Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 04:27 AM EDT

PDB ID	:	3EAO
Title	:	Crystal structure of recombinant rat selenoprotein thioredoxin reductase 1 with oxidized C-terminal tail
Authors	:	Sandalova, T.; Cheng, Q.; Lindqvist, Y.; Arner, E.
Deposited on	:	2008-08-26
Resolution	:	3.10 Å(reported)

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

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

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

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

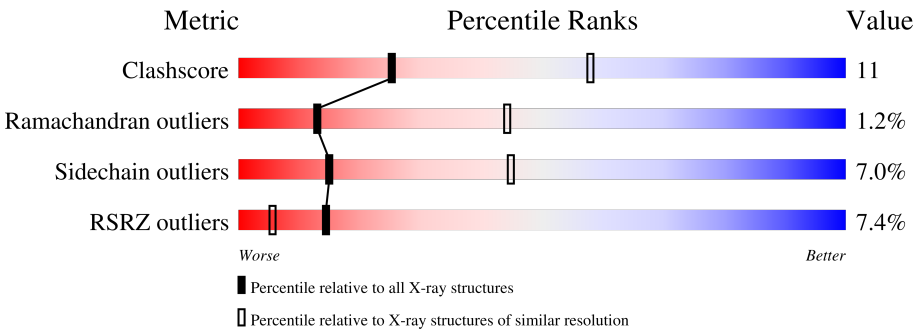
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	499	6% 74% 22% • • •
1	B	499	5% 76% 20% • • •
1	C	499	6% 72% 22% • • •
1	D	499	% 73% 22% • • •
1	E	499	4% 75% 21% • • •
1	F	499	23% 68% 27% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	F	601	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23114 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, cytoplasmic.

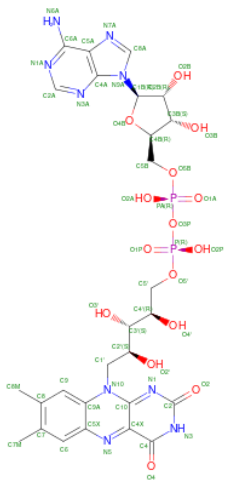
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	489	3762	2390	636	714	21	1	0	0	0
1	B	490	3768	2393	637	716	21	1	0	0	0
1	C	486	3731	2368	633	708	21	1	0	0	0
1	D	491	3777	2399	639	717	21	1	0	0	0
1	E	490	3768	2393	637	716	21	1	0	0	0
1	F	489	3762	2390	636	714	21	1	0	0	0

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: $C_{27}H_{33}N_9O_{15}P_2$).

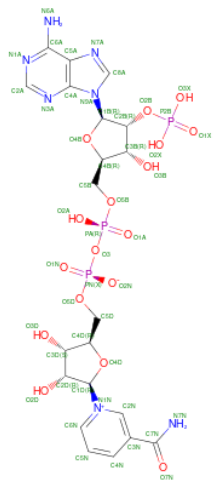
FAD



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

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

NAP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	32	11	5	13	3	0	0
3	B	1	32	11	5	13	3	0	0
3	C	1	32	11	5	13	3	0	0
3	D	1	32	11	5	13	3	0	0
3	E	1	32	11	5	13	3	0	0
3	F	1	32	11	5	13	3	0	0

- Molecule 4 is water.

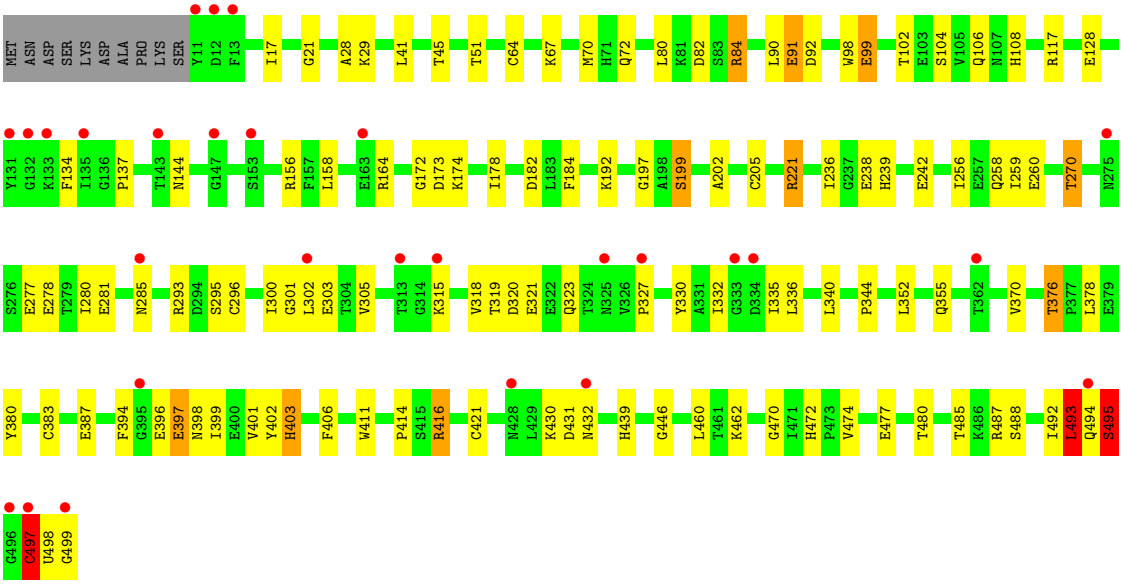
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	3	3	3	0	0
4	B	8	8	8	0	0
4	C	5	5	5	0	0
4	D	11	11	11	0	0
4	E	4	4	4	0	0
4	F	5	5	5	0	0

3 Residue-property plots (i)

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

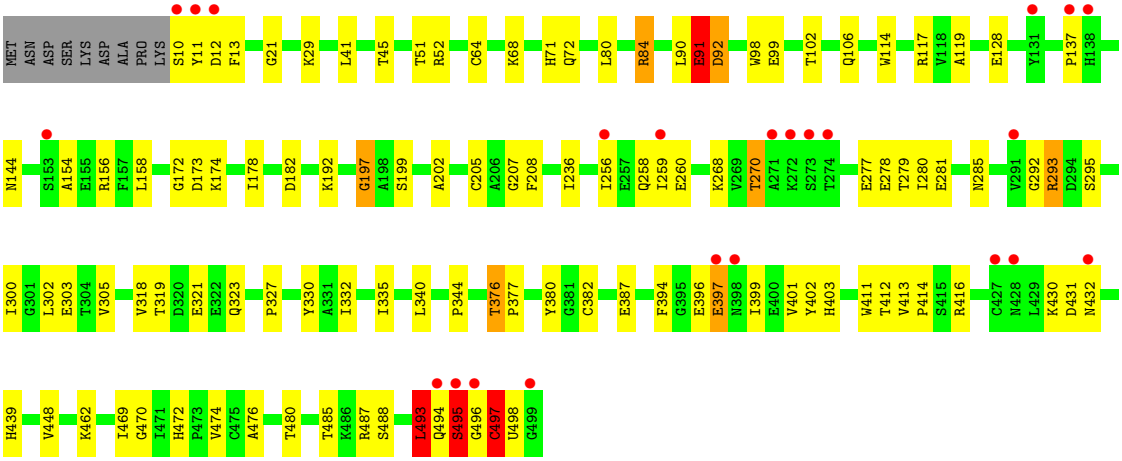
• Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain A:



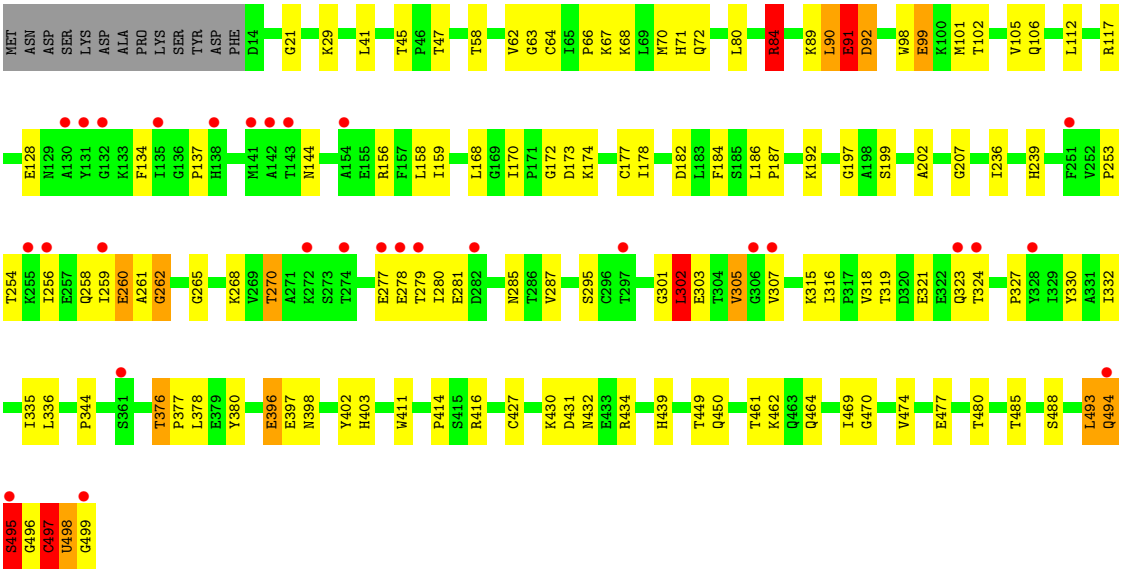
• Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain B:



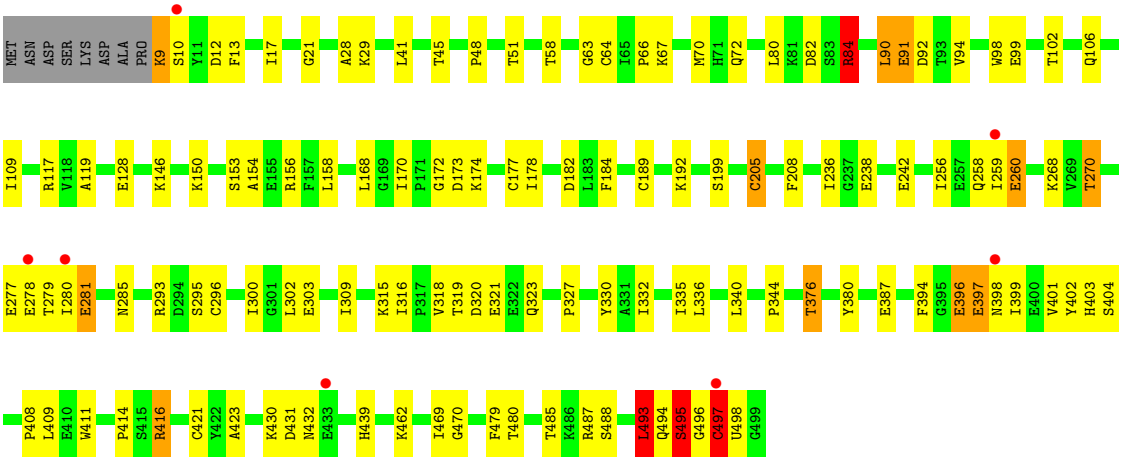
• Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain C:



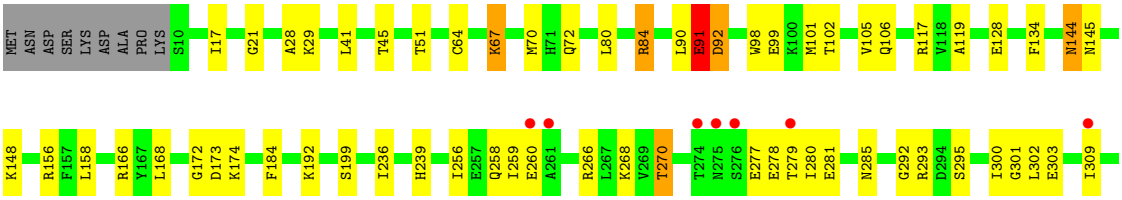
• Molecule 1: Thioredoxin reductase 1, cytoplasmic

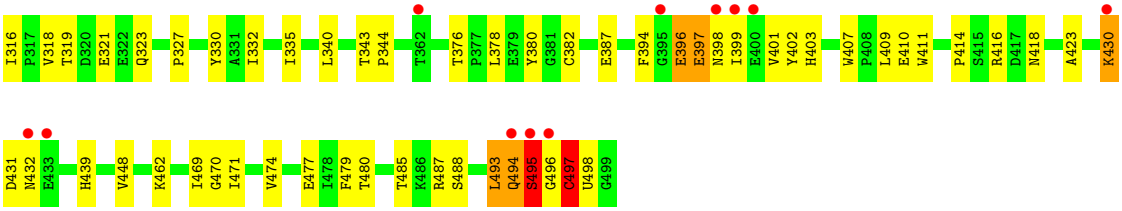
Chain D:



• Molecule 1: Thioredoxin reductase 1, cytoplasmic

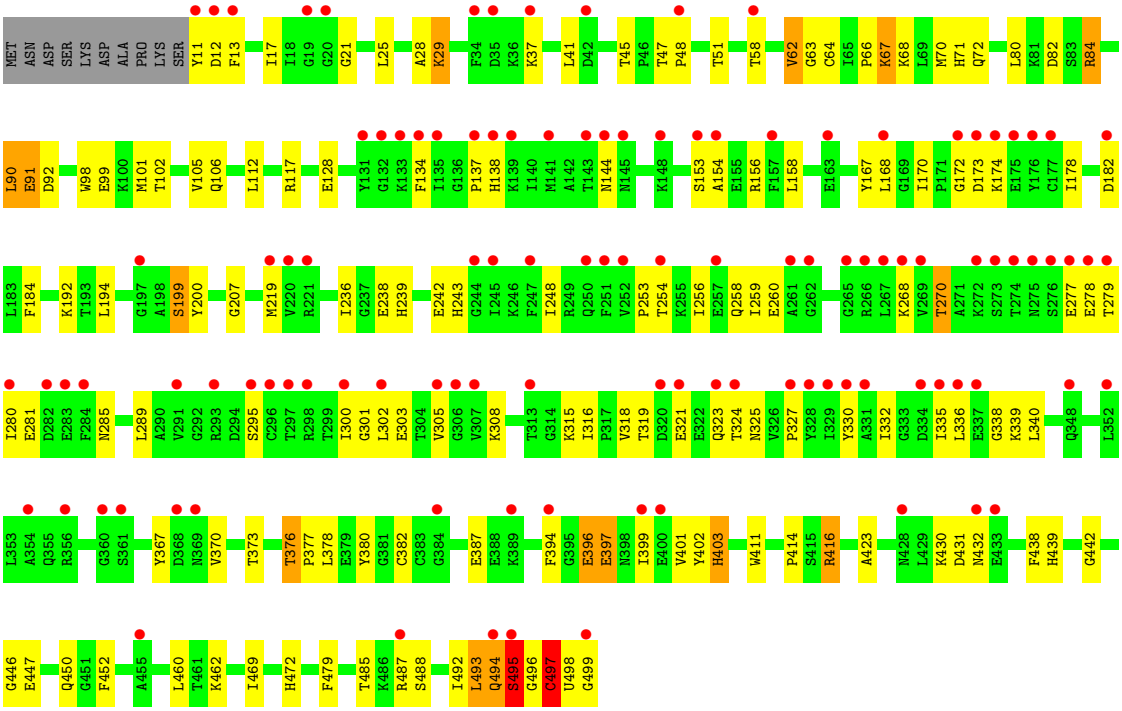
Chain E:





• Molecule 1: Thioredoxin reductase 1, cytoplasmic

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	78.23Å 137.75Å 168.95Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 64.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-3.10) 99.3 (64.35-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.256 , 0.289 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	23114	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.66	2/3829 (0.1%)	0.77	5/5177 (0.1%)
1	B	0.64	1/3835 (0.0%)	0.72	2/5185 (0.0%)
1	C	0.70	0/3796	0.80	6/5132 (0.1%)
1	D	0.69	5/3844 (0.1%)	0.76	4/5196 (0.1%)
1	E	0.67	0/3835	0.72	3/5185 (0.1%)
1	F	0.87	1/3829 (0.0%)	0.76	3/5177 (0.1%)
All	All	0.71	9/22968 (0.0%)	0.76	23/31052 (0.1%)

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	A	0	1
1	B	0	4
1	C	0	6
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	16

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	205	CYS	CB-SG	-6.33	1.71	1.82
1	D	189	CYS	CB-SG	-6.30	1.71	1.82
1	A	497	CYS	CB-SG	6.15	1.92	1.82
1	D	296	CYS	CB-SG	-5.33	1.73	1.81
1	F	497	CYS	CB-SG	5.33	1.91	1.82
1	D	421	CYS	CB-SG	-5.25	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	TRP	CB-CG	5.24	1.59	1.50
1	D	177	CYS	CB-SG	-5.06	1.73	1.81
1	A	205	CYS	CB-SG	-5.02	1.73	1.81

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	ARG	NE-CZ-NH2	15.57	128.08	120.30
1	D	84	ARG	NE-CZ-NH1	-15.24	112.68	120.30
1	A	221	ARG	NE-CZ-NH2	14.32	127.46	120.30
1	A	221	ARG	NE-CZ-NH1	-14.06	113.27	120.30
1	C	84	ARG	NE-CZ-NH1	-13.93	113.34	120.30
1	D	84	ARG	NE-CZ-NH2	13.05	126.82	120.30
1	B	84	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	E	84	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	C	84	ARG	CD-NE-CZ	8.79	135.90	123.60
1	B	84	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	F	84	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	D	84	ARG	CD-NE-CZ	7.86	134.61	123.60
1	E	84	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	84	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	84	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	F	84	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	221	ARG	CD-NE-CZ	5.66	131.52	123.60
1	C	262	GLY	N-CA-C	5.53	126.92	113.10
1	C	302	LEU	CB-CG-CD1	5.30	120.01	111.00
1	D	493	LEU	CB-CG-CD2	5.27	119.96	111.00
1	F	494	GLN	N-CA-CB	-5.21	101.23	110.60
1	E	494	GLN	N-CA-CB	-5.15	101.33	110.60
1	C	494	GLN	N-CA-CB	-5.10	101.42	110.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	493	LEU	Peptide
1	B	10	SER	Peptide
1	B	197	GLY	Peptide
1	B	493	LEU	Peptide
1	B	91	GLU	Peptide
1	C	260	GLU	Peptide
1	C	261	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	C	493	LEU	Peptide
1	C	497	CYS	Peptide
1	C	498	SEC	Peptide
1	C	91	GLU	Peptide
1	D	260	GLU	Peptide
1	D	281	GLU	Peptide
1	D	493	LEU	Peptide
1	E	493	LEU	Peptide
1	F	493	LEU	Peptide

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	3762	0	3761	86	0
1	B	3768	0	3767	73	0
1	C	3731	0	3740	90	0
1	D	3777	0	3779	89	0
1	E	3768	0	3766	87	0
1	F	3762	0	3761	111	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
2	E	53	0	31	1	0
2	F	53	0	31	1	0
3	A	32	0	11	2	0
3	B	32	0	11	0	0
3	C	32	0	11	0	0
3	D	32	0	11	0	0
3	E	32	0	11	0	0
3	F	32	0	11	0	0
4	A	3	0	0	0	0
4	B	8	0	0	0	0
4	C	5	0	0	0	0
4	D	11	0	0	0	0
4	E	4	0	0	0	0
4	F	5	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23114	0	22826	492	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 (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:CYS:SG	1:B:498:SEC:SE	2.55	1.15
1:A:493:LEU:HB3	1:A:494:GLN:HB2	1.23	1.11
1:B:197:GLY:O	1:B:202:ALA:HB1	1.55	1.06
1:F:248:ILE:HA	4:F:602:HOH:O	1.56	1.04
1:E:493:LEU:HB3	1:E:494:GLN:HB2	1.45	0.99
1:F:493:LEU:HB3	1:F:494:GLN:HB2	1.42	0.99
1:C:493:LEU:HB3	1:C:494:GLN:HB2	1.45	0.98
1:A:197:GLY:O	1:A:202:ALA:HB1	1.66	0.94
1:E:91:GLU:CD	1:E:92:ASP:H	1.72	0.93
1:B:197:GLY:O	1:B:202:ALA:CB	2.19	0.90
1:D:493:LEU:CB	1:D:494:GLN:HB2	2.04	0.86
1:A:493:LEU:HB3	1:A:494:GLN:CB	2.06	0.85
1:C:497:CYS:SG	1:C:498:SEC:SE	2.85	0.84
1:C:91:GLU:CD	1:C:92:ASP:H	1.82	0.83
1:B:91:GLU:CD	1:B:92:ASP:H	1.82	0.82
1:C:262:GLY:HA3	1:C:265:GLY:HA2	1.62	0.82
1:B:493:LEU:CB	1:B:494:GLN:HB2	2.09	0.82
1:F:338:GLY:HA2	4:F:603:HOH:O	1.79	0.81
1:F:13:PHE:HD1	1:F:37:LYS:HB3	1.46	0.80
1:F:494:GLN:HA	1:F:495:SER:HB2	1.61	0.80
1:D:258:GLN:HG3	1:D:260:GLU:O	1.81	0.80
1:E:258:GLN:HG3	1:E:260:GLU:O	1.83	0.79
1:A:499:GLY:HA2	1:B:119:ALA:HB1	1.66	0.78
1:D:493:LEU:HB3	1:D:494:GLN:HB2	1.65	0.78
1:A:84:ARG:NH2	1:A:91:GLU:O	2.17	0.78
1:E:494:GLN:HA	1:E:495:SER:HB2	1.66	0.77
1:E:494:GLN:CA	1:E:495:SER:HB2	2.14	0.77
1:F:258:GLN:HG3	1:F:260:GLU:O	1.83	0.77
1:A:197:GLY:O	1:A:202:ALA:CB	2.33	0.77
1:C:258:GLN:HG3	1:C:260:GLU:O	1.85	0.77
1:D:494:GLN:N	1:D:495:SER:HB2	2.00	0.76
1:F:494:GLN:CA	1:F:495:SER:HB2	2.15	0.76
1:C:494:GLN:HA	1:C:495:SER:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLN:OE1	1:C:260:GLU:O	2.05	0.75
1:B:494:GLN:N	1:B:495:SER:HB2	2.01	0.75
1:D:258:GLN:OE1	1:D:260:GLU:O	2.04	0.75
1:C:89:LYS:O	1:D:94:VAL:HG13	1.87	0.75
1:C:494:GLN:CA	1:C:495:SER:HB2	2.18	0.74
1:E:258:GLN:OE1	1:E:260:GLU:O	2.06	0.74
1:A:494:GLN:N	1:A:495:SER:HB2	2.02	0.73
1:D:494:GLN:CA	1:D:495:SER:HB2	2.17	0.73
1:D:158:LEU:HD11	1:D:332:ILE:HG12	1.70	0.73
1:E:158:LEU:HD11	1:E:332:ILE:HG12	1.71	0.73
1:A:493:LEU:CB	1:A:494:GLN:HB2	2.13	0.72
1:A:494:GLN:CA	1:A:495:SER:HB2	2.19	0.72
1:C:158:LEU:HD11	1:C:332:ILE:HG12	1.71	0.72
1:F:13:PHE:CD1	1:F:37:LYS:HB3	2.25	0.72
1:B:158:LEU:HD11	1:B:332:ILE:HG12	1.70	0.72
1:B:493:LEU:HB3	1:B:494:GLN:HB2	1.71	0.71
1:C:258:GLN:CG	1:C:260:GLU:O	2.37	0.71
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.73	0.70
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.72	0.70
1:E:469:ILE:HB	1:F:370:VAL:HG13	1.73	0.70
1:D:258:GLN:CG	1:D:260:GLU:O	2.40	0.70
1:F:84:ARG:NH2	1:F:91:GLU:O	2.25	0.70
1:D:493:LEU:HB2	1:D:494:GLN:HB2	1.74	0.69
1:F:472:HIS:CE1	4:F:605:HOH:O	2.45	0.69
1:B:494:GLN:CA	1:B:495:SER:HB2	2.22	0.69
1:F:258:GLN:OE1	1:F:260:GLU:O	2.12	0.68
1:B:91:GLU:CD	1:B:92:ASP:N	2.48	0.67
1:F:493:LEU:HB3	1:F:494:GLN:CB	2.23	0.67
1:E:258:GLN:CG	1:E:260:GLU:O	2.43	0.67
1:B:493:LEU:HB2	1:B:494:GLN:HB2	1.76	0.67
1:F:258:GLN:CG	1:F:260:GLU:O	2.42	0.66
1:E:485:THR:OG1	1:E:488:SER:HB3	1.96	0.66
1:F:158:LEU:HD11	1:F:332:ILE:HG12	1.77	0.66
1:E:84:ARG:NH2	1:E:91:GLU:O	2.28	0.66
1:C:91:GLU:CD	1:C:92:ASP:N	2.49	0.65
1:E:469:ILE:CG1	1:F:370:VAL:HG22	2.28	0.64
1:B:431:ASP:O	1:B:432:ASN:HB2	1.97	0.63
1:C:258:GLN:CD	1:C:260:GLU:O	2.37	0.63
1:C:380:TYR:OH	1:C:439:HIS:HD2	1.82	0.62
1:C:496:GLY:HA2	1:C:497:CYS:SG	2.38	0.62
1:F:13:PHE:HD1	1:F:37:LYS:CB	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:CB	1:D:146:LYS:HE3	2.30	0.61
1:D:258:GLN:CD	1:D:260:GLU:O	2.38	0.61
1:A:192:LYS:H	1:A:285:ASN:HD22	1.49	0.61
1:D:84:ARG:NH2	1:D:91:GLU:O	2.32	0.61
1:E:91:GLU:CD	1:E:92:ASP:N	2.49	0.61
1:F:170:ILE:HD11	1:F:256:ILE:HD12	1.83	0.61
1:A:192:LYS:N	1:A:285:ASN:HD22	1.99	0.61
1:A:80:LEU:HD22	1:B:80:LEU:HD22	1.82	0.60
1:A:485:THR:OG1	1:A:488:SER:HB3	2.01	0.60
1:A:411:TRP:C	1:A:414:PRO:HD2	2.21	0.60
1:D:493:LEU:HB3	1:D:494:GLN:CB	2.31	0.60
1:B:84:ARG:HD3	1:D:150:LYS:HE2	1.83	0.60
1:E:258:GLN:CD	1:E:260:GLU:O	2.40	0.60
1:F:497:CYS:C	1:F:498:SEC:SE	2.90	0.60
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.83	0.60
1:E:91:GLU:CG	1:E:92:ASP:N	2.64	0.60
1:C:99:GLU:OE1	1:E:148:LYS:HE3	2.02	0.60
1:D:485:THR:OG1	1:D:488:SER:HB3	2.01	0.59
1:F:11:TYR:HE2	1:F:138:HIS:ND1	1.99	0.59
1:A:323:GLN:NE2	1:A:327:PRO:HA	2.17	0.59
1:E:380:TYR:OH	1:E:439:HIS:HD2	1.85	0.59
1:F:295:SER:HB3	1:F:335:ILE:HG22	1.85	0.59
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.85	0.59
1:F:485:THR:OG1	1:F:488:SER:HB3	2.02	0.59
1:D:323:GLN:HE21	1:D:327:PRO:HA	1.68	0.59
1:F:106:GLN:NE2	1:F:184:PHE:O	2.36	0.58
1:B:173:ASP:OD1	1:B:174:LYS:N	2.38	0.57
1:A:270:THR:HG23	1:A:281:GLU:HG3	1.87	0.57
1:A:499:GLY:HA2	1:B:119:ALA:CB	2.35	0.57
1:C:80:LEU:HD22	1:D:80:LEU:HD22	1.86	0.57
1:F:315:LYS:HD2	1:F:336:LEU:O	2.04	0.57
1:E:496:GLY:HA2	1:E:497:CYS:SG	2.45	0.57
1:F:11:TYR:CE2	1:F:138:HIS:ND1	2.73	0.57
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.69	0.56
1:F:13:PHE:O	1:F:154:ALA:HA	2.05	0.56
1:C:485:THR:OG1	1:C:488:SER:HB3	2.04	0.56
1:F:323:GLN:HE21	1:F:327:PRO:HA	1.68	0.56
1:F:156:ARG:HD3	1:F:330:TYR:HE2	1.71	0.56
1:E:402:TYR:CD2	1:E:462:LYS:HE2	2.40	0.56
1:B:493:LEU:HB3	1:B:494:GLN:CB	2.35	0.56
1:A:258:GLN:OE1	1:A:260:GLU:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLY:HA3	1:C:256:ILE:O	2.06	0.56
1:E:498:SEC:SE	1:F:112:LEU:HD22	2.55	0.56
1:F:41:LEU:HD23	1:F:128:GLU:HB3	1.88	0.56
1:A:134:PHE:HB2	1:A:301:GLY:O	2.06	0.56
1:C:302:LEU:HG	1:C:307:VAL:HB	1.88	0.56
1:A:197:GLY:C	1:A:202:ALA:CB	2.74	0.55
1:E:470:GLY:HA2	1:E:480:THR:HG21	1.89	0.55
1:C:98:TRP:CE2	1:C:102:THR:HG21	2.41	0.55
1:D:494:GLN:HA	1:D:495:SER:HB2	1.87	0.55
1:A:72:GLN:HA	1:A:72:GLN:HE21	1.72	0.55
1:F:411:TRP:C	1:F:414:PRO:HD2	2.27	0.55
1:C:158:LEU:HD11	1:C:332:ILE:CG1	2.36	0.55
1:E:497:CYS:C	1:E:498:SEC:SE	2.94	0.55
1:C:402:TYR:CD2	1:C:462:LYS:HE2	2.41	0.55
1:F:258:GLN:CD	1:F:260:GLU:O	2.44	0.55
1:C:270:THR:HG23	1:C:281:GLU:HG3	1.89	0.55
1:F:259:ILE:O	1:F:259:ILE:HG22	2.07	0.55
1:F:431:ASP:O	1:F:432:ASN:HB2	2.06	0.54
1:C:259:ILE:HG22	1:C:259:ILE:O	2.08	0.54
1:F:323:GLN:NE2	1:F:327:PRO:HA	2.22	0.54
1:B:158:LEU:HD11	1:B:332:ILE:CG1	2.38	0.54
1:D:380:TYR:OH	1:D:439:HIS:HD2	1.91	0.54
1:F:102:THR:O	1:F:106:GLN:HG2	2.08	0.54
1:D:106:GLN:NE2	1:D:184:PHE:O	2.40	0.54
1:E:172:GLY:HA3	1:E:256:ILE:O	2.07	0.54
1:A:323:GLN:HE21	1:A:327:PRO:HA	1.71	0.54
1:B:397:GLU:HA	1:B:487:ARG:HH22	1.71	0.54
1:E:17:ILE:HD13	1:E:28:ALA:HB2	1.89	0.54
1:A:41:LEU:HD23	1:A:128:GLU:HB3	1.88	0.54
1:A:494:GLN:HA	1:A:495:SER:HB2	1.90	0.54
1:C:173:ASP:OD1	1:C:174:LYS:N	2.41	0.54
1:C:499:GLY:HA3	1:D:119:ALA:HB1	1.89	0.53
1:D:84:ARG:NH2	1:D:90:LEU:HB3	2.23	0.53
1:D:323:GLN:NE2	1:D:327:PRO:HA	2.23	0.53
1:C:90:LEU:HD13	1:D:94:VAL:HG21	1.88	0.53
1:D:300:ILE:HG13	1:D:302:LEU:HG	1.90	0.53
1:E:469:ILE:HG12	1:F:370:VAL:HG22	1.89	0.53
1:B:496:GLY:HA2	1:B:497:CYS:SG	2.48	0.53
1:D:72:GLN:HE21	1:D:72:GLN:HA	1.73	0.53
1:B:494:GLN:HA	1:B:495:SER:HB2	1.91	0.53
1:E:259:ILE:HG22	1:E:259:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ILE:HD11	1:F:256:ILE:CD1	2.38	0.53
1:E:72:GLN:HE21	1:E:72:GLN:HA	1.74	0.53
1:E:270:THR:HG23	1:E:281:GLU:HG3	1.91	0.53
1:B:72:GLN:HE21	1:B:72:GLN:HA	1.73	0.53
1:B:192:LYS:N	1:B:285:ASN:HD22	2.07	0.53
1:C:106:GLN:NE2	1:C:184:PHE:O	2.42	0.53
1:F:134:PHE:HB2	1:F:301:GLY:O	2.08	0.53
1:F:98:TRP:CE2	1:F:102:THR:HG21	2.44	0.52
1:A:17:ILE:HD13	1:A:28:ALA:HB2	1.91	0.52
1:A:173:ASP:OD1	1:A:174:LYS:N	2.42	0.52
1:D:295:SER:HB3	1:D:335:ILE:HG22	1.90	0.52
1:A:300:ILE:HG13	1:A:302:LEU:HG	1.91	0.52
1:E:398:ASN:OD1	1:E:430:LYS:HE3	2.09	0.52
1:F:236:ILE:HD11	1:F:380:TYR:CD2	2.44	0.52
1:D:12:ASP:HB2	1:D:153:SER:O	2.10	0.52
1:A:106:GLN:NE2	1:A:184:PHE:O	2.43	0.52
1:B:270:THR:HG23	1:B:281:GLU:HG3	1.92	0.52
1:C:21:GLY:HA3	2:C:600:FAD:O5B	2.10	0.52
1:D:397:GLU:HA	1:D:487:ARG:HH22	1.75	0.52
1:B:323:GLN:NE2	1:B:327:PRO:HA	2.24	0.52
1:E:477:GLU:HA	1:F:450:GLN:OE1	2.10	0.52
1:F:397:GLU:HA	1:F:487:ARG:HH22	1.75	0.51
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.93	0.51
1:B:411:TRP:C	1:B:414:PRO:HD2	2.31	0.51
1:C:411:TRP:C	1:C:414:PRO:HD2	2.30	0.51
1:D:192:LYS:N	1:D:285:ASN:HD22	2.08	0.51
1:C:84:ARG:NH2	1:C:90:LEU:HB3	2.25	0.51
1:A:158:LEU:HD11	1:A:332:ILE:CG1	2.41	0.51
1:C:192:LYS:N	1:C:285:ASN:HD22	2.08	0.51
1:F:21:GLY:HA3	2:F:600:FAD:O5B	2.10	0.51
1:C:268:LYS:HE2	1:C:281:GLU:HG2	1.94	0.50
1:C:497:CYS:C	1:C:498:SEC:SE	3.00	0.50
1:E:411:TRP:C	1:E:414:PRO:HD2	2.31	0.50
1:F:172:GLY:HA3	1:F:256:ILE:O	2.11	0.50
1:A:156:ARG:HD3	1:A:330:TYR:HE2	1.75	0.50
1:C:431:ASP:O	1:C:432:ASN:HB2	2.11	0.50
1:C:493:LEU:HB3	1:C:494:GLN:CB	2.30	0.50
1:D:173:ASP:OD1	1:D:174:LYS:N	2.44	0.50
1:E:494:GLN:N	1:E:495:SER:HB2	2.25	0.50
1:A:21:GLY:HA3	2:A:600:FAD:O5B	2.11	0.50
1:F:378:LEU:HD11	1:F:442:GLY:HA2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:HG22	1:B:469:ILE:HG13	1.93	0.50
1:A:497:CYS:C	1:A:498:SEC:SE	3.00	0.50
1:B:258:GLN:OE1	1:B:260:GLU:O	2.29	0.50
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.93	0.50
1:A:402:TYR:CD2	1:A:462:LYS:HE2	2.47	0.50
1:B:192:LYS:H	1:B:285:ASN:HD22	1.60	0.50
1:D:431:ASP:O	1:D:432:ASN:HB2	2.11	0.49
1:A:259:ILE:O	1:A:259:ILE:HG22	2.12	0.49
1:C:102:THR:O	1:C:106:GLN:HG2	2.12	0.49
1:A:315:LYS:HD2	1:A:336:LEU:O	2.12	0.49
1:D:497:CYS:C	1:D:498:SEC:SE	3.01	0.49
1:C:295:SER:HB3	1:C:335:ILE:HG22	1.94	0.49
1:D:170:ILE:HD11	1:D:256:ILE:HD12	1.95	0.49
1:E:300:ILE:HG13	1:E:302:LEU:HG	1.94	0.49
1:F:239:HIS:CD2	1:F:243:HIS:CE1	3.01	0.49
1:F:300:ILE:HG13	1:F:302:LEU:HG	1.94	0.49
1:C:402:TYR:CE2	1:C:462:LYS:HE2	2.48	0.49
1:F:178:ILE:HB	1:F:182:ASP:HB2	1.93	0.49
1:F:236:ILE:HG21	1:F:376:THR:HG21	1.93	0.49
1:C:178:ILE:HB	1:C:182:ASP:HB2	1.95	0.49
1:A:221:ARG:HD2	3:A:601:NAP:O2X	2.12	0.49
1:A:431:ASP:O	1:A:432:ASN:HB2	2.12	0.49
1:E:344:PRO:HB2	1:F:469:ILE:HG22	1.94	0.49
1:E:409:LEU:HD23	1:F:68:LYS:HB3	1.95	0.49
1:F:270:THR:HG23	1:F:281:GLU:HG3	1.93	0.49
1:B:268:LYS:HE2	1:B:281:GLU:HG2	1.95	0.49
1:E:158:LEU:HD11	1:E:332:ILE:CG1	2.41	0.49
1:E:431:ASP:O	1:E:432:ASN:HB2	2.12	0.49
1:F:259:ILE:O	1:F:259:ILE:CG2	2.61	0.49
1:A:99:GLU:OE1	1:D:146:LYS:HE3	2.12	0.49
1:C:315:LYS:HD2	1:C:336:LEU:O	2.13	0.49
1:D:192:LYS:H	1:D:285:ASN:HD22	1.60	0.49
1:E:173:ASP:OD1	1:E:174:LYS:N	2.46	0.49
1:F:72:GLN:HE21	1:F:72:GLN:HA	1.77	0.49
1:F:168:LEU:CD1	1:F:253:PRO:HG2	2.43	0.49
1:E:106:GLN:NE2	1:E:184:PHE:O	2.46	0.48
1:F:58:THR:O	1:F:63:GLY:N	2.46	0.48
1:F:192:LYS:N	1:F:285:ASN:HD22	2.11	0.48
1:C:112:LEU:HD22	1:D:498:SEC:SE	2.63	0.48
1:E:192:LYS:N	1:E:285:ASN:HD22	2.11	0.48
1:D:156:ARG:HD3	1:D:330:TYR:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:LEU:HD23	1:E:494:GLN:NE2	2.29	0.48
1:F:194:LEU:HD11	1:F:219:MET:HB2	1.95	0.48
1:C:493:LEU:O	1:C:495:SER:HB2	2.13	0.48
1:C:236:ILE:HD11	1:C:380:TYR:CD2	2.49	0.48
1:E:192:LYS:H	1:E:285:ASN:HD22	1.60	0.48
1:A:258:GLN:HG3	1:A:260:GLU:O	2.14	0.48
1:B:300:ILE:HG13	1:B:302:LEU:HG	1.95	0.48
1:D:259:ILE:O	1:D:259:ILE:HG22	2.14	0.48
1:E:295:SER:HB3	1:E:335:ILE:HG22	1.94	0.48
1:E:469:ILE:HG13	1:F:370:VAL:HG22	1.95	0.48
1:B:485:THR:OG1	1:B:488:SER:HB3	2.12	0.48
1:B:172:GLY:HA3	1:B:256:ILE:O	2.14	0.48
1:B:259:ILE:HG22	1:B:259:ILE:O	2.13	0.48
1:F:12:ASP:HB3	1:F:153:SER:O	2.12	0.48
1:F:137:PRO:HA	1:F:305:VAL:HG12	1.96	0.48
1:F:268:LYS:HE2	1:F:281:GLU:HG2	1.96	0.48
1:A:98:TRP:CE2	1:A:102:THR:HG21	2.48	0.47
1:C:137:PRO:HA	1:C:305:VAL:HG12	1.96	0.47
1:F:308:LYS:HD2	1:F:325:ASN:ND2	2.28	0.47
1:B:156:ARG:HD3	1:B:330:TYR:HE2	1.78	0.47
1:E:41:LEU:HD23	1:E:128:GLU:HB3	1.95	0.47
1:E:80:LEU:HD22	1:F:80:LEU:HD22	1.97	0.47
1:E:402:TYR:CE2	1:E:462:LYS:HE2	2.49	0.47
1:F:91:GLU:H	1:F:91:GLU:CD	2.16	0.47
1:F:403:HIS:CE1	1:F:492:ILE:HD13	2.49	0.47
1:E:268:LYS:HE2	1:E:281:GLU:HG2	1.96	0.47
1:C:427:CYS:HA	1:C:434:ARG:O	2.14	0.47
1:D:411:TRP:C	1:D:414:PRO:HD2	2.35	0.47
1:A:82:ASP:OD2	1:A:416:ARG:NH1	2.47	0.47
1:A:295:SER:HB3	1:A:335:ILE:HG22	1.96	0.47
1:A:319:THR:C	1:A:321:GLU:H	2.18	0.47
1:D:319:THR:C	1:D:321:GLU:H	2.16	0.47
1:F:84:ARG:NH2	1:F:90:LEU:HB3	2.30	0.47
1:C:323:GLN:NE2	1:C:327:PRO:HA	2.30	0.47
1:D:423:ALA:HB1	1:D:479:PHE:CZ	2.50	0.47
1:F:66:PRO:O	1:F:70:MET:HG3	2.14	0.47
1:F:494:GLN:HA	1:F:495:SER:CB	2.40	0.47
1:A:238:GLU:O	1:A:242:GLU:HG3	2.15	0.47
1:C:239:HIS:CE1	1:C:378:LEU:HB2	2.50	0.47
1:F:423:ALA:HB1	1:F:479:PHE:CZ	2.50	0.47
1:B:72:GLN:HA	1:B:72:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:GLU:HA	1:E:487:ARG:HH22	1.80	0.46
1:B:402:TYR:CD2	1:B:462:LYS:HE2	2.51	0.46
1:C:156:ARG:HD3	1:C:330:TYR:HE2	1.81	0.46
1:E:309:ILE:HG22	1:E:316:ILE:HG12	1.97	0.46
1:A:470:GLY:HA2	1:A:480:THR:HG21	1.97	0.46
1:F:72:GLN:HA	1:F:72:GLN:NE2	2.31	0.46
1:F:158:LEU:HD11	1:F:332:ILE:CG1	2.44	0.46
1:F:323:GLN:HG2	1:F:324:THR:O	2.16	0.46
1:A:102:THR:O	1:A:106:GLN:HG2	2.16	0.46
1:B:178:ILE:HB	1:B:182:ASP:HB2	1.95	0.46
1:D:17:ILE:HD13	1:D:28:ALA:HB2	1.96	0.46
1:D:270:THR:HG23	1:D:281:GLU:HG3	1.96	0.46
1:B:102:THR:O	1:B:106:GLN:HG2	2.15	0.46
1:C:494:GLN:N	1:C:495:SER:HB2	2.29	0.46
1:D:158:LEU:HD11	1:D:332:ILE:CG1	2.44	0.46
1:B:137:PRO:HA	1:B:305:VAL:HG12	1.98	0.46
1:E:387:GLU:OE1	1:E:401:VAL:HG21	2.16	0.46
1:A:104:SER:HB3	1:B:413:VAL:HG13	1.98	0.46
1:B:236:ILE:HG21	1:B:376:THR:HG21	1.98	0.46
1:D:387:GLU:OE1	1:D:401:VAL:HG21	2.16	0.46
1:E:70:MET:CE	1:E:102:THR:HG22	2.46	0.46
1:E:98:TRP:CE2	1:E:102:THR:HG21	2.51	0.46
1:A:323:GLN:HA	1:A:330:TYR:CD1	2.51	0.46
1:C:67:LYS:HB3	1:C:67:LYS:HE2	1.80	0.46
1:E:423:ALA:HB1	1:E:479:PHE:CZ	2.50	0.46
1:F:494:GLN:N	1:F:495:SER:HB2	2.31	0.46
1:A:493:LEU:HD23	1:A:494:GLN:NE2	2.30	0.45
1:B:41:LEU:HD23	1:B:128:GLU:HB3	1.98	0.45
1:B:98:TRP:CE2	1:B:102:THR:HG21	2.51	0.45
1:C:58:THR:O	1:C:63:GLY:N	2.49	0.45
1:D:236:ILE:HG21	1:D:376:THR:HG21	1.98	0.45
1:E:474:VAL:HG21	1:F:446:GLY:HA3	1.97	0.45
1:C:89:LYS:C	1:D:94:VAL:HG13	2.37	0.45
1:E:134:PHE:HB2	1:E:301:GLY:O	2.17	0.45
1:E:471:ILE:HG21	1:F:373:THR:OG1	2.17	0.45
1:C:72:GLN:HA	1:C:72:GLN:NE2	2.31	0.45
1:C:259:ILE:O	1:C:259:ILE:CG2	2.64	0.45
1:C:469:ILE:HG22	1:D:344:PRO:HB2	1.97	0.45
1:F:238:GLU:O	1:F:242:GLU:HG3	2.17	0.45
1:A:99:GLU:HB2	1:D:146:LYS:HE3	1.99	0.45
1:D:398:ASN:OD1	1:D:430:LYS:HE3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:HA	1:A:72:GLN:NE2	2.31	0.45
1:A:370:VAL:HG22	1:B:469:ILE:CG1	2.47	0.45
1:C:323:GLN:HE21	1:C:327:PRO:HA	1.81	0.45
1:D:98:TRP:CE2	1:D:102:THR:HG21	2.51	0.45
1:E:319:THR:C	1:E:321:GLU:H	2.18	0.45
1:C:499:GLY:HA3	1:D:119:ALA:CB	2.47	0.45
1:D:82:ASP:OD2	1:D:416:ARG:NH1	2.49	0.45
1:F:173:ASP:OD1	1:F:174:LYS:N	2.49	0.45
1:F:192:LYS:H	1:F:285:ASN:HD22	1.65	0.45
1:A:70:MET:CE	1:A:102:THR:HG22	2.47	0.45
1:A:137:PRO:HA	1:A:305:VAL:HG12	1.99	0.45
1:A:236:ILE:HG21	1:A:376:THR:HG21	1.99	0.45
1:A:236:ILE:HD11	1:A:380:TYR:CD2	2.52	0.45
1:C:41:LEU:HD23	1:C:128:GLU:HB3	1.99	0.45
1:C:398:ASN:OD1	1:C:430:LYS:HE3	2.17	0.45
1:E:67:LYS:HE2	1:E:67:LYS:HB3	1.78	0.45
1:C:192:LYS:H	1:C:285:ASN:HD22	1.63	0.45
1:E:236:ILE:HD11	1:E:380:TYR:CD2	2.52	0.45
1:B:197:GLY:C	1:B:202:ALA:CB	2.84	0.44
1:C:112:LEU:CD2	1:D:498:SEC:SE	3.15	0.44
1:E:156:ARG:HD3	1:E:330:TYR:HE2	1.83	0.44
1:E:316:ILE:HD12	1:E:335:ILE:HD12	1.99	0.44
1:A:178:ILE:HB	1:A:182:ASP:HB2	1.99	0.44
1:F:438:PHE:CE1	1:F:452:PHE:CG	3.06	0.44
1:A:259:ILE:O	1:A:259:ILE:CG2	2.65	0.44
1:E:380:TYR:CE1	1:E:382:CYS:HB3	2.53	0.44
1:A:70:MET:HE2	1:A:102:THR:HG22	1.98	0.44
1:E:493:LEU:HB3	1:E:494:GLN:CB	2.31	0.44
1:B:207:GLY:HA3	1:B:377:PRO:HD3	2.00	0.44
1:D:402:TYR:CD2	1:D:462:LYS:HE2	2.52	0.44
1:E:494:GLN:HA	1:E:495:SER:CB	2.41	0.44
1:F:319:THR:C	1:F:321:GLU:H	2.21	0.44
1:B:319:THR:C	1:B:321:GLU:H	2.21	0.44
1:A:493:LEU:HD23	1:A:494:GLN:HE21	1.83	0.44
1:C:101:MET:O	1:C:105:VAL:HG23	2.18	0.44
1:D:9:LYS:NZ	1:D:9:LYS:HB3	2.33	0.44
1:A:397:GLU:HA	1:A:487:ARG:HH22	1.82	0.44
1:D:268:LYS:HE2	1:D:281:GLU:HG2	2.00	0.44
1:D:315:LYS:HD2	1:D:336:LEU:O	2.18	0.44
1:E:259:ILE:O	1:E:259:ILE:CG2	2.65	0.44
1:F:82:ASP:OD2	1:F:416:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:SER:HB3	3:A:601:NAP:O1N	2.18	0.43
1:D:102:THR:O	1:D:106:GLN:HG2	2.18	0.43
1:D:332:ILE:HA	1:D:332:ILE:HD13	1.77	0.43
1:F:316:ILE:HD12	1:F:335:ILE:HD12	1.99	0.43
1:F:380:TYR:CE1	1:F:382:CYS:HB3	2.52	0.43
1:A:99:GLU:HB3	1:D:146:LYS:HE3	2.00	0.43
1:B:470:GLY:HA2	1:B:480:THR:HG21	2.00	0.43
1:C:449:THR:O	1:C:450:GLN:C	2.55	0.43
1:F:394:PHE:HB2	1:F:399:ILE:HD11	2.00	0.43
1:C:168:LEU:CD1	1:C:253:PRO:HG2	2.48	0.43
1:D:205:CYS:HA	1:D:208:PHE:CE2	2.53	0.43
1:E:448:VAL:HG22	1:F:447:GLU:HB3	2.00	0.43
1:F:67:LYS:HB3	1:F:67:LYS:HE2	1.81	0.43
1:A:402:TYR:CE2	1:A:462:LYS:HE2	2.53	0.43
1:C:68:LYS:O	1:C:71:HIS:HB3	2.19	0.43
1:D:41:LEU:HD23	1:D:128:GLU:HB3	2.00	0.43
1:C:207:GLY:HA3	1:C:377:PRO:HD3	2.00	0.43
1:E:70:MET:HE1	1:E:102:THR:HG22	2.01	0.43
1:E:493:LEU:O	1:E:495:SER:HB2	2.18	0.43
1:D:236:ILE:HD11	1:D:380:TYR:CD2	2.53	0.43
1:D:259:ILE:O	1:D:259:ILE:CG2	2.66	0.43
1:E:72:GLN:HA	1:E:72:GLN:NE2	2.33	0.43
1:E:343:THR:HB	1:E:344:PRO:HD3	2.00	0.43
1:C:323:GLN:HG2	1:C:324:THR:O	2.19	0.43
1:D:67:LYS:HB3	1:D:67:LYS:HE2	1.81	0.43
1:E:101:MET:O	1:E:105:VAL:HG23	2.18	0.43
1:A:406:PHE:CZ	1:A:421:CYS:HB3	2.54	0.43
1:B:497:CYS:C	1:B:498:SEC:SE	3.07	0.43
1:D:496:GLY:HA2	1:D:497:CYS:SG	2.59	0.43
1:C:170:ILE:HB	1:C:254:THR:O	2.19	0.43
1:E:102:THR:O	1:E:106:GLN:HG2	2.19	0.43
1:E:332:ILE:HD13	1:E:332:ILE:HA	1.88	0.43
1:F:259:ILE:CD1	1:F:268:LYS:HB2	2.48	0.43
1:C:134:PHE:HB2	1:C:301:GLY:O	2.19	0.42
1:C:177:CYS:SG	1:C:287:VAL:HB	2.59	0.42
1:F:17:ILE:HD13	1:F:28:ALA:HB2	2.01	0.42
1:F:339:LYS:HD2	1:F:367:TYR:CD2	2.54	0.42
1:B:258:GLN:HG3	1:B:260:GLU:O	2.18	0.42
1:A:446:GLY:HA3	1:B:474:VAL:HG21	2.00	0.42
1:C:316:ILE:HD12	1:C:335:ILE:HD12	2.00	0.42
1:D:21:GLY:HA3	2:D:600:FAD:O5B	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:GLN:NE2	1:E:327:PRO:HA	2.33	0.42
1:F:170:ILE:HB	1:F:254:THR:O	2.18	0.42
1:A:239:HIS:CE1	1:A:378:LEU:HB2	2.55	0.42
1:C:170:ILE:HD12	1:C:254:THR:C	2.40	0.42
1:E:166:ARG:HH12	1:E:292:GLY:HA3	1.84	0.42
1:E:407:TRP:CD1	1:E:418:ASN:HA	2.55	0.42
1:A:99:GLU:OE1	1:D:146:LYS:CD	2.68	0.42
1:B:21:GLY:HA3	2:B:600:FAD:O5B	2.19	0.42
1:B:259:ILE:O	1:B:259:ILE:CG2	2.66	0.42
1:B:332:ILE:HD13	1:B:332:ILE:HA	1.85	0.42
1:D:66:PRO:HB3	1:D:109:ILE:HD11	2.01	0.42
1:A:172:GLY:HA3	1:A:256:ILE:O	2.19	0.42
1:D:178:ILE:HB	1:D:182:ASP:HB2	2.02	0.42
1:E:168:LEU:O	1:E:173:ASP:OD2	2.38	0.42
1:B:68:LYS:O	1:B:71:HIS:HB3	2.20	0.42
1:C:461:THR:OG1	1:C:464:GLN:HG3	2.20	0.42
1:E:21:GLY:HA3	2:E:600:FAD:O5B	2.20	0.42
1:F:58:THR:HG23	1:F:62:VAL:HG23	2.01	0.42
1:B:292:GLY:C	1:B:293:ARG:HG2	2.38	0.42
1:B:323:GLN:HE21	1:B:327:PRO:HA	1.83	0.42
1:C:66:PRO:O	1:C:70:MET:HG3	2.19	0.42
1:D:70:MET:CE	1:D:102:THR:HG22	2.50	0.42
1:E:239:HIS:CE1	1:E:378:LEU:HB2	2.55	0.42
1:E:409:LEU:CD2	1:F:68:LYS:HB3	2.50	0.42
1:F:12:ASP:HB2	1:F:153:SER:OG	2.19	0.42
1:F:48:PRO:HG2	1:F:167:TYR:CZ	2.54	0.42
1:F:402:TYR:CD2	1:F:462:LYS:HE2	2.55	0.42
1:B:448:VAL:HG13	1:B:476:ALA:HB2	2.02	0.42
1:C:98:TRP:NE1	1:C:102:THR:HG21	2.35	0.42
1:D:13:PHE:O	1:D:154:ALA:HA	2.19	0.42
1:E:144:ASN:OD1	1:E:144:ASN:C	2.57	0.42
1:E:394:PHE:HB2	1:E:399:ILE:HD11	2.01	0.42
1:F:207:GLY:HA3	1:F:377:PRO:HD3	2.02	0.42
1:D:309:ILE:HG22	1:D:316:ILE:HG12	2.01	0.42
1:F:387:GLU:OE1	1:F:401:VAL:HG21	2.20	0.42
1:C:197:GLY:O	1:C:202:ALA:HB1	2.20	0.41
1:D:408:PRO:O	1:D:409:LEU:C	2.57	0.41
1:F:308:LYS:HD2	1:F:325:ASN:HD22	1.85	0.41
1:A:108:HIS:CE1	1:B:412:THR:HB	2.55	0.41
1:A:319:THR:C	1:A:321:GLU:N	2.74	0.41
1:A:474:VAL:O	1:A:477:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PRO:HB2	1:D:469:ILE:HG22	2.01	0.41
1:D:70:MET:HE2	1:D:102:THR:HG22	2.02	0.41
1:F:101:MET:O	1:F:105:VAL:HG23	2.19	0.41
1:A:394:PHE:HB2	1:A:399:ILE:HD11	2.02	0.41
1:C:170:ILE:HD11	1:C:256:ILE:HD12	2.01	0.41
1:D:58:THR:O	1:D:63:GLY:N	2.53	0.41
1:C:376:THR:O	1:C:377:PRO:C	2.59	0.41
1:D:238:GLU:O	1:D:242:GLU:HG3	2.21	0.41
1:D:470:GLY:HA2	1:D:480:THR:HG21	2.02	0.41
1:E:119:ALA:HB1	1:F:499:GLY:HA2	2.02	0.41
1:A:164:ARG:HG2	1:A:296:CYS:SG	2.61	0.41
1:B:323:GLN:HA	1:B:330:TYR:CD1	2.55	0.41
1:F:68:LYS:O	1:F:71:HIS:HB3	2.21	0.41
1:A:352:LEU:O	1:A:355:GLN:HB2	2.21	0.41
1:C:186:LEU:HA	1:C:187:PRO:HD3	1.83	0.41
1:C:493:LEU:HD23	1:C:494:GLN:NE2	2.35	0.41
1:D:172:GLY:HA3	1:D:256:ILE:O	2.20	0.41
1:D:416:ARG:HH11	1:D:416:ARG:HD3	1.71	0.41
1:A:332:ILE:HD13	1:A:332:ILE:HA	1.88	0.41
1:A:403:HIS:CE1	1:A:492:ILE:HD13	2.56	0.41
1:B:13:PHE:O	1:B:154:ALA:HA	2.19	0.41
1:D:319:THR:C	1:D:321:GLU:N	2.74	0.41
1:E:260:GLU:OE1	1:E:266:ARG:NH2	2.51	0.41
1:A:387:GLU:OE1	1:A:401:VAL:HG21	2.20	0.41
1:B:205:CYS:HA	1:B:208:PHE:CE2	2.56	0.41
1:B:236:ILE:HD11	1:B:380:TYR:CD2	2.55	0.41
1:B:387:GLU:OE1	1:B:401:VAL:HG21	2.21	0.41
1:C:159:ILE:HD13	1:C:302:LEU:HD11	2.03	0.41
1:C:470:GLY:HA2	1:C:480:THR:HG21	2.03	0.41
1:C:474:VAL:O	1:C:477:GLU:HG2	2.21	0.41
1:E:498:SEC:SE	1:F:112:LEU:CD2	3.19	0.41
1:F:173:ASP:HB2	1:F:289:LEU:HD11	2.03	0.41
1:F:199:SER:O	1:F:200:TYR:C	2.59	0.41
1:F:496:GLY:HA2	1:F:497:CYS:SG	2.61	0.41
1:A:398:ASN:OD1	1:A:430:LYS:HE3	2.21	0.41
1:C:469:ILE:CG2	1:D:344:PRO:HB2	2.51	0.41
1:D:168:LEU:O	1:D:173:ASP:OD2	2.39	0.41
1:D:259:ILE:CD1	1:D:268:LYS:HB2	2.51	0.41
1:E:410:GLU:OE2	1:F:68:LYS:HE2	2.20	0.40
1:B:380:TYR:CE1	1:B:382:CYS:HB3	2.56	0.40
1:C:319:THR:C	1:C:321:GLU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:HD12	1:A:493:LEU:HA	1.97	0.40
1:B:295:SER:HB3	1:B:335:ILE:HG22	2.04	0.40
1:F:25:LEU:O	1:F:29:LYS:HB3	2.21	0.40
1:F:236:ILE:CG2	1:F:376:THR:HG21	2.52	0.40
1:B:394:PHE:HB2	1:B:399:ILE:HD11	2.02	0.40
1:C:495:SER:HA	1:C:496:GLY:O	2.21	0.40
1:D:394:PHE:HB2	1:D:399:ILE:HD11	2.04	0.40
1:B:91:GLU:CG	1:B:92:ASP:N	2.83	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	486/499 (97%)	436 (90%)	44 (9%)	6 (1%)	13	44
1	B	487/499 (98%)	440 (90%)	42 (9%)	5 (1%)	15	49
1	C	483/499 (97%)	437 (90%)	42 (9%)	4 (1%)	19	54
1	D	488/499 (98%)	450 (92%)	31 (6%)	7 (1%)	11	40
1	E	487/499 (98%)	441 (91%)	40 (8%)	6 (1%)	13	44
1	F	486/499 (97%)	437 (90%)	43 (9%)	6 (1%)	13	44
All	All	2917/2994 (97%)	2641 (90%)	242 (8%)	34 (1%)	13	44

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	SER
1	B	493	LEU
1	B	495	SER
1	C	495	SER

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Mol	Chain	Res	Type
1	D	493	LEU
1	D	495	SER
1	E	495	SER
1	F	91	GLU
1	F	495	SER
1	A	493	LEU
1	C	278	GLU
1	C	497	CYS
1	D	91	GLU
1	E	430	LYS
1	A	91	GLU
1	B	278	GLU
1	B	430	LYS
1	B	497	CYS
1	C	396	GLU
1	D	278	GLU
1	E	278	GLU
1	E	396	GLU
1	F	497	CYS
1	A	320	ASP
1	A	497	CYS
1	D	396	GLU
1	D	497	CYS
1	E	91	GLU
1	E	497	CYS
1	F	278	GLU
1	F	396	GLU
1	A	278	GLU
1	D	320	ASP
1	F	430	LYS

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	404/413 (98%)	377 (93%)	27 (7%)	16 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	405/413 (98%)	376 (93%)	29 (7%)	14	44
1	C	401/413 (97%)	373 (93%)	28 (7%)	15	45
1	D	406/413 (98%)	377 (93%)	29 (7%)	14	44
1	E	405/413 (98%)	377 (93%)	28 (7%)	15	45
1	F	404/413 (98%)	376 (93%)	28 (7%)	15	45
All	All	2425/2478 (98%)	2256 (93%)	169 (7%)	15	45

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	45	THR
1	A	51	THR
1	A	64	CYS
1	A	67	LYS
1	A	90	LEU
1	A	92	ASP
1	A	99	GLU
1	A	117	ARG
1	A	144	ASN
1	A	199	SER
1	A	270	THR
1	A	277	GLU
1	A	280	ILE
1	A	293	ARG
1	A	303	GLU
1	A	318	VAL
1	A	340	LEU
1	A	376	THR
1	A	383	CYS
1	A	396	GLU
1	A	397	GLU
1	A	403	HIS
1	A	416	ARG
1	A	460	LEU
1	A	495	SER
1	A	497	CYS
1	B	11	TYR
1	B	12	ASP
1	B	29	LYS

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Mol	Chain	Res	Type
1	B	45	THR
1	B	51	THR
1	B	52	ARG
1	B	64	CYS
1	B	90	LEU
1	B	91	GLU
1	B	92	ASP
1	B	99	GLU
1	B	117	ARG
1	B	144	ASN
1	B	199	SER
1	B	270	THR
1	B	277	GLU
1	B	279	THR
1	B	280	ILE
1	B	293	ARG
1	B	303	GLU
1	B	318	VAL
1	B	340	LEU
1	B	376	THR
1	B	396	GLU
1	B	397	GLU
1	B	403	HIS
1	B	416	ARG
1	B	495	SER
1	B	497	CYS
1	C	29	LYS
1	C	45	THR
1	C	47	THR
1	C	62	VAL
1	C	64	CYS
1	C	84	ARG
1	C	90	LEU
1	C	91	GLU
1	C	92	ASP
1	C	99	GLU
1	C	117	ARG
1	C	144	ASN
1	C	199	SER
1	C	270	THR
1	C	277	GLU
1	C	279	THR

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Mol	Chain	Res	Type
1	C	280	ILE
1	C	302	LEU
1	C	303	GLU
1	C	305	VAL
1	C	318	VAL
1	C	376	THR
1	C	396	GLU
1	C	397	GLU
1	C	403	HIS
1	C	416	ARG
1	C	495	SER
1	C	497	CYS
1	D	9	LYS
1	D	10	SER
1	D	29	LYS
1	D	45	THR
1	D	48	PRO
1	D	51	THR
1	D	64	CYS
1	D	84	ARG
1	D	90	LEU
1	D	92	ASP
1	D	99	GLU
1	D	117	ARG
1	D	199	SER
1	D	270	THR
1	D	277	GLU
1	D	279	THR
1	D	280	ILE
1	D	293	ARG
1	D	303	GLU
1	D	318	VAL
1	D	340	LEU
1	D	376	THR
1	D	396	GLU
1	D	397	GLU
1	D	403	HIS
1	D	404	SER
1	D	416	ARG
1	D	495	SER
1	D	497	CYS
1	E	29	LYS

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Mol	Chain	Res	Type
1	E	45	THR
1	E	51	THR
1	E	64	CYS
1	E	67	LYS
1	E	90	LEU
1	E	91	GLU
1	E	92	ASP
1	E	99	GLU
1	E	117	ARG
1	E	144	ASN
1	E	145	ASN
1	E	199	SER
1	E	270	THR
1	E	277	GLU
1	E	279	THR
1	E	280	ILE
1	E	293	ARG
1	E	303	GLU
1	E	318	VAL
1	E	340	LEU
1	E	376	THR
1	E	396	GLU
1	E	397	GLU
1	E	403	HIS
1	E	416	ARG
1	E	495	SER
1	E	497	CYS
1	F	29	LYS
1	F	45	THR
1	F	47	THR
1	F	51	THR
1	F	62	VAL
1	F	64	CYS
1	F	67	LYS
1	F	90	LEU
1	F	92	ASP
1	F	99	GLU
1	F	117	ARG
1	F	144	ASN
1	F	199	SER
1	F	270	THR
1	F	277	GLU

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Mol	Chain	Res	Type
1	F	279	THR
1	F	280	ILE
1	F	303	GLU
1	F	318	VAL
1	F	340	LEU
1	F	376	THR
1	F	396	GLU
1	F	397	GLU
1	F	403	HIS
1	F	416	ARG
1	F	460	LEU
1	F	495	SER
1	F	497	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	85	ASN
1	A	145	ASN
1	A	258	GLN
1	A	285	ASN
1	A	323	GLN
1	A	439	HIS
1	A	494	GLN
1	B	72	GLN
1	B	106	GLN
1	B	145	ASN
1	B	258	GLN
1	B	285	ASN
1	B	439	HIS
1	C	72	GLN
1	C	106	GLN
1	C	239	HIS
1	C	258	GLN
1	C	285	ASN
1	C	323	GLN
1	C	439	HIS
1	C	494	GLN
1	D	72	GLN
1	D	85	ASN
1	D	106	GLN

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Mol	Chain	Res	Type
1	D	145	ASN
1	D	258	GLN
1	D	285	ASN
1	D	323	GLN
1	D	439	HIS
1	E	72	GLN
1	E	85	ASN
1	E	145	ASN
1	E	285	ASN
1	E	323	GLN
1	E	439	HIS
1	E	494	GLN
1	F	72	GLN
1	F	85	ASN
1	F	106	GLN
1	F	258	GLN
1	F	285	ASN
1	F	323	GLN
1	F	439	HIS
1	F	472	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	$\#\|Z\| > 2$
2	FAD	B	600	-	53,58,58	1.49	3 (5%)	68,89,89	1.34	8 (11%)
3	NAP	B	601	-	28,34,52	1.37	4 (14%)	34,53,80	1.42	5 (14%)
2	FAD	D	600	-	53,58,58	1.36	6 (11%)	68,89,89	1.32	10 (14%)
3	NAP	A	601	-	28,34,52	1.66	4 (14%)	34,53,80	1.30	2 (5%)
2	FAD	E	600	-	53,58,58	1.50	7 (13%)	68,89,89	1.36	11 (16%)
3	NAP	C	601	-	28,34,52	1.81	4 (14%)	34,53,80	1.43	3 (8%)
2	FAD	A	600	-	53,58,58	1.31	4 (7%)	68,89,89	1.38	10 (14%)
2	FAD	C	600	-	53,58,58	1.67	7 (13%)	68,89,89	1.29	9 (13%)
3	NAP	E	601	-	28,34,52	1.53	4 (14%)	34,53,80	1.40	4 (11%)
3	NAP	F	601	-	28,34,52	2.00	5 (17%)	34,53,80	1.46	4 (11%)
3	NAP	D	601	-	28,34,52	1.30	3 (10%)	34,53,80	1.37	3 (8%)
2	FAD	F	600	-	53,58,58	1.80	7 (13%)	68,89,89	1.43	8 (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
2	FAD	B	600	-	-	3/30/50/50	0/6/6/6
3	NAP	B	601	-	-	10/20/40/67	0/3/3/5
2	FAD	D	600	-	-	2/30/50/50	0/6/6/6
3	NAP	A	601	-	-	11/20/40/67	0/3/3/5
2	FAD	E	600	-	-	3/30/50/50	0/6/6/6
3	NAP	C	601	-	-	10/20/40/67	0/3/3/5
2	FAD	A	600	-	-	3/30/50/50	0/6/6/6
2	FAD	C	600	-	-	5/30/50/50	0/6/6/6
3	NAP	E	601	-	-	11/20/40/67	0/3/3/5
3	NAP	F	601	-	-	10/20/40/67	0/3/3/5
3	NAP	D	601	-	-	9/20/40/67	0/3/3/5
2	FAD	F	600	-	-	7/30/50/50	0/6/6/6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	FAD	O4B-C1B	7.67	1.51	1.41
2	C	600	FAD	O4B-C1B	6.83	1.50	1.41
2	B	600	FAD	O4B-C1B	6.14	1.49	1.41
2	F	600	FAD	C4X-N5	5.81	1.42	1.30
3	F	601	NAP	O4B-C1B	5.51	1.48	1.41
2	E	600	FAD	C4X-N5	5.47	1.41	1.30
2	E	600	FAD	O4B-C1B	5.32	1.48	1.41
2	A	600	FAD	C4X-N5	5.23	1.40	1.30
2	C	600	FAD	C4X-N5	5.20	1.40	1.30
2	F	600	FAD	C10-N1	5.18	1.43	1.33
3	F	601	NAP	P2B-O1X	5.13	1.67	1.50
2	D	600	FAD	C4X-N5	5.05	1.40	1.30
3	C	601	NAP	O4B-C1B	5.04	1.48	1.41
2	C	600	FAD	C10-N1	5.04	1.43	1.33
3	C	601	NAP	P2B-O1X	4.68	1.65	1.50
2	B	600	FAD	C4X-N5	4.61	1.39	1.30
2	A	600	FAD	C10-N1	4.56	1.42	1.33
3	F	601	NAP	P2B-O2X	4.25	1.71	1.54
3	E	601	NAP	PN-O5D	4.21	1.74	1.59
3	A	601	NAP	O4B-C1B	4.11	1.46	1.41
3	F	601	NAP	PN-O5D	4.08	1.73	1.59
3	C	601	NAP	PN-O5D	4.03	1.73	1.59
3	A	601	NAP	PN-O5D	3.92	1.73	1.59
2	B	600	FAD	C10-N1	3.82	1.41	1.33
3	B	601	NAP	O4B-C1B	3.80	1.46	1.41
2	E	600	FAD	C10-N1	3.69	1.40	1.33
3	E	601	NAP	O4B-C1B	3.67	1.46	1.41
3	A	601	NAP	P2B-O2B	3.65	1.66	1.59
3	A	601	NAP	P2B-O1X	3.64	1.62	1.50
3	B	601	NAP	PN-O5D	3.52	1.71	1.59
2	D	600	FAD	C10-N1	3.28	1.39	1.33
3	D	601	NAP	O4B-C1B	3.27	1.45	1.41
3	C	601	NAP	P2B-O2X	3.10	1.66	1.54
3	E	601	NAP	P2B-O1X	2.99	1.60	1.50
3	F	601	NAP	P2B-O2B	2.95	1.64	1.59
2	A	600	FAD	O4B-C1B	2.95	1.45	1.41
3	D	601	NAP	P2B-O1X	2.85	1.59	1.50
3	D	601	NAP	PN-O5D	2.79	1.69	1.59
2	F	600	FAD	C2-N1	2.78	1.43	1.36
2	D	600	FAD	O4B-C1B	2.74	1.44	1.41
2	E	600	FAD	C10-N10	2.73	1.43	1.37
2	C	600	FAD	PA-O5B	2.62	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAP	P2B-O1X	2.53	1.58	1.50
2	C	600	FAD	C10-N10	2.52	1.42	1.37
2	A	600	FAD	C10-N10	2.47	1.42	1.37
3	E	601	NAP	P2B-O3X	-2.38	1.45	1.54
2	F	600	FAD	C10-N10	2.36	1.42	1.37
2	F	600	FAD	C4-N3	2.35	1.43	1.38
2	D	600	FAD	PA-O2A	-2.28	1.44	1.55
2	E	600	FAD	PA-O2A	-2.23	1.44	1.55
2	D	600	FAD	C5A-N7A	-2.18	1.31	1.39
2	C	600	FAD	C2-N1	2.17	1.41	1.36
2	E	600	FAD	C2-N1	2.16	1.41	1.36
2	C	600	FAD	C5'-C4'	2.13	1.54	1.51
3	B	601	NAP	P2B-O3X	-2.10	1.46	1.54
2	F	600	FAD	PA-O5B	2.10	1.67	1.59
2	E	600	FAD	P-O2P	-2.09	1.45	1.55
2	D	600	FAD	C10-N10	2.06	1.41	1.37

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	NAP	N3A-C2A-N1A	-5.75	119.69	128.68
2	F	600	FAD	N3A-C2A-N1A	-5.63	119.87	128.68
3	F	601	NAP	N3A-C2A-N1A	-5.62	119.89	128.68
2	B	600	FAD	N3A-C2A-N1A	-5.54	120.01	128.68
3	A	601	NAP	N3A-C2A-N1A	-5.03	120.81	128.68
3	D	601	NAP	N3A-C2A-N1A	-4.86	121.08	128.68
2	A	600	FAD	N3A-C2A-N1A	-4.85	121.09	128.68
3	B	601	NAP	N3A-C2A-N1A	-4.82	121.14	128.68
3	E	601	NAP	N3A-C2A-N1A	-4.74	121.28	128.68
2	E	600	FAD	N3A-C2A-N1A	-4.73	121.29	128.68
2	C	600	FAD	N3A-C2A-N1A	-4.16	122.17	128.68
2	D	600	FAD	N3A-C2A-N1A	-4.14	122.20	128.68
2	D	600	FAD	O4B-C1B-C2B	-3.43	101.92	106.93
2	E	600	FAD	C4-N3-C2	-3.33	119.48	125.64
2	E	600	FAD	C4X-C4-N3	3.17	121.25	113.19
2	A	600	FAD	P-O3P-PA	-3.02	122.46	132.83
2	E	600	FAD	C10-C4X-N5	-2.91	118.69	124.86
2	F	600	FAD	C2A-N1A-C6A	2.90	123.72	118.75
2	A	600	FAD	C4X-C4-N3	2.89	120.53	113.19
2	F	600	FAD	C9A-C5X-N5	-2.88	119.31	122.43
2	F	600	FAD	P-O3P-PA	-2.88	122.96	132.83
3	F	601	NAP	C1B-N9A-C4A	-2.84	121.65	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	C4-N3-C2	-2.81	120.45	125.64
2	C	600	FAD	C4X-C4-N3	2.80	120.30	113.19
2	E	600	FAD	C4X-C10-N1	-2.77	118.31	124.73
2	C	600	FAD	C4-N3-C2	-2.73	120.60	125.64
2	B	600	FAD	P-O3P-PA	-2.70	123.55	132.83
3	C	601	NAP	O3X-P2B-O2X	2.69	117.92	107.64
2	F	600	FAD	C4X-C4-N3	2.68	120.00	113.19
2	F	600	FAD	O4-C4-C4X	-2.68	119.49	126.60
2	A	600	FAD	C10-C4X-N5	-2.68	119.17	124.86
2	A	600	FAD	C9A-C5X-N5	-2.66	119.54	122.43
3	B	601	NAP	C1B-N9A-C4A	-2.65	121.98	126.64
2	D	600	FAD	O4-C4-C4X	-2.64	119.60	126.60
2	C	600	FAD	C9A-C5X-N5	-2.60	119.61	122.43
2	D	600	FAD	C9A-C5X-N5	-2.60	119.61	122.43
2	B	600	FAD	O4B-C1B-C2B	-2.58	103.15	106.93
2	C	600	FAD	O4-C4-C4X	-2.55	119.84	126.60
2	B	600	FAD	C4-N3-C2	-2.53	120.97	125.64
2	F	600	FAD	C4-N3-C2	-2.51	121.00	125.64
2	A	600	FAD	C4X-C10-N1	-2.48	118.97	124.73
3	E	601	NAP	C1B-N9A-C4A	-2.48	122.28	126.64
2	D	600	FAD	C4-N3-C2	-2.43	121.16	125.64
3	A	601	NAP	C1B-N9A-C4A	-2.39	122.43	126.64
3	E	601	NAP	C4A-C5A-N7A	-2.39	106.91	109.40
2	B	600	FAD	C4-C4X-C10	2.39	120.80	116.79
2	D	600	FAD	C4-C4X-C10	2.38	120.78	116.79
3	B	601	NAP	O3X-P2B-O2X	2.38	116.72	107.64
2	D	600	FAD	C4X-C4-N3	2.38	119.22	113.19
3	D	601	NAP	C4A-C5A-N7A	-2.36	106.94	109.40
2	C	600	FAD	C10-C4X-N5	-2.35	119.87	124.86
2	E	600	FAD	C4-C4X-C10	2.35	120.73	116.79
2	B	600	FAD	C4X-C4-N3	2.34	119.14	113.19
2	B	600	FAD	O4-C4-C4X	-2.34	120.39	126.60
2	E	600	FAD	O4B-C1B-C2B	-2.31	103.55	106.93
2	E	600	FAD	C5X-N5-C4X	2.27	121.85	118.07
2	B	600	FAD	C9A-C5X-N5	-2.27	119.96	122.43
2	A	600	FAD	C5X-N5-C4X	2.26	121.83	118.07
2	D	600	FAD	C4X-C10-N1	-2.26	119.49	124.73
2	E	600	FAD	C4X-C10-N10	2.21	119.71	116.48
3	D	601	NAP	O3X-P2B-O2B	2.20	115.85	105.99
2	E	600	FAD	O4-C4-C4X	-2.19	120.80	126.60
2	E	600	FAD	C9A-C5X-N5	-2.19	120.06	122.43
2	D	600	FAD	P-O3P-PA	-2.17	125.37	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	NAP	C4A-C5A-N7A	-2.16	107.15	109.40
2	A	600	FAD	C4-C4X-C10	2.15	120.40	116.79
2	C	600	FAD	C4X-C10-N1	-2.15	119.75	124.73
3	F	601	NAP	O3X-P2B-O2X	2.14	115.83	107.64
3	B	601	NAP	O5B-PA-O1A	-2.14	100.72	109.07
3	F	601	NAP	C2A-N1A-C6A	2.13	122.39	118.75
3	E	601	NAP	C2A-N1A-C6A	2.12	122.38	118.75
2	A	600	FAD	O4B-C1B-C2B	-2.09	103.87	106.93
2	C	600	FAD	C4-C4X-C10	2.08	120.28	116.79
2	D	600	FAD	C10-C4X-N5	-2.05	120.52	124.86
2	F	600	FAD	O2A-PA-O1A	2.01	122.18	112.24
3	C	601	NAP	C2A-N1A-C6A	2.01	122.19	118.75
2	C	600	FAD	C5X-N5-C4X	2.00	121.40	118.07

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	600	FAD	O4B-C4B-C5B-O5B
2	D	600	FAD	O4B-C4B-C5B-O5B
2	E	600	FAD	O4B-C4B-C5B-O5B
2	F	600	FAD	C5B-O5B-PA-O2A
2	F	600	FAD	O4B-C4B-C5B-O5B
3	A	601	NAP	C5B-O5B-PA-O1A
3	A	601	NAP	C5B-O5B-PA-O3
3	A	601	NAP	C5D-O5D-PN-O1N
3	B	601	NAP	C5B-O5B-PA-O1A
3	B	601	NAP	C5B-O5B-PA-O3
3	B	601	NAP	C5D-O5D-PN-O1N
3	C	601	NAP	C5B-O5B-PA-O1A
3	C	601	NAP	C5B-O5B-PA-O3
3	D	601	NAP	C5B-O5B-PA-O1A
3	D	601	NAP	C5B-O5B-PA-O3
3	E	601	NAP	C5B-O5B-PA-O1A
3	E	601	NAP	C5B-O5B-PA-O3
3	E	601	NAP	C5D-O5D-PN-O1N
3	F	601	NAP	C5B-O5B-PA-O1A
3	F	601	NAP	C5B-O5B-PA-O3
3	F	601	NAP	C5D-O5D-PN-O1N
2	A	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	C3B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	600	FAD	C3B-C4B-C5B-O5B
2	D	600	FAD	C3B-C4B-C5B-O5B
2	E	600	FAD	C3B-C4B-C5B-O5B
2	F	600	FAD	C3B-C4B-C5B-O5B
2	C	600	FAD	C3B-C4B-C5B-O5B
3	C	601	NAP	C5D-O5D-PN-O1N
3	D	601	NAP	C5D-O5D-PN-O1N
2	F	600	FAD	C2'-C3'-C4'-O4'
2	B	600	FAD	PA-O3P-P-O5'
3	A	601	NAP	PA-O3-PN-O5D
3	B	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	B	601	NAP	C2B-O2B-P2B-O1X
3	D	601	NAP	C2B-O2B-P2B-O1X
3	E	601	NAP	C2B-O2B-P2B-O1X
3	D	601	NAP	C4B-C5B-O5B-PA
2	C	600	FAD	C5B-O5B-PA-O2A
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	E	601	NAP	C5B-O5B-PA-O2A
3	B	601	NAP	C4B-C5B-O5B-PA
3	C	601	NAP	C4B-C5B-O5B-PA
3	E	601	NAP	C4B-C5B-O5B-PA
2	F	600	FAD	C2'-C3'-C4'-C5'
3	F	601	NAP	C4B-C5B-O5B-PA
3	A	601	NAP	C5D-O5D-PN-O2N
3	B	601	NAP	C5D-O5D-PN-O2N
3	E	601	NAP	C5D-O5D-PN-O2N
3	F	601	NAP	C5D-O5D-PN-O2N
3	A	601	NAP	C4B-C5B-O5B-PA
2	F	600	FAD	O3'-C3'-C4'-O4'
3	C	601	NAP	PA-O3-PN-O5D
3	A	601	NAP	C2B-O2B-P2B-O1X
3	C	601	NAP	C2B-O2B-P2B-O1X
3	F	601	NAP	C2B-O2B-P2B-O1X
2	C	600	FAD	C5B-O5B-PA-O3P
3	A	601	NAP	C2B-O2B-P2B-O2X
3	A	601	NAP	C2B-O2B-P2B-O3X
3	B	601	NAP	C2B-O2B-P2B-O2X

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Mol	Chain	Res	Type	Atoms
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	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	E	601	NAP	O4B-C4B-C5B-O5B
3	F	601	NAP	O4B-C4B-C5B-O5B
2	A	600	FAD	C5B-O5B-PA-O1A
2	C	600	FAD	C5B-O5B-PA-O1A
2	E	600	FAD	C5B-O5B-PA-O1A
3	A	601	NAP	C5B-O5B-PA-O2A
3	F	601	NAP	C5B-O5B-PA-O2A
3	B	601	NAP	O4B-C4B-C5B-O5B
3	C	601	NAP	O4B-C4B-C5B-O5B
3	D	601	NAP	O4B-C4B-C5B-O5B
2	F	600	FAD	O3'-C3'-C4'-C5'

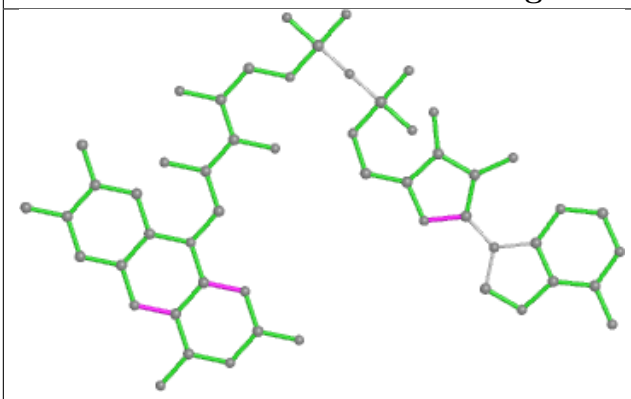
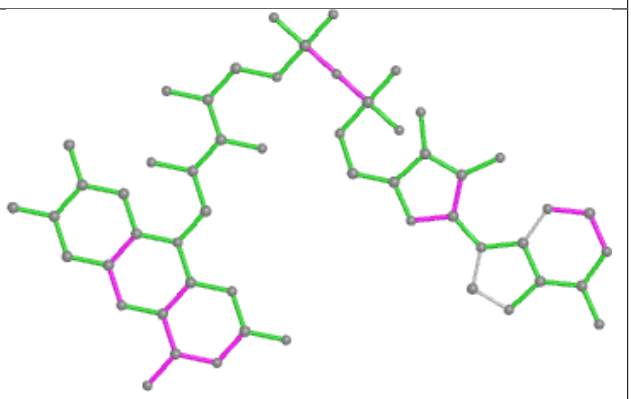
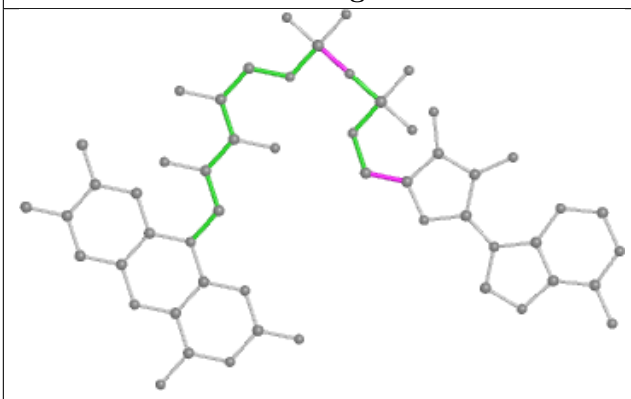
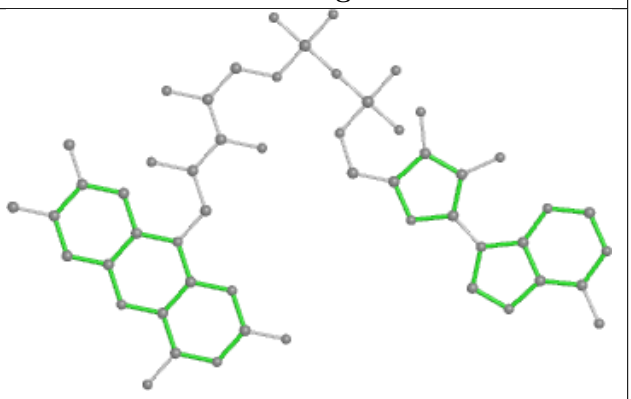
There are no ring outliers.

7 monomers are involved in 8 short contacts:

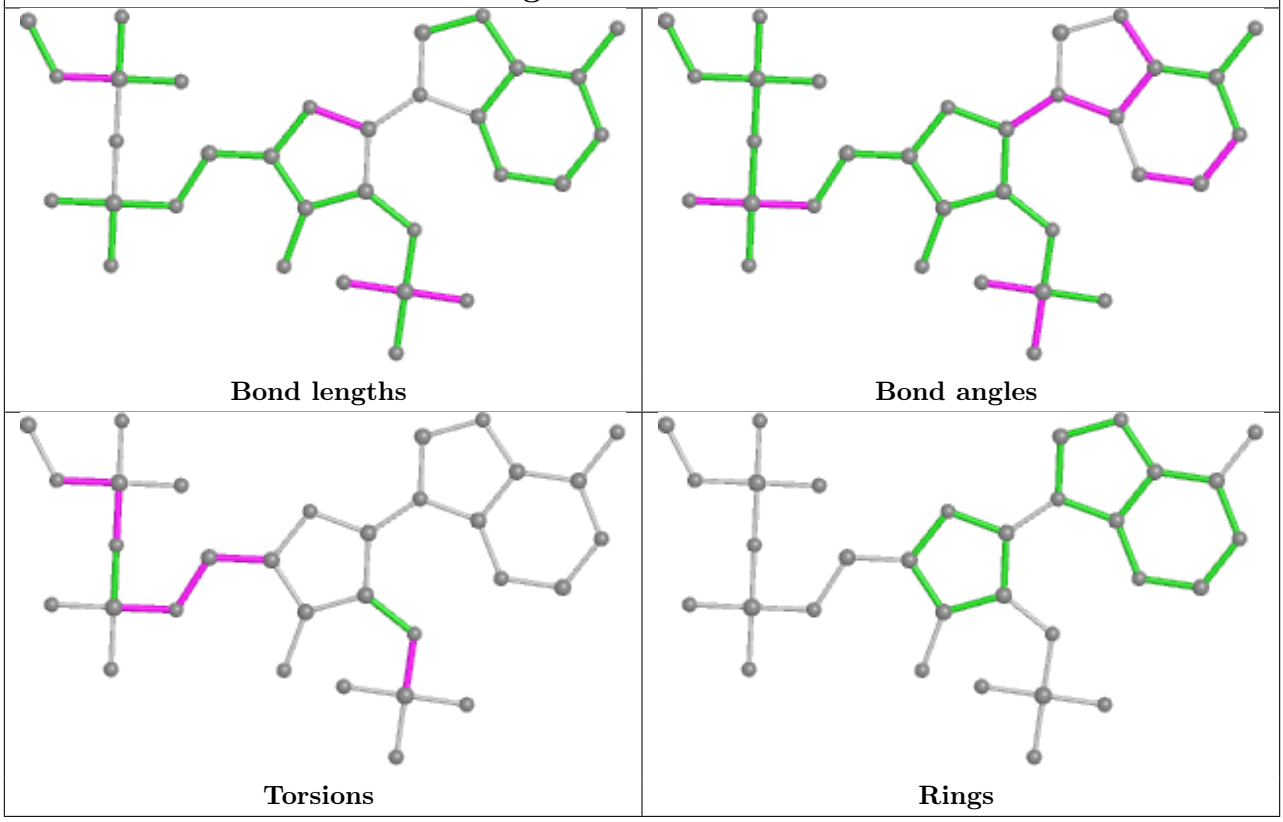
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	1	0
2	D	600	FAD	1	0
3	A	601	NAP	2	0
2	E	600	FAD	1	0
2	A	600	FAD	1	0
2	C	600	FAD	1	0
2	F	600	FAD	1	0

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

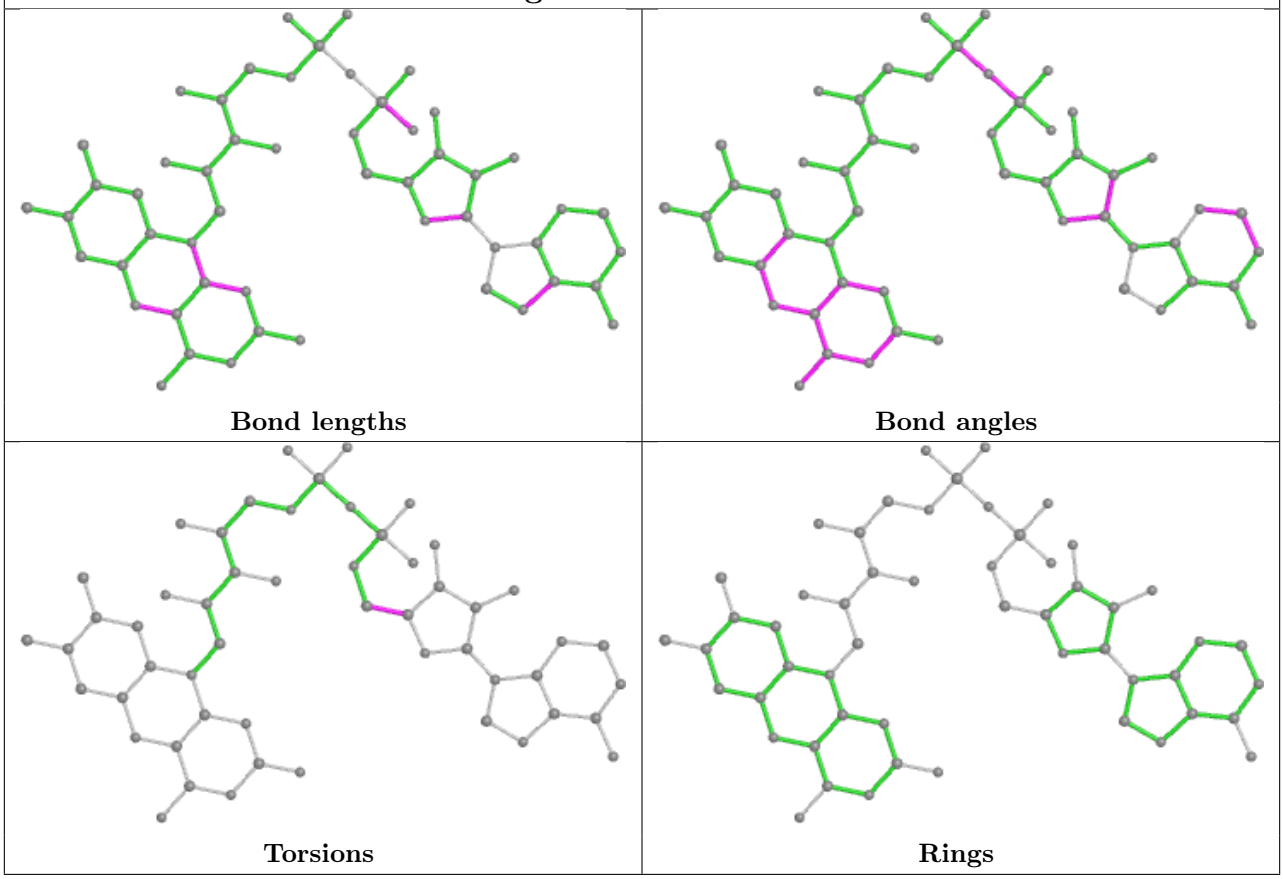
equivalents in the CSD to analyse the geometry.

Ligand FAD B 600	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

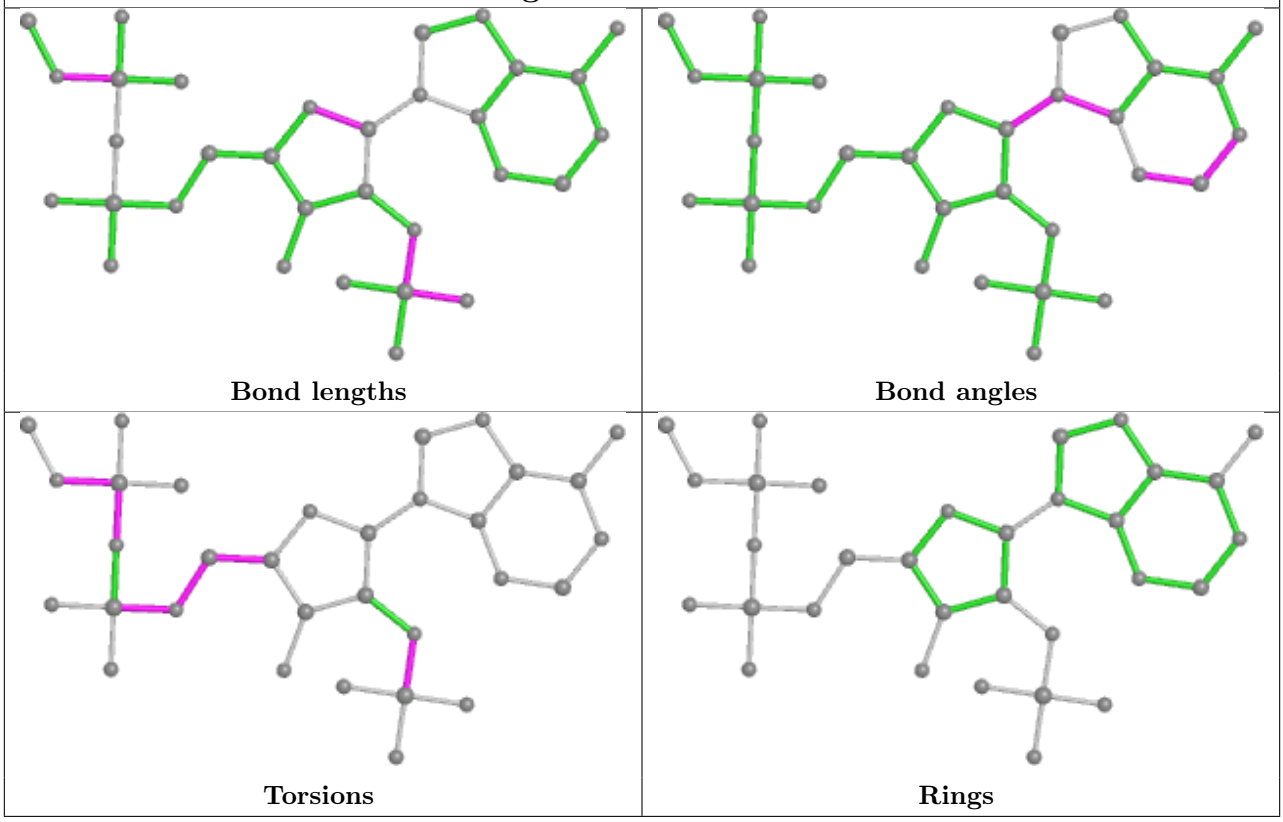
Ligand NAP B 601



Ligand FAD D 600



Ligand NAP A 601



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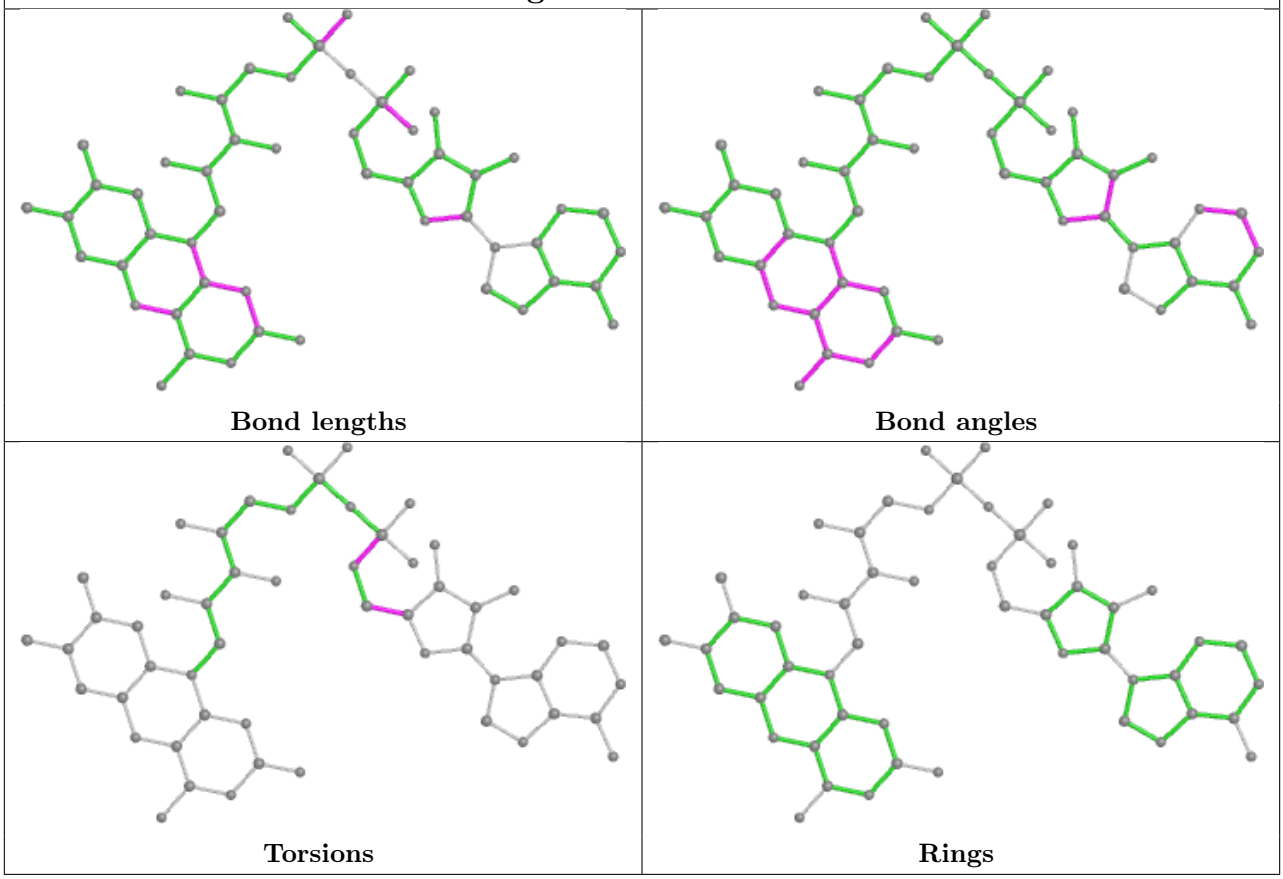

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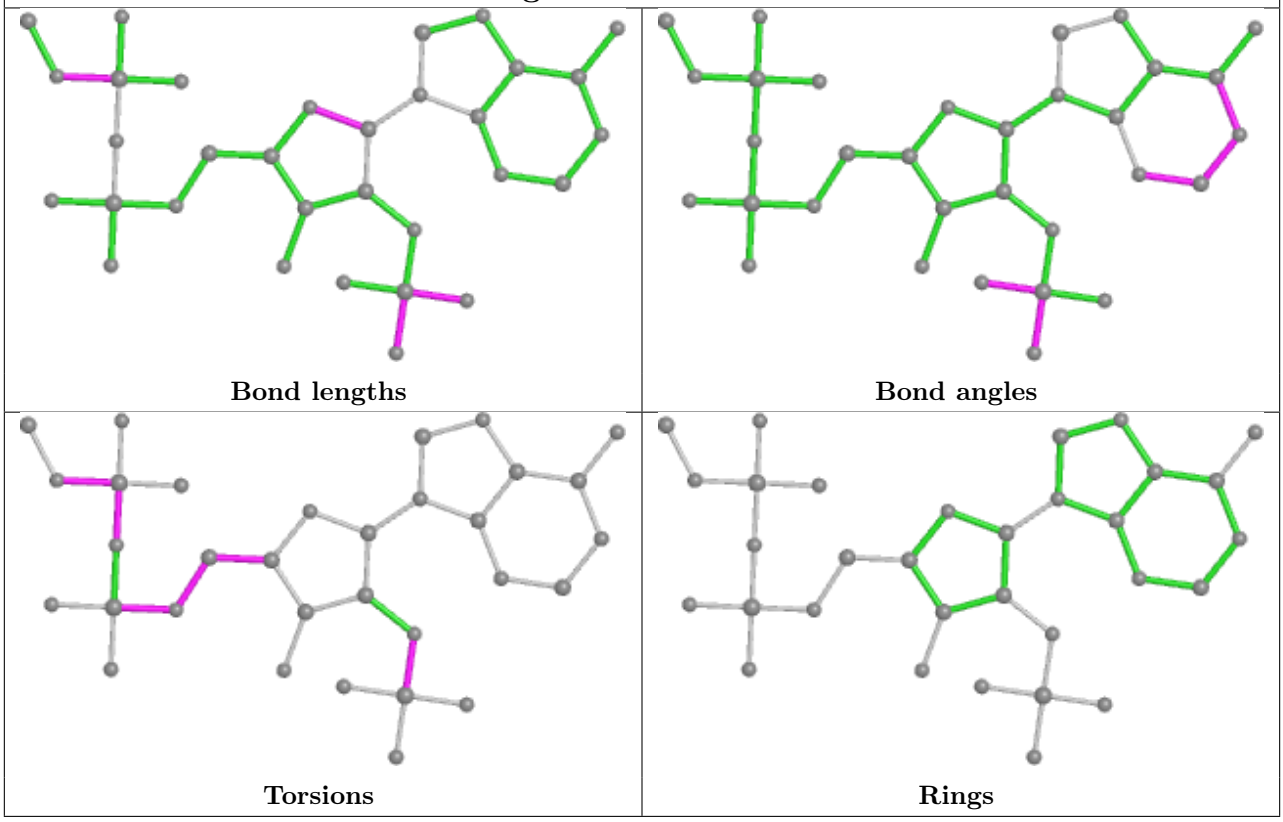

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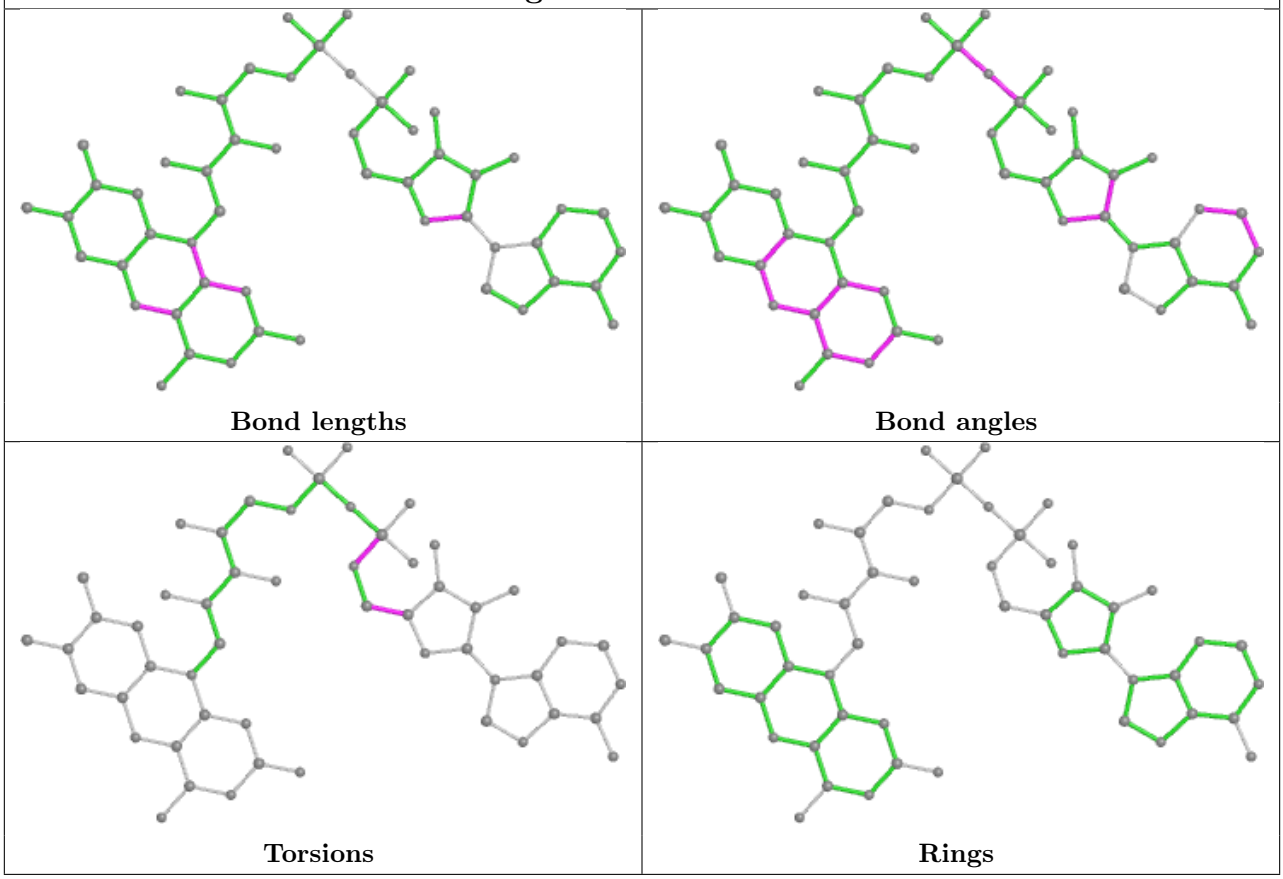

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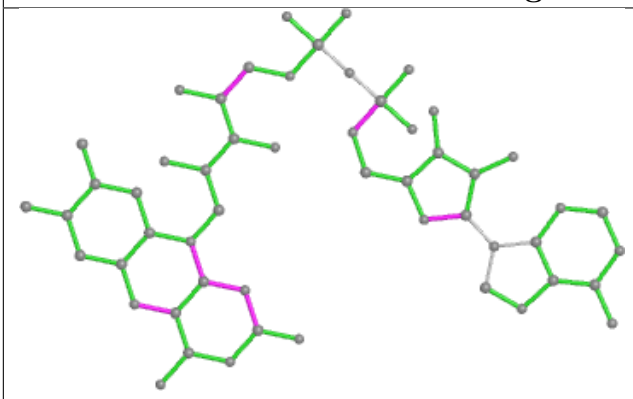
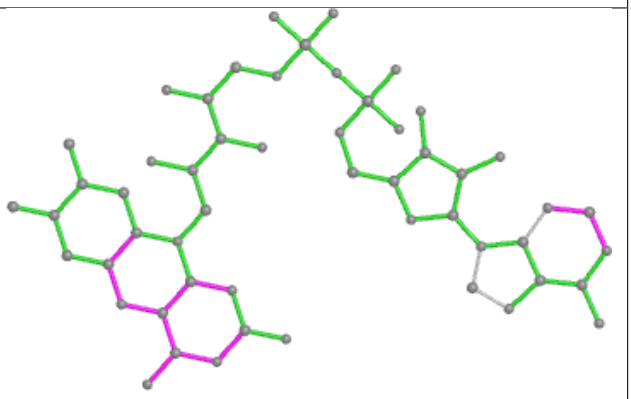
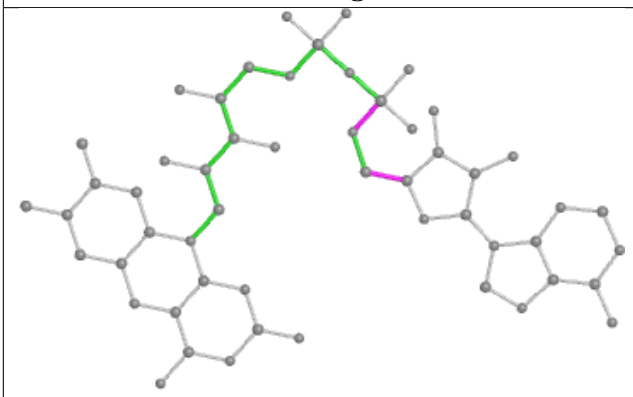


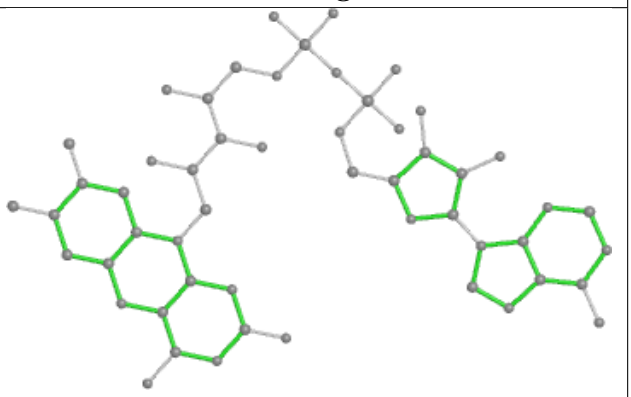
Bond lengths



Bond angles

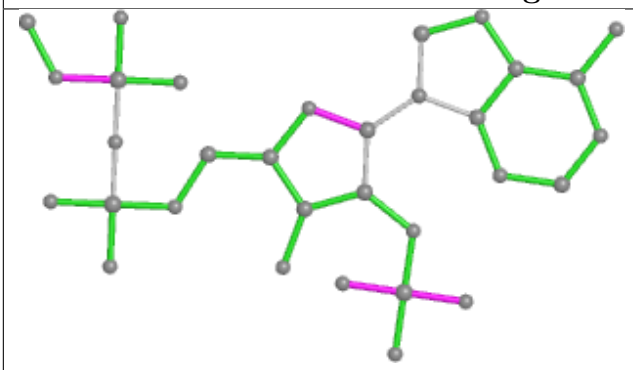


Torsions

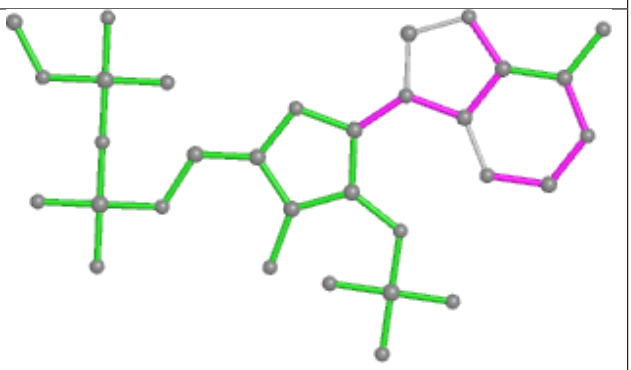


Rings

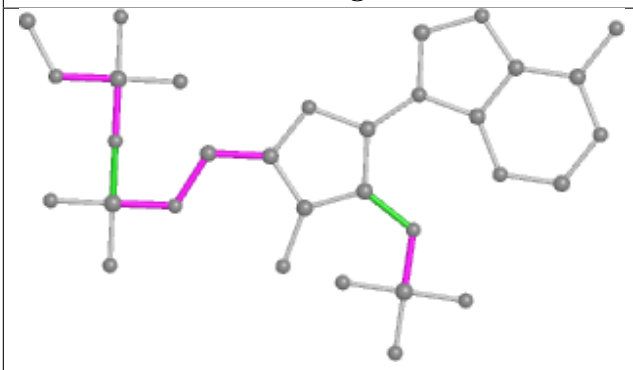
Ligand NAP E 601



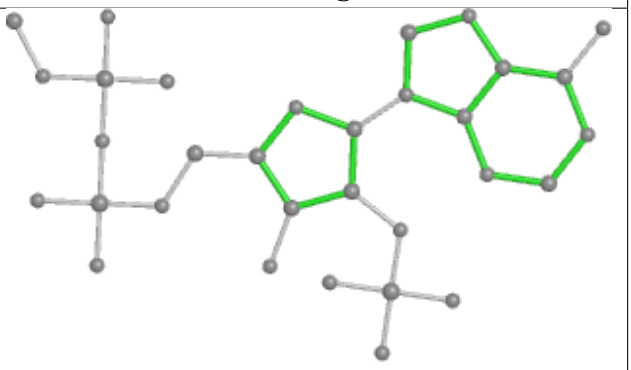
Bond lengths



Bond angles

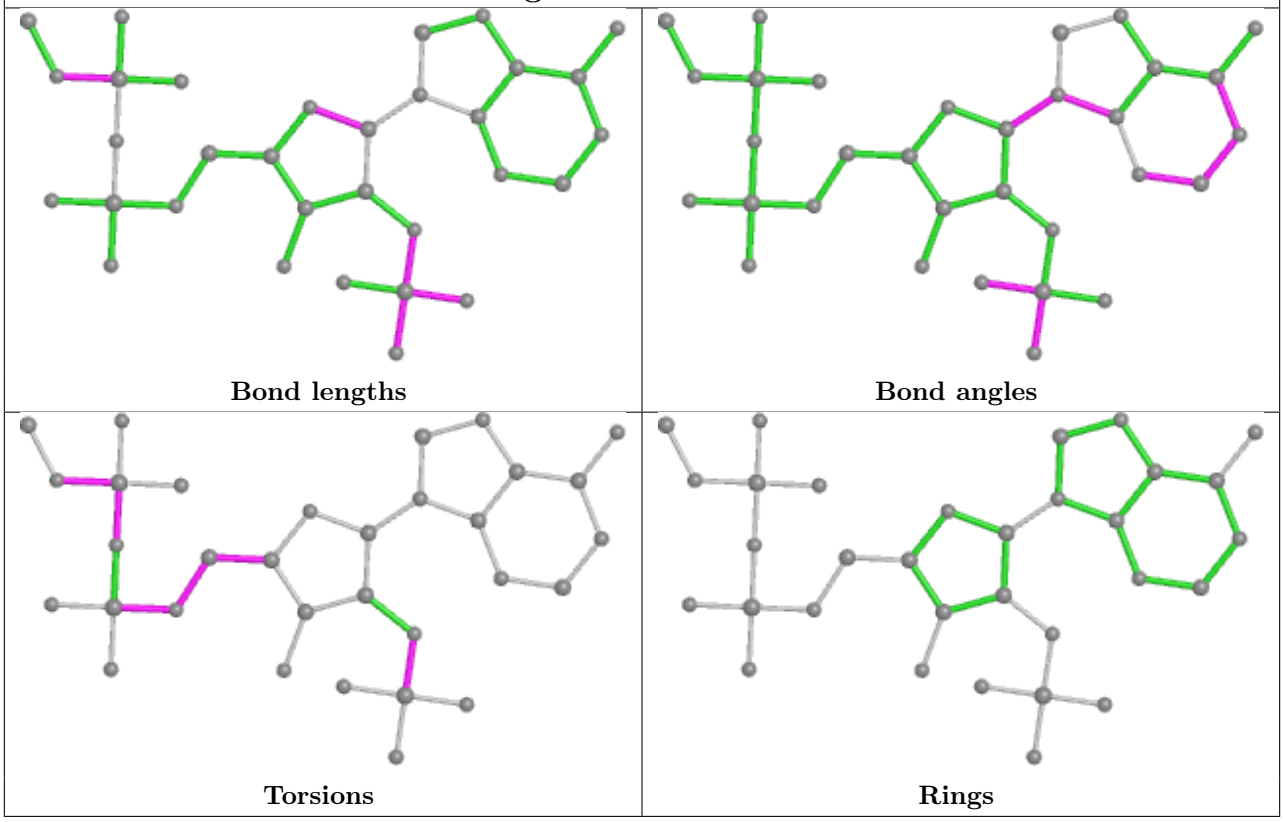


Torsions



Rings

Ligand NAP F 601



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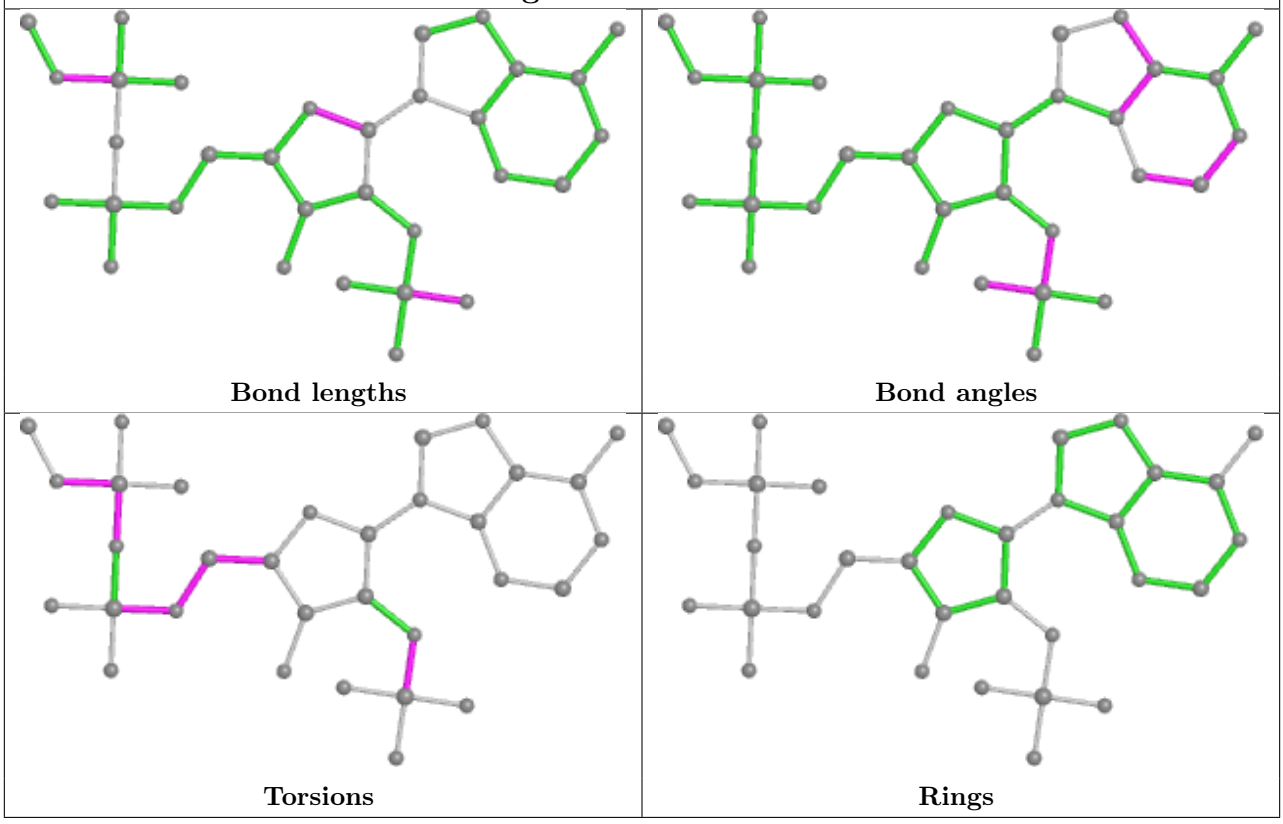
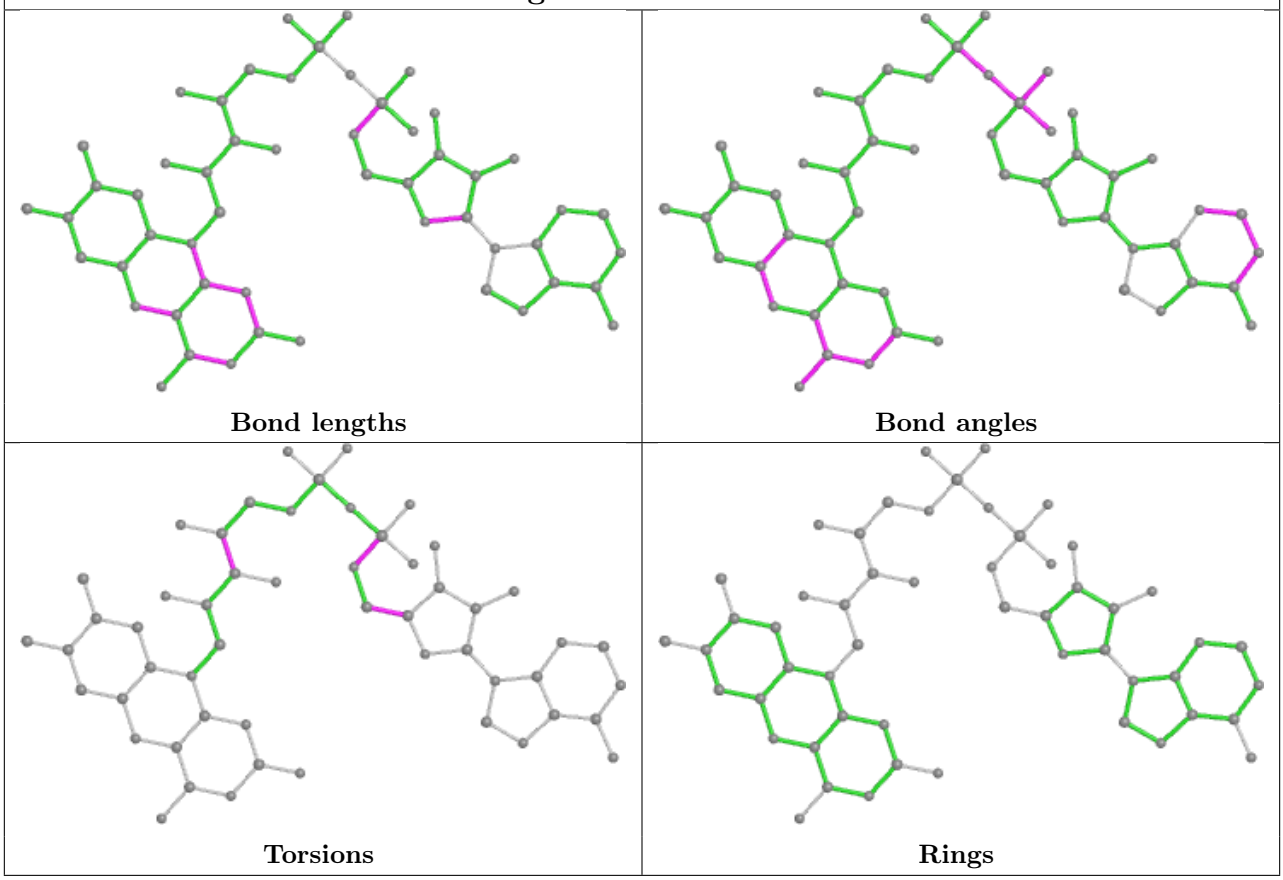


Ligand FAD F 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	488/499 (97%)	0.40	28 (5%)	23	11	23, 55, 69, 96	0
1	B	489/499 (97%)	0.31	23 (4%)	31	15	23, 55, 69, 96	0
1	C	485/499 (97%)	0.51	29 (5%)	21	10	23, 55, 68, 96	0
1	D	490/499 (98%)	0.32	7 (1%)	75	56	23, 55, 68, 96	0
1	E	489/499 (97%)	0.39	18 (3%)	41	21	23, 55, 68, 96	0
1	F	488/499 (97%)	1.04	113 (23%)	0	0	23, 55, 69, 96	0
All	All	2929/2994 (97%)	0.50	218 (7%)	14	5	23, 55, 69, 96	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	143	THR	6.1
1	F	278	GLU	4.9
1	F	282	ASP	4.8
1	A	132	GLY	4.8
1	F	177	CYS	4.7
1	E	432	ASN	4.6
1	F	277	GLU	4.5
1	E	398	ASN	4.4
1	F	307	VAL	4.4
1	E	274	THR	4.4
1	F	267	LEU	4.3
1	C	130	ALA	4.3
1	C	499	GLY	4.3
1	F	272	LYS	4.3
1	F	432	ASN	4.2
1	F	295	SER	4.0
1	F	369	ASN	3.9
1	F	283	GLU	3.9
1	B	494	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	153	SER	3.9
1	E	495	SER	3.8
1	F	132	GLY	3.8
1	F	19	GLY	3.8
1	F	154	ALA	3.8
1	F	499	GLY	3.8
1	F	251	PHE	3.8
1	F	284	PHE	3.7
1	F	306	GLY	3.6
1	B	153	SER	3.6
1	F	297	THR	3.6
1	E	494	GLN	3.5
1	A	428	ASN	3.5
1	F	163	GLU	3.5
1	F	494	GLN	3.5
1	C	277	GLU	3.4
1	F	35	ASP	3.4
1	F	197	GLY	3.4
1	F	266	ARG	3.4
1	F	244	GLY	3.4
1	F	302	LEU	3.4
1	A	334	ASP	3.3
1	F	131	TYR	3.3
1	B	12	ASP	3.3
1	F	399	ILE	3.3
1	F	324	THR	3.3
1	A	11	TYR	3.2
1	F	279	THR	3.2
1	F	298	ARG	3.2
1	F	11	TYR	3.2
1	F	331	ALA	3.2
1	F	361	SER	3.2
1	E	399	ILE	3.2
1	F	250	GLN	3.2
1	F	261	ALA	3.2
1	F	268	LYS	3.2
1	F	219	MET	3.2
1	F	276	SER	3.1
1	F	323	GLN	3.1
1	F	328	TYR	3.1
1	C	494	GLN	3.1
1	C	282	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	496	GLY	3.1
1	F	335	ILE	3.1
1	B	10	SER	3.0
1	F	141	MET	3.0
1	B	272	LYS	3.0
1	A	432	ASN	3.0
1	F	360	GLY	3.0
1	F	13	PHE	3.0
1	D	278	GLU	3.0
1	F	144	ASN	3.0
1	F	275	ASN	3.0
1	F	175	GLU	3.0
1	C	251	PHE	3.0
1	F	254	THR	3.0
1	F	327	PRO	3.0
1	F	269	VAL	2.9
1	B	273	SER	2.9
1	F	293	ARG	2.9
1	D	259	ILE	2.9
1	F	280	ILE	2.9
1	F	157	PHE	2.9
1	C	154	ALA	2.9
1	F	34	PHE	2.8
1	F	265	GLY	2.8
1	B	259	ILE	2.8
1	F	321	GLU	2.8
1	F	428	ASN	2.8
1	F	273	SER	2.8
1	C	143	THR	2.8
1	C	306	GLY	2.8
1	F	221	ARG	2.8
1	E	496	GLY	2.7
1	F	296	CYS	2.7
1	A	499	GLY	2.7
1	F	433	GLU	2.7
1	E	433	GLU	2.7
1	F	257	GLU	2.7
1	B	138	HIS	2.7
1	B	495	SER	2.7
1	D	280	ILE	2.7
1	F	337	GLU	2.7
1	A	275	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	334	ASP	2.7
1	B	499	GLY	2.7
1	F	400	GLU	2.7
1	C	307	VAL	2.6
1	F	348	GLN	2.6
1	B	131	TYR	2.6
1	A	143	THR	2.6
1	F	352	LEU	2.6
1	F	20	GLY	2.6
1	F	320	ASP	2.6
1	F	455	ALA	2.6
1	F	173	ASP	2.6
1	F	182	ASP	2.6
1	F	394	PHE	2.6
1	C	323	GLN	2.6
1	F	252	VAL	2.6
1	F	58	THR	2.6
1	F	389	LYS	2.6
1	A	285	ASN	2.6
1	F	134	PHE	2.5
1	C	135	ILE	2.5
1	C	256	ILE	2.5
1	A	497	CYS	2.5
1	F	137	PRO	2.5
1	C	272	LYS	2.5
1	D	10	SER	2.5
1	C	278	GLU	2.5
1	E	309	ILE	2.4
1	E	400	GLU	2.4
1	A	494	GLN	2.4
1	F	133	LYS	2.4
1	B	496	GLY	2.4
1	E	395	GLY	2.4
1	B	427	CYS	2.4
1	C	324	THR	2.4
1	E	275	ASN	2.4
1	B	256	ILE	2.4
1	E	430	LYS	2.4
1	A	395	GLY	2.4
1	C	132	GLY	2.4
1	C	361	SER	2.4
1	C	495	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	279	THR	2.4
1	F	336	LEU	2.4
1	F	262	GLY	2.4
1	F	356	ARG	2.4
1	D	497	CYS	2.4
1	F	139	LYS	2.4
1	F	305	VAL	2.3
1	F	384	GLY	2.3
1	A	327	PRO	2.3
1	F	330	TYR	2.3
1	A	12	ASP	2.3
1	E	276	SER	2.3
1	F	37	LYS	2.3
1	C	259	ILE	2.3
1	F	245	ILE	2.3
1	B	291	VAL	2.3
1	A	147	GLY	2.3
1	F	135	ILE	2.3
1	E	362	THR	2.3
1	A	13	PHE	2.3
1	F	176	TYR	2.3
1	C	138	HIS	2.3
1	B	11	TYR	2.3
1	B	432	ASN	2.3
1	F	220	VAL	2.3
1	C	279	THR	2.3
1	D	433	GLU	2.2
1	C	328	TYR	2.2
1	C	142	ALA	2.2
1	B	398	ASN	2.2
1	F	274	THR	2.2
1	A	315	LYS	2.2
1	C	131	TYR	2.2
1	E	260	GLU	2.2
1	F	313	THR	2.2
1	F	368	ASP	2.2
1	A	302	LEU	2.2
1	A	131	TYR	2.2
1	F	174	LYS	2.2
1	B	271	ALA	2.2
1	F	153	SER	2.2
1	F	42	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	274	THR	2.2
1	A	135	ILE	2.1
1	F	48	PRO	2.1
1	C	274	THR	2.1
1	F	145	ASN	2.1
1	F	487	ARG	2.1
1	B	137	PRO	2.1
1	F	300	ILE	2.1
1	F	329	ILE	2.1
1	C	255	LYS	2.1
1	F	354	ALA	2.1
1	F	138	HIS	2.1
1	A	133	LYS	2.1
1	F	291	VAL	2.1
1	A	362	THR	2.1
1	B	428	ASN	2.1
1	A	333	GLY	2.1
1	E	261	ALA	2.1
1	F	247	PHE	2.1
1	F	148	LYS	2.1
1	F	172	GLY	2.1
1	C	141	MET	2.0
1	F	495	SER	2.0
1	F	168	LEU	2.0
1	A	163	GLU	2.0
1	B	397	GLU	2.0
1	F	12	ASP	2.0
1	A	313	THR	2.0
1	A	325	ASN	2.0
1	C	297	THR	2.0
1	D	398	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

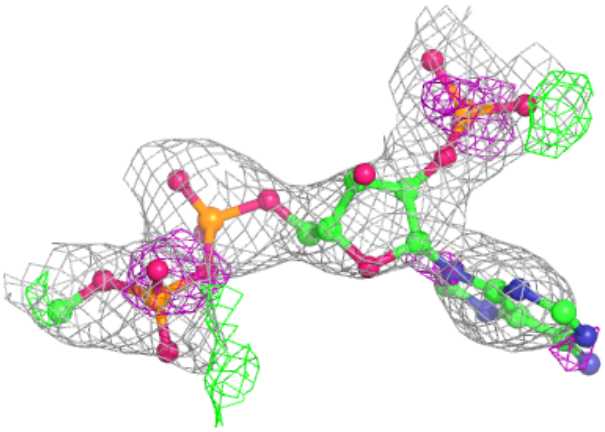
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

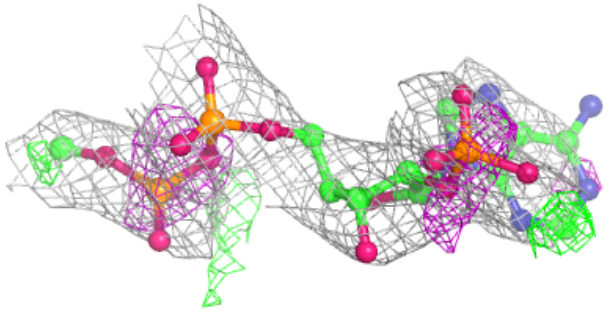
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	F	601	32/48	0.79	0.45	64,73,87,89	0
3	NAP	C	601	32/48	0.83	0.37	64,73,87,89	0
2	FAD	F	600	53/53	0.83	0.39	54,57,61,62	0
3	NAP	B	601	32/48	0.86	0.31	64,73,87,89	0
3	NAP	E	601	32/48	0.87	0.30	64,73,87,89	0
2	FAD	C	600	53/53	0.89	0.33	54,57,61,62	0
3	NAP	D	601	32/48	0.89	0.32	64,73,87,89	0
3	NAP	A	601	32/48	0.90	0.34	64,73,87,89	0
2	FAD	A	600	53/53	0.94	0.27	54,57,61,62	0
2	FAD	E	600	53/53	0.95	0.30	54,57,61,61	0
2	FAD	B	600	53/53	0.95	0.28	54,57,61,62	0
2	FAD	D	600	53/53	0.96	0.28	54,57,61,62	0

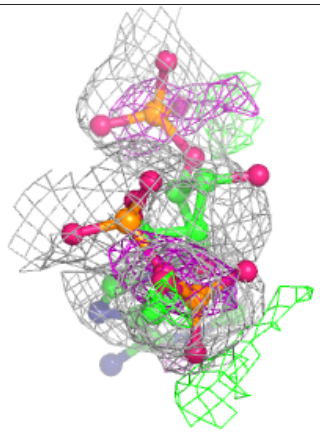
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

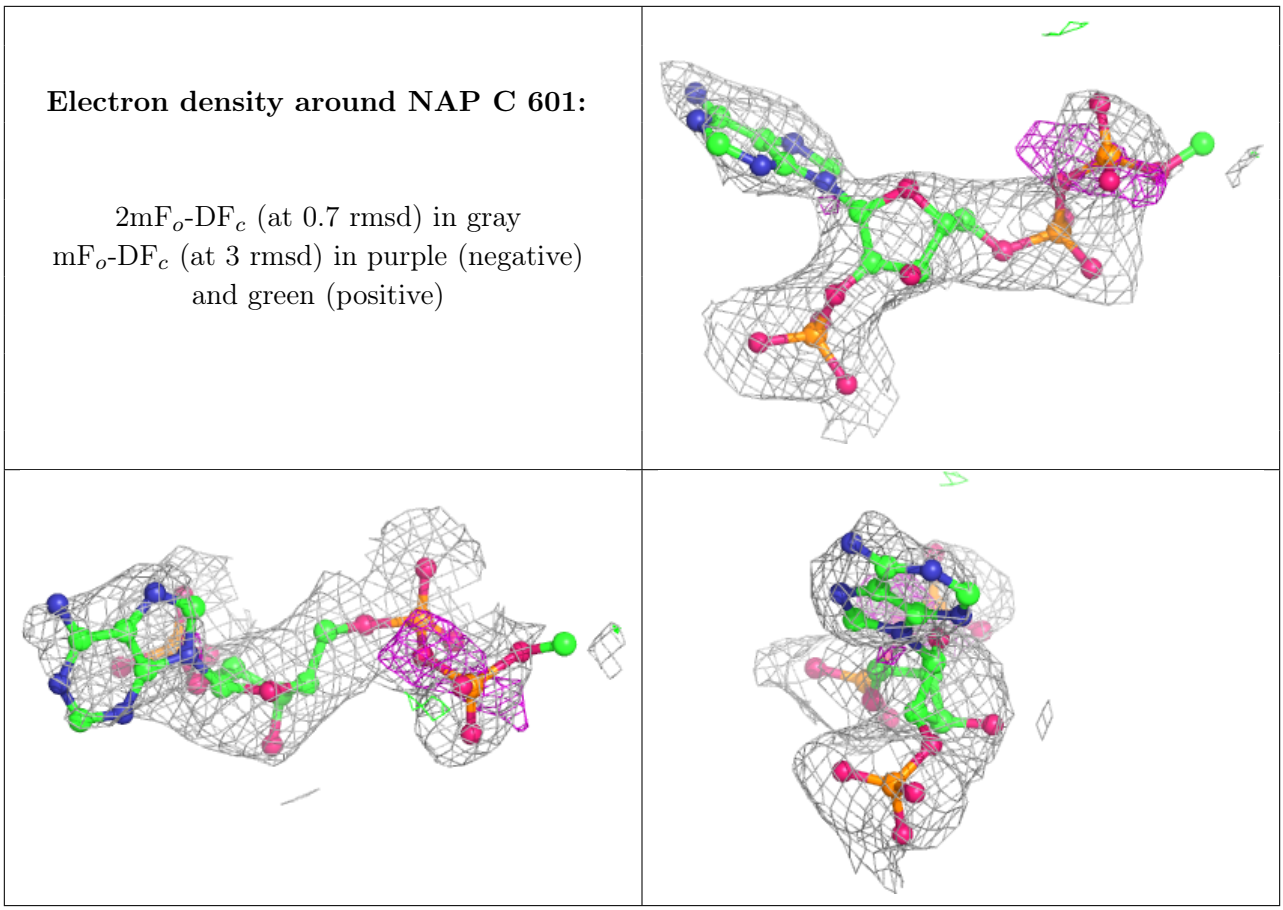






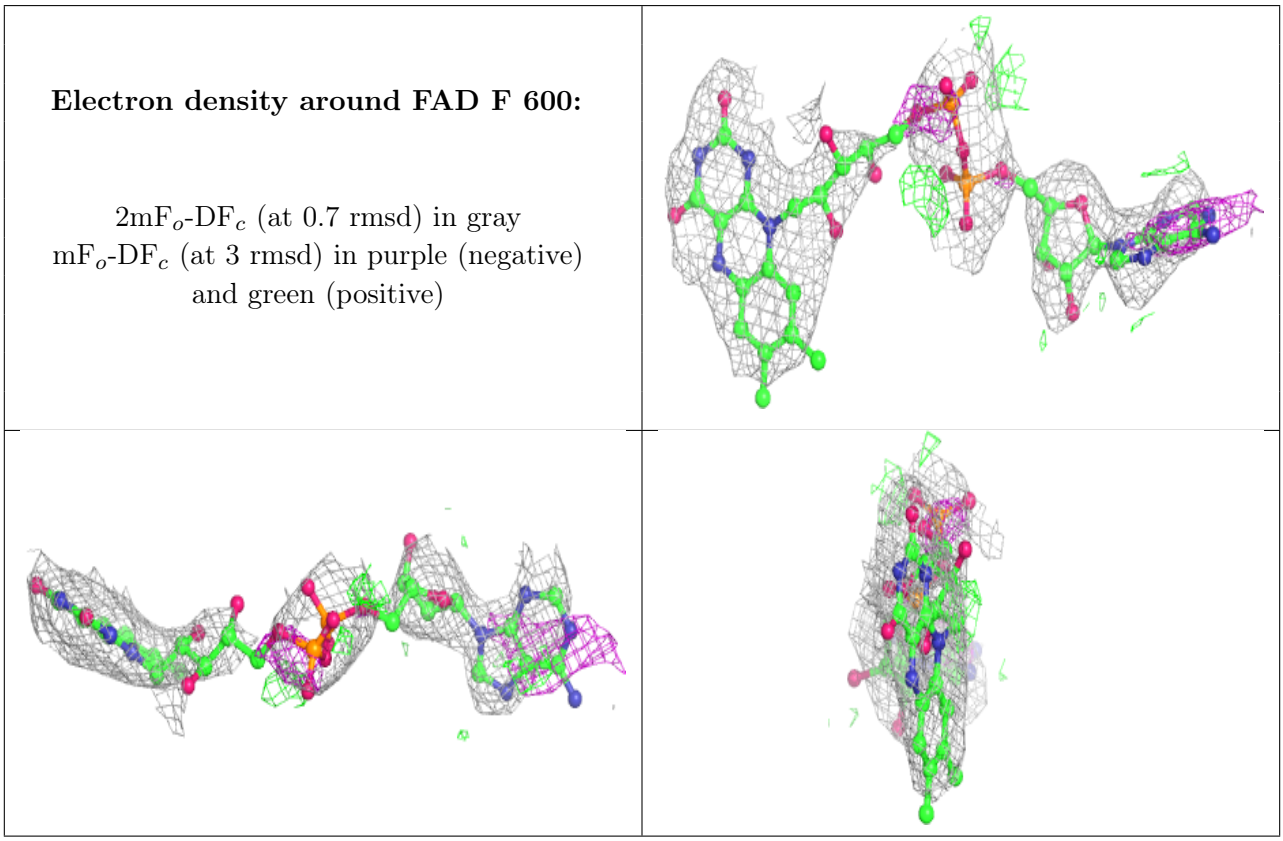
Electron density around NAP C 601:

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



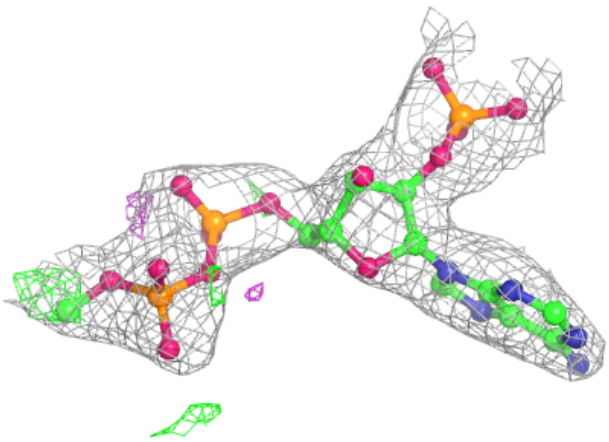
Electron density around FAD F 600:

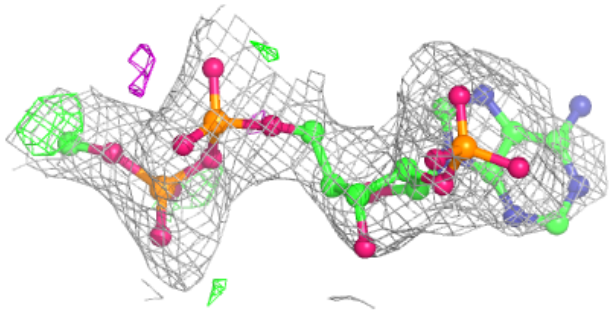
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

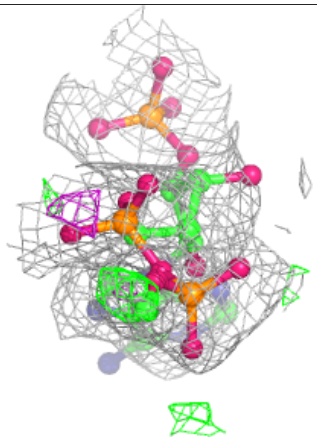


Electron density around NAP B 601:

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

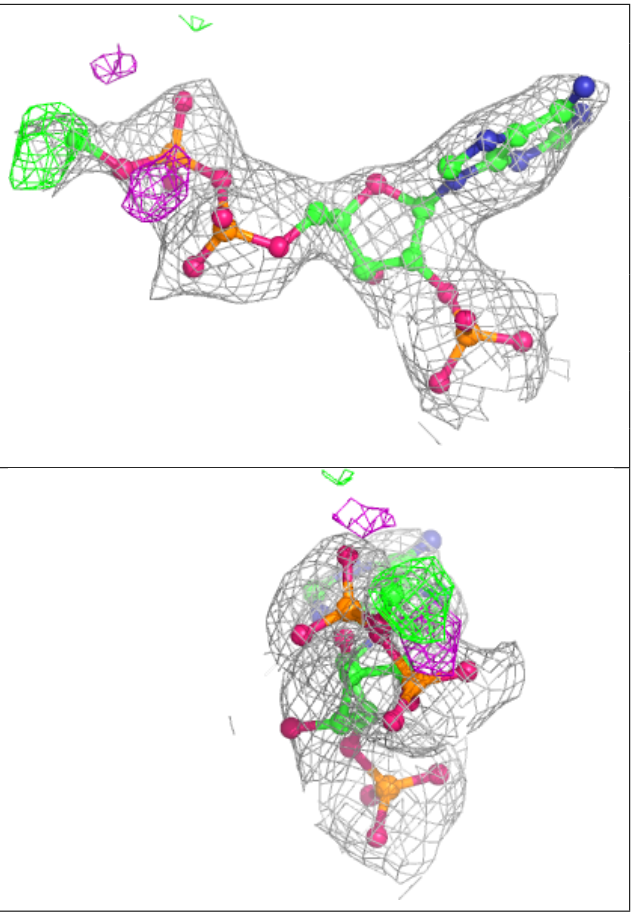






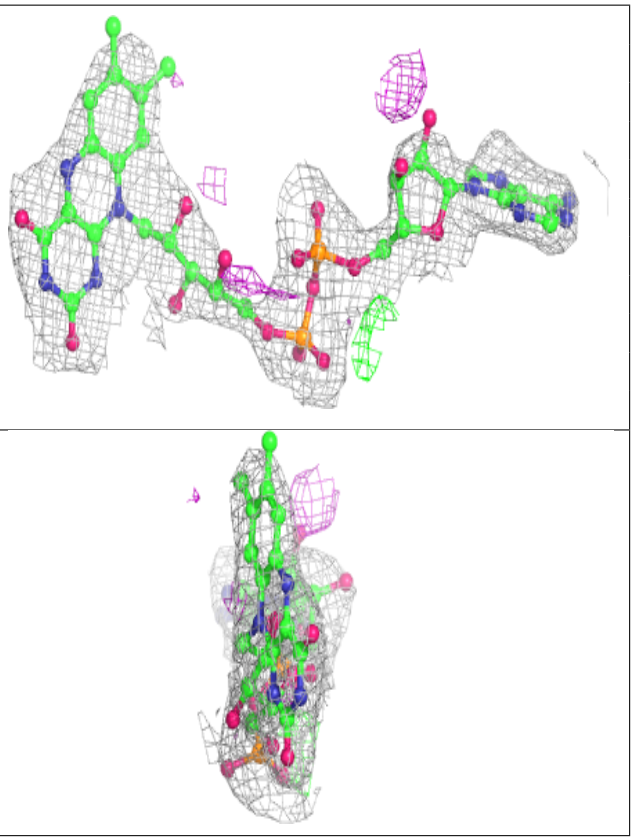
Electron density around NAP E 601:

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



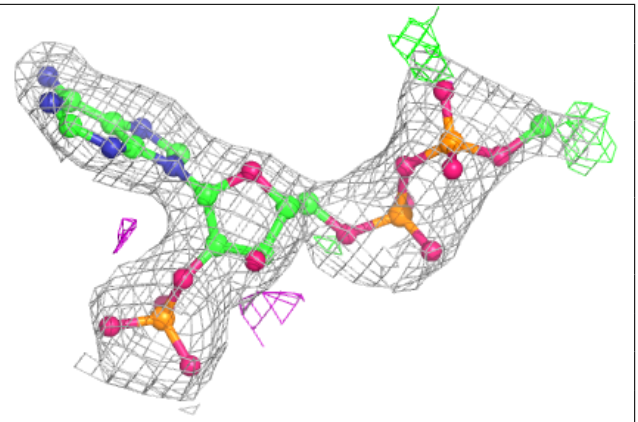
Electron density around FAD C 600:

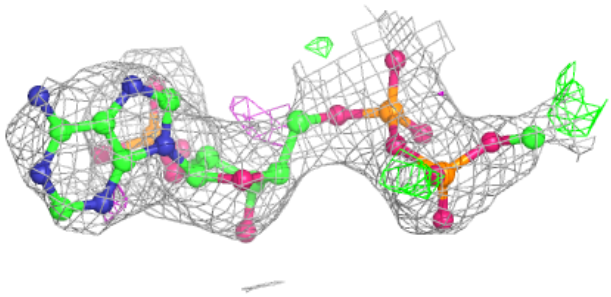
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

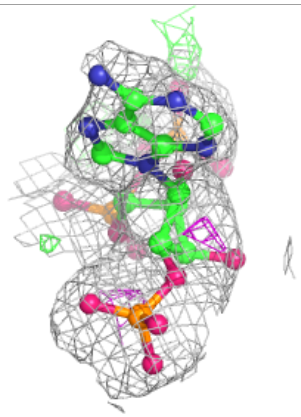


Electron density around NAP D 601:

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

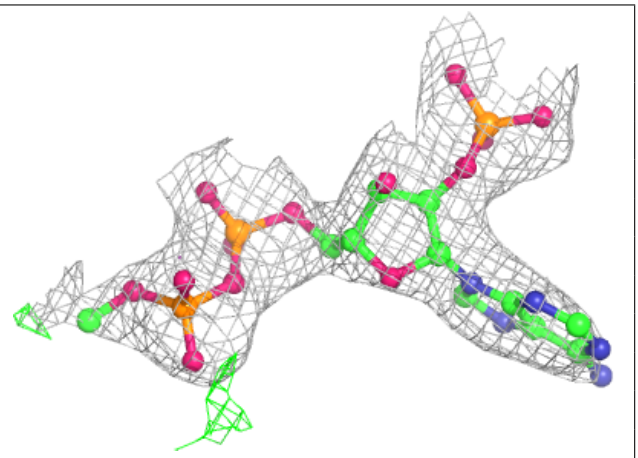


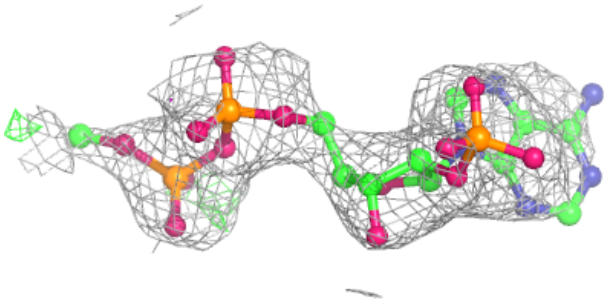


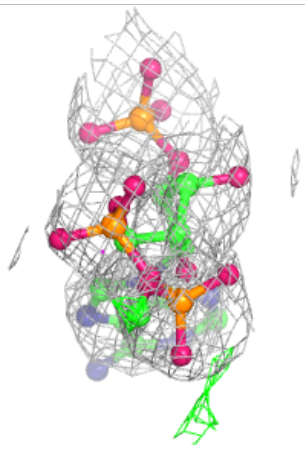


Electron density around NAP A 601:

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

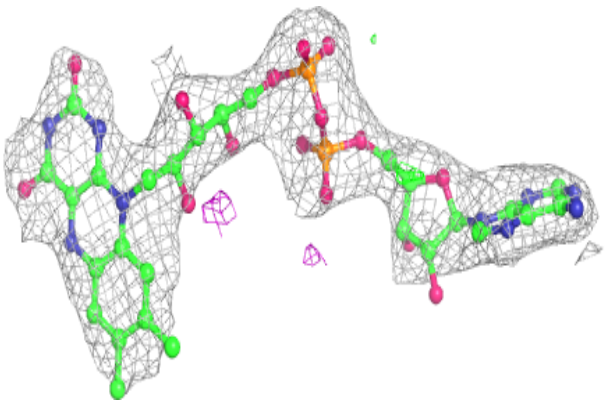


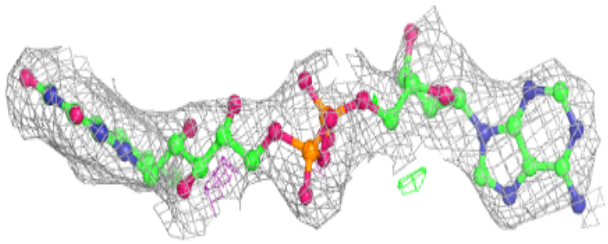


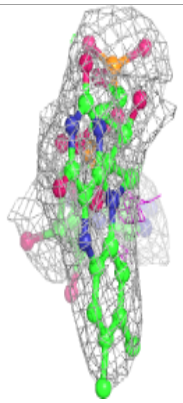


Electron density around FAD A 600:

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

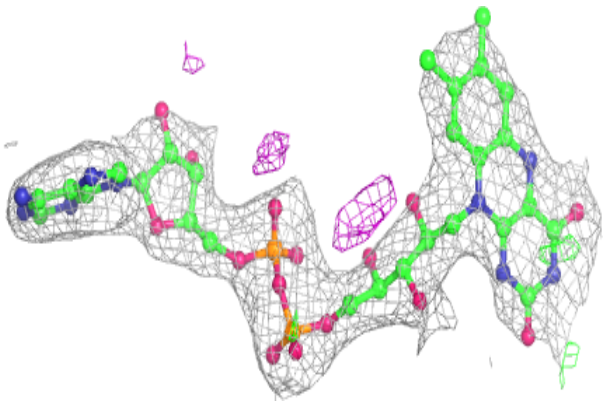


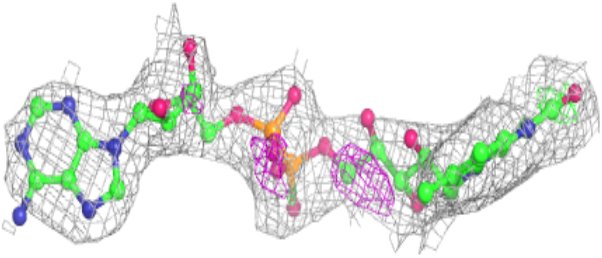


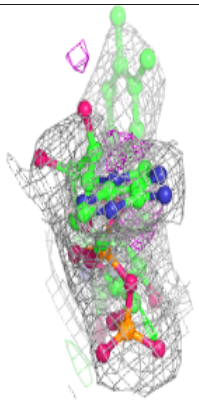


Electron density around FAD E 600:

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

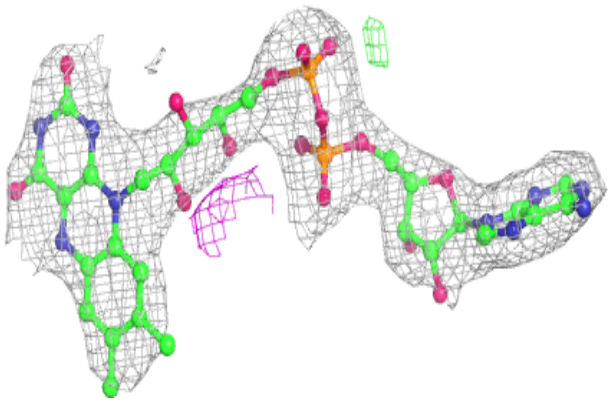


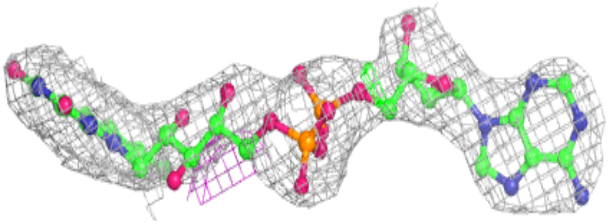


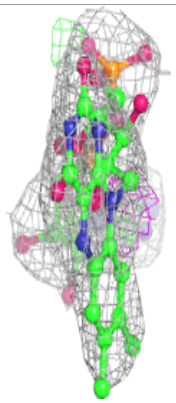


Electron density around FAD B 600:

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

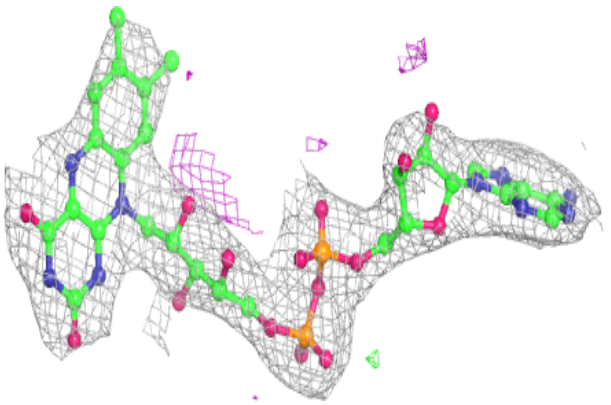


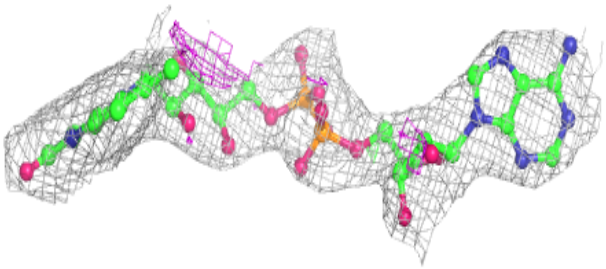


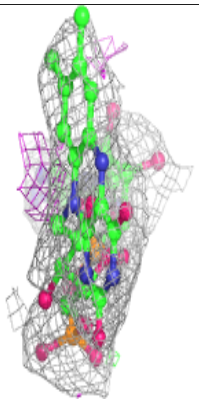


Electron density around FAD D 600:

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







6.5 Other polymers (i)

There are no such residues in this entry.