Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:18 pm BST

PDB ID	:	6SE3
Title	:	Crystal Structure of Ancestral Flavin-containing monooxygenase (FMO) 3-6
Authors	:	Nicoll, C.; Bailleul, G.; Fiorentini, F.; Mascotti, M.L.; Fraaije, M.; Mattevi, A.
Deposited on	:	2019-07-29
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

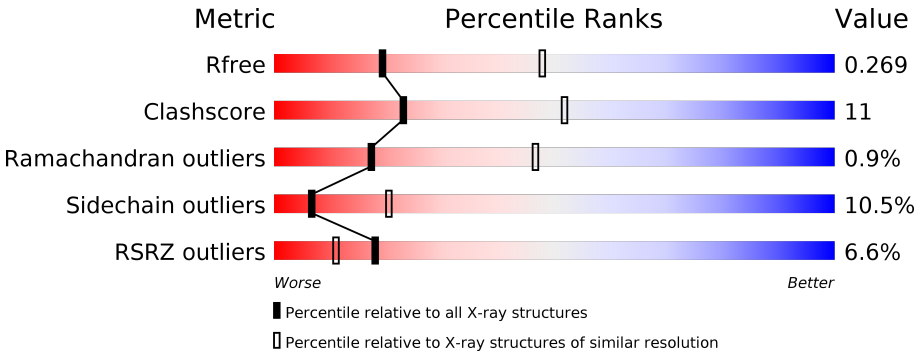
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	532	21% 70% 23% 6%
1	B	532	5% 78% 16% 5%
1	C	532	2% 79% 15%
1	D	532	3% 78% 16% 5%
1	E	532	5% 80% 15%
1	F	532	3% 79% 15%

2 Entry composition

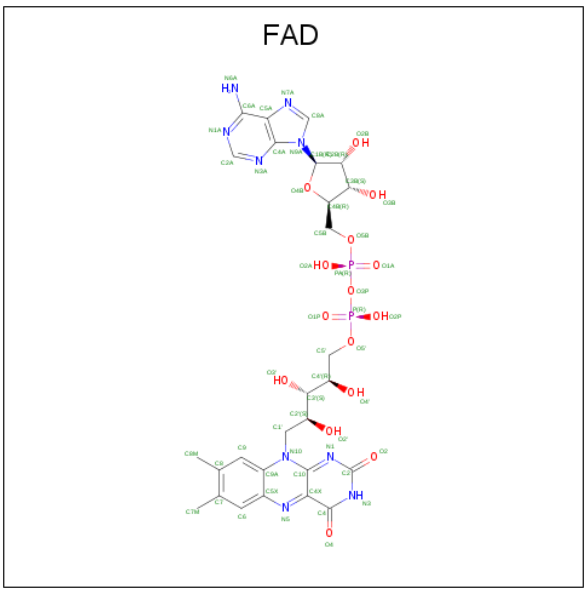
There are 5 unique types of molecules in this entry. The entry contains 26163 atoms, of which 0 are hydrogens and 0 are deuteriums.

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) 3-6.

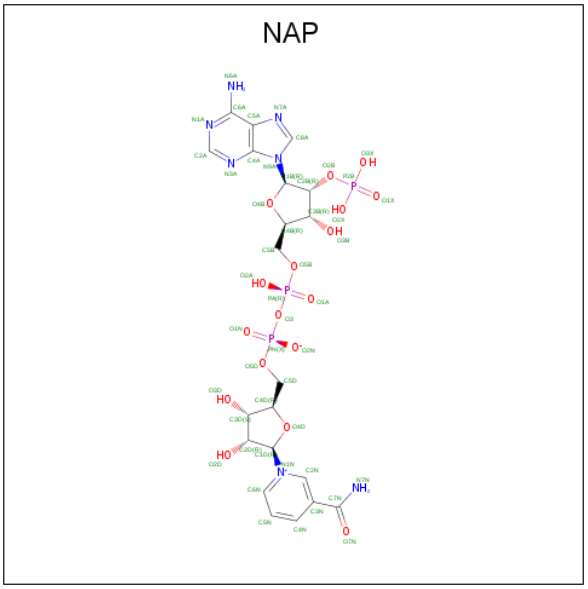
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	528	Total	C	N	O	S	0	0	0
			4198	2718	689	767	24			
1	A	528	Total	C	N	O	S	0	0	0
			4198	2718	689	767	24			
1	B	528	Total	C	N	O	S	0	0	0
			4198	2718	689	767	24			
1	C	528	Total	C	N	O	S	0	0	0
			4198	2718	689	767	24			
1	E	528	Total	C	N	O	S	0	0	0
			4198	2718	689	767	24			
1	F	528	Total	C	N	O	S	0	0	0
			4198	2718	689	767	24			

- 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
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	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
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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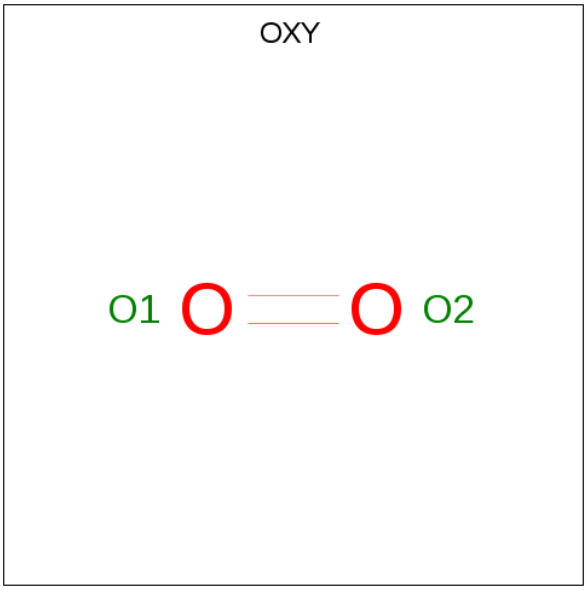
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			2	2		
4	A	1	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	74	Total	O	0	0
			74	74		
5	A	32	Total	O	0	0
			32	32		

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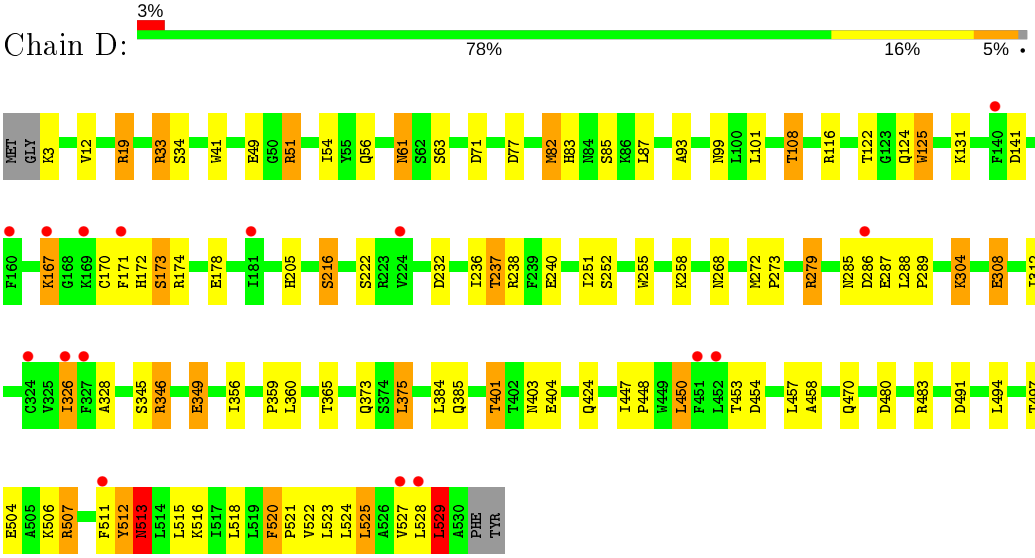
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	52	Total O 52 52	0	0
5	C	75	Total O 75 75	0	0
5	E	56	Total O 56 56	0	0
5	F	68	Total O 68 68	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

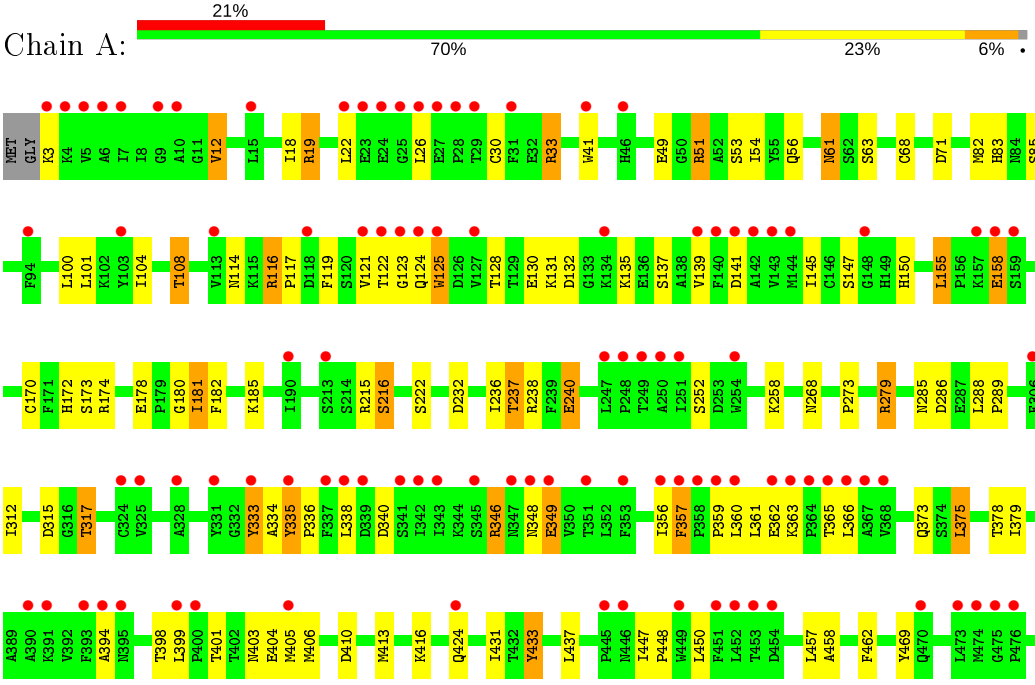
- Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6

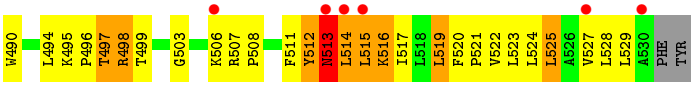
Chain D:



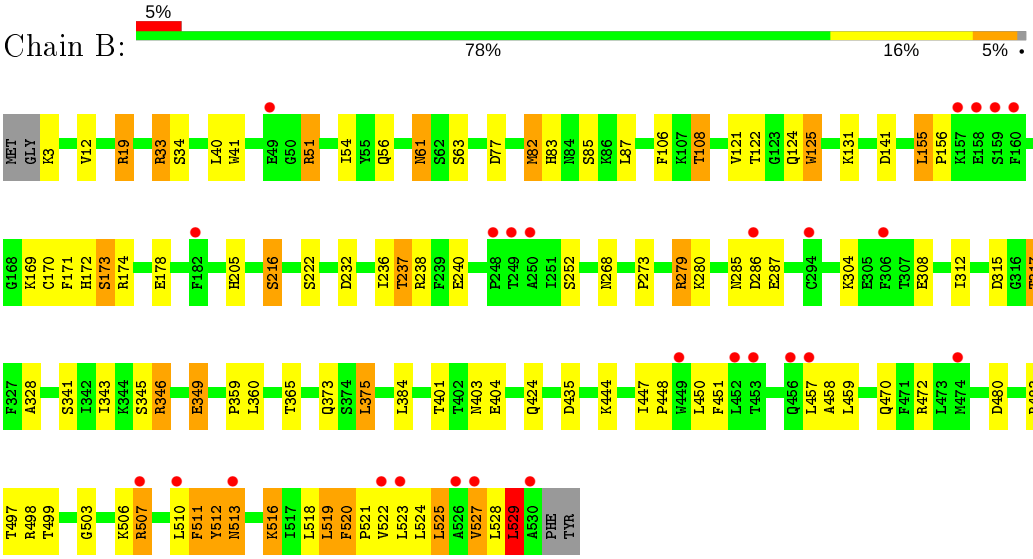
- Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6

Chain A:

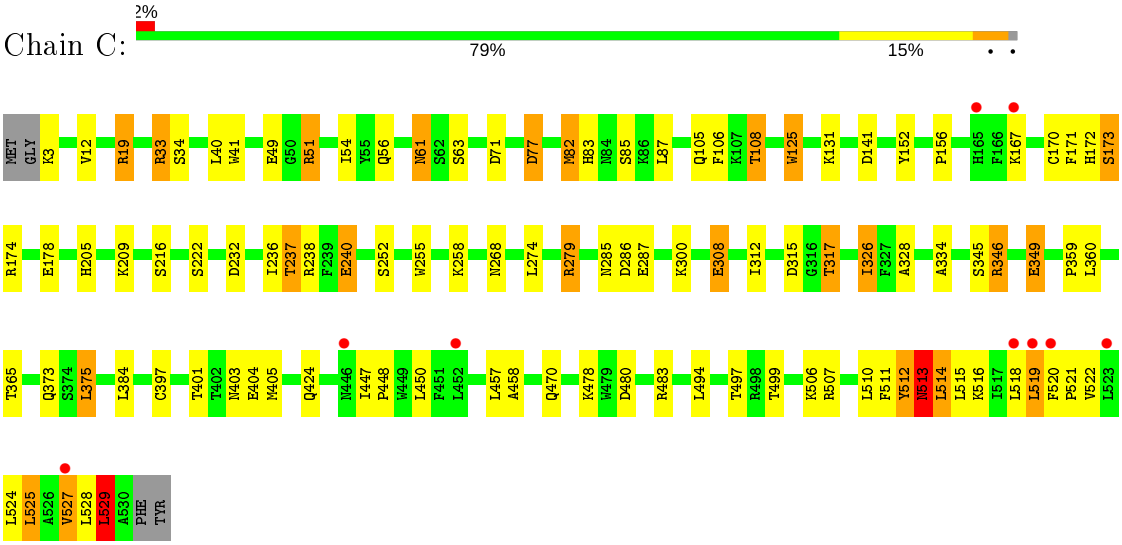




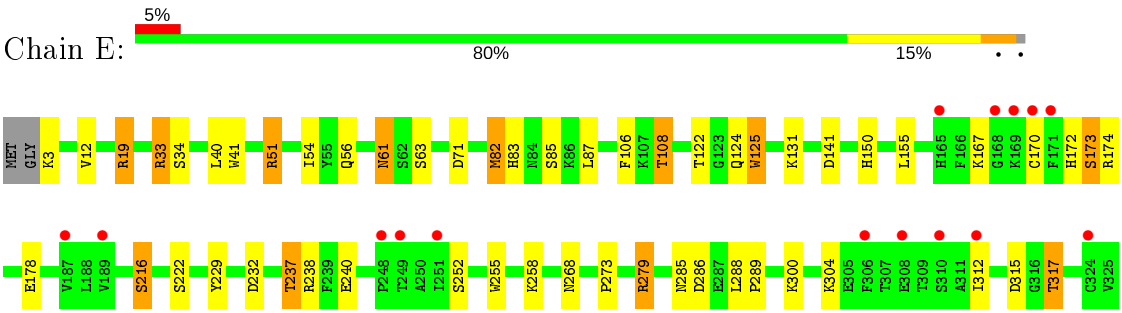
• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6

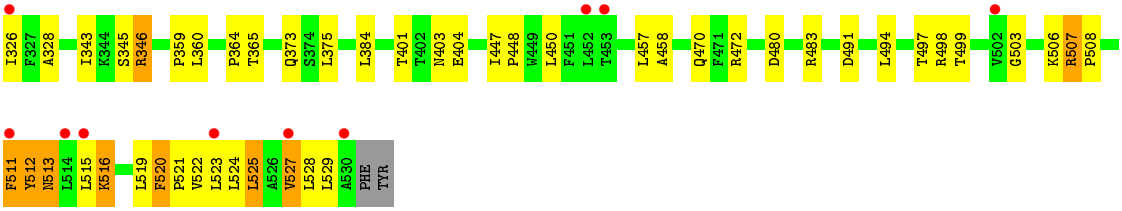


• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6

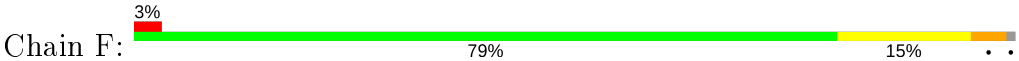


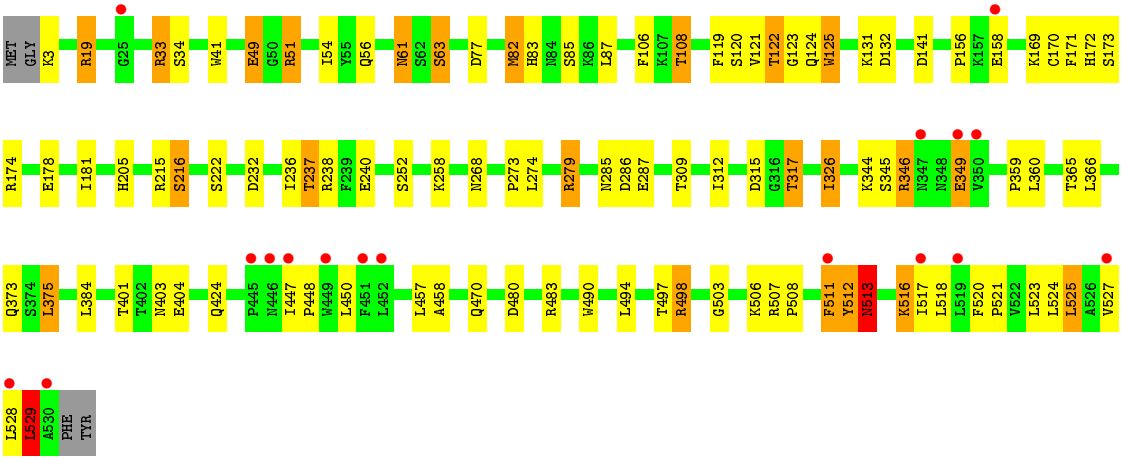
• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6





• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	156.09Å 156.09Å 370.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.30 – 2.80 49.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.30-2.80) 100.0 (49.30-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.217 , 0.266 0.220 , 0.269	Depositor DCC
R_{free} test set	6492 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	26163	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.54	0/4312	0.77	4/5843 (0.1%)
1	B	0.53	1/4312 (0.0%)	0.73	0/5843
1	C	0.53	0/4312	0.73	0/5843
1	D	0.52	0/4312	0.71	0/5843
1	E	0.52	0/4312	0.72	0/5843
1	F	0.54	0/4312	0.73	0/5843
All	All	0.53	1/25872 (0.0%)	0.73	4/35058 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	507	ARG	C-N	8.65	1.50	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	335	TYR	CB-CG-CD2	6.66	124.99	121.00
1	A	335	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	A	357	PHE	CB-CG-CD1	5.63	124.74	120.80
1	A	357	PHE	CB-CG-CD2	-5.63	116.86	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4198	0	4172	147	0
1	B	4198	0	4172	93	0
1	C	4198	0	4172	97	0
1	D	4198	0	4172	98	0
1	E	4198	0	4172	68	0
1	F	4198	0	4172	86	0
2	A	53	0	31	18	0
2	B	53	0	31	2	0
2	C	53	0	31	4	0
2	D	53	0	31	2	0
2	E	53	0	31	3	0
2	F	53	0	31	4	0
3	A	48	0	25	4	0
3	B	48	0	25	3	0
3	C	48	0	25	3	0
3	D	48	0	25	5	0
3	E	48	0	25	2	0
3	F	48	0	25	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	32	0	0	19	0
5	B	52	0	0	5	0
5	C	75	0	0	11	0
5	D	74	0	0	8	0
5	E	56	0	0	2	0
5	F	68	0	0	6	0
All	All	26163	0	25368	584	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 11.

All (584) 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:A:145:ILE:CG2	1:A:335:TYR:HE1	1.61	1.14
1:A:145:ILE:CG2	1:A:335:TYR:CE1	2.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ARG:HE	1:C:470:GLN:NE2	1.51	1.08
1:A:145:ILE:HG21	1:A:335:TYR:CE1	1.89	1.07
1:A:145:ILE:HG22	1:A:335:TYR:HE1	1.16	1.05
1:A:51:ARG:HH11	1:A:51:ARG:HB3	1.24	1.03
1:E:238:ARG:HE	1:E:470:GLN:NE2	1.59	1.00
1:C:268:ASN:O	1:F:497:THR:HG23	1.61	1.00
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.29	0.98
1:D:238:ARG:HH11	1:D:470:GLN:HE21	1.07	0.98
1:F:19:ARG:HG2	1:F:19:ARG:HH11	1.30	0.97
1:F:238:ARG:HE	1:F:470:GLN:NE2	1.66	0.94
1:F:521:PRO:HA	5:F:713:HOH:O	1.67	0.93
1:C:359:PRO:HB3	1:C:405:MET:HE3	1.51	0.92
1:D:33:ARG:HH11	1:D:33:ARG:HG3	1.34	0.92
1:A:33:ARG:HB2	1:A:33:ARG:HH11	1.35	0.92
1:F:19:ARG:HG2	1:F:19:ARG:NH1	1.83	0.90
1:D:497:THR:HG23	1:B:268:ASN:O	1.73	0.89
1:C:300:LYS:HE3	5:C:752:HOH:O	1.72	0.88
1:A:33:ARG:CD	2:A:601:FAD:C5A	2.51	0.87
1:F:238:ARG:HH11	1:F:470:GLN:HE21	1.19	0.86
1:A:33:ARG:HD3	2:A:601:FAD:C4A	2.06	0.86
1:A:497:THR:HG23	1:E:268:ASN:O	1.76	0.85
1:A:51:ARG:CB	1:A:51:ARG:HH11	1.88	0.85
1:A:33:ARG:CB	1:A:33:ARG:HH11	1.89	0.85
1:C:238:ARG:HE	1:C:470:GLN:HE21	1.18	0.85
1:D:238:ARG:NH1	1:D:470:GLN:HE21	1.74	0.84
1:F:19:ARG:CG	1:F:19:ARG:HH11	1.90	0.84
1:D:167:LYS:HD2	1:D:308:GLU:HG3	1.60	0.84
1:A:145:ILE:HG21	1:A:335:TYR:CD1	2.13	0.83
1:C:238:ARG:NE	1:C:470:GLN:NE2	2.28	0.82
1:E:238:ARG:HE	1:E:470:GLN:HE21	1.26	0.80
1:F:309:THR:HG23	5:F:710:HOH:O	1.81	0.79
1:A:33:ARG:HD2	2:A:601:FAD:C5A	2.12	0.79
1:A:268:ASN:O	1:E:497:THR:HG23	1.82	0.79
1:C:359:PRO:HB3	1:C:405:MET:CE	2.13	0.79
1:A:145:ILE:HG22	1:A:335:TYR:CE1	2.07	0.78
1:B:19:ARG:HH12	1:B:472:ARG:NH2	1.82	0.77
1:E:524:LEU:O	1:E:528:LEU:HD23	1.84	0.77
1:D:99:ASN:HB2	5:D:753:HOH:O	1.85	0.77
1:A:19:ARG:HG2	1:A:19:ARG:HH11	1.51	0.76
1:A:33:ARG:CD	2:A:601:FAD:C4A	2.64	0.76
1:E:33:ARG:HH11	1:E:33:ARG:HG3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ARG:NH1	1:D:33:ARG:HG3	1.99	0.76
1:B:237:THR:HG22	1:B:240:GLU:H	1.51	0.75
1:F:237:THR:HG22	1:F:240:GLU:H	1.51	0.75
1:D:237:THR:HG22	1:D:240:GLU:H	1.52	0.75
1:C:238:ARG:HH21	1:C:238:ARG:HG2	1.51	0.74
1:E:237:THR:HG22	1:E:240:GLU:H	1.52	0.74
1:E:108:THR:HG22	1:E:131:LYS:HD3	1.67	0.74
1:A:51:ARG:NH1	1:A:51:ARG:HB3	2.01	0.73
1:C:237:THR:HG22	1:C:240:GLU:H	1.52	0.73
1:A:447:ILE:HB	1:A:448:PRO:HD3	1.71	0.73
2:A:601:FAD:C6	3:A:602:NAP:C2N	2.66	0.73
1:A:237:THR:HG22	1:A:240:GLU:H	1.52	0.73
1:F:524:LEU:O	1:F:528:LEU:HD12	1.89	0.73
1:D:268:ASN:O	1:B:497:THR:HG23	1.88	0.72
1:F:238:ARG:NH1	1:F:470:GLN:HE21	1.87	0.72
1:B:33:ARG:NH1	1:B:33:ARG:HG3	1.99	0.72
1:A:33:ARG:HD3	2:A:601:FAD:N9A	2.04	0.72
1:C:497:THR:HG23	1:F:268:ASN:O	1.90	0.72
1:A:128:THR:HG23	5:A:722:HOH:O	1.90	0.71
1:C:77:ASP:CB	5:C:746:HOH:O	2.38	0.71
1:F:524:LEU:O	1:F:528:LEU:HB2	1.90	0.71
1:D:529:LEU:HD11	1:F:518:LEU:HD13	1.72	0.71
1:B:125:TRP:HZ3	1:B:365:THR:HG1	1.39	0.71
1:B:457:LEU:HD22	1:B:483:ARG:HG3	1.73	0.71
1:A:19:ARG:CG	1:A:19:ARG:HH11	2.04	0.70
1:D:498:ARG:NH2	1:D:503:GLY:O	2.23	0.70
1:E:457:LEU:HD22	1:E:483:ARG:HG3	1.73	0.70
1:C:125:TRP:HZ3	1:C:365:THR:HG1	1.40	0.70
1:A:512:TYR:CZ	5:A:701:HOH:O	2.44	0.70
1:A:524:LEU:O	1:A:528:LEU:HB2	1.92	0.69
1:F:457:LEU:HD22	1:F:483:ARG:HG3	1.74	0.69
1:D:125:TRP:HZ3	1:D:365:THR:HG1	1.37	0.69
1:A:498:ARG:NH2	1:A:503:GLY:O	2.25	0.69
1:B:19:ARG:HH12	1:B:472:ARG:HH21	1.37	0.69
1:D:457:LEU:HD22	1:D:483:ARG:HG3	1.74	0.69
1:B:19:ARG:NH1	1:B:472:ARG:NH2	2.41	0.69
2:E:601:FAD:HM73	3:E:602:NAP:C5N	2.23	0.69
1:A:119:PHE:CE2	1:A:362:GLU:HB2	2.27	0.69
1:F:106:PHE:O	1:F:108:THR:HG23	1.93	0.69
1:A:19:ARG:NH2	1:A:71:ASP:OD2	2.25	0.68
1:A:33:ARG:HD3	2:A:601:FAD:C8A	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:LEU:HD13	1:B:519:LEU:H	1.59	0.68
1:D:524:LEU:O	1:D:528:LEU:HG	1.93	0.68
1:E:125:TRP:HZ3	1:E:365:THR:HG1	1.39	0.68
1:A:130:GLU:HB2	1:A:135:LYS:NZ	2.09	0.68
1:A:433:TYR:HE2	1:A:437:LEU:HD22	1.58	0.68
1:C:457:LEU:HD22	1:C:483:ARG:HG3	1.75	0.68
1:A:33:ARG:CG	1:A:33:ARG:HH11	2.05	0.68
1:F:63:SER:HB3	1:F:232:ASP:OD1	1.94	0.67
1:A:181:ILE:H	1:A:181:ILE:HD13	1.60	0.67
1:C:172:HIS:HD2	1:C:174:ARG:HB2	1.58	0.67
1:F:450:LEU:HB3	1:F:458:ALA:HB2	1.77	0.67
1:A:51:ARG:HH11	1:A:51:ARG:CG	2.07	0.67
1:D:167:LYS:CD	1:D:308:GLU:HG3	2.25	0.66
1:C:106:PHE:O	1:C:108:THR:HG23	1.95	0.66
1:A:309:THR:HG22	5:A:711:HOH:O	1.95	0.66
1:A:457:LEU:HD22	1:A:483:ARG:HG3	1.76	0.66
1:A:361:LEU:HD23	1:A:363:LYS:O	1.95	0.66
1:E:106:PHE:O	1:E:108:THR:HG23	1.95	0.66
1:A:125:TRP:HZ3	1:A:365:THR:HG1	1.43	0.66
1:F:122:THR:HB	1:F:124:GLN:HG3	1.76	0.66
1:F:125:TRP:HZ3	1:F:365:THR:HG1	1.41	0.66
1:C:238:ARG:NH2	1:C:238:ARG:HG2	2.11	0.65
1:B:279:ARG:HH11	1:B:279:ARG:CG	2.10	0.65
1:B:106:PHE:O	1:B:108:THR:HG23	1.96	0.65
1:C:450:LEU:HB3	1:C:458:ALA:HB2	1.77	0.65
1:D:450:LEU:HB3	1:D:458:ALA:HB2	1.78	0.65
1:C:513:ASN:HB3	1:C:516:LYS:HB3	1.79	0.65
1:D:447:ILE:HB	1:D:448:PRO:HD3	1.79	0.65
1:C:279:ARG:CG	1:C:279:ARG:HH11	2.09	0.64
1:F:238:ARG:NE	1:F:470:GLN:NE2	2.40	0.64
1:D:122:THR:HB	1:D:124:GLN:HG3	1.80	0.64
1:B:519:LEU:HD22	1:B:520:PHE:H	1.62	0.64
1:E:513:ASN:HB3	1:E:516:LYS:HB3	1.81	0.63
1:A:410:ASP:HA	5:A:712:HOH:O	1.97	0.63
1:D:521:PRO:HB2	5:D:711:HOH:O	1.97	0.63
1:F:279:ARG:CG	1:F:279:ARG:HH11	2.11	0.63
1:A:19:ARG:HG2	1:A:19:ARG:NH1	2.11	0.63
1:A:119:PHE:HE2	1:A:362:GLU:HB2	1.61	0.63
1:C:519:LEU:N	1:C:519:LEU:HD13	2.14	0.63
1:E:33:ARG:HG3	1:E:33:ARG:NH1	2.11	0.63
1:F:172:HIS:HD2	1:F:174:ARG:HB2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:HIS:HD2	1:E:174:ARG:HB2	1.63	0.62
1:B:518:LEU:HD13	1:C:529:LEU:HD13	1.81	0.62
1:D:172:HIS:HD2	1:D:174:ARG:HB2	1.63	0.62
1:D:516:LYS:HD2	5:D:719:HOH:O	1.98	0.62
1:B:172:HIS:HD2	1:B:174:ARG:HB2	1.64	0.62
1:D:279:ARG:HH11	1:D:279:ARG:CG	2.12	0.62
1:B:519:LEU:HD13	1:B:519:LEU:N	2.15	0.62
1:D:524:LEU:O	1:D:528:LEU:CG	2.47	0.62
1:E:279:ARG:HH11	1:E:279:ARG:CG	2.13	0.62
1:A:515:LEU:C	1:A:519:LEU:HD21	2.19	0.62
1:D:238:ARG:HE	1:D:470:GLN:NE2	1.97	0.61
1:A:416:LYS:HG3	5:A:730:HOH:O	2.00	0.61
1:B:516:LYS:HA	1:B:519:LEU:HD21	1.82	0.61
1:A:33:ARG:HD3	2:A:601:FAD:C5A	2.28	0.61
1:C:447:ILE:HB	1:C:448:PRO:HD3	1.82	0.61
1:E:450:LEU:HB3	1:E:458:ALA:HB2	1.81	0.61
1:A:12:VAL:HG11	1:A:379:ILE:HG12	1.82	0.61
1:D:19:ARG:HH11	1:D:19:ARG:CG	2.14	0.61
1:D:156:PRO:HG2	3:D:602:NAP:N6A	2.16	0.61
1:F:238:ARG:HE	1:F:470:GLN:HE22	1.44	0.61
1:A:238:ARG:HH21	1:A:431:ILE:HG23	1.65	0.60
1:E:447:ILE:HB	1:E:448:PRO:HD3	1.82	0.60
1:C:82:MET:HE1	1:C:87:LEU:HA	1.83	0.60
1:A:238:ARG:HH21	1:A:431:ILE:CG2	2.14	0.60
1:B:450:LEU:HB3	1:B:458:ALA:HB2	1.82	0.60
1:D:82:MET:HE1	1:D:87:LEU:HA	1.84	0.60
1:F:516:LYS:HE2	5:F:762:HOH:O	1.99	0.60
1:E:255:TRP:HZ2	1:E:515:LEU:HD13	1.65	0.60
1:A:450:LEU:HB3	1:A:458:ALA:HB2	1.82	0.60
1:B:82:MET:HE1	1:B:87:LEU:HA	1.84	0.60
1:F:447:ILE:HB	1:F:448:PRO:HD3	1.84	0.60
1:A:498:ARG:O	1:A:498:ARG:HG2	2.02	0.60
1:A:333:TYR:CD1	1:A:333:TYR:N	2.68	0.59
1:A:238:ARG:HG3	1:A:462:PHE:HA	1.84	0.59
1:E:82:MET:HE1	1:E:87:LEU:HA	1.83	0.59
1:D:349:GLU:HG3	1:D:424:GLN:HE22	1.67	0.59
1:A:399:LEU:HD22	1:A:405:MET:SD	2.42	0.59
1:A:279:ARG:HH11	1:A:279:ARG:CG	2.16	0.59
1:F:82:MET:HE1	1:F:87:LEU:HA	1.83	0.59
1:F:222:SER:HB2	1:F:286:ASP:OD1	2.03	0.58
1:F:498:ARG:NH2	1:F:503:GLY:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:FAD:HM73	3:A:602:NAP:C5N	2.33	0.58
1:A:516:LYS:O	1:A:521:PRO:HD3	2.03	0.58
1:D:255:TRP:HZ2	1:D:515:LEU:HD13	1.68	0.58
1:D:222:SER:HB2	1:D:286:ASP:OD1	2.03	0.58
1:B:315:ASP:OD1	1:B:317:THR:OG1	2.21	0.58
1:B:451:PHE:HD1	1:B:458:ALA:HB1	1.67	0.58
1:A:182:PHE:HA	1:A:185:LYS:HD2	1.86	0.57
1:A:222:SER:HB2	1:A:286:ASP:OD1	2.04	0.57
1:B:447:ILE:HB	1:B:448:PRO:HD3	1.85	0.57
1:E:222:SER:HB2	1:E:286:ASP:OD1	2.04	0.57
1:A:19:ARG:HH22	1:A:71:ASP:CG	2.08	0.57
1:B:349:GLU:HG3	1:B:424:GLN:HE22	1.68	0.57
1:C:222:SER:HB2	1:C:286:ASP:OD1	2.04	0.57
1:A:520:PHE:O	1:A:524:LEU:HB2	2.05	0.57
1:B:451:PHE:CD1	1:B:458:ALA:HB1	2.40	0.57
1:D:167:LYS:HD2	1:D:308:GLU:CG	2.33	0.57
1:C:255:TRP:CZ2	1:C:515:LEU:HD22	2.40	0.57
1:A:333:TYR:N	1:A:333:TYR:HD1	2.02	0.57
1:A:336:PRO:HA	5:A:717:HOH:O	2.04	0.57
1:A:108:THR:HG23	1:A:131:LYS:HD3	1.86	0.56
1:E:520:PHE:O	1:E:524:LEU:HB2	2.05	0.56
1:B:518:LEU:HD13	1:C:529:LEU:CD1	2.35	0.56
1:D:125:TRP:HZ3	1:D:365:THR:OG1	1.88	0.56
1:A:180:GLY:N	5:A:704:HOH:O	2.31	0.56
1:A:33:ARG:HD2	2:A:601:FAD:C4A	2.35	0.56
1:E:125:TRP:HZ3	1:E:365:THR:OG1	1.88	0.56
1:B:19:ARG:CG	1:B:19:ARG:HH11	2.17	0.56
1:D:453:THR:HB	5:D:706:HOH:O	2.06	0.56
1:B:222:SER:HB2	1:B:286:ASP:OD1	2.04	0.56
1:C:19:ARG:NH2	1:C:71:ASP:OD1	2.38	0.56
1:F:34:SER:HB3	1:F:51:ARG:HE	1.71	0.56
1:F:520:PHE:O	1:F:524:LEU:HB2	2.06	0.56
1:C:238:ARG:NH2	5:C:703:HOH:O	2.39	0.56
1:C:34:SER:HB3	1:C:51:ARG:HE	1.70	0.56
1:B:359:PRO:O	1:B:360:LEU:HB2	2.05	0.56
1:E:524:LEU:O	1:E:528:LEU:HB2	2.06	0.56
1:F:513:ASN:HB3	1:F:516:LYS:HB3	1.88	0.56
1:C:506:LYS:HE3	5:C:725:HOH:O	2.05	0.56
1:E:172:HIS:CD2	1:E:174:ARG:H	2.24	0.56
1:A:172:HIS:CD2	1:A:174:ARG:H	2.24	0.55
1:B:172:HIS:CD2	1:B:174:ARG:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:HIS:CD2	1:F:174:ARG:H	2.24	0.55
1:C:125:TRP:HZ3	1:C:365:THR:OG1	1.89	0.55
1:D:359:PRO:O	1:D:360:LEU:HB2	2.06	0.55
1:B:238:ARG:HD3	5:B:747:HOH:O	2.07	0.55
1:D:172:HIS:CD2	1:D:174:ARG:H	2.25	0.55
1:A:18:ILE:HD11	1:A:30:CYS:HB2	1.89	0.55
1:C:172:HIS:CD2	1:C:174:ARG:H	2.25	0.55
1:A:334:ALA:O	1:A:335:TYR:HB2	2.07	0.55
1:D:527:VAL:O	1:D:528:LEU:HD23	2.06	0.55
1:B:122:THR:HB	1:B:124:GLN:HG3	1.88	0.55
1:F:125:TRP:HZ3	1:F:365:THR:OG1	1.90	0.55
1:A:348:ASN:HA	5:A:703:HOH:O	2.06	0.54
1:A:490:TRP:CE2	1:A:508:PRO:HG2	2.41	0.54
1:A:525:LEU:C	1:A:525:LEU:HD22	2.28	0.54
1:E:315:ASP:OD1	1:E:317:THR:OG1	2.24	0.54
1:E:359:PRO:O	1:E:360:LEU:HB2	2.06	0.54
1:F:525:LEU:HD22	1:F:525:LEU:C	2.28	0.54
1:F:527:VAL:O	1:F:527:VAL:HG12	2.07	0.54
1:C:359:PRO:CB	1:C:405:MET:CE	2.85	0.54
1:D:525:LEU:C	1:D:525:LEU:HD22	2.28	0.54
1:E:497:THR:HG21	5:E:705:HOH:O	2.07	0.54
1:E:525:LEU:C	1:E:525:LEU:HD22	2.28	0.54
1:B:524:LEU:O	1:B:528:LEU:HB2	2.07	0.54
1:E:34:SER:HB3	1:E:51:ARG:HE	1.73	0.54
1:B:125:TRP:HZ3	1:B:365:THR:OG1	1.89	0.54
1:E:19:ARG:NH2	1:E:71:ASP:OD1	2.41	0.54
1:A:150:HIS:HD2	2:A:601:FAD:O2'	1.90	0.54
1:B:525:LEU:C	1:B:525:LEU:HD22	2.28	0.54
1:E:527:VAL:HG12	1:E:527:VAL:O	2.08	0.54
1:F:315:ASP:OD1	1:F:317:THR:OG1	2.25	0.54
1:B:34:SER:HB3	1:B:51:ARG:HE	1.73	0.54
1:B:525:LEU:HD21	1:C:522:VAL:HG21	1.90	0.54
1:C:527:VAL:HG12	1:C:527:VAL:O	2.08	0.54
1:D:527:VAL:HG12	1:D:527:VAL:O	2.08	0.54
1:A:117:PRO:HA	5:A:713:HOH:O	2.08	0.54
1:D:51:ARG:HB3	1:D:51:ARG:HH11	1.72	0.54
1:A:527:VAL:O	1:A:527:VAL:HG12	2.08	0.53
1:B:279:ARG:HH11	1:B:279:ARG:HG2	1.73	0.53
1:A:515:LEU:HD13	1:A:519:LEU:HD22	1.91	0.53
1:D:315:ASP:OD1	1:D:317:THR:OG1	2.27	0.53
1:D:19:ARG:NH2	1:D:71:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:VAL:HA	1:A:525:LEU:CD1	2.38	0.53
1:C:19:ARG:HH11	1:C:19:ARG:CG	2.20	0.53
1:E:527:VAL:O	1:E:528:LEU:HD22	2.09	0.53
1:A:18:ILE:HD11	1:A:30:CYS:CB	2.39	0.53
1:B:525:LEU:HD21	1:C:522:VAL:CG2	2.39	0.53
1:D:34:SER:HB3	1:D:51:ARG:HE	1.73	0.53
1:A:125:TRP:HZ3	1:A:365:THR:OG1	1.91	0.53
1:A:135:LYS:CG	5:A:716:HOH:O	2.56	0.53
1:A:90:TYR:HA	5:A:728:HOH:O	2.08	0.53
1:A:145:ILE:CG2	1:A:335:TYR:CD1	2.85	0.53
1:C:349:GLU:HG3	1:C:424:GLN:HE22	1.73	0.53
1:C:524:LEU:HA	1:C:528:LEU:HD23	1.91	0.52
1:D:19:ARG:NH1	1:D:19:ARG:HG2	2.24	0.52
1:C:512:TYR:CE1	1:C:514:LEU:HB2	2.45	0.52
1:A:433:TYR:CD2	1:A:433:TYR:C	2.81	0.52
1:A:359:PRO:O	1:A:360:LEU:HB2	2.09	0.52
1:C:524:LEU:O	1:C:528:LEU:HB2	2.10	0.52
1:F:401:THR:HG22	1:F:404:GLU:CG	2.39	0.52
1:B:238:ARG:HH22	1:B:435:ASP:CG	2.12	0.52
1:C:359:PRO:O	1:C:360:LEU:HB2	2.08	0.52
1:E:51:ARG:HH11	1:E:51:ARG:HB3	1.75	0.52
1:F:119:PHE:CD1	1:F:123:GLY:HA2	2.45	0.52
1:B:527:VAL:O	1:B:527:VAL:HG12	2.10	0.52
1:F:108:THR:HG22	1:F:131:LYS:HD3	1.92	0.52
1:D:401:THR:HG22	1:D:404:GLU:CG	2.40	0.52
1:A:346:ARG:NH1	1:A:406:MET:HE3	2.25	0.52
1:C:300:LYS:CE	5:C:752:HOH:O	2.45	0.52
1:C:167:LYS:HD2	1:C:308:GLU:HG2	1.92	0.51
1:C:315:ASP:OD1	1:C:317:THR:OG1	2.27	0.51
1:D:61:ASN:HD22	1:D:61:ASN:C	2.14	0.51
1:A:33:ARG:HB2	1:A:33:ARG:NH1	2.16	0.51
1:C:156:PRO:HG3	3:C:602:NAP:N6A	2.26	0.51
1:A:172:HIS:HD2	1:A:174:ARG:H	1.59	0.51
1:A:53:SER:OG	1:A:174:ARG:O	2.26	0.51
1:C:401:THR:HG22	1:C:404:GLU:CG	2.41	0.51
1:F:61:ASN:C	1:F:61:ASN:HD22	2.14	0.51
1:B:51:ARG:HB3	1:B:51:ARG:HH11	1.76	0.51
1:A:401:THR:HG22	1:A:404:GLU:CG	2.40	0.51
1:A:33:ARG:HD2	2:A:601:FAD:C6A	2.40	0.51
1:B:108:THR:HG22	1:B:131:LYS:HD3	1.93	0.51
1:B:19:ARG:NH1	1:B:19:ARG:CG	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:TRP:HZ2	1:C:515:LEU:HD22	1.75	0.51
1:D:522:VAL:HG23	5:D:711:HOH:O	2.10	0.51
1:A:315:ASP:OD1	1:A:317:THR:OG1	2.29	0.51
1:B:401:THR:HG22	1:B:404:GLU:CG	2.41	0.51
1:C:41:TRP:CD2	1:C:87:LEU:HD23	2.45	0.51
1:E:229:TYR:CE2	1:E:508:PRO:HG3	2.46	0.51
1:F:41:TRP:CD2	1:F:87:LEU:HD23	2.46	0.51
1:D:167:LYS:CD	1:D:308:GLU:CG	2.88	0.50
1:A:279:ARG:HH11	1:A:279:ARG:HG3	1.76	0.50
1:D:41:TRP:CD2	1:D:87:LEU:HD23	2.46	0.50
1:D:524:LEU:O	1:D:528:LEU:HD12	2.11	0.50
1:E:19:ARG:CG	1:E:19:ARG:HH11	2.23	0.50
1:E:401:THR:HG22	1:E:404:GLU:CG	2.40	0.50
1:E:522:VAL:HA	1:E:525:LEU:CD1	2.41	0.50
1:E:41:TRP:CD2	1:E:87:LEU:HD23	2.46	0.50
1:F:172:HIS:HD2	1:F:174:ARG:H	1.59	0.50
1:F:490:TRP:CZ2	1:F:508:PRO:HG2	2.47	0.50
1:A:3:LYS:N	1:A:141:ASP:OD2	2.45	0.50
1:A:33:ARG:CG	1:A:33:ARG:NH1	2.72	0.50
1:A:349:GLU:CD	1:A:424:GLN:HE22	2.15	0.50
1:B:155:LEU:CD2	1:B:172:HIS:HB2	2.42	0.50
1:A:19:ARG:NH2	1:A:71:ASP:CG	2.65	0.50
1:B:41:TRP:CD2	1:B:87:LEU:HD23	2.45	0.50
1:B:516:LYS:HG2	1:B:519:LEU:HD21	1.92	0.50
1:F:156:PRO:HG2	3:F:602:NAP:H61A	1.77	0.50
1:F:359:PRO:O	1:F:360:LEU:HB2	2.11	0.50
2:D:601:FAD:C6	3:D:602:NAP:C2N	2.90	0.50
1:C:108:THR:HG22	1:C:131:LYS:HD3	1.94	0.50
1:F:51:ARG:HB3	1:F:51:ARG:HH11	1.77	0.50
1:A:19:ARG:O	1:A:19:ARG:HD2	2.12	0.50
1:A:490:TRP:CZ2	1:A:508:PRO:HG2	2.46	0.50
1:C:519:LEU:HD13	1:C:519:LEU:H	1.77	0.50
1:A:114:ASN:HB2	5:A:706:HOH:O	2.12	0.50
1:D:238:ARG:NE	1:D:470:GLN:NE2	2.60	0.50
1:A:433:TYR:HD2	1:A:433:TYR:C	2.15	0.50
1:A:68:CYS:HG	1:A:469:TYR:HE1	1.58	0.50
1:F:524:LEU:HB2	5:F:713:HOH:O	2.10	0.50
1:A:527:VAL:O	1:A:528:LEU:HD22	2.12	0.49
1:A:61:ASN:C	1:A:61:ASN:HD22	2.15	0.49
1:C:238:ARG:NE	1:C:470:GLN:HE21	1.96	0.49
1:E:172:HIS:HD2	1:E:174:ARG:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ARG:HB3	1:C:51:ARG:HH11	1.76	0.49
1:F:215:ARG:NH1	5:F:703:HOH:O	2.42	0.49
1:A:41:TRP:CD2	1:A:87:LEU:HD23	2.47	0.49
1:B:238:ARG:NH2	1:B:435:ASP:OD2	2.45	0.49
1:A:346:ARG:HD3	1:A:406:MET:HE1	1.95	0.49
2:C:601:FAD:HM73	3:C:602:NAP:C5N	2.42	0.49
1:F:345:SER:O	1:F:346:ARG:HB2	2.13	0.49
1:D:518:LEU:CD2	1:F:525:LEU:HD23	2.43	0.49
1:A:51:ARG:NH1	1:A:51:ARG:CG	2.72	0.49
2:B:601:FAD:C6	3:B:602:NAP:C2N	2.91	0.49
1:E:238:ARG:HE	1:E:470:GLN:HE22	1.51	0.49
1:C:172:HIS:HD2	1:C:174:ARG:H	1.60	0.49
1:D:172:HIS:HD2	1:D:174:ARG:H	1.60	0.49
1:B:238:ARG:HH11	1:B:470:GLN:HE21	1.59	0.48
1:C:527:VAL:O	1:C:528:LEU:HD22	2.12	0.48
1:A:123:GLY:O	1:A:141:ASP:O	2.30	0.48
1:B:61:ASN:C	1:B:61:ASN:HD22	2.16	0.48
1:F:238:ARG:HE	1:F:470:GLN:HE21	1.58	0.48
1:F:401:THR:HG22	1:F:404:GLU:HG3	1.95	0.48
1:A:180:GLY:CA	5:A:704:HOH:O	2.60	0.48
1:A:522:VAL:HA	1:A:525:LEU:HD12	1.95	0.48
1:B:451:PHE:HD1	1:B:458:ALA:CB	2.26	0.48
1:C:172:HIS:CD2	1:C:174:ARG:HB2	2.45	0.48
1:C:61:ASN:C	1:C:61:ASN:HD22	2.16	0.48
1:D:516:LYS:O	1:D:521:PRO:HD3	2.13	0.48
1:E:491:ASP:OD1	1:E:507:ARG:NH2	2.40	0.48
1:B:172:HIS:HD2	1:B:174:ARG:H	1.59	0.48
1:D:108:THR:HG23	1:D:131:LYS:HD3	1.94	0.48
1:D:518:LEU:HD13	1:F:529:LEU:CD1	2.44	0.48
2:D:601:FAD:HM73	3:D:602:NAP:C5N	2.43	0.48
1:C:522:VAL:HG23	5:C:747:HOH:O	2.14	0.48
1:A:356:ILE:HD11	1:A:385:GLN:HG2	1.96	0.48
1:B:510:LEU:HD21	5:B:712:HOH:O	2.13	0.48
1:D:518:LEU:HD22	1:F:529:LEU:HD13	1.96	0.48
1:A:348:ASN:CA	5:A:703:HOH:O	2.61	0.47
1:C:238:ARG:NE	1:C:470:GLN:HE22	2.07	0.47
1:C:77:ASP:HB3	5:C:746:HOH:O	2.06	0.47
1:C:519:LEU:HD22	1:C:520:PHE:H	1.78	0.47
1:E:401:THR:HG22	1:E:404:GLU:HB2	1.96	0.47
1:A:137:SER:HB2	5:A:722:HOH:O	2.14	0.47
1:F:156:PRO:HG2	3:F:602:NAP:N6A	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ARG:HH11	1:C:279:ARG:HG2	1.79	0.47
1:D:19:ARG:CG	1:D:19:ARG:NH1	2.73	0.47
1:F:349:GLU:HG3	1:F:424:GLN:HE22	1.80	0.47
1:B:33:ARG:CG	1:B:33:ARG:HH11	2.10	0.47
1:C:512:TYR:CD2	1:C:513:ASN:N	2.83	0.47
1:D:520:PHE:N	1:D:521:PRO:CD	2.78	0.47
1:E:61:ASN:HD22	1:E:61:ASN:C	2.16	0.47
1:F:279:ARG:CG	1:F:279:ARG:NH1	2.78	0.47
1:A:33:ARG:NE	2:A:601:FAD:N7A	2.62	0.47
2:C:601:FAD:C6	3:C:602:NAP:C2N	2.93	0.47
1:A:101:LEU:HA	1:A:104:ILE:HD12	1.96	0.47
1:B:401:THR:HG22	1:B:404:GLU:HB2	1.97	0.47
5:B:715:HOH:O	1:C:529:LEU:HD21	2.14	0.47
1:A:130:GLU:HB2	1:A:135:LYS:HZ1	1.76	0.47
1:A:150:HIS:CD2	2:A:601:FAD:O2'	2.67	0.47
1:C:397:CYS:HA	5:C:713:HOH:O	2.15	0.47
1:D:101:LEU:HD12	5:D:774:HOH:O	2.15	0.47
1:D:345:SER:O	1:D:346:ARG:HB2	2.15	0.47
1:E:512:TYR:CD2	1:E:513:ASN:N	2.82	0.47
1:B:527:VAL:O	1:B:528:LEU:HD22	2.14	0.46
1:D:522:VAL:HA	1:D:525:LEU:CD1	2.45	0.46
1:D:454:ASP:N	5:D:706:HOH:O	2.47	0.46
1:A:236:ILE:HD11	1:A:375:LEU:HB3	1.98	0.46
1:C:40:LEU:HD11	2:C:601:FAD:C8M	2.46	0.46
1:D:156:PRO:HG2	3:D:602:NAP:H61A	1.79	0.46
1:D:3:LYS:N	1:D:141:ASP:OD2	2.48	0.46
1:D:516:LYS:O	1:D:516:LYS:HG2	2.14	0.46
1:B:522:VAL:HA	1:B:525:LEU:CD1	2.45	0.46
1:C:345:SER:O	1:C:346:ARG:HB2	2.15	0.46
1:D:304:LYS:HA	1:D:304:LYS:HD2	1.76	0.46
1:B:520:PHE:O	1:B:524:LEU:HB2	2.15	0.46
1:D:401:THR:HG22	1:D:404:GLU:HG3	1.97	0.46
1:D:216:SER:OG	3:D:602:NAP:O2X	2.34	0.46
1:F:512:TYR:CD2	1:F:513:ASN:N	2.82	0.46
1:E:238:ARG:NE	1:E:470:GLN:NE2	2.43	0.46
1:B:512:TYR:CD2	1:B:513:ASN:N	2.83	0.46
1:B:519:LEU:HD22	1:B:520:PHE:N	2.30	0.46
1:C:279:ARG:NH1	1:C:279:ARG:CG	2.76	0.46
1:D:512:TYR:CD2	1:D:513:ASN:N	2.83	0.46
2:E:601:FAD:C6	3:E:602:NAP:C2N	2.93	0.46
1:D:524:LEU:O	1:D:528:LEU:CD1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ARG:CG	1:C:19:ARG:NH1	2.78	0.46
1:E:229:TYR:CZ	1:E:508:PRO:HG3	2.51	0.46
2:F:601:FAD:HM73	3:F:602:NAP:C5N	2.46	0.46
1:B:156:PRO:HG2	3:B:602:NAP:H61A	1.80	0.45
1:C:359:PRO:CB	1:C:405:MET:HE3	2.33	0.45
1:B:345:SER:O	1:B:346:ARG:HB2	2.16	0.45
1:A:512:TYR:CE1	1:A:514:LEU:HB2	2.51	0.45
1:D:49:GLU:OE2	1:D:49:GLU:HA	2.16	0.45
1:C:521:PRO:HB2	5:C:747:HOH:O	2.16	0.45
1:A:33:ARG:CD	2:A:601:FAD:N7A	2.79	0.45
1:A:512:TYR:CD2	1:A:513:ASN:N	2.83	0.45
1:E:401:THR:HG22	1:E:404:GLU:HG3	1.99	0.45
1:A:401:THR:HG22	1:A:404:GLU:HG3	1.99	0.45
1:B:173:SER:HB3	1:B:328:ALA:HA	1.99	0.45
1:C:33:ARG:HG2	2:C:601:FAD:C4A	2.46	0.45
1:D:401:THR:HG22	1:D:404:GLU:HB2	1.98	0.45
1:D:83:HIS:HD2	1:D:85:SER:OG	2.00	0.45
1:F:158:GLU:O	1:F:158:GLU:HG3	2.17	0.45
1:C:3:LYS:N	1:C:141:ASP:OD2	2.50	0.45
1:C:516:LYS:HA	1:C:519:LEU:HD21	1.99	0.45
1:B:516:LYS:HA	1:B:519:LEU:HD11	1.99	0.45
2:B:601:FAD:HM73	3:B:602:NAP:C5N	2.46	0.45
1:E:498:ARG:NH2	1:E:503:GLY:O	2.50	0.45
1:A:119:PHE:O	1:A:122:THR:O	2.34	0.44
1:B:520:PHE:N	1:B:521:PRO:CD	2.80	0.44
1:D:19:ARG:HH11	1:D:19:ARG:HG2	1.82	0.44
1:D:63:SER:HB3	1:D:232:ASP:OD1	2.17	0.44
1:B:529:LEU:CD1	1:C:518:LEU:HD22	2.48	0.44
1:E:122:THR:HB	1:E:124:GLN:HG3	1.98	0.44
1:A:357:PHE:CD2	1:A:399:LEU:HD21	2.52	0.44
1:C:19:ARG:HG2	1:C:19:ARG:NH1	2.33	0.44
1:C:401:THR:HG22	1:C:404:GLU:HB2	1.98	0.44
1:B:529:LEU:HD22	5:C:757:HOH:O	2.17	0.44
1:E:522:VAL:HA	1:E:525:LEU:HD12	1.98	0.44
1:F:171:PHE:CZ	1:F:326:ILE:HD13	2.52	0.44
1:F:401:THR:HG22	1:F:404:GLU:HB2	2.00	0.44
1:C:205:HIS:HE1	1:C:287:GLU:OE1	2.01	0.44
1:E:19:ARG:CG	1:E:19:ARG:NH1	2.79	0.44
2:F:601:FAD:C6	3:F:602:NAP:C2N	2.95	0.44
1:A:63:SER:HB3	1:A:232:ASP:OD1	2.18	0.44
1:B:63:SER:HB3	1:B:232:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:SER:HB3	1:E:328:ALA:HA	2.00	0.44
1:D:279:ARG:HH11	1:D:279:ARG:HG2	1.81	0.44
1:A:181:ILE:H	1:A:181:ILE:CD1	2.21	0.44
3:A:602:NAP:O5D	3:A:602:NAP:O2A	2.35	0.44
1:C:63:SER:HB3	1:C:232:ASP:OD1	2.18	0.44
1:C:520:PHE:O	1:C:524:LEU:HB2	2.18	0.44
1:E:345:SER:O	1:E:346:ARG:HB2	2.18	0.44
1:E:520:PHE:N	1:E:521:PRO:CD	2.81	0.44
1:F:524:LEU:CB	5:F:713:HOH:O	2.66	0.44
1:A:135:LYS:HB2	5:A:716:HOH:O	2.18	0.43
1:A:401:THR:HG22	1:A:404:GLU:HB2	2.00	0.43
1:E:3:LYS:N	1:E:141:ASP:OD2	2.51	0.43
1:B:3:LYS:N	1:B:141:ASP:OD2	2.51	0.43
1:B:495:LYS:HB3	1:B:496:PRO:HD3	2.00	0.43
5:B:715:HOH:O	1:C:529:LEU:CD2	2.65	0.43
1:D:93:ALA:HA	5:D:758:HOH:O	2.16	0.43
1:E:83:HIS:HD2	1:E:85:SER:OG	2.01	0.43
1:B:82:MET:HE2	1:B:87:LEU:HB2	2.00	0.43
1:D:173:SER:HB3	1:D:328:ALA:HA	1.99	0.43
1:D:238:ARG:CZ	1:D:470:GLN:HE21	2.29	0.43
1:F:279:ARG:HG2	1:F:279:ARG:HH11	1.80	0.43
1:B:516:LYS:HA	1:B:519:LEU:CD2	2.46	0.43
1:D:529:LEU:CD1	1:F:518:LEU:HD13	2.45	0.43
1:B:345:SER:HB3	5:B:704:HOH:O	2.19	0.43
1:B:359:PRO:O	1:B:360:LEU:CB	2.66	0.43
1:F:401:THR:HG22	1:F:404:GLU:CB	2.49	0.43
1:F:238:ARG:CZ	1:F:470:GLN:HE21	2.32	0.43
1:B:519:LEU:CD1	1:B:519:LEU:N	2.79	0.43
1:E:63:SER:HB3	1:E:232:ASP:OD1	2.18	0.43
1:A:26:LEU:HD21	1:A:394:ALA:HB2	2.00	0.43
1:B:236:ILE:HD11	1:B:375:LEU:HB3	2.01	0.43
1:C:401:THR:HG22	1:C:404:GLU:HG3	2.00	0.43
2:A:601:FAD:HM73	3:A:602:NAP:C6N	2.49	0.43
1:B:401:THR:HG22	1:B:404:GLU:CB	2.48	0.43
1:D:529:LEU:HD11	1:F:518:LEU:CD1	2.45	0.43
1:E:288:LEU:HB3	1:E:289:PRO:HD3	2.01	0.43
1:F:238:ARG:NE	1:F:470:GLN:HE22	2.12	0.43
1:B:19:ARG:NH1	1:B:19:ARG:HG2	2.33	0.42
1:E:279:ARG:NH1	1:E:279:ARG:CG	2.79	0.42
1:E:359:PRO:O	1:E:360:LEU:CB	2.67	0.42
1:F:216:SER:O	1:F:273:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:HIS:HD2	1:F:85:SER:OG	2.02	0.42
1:D:288:LEU:HB3	1:D:289:PRO:HD3	2.01	0.42
1:D:33:ARG:HH11	1:D:33:ARG:CG	2.12	0.42
1:D:520:PHE:O	1:D:524:LEU:HB2	2.19	0.42
1:E:19:ARG:NH1	1:E:472:ARG:NH2	2.67	0.42
1:F:520:PHE:N	1:F:521:PRO:CD	2.82	0.42
1:A:83:HIS:HD2	1:A:85:SER:OG	2.02	0.42
1:C:173:SER:HB3	1:C:328:ALA:HA	2.01	0.42
1:C:516:LYS:HA	1:C:519:LEU:CD2	2.49	0.42
1:E:401:THR:HG22	1:E:404:GLU:CB	2.48	0.42
1:A:520:PHE:N	1:A:521:PRO:CD	2.82	0.42
1:D:401:THR:HG22	1:D:404:GLU:CB	2.48	0.42
1:B:401:THR:HG22	1:B:404:GLU:HG3	2.00	0.42
1:B:83:HIS:HD2	1:B:85:SER:OG	2.02	0.42
1:D:205:HIS:HE1	1:D:287:GLU:OE1	2.03	0.42
1:F:172:HIS:CD2	1:F:174:ARG:HB2	2.50	0.42
1:F:205:HIS:HE1	1:F:287:GLU:OE1	2.02	0.42
1:F:513:ASN:O	1:F:517:ILE:HD13	2.19	0.42
1:F:33:ARG:HG2	2:F:601:FAD:C4A	2.49	0.42
1:D:359:PRO:O	1:D:360:LEU:CB	2.67	0.42
1:F:3:LYS:N	1:F:141:ASP:OD2	2.53	0.42
1:F:158:GLU:O	1:F:158:GLU:CG	2.67	0.42
1:B:172:HIS:CD2	1:B:174:ARG:HB2	2.50	0.42
1:C:401:THR:HG22	1:C:404:GLU:CB	2.49	0.42
1:C:83:HIS:HD2	1:C:85:SER:OG	2.03	0.42
1:A:359:PRO:O	1:A:360:LEU:CB	2.68	0.42
1:E:364:PRO:HA	5:E:741:HOH:O	2.19	0.42
1:F:236:ILE:HD11	1:F:375:LEU:HB3	2.02	0.42
1:A:135:LYS:CB	5:A:716:HOH:O	2.68	0.42
1:B:498:ARG:NH2	1:B:503:GLY:O	2.53	0.42
1:C:105:GLN:HG3	5:C:739:HOH:O	2.20	0.42
1:C:520:PHE:N	1:C:521:PRO:CD	2.83	0.42
1:A:18:ILE:HG22	1:A:100:LEU:HD22	2.01	0.41
1:A:401:THR:HG22	1:A:404:GLU:CB	2.50	0.41
1:A:495:LYS:N	1:A:496:PRO:HD2	2.35	0.41
1:A:507:ARG:H	1:A:507:ARG:HG2	1.47	0.41
1:D:171:PHE:CZ	1:D:326:ILE:HD13	2.55	0.41
1:D:236:ILE:HD11	1:D:375:LEU:HB3	2.01	0.41
1:F:125:TRP:CH2	1:F:366:LEU:HB2	2.55	0.41
1:A:116:ARG:NH2	1:A:139:VAL:HG21	2.35	0.41
1:B:33:ARG:NH1	1:B:33:ARG:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LEU:HD13	1:C:518:LEU:HD22	2.01	0.41
1:D:116:ARG:HG3	1:D:124:GLN:HB2	2.03	0.41
1:A:116:ARG:HB2	1:A:124:GLN:O	2.21	0.41
1:A:82:MET:HE2	1:A:82:MET:HB2	1.68	0.41
1:F:279:ARG:HG3	1:F:279:ARG:HH11	1.85	0.41
1:A:378:THR:HG21	2:A:601:FAD:C5'	2.50	0.41
1:C:83:HIS:CD2	1:C:85:SER:H	2.39	0.41
1:D:216:SER:O	1:D:273:PRO:HA	2.21	0.41
1:D:491:ASP:HA	1:D:507:ARG:HH12	1.86	0.41
1:E:279:ARG:HG3	1:E:279:ARG:HH11	1.85	0.41
1:A:155:LEU:CD2	1:A:172:HIS:HB2	2.50	0.41
1:A:288:LEU:HB3	1:A:289:PRO:HD3	2.02	0.41
1:B:495:LYS:N	1:B:496:PRO:HD2	2.36	0.41
1:C:236:ILE:HD11	1:C:375:LEU:HB3	2.03	0.41
1:D:522:VAL:HA	1:D:525:LEU:HD12	2.03	0.41
1:F:49:GLU:OE2	1:F:49:GLU:HA	2.21	0.41
1:A:512:TYR:OH	5:A:701:HOH:O	2.22	0.41
1:B:279:ARG:HG2	1:B:279:ARG:NH1	2.34	0.41
1:B:205:HIS:HE1	1:B:287:GLU:OE1	2.02	0.41
1:E:83:HIS:CD2	1:E:85:SER:H	2.39	0.41
1:B:216:SER:O	1:B:273:PRO:HA	2.20	0.41
1:B:516:LYS:HE3	1:B:516:LYS:HB3	1.92	0.41
1:C:152:TYR:CE2	1:C:334:ALA:HB3	2.56	0.41
1:C:49:GLU:OE2	1:C:49:GLU:HA	2.20	0.41
1:D:356:ILE:HD11	1:D:385:GLN:HG2	2.03	0.41
1:E:216:SER:O	1:E:273:PRO:HA	2.20	0.41
1:F:516:LYS:HG2	1:F:516:LYS:O	2.21	0.41
1:B:451:PHE:CE1	1:B:459:LEU:HD23	2.56	0.41
1:F:238:ARG:NE	1:F:470:GLN:HE21	2.16	0.41
1:A:158:GLU:CG	1:A:158:GLU:O	2.68	0.40
1:A:216:SER:O	1:A:273:PRO:HA	2.21	0.40
1:A:519:LEU:HD23	1:A:519:LEU:N	2.36	0.40
1:B:171:PHE:CZ	1:B:326:ILE:HD13	2.56	0.40
1:A:125:TRP:CH2	1:A:366:LEU:HB2	2.56	0.40
1:C:279:ARG:HG3	1:C:279:ARG:HH11	1.83	0.40
1:D:41:TRP:CE2	1:D:87:LEU:HD23	2.56	0.40
1:A:125:TRP:HH2	1:A:361:LEU:HD21	1.85	0.40
1:D:504:GLU:O	1:D:506:LYS:HD3	2.21	0.40
1:A:164:LYS:HE3	5:A:727:HOH:O	2.21	0.40
1:A:33:ARG:NE	2:A:601:FAD:C5A	2.85	0.40
1:C:510:LEU:O	1:C:512:TYR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ARG:NH1	1:D:470:GLN:NE2	2.56	0.40
1:D:529:LEU:CD1	1:F:518:LEU:CD1	2.99	0.40
1:E:82:MET:HE2	1:E:87:LEU:HB2	2.04	0.40
1:F:359:PRO:O	1:F:360:LEU:CB	2.69	0.40
1:C:171:PHE:CZ	1:C:326:ILE:HD13	2.56	0.40
1:B:518:LEU:HD21	1:C:525:LEU:HD12	2.04	0.40
1:E:150:HIS:HD2	2:E:601:FAD:O2'	2.04	0.40
2:F:601:FAD:O2'	2:F:601:FAD:H5'1	2.22	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	526/532 (99%)	481 (91%)	41 (8%)	4 (1%)	19	49
1	B	526/532 (99%)	487 (93%)	34 (6%)	5 (1%)	15	44
1	C	526/532 (99%)	489 (93%)	32 (6%)	5 (1%)	15	44
1	D	526/532 (99%)	484 (92%)	38 (7%)	4 (1%)	19	49
1	E	526/532 (99%)	487 (93%)	34 (6%)	5 (1%)	15	44
1	F	526/532 (99%)	485 (92%)	37 (7%)	4 (1%)	19	49
All	All	3156/3192 (99%)	2913 (92%)	216 (7%)	27 (1%)	17	46

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	511	PHE
1	A	511	PHE
1	B	511	PHE
1	C	511	PHE

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Mol	Chain	Res	Type
1	E	511	PHE
1	D	346	ARG
1	D	529	LEU
1	A	529	LEU
1	B	346	ARG
1	B	529	LEU
1	C	346	ARG
1	C	529	LEU
1	E	346	ARG
1	E	529	LEU
1	F	346	ARG
1	F	511	PHE
1	F	529	LEU
1	B	513	ASN
1	C	513	ASN
1	E	513	ASN
1	D	513	ASN
1	A	513	ASN
1	A	346	ARG
1	F	513	ASN
1	E	527	VAL
1	C	527	VAL
1	B	527	VAL

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	459/462 (99%)	402 (88%)	57 (12%)	4 14
1	B	459/462 (99%)	408 (89%)	51 (11%)	6 19
1	C	459/462 (99%)	416 (91%)	43 (9%)	8 26
1	D	459/462 (99%)	414 (90%)	45 (10%)	8 24
1	E	459/462 (99%)	415 (90%)	44 (10%)	8 24
1	F	459/462 (99%)	410 (89%)	49 (11%)	6 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2754/2772 (99%)	2465 (90%)	289 (10%)	7 20

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	12	VAL
1	D	19	ARG
1	D	33	ARG
1	D	51	ARG
1	D	54	ILE
1	D	56	GLN
1	D	61	ASN
1	D	77	ASP
1	D	82	MET
1	D	108	THR
1	D	125	TRP
1	D	167	LYS
1	D	170	CYS
1	D	173	SER
1	D	178	GLU
1	D	216	SER
1	D	237	THR
1	D	251	ILE
1	D	252	SER
1	D	258	LYS
1	D	272	MET
1	D	279	ARG
1	D	285	ASN
1	D	304	LYS
1	D	308	GLU
1	D	312	ILE
1	D	317	THR
1	D	326	ILE
1	D	349	GLU
1	D	373	GLN
1	D	375	LEU
1	D	384	LEU
1	D	401	THR
1	D	403	ASN
1	D	450	LEU
1	D	480	ASP
1	D	494	LEU

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Mol	Chain	Res	Type
1	D	499	THR
1	D	507	ARG
1	D	512	TYR
1	D	513	ASN
1	D	520	PHE
1	D	523	LEU
1	D	525	LEU
1	D	529	LEU
1	A	12	VAL
1	A	19	ARG
1	A	22	LEU
1	A	33	ARG
1	A	49	GLU
1	A	51	ARG
1	A	54	ILE
1	A	56	GLN
1	A	61	ASN
1	A	108	THR
1	A	116	ARG
1	A	121	VAL
1	A	125	TRP
1	A	132	ASP
1	A	147	SER
1	A	155	LEU
1	A	158	GLU
1	A	170	CYS
1	A	173	SER
1	A	178	GLU
1	A	181	ILE
1	A	215	ARG
1	A	216	SER
1	A	237	THR
1	A	240	GLU
1	A	252	SER
1	A	258	LYS
1	A	279	ARG
1	A	285	ASN
1	A	312	ILE
1	A	317	THR
1	A	333	TYR
1	A	338	LEU
1	A	340	ASP

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Mol	Chain	Res	Type
1	A	349	GLU
1	A	373	GLN
1	A	375	LEU
1	A	384	LEU
1	A	398	THR
1	A	403	ASN
1	A	413	MET
1	A	433	TYR
1	A	480	ASP
1	A	494	LEU
1	A	497	THR
1	A	498	ARG
1	A	499	THR
1	A	506	LYS
1	A	512	TYR
1	A	513	ASN
1	A	514	LEU
1	A	515	LEU
1	A	516	LYS
1	A	517	ILE
1	A	519	LEU
1	A	523	LEU
1	A	525	LEU
1	B	12	VAL
1	B	19	ARG
1	B	33	ARG
1	B	40	LEU
1	B	51	ARG
1	B	54	ILE
1	B	56	GLN
1	B	61	ASN
1	B	77	ASP
1	B	82	MET
1	B	108	THR
1	B	121	VAL
1	B	125	TRP
1	B	155	LEU
1	B	167	LYS
1	B	169	LYS
1	B	170	CYS
1	B	173	SER
1	B	178	GLU

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Mol	Chain	Res	Type
1	B	216	SER
1	B	237	THR
1	B	252	SER
1	B	279	ARG
1	B	280	LYS
1	B	285	ASN
1	B	304	LYS
1	B	308	GLU
1	B	312	ILE
1	B	317	THR
1	B	326	ILE
1	B	341	SER
1	B	343	ILE
1	B	349	GLU
1	B	373	GLN
1	B	375	LEU
1	B	384	LEU
1	B	403	ASN
1	B	444	LYS
1	B	480	ASP
1	B	494	LEU
1	B	499	THR
1	B	506	LYS
1	B	507	ARG
1	B	511	PHE
1	B	512	TYR
1	B	516	LYS
1	B	519	LEU
1	B	520	PHE
1	B	523	LEU
1	B	525	LEU
1	B	529	LEU
1	C	12	VAL
1	C	19	ARG
1	C	33	ARG
1	C	51	ARG
1	C	54	ILE
1	C	56	GLN
1	C	61	ASN
1	C	77	ASP
1	C	82	MET
1	C	108	THR

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Mol	Chain	Res	Type
1	C	125	TRP
1	C	170	CYS
1	C	173	SER
1	C	178	GLU
1	C	209	LYS
1	C	216	SER
1	C	237	THR
1	C	240	GLU
1	C	252	SER
1	C	258	LYS
1	C	274	LEU
1	C	279	ARG
1	C	285	ASN
1	C	308	GLU
1	C	312	ILE
1	C	317	THR
1	C	326	ILE
1	C	349	GLU
1	C	373	GLN
1	C	375	LEU
1	C	384	LEU
1	C	403	ASN
1	C	478	LYS
1	C	480	ASP
1	C	494	LEU
1	C	499	THR
1	C	507	ARG
1	C	512	TYR
1	C	513	ASN
1	C	514	LEU
1	C	519	LEU
1	C	525	LEU
1	C	529	LEU
1	E	12	VAL
1	E	19	ARG
1	E	33	ARG
1	E	40	LEU
1	E	51	ARG
1	E	54	ILE
1	E	56	GLN
1	E	61	ASN
1	E	82	MET

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Mol	Chain	Res	Type
1	E	108	THR
1	E	125	TRP
1	E	155	LEU
1	E	167	LYS
1	E	170	CYS
1	E	173	SER
1	E	178	GLU
1	E	216	SER
1	E	237	THR
1	E	252	SER
1	E	258	LYS
1	E	279	ARG
1	E	285	ASN
1	E	300	LYS
1	E	304	LYS
1	E	312	ILE
1	E	317	THR
1	E	326	ILE
1	E	343	ILE
1	E	373	GLN
1	E	375	LEU
1	E	384	LEU
1	E	403	ASN
1	E	480	ASP
1	E	494	LEU
1	E	499	THR
1	E	506	LYS
1	E	507	ARG
1	E	511	PHE
1	E	512	TYR
1	E	516	LYS
1	E	519	LEU
1	E	520	PHE
1	E	523	LEU
1	E	525	LEU
1	F	19	ARG
1	F	33	ARG
1	F	49	GLU
1	F	51	ARG
1	F	54	ILE
1	F	56	GLN
1	F	61	ASN

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Mol	Chain	Res	Type
1	F	63	SER
1	F	77	ASP
1	F	82	MET
1	F	108	THR
1	F	120	SER
1	F	121	VAL
1	F	122	THR
1	F	125	TRP
1	F	132	ASP
1	F	169	LYS
1	F	170	CYS
1	F	173	SER
1	F	178	GLU
1	F	181	ILE
1	F	216	SER
1	F	237	THR
1	F	252	SER
1	F	258	LYS
1	F	274	LEU
1	F	279	ARG
1	F	285	ASN
1	F	312	ILE
1	F	317	THR
1	F	326	ILE
1	F	344	LYS
1	F	349	GLU
1	F	373	GLN
1	F	375	LEU
1	F	384	LEU
1	F	403	ASN
1	F	480	ASP
1	F	494	LEU
1	F	498	ARG
1	F	506	LYS
1	F	507	ARG
1	F	511	PHE
1	F	512	TYR
1	F	513	ASN
1	F	516	LYS
1	F	523	LEU
1	F	525	LEU
1	F	529	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	56	GLN
1	D	61	ASN
1	D	83	HIS
1	D	150	HIS
1	D	172	HIS
1	D	205	HIS
1	D	285	ASN
1	D	373	GLN
1	D	470	GLN
1	A	56	GLN
1	A	83	HIS
1	A	150	HIS
1	A	172	HIS
1	A	205	HIS
1	A	285	ASN
1	A	395	ASN
1	B	56	GLN
1	B	61	ASN
1	B	83	HIS
1	B	150	HIS
1	B	172	HIS
1	B	205	HIS
1	B	285	ASN
1	B	373	GLN
1	B	470	GLN
1	B	513	ASN
1	C	56	GLN
1	C	61	ASN
1	C	83	HIS
1	C	150	HIS
1	C	172	HIS
1	C	205	HIS
1	C	285	ASN
1	C	470	GLN
1	E	56	GLN
1	E	61	ASN
1	E	83	HIS
1	E	150	HIS
1	E	172	HIS
1	E	205	HIS
1	E	285	ASN

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Mol	Chain	Res	Type
1	E	470	GLN
1	F	56	GLN
1	F	61	ASN
1	F	83	HIS
1	F	150	HIS
1	F	172	HIS
1	F	205	HIS
1	F	285	ASN
1	F	470	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

18 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	$\#\|Z\| > 2$
2	FAD	A	601	-	51,58,58	2.10	13 (25%)	60,89,89	3.04	25 (41%)
4	OXY	C	603	-	1,1,1	0.01	0	-		
3	NAP	D	602	-	45,52,52	0.99	2 (4%)	56,80,80	1.37	8 (14%)
4	OXY	A	603	-	1,1,1	0.00	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAP	F	602	-	45,52,52	0.88	0	56,80,80	1.58	14 (25%)
3	NAP	C	602	-	45,52,52	0.91	1 (2%)	56,80,80	1.69	11 (19%)
4	OXY	D	603	-	1,1,1	0.12	0	-		
3	NAP	E	602	-	45,52,52	1.15	4 (8%)	56,80,80	1.67	11 (19%)
3	NAP	B	602	-	45,52,52	0.96	2 (4%)	56,80,80	1.40	4 (7%)
4	OXY	F	603	-	1,1,1	0.01	0	-		
3	NAP	A	602	-	45,52,52	1.18	5 (11%)	56,80,80	1.86	16 (28%)
2	FAD	B	601	-	51,58,58	1.84	10 (19%)	60,89,89	2.78	17 (28%)
4	OXY	B	603	-	1,1,1	0.03	0	-		
2	FAD	F	601	-	51,58,58	1.79	10 (19%)	60,89,89	2.14	16 (26%)
2	FAD	C	601	-	51,58,58	1.97	8 (15%)	60,89,89	2.61	19 (31%)
2	FAD	D	601	-	51,58,58	1.99	11 (21%)	60,89,89	2.68	15 (25%)
2	FAD	E	601	-	51,58,58	1.66	6 (11%)	60,89,89	2.32	13 (21%)
4	OXY	E	603	-	1,1,1	0.02	0	-		

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	-	-	2/31/67/67	0/5/5/5
3	NAP	F	602	-	-	6/31/67/67	0/5/5/5
3	NAP	C	602	-	-	7/31/67/67	0/5/5/5
3	NAP	E	602	-	-	5/31/67/67	0/5/5/5
3	NAP	B	602	-	-	4/31/67/67	0/5/5/5
3	NAP	A	602	-	-	9/31/67/67	0/5/5/5
2	FAD	B	601	-	-	4/30/50/50	0/6/6/6
2	FAD	C	601	-	-	6/30/50/50	0/6/6/6
2	FAD	F	601	-	-	8/30/50/50	0/6/6/6
2	FAD	A	601	-	-	15/30/50/50	0/6/6/6
2	FAD	D	601	-	-	7/30/50/50	0/6/6/6
2	FAD	E	601	-	-	6/30/50/50	0/6/6/6

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C4X-C10	9.74	1.48	1.38
2	D	601	FAD	C4X-C10	8.96	1.47	1.38
2	A	601	FAD	C4X-C10	8.62	1.47	1.38
2	B	601	FAD	C4X-C10	8.37	1.47	1.38
2	F	601	FAD	C4X-C10	7.86	1.46	1.38
2	E	601	FAD	C4X-C10	7.78	1.46	1.38
2	D	601	FAD	C4-C4X	5.19	1.50	1.41
2	A	601	FAD	C5'-C4'	4.57	1.58	1.51
2	B	601	FAD	C6-C5X	-4.10	1.35	1.41
2	A	601	FAD	C9A-C5X	4.01	1.50	1.42
2	F	601	FAD	C1'-N10	-3.95	1.44	1.48
3	E	602	NAP	C2D-C1D	-3.86	1.47	1.53
2	D	601	FAD	C1'-N10	-3.84	1.44	1.48
2	F	601	FAD	C6-C5X	-3.83	1.35	1.41
2	E	601	FAD	C1'-N10	-3.76	1.44	1.48
2	C	601	FAD	C9A-C5X	3.74	1.50	1.42
2	C	601	FAD	C8-C7	3.71	1.50	1.40
2	A	601	FAD	C8-C7	3.53	1.49	1.40
2	C	601	FAD	C4-C4X	3.49	1.47	1.41
2	F	601	FAD	C2B-C1B	-3.49	1.48	1.53
2	C	601	FAD	C10-N1	3.45	1.37	1.33
2	B	601	FAD	C9A-N10	3.44	1.43	1.38
2	E	601	FAD	C9A-C5X	3.32	1.49	1.42
2	A	601	FAD	C4-C4X	3.25	1.47	1.41
2	D	601	FAD	O4B-C1B	3.22	1.45	1.41
2	A	601	FAD	C5A-C4A	3.17	1.49	1.40
2	B	601	FAD	C9A-C5X	3.06	1.48	1.42
2	A	601	FAD	O4B-C1B	2.98	1.45	1.41
3	A	602	NAP	O4D-C1D	2.85	1.45	1.41
3	A	602	NAP	C2A-N3A	2.84	1.36	1.32
2	E	601	FAD	C4-C4X	2.80	1.46	1.41
2	A	601	FAD	C9A-N10	2.76	1.42	1.38
2	D	601	FAD	C9A-C5X	2.75	1.48	1.42
3	B	602	NAP	C2D-C1D	-2.65	1.49	1.53
2	B	601	FAD	C4-C4X	2.63	1.45	1.41
3	A	602	NAP	C5A-C4A	2.61	1.47	1.40
2	F	601	FAD	C4-C4X	2.61	1.45	1.41
3	E	602	NAP	O4D-C1D	2.61	1.44	1.41
2	E	601	FAD	C8-C7	2.50	1.47	1.40
3	D	602	NAP	C5A-C4A	2.50	1.47	1.40
2	A	601	FAD	C4-N3	2.46	1.37	1.33
2	D	601	FAD	C8-C7	2.44	1.47	1.40
3	B	602	NAP	C5A-C4A	2.40	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4A-N3A	2.37	1.38	1.35
2	D	601	FAD	C5A-C4A	2.34	1.47	1.40
2	D	601	FAD	C2-N3	-2.33	1.33	1.38
2	F	601	FAD	C9A-C5X	2.33	1.47	1.42
2	B	601	FAD	C10-N1	2.30	1.36	1.33
2	C	601	FAD	C6-C5X	-2.30	1.38	1.41
2	C	601	FAD	C4'-C3'	-2.29	1.49	1.53
3	C	602	NAP	C2D-C3D	-2.26	1.47	1.53
2	B	601	FAD	C8-C7	2.23	1.46	1.40
2	D	601	FAD	C2A-N3A	2.22	1.35	1.32
3	E	602	NAP	C5D-C4D	2.18	1.58	1.51
2	F	601	FAD	C9-C9A	-2.18	1.36	1.40
2	B	601	FAD	C2B-C1B	-2.17	1.50	1.53
3	A	602	NAP	C8A-N7A	2.17	1.38	1.34
2	A	601	FAD	C2A-N3A	2.17	1.35	1.32
2	D	601	FAD	C2-N1	-2.17	1.33	1.38
3	D	602	NAP	C2A-N3A	2.14	1.35	1.32
2	D	601	FAD	C5'-C4'	2.13	1.54	1.51
2	B	601	FAD	C5'-C4'	2.10	1.54	1.51
2	F	601	FAD	C8-C7	2.09	1.46	1.40
2	B	601	FAD	C5A-C4A	2.09	1.46	1.40
2	F	601	FAD	C9A-N10	2.08	1.41	1.38
2	A	601	FAD	C10-N1	2.08	1.35	1.33
3	A	602	NAP	PN-O5D	2.07	1.67	1.59
2	F	601	FAD	C5A-C4A	2.06	1.46	1.40
2	C	601	FAD	C9A-N10	2.05	1.41	1.38
2	E	601	FAD	C2B-C1B	-2.04	1.50	1.53
3	E	602	NAP	C2N-C3N	2.02	1.42	1.39
2	A	601	FAD	C2'-C3'	2.00	1.57	1.53

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	FAD	C4-N3-C2	12.04	125.30	115.14
2	E	601	FAD	C4-N3-C2	10.19	123.75	115.14
2	B	601	FAD	C4-C4X-C10	-10.05	113.30	119.95
2	B	601	FAD	C1'-N10-C9A	9.51	125.78	118.29
2	A	601	FAD	C1'-N10-C9A	9.41	125.70	118.29
2	B	601	FAD	C4-N3-C2	9.19	122.91	115.14
2	D	601	FAD	C1'-N10-C9A	8.81	125.23	118.29
2	A	601	FAD	C4-C4X-C10	-8.77	114.14	119.95
2	D	601	FAD	C4-N3-C2	8.71	122.50	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	C4-N3-C2	8.36	122.20	115.14
2	C	601	FAD	C4-C4X-C10	-7.94	114.69	119.95
2	E	601	FAD	C4-C4X-C10	-7.92	114.71	119.95
2	D	601	FAD	C4X-N5-C5X	6.98	123.75	116.77
2	F	601	FAD	C1'-N10-C9A	6.82	123.66	118.29
2	D	601	FAD	C10-C4X-N5	-6.73	116.60	121.26
2	F	601	FAD	C4-N3-C2	6.66	120.76	115.14
2	F	601	FAD	C4-C4X-C10	-6.63	115.56	119.95
2	D	601	FAD	C4-C4X-N5	6.59	126.13	118.60
2	A	601	FAD	P-O3P-PA	-5.76	113.08	132.83
3	C	602	NAP	O7N-C7N-C3N	-5.59	112.94	119.63
2	A	601	FAD	O5'-C5'-C4'	5.14	123.08	109.36
3	A	602	NAP	N3A-C2A-N1A	-5.13	120.66	128.68
2	A	601	FAD	N3A-C2A-N1A	-4.97	120.91	128.68
2	F	601	FAD	N3A-C2A-N1A	-4.90	121.02	128.68
2	C	601	FAD	C1'-N10-C9A	4.77	122.04	118.29
2	D	601	FAD	C4X-C4-N3	-4.74	116.95	123.43
2	E	601	FAD	O2'-C2'-C1'	-4.72	98.24	109.59
2	C	601	FAD	N3A-C2A-N1A	-4.70	121.34	128.68
3	E	602	NAP	N3A-C2A-N1A	-4.67	121.38	128.68
2	B	601	FAD	C4-C4X-N5	4.64	123.91	118.60
2	A	601	FAD	O5'-P-O1P	-4.60	91.08	109.07
3	A	602	NAP	PN-O3-PA	-4.47	117.47	132.83
3	C	602	NAP	N3A-C2A-N1A	-4.42	121.77	128.68
3	F	602	NAP	C1B-N9A-C4A	-4.37	118.97	126.64
2	E	601	FAD	C1'-N10-C9A	4.35	121.71	118.29
3	B	602	NAP	N3A-C2A-N1A	-4.20	122.11	128.68
3	F	602	NAP	N3A-C2A-N1A	-4.19	122.13	128.68
2	A	601	FAD	C1B-N9A-C4A	-4.19	119.28	126.64
3	C	602	NAP	C1B-N9A-C4A	-4.17	119.31	126.64
2	D	601	FAD	C4-C4X-C10	-4.12	117.23	119.95
2	A	601	FAD	O2'-C2'-C3'	4.09	119.05	109.10
3	D	602	NAP	N3A-C2A-N1A	-4.05	122.35	128.68
3	A	602	NAP	C3N-C7N-N7N	4.05	122.61	117.75
2	D	601	FAD	C1'-N10-C10	-4.04	114.79	118.41
2	C	601	FAD	O2'-C2'-C1'	-4.03	99.89	109.59
2	B	601	FAD	C4X-N5-C5X	4.01	120.78	116.77
2	B	601	FAD	O2'-C2'-C1'	-4.00	99.97	109.59
2	A	601	FAD	C4-C4X-N5	3.99	123.16	118.60
2	A	601	FAD	C2A-N1A-C6A	3.82	125.29	118.75
3	A	602	NAP	C6N-N1N-C2N	-3.79	118.52	121.97
2	C	601	FAD	C10-C4X-N5	3.72	123.83	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C4A-C5A-N7A	-3.71	105.53	109.40
2	B	601	FAD	C5'-C4'-C3'	3.71	119.36	112.20
2	A	601	FAD	O2'-C2'-C1'	-3.71	100.67	109.59
2	A	601	FAD	C4X-N5-C5X	3.67	120.44	116.77
3	E	602	NAP	C1B-N9A-C4A	-3.60	120.32	126.64
2	A	601	FAD	C1'-N10-C10	-3.59	115.19	118.41
2	F	601	FAD	C10-C4X-N5	3.51	123.69	121.26
2	A	601	FAD	C3B-C2B-C1B	-3.49	95.73	100.98
3	B	602	NAP	C3N-C7N-N7N	3.41	121.85	117.75
3	E	602	NAP	C2A-N1A-C6A	3.39	124.56	118.75
2	F	601	FAD	O2'-C2'-C1'	-3.35	101.54	109.59
3	A	602	NAP	C1B-N9A-C4A	-3.33	120.79	126.64
2	B	601	FAD	O4'-C4'-C5'	-3.31	102.47	109.92
2	B	601	FAD	C1'-N10-C10	-3.30	115.46	118.41
3	A	602	NAP	O7N-C7N-C3N	-3.26	115.73	119.63
2	C	601	FAD	C4X-C10-N10	-3.25	116.96	120.30
2	E	601	FAD	C4X-C4-N3	-3.24	119.00	123.43
2	C	601	FAD	C4X-C4-N3	-3.21	119.04	123.43
3	A	602	NAP	C4A-C5A-N7A	-3.19	106.08	109.40
3	E	602	NAP	PN-O3-PA	-3.14	122.05	132.83
2	E	601	FAD	C4-C4X-N5	3.12	122.16	118.60
3	C	602	NAP	O3X-P2B-O2X	3.09	119.45	107.64
2	A	601	FAD	O3'-C3'-C2'	3.08	116.24	108.81
2	D	601	FAD	O4'-C4'-C5'	-3.03	103.11	109.92
2	E	601	FAD	C3B-C2B-C1B	2.98	105.47	100.98
3	B	602	NAP	C1B-N9A-C4A	-2.95	121.45	126.64
2	E	601	FAD	C4X-N5-C5X	2.95	119.72	116.77
2	B	601	FAD	C1'-C2'-C3'	2.95	118.03	109.79
2	D	601	FAD	C5'-C4'-C3'	2.94	117.89	112.20
2	B	601	FAD	N3A-C2A-N1A	-2.93	124.11	128.68
3	A	602	NAP	O3X-P2B-O2X	2.92	118.81	107.64
2	A	601	FAD	O2A-PA-O5B	-2.91	94.24	107.75
3	C	602	NAP	O7N-C7N-N7N	2.89	126.68	122.58
3	E	602	NAP	N6A-C6A-N1A	2.89	124.56	118.57
2	F	601	FAD	C5X-C9A-N10	2.83	119.77	117.72
2	E	601	FAD	C4A-C5A-N7A	-2.83	106.45	109.40
2	C	601	FAD	C5'-C4'-C3'	2.79	117.59	112.20
2	C	601	FAD	C2A-N1A-C6A	2.78	123.52	118.75
3	E	602	NAP	O4B-C4B-C3B	2.77	110.60	105.11
3	F	602	NAP	O7N-C7N-C3N	-2.75	116.34	119.63
3	F	602	NAP	O3X-P2B-O1X	2.75	121.44	110.68
2	C	601	FAD	P-O3P-PA	-2.73	123.46	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	FAD	C10-C4X-N5	2.70	123.12	121.26
3	C	602	NAP	C2N-C3N-C4N	2.70	121.31	118.26
3	A	602	NAP	C3B-C2B-C1B	2.68	107.92	102.89
3	D	602	NAP	O3X-P2B-O2X	2.66	117.81	107.64
3	D	602	NAP	C3D-C2D-C1D	2.66	104.98	100.98
3	A	602	NAP	O5D-C5D-C4D	2.65	118.10	108.99
2	E	601	FAD	O2'-C2'-C3'	2.64	115.52	109.10
3	D	602	NAP	C5N-C4N-C3N	-2.63	117.23	120.34
2	E	601	FAD	O4B-C4B-C3B	2.59	110.25	105.11
2	B	601	FAD	C1B-N9A-C4A	-2.59	122.10	126.64
3	C	602	NAP	C3D-C2D-C1D	2.58	104.86	100.98
2	F	601	FAD	C3B-C2B-C1B	2.53	104.79	100.98
3	F	602	NAP	O4D-C4D-C3D	2.52	110.11	105.11
2	C	601	FAD	C4-C4X-N5	2.52	121.48	118.60
3	E	602	NAP	O2A-PA-O1A	2.52	124.70	112.24
2	F	601	FAD	C9A-N10-C10	-2.50	118.64	121.91
3	B	602	NAP	O3X-P2B-O1X	2.49	120.44	110.68
3	F	602	NAP	O2A-PA-O1A	2.47	124.44	112.24
3	F	602	NAP	O3X-P2B-O2B	-2.46	94.95	105.99
3	C	602	NAP	O3X-P2B-O2B	-2.46	94.97	105.99
2	B	601	FAD	C9A-N10-C10	-2.46	118.69	121.91
2	D	601	FAD	N3A-C2A-N1A	-2.45	124.86	128.68
2	F	601	FAD	C2A-N1A-C6A	2.43	122.91	118.75
2	A	601	FAD	C4X-C4-N3	-2.42	120.11	123.43
3	E	602	NAP	O3B-C3B-C2B	2.41	118.00	111.17
2	A	601	FAD	C5X-C9A-N10	2.40	119.46	117.72
3	C	602	NAP	O5D-PN-O1N	2.40	118.43	109.07
3	D	602	NAP	C6N-N1N-C2N	-2.38	119.81	121.97
2	C	601	FAD	C4X-N5-C5X	2.36	119.13	116.77
3	E	602	NAP	O7N-C7N-N7N	2.35	125.91	122.58
2	C	601	FAD	C4'-C3'-C2'	-2.34	108.50	113.36
2	C	601	FAD	O4'-C4'-C5'	-2.31	104.73	109.92
3	A	602	NAP	O4D-C1D-C2D	-2.31	103.55	106.93
3	C	602	NAP	O2A-PA-O1A	2.31	123.64	112.24
3	F	602	NAP	O2B-P2B-O1X	-2.29	100.54	109.39
2	D	601	FAD	O2'-C2'-C1'	-2.27	104.12	109.59
2	F	601	FAD	O2A-PA-O1A	2.27	123.45	112.24
3	F	602	NAP	N6A-C6A-N1A	2.27	123.28	118.57
2	B	601	FAD	C4X-C10-N10	-2.27	117.97	120.30
3	D	602	NAP	C1B-N9A-C4A	-2.25	122.68	126.64
3	A	602	NAP	O2N-PN-O5D	2.25	118.19	107.75
2	D	601	FAD	C8M-C8-C7	-2.25	116.13	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	FAD	C1B-N9A-C4A	-2.24	122.71	126.64
3	F	602	NAP	O2B-C2B-C1B	-2.22	102.10	110.10
2	D	601	FAD	C4A-C5A-N7A	-2.21	107.09	109.40
2	B	601	FAD	C10-C4X-N5	2.20	122.78	121.26
2	F	601	FAD	C5'-C4'-C3'	2.20	116.45	112.20
2	C	601	FAD	N6A-C6A-N1A	2.20	123.13	118.57
3	F	602	NAP	O3X-P2B-O2X	2.19	116.00	107.64
2	F	601	FAD	O5'-C5'-C4'	-2.19	103.52	109.36
2	C	601	FAD	O2A-PA-O1A	2.18	123.04	112.24
2	C	601	FAD	O2P-P-O1P	2.17	122.98	112.24
3	E	602	NAP	O4B-C4B-C5B	-2.17	102.23	109.37
2	A	601	FAD	O5B-C5B-C4B	2.16	116.42	108.99
2	A	601	FAD	C9A-N10-C10	-2.15	119.09	121.91
3	A	602	NAP	O4B-C1B-C2B	-2.15	102.85	106.59
3	F	602	NAP	O7N-C7N-N7N	2.14	125.62	122.58
2	A	601	FAD	C7M-C7-C8	-2.14	116.34	120.74
3	A	602	NAP	O2D-C2D-C3D	2.13	118.70	111.82
3	D	602	NAP	C2A-N1A-C6A	2.12	122.38	118.75
2	E	601	FAD	N3A-C2A-N1A	-2.11	125.38	128.68
3	F	602	NAP	C2A-N1A-C6A	2.10	122.34	118.75
2	A	601	FAD	O2A-PA-O1A	2.08	122.50	112.24
2	D	601	FAD	C5X-C9A-N10	-2.07	116.21	117.72
3	C	602	NAP	C3N-C7N-N7N	2.06	120.23	117.75
3	A	602	NAP	O2X-P2B-O2B	-2.06	96.76	105.99
2	A	601	FAD	C10-C4X-N5	2.06	122.68	121.26
2	A	601	FAD	N6A-C6A-N1A	2.05	122.83	118.57
2	C	601	FAD	C1'-C2'-C3'	2.05	115.52	109.79
2	F	601	FAD	C4'-C3'-C2'	-2.04	109.12	113.36
3	E	602	NAP	C2D-C3D-C4D	2.03	106.60	102.64
2	F	601	FAD	P-O3P-PA	-2.03	125.85	132.83
3	D	602	NAP	C2N-C3N-C4N	2.03	120.56	118.26
3	A	602	NAP	C2A-N1A-C6A	2.01	122.19	118.75
3	F	602	NAP	C3D-C2D-C1D	2.00	104.00	100.98
2	B	601	FAD	C5X-C9A-N10	2.00	119.17	117.72

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	NAP	C5B-O5B-PA-O1A
3	A	602	NAP	O4D-C4D-C5D-O5D
2	B	601	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
2	C	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	N10-C1'-C2'-O2'
2	F	601	FAD	N10-C1'-C2'-O2'
2	F	601	FAD	C5'-O5'-P-O2P
2	F	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	C5B-O5B-PA-O1A
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	C2'-C3'-C4'-C5'
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-C3'
2	E	601	FAD	C5B-O5B-PA-O1A
2	E	601	FAD	O4B-C4B-C5B-O5B
2	E	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	O3'-C3'-C4'-O4'
3	A	602	NAP	C3D-C4D-C5D-O5D
2	C	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
2	E	601	FAD	C3B-C4B-C5B-O5B
3	B	602	NAP	C3B-C2B-O2B-P2B
3	A	602	NAP	C3B-C2B-O2B-P2B
2	A	601	FAD	O3'-C3'-C4'-C5'
2	C	601	FAD	C3B-C4B-C5B-O5B
3	B	602	NAP	C1B-C2B-O2B-P2B
2	D	601	FAD	C3B-C4B-C5B-O5B
3	C	602	NAP	PN-O3-PA-O1A
2	F	601	FAD	P-O3P-PA-O1A
2	A	601	FAD	C4'-C5'-O5'-P
3	C	602	NAP	C2N-C3N-C7N-O7N
3	C	602	NAP	PA-O3-PN-O5D
3	B	602	NAP	PA-O3-PN-O5D
3	A	602	NAP	PA-O3-PN-O5D
2	B	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	P-O3P-PA-O5B
3	E	602	NAP	C4N-C3N-C7N-N7N
2	A	601	FAD	O4B-C4B-C5B-O5B
3	F	602	NAP	C2B-O2B-P2B-O1X
3	F	602	NAP	C5B-O5B-PA-O3
2	D	601	FAD	C5B-O5B-PA-O3P
2	E	601	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	A	601	FAD	PA-O3P-P-O1P
3	F	602	NAP	C5B-O5B-PA-O2A
2	A	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O2A
3	F	602	NAP	O4B-C4B-C5B-O5B
2	B	601	FAD	N10-C1'-C2'-C3'
2	C	601	FAD	N10-C1'-C2'-C3'
2	F	601	FAD	N10-C1'-C2'-C3'
2	E	601	FAD	N10-C1'-C2'-C3'
3	E	602	NAP	C2N-C3N-C7N-N7N
3	E	602	NAP	C4N-C3N-C7N-O7N
2	F	601	FAD	P-O3P-PA-O2A
3	E	602	NAP	O4B-C4B-C5B-O5B
3	D	602	NAP	O4B-C4B-C5B-O5B
3	B	602	NAP	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
3	A	602	NAP	C1B-C2B-O2B-P2B
3	C	602	NAP	C4N-C3N-C7N-O7N
3	A	602	NAP	C2B-O2B-P2B-O1X
2	C	601	FAD	O4'-C4'-C5'-O5'
3	E	602	NAP	C2N-C3N-C7N-O7N
2	F	601	FAD	O4B-C4B-C5B-O5B
3	D	602	NAP	C2B-O2B-P2B-O2X
3	C	602	NAP	C2B-O2B-P2B-O2X
3	A	602	NAP	C5B-O5B-PA-O3
2	F	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	C5B-O5B-PA-O3P
3	C	602	NAP	O4B-C4B-C5B-O5B
3	A	602	NAP	O4B-C4B-C5B-O5B
3	C	602	NAP	PN-O3-PA-O2A
2	A	601	FAD	PA-O3P-P-O2P
3	A	602	NAP	C5B-O5B-PA-O1A
3	F	602	NAP	C3B-C4B-C5B-O5B

There are no ring outliers.

12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	18	0
3	D	602	NAP	5	0
3	F	602	NAP	4	0

Continued on next page...

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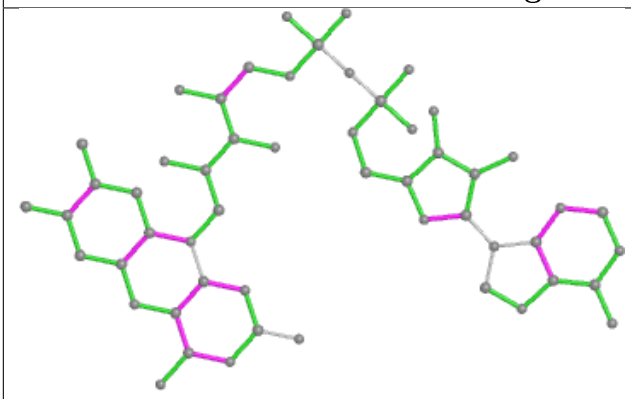
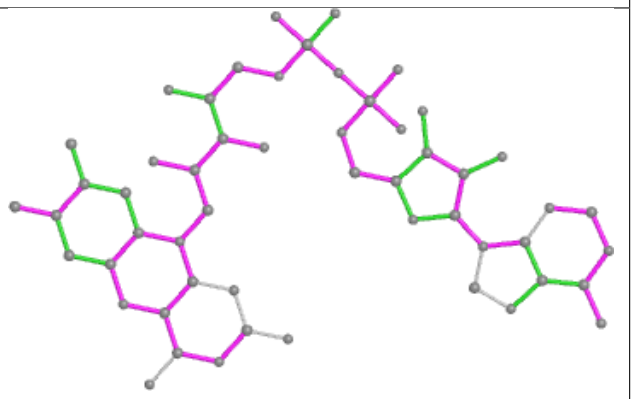
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	NAP	3	0
3	E	602	NAP	2	0
3	B	602	NAP	3	0
3	A	602	NAP	4	0
2	B	601	FAD	2	0
2	F	601	FAD	4	0
2	C	601	FAD	4	0
2	D	601	FAD	2	0
2	E	601	FAD	3	0

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

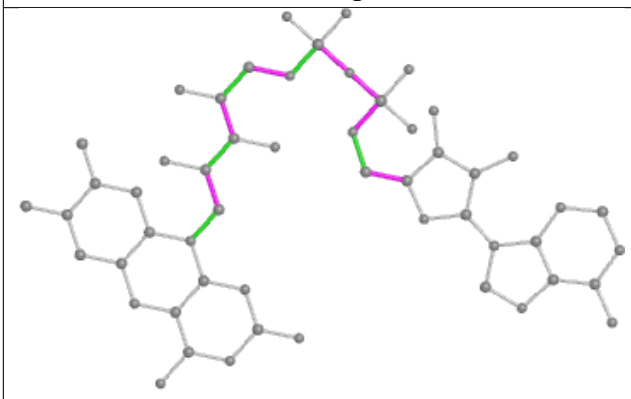
Ligand FAD A 601



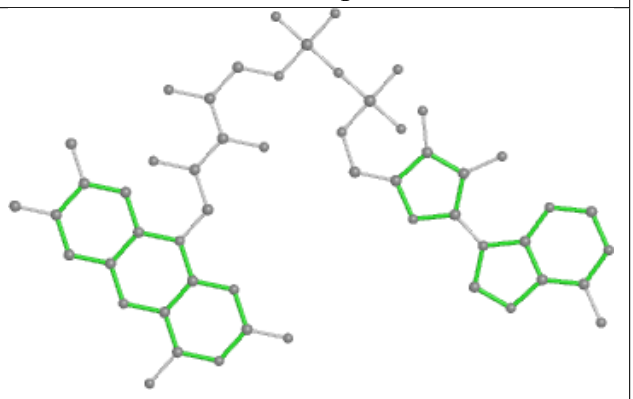
Bond lengths



Bond angles

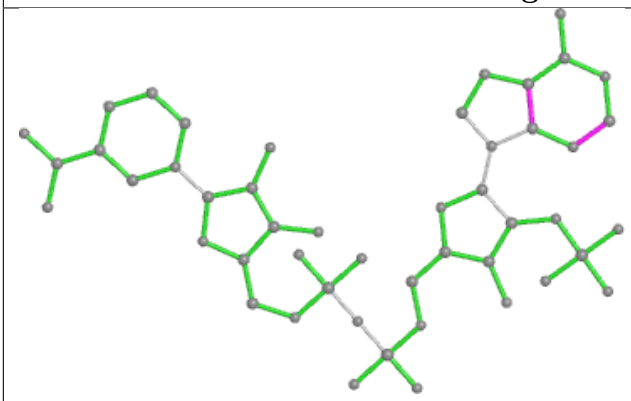


Torsions

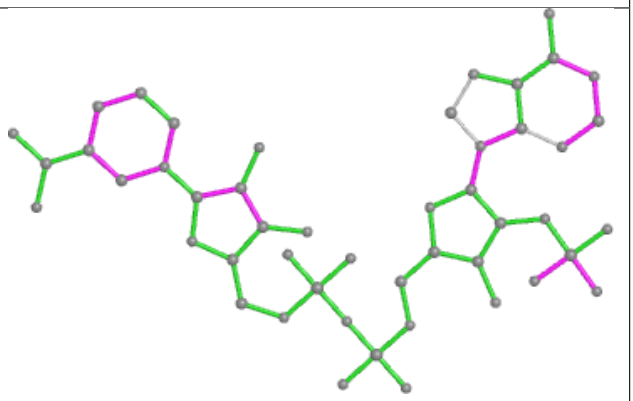


Rings

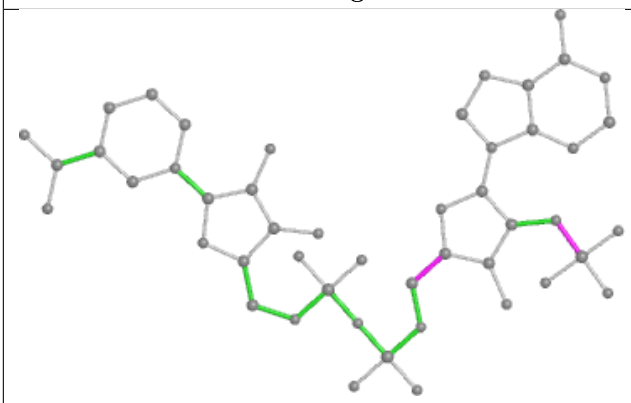
Ligand NAP D 602



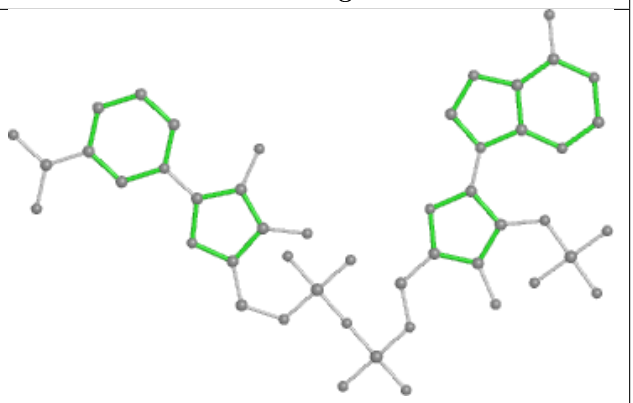
Bond lengths



Bond angles

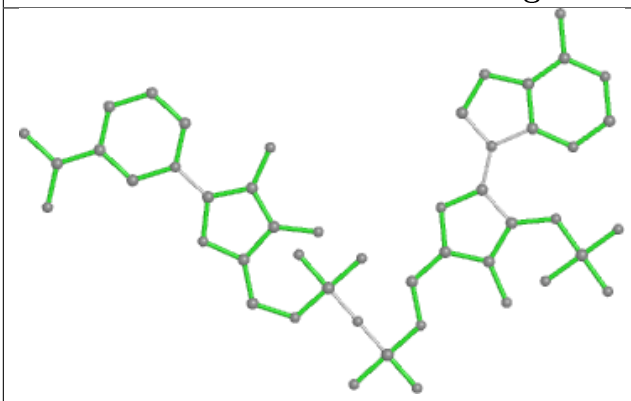


Torsions

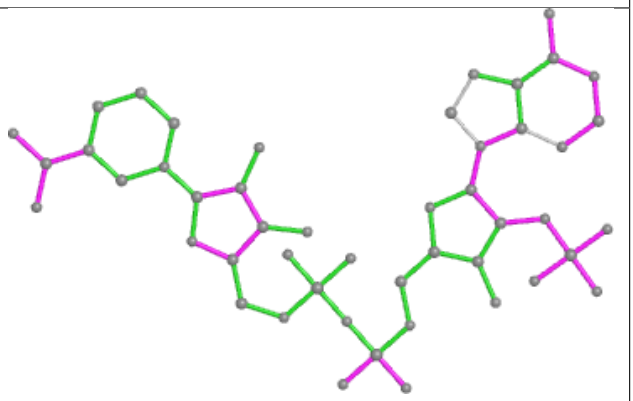


Rings

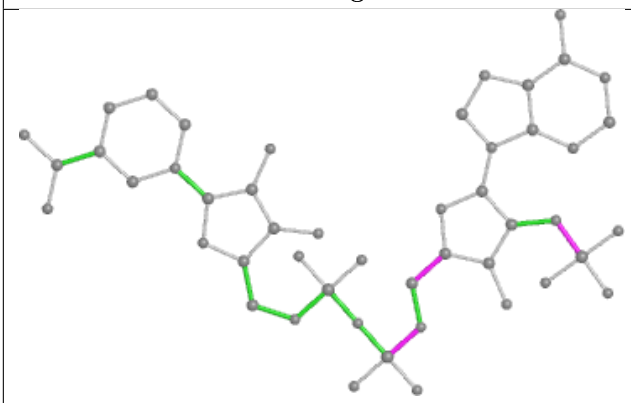
Ligand NAP F 602



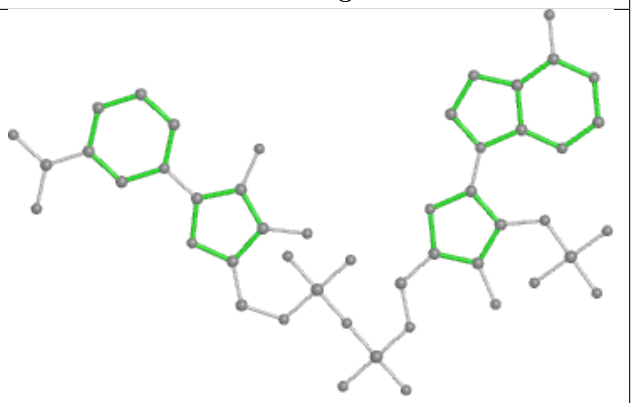
Bond lengths



Bond angles

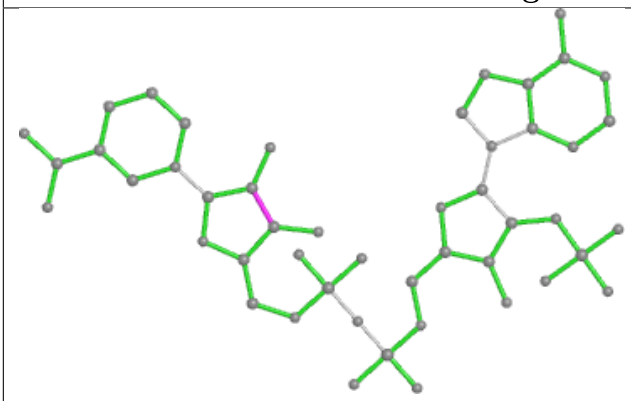


Torsions

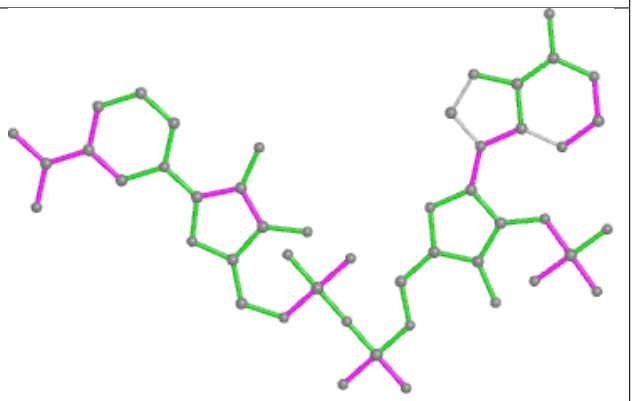


Rings

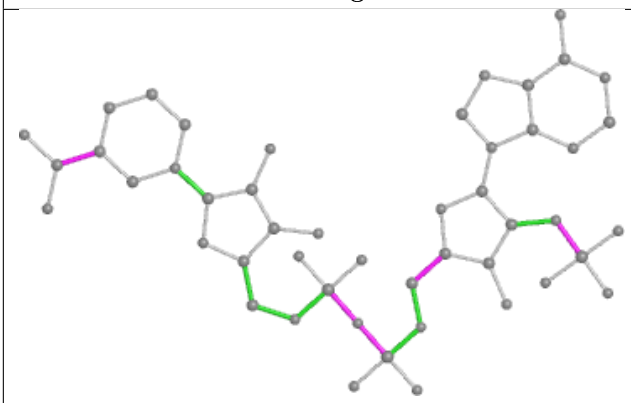
Ligand NAP C 602



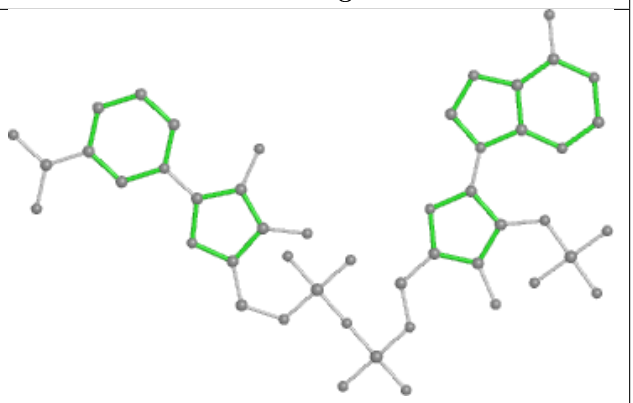
Bond lengths



Bond angles

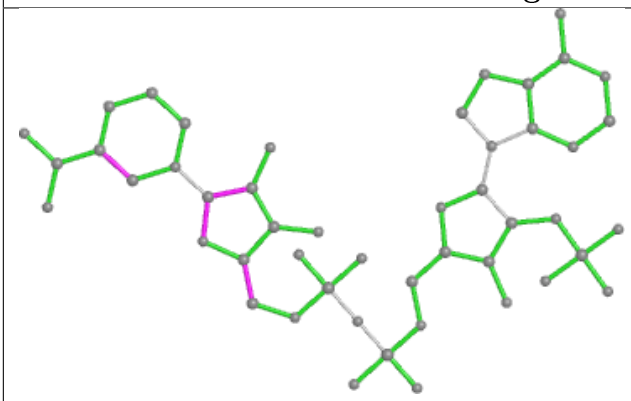


Torsions

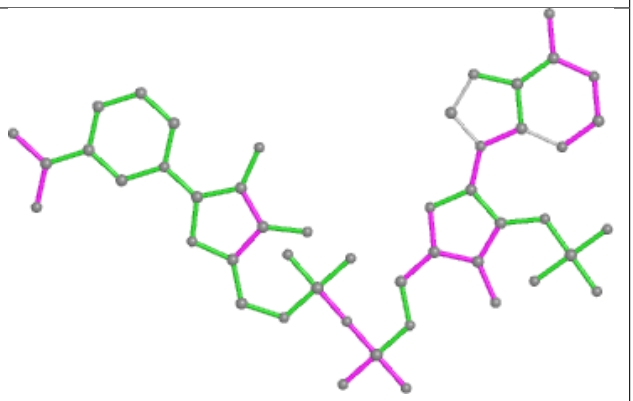


Rings

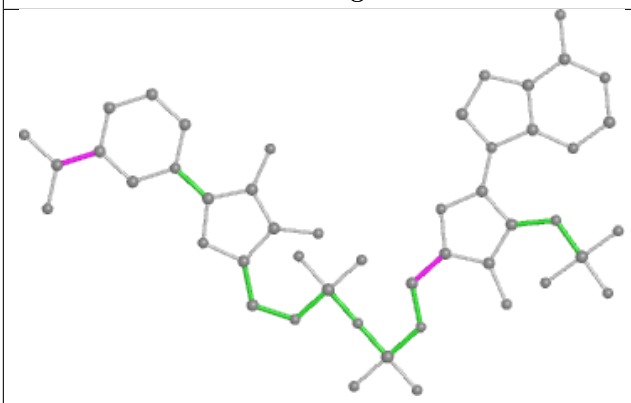
Ligand NAP E 602



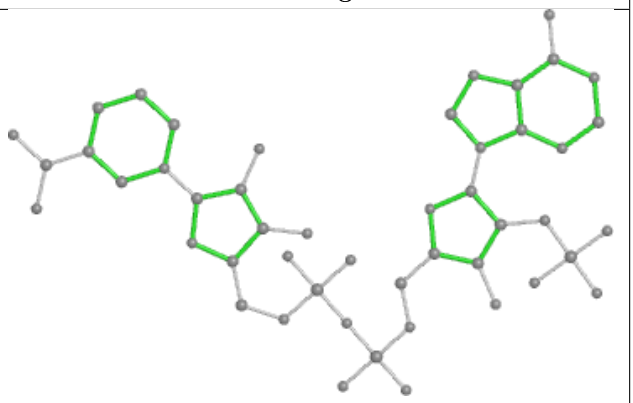
Bond lengths



Bond angles

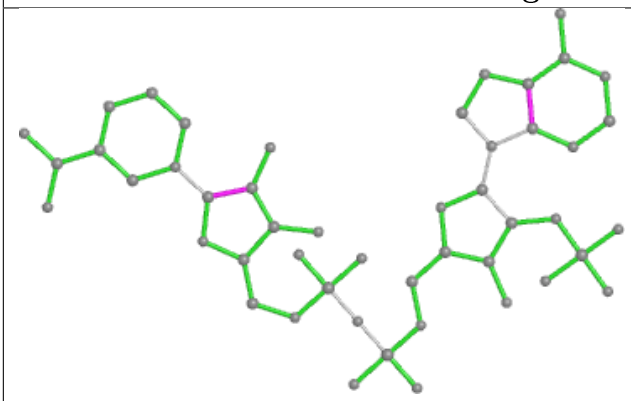


Torsions

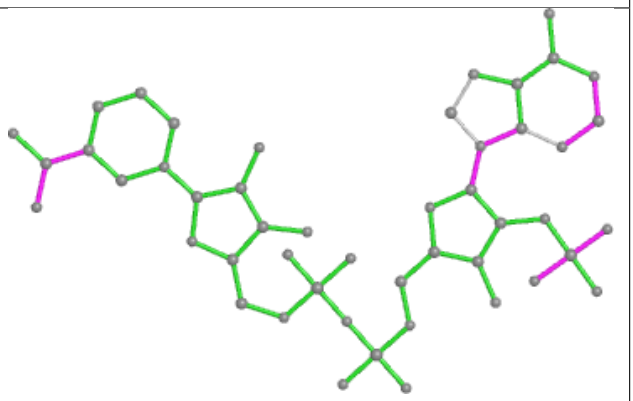


Rings

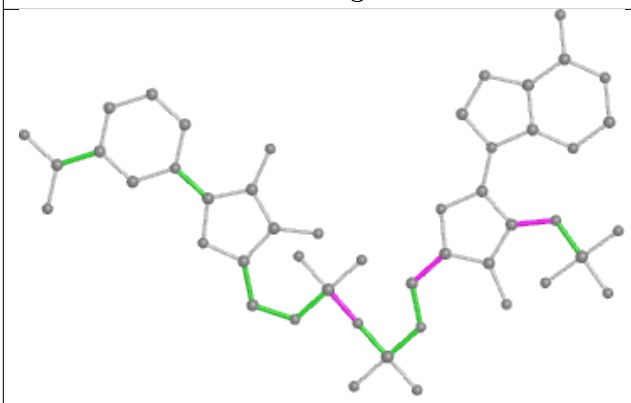
Ligand NAP B 602



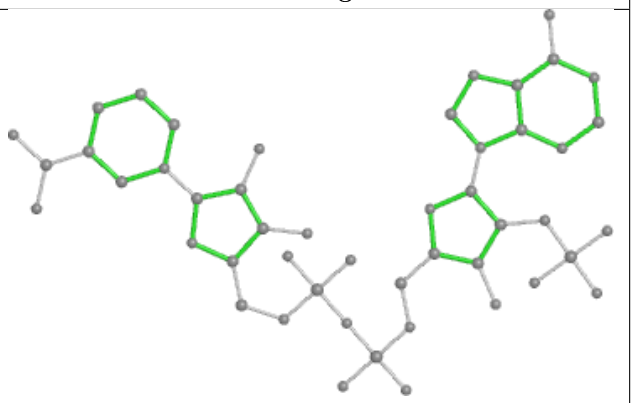
Bond lengths



Bond angles

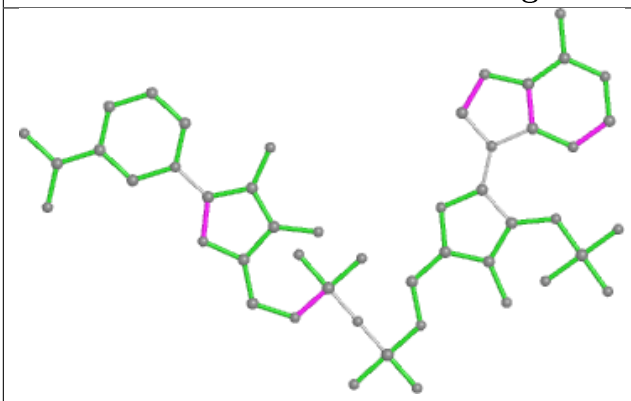


Torsions

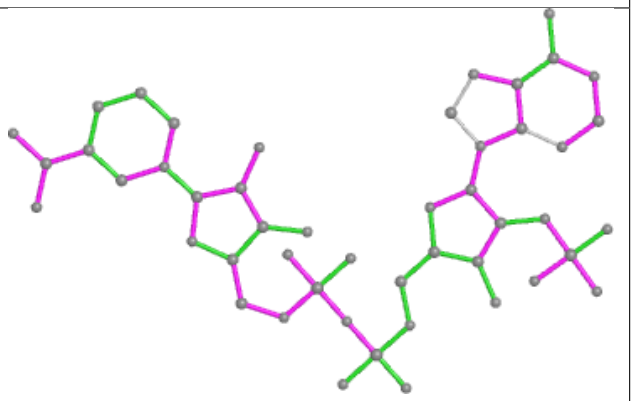


Rings

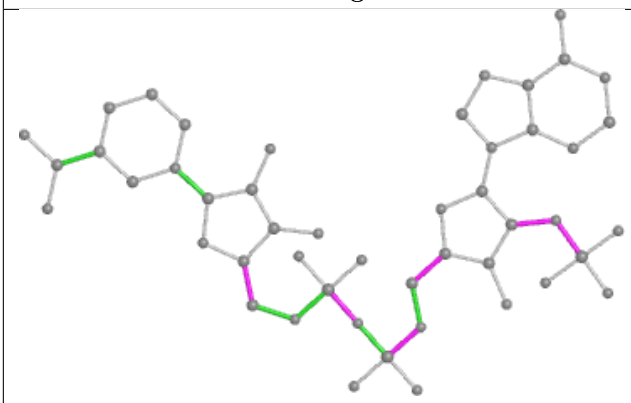
Ligand NAP A 602



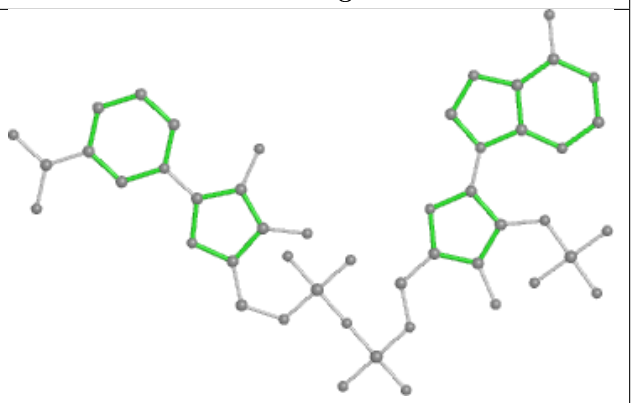
Bond lengths



Bond angles

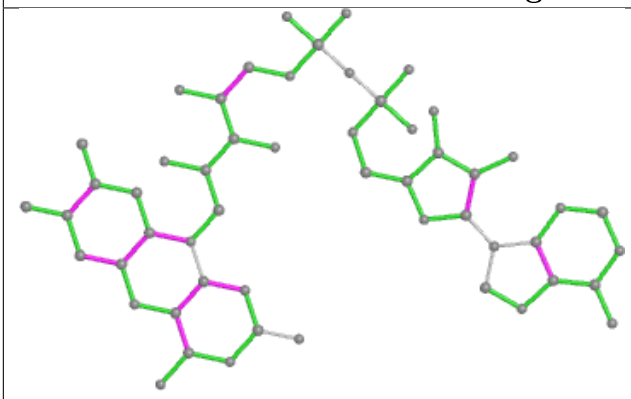


Torsions

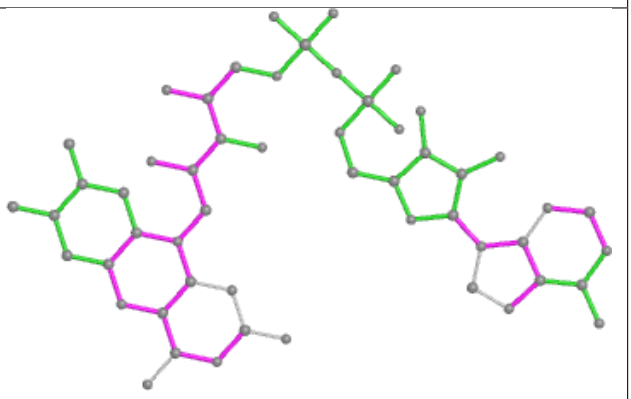


Rings

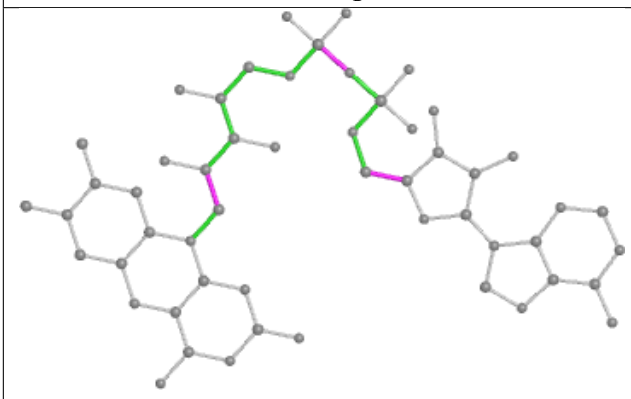
Ligand FAD B 601



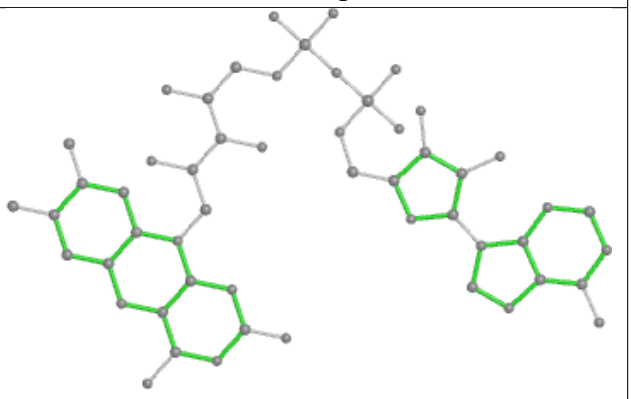
Bond lengths



Bond angles

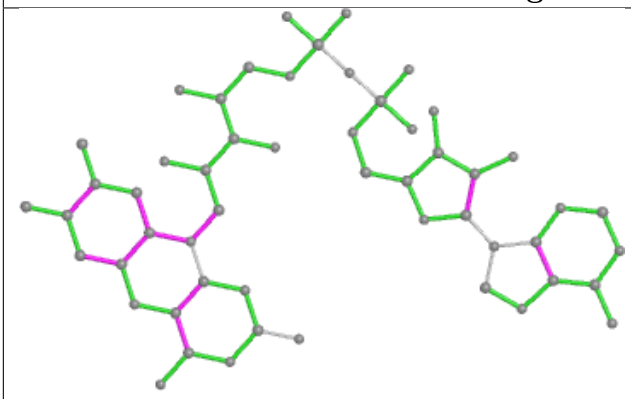


Torsions

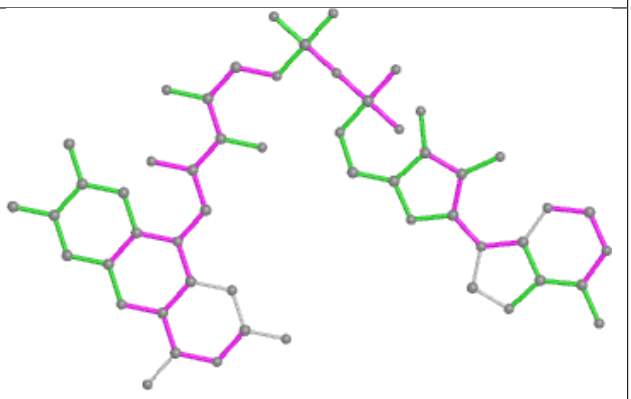


Rings

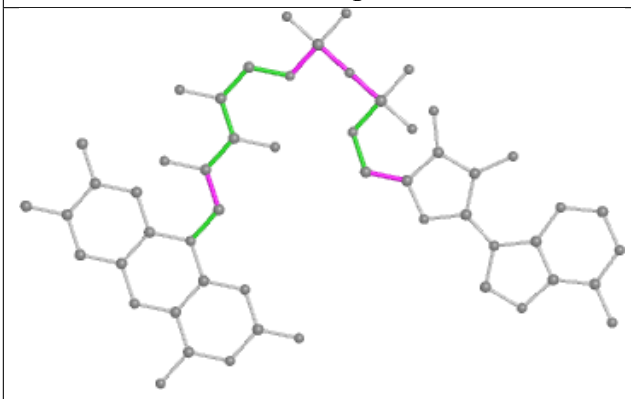
Ligand FAD F 601



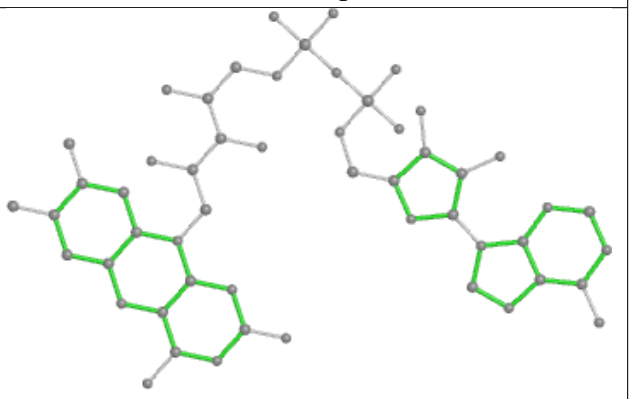
Bond lengths



Bond angles

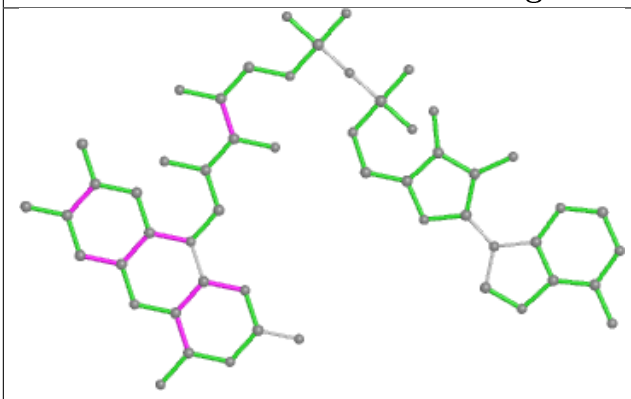


Torsions

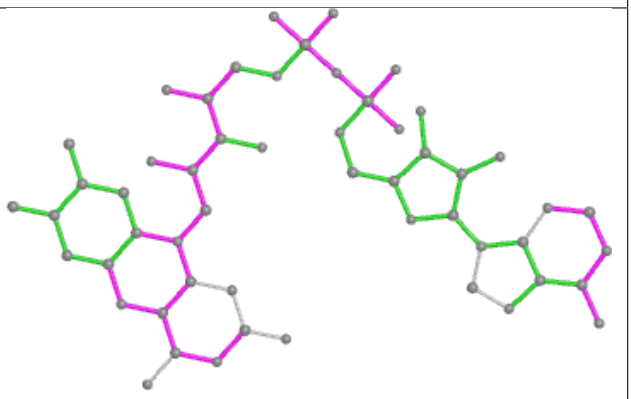


Rings

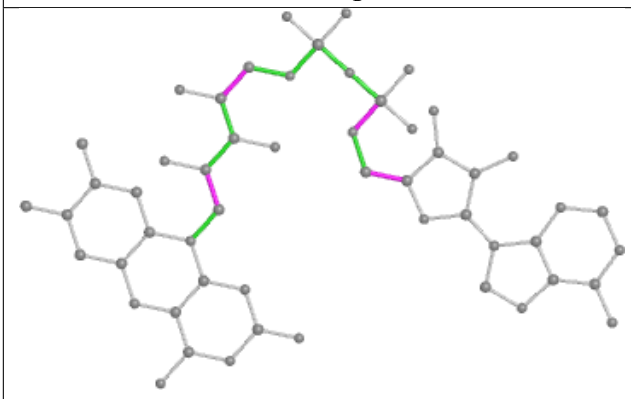
Ligand FAD C 601



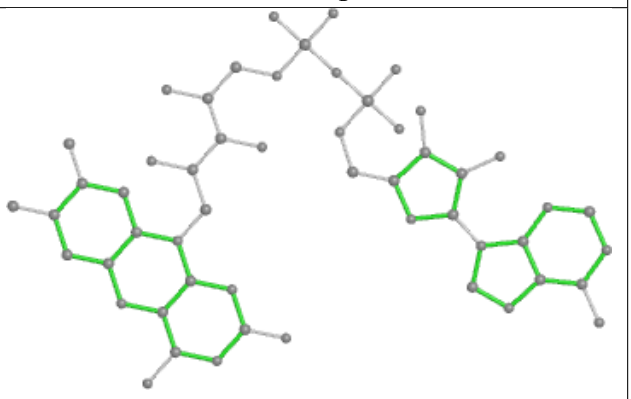
Bond lengths



Bond angles

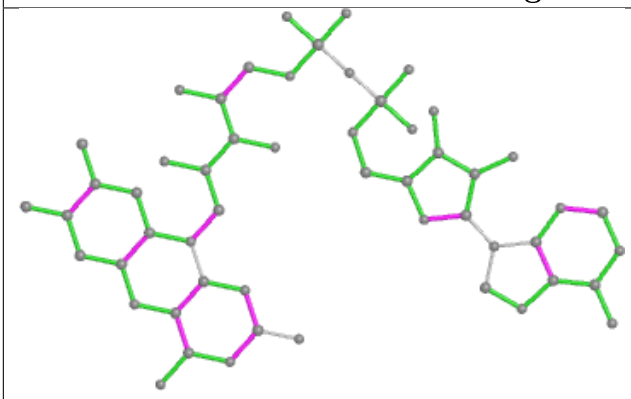


Torsions

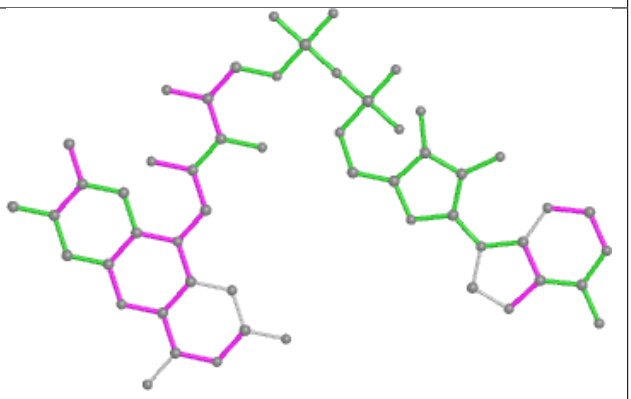


Rings

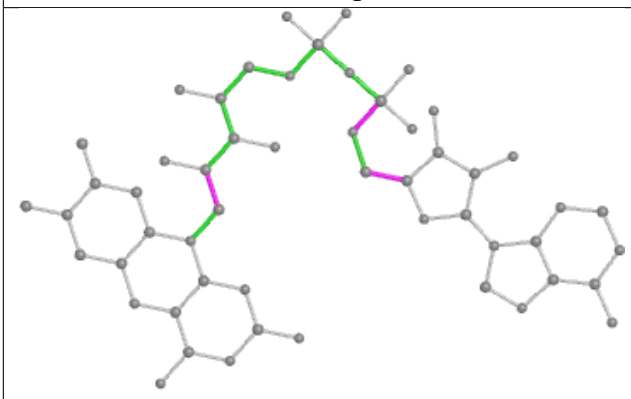
Ligand FAD D 601



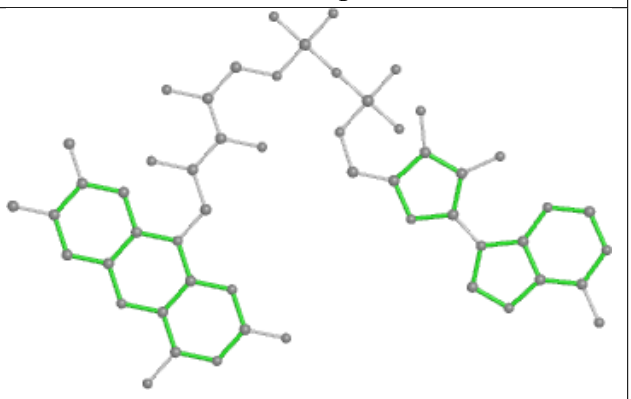
Bond lengths



Bond angles

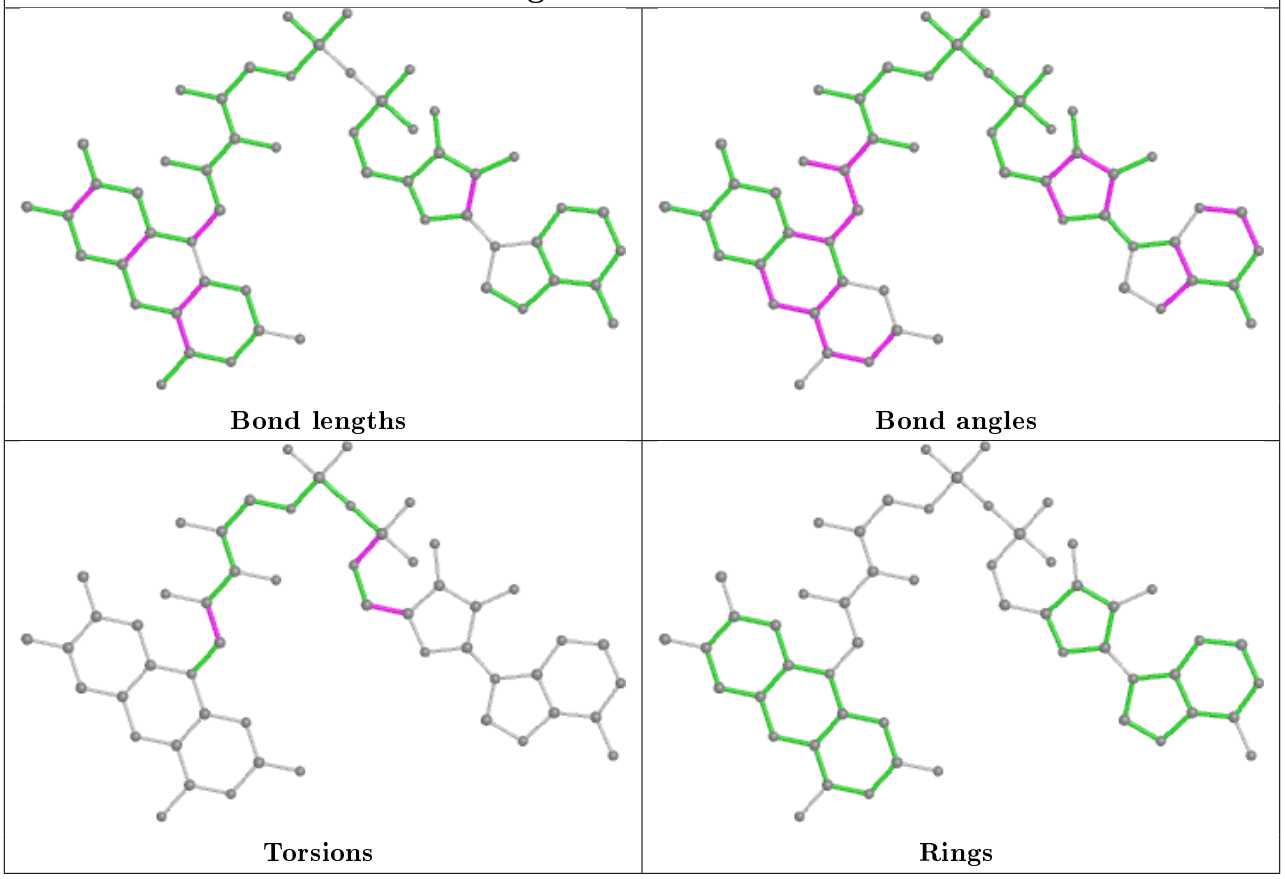


Torsions



Rings

Ligand FAD E 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	528/532 (99%)	1.25	112 (21%) 0 0	44, 110, 162, 232	0
1	B	528/532 (99%)	0.16	29 (5%) 25 16	41, 65, 112, 180	0
1	C	528/532 (99%)	-0.02	9 (1%) 70 63	35, 59, 100, 163	0
1	D	528/532 (99%)	0.10	18 (3%) 45 35	39, 62, 115, 155	0
1	E	528/532 (99%)	0.04	25 (4%) 31 22	37, 62, 111, 184	0
1	F	528/532 (99%)	-0.01	17 (3%) 47 37	36, 59, 100, 169	0
All	All	3168/3192 (99%)	0.25	210 (6%) 18 11	35, 65, 139, 232	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ALA	11.6
1	A	367	ALA	10.2
1	A	405	MET	9.8
1	A	365	THR	8.8
1	A	25	GLY	8.3
1	C	527	VAL	8.3
1	A	359	PRO	8.2
1	A	113	VAL	7.6
1	A	474	MET	7.4
1	F	530	ALA	6.4
1	E	514	LEU	6.3
1	A	143	VAL	6.2
1	A	343	ILE	6.0
1	A	390	ALA	5.9
1	A	351	THR	5.7
1	A	5	VAL	5.3
1	A	530	ALA	5.3
1	A	251	ILE	5.1
1	A	342	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	VAL	5.1
1	D	527	VAL	5.0
1	B	527	VAL	4.9
1	A	22	LEU	4.9
1	A	451	PHE	4.9
1	A	24	GLU	4.9
1	A	27	GLU	4.9
1	A	10	ALA	4.9
1	A	353	PHE	4.7
1	A	140	PHE	4.7
1	A	388	TRP	4.7
1	A	123	GLY	4.6
1	A	452	LEU	4.6
1	A	366	LEU	4.6
1	F	449	TRP	4.5
1	A	345	SER	4.4
1	B	523	LEU	4.4
1	E	530	ALA	4.4
1	A	338	LEU	4.3
1	A	141	ASP	4.3
1	B	530	ALA	4.3
1	A	364	PRO	4.3
1	A	3	LYS	4.3
1	B	457	LEU	4.3
1	A	306	PHE	4.3
1	A	360	LEU	4.3
1	A	341	SER	4.3
1	A	158	GLU	4.2
1	B	158	GLU	4.2
1	A	449	TRP	4.2
1	A	445	PRO	4.2
1	F	527	VAL	4.2
1	A	339	ASP	4.2
1	A	26	LEU	4.1
1	A	134	LYS	4.1
1	F	528	LEU	4.0
1	A	121	VAL	4.0
1	B	452	LEU	4.0
1	A	6	ALA	4.0
1	A	7	ILE	3.9
1	A	139	VAL	3.9
1	A	357	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLU	3.9
1	F	347	ASN	3.8
1	E	527	VAL	3.8
1	A	94	PHE	3.7
1	A	363	LYS	3.7
1	B	157	LYS	3.7
1	A	31	PHE	3.7
1	E	306	PHE	3.6
1	A	28	PRO	3.6
1	A	250	ALA	3.6
1	D	160	PHE	3.6
1	A	41	TRP	3.6
1	A	164	LYS	3.6
1	A	4	LYS	3.5
1	A	453	THR	3.5
1	B	164	LYS	3.5
1	E	511	PHE	3.5
1	D	169	LYS	3.5
1	B	456	GLN	3.5
1	A	368	VAL	3.4
1	B	453	THR	3.4
1	C	165	HIS	3.4
1	A	347	ASN	3.4
1	A	124	GLN	3.3
1	A	335	TYR	3.3
1	D	324	CYS	3.3
1	B	160	PHE	3.3
1	A	470	GLN	3.3
1	F	447	ILE	3.3
1	A	23	GLU	3.3
1	A	29	THR	3.3
1	F	445	PRO	3.2
1	C	519	LEU	3.2
1	E	310	SER	3.2
1	A	476	PRO	3.2
1	E	452	LEU	3.2
1	F	446	ASN	3.2
1	B	449	TRP	3.2
1	A	395	ASN	3.1
1	F	519	LEU	3.1
1	A	475	GLY	3.1
1	E	187	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	473	LEU	3.1
1	A	446	ASN	3.1
1	F	452	LEU	3.1
1	D	326	ILE	3.0
1	A	515	LEU	3.0
1	E	171	PHE	3.0
1	A	333	TYR	3.0
1	A	159	SER	3.0
1	B	526	ALA	2.9
1	A	166	PHE	2.9
1	F	158	GLU	2.9
1	A	122	THR	2.9
1	E	165	HIS	2.9
1	B	182	PHE	2.9
1	A	349	GLU	2.9
1	A	514	LEU	2.9
1	C	167	LYS	2.8
1	B	249	THR	2.8
1	A	331	TYR	2.8
1	A	125	TRP	2.8
1	A	358	PRO	2.8
1	A	118	ASP	2.8
1	A	399	LEU	2.8
1	E	168	GLY	2.8
1	A	348	ASN	2.7
1	E	453	THR	2.7
1	E	170	CYS	2.7
1	A	400	PRO	2.7
1	A	213	SER	2.7
1	A	424	GLN	2.7
1	B	510	LEU	2.7
1	F	511	PHE	2.7
1	A	249	THR	2.7
1	F	25	GLY	2.6
1	A	127	VAL	2.6
1	A	165	HIS	2.6
1	D	286	ASP	2.6
1	D	171	PHE	2.6
1	E	326	ILE	2.6
1	A	394	ALA	2.6
1	E	308	GLU	2.6
1	F	517	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	2.6
1	D	167	LYS	2.5
1	E	251	ILE	2.5
1	A	254	TRP	2.5
1	A	324	CYS	2.5
1	B	294	CYS	2.5
1	E	324	CYS	2.5
1	A	506	LYS	2.5
1	D	327	PHE	2.5
1	D	451	PHE	2.4
1	A	144	MET	2.4
1	B	250	ALA	2.4
1	C	518	LEU	2.4
1	F	350	VAL	2.4
1	B	286	ASP	2.4
1	A	393	PHE	2.4
1	A	337	PHE	2.4
1	A	9	GLY	2.4
1	A	328	ALA	2.4
1	A	247	LEU	2.4
1	A	391	LYS	2.4
1	D	511	PHE	2.4
1	A	356	ILE	2.4
1	A	15	LEU	2.3
1	D	157	LYS	2.3
1	E	248	PRO	2.3
1	A	190	ILE	2.3
1	B	159	SER	2.3
1	D	224	VAL	2.3
1	D	452	LEU	2.3
1	A	310	SER	2.3
1	C	520	PHE	2.2
1	F	349	GLU	2.2
1	C	523	LEU	2.2
1	B	474	MET	2.2
1	B	324	CYS	2.2
1	A	103	TYR	2.2
1	E	249	THR	2.1
1	A	163	LEU	2.1
1	E	515	LEU	2.1
1	D	181	ILE	2.1
1	E	312	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	446	ASN	2.1
1	E	169	LYS	2.1
1	B	49	GLU	2.1
1	B	166	PHE	2.1
1	F	451	PHE	2.1
1	B	522	VAL	2.1
1	C	452	LEU	2.1
1	A	454	ASP	2.1
1	B	248	PRO	2.1
1	E	502	VAL	2.1
1	B	306	PHE	2.1
1	A	513	ASN	2.1
1	D	140	PHE	2.1
1	A	148	GLY	2.0
1	D	158	GLU	2.0
1	A	157	LYS	2.0
1	A	46	HIS	2.0
1	A	325	VAL	2.0
1	B	507	ARG	2.0
1	E	189	VAL	2.0
1	D	528	LEU	2.0
1	B	513	ASN	2.0
1	E	523	LEU	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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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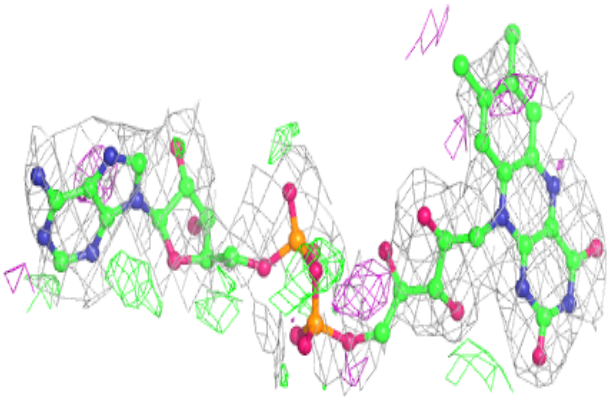
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

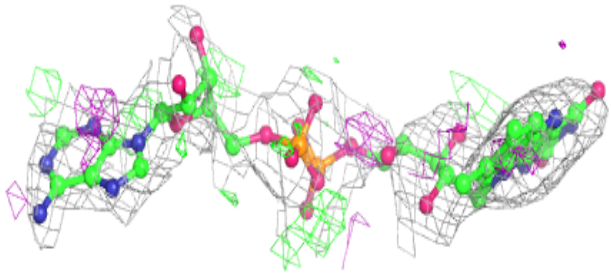
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OXY	A	603	2/2	0.71	0.37	72,72,72,74	0
2	FAD	A	601	53/53	0.83	0.24	55,88,147,158	0
4	OXY	B	603	2/2	0.86	0.52	58,58,58,59	0
3	NAP	A	602	48/48	0.88	0.19	65,94,126,138	0
4	OXY	C	603	2/2	0.91	0.50	52,52,52,56	0
3	NAP	B	602	48/48	0.93	0.18	45,57,75,77	0
2	FAD	B	601	53/53	0.94	0.19	44,54,62,69	0
3	NAP	E	602	48/48	0.95	0.17	45,67,99,105	0
2	FAD	C	601	53/53	0.95	0.17	32,50,63,69	0
3	NAP	D	602	48/48	0.95	0.15	45,64,86,94	0
2	FAD	D	601	53/53	0.95	0.17	37,48,62,67	0
4	OXY	F	603	2/2	0.95	0.41	47,47,47,51	0
4	OXY	D	603	2/2	0.95	0.50	54,54,54,60	0
3	NAP	F	602	48/48	0.96	0.15	35,55,74,79	0
2	FAD	E	601	53/53	0.96	0.19	33,42,50,52	0
2	FAD	F	601	53/53	0.97	0.14	39,47,56,61	0
4	OXY	E	603	2/2	0.97	0.42	52,52,52,56	0
3	NAP	C	602	48/48	0.97	0.14	47,57,72,79	0

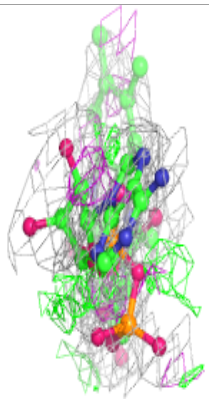
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

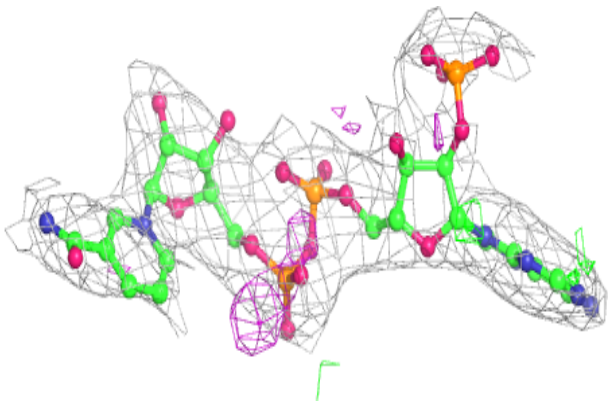


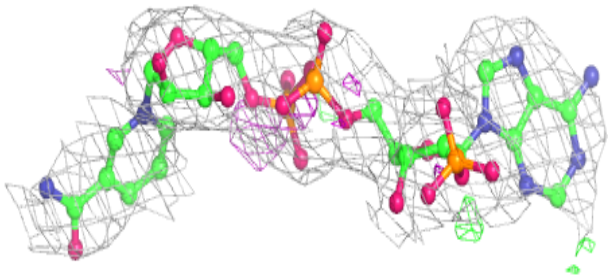


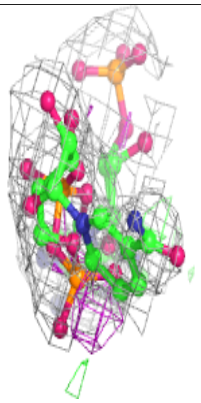


Electron density around NAP A 602:

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

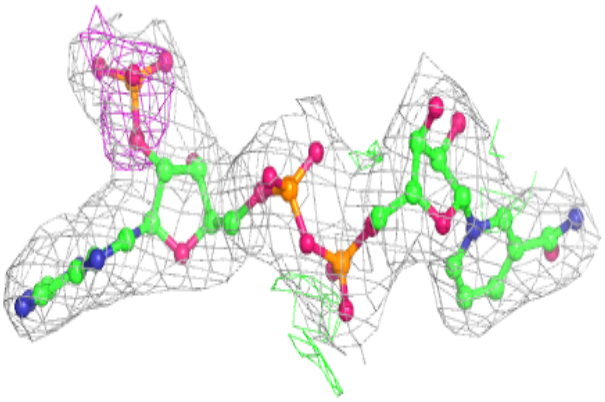


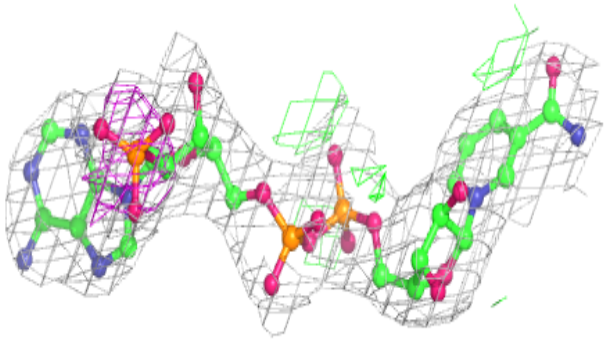


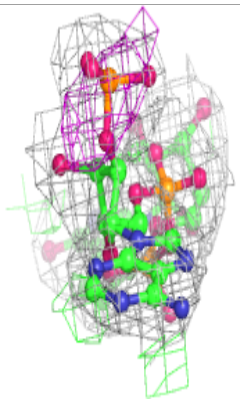


Electron density around NAP B 602:

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

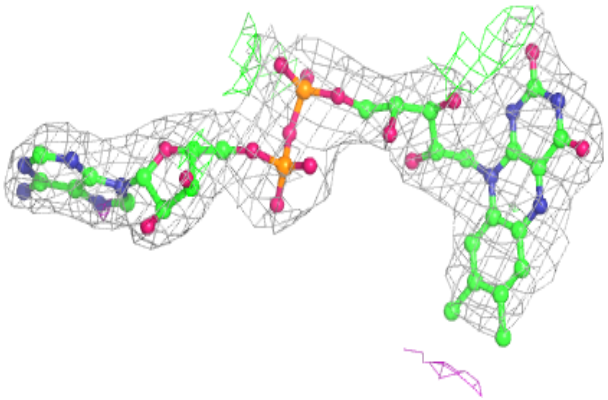


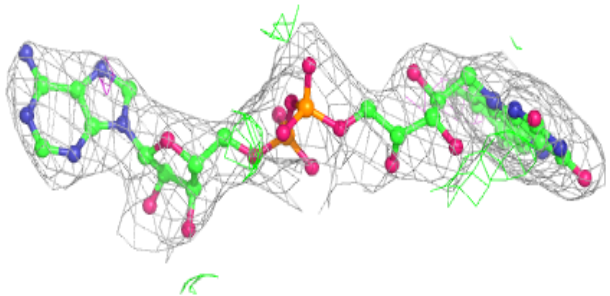




Electron density around FAD B 601:

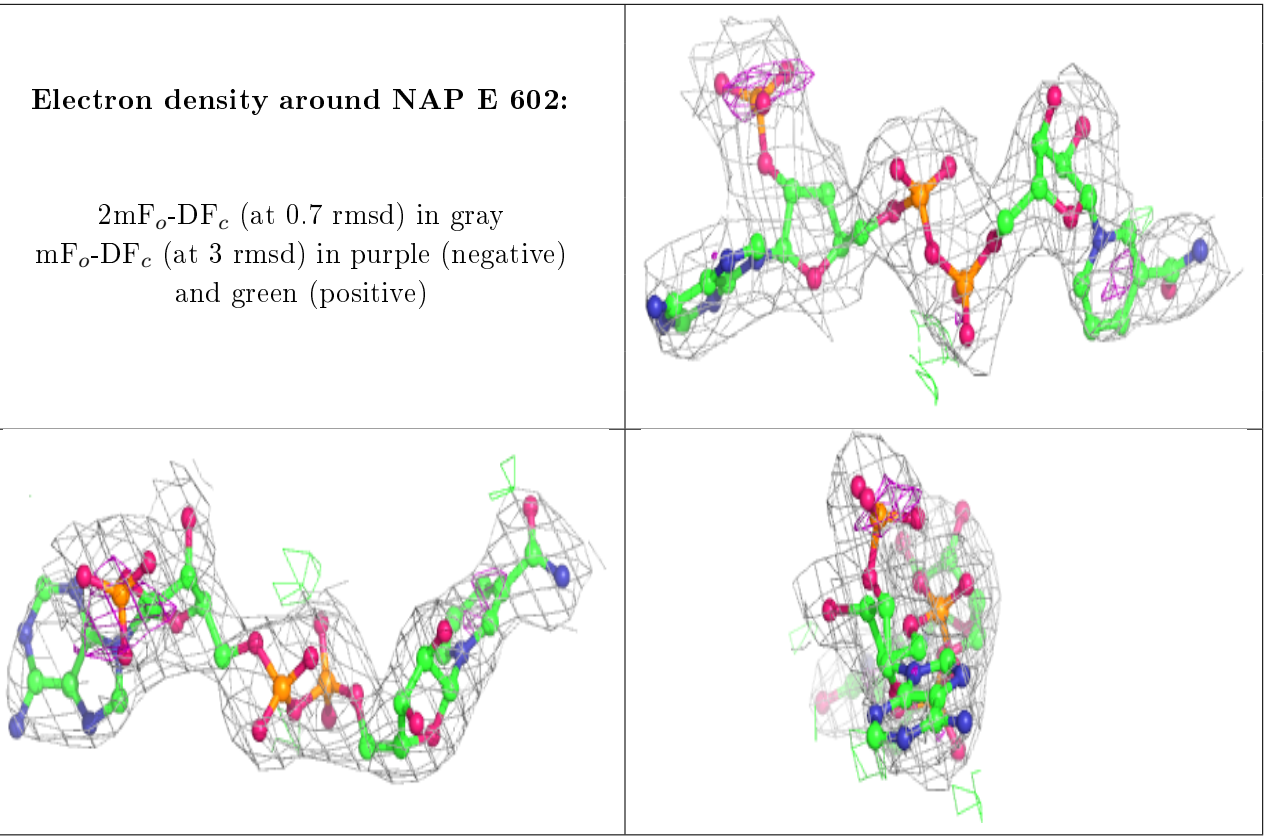
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





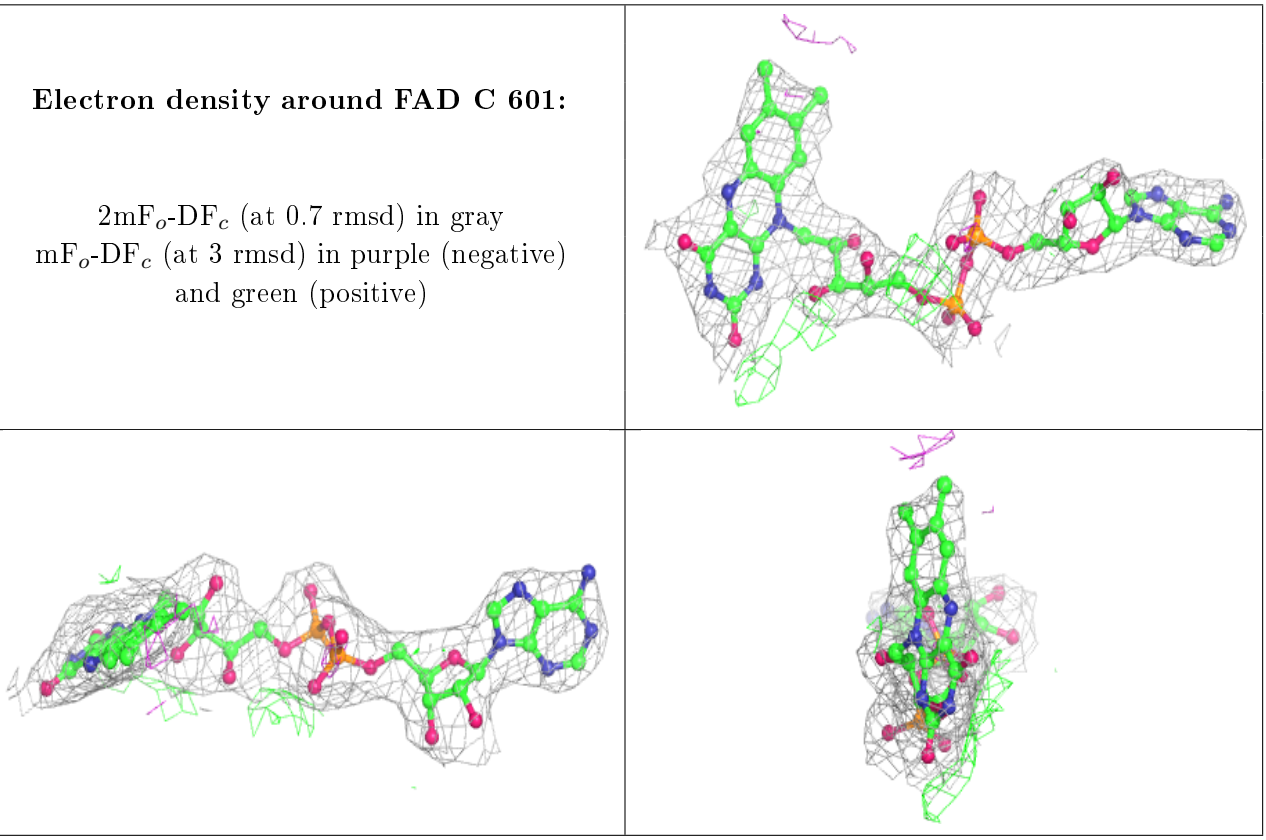
Electron density around NAP E 602:

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



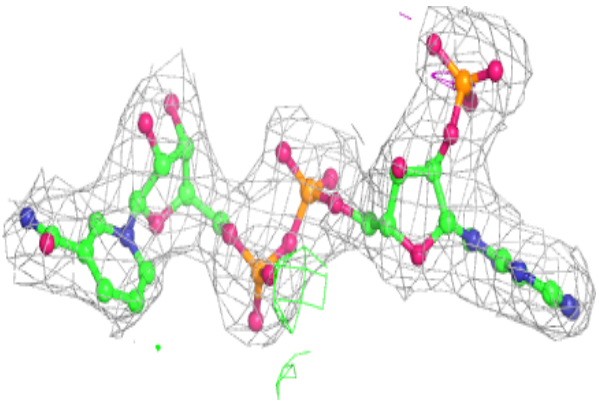
Electron density around FAD C 601:

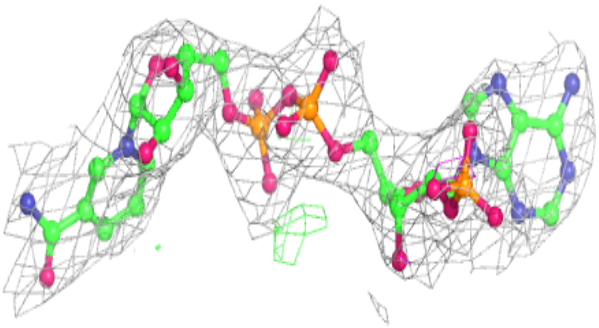
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

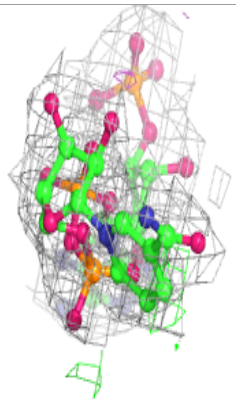


Electron density around NAP D 602:

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

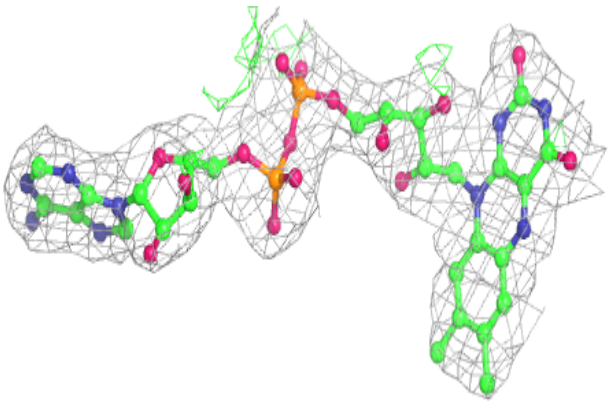


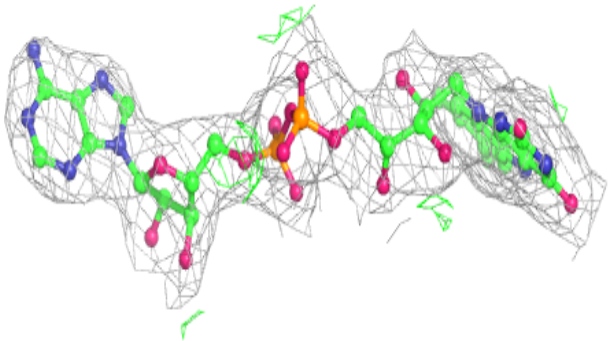


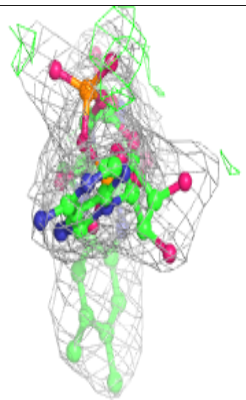


Electron density around FAD D 601:

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

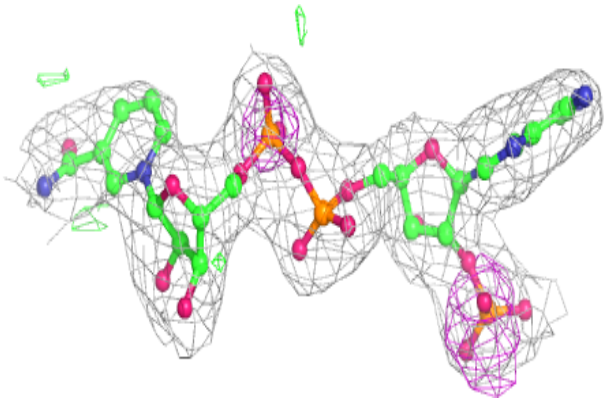


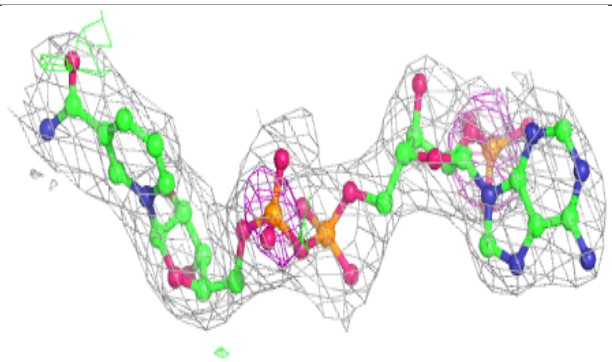


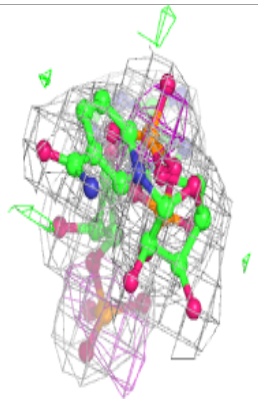


Electron density around NAP F 602:

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

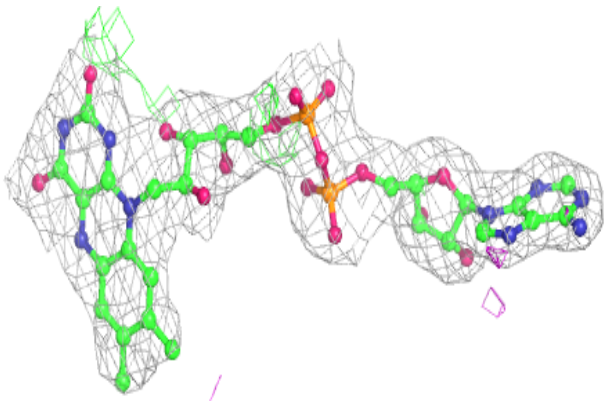


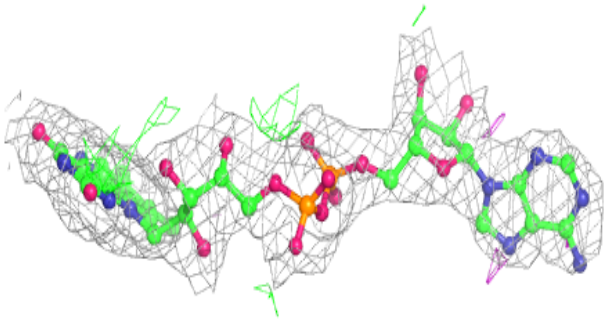


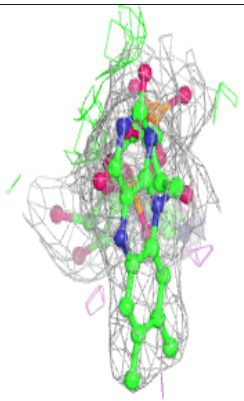


Electron density around FAD E 601:

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

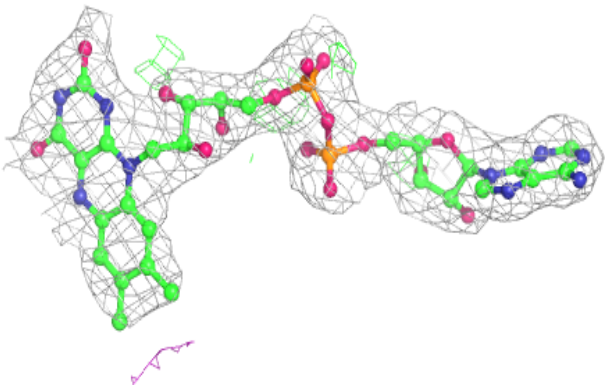


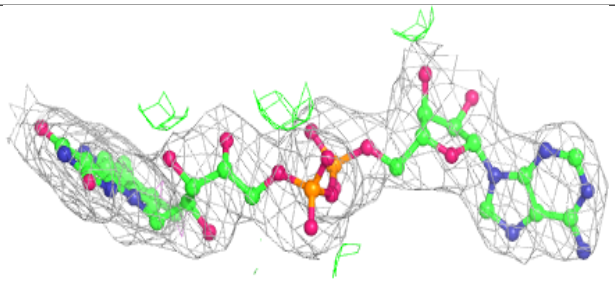




Electron density around FAD F 601:

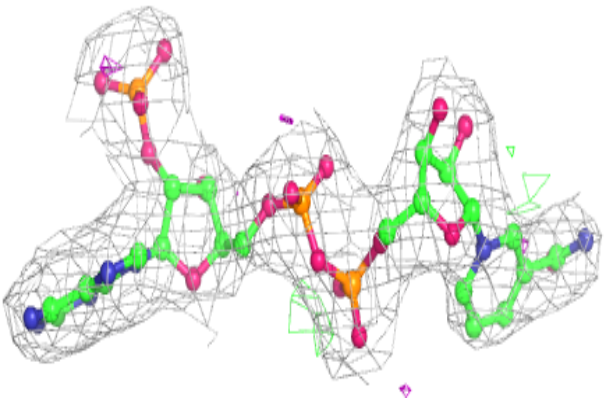
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

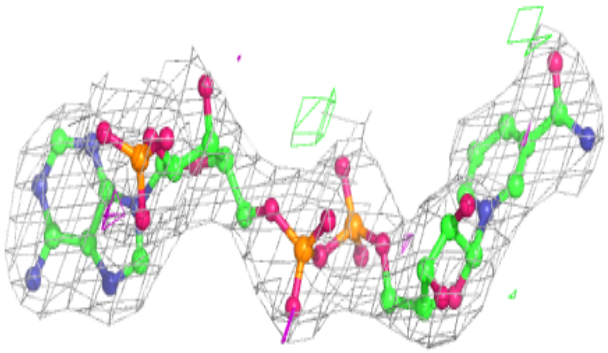


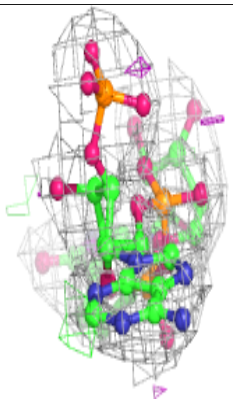


Electron density around NAP C 602:

$2mF_o$-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.