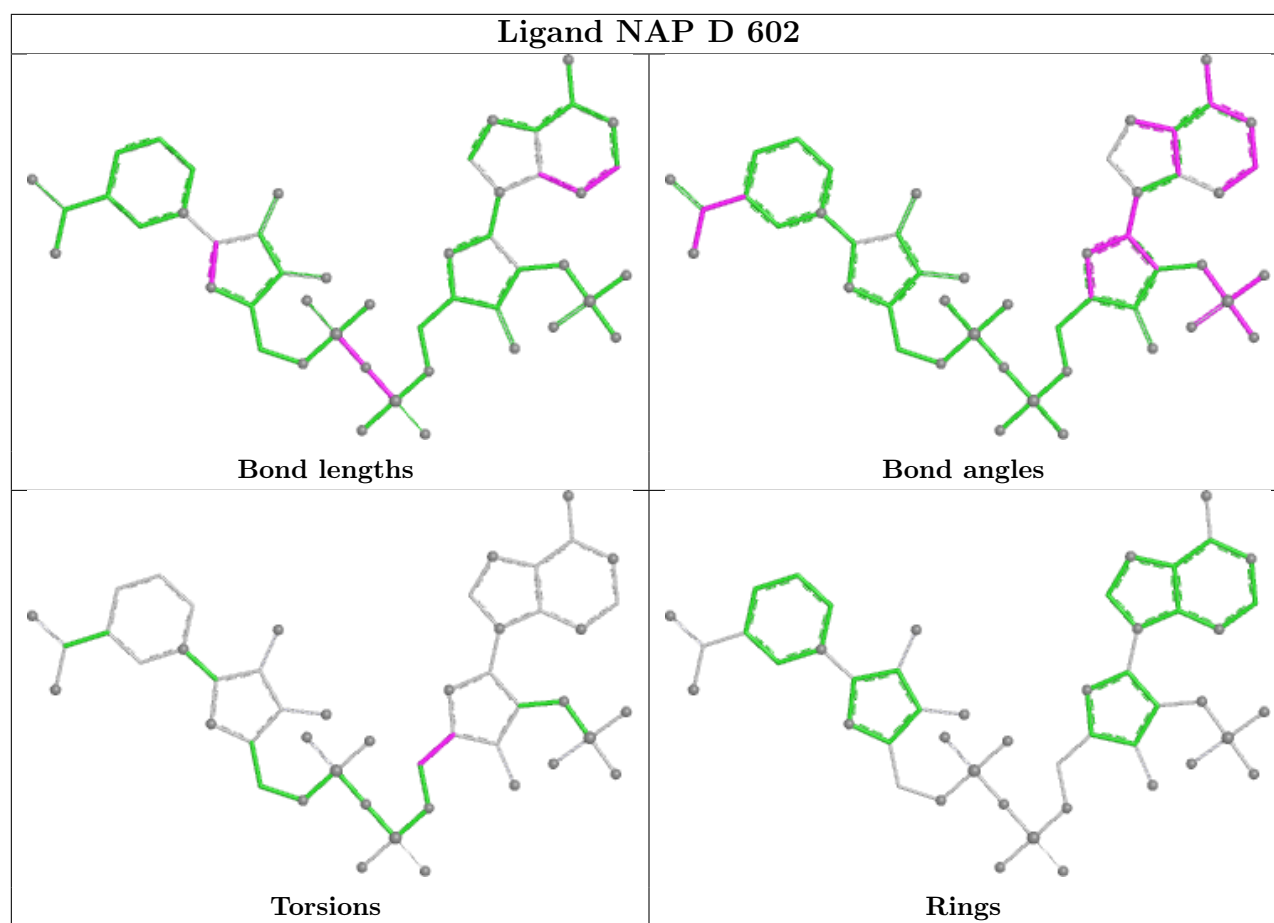
Mol	Chain	Res	Type	Atoms
3	A	602	NAP	C5D-O5D-PN-O1N
4	D	603	MA4	O50-C10-O10-C11
4	D	603	MA4	C20-C10-O10-C11
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
3	B	602	NAP	O4D-C4D-C5D-O5D
3	A	602	NAP	O4D-C4D-C5D-O5D
2	B	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	D	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
3	A	602	NAP	C3D-C4D-C5D-O5D
4	D	603	MA4	C4-C5-C6-O6
4	D	603	MA4	O5-C5-C6-O6
3	C	602	NAP	O4D-C4D-C5D-O5D
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
3	B	602	NAP	O4B-C4B-C5B-O5B
3	C	602	NAP	C3D-C4D-C5D-O5D
3	B	602	NAP	PA-O3-PN-O5D
4	D	603	MA4	O50-C50-C60-O60
2	C	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	C5B-O5B-PA-O1A
3	B	602	NAP	C5B-O5B-PA-O1A
3	B	602	NAP	C5D-O5D-PN-O1N
3	A	602	NAP	C5B-O5B-PA-O2A
3	C	602	NAP	C4N-C3N-C7N-O7N
3	C	602	NAP	C4N-C3N-C7N-N7N
4	D	603	MA4	C40-C50-C60-O60
3	C	602	NAP	C2B-O2B-P2B-O1X
3	C	602	NAP	C2N-C3N-C7N-O7N
3	A	602	NAP	PA-O3-PN-O5D
3	C	602	NAP	C2N-C3N-C7N-N7N
3	D	602	NAP	O4B-C4B-C5B-O5B
3	B	602	NAP	C2B-O2B-P2B-O1X
3	A	602	NAP	C2B-O2B-P2B-O1X
3	B	602	NAP	PA-O3-PN-O2N
3	A	602	NAP	PA-O3-PN-O2N

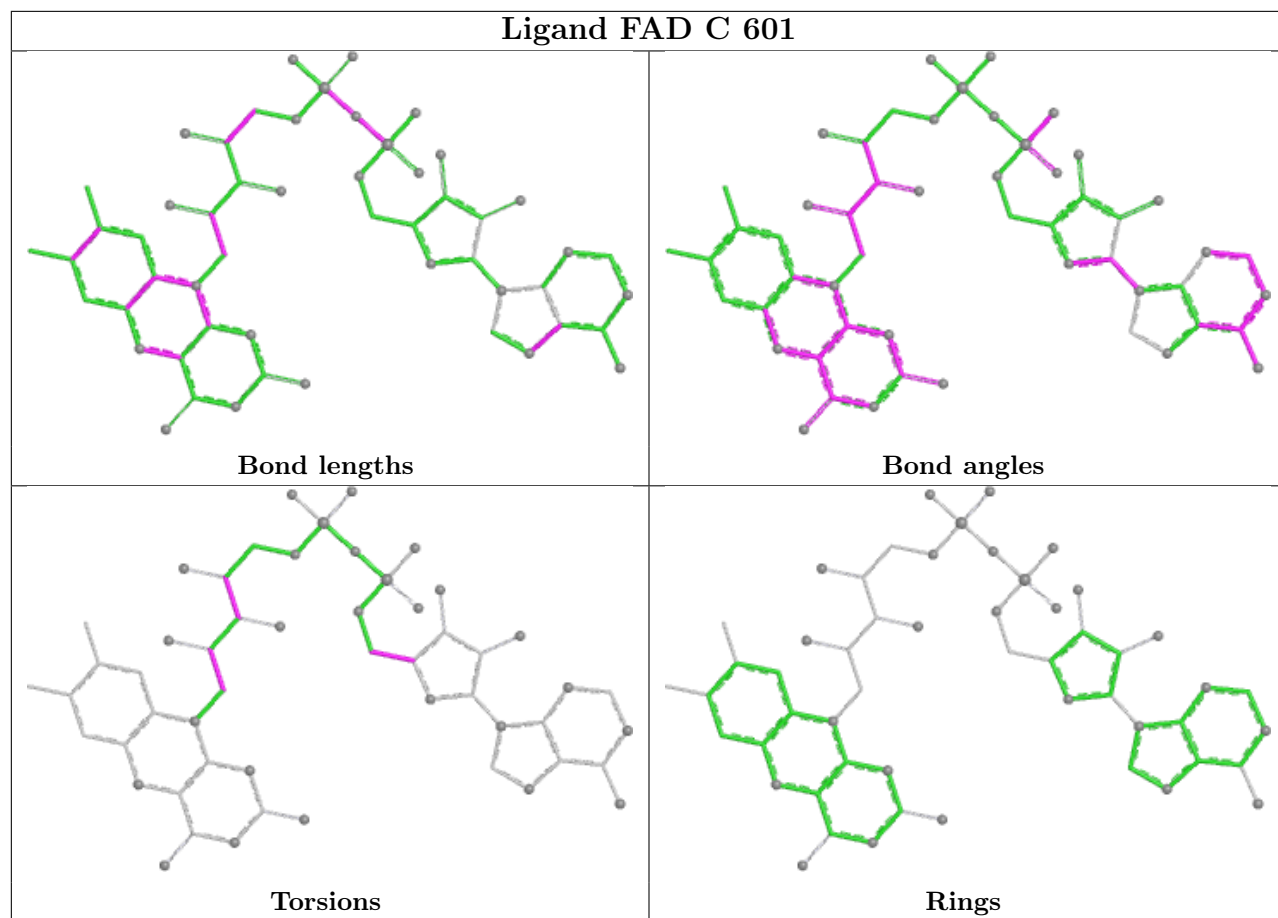
There are no ring outliers.

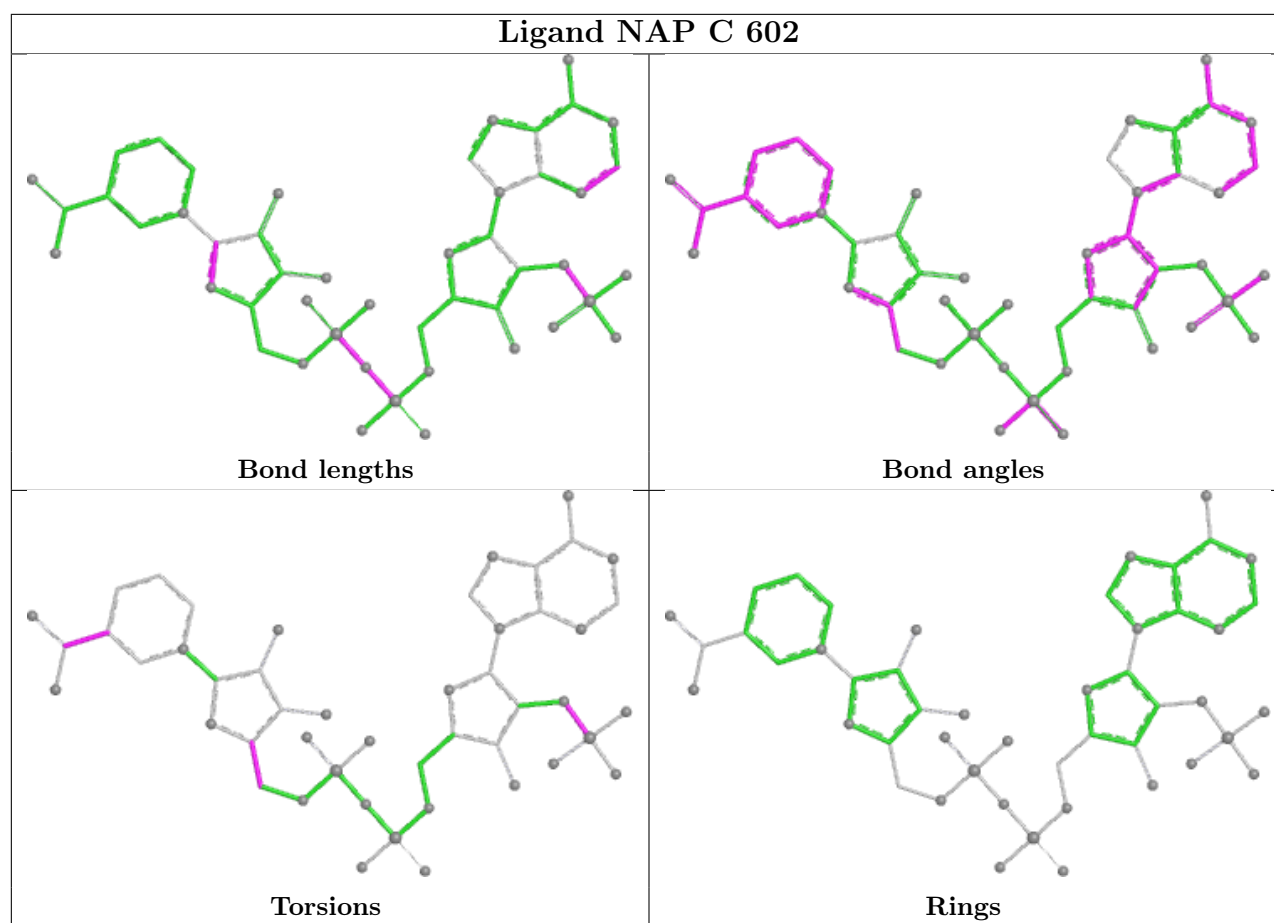
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	NAP	5	0
2	C	601	FAD	3	0
3	C	602	NAP	4	0
2	B	601	FAD	8	0
2	D	601	FAD	4	0
2	A	601	FAD	3	0
3	B	602	NAP	7	0
3	A	602	NAP	2	0

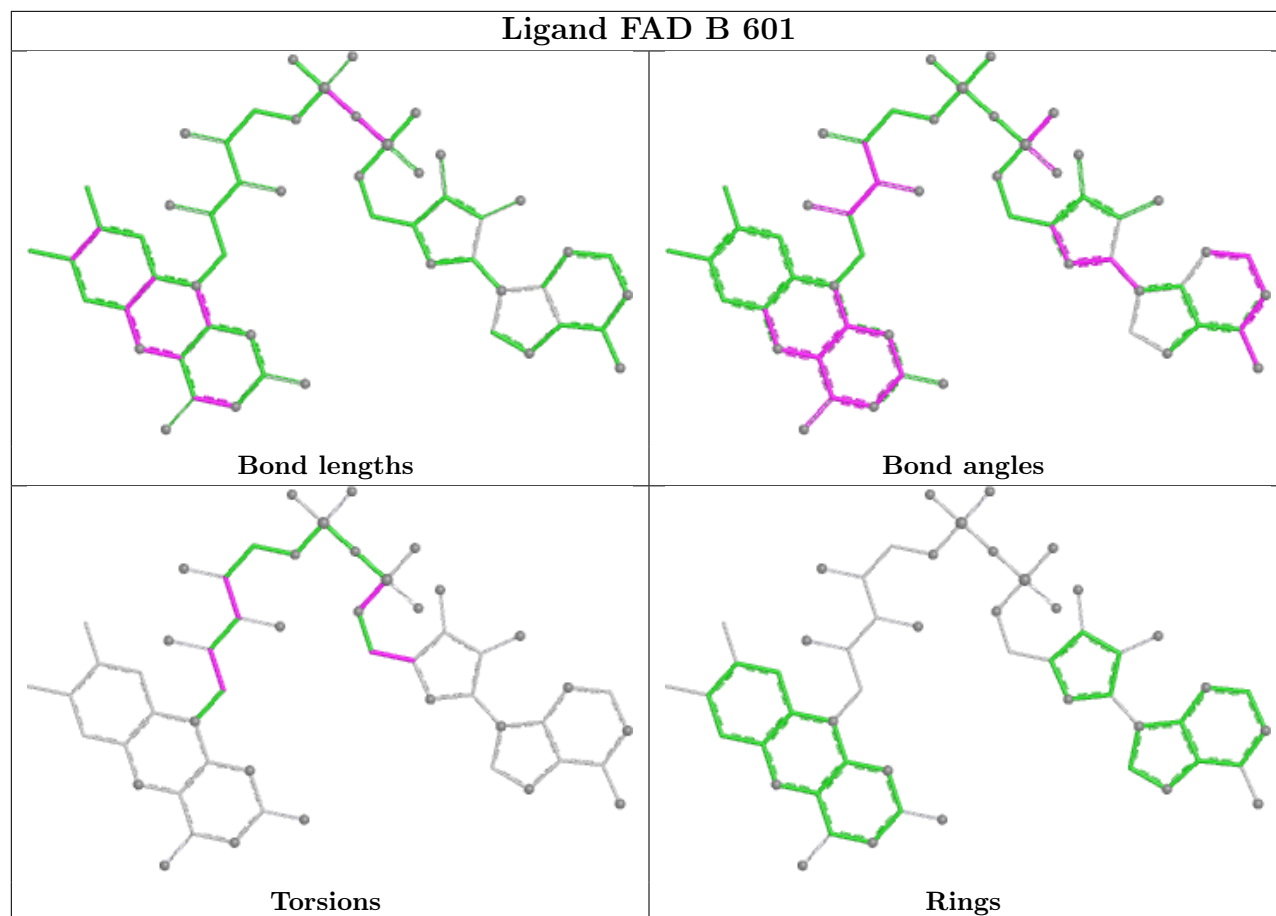
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



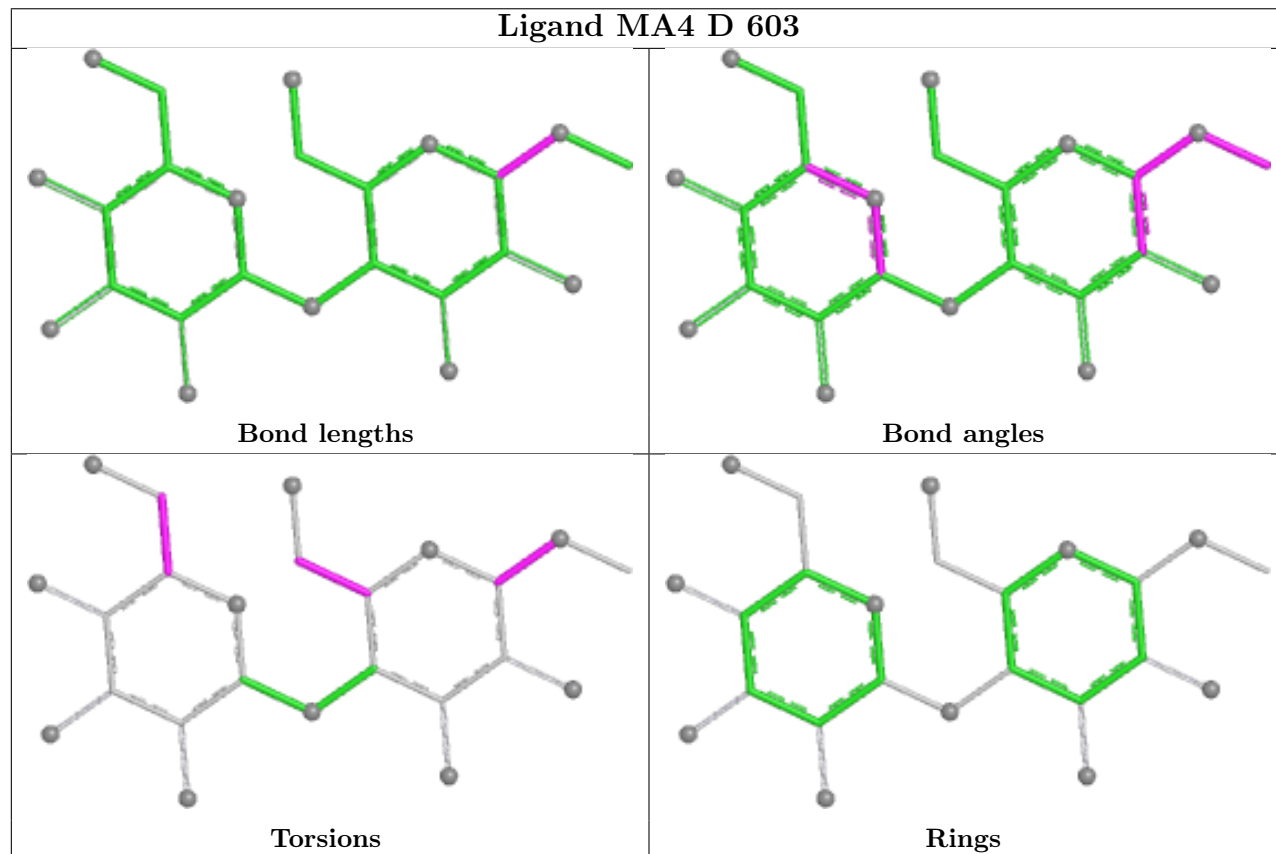


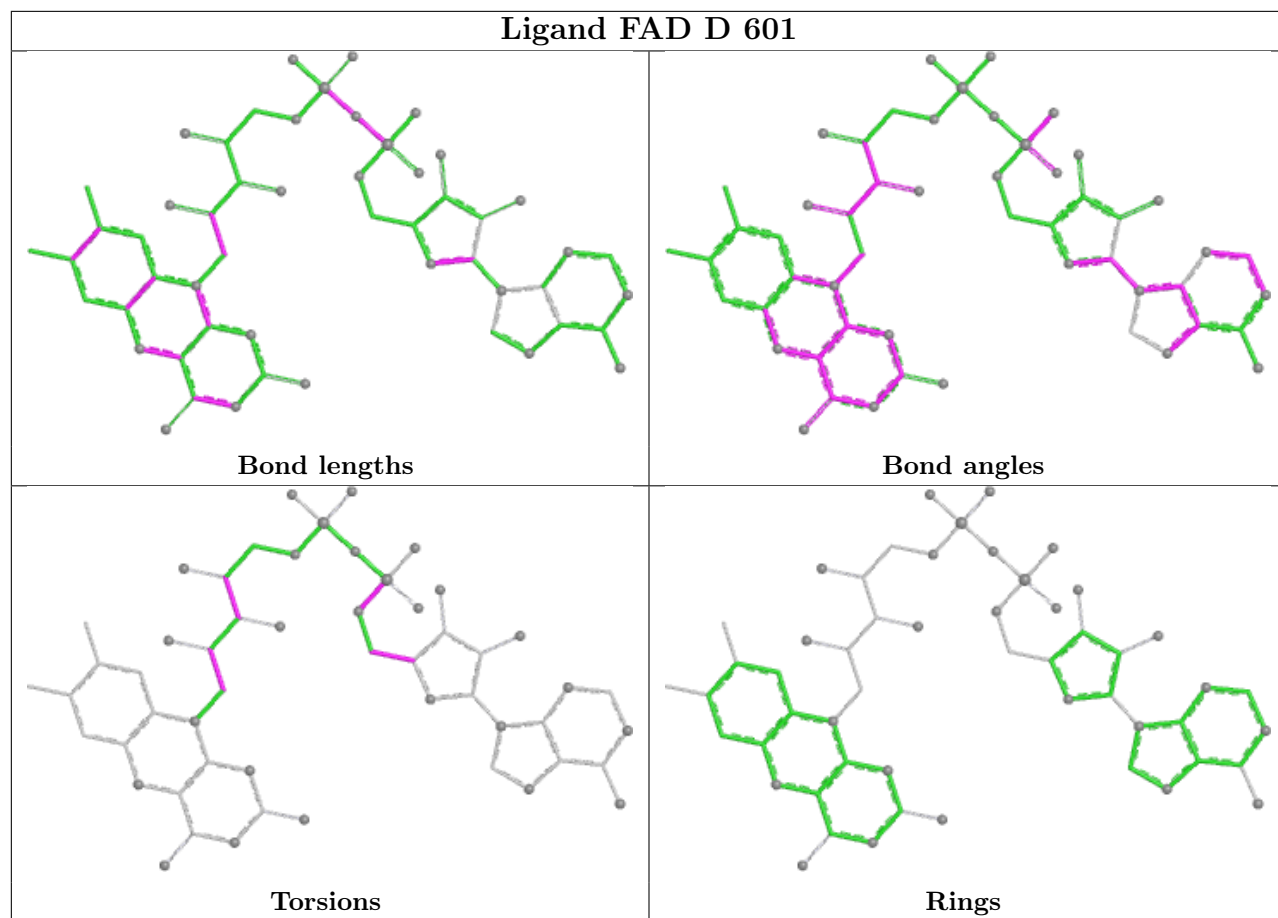


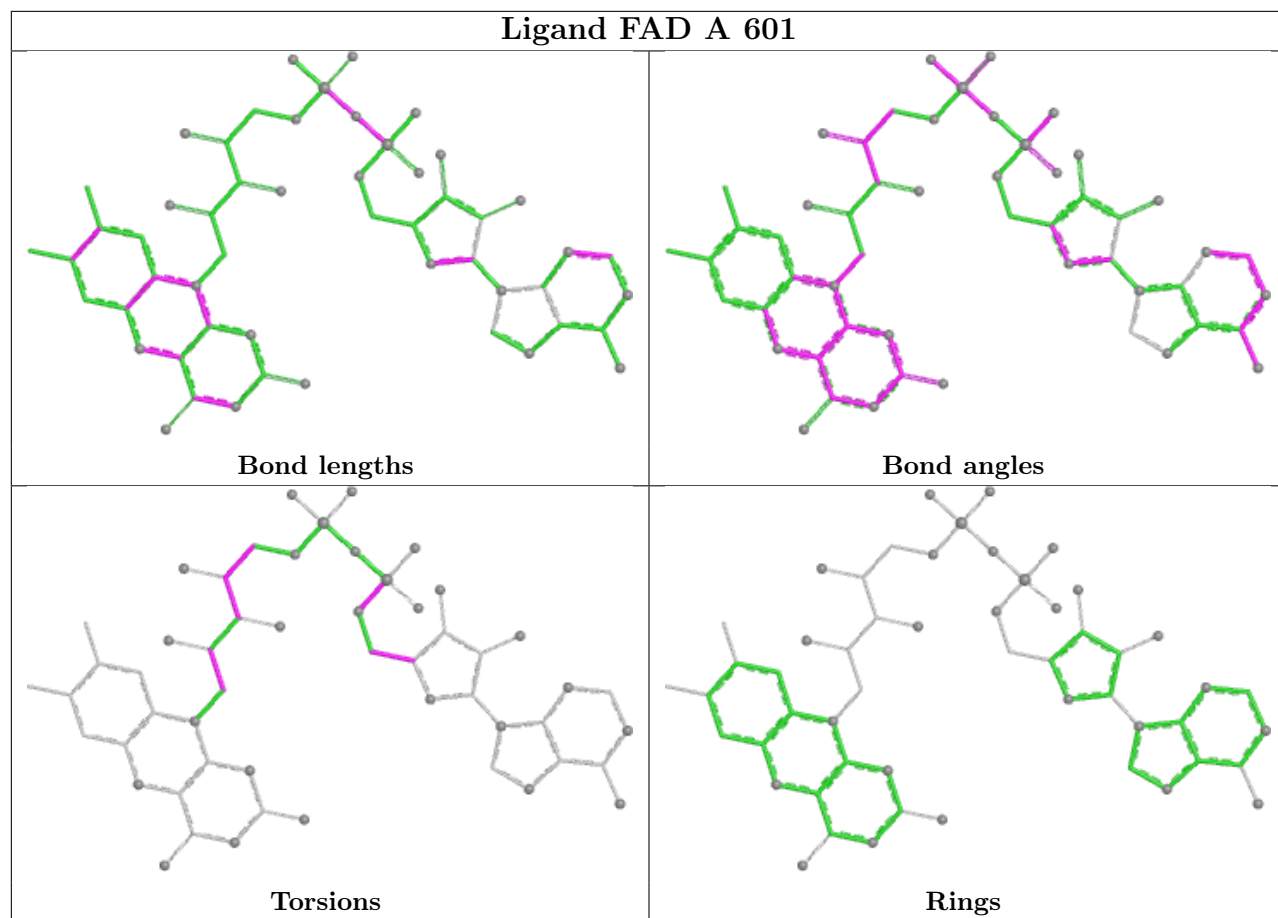
Ligand FAD B 601

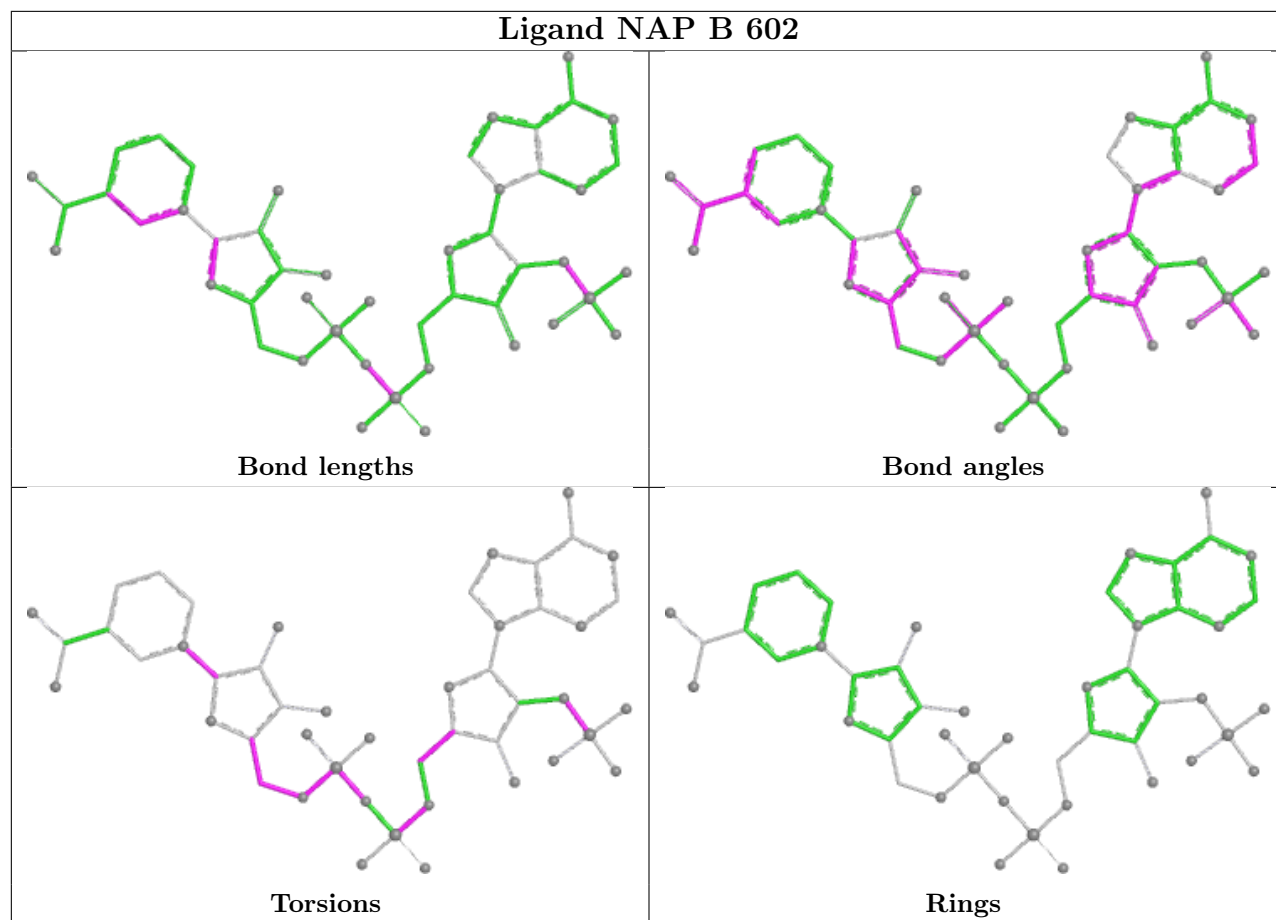


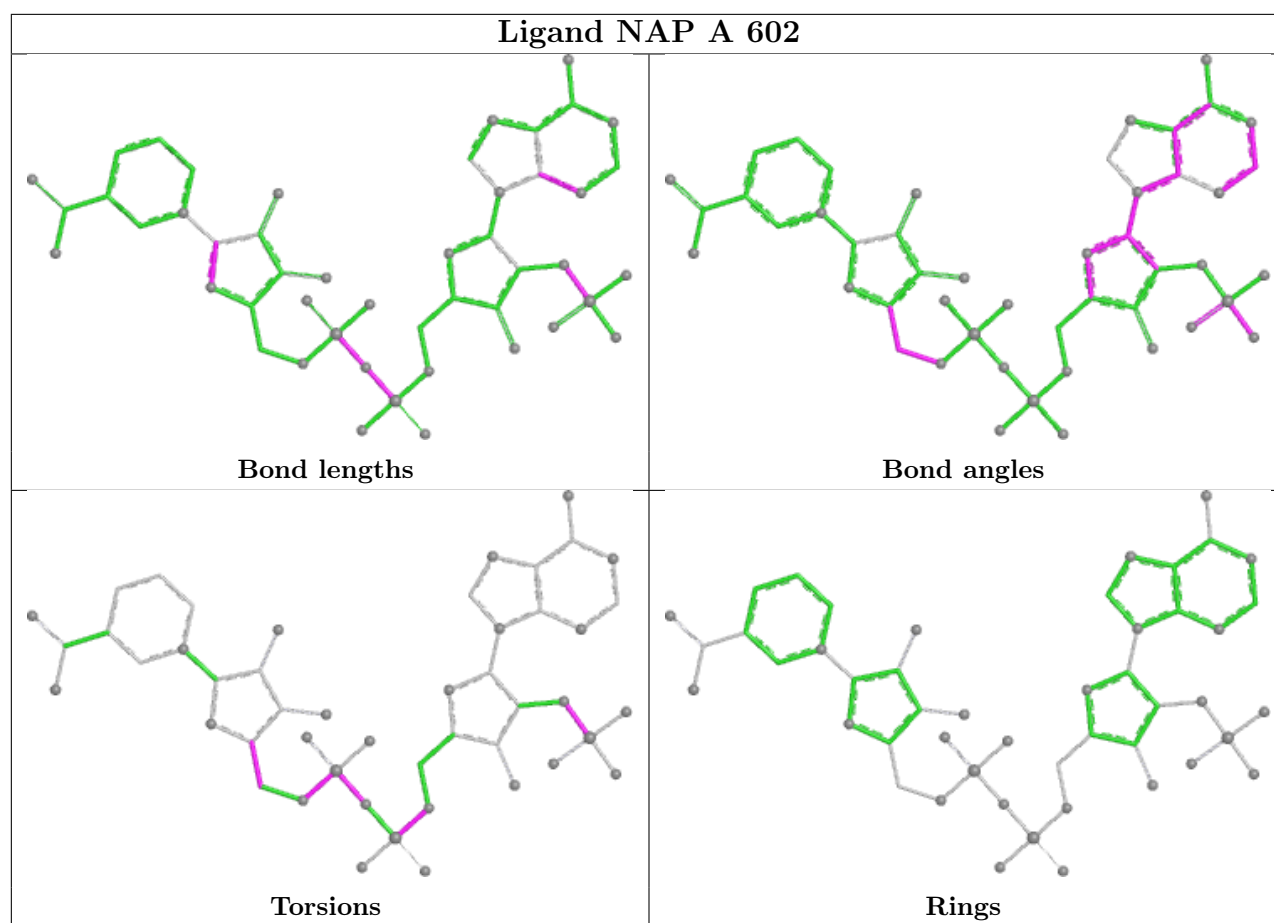
Ligand MA4 D 603











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	530/535 (99%)	-0.05	12 (2%) 60 31	55, 105, 163, 205	0
1	B	530/535 (99%)	-0.21	5 (0%) 84 62	51, 92, 151, 211	0
1	C	530/535 (99%)	-0.07	10 (1%) 66 37	48, 85, 165, 260	0
1	D	530/535 (99%)	-0.17	12 (2%) 60 31	47, 94, 161, 235	0
All	All	2120/2140 (99%)	-0.13	39 (1%) 68 39	47, 94, 158, 260	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	509	ASN	7.6
1	D	535	PHE	5.8
1	C	508	SER	5.4
1	D	530	PHE	4.5
1	A	2	ALA	4.4
1	C	530	PHE	4.3
1	D	135	GLU	4.3
1	A	134	LYS	3.8
1	A	432	TYR	3.5
1	D	134	LYS	3.4
1	A	507	SER	3.4
1	D	508	SER	3.4
1	B	262	ARG	3.3
1	A	341	SER	3.1
1	B	258	GLN	3.1
1	D	528	PHE	2.9
1	D	534	TRP	2.8
1	B	259	GLN	2.8
1	A	512	VAL	2.6
1	D	144	MET	2.6
1	A	279	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	534	TRP	2.5
1	A	246	VAL	2.4
1	D	529	PHE	2.4
1	C	436	LEU	2.4
1	D	454	LEU	2.4
1	A	107	GLN	2.3
1	C	507	SER	2.3
1	A	342	LEU	2.3
1	C	132	ASN	2.2
1	C	236	HIS	2.2
1	C	2	ALA	2.1
1	C	510	PHE	2.1
1	A	360	HIS	2.1
1	D	512	VAL	2.1
1	B	2	ALA	2.1
1	B	530	PHE	2.0
1	D	336	PRO	2.0
1	A	391	ARG	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.

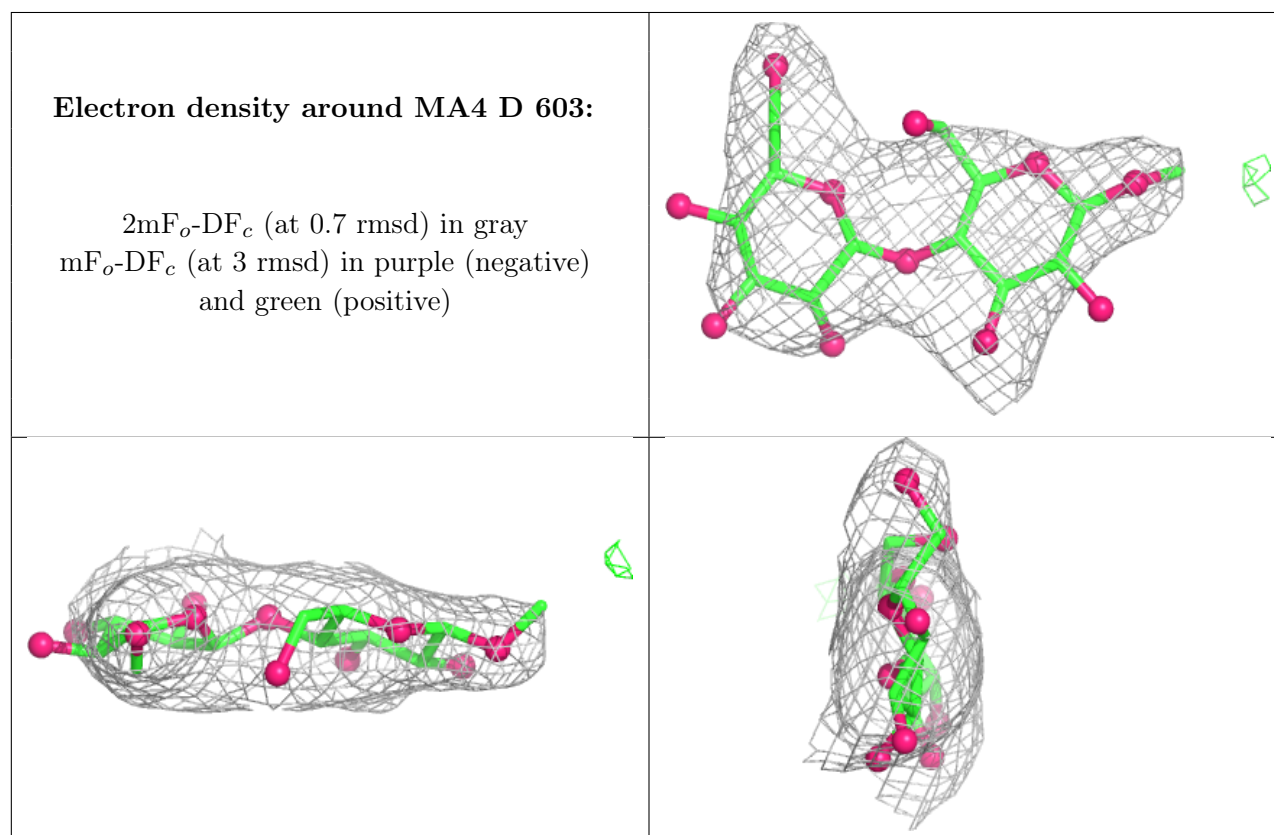
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MA4	D	603	24/35	0.85	0.28	100,160,176,194	0
2	FAD	B	601	53/53	0.95	0.22	63,85,115,122	0
2	FAD	C	601	53/53	0.96	0.25	53,77,114,121	0
3	NAP	A	602	48/48	0.96	0.15	75,95,114,122	0
3	NAP	D	602	48/48	0.96	0.17	62,89,104,114	0

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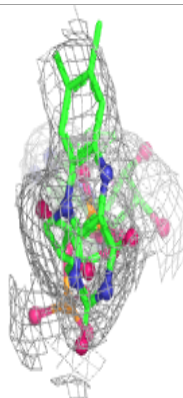
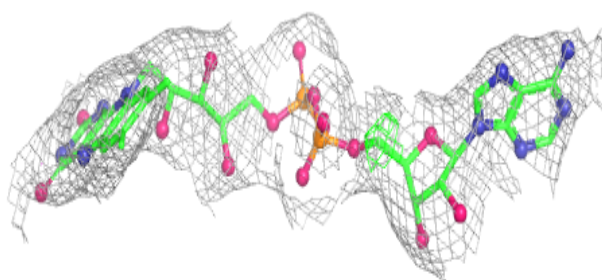
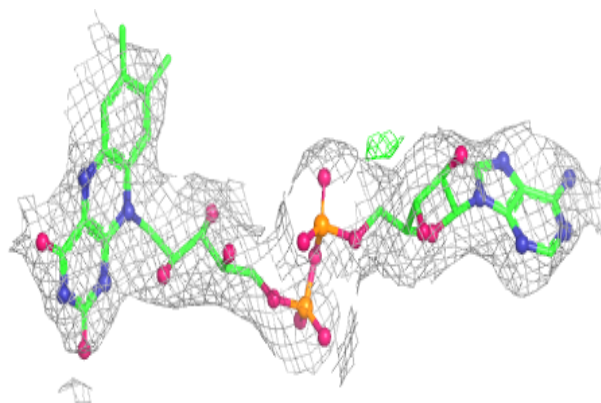
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	A	601	53/53	0.96	0.22	81,115,139,165	0
3	NAP	B	602	48/48	0.97	0.17	64,82,126,148	0
2	FAD	D	601	53/53	0.97	0.26	70,102,140,149	0
3	NAP	C	602	48/48	0.98	0.21	48,62,89,92	0

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.

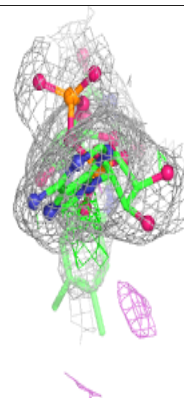
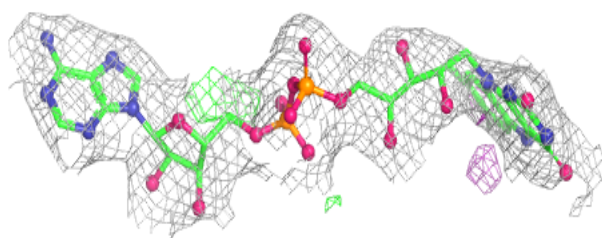
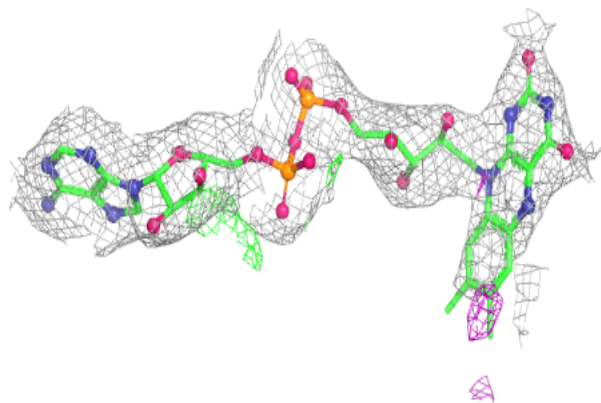


Electron density around FAD B 601:

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

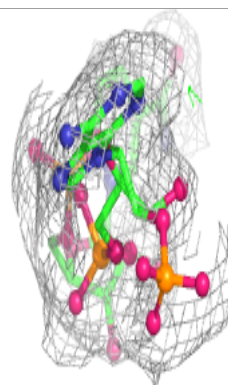
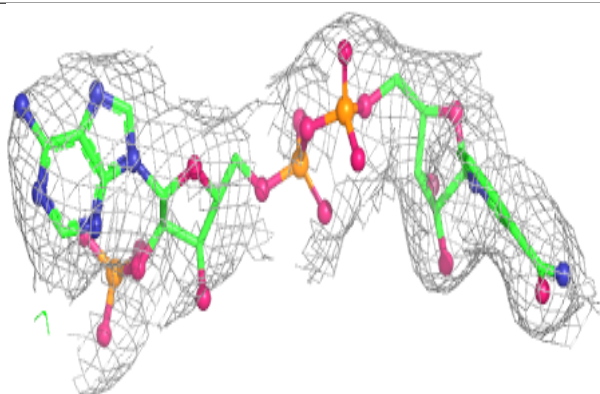
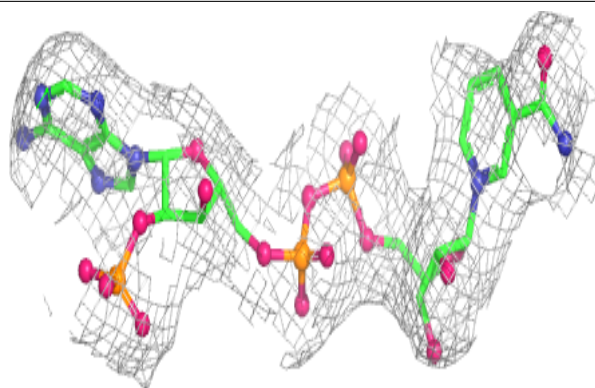
**Electron density around FAD C 601:**

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

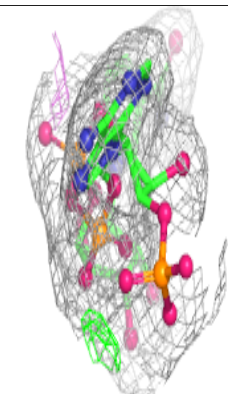
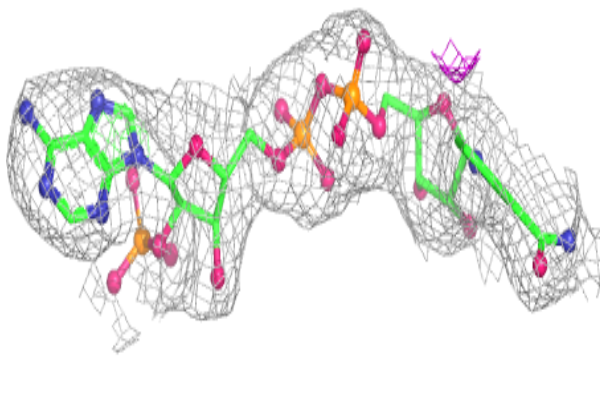
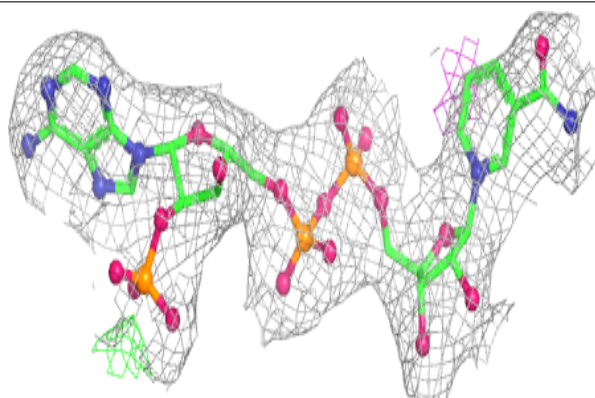


Electron density around NAP A 602:

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

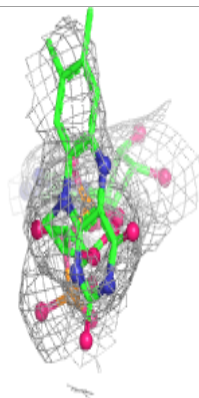
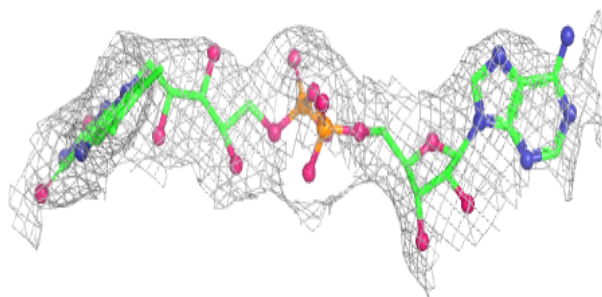
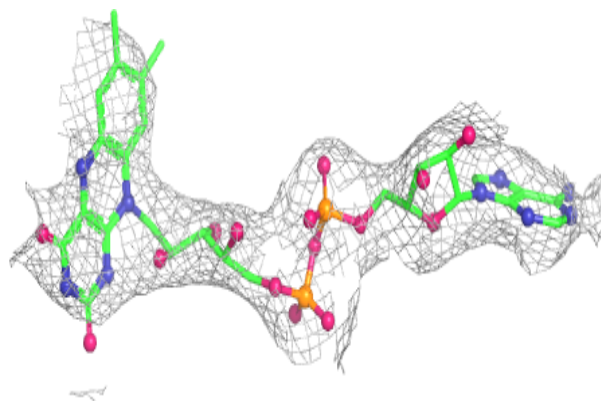
**Electron density around NAP D 602:**

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

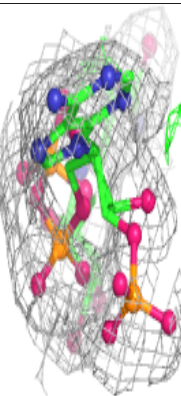
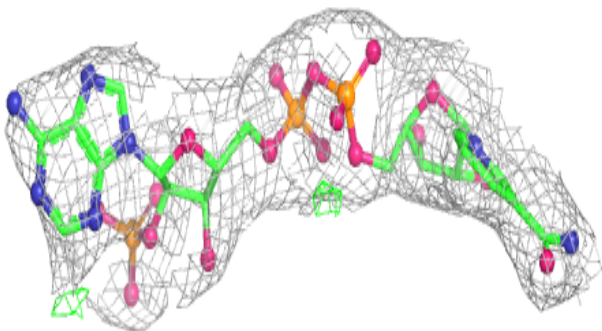
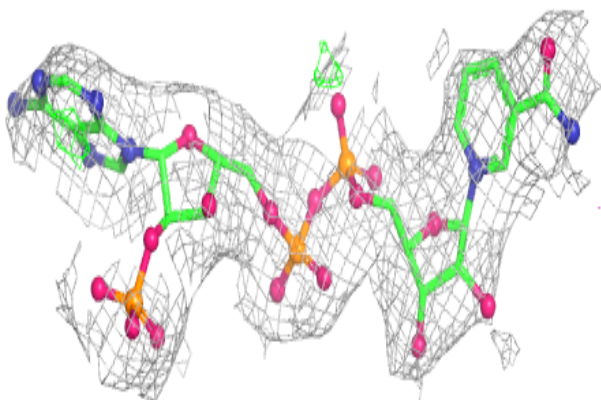


Electron density around FAD A 601:

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

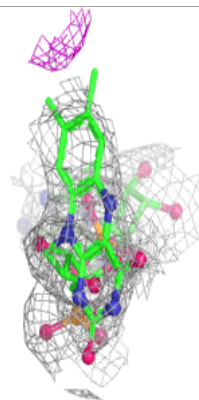
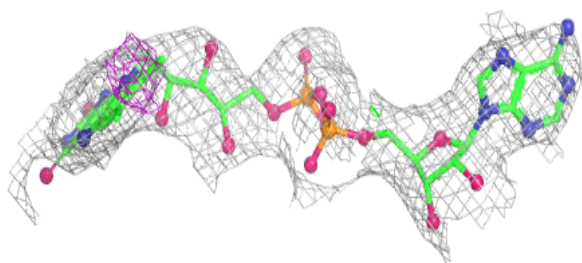
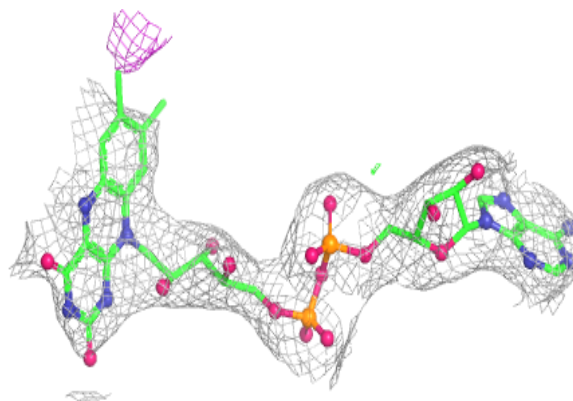
**Electron density around NAP B 602:**

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

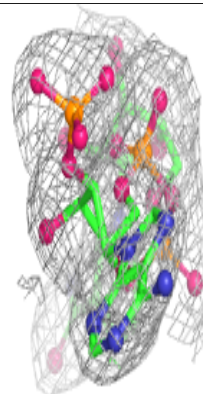
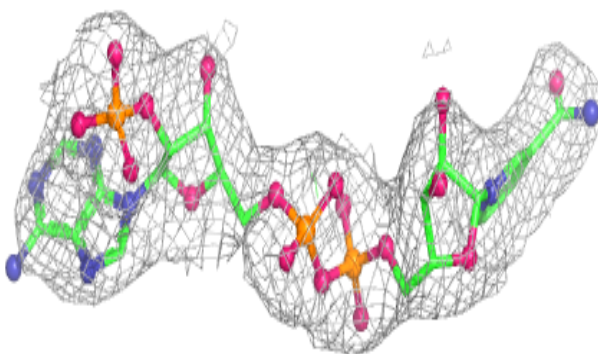
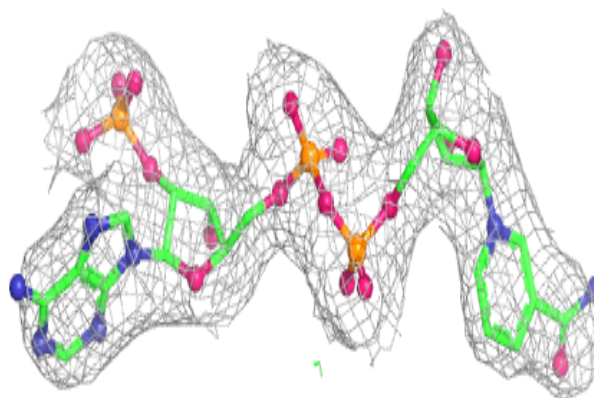


Electron density around FAD D 601:

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

**Electron density around NAP C 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.