Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 12:46 AM EDT

PDB ID	:	3EAN
Title	:	Crystal structure of recombinant rat selenoprotein thioredoxin reductase 1 with reduced C-terminal tail
Authors	:	Sandalova, T.; Cheng, Q.; Lindqvist, Y.; Arner, E.
Deposited on	:	2008-08-26
Resolution	:	2.75 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:

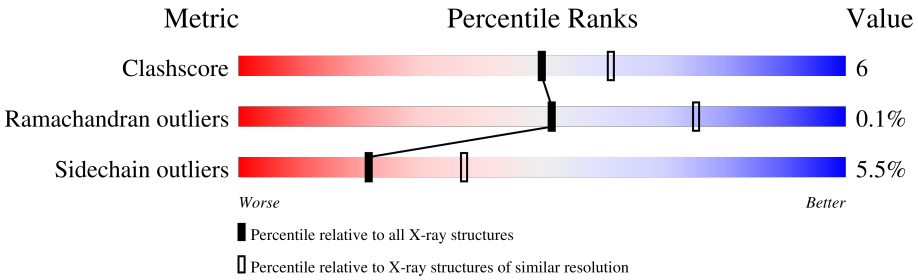
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.75 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))
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	499	83% 13% • •
1	B	499	84% 12% • •
1	C	499	84% 12% • •
1	D	499	86% 10% • •
1	E	499	83% 13% • • •
1	F	499	84% 12% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23214 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.

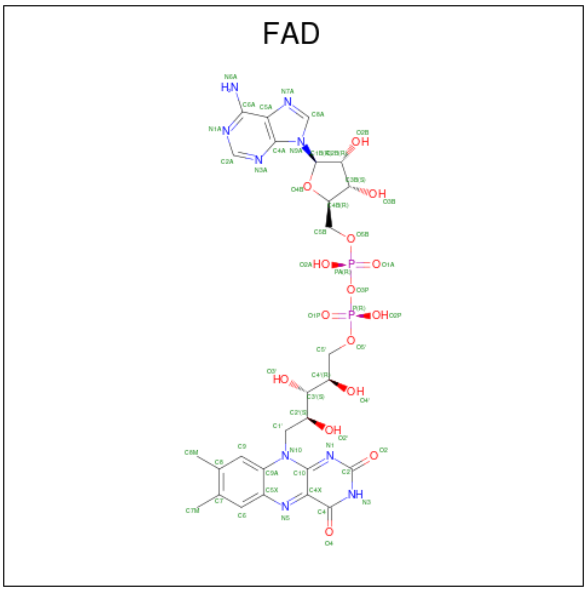
- Molecule 1 is a protein called Thioredoxin reductase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	B	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	C	486	Total	C	N	O	S	Se	0	0	0
			3731	2368	633	708	21	1			
1	D	491	Total	C	N	O	S	Se	0	0	0
			3777	2399	639	717	21	1			
1	E	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	F	489	Total	C	N	O	S	Se	0	0	0
			3762	2390	636	714	21	1			

There are 12 discrepancies between the modelled and reference sequences:

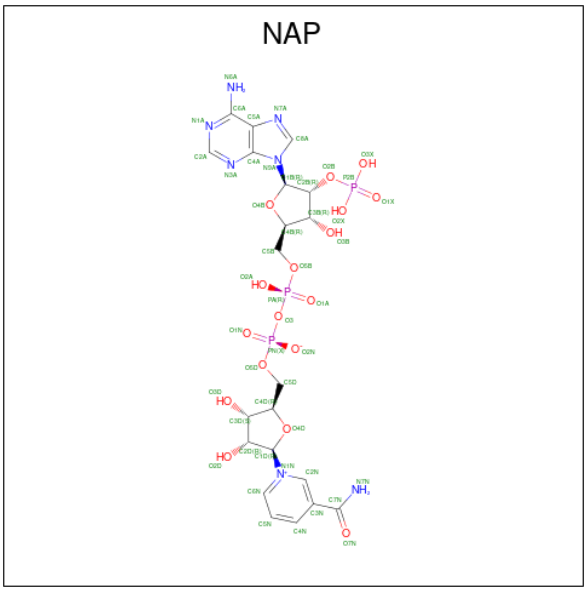
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ARG	ASN	conflict	UNP O89049
A	53	TRP	GLY	conflict	UNP O89049
B	52	ARG	ASN	conflict	UNP O89049
B	53	TRP	GLY	conflict	UNP O89049
C	52	ARG	ASN	conflict	UNP O89049
C	53	TRP	GLY	conflict	UNP O89049
D	52	ARG	ASN	conflict	UNP O89049
D	53	TRP	GLY	conflict	UNP O89049
E	52	ARG	ASN	conflict	UNP O89049
E	53	TRP	GLY	conflict	UNP O89049
F	52	ARG	ASN	conflict	UNP O89049
F	53	TRP	GLY	conflict	UNP O89049

- 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	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	D	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	A	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 4 is water.

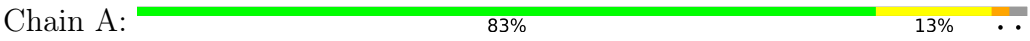
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	20	Total	O	0	0
			20	20		
4	C	14	Total	O	0	0
			14	14		
4	D	35	Total	O	0	0
			35	35		
4	E	26	Total	O	0	0
			26	26		
4	F	12	Total	O	0	0
			12	12		

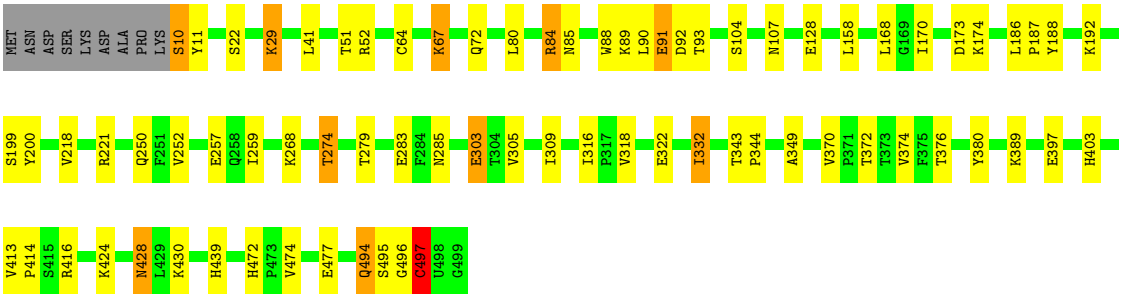
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Thioredoxin reductase 1

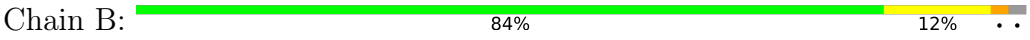
Chain A:





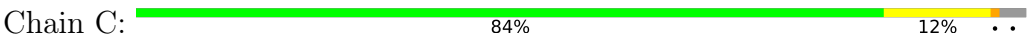
• Molecule 1: Thioredoxin reductase 1

Chain B:



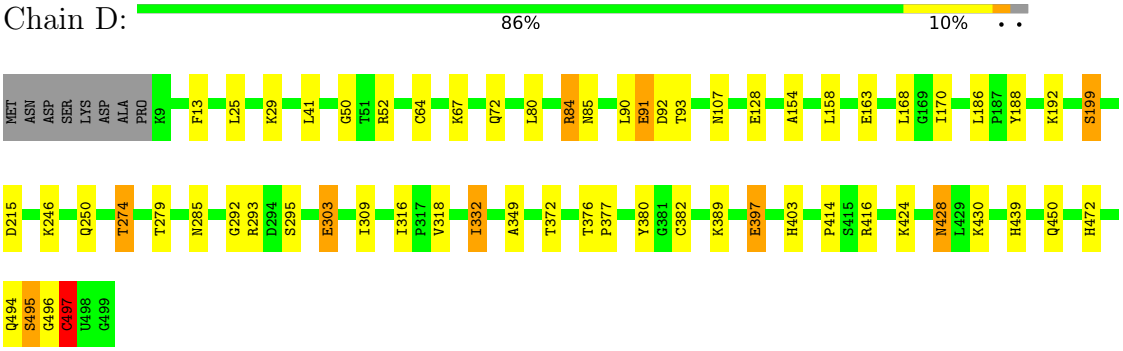
• Molecule 1: Thioredoxin reductase 1

Chain C:



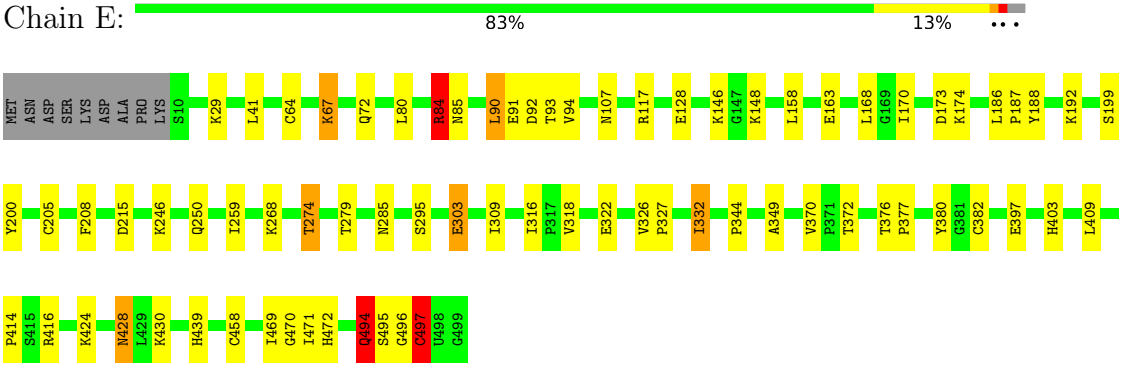
• Molecule 1: Thioredoxin reductase 1

Chain D:



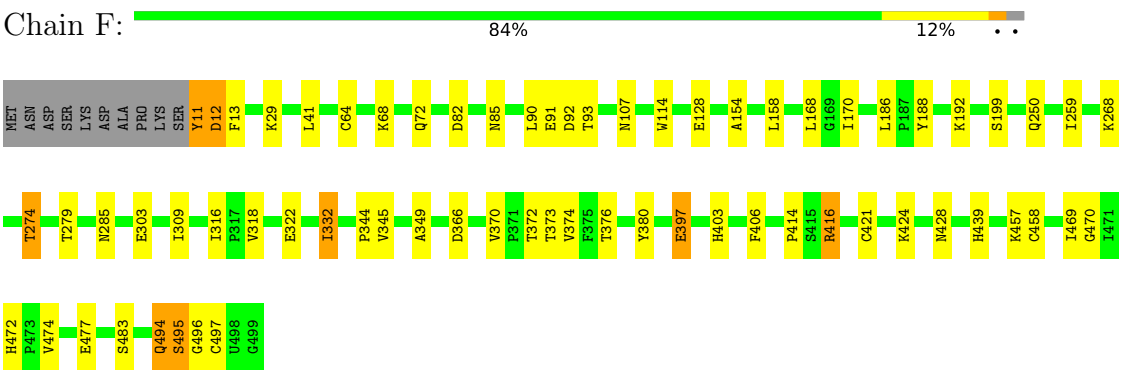
• Molecule 1: Thioredoxin reductase 1

Chain E:



• Molecule 1: Thioredoxin reductase 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.57Å 140.67Å 171.17Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	29.74 – 2.75 29.74 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.74-2.75) 99.5 (29.74-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.236 0.278 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	23214	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: FAD, NAP, SEC

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	0.77	3/3835 (0.1%)	0.70	0/5185
1	B	0.78	1/3835 (0.0%)	0.71	0/5185
1	C	0.65	1/3796 (0.0%)	0.67	1/5132 (0.0%)
1	D	0.79	2/3844 (0.1%)	0.73	0/5196
1	E	0.75	3/3835 (0.1%)	0.71	2/5185 (0.0%)
1	F	0.63	1/3829 (0.0%)	0.66	1/5177 (0.0%)
All	All	0.73	11/22974 (0.0%)	0.70	4/31060 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
1	F	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	495	SER	CB-OG	5.96	1.50	1.42
1	F	11	TYR	N-CA	5.94	1.58	1.46
1	E	200	TYR	CD2-CE2	5.79	1.48	1.39
1	D	495	SER	CB-OG	5.78	1.49	1.42
1	E	382	CYS	CB-SG	-5.63	1.72	1.81
1	E	200	TYR	CD1-CE1	5.54	1.47	1.39
1	A	200	TYR	CE2-CZ	5.36	1.45	1.38
1	A	200	TYR	CD2-CE2	5.34	1.47	1.39
1	C	427	CYS	CB-SG	-5.28	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	VAL	CB-CG2	-5.15	1.42	1.52
1	D	382	CYS	CB-SG	-5.01	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	114	TRP	CA-CB-CG	-7.31	99.81	113.70
1	E	84	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	E	117	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	221	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	494	GLN	Peptide
1	C	496	GLY	Peptide
1	E	494	GLN	Peptide
1	F	11	TYR	Mainchain

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	3768	0	3767	56	0
1	B	3768	0	3769	50	0
1	C	3731	0	3740	53	0
1	D	3777	0	3780	34	0
1	E	3768	0	3767	55	0
1	F	3762	0	3762	46	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
3	A	32	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	11	2	0
3	C	32	0	11	1	0
3	D	32	0	11	1	0
3	E	32	0	11	1	0
3	F	32	0	11	1	0
4	A	23	0	0	2	0
4	B	20	0	0	5	0
4	C	14	0	0	7	0
4	D	35	0	0	0	0
4	E	26	0	0	0	0
4	F	12	0	0	1	0
All	All	23214	0	22837	266	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 6.

All (266) 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:C:192:LYS:H	1:C:285:ASN:HD22	1.24	0.85
1:E:496:GLY:N	1:E:497:CYS:HB2	1.92	0.84
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.62	0.83
1:A:10:SER:O	1:A:11:TYR:CG	2.35	0.80
1:B:192:LYS:H	1:B:285:ASN:HD22	1.28	0.78
1:E:380:TYR:OH	1:E:439:HIS:HD2	1.64	0.78
1:A:192:LYS:H	1:A:285:ASN:HD22	1.28	0.77
1:A:10:SER:O	1:A:11:TYR:CD1	2.38	0.77
1:E:192:LYS:H	1:E:285:ASN:HD22	1.30	0.76
1:C:380:TYR:OH	1:C:439:HIS:HD2	1.70	0.75
1:C:494:GLN:HE21	1:C:494:GLN:HA	1.52	0.74
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.71	0.74
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.70	0.73
1:E:469:ILE:HB	1:F:370:VAL:HG13	1.70	0.72
1:D:192:LYS:H	1:D:285:ASN:HD22	1.38	0.71
1:A:221:ARG:HG3	1:A:252:VAL:CG2	2.21	0.70
1:C:84:ARG:HH22	1:C:90:LEU:HB3	1.57	0.70
1:C:46:PRO:HB3	1:C:52:ARG:NH1	2.06	0.69
1:C:138:HIS:HB3	4:C:613:HOH:O	1.93	0.69
1:C:84:ARG:NH2	1:C:90:LEU:HB3	2.07	0.69
1:C:90:LEU:HD11	1:D:90:LEU:HD11	1.75	0.69
1:A:494:GLN:HB3	1:A:495:SER:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:TYR:OH	1:D:439:HIS:HD2	1.77	0.68
1:F:192:LYS:H	1:F:285:ASN:HD22	1.42	0.67
1:E:72:GLN:HA	1:E:72:GLN:NE2	2.10	0.67
1:D:84:ARG:NH2	1:D:90:LEU:HB3	2.11	0.66
1:C:494:GLN:HA	1:C:494:GLN:NE2	2.10	0.66
1:E:496:GLY:H	1:E:497:CYS:CB	2.09	0.66
1:C:494:GLN:HE21	1:C:494:GLN:CA	2.09	0.65
1:B:494:GLN:HE21	1:B:494:GLN:HA	1.61	0.65
1:E:72:GLN:HA	1:E:72:GLN:HE21	1.60	0.65
1:D:50:GLY:O	1:D:52:ARG:NH1	2.30	0.64
1:F:494:GLN:HB3	1:F:495:SER:HB2	1.79	0.64
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.80	0.64
1:E:496:GLY:H	1:E:497:CYS:HB2	1.62	0.63
1:E:84:ARG:NH2	1:E:90:LEU:HB3	2.15	0.62
1:F:494:GLN:HE21	1:F:494:GLN:HA	1.65	0.61
1:D:186:LEU:HD11	1:D:188:TYR:CZ	2.35	0.61
1:B:486:LYS:CE	4:B:603:HOH:O	2.47	0.61
1:C:46:PRO:CG	1:C:52:ARG:NH1	2.65	0.60
1:C:158:LEU:HD11	1:C:332:ILE:HG12	1.82	0.60
1:E:344:PRO:HG3	1:F:472:HIS:HB2	1.85	0.59
1:D:84:ARG:HH22	1:D:90:LEU:HB3	1.67	0.59
1:A:91:GLU:CD	1:A:92:ASP:H	2.07	0.58
1:E:84:ARG:HH22	1:E:90:LEU:HB3	1.68	0.58
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.86	0.58
1:E:332:ILE:HD12	1:E:349:ALA:HB1	1.86	0.58
1:F:85:ASN:HD22	1:F:414:PRO:HA	1.69	0.57
1:E:380:TYR:OH	1:E:439:HIS:CD2	2.54	0.57
1:C:192:LYS:N	1:C:285:ASN:HD22	2.00	0.57
1:A:85:ASN:HD22	1:A:414:PRO:HA	1.70	0.57
1:C:46:PRO:CB	1:C:52:ARG:NH1	2.68	0.56
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.86	0.56
1:B:332:ILE:HD12	1:B:349:ALA:CB	2.35	0.56
1:D:309:ILE:HG22	1:D:316:ILE:HG12	1.87	0.56
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.87	0.56
1:F:158:LEU:HD11	1:F:332:ILE:HG12	1.88	0.56
1:B:332:ILE:HD12	1:B:349:ALA:HB1	1.86	0.56
1:E:309:ILE:HG22	1:E:316:ILE:HG12	1.88	0.55
1:E:496:GLY:N	1:E:497:CYS:CB	2.64	0.55
3:B:601:NAP:H51A	4:B:612:HOH:O	2.05	0.55
1:F:332:ILE:HD12	1:F:349:ALA:HB1	1.89	0.55
1:B:380:TYR:OH	1:B:439:HIS:CD2	2.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:PHE:CZ	1:C:421:CYS:HB3	2.42	0.55
1:F:309:ILE:HG22	1:F:316:ILE:HG12	1.89	0.55
3:B:601:NAP:C5B	4:B:612:HOH:O	2.55	0.54
1:D:158:LEU:HD11	1:D:332:ILE:HG12	1.89	0.54
1:A:72:GLN:HA	1:A:72:GLN:NE2	2.23	0.54
1:B:486:LYS:HE3	4:B:603:HOH:O	2.06	0.54
1:A:221:ARG:HG3	1:A:252:VAL:HG22	1.89	0.54
1:B:22:SER:OG	1:B:343:THR:HG23	2.07	0.54
1:A:84:ARG:NH2	1:A:90:LEU:HB3	2.23	0.54
1:D:84:ARG:CZ	1:D:84:ARG:HB2	2.38	0.54
1:E:192:LYS:N	1:E:285:ASN:HD22	2.04	0.54
1:A:259:ILE:HD11	1:A:268:LYS:HB2	1.89	0.54
1:B:332:ILE:CD1	1:B:349:ALA:HB1	2.37	0.54
1:C:72:GLN:HA	1:C:72:GLN:NE2	2.22	0.53
1:C:138:HIS:CB	4:C:613:HOH:O	2.55	0.53
1:D:199:SER:HB3	3:D:601:NAP:O1N	2.09	0.52
1:F:332:ILE:HD12	1:F:349:ALA:CB	2.39	0.52
1:E:332:ILE:HD12	1:E:349:ALA:CB	2.39	0.52
1:E:85:ASN:HD22	1:E:414:PRO:HA	1.74	0.52
1:A:29:LYS:NZ	1:B:498:SEC:SE	2.93	0.52
1:C:72:GLN:HA	1:C:72:GLN:HE21	1.75	0.52
1:C:380:TYR:OH	1:C:439:HIS:CD2	2.57	0.52
1:C:428:ASN:ND2	1:C:430:LYS:H	2.07	0.52
1:B:308:LYS:HD2	4:B:614:HOH:O	2.09	0.51
1:B:259:ILE:HD11	1:B:268:LYS:HB2	1.92	0.51
1:F:72:GLN:NE2	1:F:72:GLN:HA	2.25	0.51
1:A:168:LEU:HB2	1:A:170:ILE:HG12	1.92	0.51
1:C:199:SER:HB3	3:C:601:NAP:O1N	2.10	0.51
1:A:380:TYR:OH	1:A:439:HIS:CD2	2.60	0.51
1:D:496:GLY:N	1:D:497:CYS:HB2	2.25	0.51
1:C:84:ARG:HB2	1:C:84:ARG:CZ	2.40	0.51
1:F:494:GLN:HE21	1:F:494:GLN:CA	2.23	0.51
1:A:374:VAL:HG12	1:A:376:THR:HG23	1.93	0.51
1:E:332:ILE:CD1	1:E:349:ALA:HB1	2.40	0.51
1:A:89:LYS:HE3	1:B:97:ASP:HB2	1.93	0.51
1:C:46:PRO:HG3	1:C:52:ARG:NH1	2.26	0.51
1:B:59:CYS:CB	1:B:64:CYS:HG	2.23	0.50
1:F:494:GLN:HB3	1:F:495:SER:CB	2.41	0.50
1:F:13:PHE:O	1:F:154:ALA:HA	2.11	0.50
1:C:309:ILE:HG22	1:C:316:ILE:HG12	1.94	0.50
1:F:406:PHE:CZ	1:F:421:CYS:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLN:HA	1:B:72:GLN:NE2	2.26	0.50
1:C:259:ILE:HD11	1:C:268:LYS:HB2	1.93	0.50
1:A:84:ARG:HB2	1:A:84:ARG:CZ	2.41	0.49
1:A:104:SER:HB3	1:B:413:VAL:HG13	1.94	0.49
1:E:163:GLU:HG2	1:E:295:SER:HA	1.94	0.49
1:B:494:GLN:HE21	1:B:494:GLN:CA	2.24	0.49
1:D:91:GLU:CD	1:D:92:ASP:H	2.15	0.49
1:F:374:VAL:HG12	1:F:376:THR:HG23	1.94	0.49
1:F:494:GLN:HA	1:F:494:GLN:NE2	2.26	0.49
1:A:41:LEU:HD23	1:A:128:GLU:HB3	1.95	0.49
1:B:85:ASN:HD22	1:B:414:PRO:HA	1.77	0.49
1:D:303:GLU:CD	1:D:303:GLU:H	2.17	0.48
1:F:72:GLN:HA	1:F:72:GLN:HE21	1.78	0.48
1:B:366:ASP:OD2	1:B:457:LYS:HE3	2.13	0.48
1:D:13:PHE:O	1:D:154:ALA:HA	2.14	0.48
1:D:85:ASN:HD22	1:D:414:PRO:HA	1.78	0.48
1:C:186:LEU:HD11	1:C:188:TYR:CZ	2.48	0.47
1:B:474:VAL:O	1:B:477:GLU:HG2	2.14	0.47
1:F:168:LEU:HB2	1:F:170:ILE:HG12	1.95	0.47
1:A:67:LYS:HE2	1:A:67:LYS:HB3	1.75	0.47
1:A:428:ASN:ND2	1:A:430:LYS:H	2.13	0.47
1:F:41:LEU:HD23	1:F:128:GLU:HB3	1.95	0.47
1:C:168:LEU:HB2	1:C:170:ILE:HG12	1.97	0.47
1:E:471:ILE:HG21	1:F:373:THR:OG1	2.14	0.47
1:A:199:SER:HB3	3:A:601:NAP:O1N	2.15	0.46
1:D:332:ILE:HD12	1:D:349:ALA:HB1	1.97	0.46
1:A:494:GLN:HE21	1:A:494:GLN:N	2.13	0.46
1:C:46:PRO:CG	1:C:52:ARG:HH12	2.28	0.46
1:C:41:LEU:HD23	1:C:128:GLU:HB3	1.98	0.46
1:B:332:ILE:HD13	1:B:332:ILE:HA	1.70	0.46
1:D:84:ARG:NH2	1:D:84:ARG:HB2	2.31	0.46
1:F:474:VAL:O	1:F:477:GLU:HG2	2.16	0.46
1:F:332:ILE:CD1	1:F:349:ALA:HB1	2.45	0.46
1:A:22:SER:OG	1:A:343:THR:HG23	2.16	0.46
1:A:332:ILE:HD12	1:A:349:ALA:HB1	1.97	0.46
1:B:158:LEU:HD11	1:B:332:ILE:HG12	1.98	0.46
1:D:72:GLN:HA	1:D:72:GLN:NE2	2.31	0.46
1:C:332:ILE:HD12	1:C:349:ALA:HB1	1.98	0.46
1:D:72:GLN:HA	1:D:72:GLN:HE21	1.79	0.46
1:C:35:ASP:CB	4:C:614:HOH:O	2.63	0.46
1:A:413:VAL:HG13	1:B:104:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLN:HB3	1:D:274:THR:HB	1.97	0.45
1:D:397:GLU:O	1:D:397:GLU:HG2	2.16	0.45
1:E:322:GLU:HG2	1:E:332:ILE:CD1	2.46	0.45
1:E:496:GLY:H	1:E:497:CYS:HB3	1.80	0.45
1:A:370:VAL:HG13	1:B:469:ILE:HB	1.99	0.45
1:B:67:LYS:HB3	1:B:67:LYS:HE2	1.82	0.45
1:E:158:LEU:HD11	1:E:332:ILE:HG12	1.97	0.45
1:E:303:GLU:CD	1:E:303:GLU:H	2.19	0.45
1:F:250:GLN:HB3	1:F:274:THR:HB	1.98	0.45
1:B:322:GLU:HG2	1:B:332:ILE:HD13	1.98	0.45
1:C:67:LYS:HB3	1:C:67:LYS:HE2	1.67	0.45
1:C:160:ALA:HB1	4:C:605:HOH:O	2.16	0.45
1:A:84:ARG:HH22	1:A:90:LEU:HB3	1.79	0.45
1:B:406:PHE:CZ	1:B:421:CYS:HB3	2.51	0.45
1:B:91:GLU:CD	1:B:92:ASP:H	2.20	0.45
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.99	0.45
1:B:309:ILE:HG22	1:B:316:ILE:HG12	1.98	0.45
1:E:322:GLU:HG2	1:E:332:ILE:HD13	1.98	0.45
1:A:332:ILE:HD12	1:A:349:ALA:CB	2.46	0.45
1:B:173:ASP:OD1	1:B:174:LYS:N	2.50	0.45
1:B:494:GLN:HB3	1:B:495:SER:HA	1.99	0.45
1:E:84:ARG:HB2	1:E:84:ARG:CZ	2.47	0.44
1:B:163:GLU:HG2	1:B:295:SER:HA	2.00	0.44
1:E:205:CYS:HA	1:E:208:PHE:CE2	2.52	0.44
1:E:332:ILE:HD13	1:E:332:ILE:HA	1.70	0.44
1:A:186:LEU:HD11	1:A:188:TYR:CZ	2.53	0.44
1:A:389:LYS:HD2	1:A:389:LYS:HA	1.82	0.44
1:E:173:ASP:OD1	1:E:174:LYS:N	2.51	0.44
1:E:250:GLN:HB3	1:E:274:THR:HB	1.99	0.44
1:E:494:GLN:HB3	1:E:495:SER:HA	2.00	0.44
1:C:99:GLU:OE1	1:E:148:LYS:HE3	2.18	0.44
1:B:322:GLU:HG2	1:B:332:ILE:CD1	2.47	0.44
1:C:322:GLU:HG2	1:C:332:ILE:CD1	2.48	0.43
1:D:168:LEU:HB2	1:D:170:ILE:HG12	2.00	0.43
1:E:67:LYS:HB3	1:E:67:LYS:HE2	1.67	0.43
1:E:469:ILE:HG21	1:F:345:VAL:HG23	1.99	0.43
1:A:84:ARG:NH2	1:A:84:ARG:HB2	2.33	0.43
1:B:41:LEU:HD23	1:B:128:GLU:HB3	2.00	0.43
1:E:458:CYS:HB2	1:F:458:CYS:HB2	2.01	0.43
1:A:173:ASP:OD1	1:A:174:LYS:N	2.51	0.43
1:C:187:PRO:HB3	1:E:146:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:VAL:HG13	1:F:469:ILE:HB	2.00	0.43
1:E:469:ILE:CB	1:F:370:VAL:HG13	2.44	0.43
1:F:186:LEU:HD11	1:F:188:TYR:CZ	2.52	0.43
1:A:72:GLN:HA	1:A:72:GLN:HE21	1.81	0.43
1:A:494:GLN:HB3	1:A:495:SER:CA	2.44	0.43
1:B:72:GLN:HA	1:B:72:GLN:HE21	1.83	0.43
1:B:389:LYS:HD2	1:B:389:LYS:HA	1.78	0.43
1:E:428:ASN:ND2	1:E:430:LYS:H	2.16	0.43
1:A:250:GLN:HB3	1:A:274:THR:HB	2.01	0.43
1:C:85:ASN:HD22	1:C:414:PRO:HA	1.83	0.43
1:C:318:VAL:HG13	1:C:319:THR:O	2.19	0.43
1:F:199:SER:HB3	3:F:601:NAP:O1N	2.19	0.43
1:F:397:GLU:O	1:F:397:GLU:HG2	2.17	0.43
1:C:80:LEU:HD23	1:D:80:LEU:HD23	2.00	0.43
1:C:186:LEU:HA	1:C:187:PRO:HD3	1.80	0.43
1:D:41:LEU:HD23	1:D:128:GLU:HB3	1.99	0.43
1:D:428:ASN:ND2	1:D:430:LYS:H	2.16	0.43
1:E:472:HIS:HB2	1:F:344:PRO:HG3	1.99	0.43
1:F:322:GLU:HG2	1:F:332:ILE:HD13	2.00	0.43
1:C:35:ASP:HB2	4:C:614:HOH:O	2.19	0.43
1:F:259:ILE:HD11	1:F:268:LYS:HB2	2.01	0.43
1:A:283:GLU:HG3	4:A:620:HOH:O	2.18	0.43
1:C:138:HIS:CG	4:C:613:HOH:O	2.71	0.43
1:A:309:ILE:HG22	1:A:316:ILE:HG12	2.01	0.43
1:B:292:GLY:C	1:B:293:ARG:HG2	2.39	0.43
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.88	0.43
1:D:163:GLU:HG2	1:D:295:SER:HA	2.01	0.42
1:E:90:LEU:HD11	1:F:90:LEU:HD11	2.01	0.42
1:C:163:GLU:HG2	1:C:295:SER:HA	2.01	0.42
1:A:303:GLU:CD	1:A:303:GLU:H	2.21	0.42
1:E:41:LEU:HD23	1:E:128:GLU:HB3	2.02	0.42
1:F:483:SER:N	4:F:606:HOH:O	2.50	0.42
1:F:496:GLY:N	1:F:497:CYS:HB3	2.34	0.42
1:A:322:GLU:HG2	1:A:332:ILE:CD1	2.50	0.42
1:C:389:LYS:HD2	1:C:389:LYS:HA	1.82	0.42
1:D:292:GLY:C	1:D:293:ARG:HG2	2.40	0.42
1:E:470:GLY:O	1:F:344:PRO:HG2	2.20	0.42
1:B:428:ASN:ND2	1:B:430:LYS:H	2.18	0.42
1:C:322:GLU:HG2	1:C:332:ILE:HD13	2.01	0.42
1:E:215:ASP:OD1	1:E:246:LYS:NZ	2.52	0.42
1:C:332:ILE:HD13	1:C:332:ILE:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:LEU:HA	1:E:187:PRO:HD3	1.73	0.42
1:A:332:ILE:CD1	1:A:349:ALA:HB1	2.50	0.41
1:E:199:SER:HB3	3:E:601:NAP:O1N	2.20	0.41
1:F:366:ASP:OD2	1:F:457:LYS:HE3	2.20	0.41
1:E:259:ILE:HD11	1:E:268:LYS:HB2	2.02	0.41
1:C:378:LEU:CD2	1:C:441:LEU:HG	2.50	0.41
1:E:326:VAL:HA	1:E:327:PRO:HD3	1.93	0.41
1:B:376:THR:O	1:B:377:PRO:C	2.59	0.41
1:E:168:LEU:HB2	1:E:170:ILE:HG12	2.03	0.41
1:A:186:LEU:HA	1:A:187:PRO:HD3	1.81	0.41
1:C:46:PRO:CB	1:C:52:ARG:HH12	2.32	0.41
1:D:376:THR:O	1:D:377:PRO:C	2.57	0.41
1:A:51:THR:HA	4:A:611:HOH:O	2.19	0.41
1:B:397:GLU:O	1:B:397:GLU:HG2	2.20	0.41
1:D:215:ASP:OD1	1:D:246:LYS:NZ	2.53	0.41
1:D:389:LYS:HD2	1:D:389:LYS:HA	1.82	0.41
1:E:409:LEU:HD23	1:F:68:LYS:HG2	2.02	0.41
1:E:186:LEU:HD11	1:E:188:TYR:CZ	2.55	0.41
1:A:29:LYS:HZ3	1:B:498:SEC:SE	2.53	0.41
1:B:91:GLU:CD	1:B:92:ASP:N	2.74	0.41
1:C:332:ILE:HD12	1:C:349:ALA:CB	2.50	0.41
1:E:376:THR:O	1:E:377:PRO:C	2.59	0.41
1:A:29:LYS:HZ2	1:B:498:SEC:SE	2.54	0.41
1:A:80:LEU:CD2	1:B:80:LEU:HD23	2.51	0.41
1:A:496:GLY:H	1:A:497:CYS:HB3	1.85	0.41
1:F:12:ASP:HB3	1:F:13:PHE:CD2	2.56	0.40
1:A:88:TRP:CZ3	1:B:96:HIS:HB2	2.56	0.40
1:A:474:VAL:O	1:A:477:GLU:HG2	2.22	0.40
1:C:46:PRO:HG3	1:C:52:ARG:CZ	2.50	0.40
1:C:470:GLY:HA2	1:D:450:GLN:OE1	2.21	0.40
1:F:322:GLU:HG2	1:F:332:ILE:CD1	2.51	0.40
1:A:259:ILE:CD1	1:A:268:LYS:HB2	2.51	0.40
1:E:344:PRO:HG2	1:F:470:GLY:O	2.21	0.40
1:A:322:GLU:HG2	1:A:332:ILE:HD13	2.02	0.40
1:B:399:ILE:HD13	1:B:399:ILE:HA	1.91	0.40
1:C:34:PHE:C	4:C:614:HOH:O	2.60	0.40
1:E:80:LEU:HD13	1:E:94:VAL:HG21	2.04	0.40
1:F:82:ASP:OD2	1:F:416:ARG:NH1	2.55	0.40
1:F:332:ILE:HD13	1:F:332:ILE:HA	1.81	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	487/499 (98%)	460 (94%)	26 (5%)	1 (0%)	47 69
1	B	487/499 (98%)	463 (95%)	24 (5%)	0	100 100
1	C	483/499 (97%)	456 (94%)	26 (5%)	1 (0%)	47 69
1	D	488/499 (98%)	461 (94%)	26 (5%)	1 (0%)	47 69
1	E	487/499 (98%)	462 (95%)	24 (5%)	1 (0%)	47 69
1	F	486/499 (97%)	461 (95%)	25 (5%)	0	100 100
All	All	2918/2994 (98%)	2763 (95%)	151 (5%)	4 (0%)	51 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	497	CYS
1	D	497	CYS
1	E	497	CYS
1	A	497	CYS

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	405/413 (98%)	381 (94%)	24 (6%)	19 34
1	B	405/413 (98%)	382 (94%)	23 (6%)	20 36
1	C	401/413 (97%)	378 (94%)	23 (6%)	20 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	406/413 (98%)	384 (95%)	22 (5%)	22 38
1	E	405/413 (98%)	383 (95%)	22 (5%)	22 38
1	F	404/413 (98%)	384 (95%)	20 (5%)	24 42
All	All	2426/2478 (98%)	2292 (94%)	134 (6%)	21 37

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	29	LYS
1	A	52	ARG
1	A	64	CYS
1	A	67	LYS
1	A	84	ARG
1	A	91	GLU
1	A	93	THR
1	A	107	ASN
1	A	257	GLU
1	A	274	THR
1	A	279	THR
1	A	303	GLU
1	A	305	VAL
1	A	318	VAL
1	A	332	ILE
1	A	372	THR
1	A	397	GLU
1	A	403	HIS
1	A	416	ARG
1	A	424	LYS
1	A	428	ASN
1	A	494	GLN
1	A	497	CYS
1	B	29	LYS
1	B	64	CYS
1	B	91	GLU
1	B	92	ASP
1	B	93	THR
1	B	107	ASN
1	B	199	SER
1	B	257	GLU
1	B	274	THR

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Mol	Chain	Res	Type
1	B	279	THR
1	B	303	GLU
1	B	305	VAL
1	B	318	VAL
1	B	332	ILE
1	B	372	THR
1	B	376	THR
1	B	397	GLU
1	B	403	HIS
1	B	416	ARG
1	B	424	LYS
1	B	428	ASN
1	B	494	GLN
1	B	495	SER
1	C	29	LYS
1	C	64	CYS
1	C	67	LYS
1	C	84	ARG
1	C	91	GLU
1	C	92	ASP
1	C	93	THR
1	C	107	ASN
1	C	274	THR
1	C	279	THR
1	C	303	GLU
1	C	305	VAL
1	C	318	VAL
1	C	332	ILE
1	C	372	THR
1	C	397	GLU
1	C	403	HIS
1	C	416	ARG
1	C	424	LYS
1	C	428	ASN
1	C	494	GLN
1	C	495	SER
1	C	497	CYS
1	D	29	LYS
1	D	64	CYS
1	D	67	LYS
1	D	84	ARG
1	D	91	GLU

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Mol	Chain	Res	Type
1	D	93	THR
1	D	107	ASN
1	D	199	SER
1	D	274	THR
1	D	279	THR
1	D	303	GLU
1	D	318	VAL
1	D	332	ILE
1	D	372	THR
1	D	397	GLU
1	D	403	HIS
1	D	416	ARG
1	D	424	LYS
1	D	428	ASN
1	D	494	GLN
1	D	495	SER
1	D	497	CYS
1	E	29	LYS
1	E	64	CYS
1	E	67	LYS
1	E	84	ARG
1	E	90	LEU
1	E	91	GLU
1	E	92	ASP
1	E	93	THR
1	E	107	ASN
1	E	274	THR
1	E	279	THR
1	E	303	GLU
1	E	318	VAL
1	E	332	ILE
1	E	372	THR
1	E	397	GLU
1	E	403	HIS
1	E	416	ARG
1	E	424	LYS
1	E	428	ASN
1	E	494	GLN
1	E	497	CYS
1	F	12	ASP
1	F	29	LYS
1	F	64	CYS

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Mol	Chain	Res	Type
1	F	91	GLU
1	F	92	ASP
1	F	93	THR
1	F	107	ASN
1	F	274	THR
1	F	279	THR
1	F	303	GLU
1	F	318	VAL
1	F	332	ILE
1	F	372	THR
1	F	397	GLU
1	F	403	HIS
1	F	416	ARG
1	F	424	LYS
1	F	428	ASN
1	F	494	GLN
1	F	495	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	285	ASN
1	A	428	ASN
1	A	439	HIS
1	A	494	GLN
1	B	72	GLN
1	B	285	ASN
1	B	428	ASN
1	B	439	HIS
1	B	494	GLN
1	C	72	GLN
1	C	285	ASN
1	C	428	ASN
1	C	439	HIS
1	C	494	GLN
1	D	72	GLN
1	D	285	ASN
1	D	428	ASN
1	D	439	HIS
1	E	72	GLN
1	E	285	ASN

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Mol	Chain	Res	Type
1	E	428	ASN
1	E	439	HIS
1	E	494	GLN
1	F	72	GLN
1	F	285	ASN
1	F	428	ASN
1	F	439	HIS
1	F	494	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	F	601	-	28,34,52	1.22	2 (7%)	34,53,80	1.31	1 (2%)
2	FAD	E	600	-	53,58,58	1.50	4 (7%)	68,89,89	1.50	18 (26%)
2	FAD	C	600	-	53,58,58	1.35	4 (7%)	68,89,89	1.37	11 (16%)
2	FAD	A	600	-	53,58,58	1.27	4 (7%)	68,89,89	1.39	10 (14%)
2	FAD	F	600	-	53,58,58	1.36	4 (7%)	68,89,89	1.37	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAP	E	601	-	28,34,52	1.36	3 (10%)	34,53,80	1.39	2 (5%)
3	NAP	A	601	-	28,34,52	1.32	3 (10%)	34,53,80	1.38	3 (8%)
2	FAD	B	600	-	53,58,58	1.55	4 (7%)	68,89,89	1.40	12 (17%)
3	NAP	C	601	-	28,34,52	1.22	3 (10%)	34,53,80	1.30	3 (8%)
2	FAD	D	600	-	53,58,58	1.44	4 (7%)	68,89,89	1.60	13 (19%)
3	NAP	B	601	-	28,34,52	1.24	4 (14%)	34,53,80	1.47	2 (5%)
3	NAP	D	601	-	28,34,52	1.34	4 (14%)	34,53,80	1.47	4 (11%)

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	F	601	-	-	8/20/40/67	0/3/3/5
2	FAD	E	600	-	-	2/30/50/50	0/6/6/6
2	FAD	C	600	-	-	2/30/50/50	0/6/6/6
2	FAD	A	600	-	-	2/30/50/50	0/6/6/6
2	FAD	F	600	-	-	2/30/50/50	0/6/6/6
3	NAP	E	601	-	-	10/20/40/67	0/3/3/5
3	NAP	A	601	-	-	8/20/40/67	0/3/3/5
2	FAD	B	600	-	-	2/30/50/50	0/6/6/6
3	NAP	C	601	-	-	10/20/40/67	0/3/3/5
2	FAD	D	600	-	-	2/30/50/50	0/6/6/6
3	NAP	B	601	-	-	9/20/40/67	0/3/3/5
3	NAP	D	601	-	-	10/20/40/67	0/3/3/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	FAD	C4X-N5	6.14	1.42	1.30
2	B	600	FAD	O4B-C1B	6.08	1.49	1.41
2	D	600	FAD	C4X-N5	5.80	1.42	1.30
2	B	600	FAD	C4X-N5	5.62	1.41	1.30
2	C	600	FAD	C4X-N5	5.49	1.41	1.30
2	F	600	FAD	C4X-N5	5.35	1.41	1.30
2	A	600	FAD	C4X-N5	4.96	1.40	1.30
2	F	600	FAD	C10-N1	4.55	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	O4B-C1B	4.34	1.47	1.41
3	E	601	NAP	PN-O5D	4.28	1.74	1.59
2	E	600	FAD	O4B-C1B	4.26	1.47	1.41
2	C	600	FAD	C10-N1	3.87	1.41	1.33
3	F	601	NAP	P2B-O1X	3.80	1.62	1.50
2	A	600	FAD	C10-N1	3.76	1.40	1.33
3	B	601	NAP	P2B-O1X	3.72	1.62	1.50
3	D	601	NAP	O4B-C1B	3.63	1.46	1.41
3	A	601	NAP	PN-O5D	3.62	1.72	1.59
3	C	601	NAP	P2B-O1X	3.50	1.61	1.50
2	E	600	FAD	C10-N1	3.38	1.40	1.33
3	A	601	NAP	O4B-C1B	3.34	1.45	1.41
3	E	601	NAP	P2B-O1X	3.16	1.60	1.50
2	B	600	FAD	C10-N1	3.11	1.39	1.33
2	D	600	FAD	C10-N1	3.05	1.39	1.33
3	D	601	NAP	P2B-O1X	3.02	1.60	1.50
3	D	601	NAP	PN-O5D	2.91	1.69	1.59
2	E	600	FAD	C2B-C1B	-2.90	1.49	1.53
2	F	600	FAD	C2-N1	2.77	1.43	1.36
2	F	600	FAD	O4B-C1B	2.73	1.44	1.41
2	C	600	FAD	O4B-C1B	2.69	1.44	1.41
3	B	601	NAP	PN-O5D	2.63	1.68	1.59
3	F	601	NAP	O4B-C1B	2.62	1.44	1.41
2	C	600	FAD	C1'-C2'	2.37	1.56	1.52
3	C	601	NAP	O4B-C1B	2.37	1.44	1.41
2	A	600	FAD	O4B-C1B	2.34	1.44	1.41
2	D	600	FAD	C4A-N3A	-2.31	1.32	1.35
2	B	600	FAD	C2B-C1B	-2.30	1.50	1.53
3	A	601	NAP	P2B-O1X	2.29	1.57	1.50
3	E	601	NAP	O4B-C1B	2.26	1.44	1.41
3	C	601	NAP	PN-O5D	2.20	1.67	1.59
3	B	601	NAP	O4B-C1B	2.18	1.44	1.41
3	D	601	NAP	P2B-O3X	-2.16	1.46	1.54
2	A	600	FAD	C10-N10	2.12	1.42	1.37
3	B	601	NAP	P2B-O3X	-2.00	1.47	1.54

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	NAP	N3A-C2A-N1A	-5.60	119.93	128.68
3	D	601	NAP	N3A-C2A-N1A	-5.38	120.27	128.68
2	D	600	FAD	O4B-C1B-C2B	-5.35	99.10	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	N3A-C2A-N1A	-4.98	120.89	128.68
3	A	601	NAP	N3A-C2A-N1A	-4.88	121.04	128.68
3	F	601	NAP	N3A-C2A-N1A	-4.88	121.05	128.68
2	D	600	FAD	N3A-C2A-N1A	-4.85	121.10	128.68
3	E	601	NAP	N3A-C2A-N1A	-4.84	121.11	128.68
3	C	601	NAP	N3A-C2A-N1A	-4.70	121.33	128.68
2	F	600	FAD	N3A-C2A-N1A	-4.62	121.46	128.68
2	C	600	FAD	N3A-C2A-N1A	-4.50	121.64	128.68
2	B	600	FAD	N3A-C2A-N1A	-4.40	121.80	128.68
2	E	600	FAD	N3A-C2A-N1A	-3.81	122.72	128.68
2	F	600	FAD	O4B-C1B-C2B	-3.70	101.52	106.93
2	B	600	FAD	C5B-C4B-C3B	-3.41	102.41	115.18
2	E	600	FAD	P-O3P-PA	-3.15	122.00	132.83
2	C	600	FAD	O4B-C1B-C2B	-3.12	102.36	106.93
2	D	600	FAD	C4X-C4-N3	3.06	120.97	113.19
2	E	600	FAD	O4B-C1B-C2B	-3.02	102.52	106.93
2	A	600	FAD	C4X-C10-N10	2.99	120.85	116.48
2	D	600	FAD	C9A-C5X-N5	-2.98	119.19	122.43
2	E	600	FAD	C4X-C4-N3	2.94	120.65	113.19
2	D	600	FAD	C4X-C10-N10	2.85	120.65	116.48
2	F	600	FAD	C4X-C4-N3	2.85	120.42	113.19
2	C	600	FAD	C9A-C5X-N5	-2.81	119.38	122.43
2	F	600	FAD	C9A-C5X-N5	-2.77	119.42	122.43
2	C	600	FAD	P-O3P-PA	-2.76	123.37	132.83
2	F	600	FAD	P-O3P-PA	-2.73	123.47	132.83
2	A	600	FAD	C5'-C4'-C3'	-2.69	107.00	112.20
2	E	600	FAD	C4-N3-C2	-2.67	120.70	125.64
2	E	600	FAD	O3'-C3'-C2'	-2.67	102.36	108.81
2	C	600	FAD	C4-N3-C2	-2.66	120.72	125.64
2	B	600	FAD	O3B-C3B-C4B	-2.64	103.40	111.05
2	D	600	FAD	C4-N3-C2	-2.64	120.77	125.64
2	C	600	FAD	C4X-C4-N3	2.63	119.86	113.19
3	B	601	NAP	O3X-P2B-O2X	2.63	117.67	107.64
2	C	600	FAD	C10-C4X-N5	-2.54	119.47	124.86
2	A	600	FAD	C4X-C4-N3	2.53	119.62	113.19
2	B	600	FAD	O4B-C1B-C2B	-2.51	103.26	106.93
2	B	600	FAD	C9A-C5X-N5	-2.48	119.74	122.43
2	A	600	FAD	O4B-C1B-C2B	-2.46	103.33	106.93
2	C	600	FAD	C4X-C10-N10	2.44	120.05	116.48
2	C	600	FAD	C5'-C4'-C3'	-2.44	107.49	112.20
2	B	600	FAD	P-O3P-PA	-2.43	124.48	132.83
2	A	600	FAD	P-O3P-PA	-2.41	124.57	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	FAD	C4X-C10-N1	-2.40	119.15	124.73
2	B	600	FAD	C4X-C4-N3	2.40	119.29	113.19
3	D	601	NAP	O5B-PA-O1A	-2.40	99.69	109.07
2	E	600	FAD	O4-C4-C4X	-2.38	120.28	126.60
2	D	600	FAD	C10-C4X-N5	-2.37	119.82	124.86
2	E	600	FAD	C10-C4X-N5	-2.37	119.82	124.86
2	B	600	FAD	N6A-C6A-N1A	2.36	123.47	118.57
2	F	600	FAD	C4-N3-C2	-2.35	121.30	125.64
2	F	600	FAD	O4-C4-C4X	-2.34	120.39	126.60
2	E	600	FAD	C4X-C10-N10	2.33	119.88	116.48
2	E	600	FAD	C9A-C5X-N5	-2.32	119.91	122.43
2	D	600	FAD	P-O3P-PA	-2.32	124.88	132.83
2	F	600	FAD	C5B-C4B-C3B	-2.30	106.56	115.18
2	F	600	FAD	C10-C4X-N5	-2.27	120.04	124.86
2	B	600	FAD	C5'-C4'-C3'	-2.25	107.86	112.20
2	B	600	FAD	C10-C4X-N5	-2.24	120.09	124.86
2	E	600	FAD	O4'-C4'-C3'	2.24	114.54	109.10
2	E	600	FAD	O2P-P-O1P	2.23	123.28	112.24
2	D	600	FAD	C5B-C4B-C3B	-2.22	106.88	115.18
2	B	600	FAD	C4X-C10-N10	2.21	119.72	116.48
2	A	600	FAD	C5B-C4B-C3B	-2.19	106.99	115.18
2	C	600	FAD	C5B-C4B-C3B	-2.18	107.02	115.18
2	B	600	FAD	C4-N3-C2	-2.17	121.64	125.64
2	E	600	FAD	O2'-C2'-C3'	2.16	114.36	109.10
2	A	600	FAD	O2P-P-O1P	2.15	122.86	112.24
3	D	601	NAP	O3X-P2B-O2B	2.13	115.56	105.99
2	D	600	FAD	O3'-C3'-C2'	-2.12	103.68	108.81
3	E	601	NAP	O3X-P2B-O2X	2.11	115.71	107.64
2	D	600	FAD	O2P-P-O1P	2.11	122.68	112.24
2	E	600	FAD	O3B-C3B-C4B	-2.11	104.95	111.05
2	E	600	FAD	C10-N1-C2	2.11	121.12	116.90
2	D	600	FAD	C10-N1-C2	2.10	121.11	116.90
3	A	601	NAP	C3B-C2B-C1B	-2.09	98.95	102.89
2	E	600	FAD	C5'-C4'-C3'	-2.08	108.19	112.20
2	A	600	FAD	C10-C4X-N5	-2.07	120.45	124.86
2	A	600	FAD	C4X-C10-N1	-2.04	120.00	124.73
3	C	601	NAP	C3B-C2B-C1B	-2.04	99.06	102.89
3	D	601	NAP	O2A-PA-O1A	2.03	122.28	112.24
2	C	600	FAD	O4-C4-C4X	-2.02	121.24	126.60
3	A	601	NAP	O3X-P2B-O2X	2.01	115.32	107.64
2	E	600	FAD	C4-C4X-N5	2.01	121.09	118.23
3	C	601	NAP	O2A-PA-O1A	2.00	122.15	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	600	FAD	C4X-C10-N1	-2.00	120.09	124.73

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O4B-C4B-C5B-O5B
2	D	600	FAD	O4B-C4B-C5B-O5B
2	F	600	FAD	O4B-C4B-C5B-O5B
3	A	601	NAP	C5B-O5B-PA-O1A
3	B	601	NAP	C5B-O5B-PA-O1A
3	B	601	NAP	C5B-O5B-PA-O3
3	C	601	NAP	C5B-O5B-PA-O1A
3	D	601	NAP	C5B-O5B-PA-O1A
3	E	601	NAP	C5B-O5B-PA-O1A
3	F	601	NAP	C5B-O5B-PA-O1A
2	A	600	FAD	C3B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	C3B-C4B-C5B-O5B
2	C	600	FAD	O4B-C4B-C5B-O5B
2	C	600	FAD	C3B-C4B-C5B-O5B
2	D	600	FAD	C3B-C4B-C5B-O5B
2	E	600	FAD	O4B-C4B-C5B-O5B
2	E	600	FAD	C3B-C4B-C5B-O5B
2	F	600	FAD	C3B-C4B-C5B-O5B
3	A	601	NAP	C5D-O5D-PN-O1N
3	B	601	NAP	C5D-O5D-PN-O1N
3	C	601	NAP	C5D-O5D-PN-O1N
3	D	601	NAP	C5D-O5D-PN-O1N
3	E	601	NAP	C5D-O5D-PN-O1N
3	F	601	NAP	C5D-O5D-PN-O1N
3	A	601	NAP	PA-O3-PN-O5D
3	B	601	NAP	PA-O3-PN-O5D
3	C	601	NAP	PA-O3-PN-O5D
3	D	601	NAP	PA-O3-PN-O5D
3	E	601	NAP	PA-O3-PN-O5D
3	F	601	NAP	PA-O3-PN-O5D
3	A	601	NAP	C2B-O2B-P2B-O1X
3	B	601	NAP	C2B-O2B-P2B-O1X
3	C	601	NAP	C2B-O2B-P2B-O1X
3	D	601	NAP	C2B-O2B-P2B-O1X
3	E	601	NAP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	F	601	NAP	C2B-O2B-P2B-O1X
3	C	601	NAP	C5B-O5B-PA-O3
3	D	601	NAP	C5B-O5B-PA-O3
3	E	601	NAP	C5B-O5B-PA-O3
3	F	601	NAP	C5B-O5B-PA-O3
3	B	601	NAP	C5B-O5B-PA-O2A
3	C	601	NAP	C5B-O5B-PA-O2A
3	D	601	NAP	C5B-O5B-PA-O2A
3	B	601	NAP	O4B-C4B-C5B-O5B
3	E	601	NAP	O4B-C4B-C5B-O5B
3	D	601	NAP	PN-O3-PA-O2A
3	C	601	NAP	O4B-C4B-C5B-O5B
3	F	601	NAP	O4B-C4B-C5B-O5B
3	A	601	NAP	C5B-O5B-PA-O3
3	A	601	NAP	C2B-O2B-P2B-O2X
3	A	601	NAP	C2B-O2B-P2B-O3X
3	B	601	NAP	C2B-O2B-P2B-O2X
3	C	601	NAP	C2B-O2B-P2B-O2X
3	C	601	NAP	C2B-O2B-P2B-O3X
3	D	601	NAP	C2B-O2B-P2B-O2X
3	D	601	NAP	C2B-O2B-P2B-O3X
3	E	601	NAP	C2B-O2B-P2B-O2X
3	E	601	NAP	C2B-O2B-P2B-O3X
3	F	601	NAP	C2B-O2B-P2B-O2X
3	A	601	NAP	O4B-C4B-C5B-O5B
3	D	601	NAP	O4B-C4B-C5B-O5B
3	B	601	NAP	PN-O3-PA-O1A
3	C	601	NAP	PN-O3-PA-O2A
3	E	601	NAP	PN-O3-PA-O1A
3	F	601	NAP	PN-O3-PA-O1A
3	E	601	NAP	C5B-O5B-PA-O2A

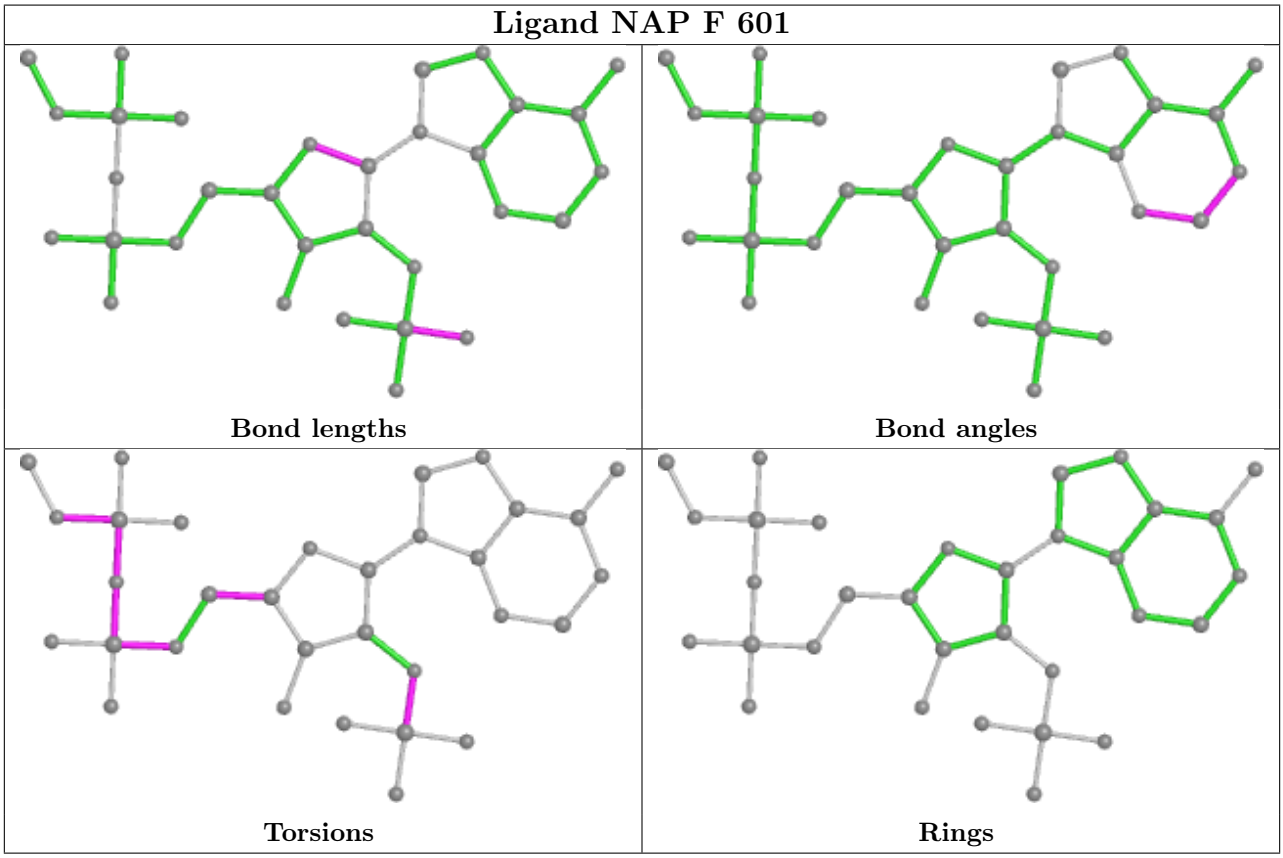
There are no ring outliers.

6 monomers are involved in 7 short contacts:

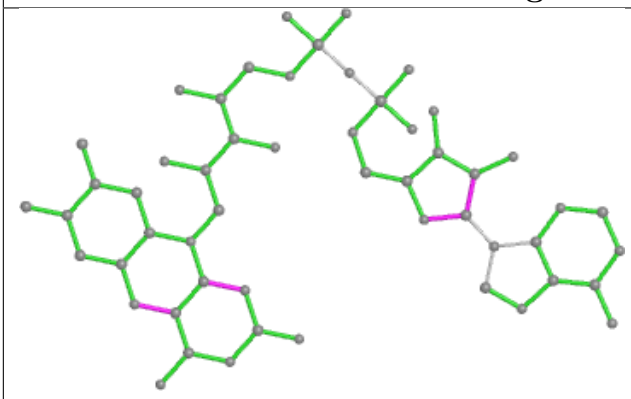
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	601	NAP	1	0
3	E	601	NAP	1	0
3	A	601	NAP	1	0
3	C	601	NAP	1	0
3	B	601	NAP	2	0
3	D	601	NAP	1	0

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

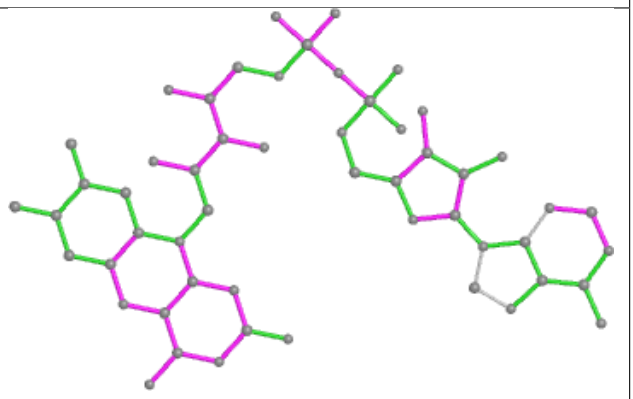
Ligand NAP F 601



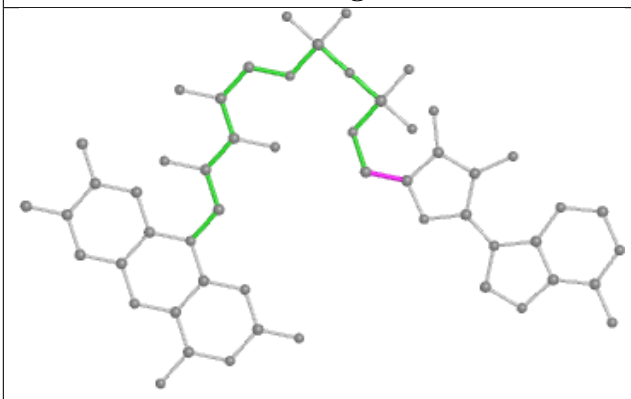
Ligand FAD E 600



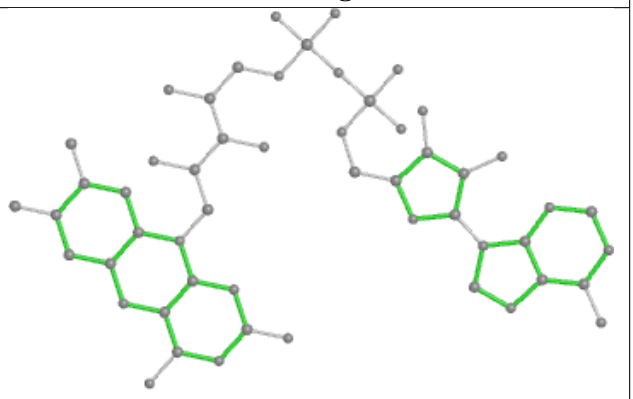
Bond lengths



Bond angles

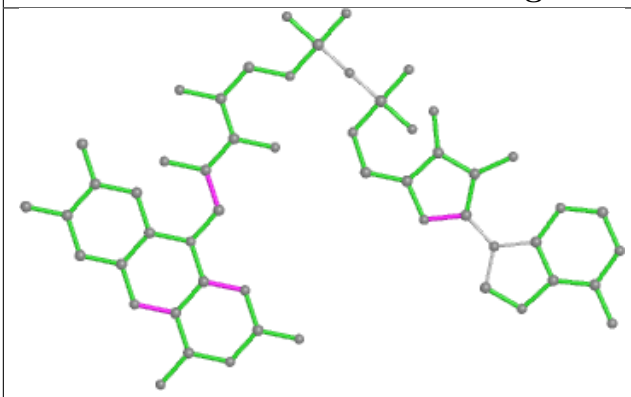


Torsions

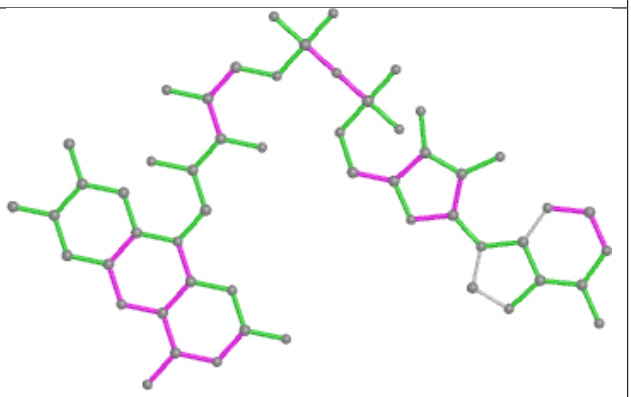


Rings

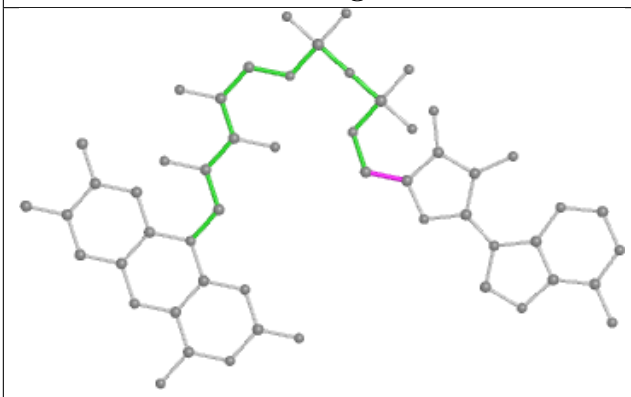
Ligand FAD C 600



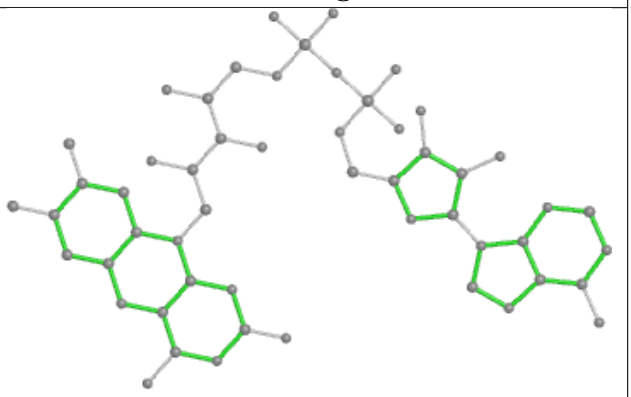
Bond lengths



Bond angles

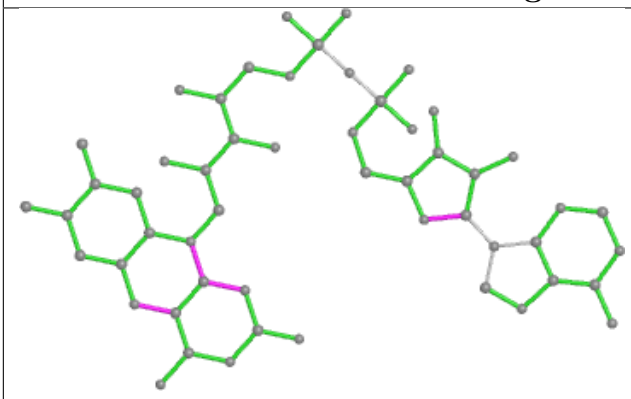


Torsions

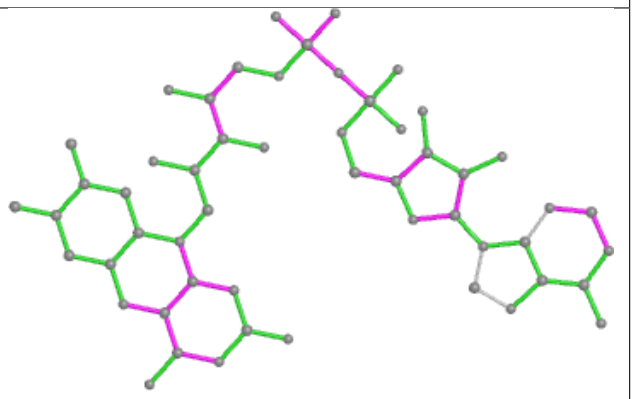


Rings

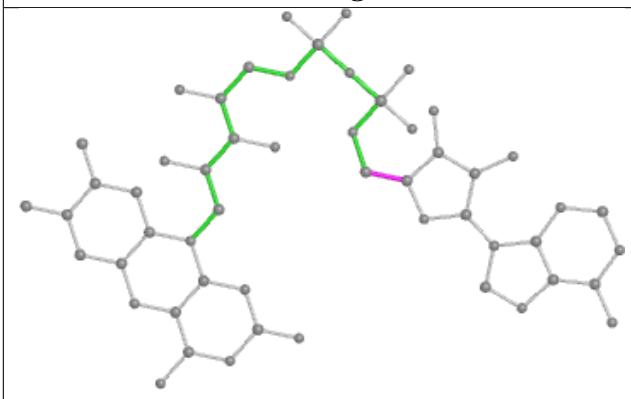
Ligand FAD A 600



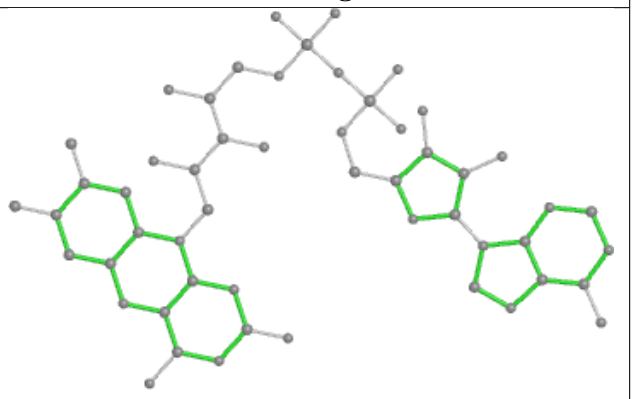
Bond lengths



Bond angles

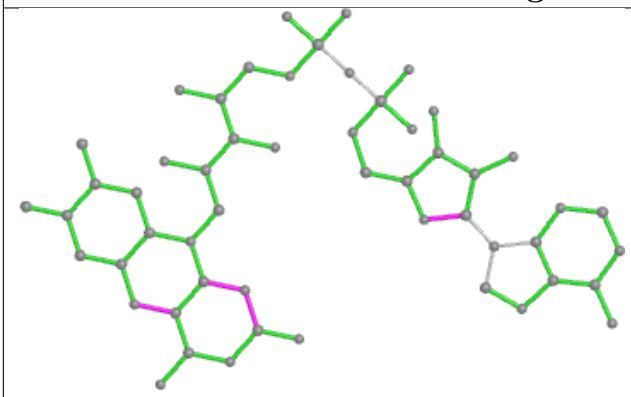


Torsions

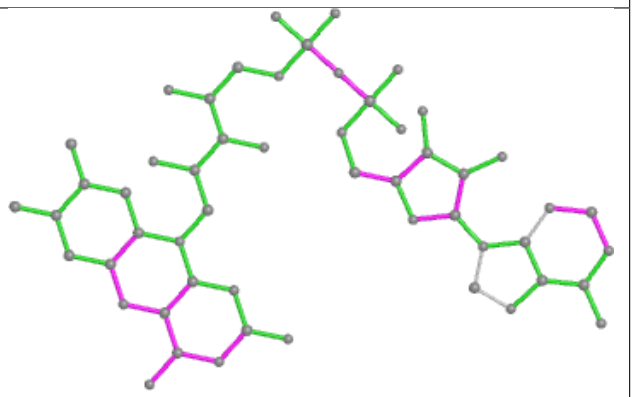


Rings

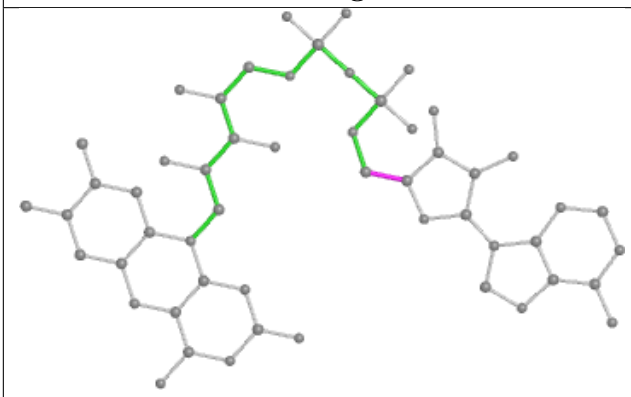
Ligand FAD F 600



Bond lengths



Bond angles



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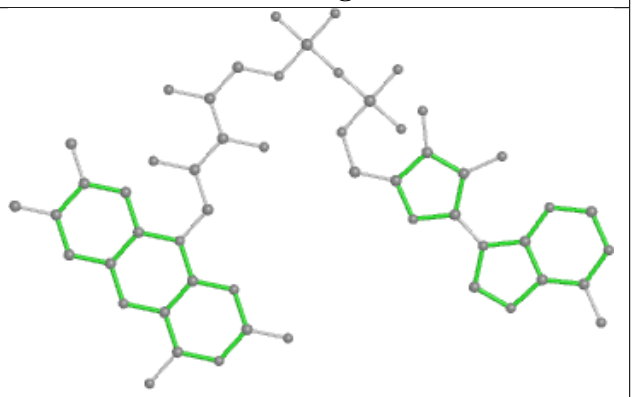
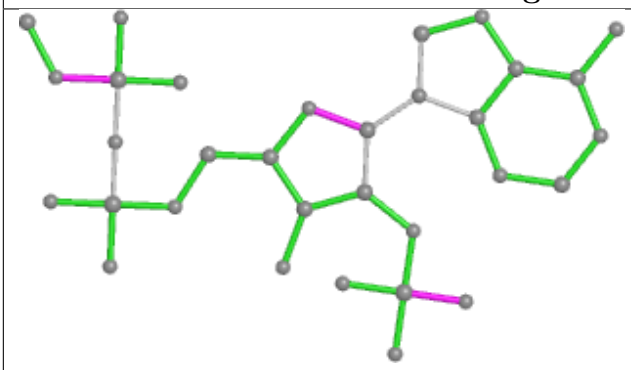
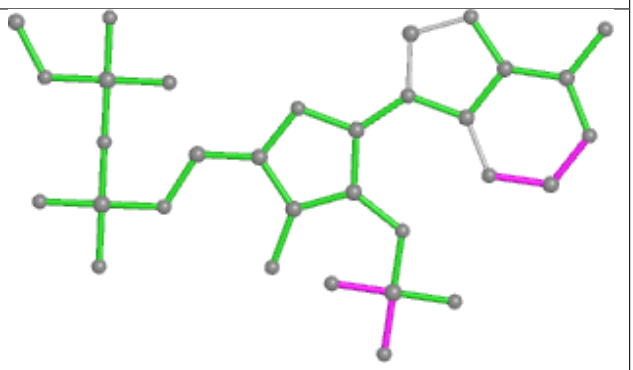


Rings

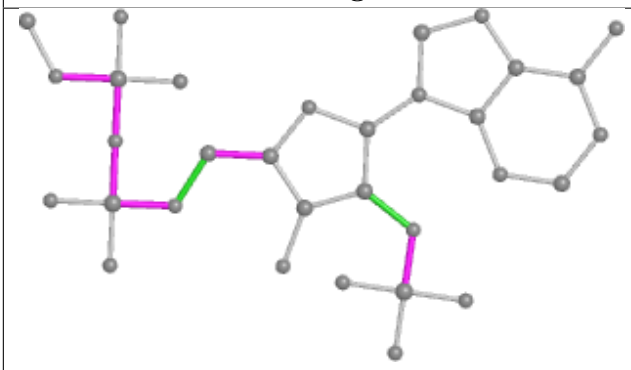
Ligand NAP E 601



Bond lengths



Bond angles



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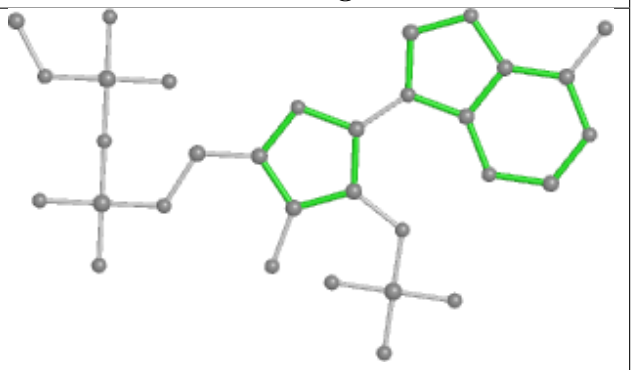
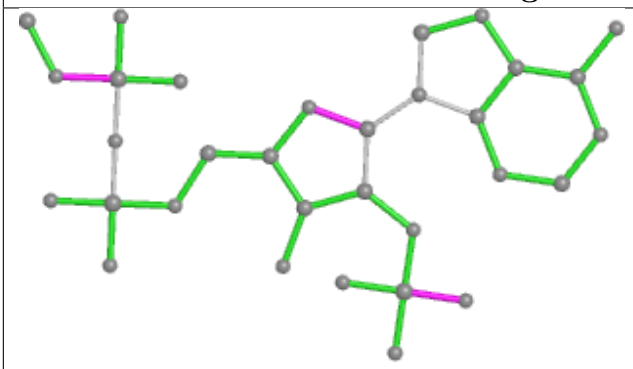
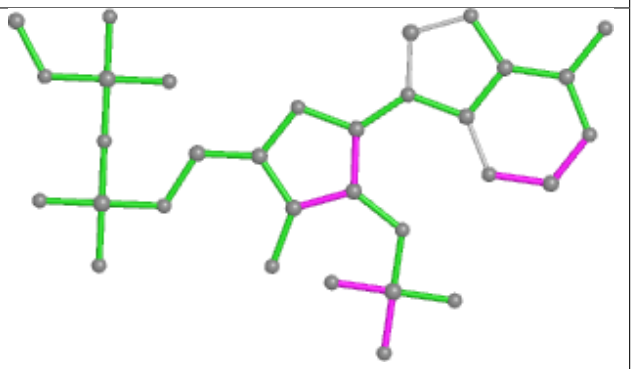


Rings

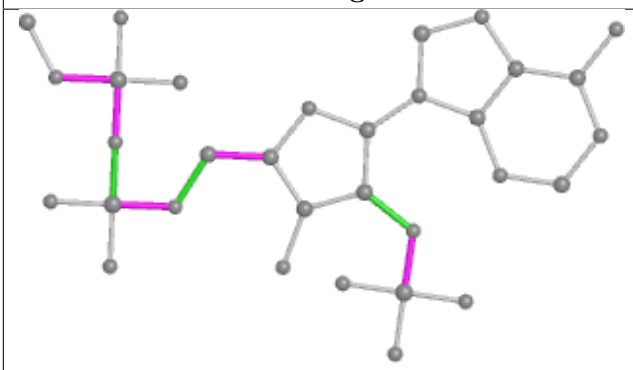
Ligand NAP A 601



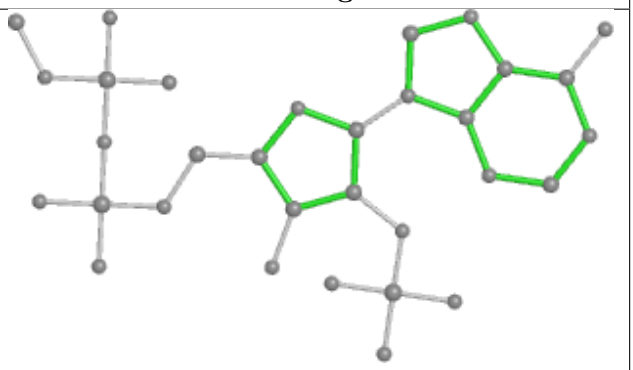
Bond lengths



Bond angles

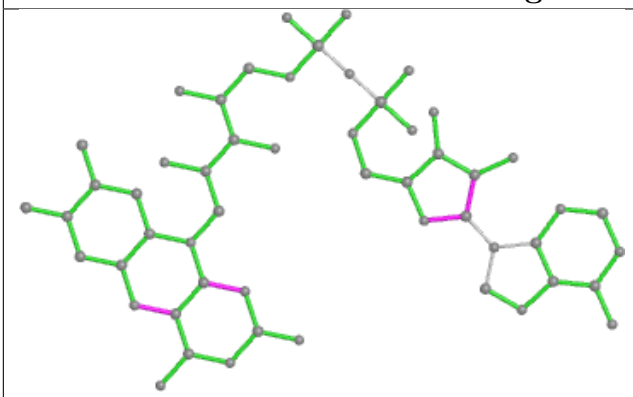


Torsions



Rings

Ligand FAD B 600



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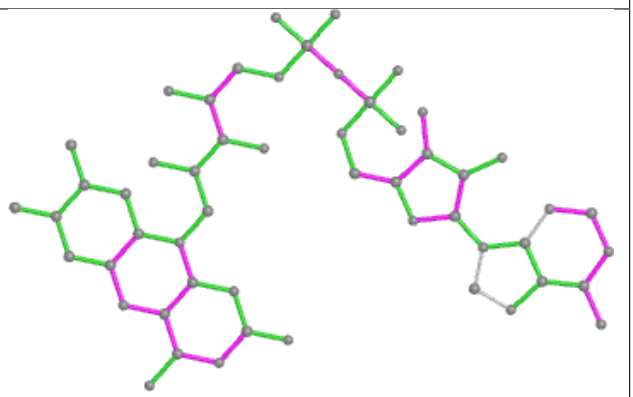
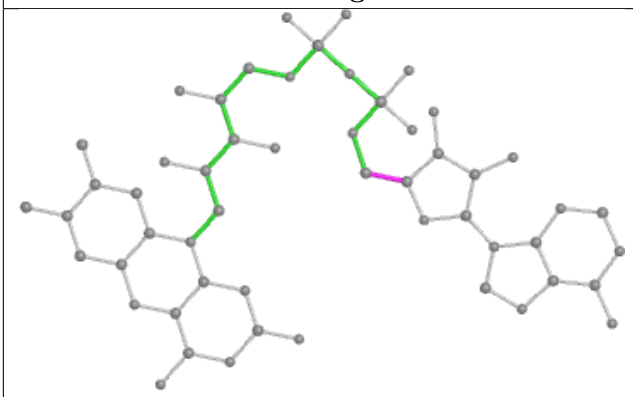


Bond angles



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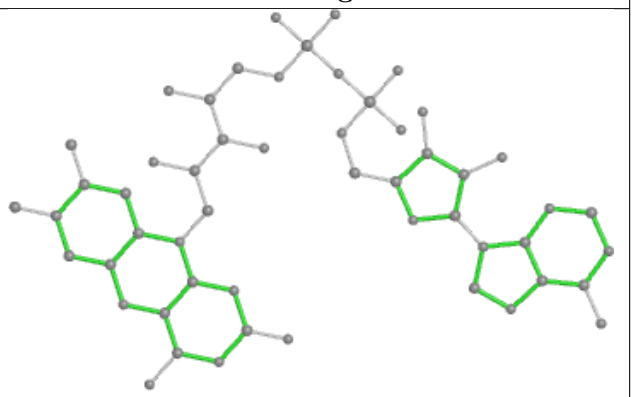
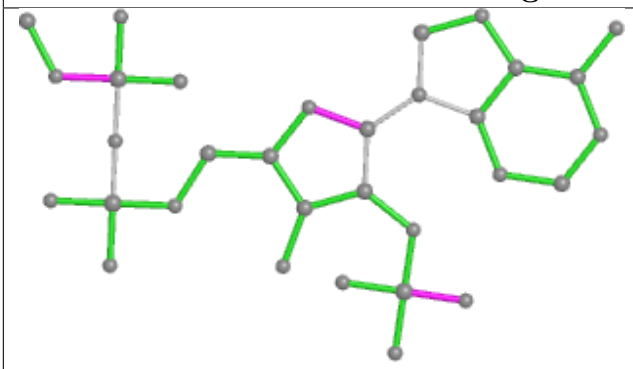
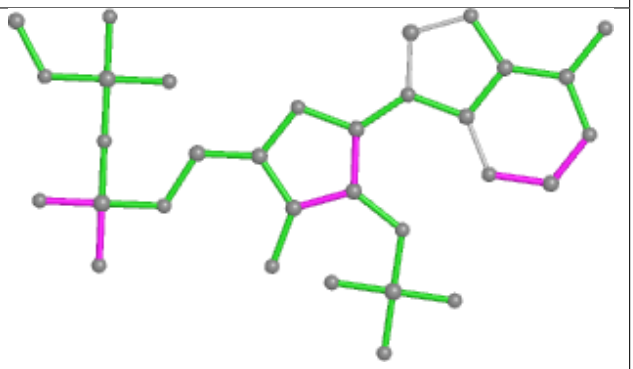


Rings

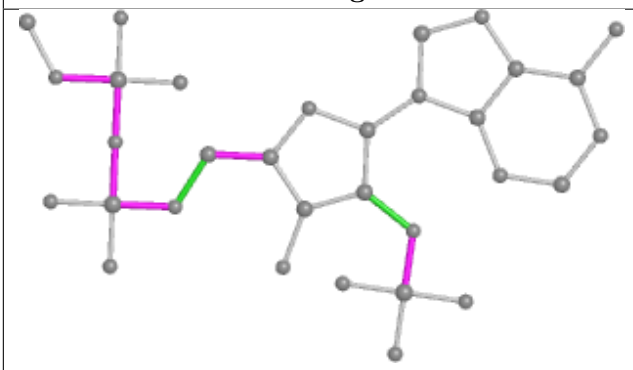
Ligand NAP C 601



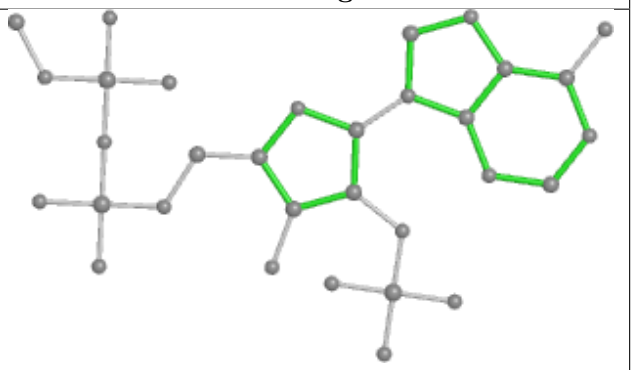
Bond lengths



Bond angles

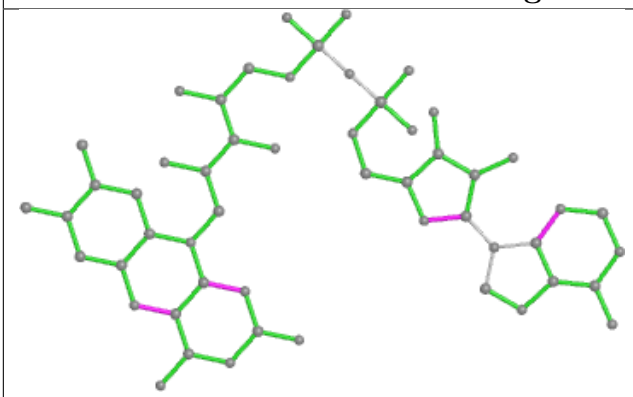


Torsions

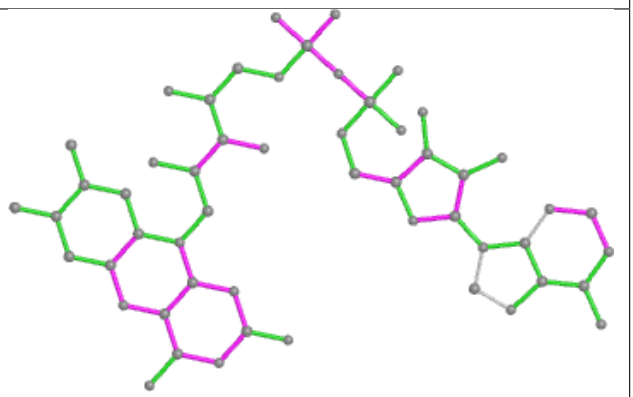


Rings

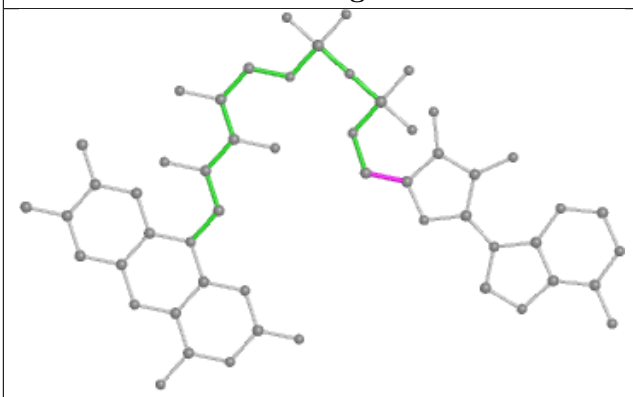
Ligand FAD D 600



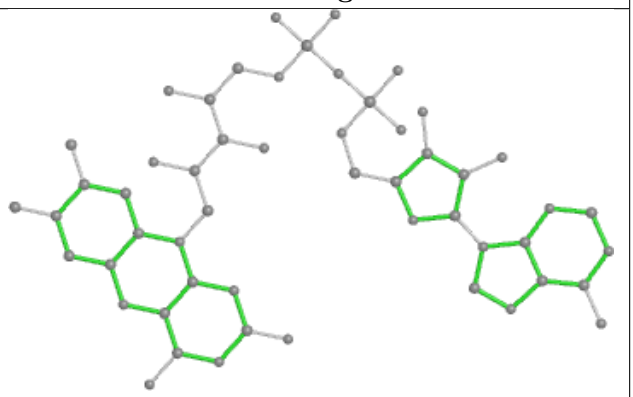
Bond lengths



Bond angles

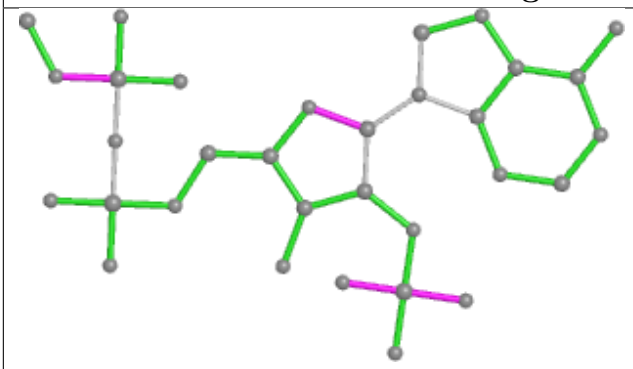


Torsions

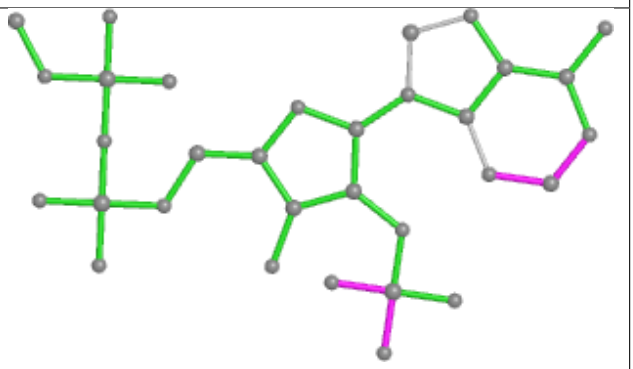


Rings

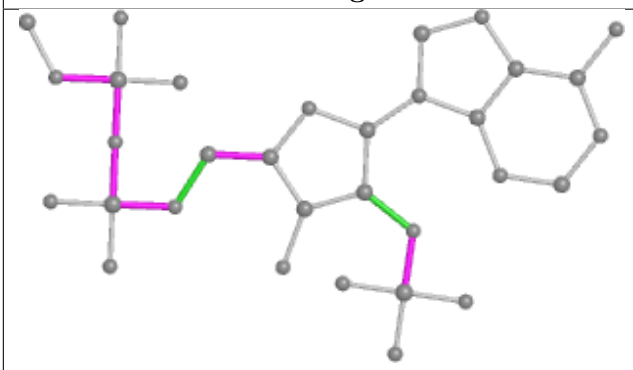
Ligand NAP B 601



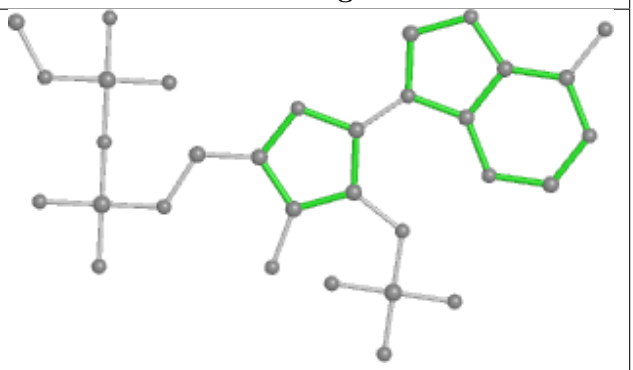
Bond lengths



Bond angles

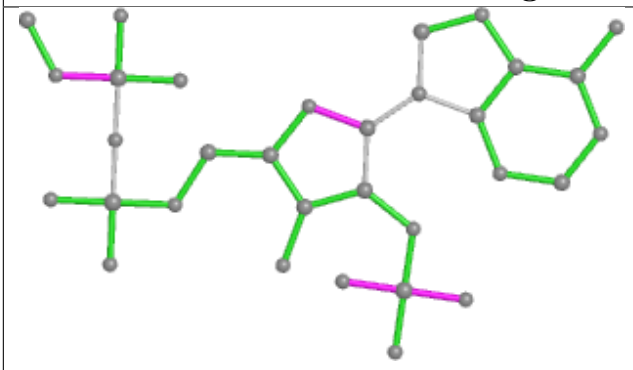


Torsions

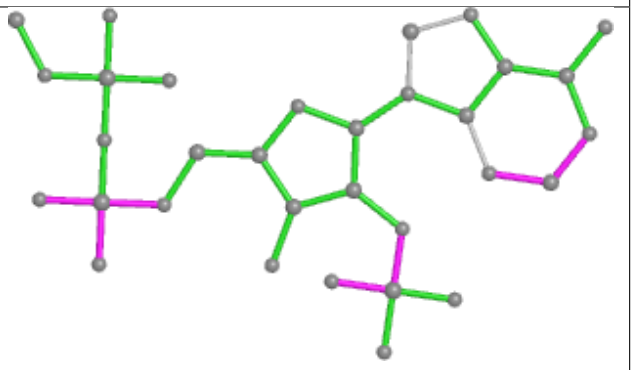


Rings

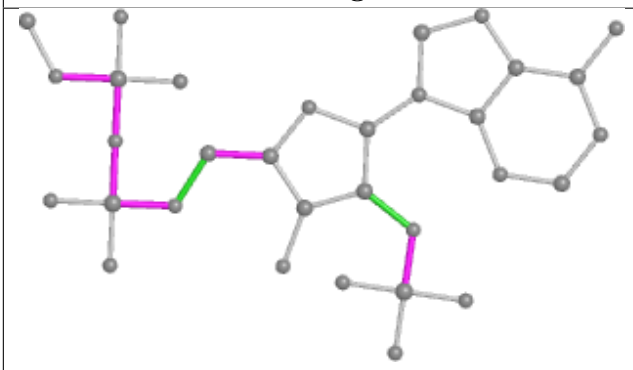
Ligand NAP D 601



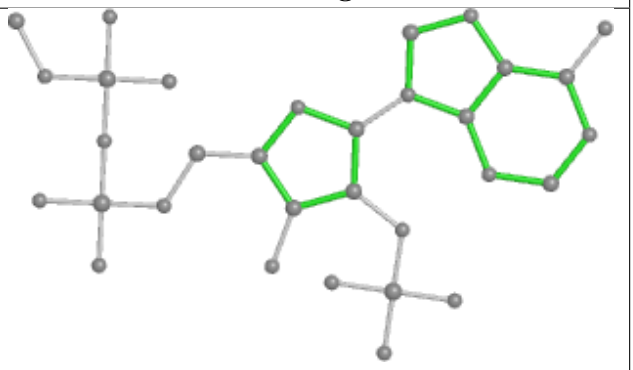
Bond lengths



Bond angles



Torsions



Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

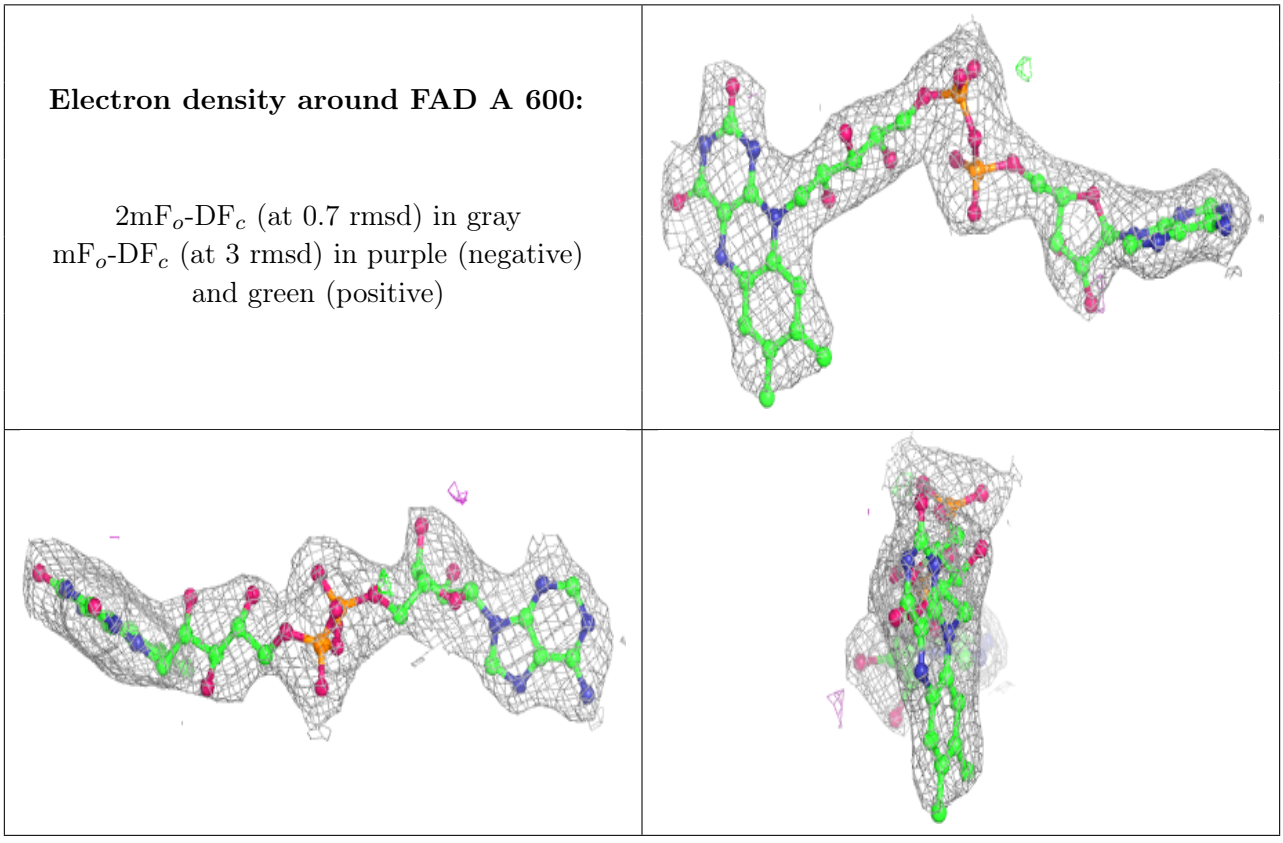
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

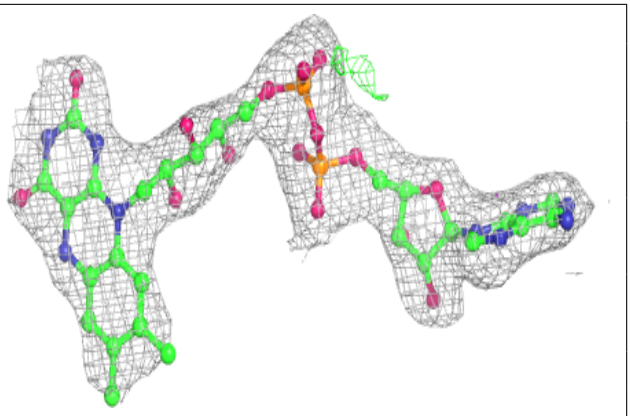
Electron density around FAD A 600:

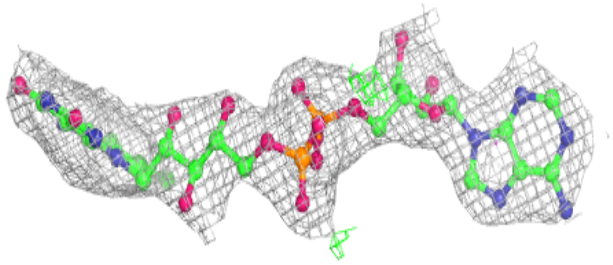
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

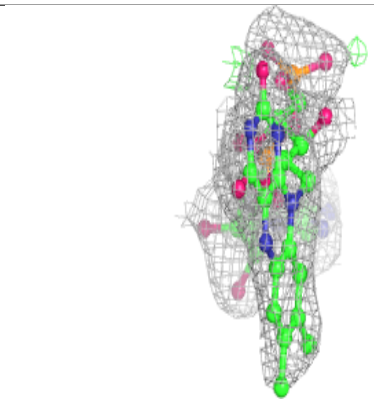


Electron density around FAD B 600:

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

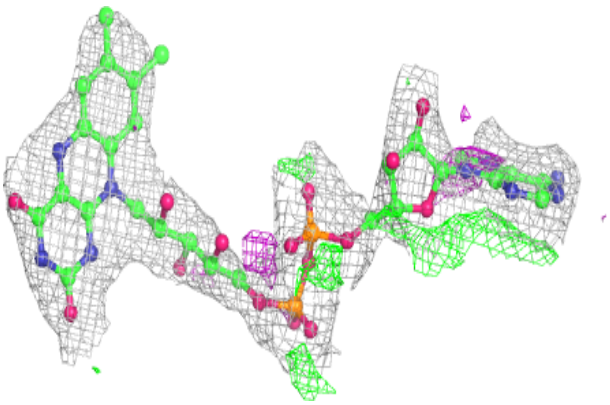


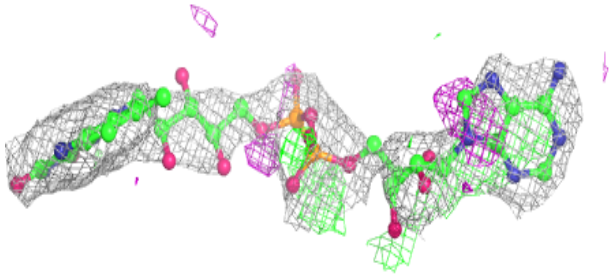


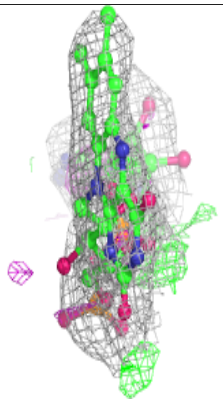


Electron density around FAD C 600:

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

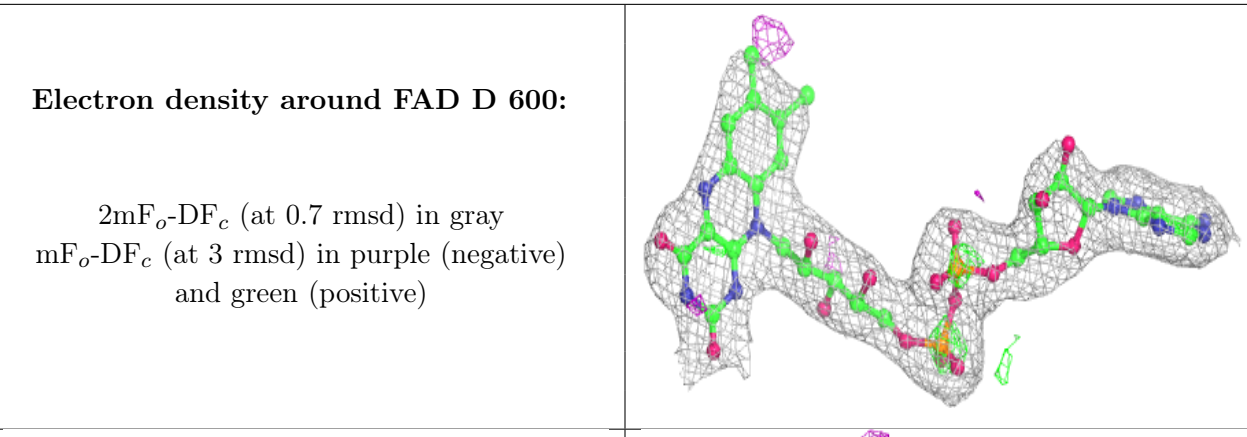






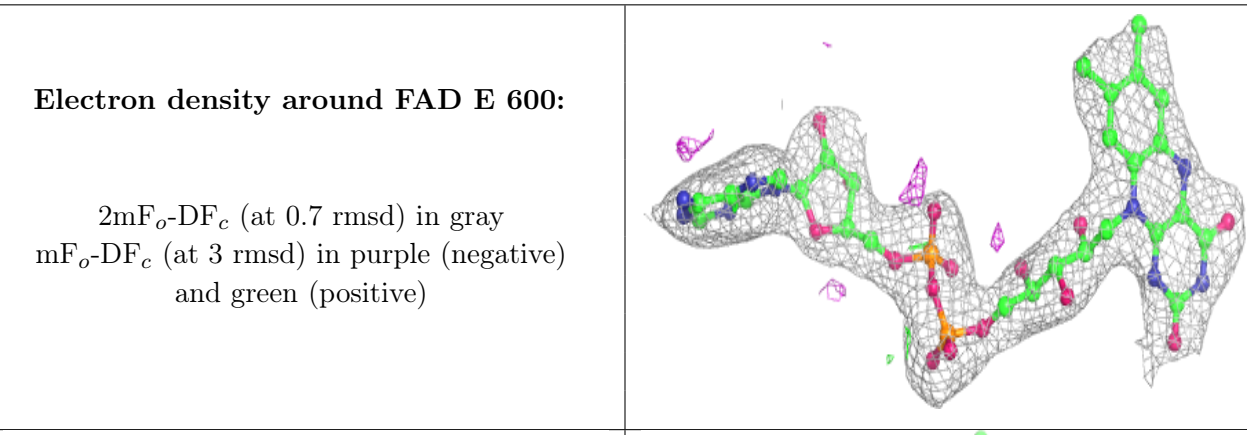
Electron density around FAD D 600:

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



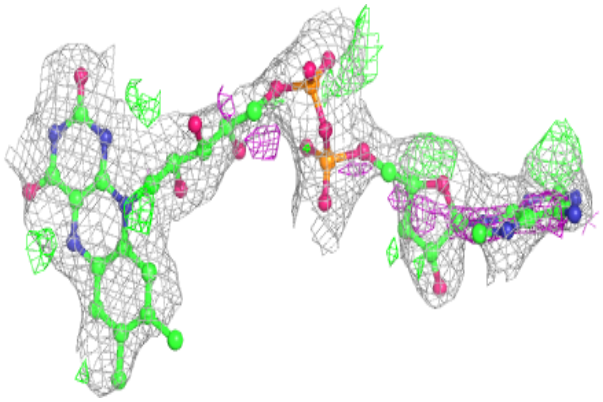
Electron density around FAD E 600:

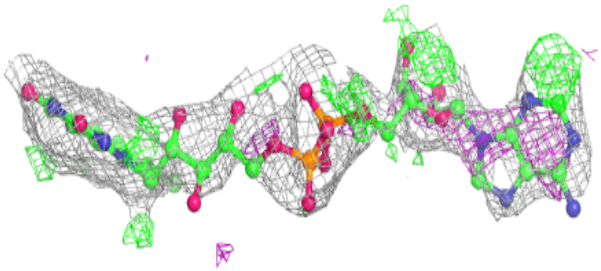
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

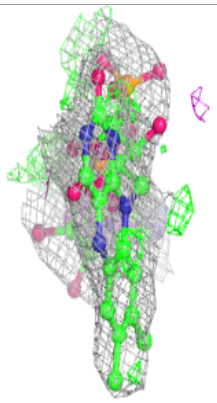


Electron density around FAD F 600:

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

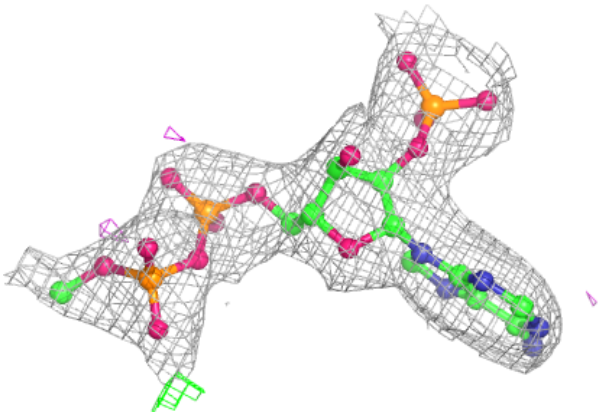


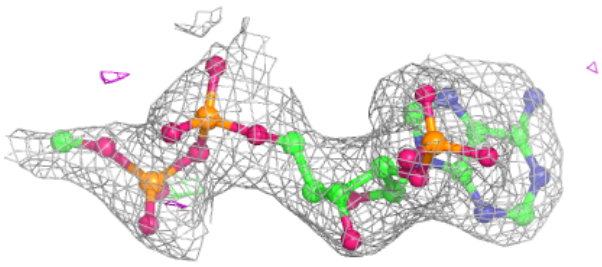


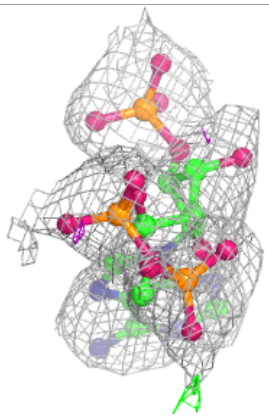


Electron density around NAP A 601:

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

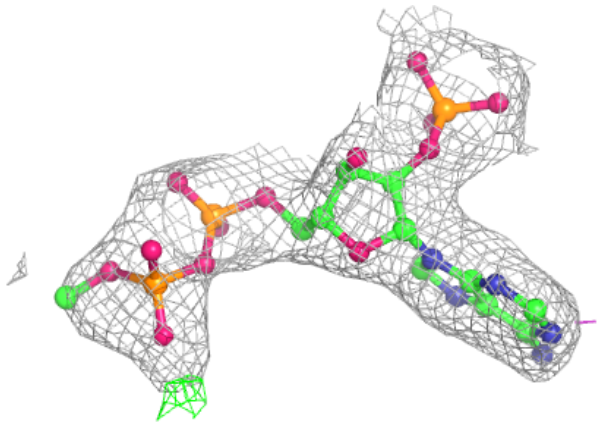


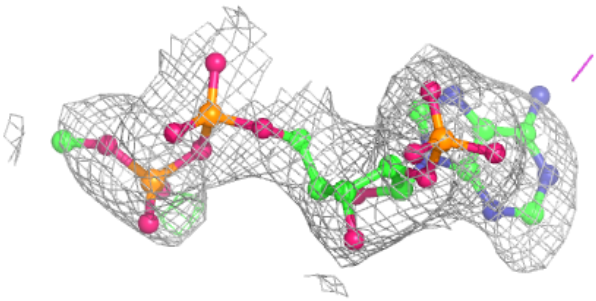


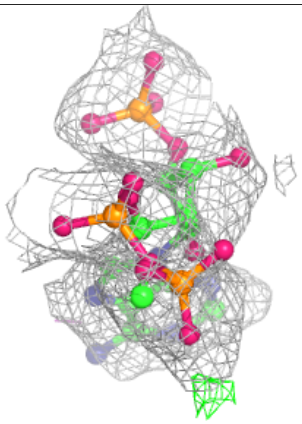


Electron density around NAP B 601:

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

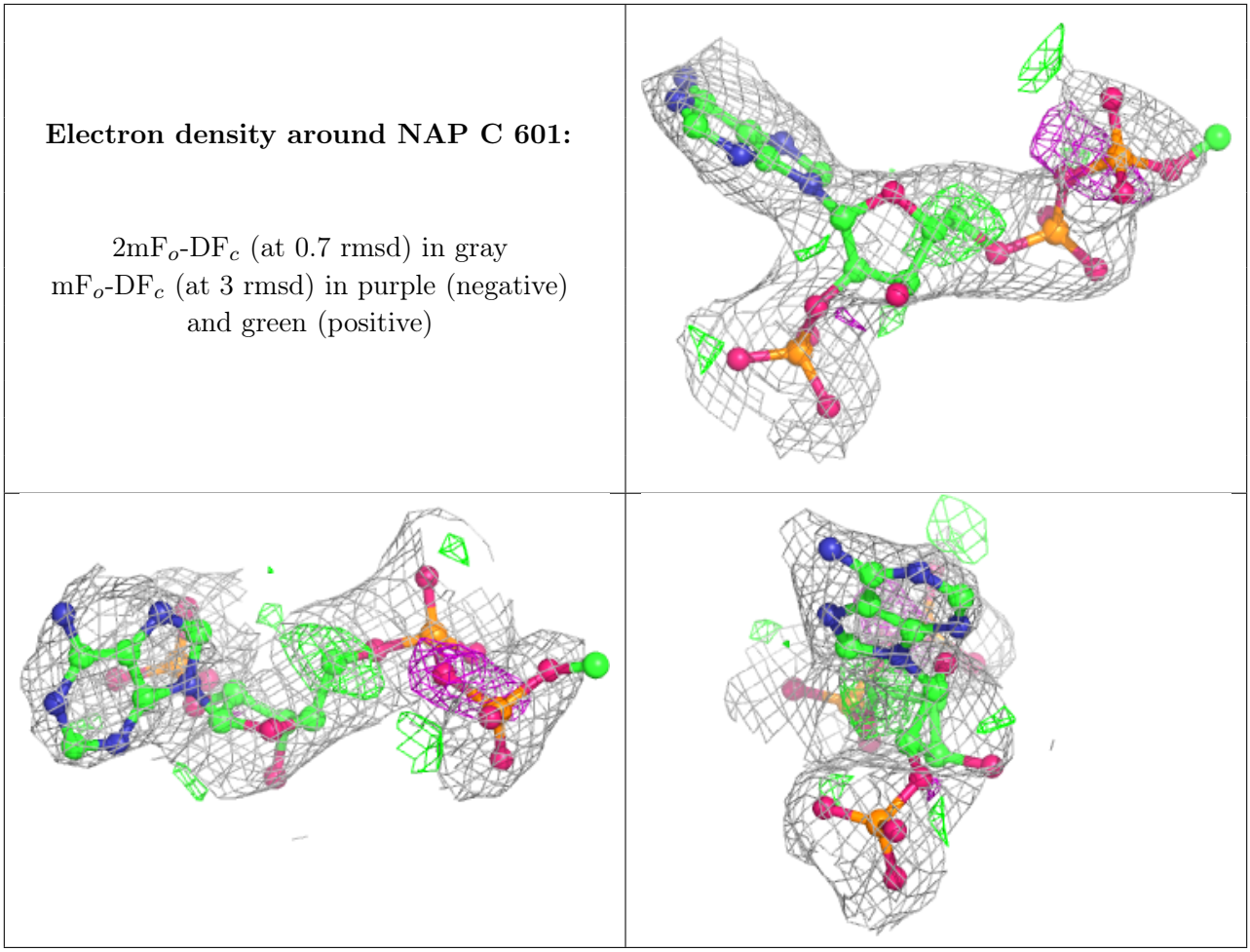






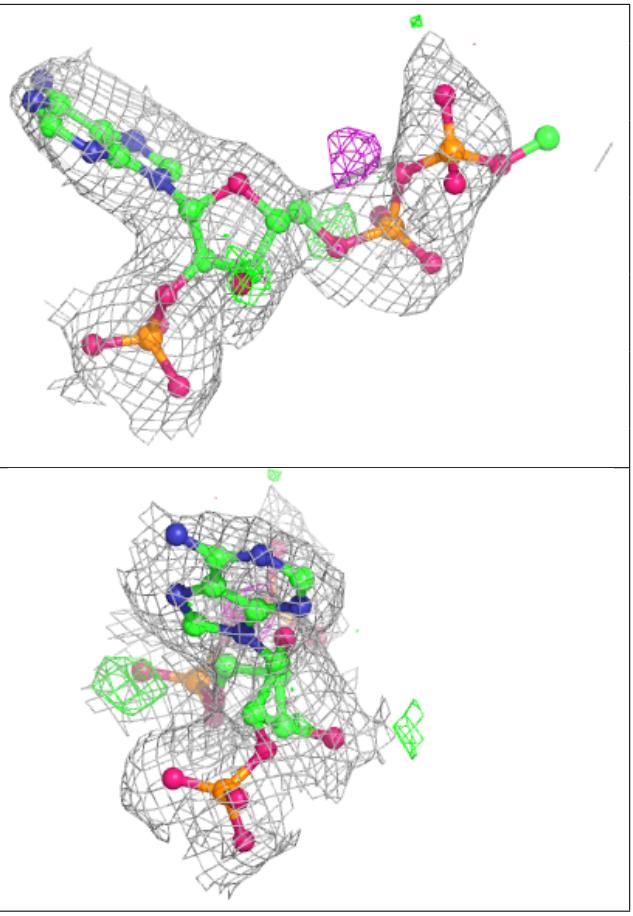
Electron density around NAP C 601:

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



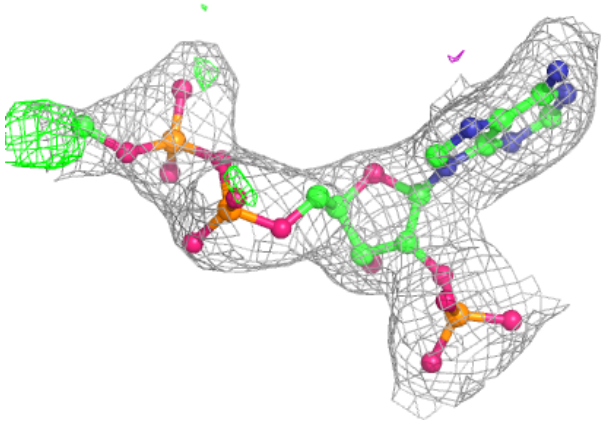
Electron density around NAP D 601:

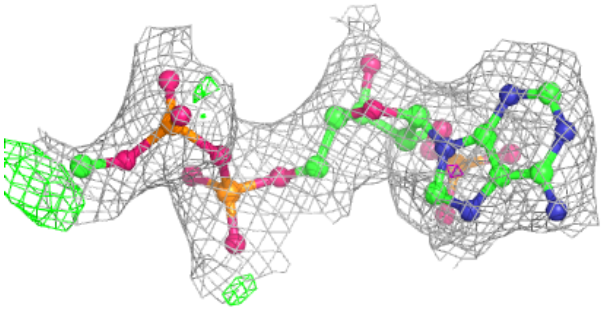
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

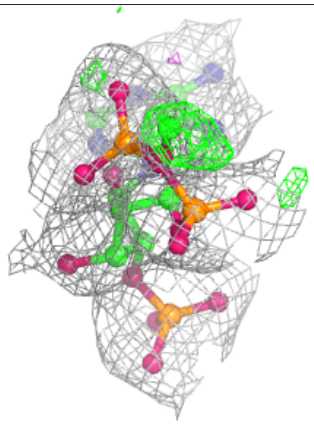


Electron density around NAP E 601:

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

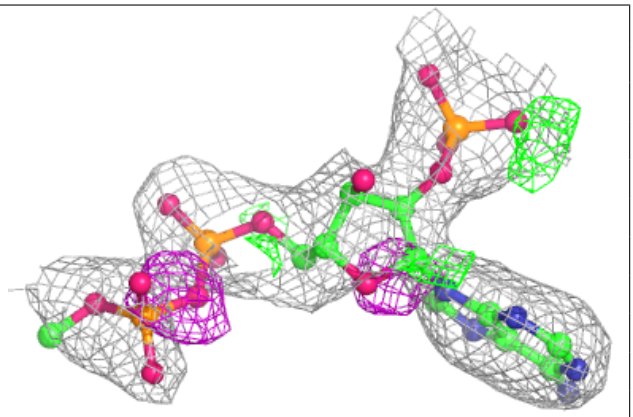


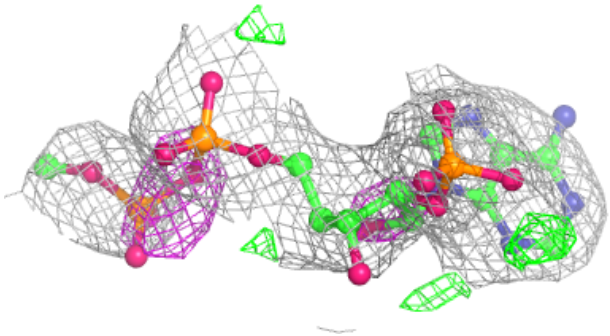


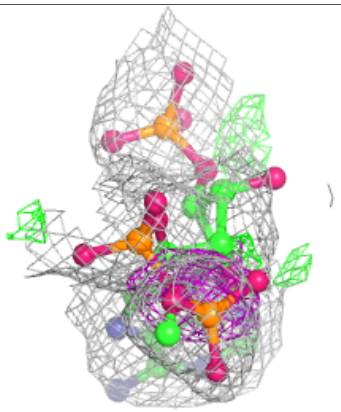


Electron density around NAP F 601:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.