



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:15 PM UTC

PDB ID : 3EAO / pdb_00003eao
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

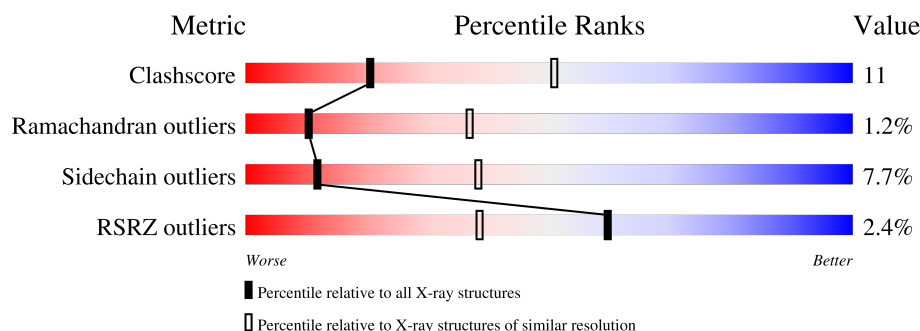
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	0% 72% 23% ...
1	B	499	0% 75% 20% ...
1	C	499	3% 70% 23% ...
1	D	499	2% 72% 22% ...
1	E	499	2% 74% 21% ...
1	F	499	6% 65% 30% ...

2 Entry composition

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.

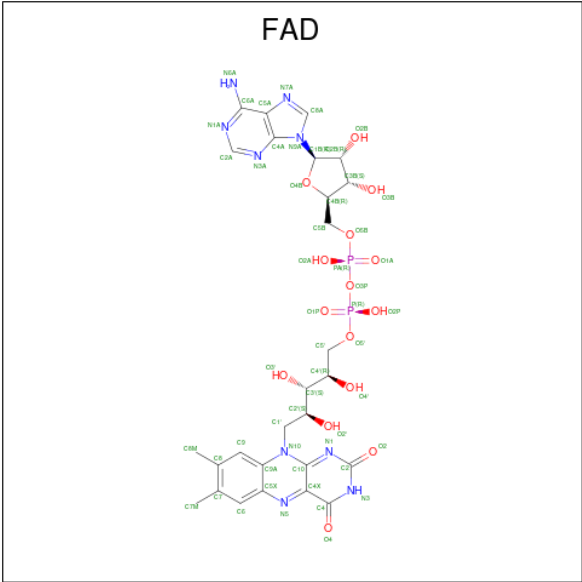
- Molecule 1 is a protein called Thioredoxin reductase 1, cytoplasmic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	Se	0	0	0
			3762	2390	636	714	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:

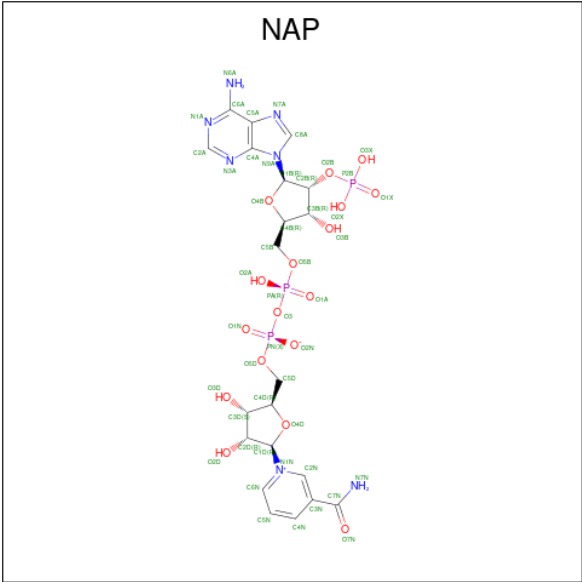
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ARG	ASN	conflict	UNP O89049
A	53	TRP	GLY	conflict	UNP O89049
B	52	ARG	ASN	conflict	UNP O89049
B	53	TRP	GLY	conflict	UNP O89049
C	52	ARG	ASN	conflict	UNP O89049
C	53	TRP	GLY	conflict	UNP O89049
D	52	ARG	ASN	conflict	UNP O89049
D	53	TRP	GLY	conflict	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 (CCD ID: 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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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		

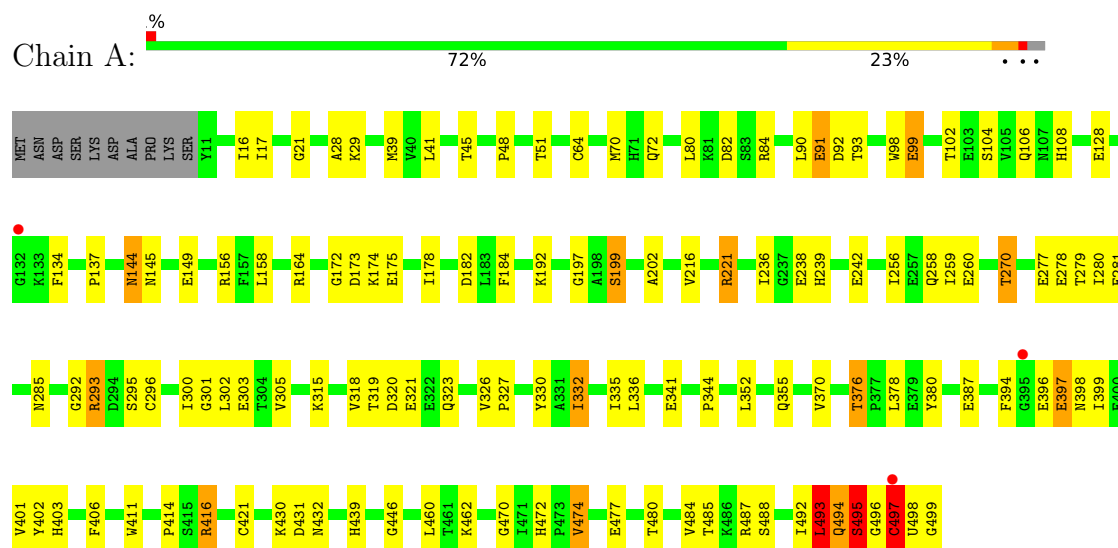
- Molecule 4 is water.

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

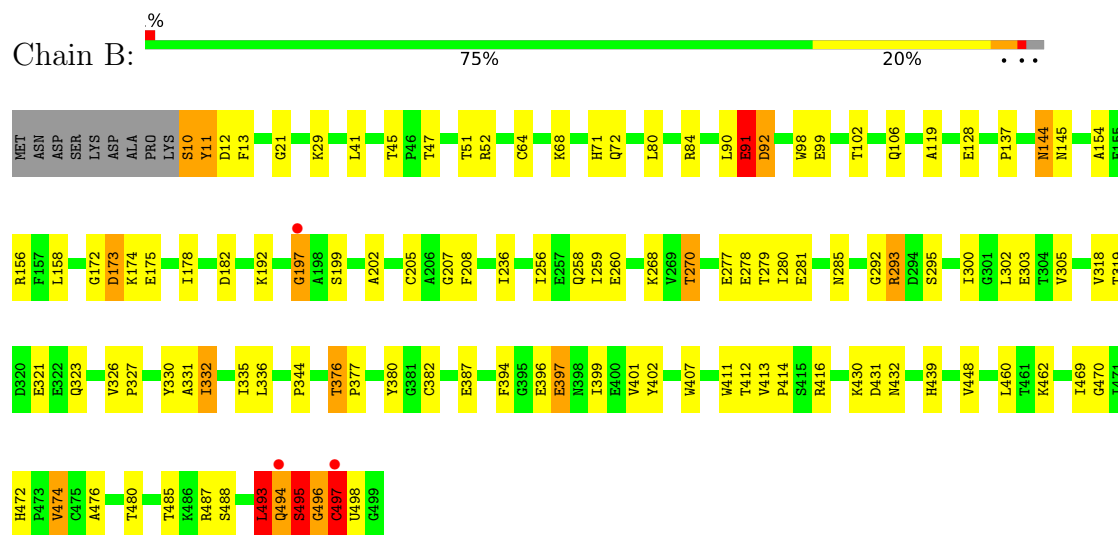
3 Residue-property plots

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

• Molecule 1: Thioredoxin reductase 1, cytoplasmic

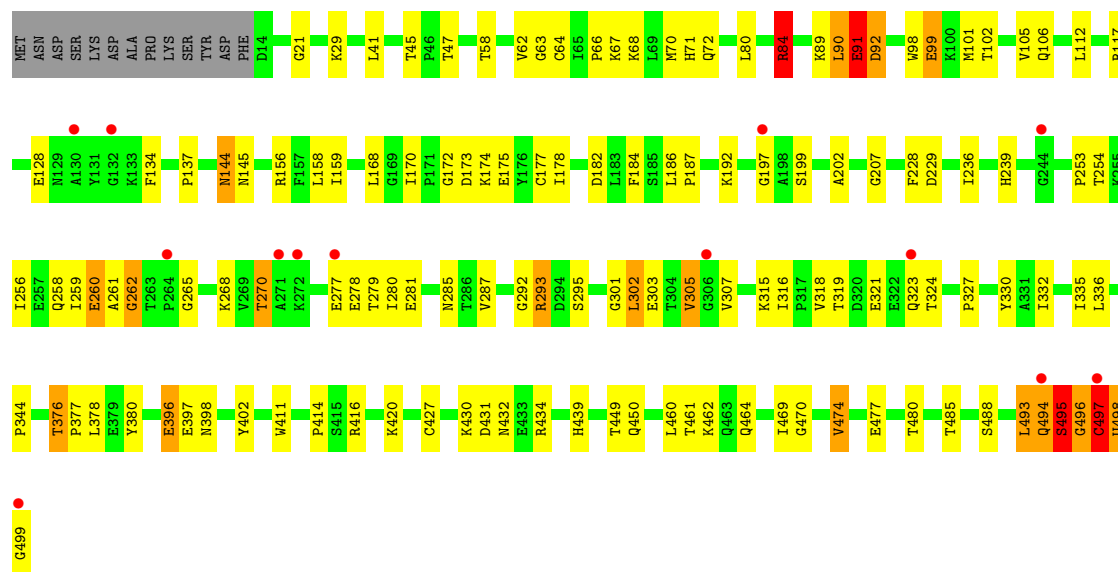


• Molecule 1: Thioredoxin reductase 1, cytoplasmic

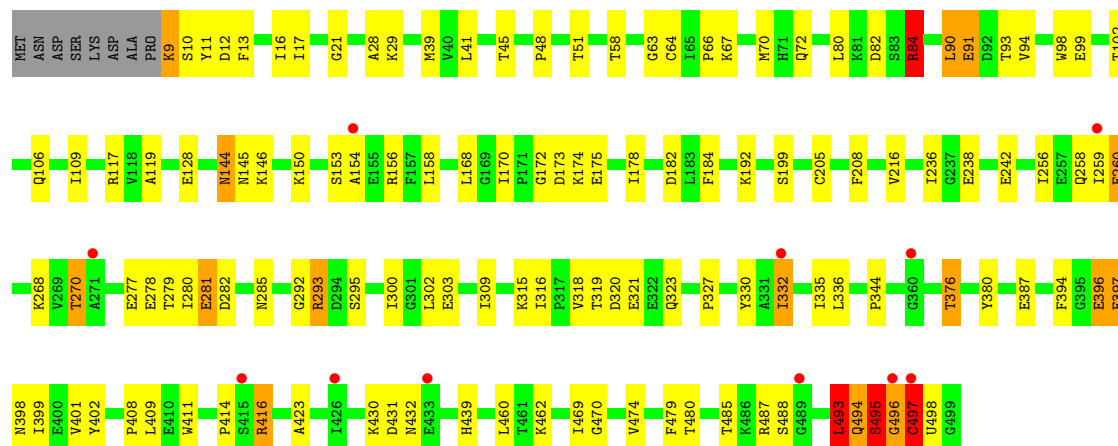


• Molecule 1: Thioredoxin reductase 1, cytoplasmic

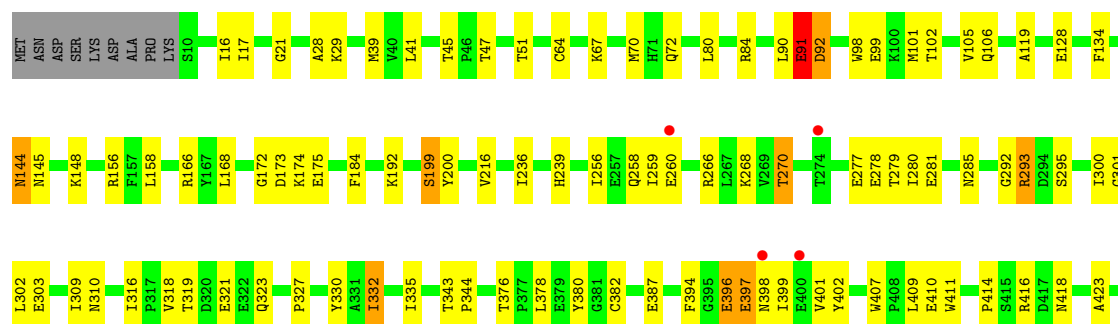
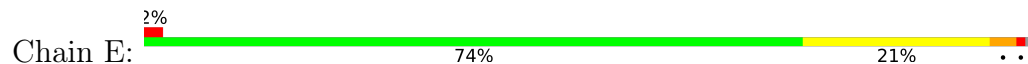




- Molecule 1: Thioredoxin reductase 1, cytoplasmic

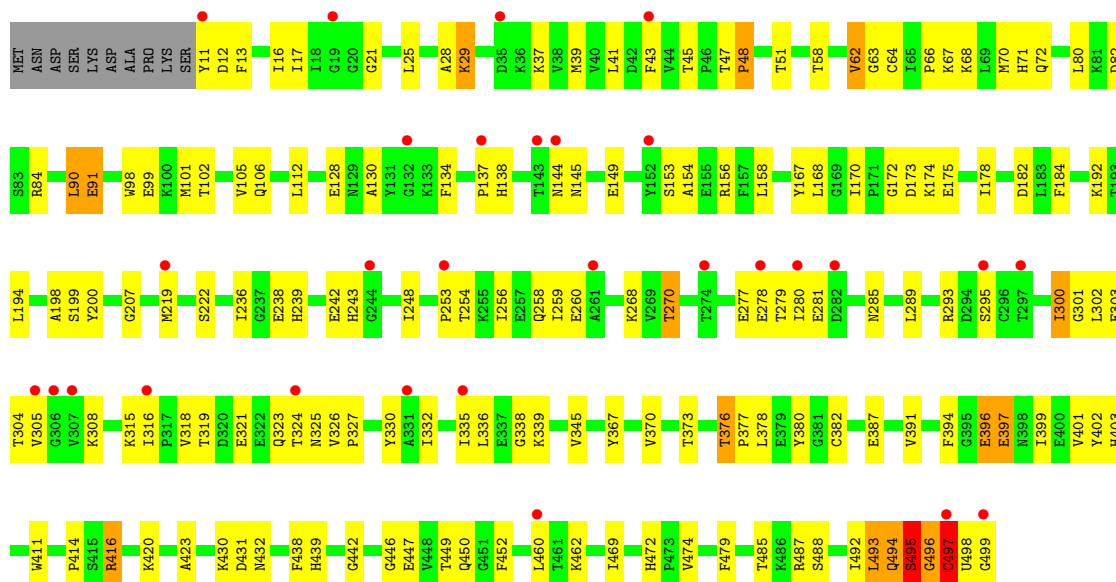


- Molecule 1: Thioredoxin reductase 1, cytoplasmic





- Molecule 1: Thioredoxin reductase 1, cytoplasmic



4 Data and refinement statistics

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 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-3.10) 99.2 (30.00-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.38 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SEC, 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	0.79	0/3829	1.01	11/5177 (0.2%)
1	B	0.81	1/3835 (0.0%)	1.01	10/5185 (0.2%)
1	C	0.86	0/3796	1.03	11/5132 (0.2%)
1	D	0.86	0/3844	1.00	11/5196 (0.2%)
1	E	0.83	0/3835	0.99	7/5185 (0.1%)
1	F	1.03	4/3829 (0.1%)	1.06	11/5177 (0.2%)
All	All	0.87	5/22968 (0.0%)	1.02	61/31052 (0.2%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	222	SER	CA-C	7.31	1.56	1.52
1	F	345	VAL	CA-CB	5.71	1.60	1.54
1	F	198	ALA	CA-CB	5.57	1.60	1.53
1	B	407	TRP	C-O	-5.28	1.20	1.25
1	F	300	ILE	CA-CB	5.17	1.60	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ARG	NE-CZ-NH2	9.87	128.08	119.20
1	B	11	TYR	N-CA-C	9.62	123.03	110.43
1	A	221	ARG	NE-CZ-NH2	9.18	127.46	119.20
1	D	84	ARG	NE-CZ-NH1	-8.82	112.68	121.50
1	D	84	ARG	NE-CZ-NH2	8.47	126.82	119.20
1	A	221	ARG	NE-CZ-NH1	-8.23	113.27	121.50
1	C	84	ARG	CD-NE-CZ	8.22	135.90	124.40
1	C	84	ARG	NE-CZ-NH1	-8.16	113.34	121.50
1	F	494	GLN	N-CA-C	7.36	123.20	107.67
1	D	84	ARG	CD-NE-CZ	7.29	134.61	124.40
1	D	282	ASP	N-CA-C	6.99	119.75	109.69
1	B	494	GLN	CA-C-N	6.85	134.03	121.70
1	B	494	GLN	C-N-CA	6.85	134.03	121.70
1	A	494	GLN	CA-C-N	6.83	134.00	121.70
1	A	494	GLN	C-N-CA	6.83	134.00	121.70
1	D	494	GLN	CA-C-N	6.61	133.61	121.70
1	D	494	GLN	C-N-CA	6.61	133.61	121.70
1	E	494	GLN	CA-C-N	6.54	133.48	121.70
1	E	494	GLN	C-N-CA	6.54	133.48	121.70
1	F	494	GLN	CA-C-N	6.53	133.45	121.70
1	F	494	GLN	C-N-CA	6.53	133.45	121.70
1	C	494	GLN	CA-C-N	6.52	133.43	121.70
1	C	494	GLN	C-N-CA	6.52	133.43	121.70
1	F	494	GLN	N-CA-CB	-6.39	101.23	111.58
1	A	496	GLY	CA-C-N	6.35	133.13	121.70
1	A	496	GLY	C-N-CA	6.35	133.13	121.70
1	C	494	GLN	N-CA-C	6.34	121.05	107.67
1	E	494	GLN	N-CA-C	6.33	121.03	107.67
1	E	494	GLN	N-CA-CB	-6.33	101.33	111.58
1	C	494	GLN	N-CA-CB	-6.27	101.42	111.58
1	F	496	GLY	CA-C-N	6.21	132.87	121.70
1	F	496	GLY	C-N-CA	6.21	132.87	121.70
1	D	496	GLY	CA-C-N	6.16	132.79	121.70
1	D	496	GLY	C-N-CA	6.16	132.79	121.70
1	F	420	LYS	N-CA-C	-6.14	105.81	113.55
1	B	496	GLY	CA-C-N	6.12	132.72	121.70
1	B	496	GLY	C-N-CA	6.12	132.72	121.70
1	D	282	ASP	N-CA-CB	-6.02	101.77	110.87
1	D	11	TYR	N-CA-C	5.99	118.32	109.69
1	A	216	VAL	N-CA-C	5.97	116.46	108.11
1	F	326	VAL	CA-C-N	5.87	126.28	119.47
1	F	326	VAL	C-N-CA	5.87	126.28	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	LYS	N-CA-C	-5.84	106.19	113.55
1	C	262	GLY	N-CA-C	5.80	126.92	113.18
1	E	496	GLY	CA-C-N	5.76	132.07	121.70
1	E	496	GLY	C-N-CA	5.76	132.07	121.70
1	D	216	VAL	N-CA-C	5.70	116.09	108.11
1	B	11	TYR	CA-C-N	5.69	127.91	120.28
1	B	11	TYR	C-N-CA	5.69	127.91	120.28
1	A	484	VAL	N-CA-C	5.57	116.79	108.54
1	B	326	VAL	CA-C-N	5.51	125.87	119.47
1	B	326	VAL	C-N-CA	5.51	125.87	119.47
1	C	496	GLY	CA-C-N	5.35	131.34	121.70
1	C	496	GLY	C-N-CA	5.35	131.34	121.70
1	E	216	VAL	N-CA-C	5.25	115.46	108.11
1	B	173	ASP	N-CA-C	5.15	116.58	111.07
1	F	391	VAL	N-CA-C	-5.09	105.36	110.30
1	A	221	ARG	CD-NE-CZ	5.08	131.52	124.40
1	F	449	THR	N-CA-C	5.08	116.50	111.07
1	A	326	VAL	CA-C-N	5.03	126.12	119.84
1	A	326	VAL	C-N-CA	5.03	126.12	119.84

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
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 ⓘ

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	88	0
1	B	3768	0	3767	76	0
1	C	3731	0	3740	95	0
1	D	3777	0	3779	91	0
1	E	3768	0	3766	93	0
1	F	3762	0	3761	115	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
All	All	23114	0	22826	514	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 (514) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:91:GLU:CD	1:E:92:ASP:H	1.72	0.98
1:A:197:GLY:O	1:A:202:ALA:HB1	1.66	0.94
1:B:197:GLY:O	1:B:202:ALA:CB	2.19	0.90
1:C:91:GLU:CD	1:C:92:ASP:H	1.82	0.88
1:B:91:GLU:CD	1:B:92:ASP:H	1.82	0.87
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:GLU:CD	1:B:92:ASP:N	2.48	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:C:91:GLU:CD	1:C:92:ASP:N	2.49	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:C:258:GLN:CD	1:C:260:GLU:O	2.37	0.68
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:D:258:GLN:CD	1:D:260:GLU:O	2.38	0.66
1:E:84:ARG:NH2	1:E:91:GLU:O	2.28	0.66
1:E:91:GLU:CD	1:E:92:ASP:N	2.49	0.65
1:E:258:GLN:CD	1:E:260:GLU:O	2.40	0.65
1:A:411:TRP:C	1:A:414:PRO:HD2	2.21	0.64
1:E:469:ILE:CG1	1:F:370:VAL:HG22	2.28	0.64
1:F:497:CYS:C	1:F:498:SEC:SE	2.90	0.64
1:B:431:ASP:O	1:B:432:ASN:HB2	1.97	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
1:A:99:GLU:CB	1:D:146:LYS:HE3	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:THR:OG1	1:A:488:SER:HB3	2.01	0.60
1:D:493:LEU:HB3	1:D:494:GLN:CB	2.31	0.60
1:A:197:GLY:C	1:A:202:ALA:CB	2.74	0.60
1:B:84:ARG:HD3	1:D:150:LYS:HE2	1.83	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:F:411:TRP:C	1:F:414:PRO:HD2	2.27	0.60
1:C:99:GLU:OE1	1:E:148:LYS:HE3	2.02	0.60
1:F:258:GLN:CD	1:F:260:GLU:O	2.44	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:497:CYS:C	1:E:498:SEC:SE	2.94	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
1:B:411:TRP:C	1:B:414:PRO:HD2	2.31	0.56
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:F:16:ILE:HG12	1:F:39:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:TRP:C	1:C:414:PRO:HD2	2.30	0.56
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:C:497:CYS:C	1:C:498:SEC:SE	3.00	0.55
1:E:411:TRP:C	1:E:414:PRO:HD2	2.31	0.55
1:C:158:LEU:HD11	1:C:332:ILE:CG1	2.36	0.55
1:C:402:TYR:CD2	1:C:462:LYS:HE2	2.41	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: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:F:431:ASP:O	1:F:432:ASN:HB2	2.06	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:A:497:CYS:C	1:A:498:SEC:SE	3.00	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:D:497:CYS:C	1:D:498:SEC:SE	3.01	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:D:319:THR:C	1:D:321:GLU:H	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:91:GLU:H	1:F:91:GLU:CD	2.16	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:D:411:TRP:C	1:D:414:PRO:HD2	2.35	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:A:319:THR:C	1:A:321:GLU:H	2.18	0.51
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: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: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:89:LYS:C	1:D:94:VAL:HG13	2.37	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
1:A:370:VAL:HG22	1:B:469:ILE:HG13	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:319:THR:C	1:E:321:GLU:H	2.18	0.50
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: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:B:197:GLY:C	1:B:202:ALA:CB	2.84	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:D:431:ASP:O	1:D:432:ASN:HB2	2.11	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:F:319:THR:C	1:F:321:GLU:H	2.21	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:B:319:THR:C	1:B:321:GLU:H	2.21	0.48
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
1:E:493:LEU:HD23	1:E:494:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:449:THR:O	1:C:450:GLN:C	2.55	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:O	1:B:259:ILE:HG22	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:B:497:CYS:C	1:B:498:SEC:SE	3.07	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: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: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:C:170:ILE:HD12	1:C:254:THR:C	2.40	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
1:E:144:ASN:OD1	1:E:144:ASN:C	2.57	0.46
1:E:397:GLU:HA	1:E:487:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:408:PRO:O	1:D:409:LEU:C	2.57	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:B:292:GLY:C	1:B:293:ARG:HG2	2.38	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:A:319:THR:C	1:A:321:GLU:N	2.74	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:376:THR:O	1:C:377:PRO:C	2.59	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:D:319:THR:C	1:D:321:GLU:N	2.74	0.46
1:E:16:ILE:HG12	1:E:39:MET:HE2	1.98	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: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:F:199:SER:O	1:F:200:TYR:C	2.59	0.45
1:C:72:GLN:HA	1:C:72:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:292:GLY:C	1:E:293:ARG:HG2	2.42	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:B:144:ASN:C	1:B:144:ASN:OD1	2.59	0.45
1:C:319:THR:C	1:C:321:GLU:H	2.24	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:F:319:THR:C	1:F:321:GLU:N	2.75	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: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:E:319:THR:C	1:E:321:GLU:N	2.76	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:170:ILE:HD12	1:F:254:THR:C	2.43	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:C:228:PHE:O	1:C:229:ASP:C	2.61	0.43
1:E:310:ASN:OD1	1:E:310:ASN:C	2.61	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:144:ASN:OD1	1:A:144:ASN:C	2.62	0.43
1:A:406:PHE:CZ	1:A:421:CYS:HB3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:144:ASN:OD1	1:C:144:ASN:C	2.62	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
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: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:C:493:LEU:C	1:C:495:SER:HB2	2.45	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:E:199:SER:O	1:E:200:TYR:C	2.62	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: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:319:THR:C	1:B:321:GLU:N	2.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:MET:HE1	1:E:102:THR:HG22	2.02	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:144:ASN:OD1	1:D:144:ASN:C	2.63	0.41
1:F:308:LYS:HD2	1:F:325:ASN:HD22	1.85	0.41
1:A:292:GLY:C	1:A:293:ARG:HG2	2.44	0.41
1:A:108:HIS:CE1	1:B:412:THR:HB	2.55	0.41
1:A:474:VAL:O	1:A:477:GLU:HG2	2.20	0.41
1:C:344:PRO:HB2	1:D:469:ILE:HG22	2.01	0.41
1:D:292:GLY:C	1:D:293:ARG:HG2	2.45	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: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:C:292:GLY:C	1:C:293:ARG:HG2	2.44	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: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:319:THR:C	1:C:321:GLU:N	2.79	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:D:16:ILE:HG12	1:D:39:MET:HE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:496:GLY:HA2	1:F:497:CYS:SG	2.61	0.41
1:A:16:ILE:HG12	1:A:39:MET:HE2	2.03	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:493:LEU:C	1:E:495:SER:HB2	2.46	0.41
1:E:410:GLU:OE2	1:F:68:LYS:HE2	2.20	0.40
1:F:43:PHE:HB2	1:F:130:ALA:C	2.46	0.40
1:B:331:ALA:C	1:B:336:LEU:HD21	2.47	0.40
1:B:380:TYR:CE1	1:B:382:CYS:HB3	2.56	0.40
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%)	10	37
1	B	487/499 (98%)	440 (90%)	42 (9%)	5 (1%)	12	41
1	C	483/499 (97%)	437 (90%)	42 (9%)	4 (1%)	16	47
1	D	488/499 (98%)	450 (92%)	31 (6%)	7 (1%)	9	34
1	E	487/499 (98%)	441 (91%)	40 (8%)	6 (1%)	10	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	486/499 (97%)	437 (90%)	43 (9%)	6 (1%)	10	37
All	All	2917/2994 (97%)	2641 (90%)	242 (8%)	34 (1%)	10	37

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
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 ⓘ

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%)	372 (92%)	32 (8%)	11	37
1	B	405/413 (98%)	372 (92%)	33 (8%)	11	36
1	C	401/413 (97%)	369 (92%)	32 (8%)	11	37
1	D	406/413 (98%)	374 (92%)	32 (8%)	11	37
1	E	405/413 (98%)	376 (93%)	29 (7%)	13	40
1	F	404/413 (98%)	375 (93%)	29 (7%)	13	40
All	All	2425/2478 (98%)	2238 (92%)	187 (8%)	12	38

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	45	THR
1	A	48	PRO
1	A	51	THR
1	A	64	CYS
1	A	90	LEU
1	A	92	ASP
1	A	93	THR
1	A	99	GLU
1	A	144	ASN
1	A	145	ASN
1	A	149	GLU
1	A	175	GLU
1	A	199	SER
1	A	270	THR
1	A	277	GLU
1	A	279	THR
1	A	280	ILE
1	A	293	ARG
1	A	303	GLU
1	A	318	VAL
1	A	332	ILE

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Mol	Chain	Res	Type
1	A	341	GLU
1	A	376	THR
1	A	396	GLU
1	A	397	GLU
1	A	416	ARG
1	A	460	LEU
1	A	474	VAL
1	A	493	LEU
1	A	495	SER
1	A	497	CYS
1	B	10	SER
1	B	11	TYR
1	B	12	ASP
1	B	29	LYS
1	B	45	THR
1	B	47	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	144	ASN
1	B	145	ASN
1	B	175	GLU
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	332	ILE
1	B	376	THR
1	B	396	GLU
1	B	397	GLU
1	B	416	ARG
1	B	460	LEU
1	B	474	VAL
1	B	495	SER

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Mol	Chain	Res	Type
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	145	ASN
1	C	175	GLU
1	C	199	SER
1	C	270	THR
1	C	277	GLU
1	C	279	THR
1	C	280	ILE
1	C	293	ARG
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	416	ARG
1	C	460	LEU
1	C	474	VAL
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

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Mol	Chain	Res	Type
1	D	93	THR
1	D	99	GLU
1	D	117	ARG
1	D	144	ASN
1	D	145	ASN
1	D	175	GLU
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	332	ILE
1	D	376	THR
1	D	396	GLU
1	D	397	GLU
1	D	416	ARG
1	D	460	LEU
1	D	474	VAL
1	D	495	SER
1	D	497	CYS
1	E	29	LYS
1	E	45	THR
1	E	47	THR
1	E	51	THR
1	E	64	CYS
1	E	90	LEU
1	E	91	GLU
1	E	92	ASP
1	E	99	GLU
1	E	144	ASN
1	E	145	ASN
1	E	175	GLU
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

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Mol	Chain	Res	Type
1	E	318	VAL
1	E	332	ILE
1	E	376	THR
1	E	396	GLU
1	E	397	GLU
1	E	416	ARG
1	E	460	LEU
1	E	474	VAL
1	E	495	SER
1	E	497	CYS
1	F	29	LYS
1	F	45	THR
1	F	47	THR
1	F	48	PRO
1	F	51	THR
1	F	62	VAL
1	F	64	CYS
1	F	90	LEU
1	F	99	GLU
1	F	144	ASN
1	F	145	ASN
1	F	149	GLU
1	F	175	GLU
1	F	270	THR
1	F	277	GLU
1	F	279	THR
1	F	280	ILE
1	F	293	ARG
1	F	303	GLU
1	F	304	THR
1	F	318	VAL
1	F	376	THR
1	F	396	GLU
1	F	397	GLU
1	F	416	ARG
1	F	460	LEU
1	F	474	VAL
1	F	495	SER
1	F	497	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	85	ASN
1	A	108	HIS
1	A	113	ASN
1	A	145	ASN
1	A	258	GLN
1	A	285	ASN
1	A	323	GLN
1	A	439	HIS
1	A	444	ASN
1	A	494	GLN
1	B	72	GLN
1	B	85	ASN
1	B	106	GLN
1	B	108	HIS
1	B	145	ASN
1	B	258	GLN
1	B	285	ASN
1	B	323	GLN
1	B	439	HIS
1	C	72	GLN
1	C	106	GLN
1	C	108	HIS
1	C	138	HIS
1	C	145	ASN
1	C	239	HIS
1	C	258	GLN
1	C	285	ASN
1	C	439	HIS
1	C	494	GLN
1	D	72	GLN
1	D	85	ASN
1	D	113	ASN
1	D	138	HIS
1	D	145	ASN
1	D	239	HIS
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	106	GLN

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Mol	Chain	Res	Type
1	E	113	ASN
1	E	138	HIS
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	113	ASN
1	F	145	ASN
1	F	285	ASN
1	F	323	GLN
1	F	418	ASN
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 oligosaccharides 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	D	601	-	34,34,52	2.36	7 (20%)	50,53,80	1.74	9 (18%)
3	NAP	A	601	-	34,34,52	2.97	8 (23%)	50,53,80	1.64	8 (16%)
3	NAP	C	601	-	34,34,52	3.04	8 (23%)	50,53,80	1.76	11 (22%)
2	FAD	C	600	-	58,58,58	1.90	11 (18%)	85,89,89	1.45	15 (17%)
2	FAD	B	600	-	58,58,58	1.43	8 (13%)	85,89,89	1.52	14 (16%)
2	FAD	F	600	-	58,58,58	2.06	10 (17%)	85,89,89	1.56	13 (15%)
2	FAD	E	600	-	58,58,58	1.45	11 (18%)	85,89,89	1.51	16 (18%)
2	FAD	A	600	-	58,58,58	1.38	8 (13%)	85,89,89	1.48	13 (15%)
3	NAP	B	601	-	34,34,52	2.64	8 (23%)	50,53,80	1.78	11 (22%)
3	NAP	E	601	-	34,34,52	2.82	7 (20%)	50,53,80	1.65	10 (20%)
2	FAD	D	600	-	58,58,58	1.44	8 (13%)	85,89,89	1.42	16 (18%)
3	NAP	F	601	-	34,34,52	3.17	7 (20%)	50,53,80	1.79	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	D	601	-	-	8/24/40/67	0/3/3/5
3	NAP	A	601	-	-	8/24/40/67	0/3/3/5
3	NAP	C	601	-	-	8/24/40/67	0/3/3/5
2	FAD	C	600	-	-	7/34/50/50	0/6/6/6
2	FAD	B	600	-	-	6/34/50/50	0/6/6/6
2	FAD	F	600	-	-	10/34/50/50	0/6/6/6
2	FAD	E	600	-	-	5/34/50/50	0/6/6/6
2	FAD	A	600	-	-	5/34/50/50	0/6/6/6
3	NAP	B	601	-	-	8/24/40/67	0/3/3/5
3	NAP	E	601	-	-	9/24/40/67	0/3/3/5
2	FAD	D	600	-	-	5/34/50/50	0/6/6/6
3	NAP	F	601	-	-	6/24/40/67	0/3/3/5

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NAP	PN-O3	12.15	1.72	1.59
3	F	601	NAP	PN-O3	11.90	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	NAP	PN-O3	11.21	1.71	1.59
3	A	601	NAP	PN-O3	10.71	1.71	1.59
3	B	601	NAP	PN-O3	10.34	1.70	1.59
3	A	601	NAP	PA-O3	9.99	1.70	1.59
2	F	600	FAD	P-O3P	9.82	1.70	1.59
3	F	601	NAP	PA-O3	9.45	1.69	1.59
3	D	601	NAP	PN-O3	9.19	1.69	1.59
3	C	601	NAP	PA-O3	8.32	1.68	1.59
3	E	601	NAP	PA-O3	8.23	1.68	1.59
3	B	601	NAP	PA-O3	8.13	1.68	1.59
2	C	600	FAD	P-O3P	7.66	1.67	1.59
3	D	601	NAP	PA-O3	6.52	1.66	1.59
3	F	601	NAP	P2B-O1X	5.34	1.67	1.50
2	F	600	FAD	C10-N1	5.24	1.43	1.33
2	F	600	FAD	C4X-N5	5.23	1.42	1.30
2	C	600	FAD	C10-N1	5.10	1.43	1.33
2	E	600	FAD	C4X-N5	4.92	1.41	1.30
3	C	601	NAP	P2B-O1X	4.87	1.65	1.50
2	C	600	FAD	PA-O3P	4.73	1.64	1.59
2	A	600	FAD	C4X-N5	4.71	1.40	1.30
2	C	600	FAD	C4X-N5	4.68	1.40	1.30
3	E	601	NAP	PN-O5D	4.66	1.74	1.58
2	A	600	FAD	C10-N1	4.61	1.42	1.33
2	D	600	FAD	C4X-N5	4.55	1.40	1.30
3	F	601	NAP	PN-O5D	4.53	1.73	1.58
3	C	601	NAP	PN-O5D	4.47	1.73	1.58
3	F	601	NAP	P2B-O2X	4.42	1.71	1.54
3	A	601	NAP	PN-O5D	4.36	1.73	1.58
2	F	600	FAD	O4B-C1B	4.23	1.51	1.42
2	B	600	FAD	C4X-N5	4.15	1.39	1.30
2	D	600	FAD	C5A-N7A	-3.97	1.31	1.39
3	B	601	NAP	PN-O5D	3.93	1.71	1.58
2	B	600	FAD	C10-N1	3.87	1.41	1.33
3	A	601	NAP	P2B-O2B	3.81	1.66	1.59
3	A	601	NAP	P2B-O1X	3.80	1.62	1.50
2	E	600	FAD	C10-N1	3.73	1.40	1.33
2	C	600	FAD	O4B-C1B	3.72	1.50	1.42
2	D	600	FAD	C10-N1	3.31	1.39	1.33
2	B	600	FAD	O4B-C1B	3.31	1.49	1.42
3	C	601	NAP	P2B-O2X	3.23	1.66	1.54
2	E	600	FAD	C5A-N7A	-3.18	1.33	1.39
3	D	601	NAP	PN-O5D	3.16	1.69	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	NAP	C5A-N7A	-3.14	1.33	1.39
3	E	601	NAP	P2B-O1X	3.12	1.60	1.50
3	F	601	NAP	P2B-O2B	3.06	1.64	1.59
2	B	600	FAD	C5A-N7A	-3.05	1.33	1.39
2	A	600	FAD	C5A-N7A	-2.99	1.33	1.39
3	C	601	NAP	C1B-N9A	2.99	1.54	1.46
3	D	601	NAP	P2B-O1X	2.98	1.59	1.50
2	F	600	FAD	C2-N1	2.98	1.43	1.36
3	B	601	NAP	C5A-N7A	-2.97	1.33	1.39
2	D	600	FAD	PA-O3P	2.95	1.62	1.59
3	F	601	NAP	O4B-C1B	2.93	1.48	1.42
2	E	600	FAD	O4B-C1B	2.81	1.48	1.42
2	F	600	FAD	PA-O3P	2.79	1.62	1.59
3	E	601	NAP	C5A-N7A	-2.77	1.34	1.39
2	E	600	FAD	C10-N10	2.77	1.43	1.37
2	C	600	FAD	PA-O5B	2.69	1.69	1.59
2	F	600	FAD	C1B-N9A	2.68	1.53	1.46
2	A	600	FAD	P-O3P	2.67	1.62	1.59
3	A	601	NAP	C5A-N7A	-2.66	1.34	1.39
3	B	601	NAP	P2B-O1X	2.65	1.58	1.50
3	C	601	NAP	O4B-C1B	2.65	1.48	1.42
2	B	600	FAD	C1B-N9A	2.64	1.53	1.46
2	D	600	FAD	C4A-N9A	-2.62	1.32	1.37
3	A	601	NAP	C4A-N9A	-2.59	1.32	1.37
2	C	600	FAD	C10-N10	2.55	1.42	1.37
2	E	600	FAD	C4A-N9A	-2.50	1.32	1.37
2	A	600	FAD	C10-N10	2.50	1.42	1.37
3	E	601	NAP	P2B-O3X	-2.45	1.45	1.54
2	E	600	FAD	C1B-N9A	2.44	1.53	1.46
3	E	601	NAP	C4A-N9A	-2.44	1.32	1.37
2	B	600	FAD	PA-O3P	2.42	1.62	1.59
2	F	600	FAD	C10-N10	2.38	1.42	1.37
3	C	601	NAP	C5A-N7A	-2.34	1.34	1.39
2	C	600	FAD	C2-N1	2.33	1.41	1.36
2	F	600	FAD	C4-N3	2.32	1.43	1.38
2	E	600	FAD	C2-N1	2.32	1.41	1.36
2	D	600	FAD	PA-O2A	-2.32	1.44	1.55
2	A	600	FAD	PA-O3P	2.31	1.62	1.59
3	B	601	NAP	C4A-N9A	-2.28	1.33	1.37
2	E	600	FAD	PA-O2A	-2.26	1.44	1.55
2	C	600	FAD	C5A-N7A	-2.26	1.35	1.39
2	C	600	FAD	C1B-N9A	2.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAP	C8A-N9A	-2.24	1.33	1.37
2	E	600	FAD	PA-O3P	2.23	1.61	1.59
2	C	600	FAD	C5'-C4'	2.21	1.54	1.51
3	D	601	NAP	C8A-N9A	-2.20	1.33	1.37
2	D	600	FAD	C8A-N9A	-2.20	1.33	1.37
2	A	600	FAD	C4A-N9A	-2.20	1.33	1.37
3	B	601	NAP	P2B-O3X	-2.17	1.46	1.54
2	F	600	FAD	PA-O5B	2.15	1.67	1.59
2	A	600	FAD	C2-N1	2.14	1.41	1.36
3	D	601	NAP	C4A-N9A	-2.14	1.33	1.37
2	E	600	FAD	P-O2P	-2.13	1.45	1.55
3	A	601	NAP	O4B-C1B	2.09	1.46	1.42
2	B	600	FAD	C4'-C3'	2.08	1.57	1.53
2	D	600	FAD	C10-N10	2.08	1.41	1.37
2	B	600	FAD	P-O3P	2.01	1.61	1.59

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	NAP	N3A-C2A-N1A	-5.87	119.69	128.58
2	F	600	FAD	N3A-C2A-N1A	-5.75	119.87	128.58
3	F	601	NAP	N3A-C2A-N1A	-5.74	119.89	128.58
2	B	600	FAD	N3A-C2A-N1A	-5.66	120.01	128.58
3	A	601	NAP	N3A-C2A-N1A	-5.13	120.81	128.58
2	B	600	FAD	C5A-C4A-N3A	-5.09	119.71	126.72
3	D	601	NAP	N3A-C2A-N1A	-4.96	121.08	128.58
2	A	600	FAD	N3A-C2A-N1A	-4.95	121.09	128.58
3	B	601	NAP	N3A-C2A-N1A	-4.92	121.14	128.58
3	D	601	NAP	C5A-C4A-N3A	-4.88	119.99	126.72
2	E	600	FAD	C5A-C4A-N3A	-4.87	120.01	126.72
2	D	600	FAD	C5A-C4A-N3A	-4.85	120.04	126.72
3	E	601	NAP	N3A-C2A-N1A	-4.83	121.28	128.58
2	E	600	FAD	N3A-C2A-N1A	-4.82	121.29	128.58
2	A	600	FAD	C5A-C4A-N3A	-4.75	120.17	126.72
3	B	601	NAP	C5A-C4A-N3A	-4.48	120.55	126.72
3	C	601	NAP	C5A-C4A-N3A	-4.42	120.63	126.72
2	C	600	FAD	N3A-C2A-N1A	-4.24	122.17	128.58
2	D	600	FAD	N3A-C2A-N1A	-4.22	122.20	128.58
2	C	600	FAD	C5A-C4A-N3A	-4.21	120.92	126.72
3	A	601	NAP	C5A-C4A-N3A	-4.19	120.95	126.72
2	B	600	FAD	C2A-N3A-C4A	3.93	121.43	111.83
3	C	601	NAP	C2A-N3A-C4A	3.88	121.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NAP	C5A-C4A-N3A	-3.87	121.39	126.72
3	F	601	NAP	C5A-C4A-N3A	-3.79	121.49	126.72
2	F	600	FAD	C5A-C4A-N3A	-3.73	121.58	126.72
3	B	601	NAP	N9A-C8A-N7A	-3.71	108.67	113.94
3	F	601	NAP	N9A-C8A-N7A	-3.61	108.81	113.94
3	F	601	NAP	C2A-N3A-C4A	3.61	120.65	111.83
2	E	600	FAD	C2A-N3A-C4A	3.61	120.64	111.83
2	F	600	FAD	N3A-C4A-N9A	3.58	133.25	127.17
2	B	600	FAD	N3A-C4A-N9A	3.56	133.22	127.17
3	D	601	NAP	C2A-N3A-C4A	3.54	120.48	111.83
2	A	600	FAD	C2A-N3A-C4A	3.50	120.39	111.83
3	A	601	NAP	C2A-N3A-C4A	3.49	120.36	111.83
3	B	601	NAP	C2A-N3A-C4A	3.49	120.35	111.83
2	E	600	FAD	C4-N3-C2	-3.47	119.48	125.64
3	E	601	NAP	N9A-C8A-N7A	-3.46	109.03	113.94
3	A	601	NAP	N9A-C8A-N7A	-3.46	109.03	113.94
2	F	600	FAD	C2A-N3A-C4A	3.44	120.23	111.83
2	F	600	FAD	C4A-N9A-C8A	3.44	109.35	105.74
3	D	601	NAP	N9A-C8A-N7A	-3.26	109.31	113.94
3	F	601	NAP	C4A-N9A-C8A	3.24	109.14	105.74
3	E	601	NAP	C4A-C5A-N7A	-3.21	106.91	110.58
3	D	601	NAP	C4A-C5A-N7A	-3.18	106.94	110.58
3	C	601	NAP	N3A-C4A-N9A	3.16	132.54	127.17
2	E	600	FAD	C4X-C4-N3	3.14	121.25	113.25
2	A	600	FAD	N3A-C4A-N9A	3.14	132.51	127.17
2	E	600	FAD	N3A-C4A-N9A	3.14	132.50	127.17
2	C	600	FAD	N3A-C4A-N9A	3.10	132.44	127.17
2	F	600	FAD	N9A-C8A-N7A	-3.10	109.54	113.94
2	D	600	FAD	C2A-N3A-C4A	3.08	119.34	111.83
3	E	601	NAP	C5A-N7A-C8A	3.07	108.27	103.45
3	B	601	NAP	C5A-N7A-C8A	3.06	108.25	103.45
2	F	600	FAD	C2A-N1A-C6A	3.04	123.72	118.73
3	D	601	NAP	C5A-N7A-C8A	3.03	108.21	103.45
3	E	601	NAP	C2A-N3A-C4A	3.02	119.22	111.83
3	B	601	NAP	C4A-C5A-N7A	-3.00	107.15	110.58
2	E	600	FAD	C10-C4X-N5	-3.00	118.69	124.81
3	D	601	NAP	N3A-C4A-N9A	3.00	132.26	127.17
3	B	601	NAP	N3A-C4A-N9A	2.99	132.24	127.17
3	F	601	NAP	N3A-C4A-N9A	2.97	132.23	127.17
2	F	600	FAD	C9A-C5X-N5	-2.97	119.31	122.45
2	C	600	FAD	N9A-C8A-N7A	-2.95	109.75	113.94
2	A	600	FAD	C4-N3-C2	-2.93	120.45	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	FAD	C2A-N3A-C4A	2.88	118.86	111.83
3	C	601	NAP	N9A-C8A-N7A	-2.87	109.87	113.94
2	A	600	FAD	C4X-C4-N3	2.86	120.53	113.25
3	B	601	NAP	C4A-N9A-C8A	2.84	108.72	105.74
2	C	600	FAD	C4-N3-C2	-2.84	120.60	125.64
3	A	601	NAP	N3A-C4A-N9A	2.77	131.89	127.17
2	C	600	FAD	C4X-C4-N3	2.77	120.30	113.25
2	A	600	FAD	C10-C4X-N5	-2.76	119.17	124.81
2	A	600	FAD	C9A-C5X-N5	-2.74	119.54	122.45
2	B	600	FAD	N9A-C8A-N7A	-2.73	110.07	113.94
3	A	601	NAP	C4A-N9A-C8A	2.72	108.59	105.74
3	C	601	NAP	O3X-P2B-O2X	2.70	117.92	107.80
2	C	600	FAD	C9A-C5X-N5	-2.69	119.61	122.45
2	D	600	FAD	C9A-C5X-N5	-2.69	119.61	122.45
2	D	600	FAD	C4A-C5A-N7A	-2.68	107.52	110.58
2	F	600	FAD	O4-C4-C4X	-2.67	119.49	126.53
2	D	600	FAD	N3A-C4A-N9A	2.67	131.70	127.17
2	E	600	FAD	N9A-C8A-N7A	-2.66	110.16	113.94
3	F	601	NAP	C5A-N7A-C8A	2.66	107.62	103.45
2	F	600	FAD	C4X-C4-N3	2.65	120.00	113.25
2	B	600	FAD	C4-N3-C2	-2.63	120.97	125.64
2	D	600	FAD	O4-C4-C4X	-2.62	119.60	126.53
2	F	600	FAD	C4-N3-C2	-2.61	121.00	125.64
3	A	601	NAP	C5A-N7A-C8A	2.60	107.53	103.45
3	D	601	NAP	O3X-P2B-O2B	2.57	115.85	105.85
3	E	601	NAP	C4A-N9A-C8A	2.56	108.43	105.74
2	E	600	FAD	C4X-C10-N1	-2.56	118.31	124.59
3	A	601	NAP	C4A-C5A-N7A	-2.54	107.67	110.58
2	C	600	FAD	O4-C4-C4X	-2.53	119.84	126.53
2	D	600	FAD	C4-N3-C2	-2.52	121.16	125.64
2	C	600	FAD	C4A-N9A-C8A	2.49	108.35	105.74
3	F	601	NAP	O4B-C1B-N9A	2.45	112.79	108.09
2	B	600	FAD	C5A-N7A-C8A	2.44	107.29	103.45
2	C	600	FAD	C5A-N7A-C8A	2.44	107.28	103.45
2	C	600	FAD	C10-C4X-N5	-2.42	119.87	124.81
3	E	601	NAP	N3A-C4A-N9A	2.40	131.24	127.17
3	C	601	NAP	C5A-N7A-C8A	2.39	107.20	103.45
3	B	601	NAP	O3X-P2B-O2X	2.38	116.72	107.80
2	A	600	FAD	N9A-C8A-N7A	-2.37	110.57	113.94
3	D	601	NAP	O3-PN-O1N	-2.36	103.62	110.70
2	B	600	FAD	C9A-C5X-N5	-2.35	119.96	122.45
2	D	600	FAD	C4X-C4-N3	2.35	119.22	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O4-C4-C4X	-2.33	120.39	126.53
2	E	600	FAD	C5X-N5-C4X	2.33	121.85	118.09
3	E	601	NAP	O3X-P2B-O2B	2.32	114.91	105.85
2	A	600	FAD	C5X-N5-C4X	2.32	121.83	118.09
2	B	600	FAD	C4X-C4-N3	2.31	119.14	113.25
2	A	600	FAD	C4X-C10-N1	-2.29	118.97	124.59
2	C	600	FAD	C4A-C5A-N7A	-2.29	107.97	110.58
2	D	600	FAD	C5A-N7A-C8A	2.28	107.03	103.45
2	E	600	FAD	C9A-C5X-N5	-2.26	120.06	122.45
2	B	600	FAD	C4-C4X-C10	2.26	120.80	116.93
2	E	600	FAD	C4X-C10-N10	2.25	119.71	116.48
2	D	600	FAD	C4-C4X-C10	2.25	120.78	116.93
2	D	600	FAD	C5A-C4A-N9A	2.24	108.25	105.81
2	D	600	FAD	N9A-C8A-N7A	-2.24	110.76	113.94
3	F	601	NAP	C2A-N1A-C6A	2.23	122.39	118.73
3	E	601	NAP	C2A-N1A-C6A	2.22	122.38	118.73
2	F	600	FAD	C5A-N7A-C8A	2.22	106.94	103.45
2	E	600	FAD	C4-C4X-C10	2.22	120.73	116.93
3	B	601	NAP	O3X-P2B-O2B	2.20	114.42	105.85
2	D	600	FAD	O4B-C1B-C2B	-2.20	101.92	106.62
2	B	600	FAD	C4A-C5A-N7A	-2.18	108.09	110.58
2	E	600	FAD	O4-C4-C4X	-2.17	120.80	126.53
3	F	601	NAP	O3X-P2B-O2X	2.14	115.83	107.80
3	F	601	NAP	C4A-C5A-N7A	-2.14	108.14	110.58
3	F	601	NAP	C4A-N9A-C1B	-2.13	121.65	126.63
3	C	601	NAP	O3-PN-O1N	-2.12	104.32	110.70
3	C	601	NAP	C2A-N1A-C6A	2.10	122.19	118.73
2	D	600	FAD	C10-C4X-N5	-2.10	120.52	124.81
2	E	600	FAD	C5A-N7A-C8A	2.10	106.75	103.45
2	F	600	FAD	O2A-PA-O1A	2.09	122.18	112.44
3	C	601	NAP	O3X-P2B-O2B	2.09	114.00	105.85
2	D	600	FAD	C4X-C10-N1	-2.08	119.49	124.59
3	B	601	NAP	O5B-PA-O1A	-2.07	100.72	108.94
2	A	600	FAD	C4A-C5A-N7A	-2.06	108.23	110.58
3	F	601	NAP	O3X-P2B-O2B	2.06	113.87	105.85
2	C	600	FAD	C5X-N5-C4X	2.05	121.40	118.09
2	B	600	FAD	O4B-C1B-N9A	2.05	112.02	108.09
2	B	600	FAD	C2A-N1A-C6A	2.04	122.08	118.73
2	A	600	FAD	C4-C4X-C10	2.02	120.40	116.93
2	E	600	FAD	C4A-C5A-N7A	-2.02	108.27	110.58
3	C	601	NAP	C4A-C5A-N7A	-2.01	108.28	110.58
2	C	600	FAD	C2A-N1A-C6A	2.01	122.03	118.73

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	600	FAD	C5B-O5B-PA-O2A
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	C3B-C4B-C5B-O5B
2	B	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	C	601	NAP	C5D-O5D-PN-O1N
3	D	601	NAP	C5D-O5D-PN-O1N
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B
2	C	600	FAD	O4B-C4B-C5B-O5B
2	C	600	FAD	C3B-C4B-C5B-O5B
2	D	600	FAD	O4B-C4B-C5B-O5B
2	F	600	FAD	O4B-C4B-C5B-O5B
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
2	D	600	FAD	C2B-C1B-N9A-C8A
2	A	600	FAD	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	B	600	FAD	C2B-C1B-N9A-C8A
2	C	600	FAD	C2B-C1B-N9A-C8A
2	E	600	FAD	C2B-C1B-N9A-C8A
2	F	600	FAD	C2B-C1B-N9A-C8A
3	B	601	NAP	C2B-O2B-P2B-O1X
3	E	601	NAP	C2B-O2B-P2B-O1X
2	F	600	FAD	C2'-C3'-C4'-C5'
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	A	601	NAP	C5D-O5D-PN-O2N
2	B	600	FAD	C2B-C1B-N9A-C4A
2	C	600	FAD	C2B-C1B-N9A-C4A
2	D	600	FAD	C2B-C1B-N9A-C4A
2	F	600	FAD	C2B-C1B-N9A-C4A
2	F	600	FAD	O3'-C3'-C4'-O4'
3	D	601	NAP	C4B-C5B-O5B-PA
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	O3'-C3'-C4'-C5'
3	A	601	NAP	C2B-O2B-P2B-O1X
3	C	601	NAP	C2B-O2B-P2B-O1X
3	F	601	NAP	C2B-O2B-P2B-O1X
3	C	601	NAP	PA-O3-PN-O5D
2	B	600	FAD	O4B-C1B-N9A-C8A
2	D	600	FAD	O4B-C1B-N9A-C8A
3	F	601	NAP	C4B-C5B-O5B-PA
2	A	600	FAD	O4B-C1B-N9A-C8A
2	C	600	FAD	O4B-C1B-N9A-C8A
3	A	601	NAP	C4B-C5B-O5B-PA
2	F	600	FAD	O4B-C1B-N9A-C8A
2	C	600	FAD	C2'-C3'-C4'-O4'
2	E	600	FAD	O4B-C1B-N9A-C8A
3	A	601	NAP	C2B-O2B-P2B-O3X
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
2	A	600	FAD	C2B-C1B-N9A-C4A

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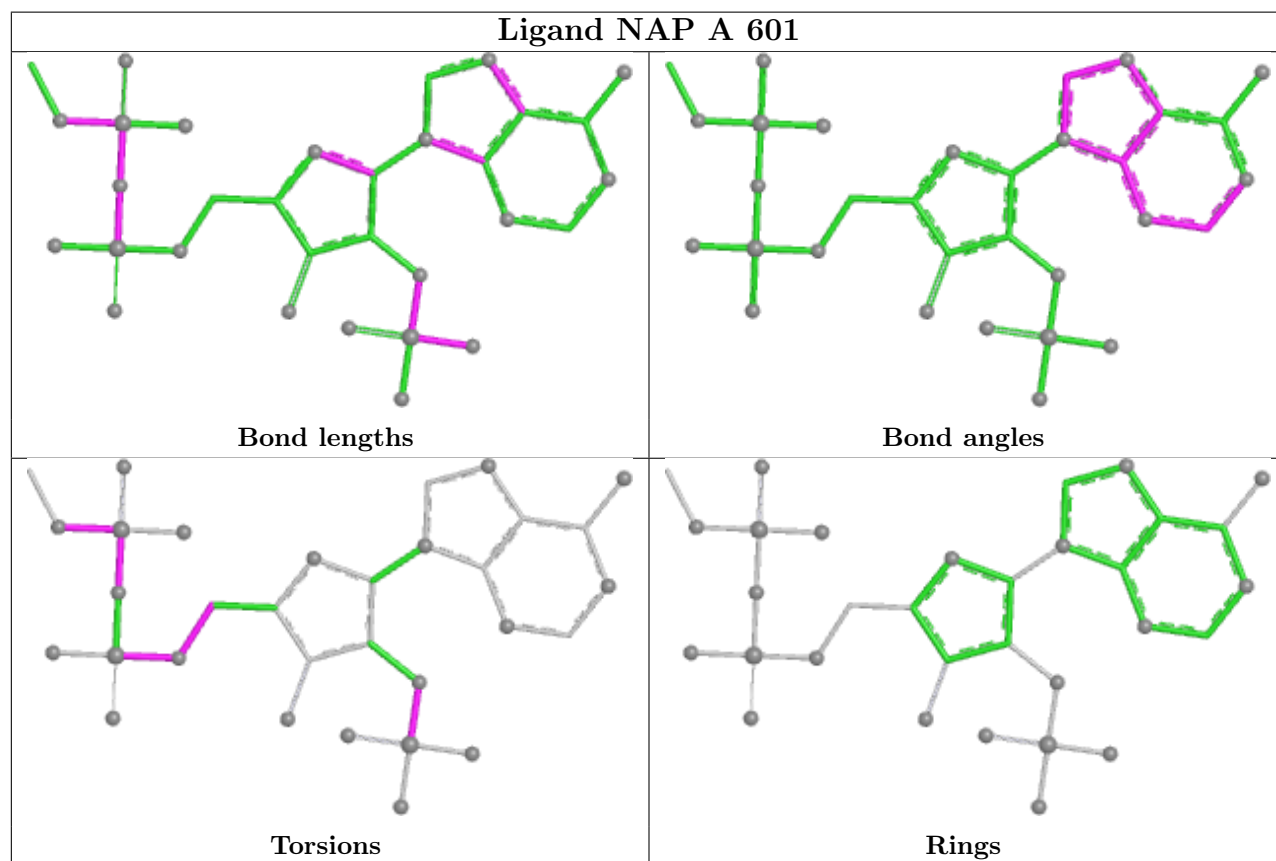
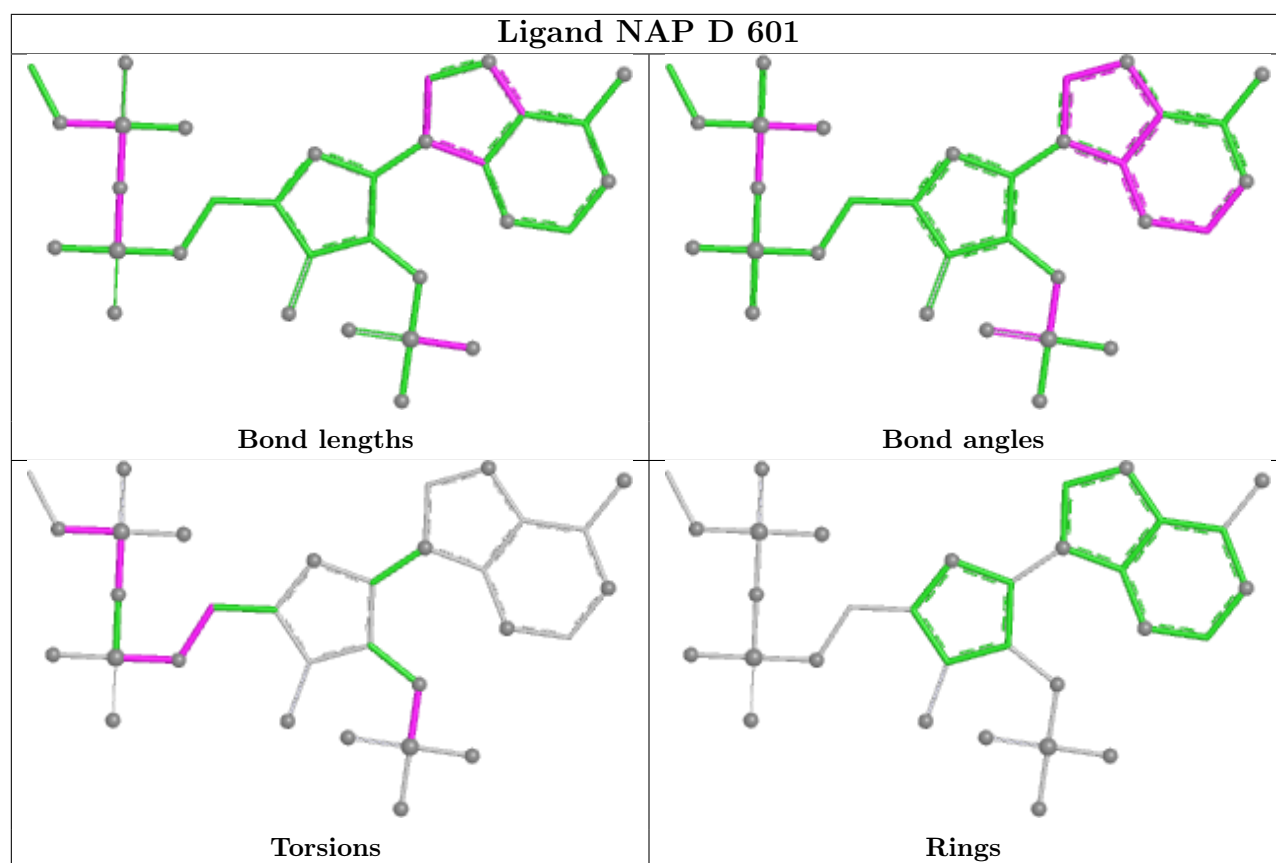
Mol	Chain	Res	Type	Atoms
2	E	600	FAD	C2B-C1B-N9A-C4A
3	D	601	NAP	C2B-O2B-P2B-O1X
3	B	601	NAP	PA-O3-PN-O2N

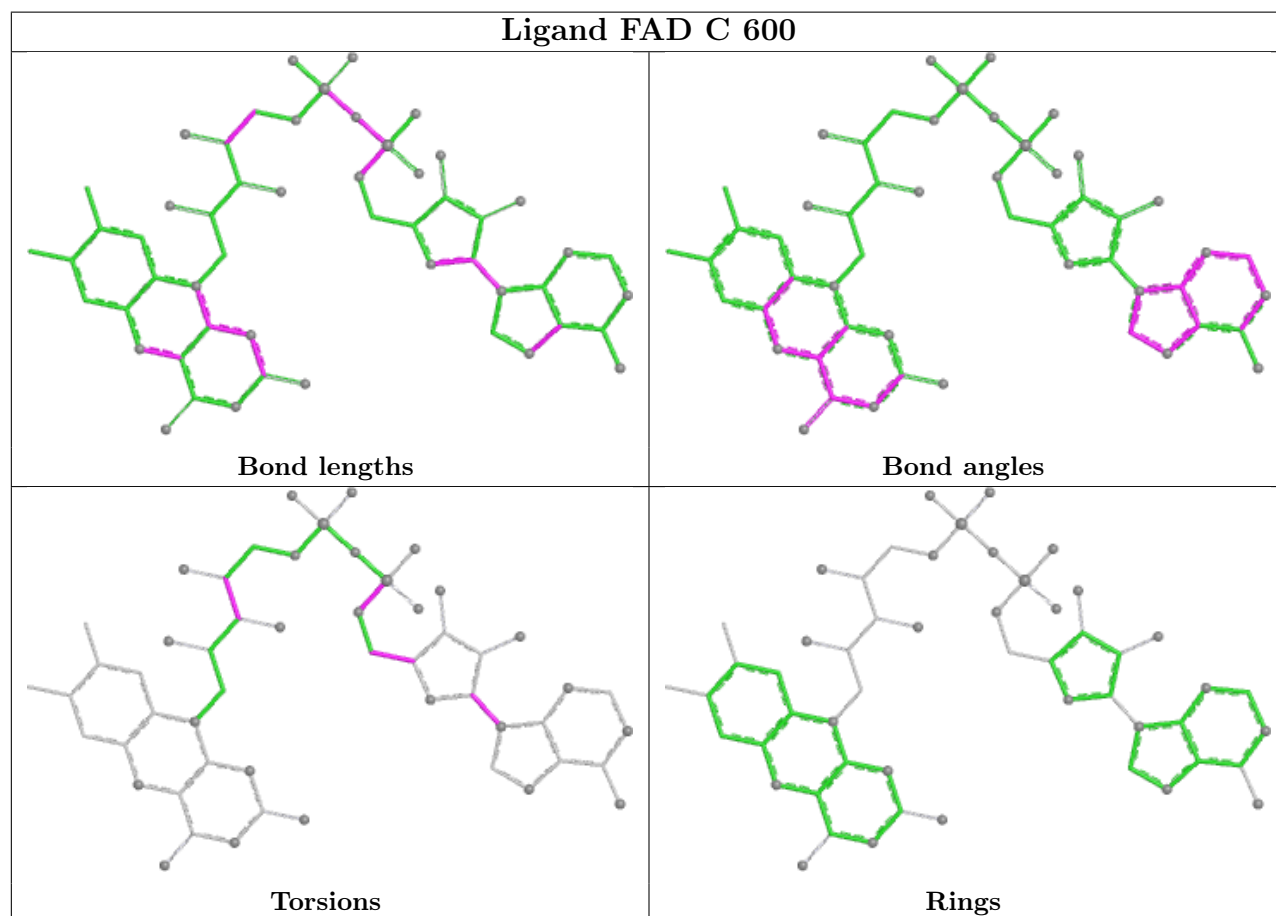
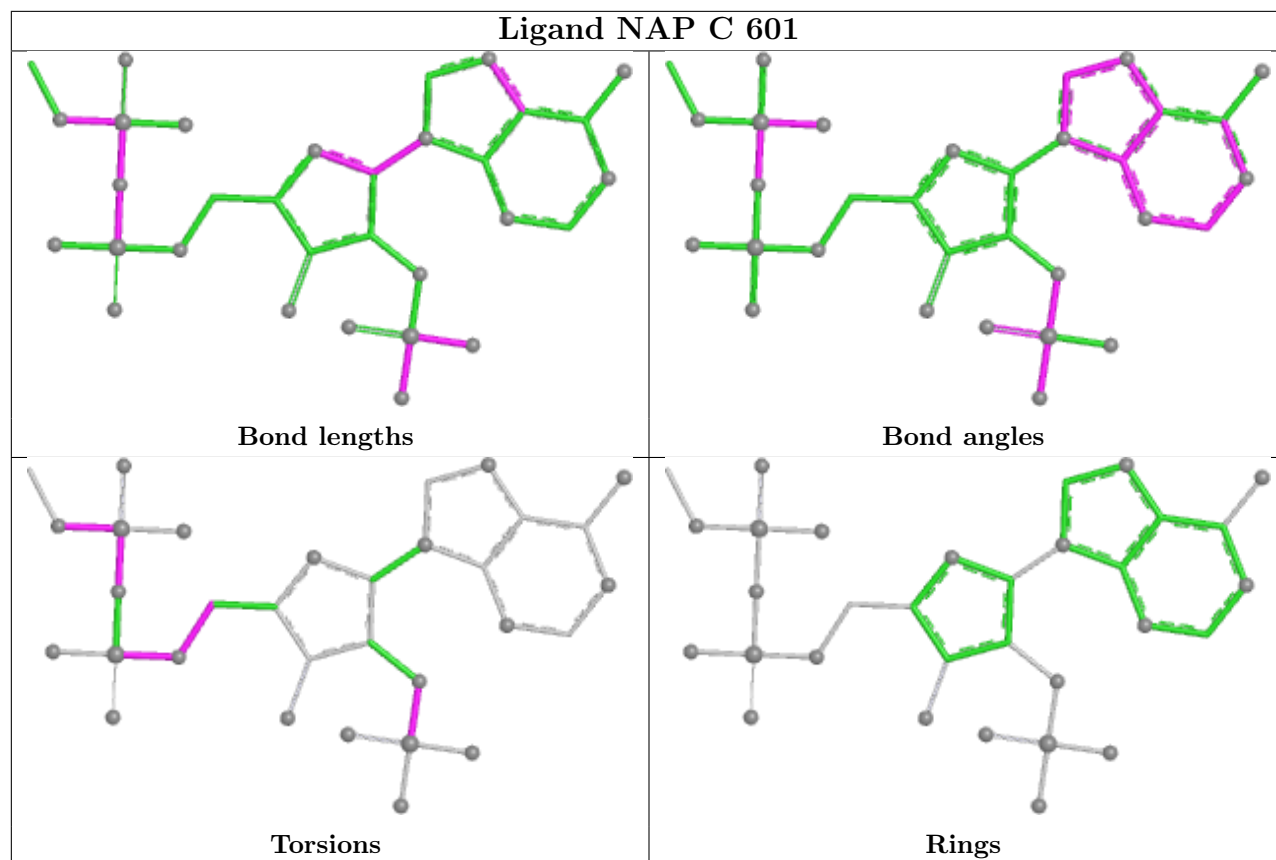
There are no ring outliers.

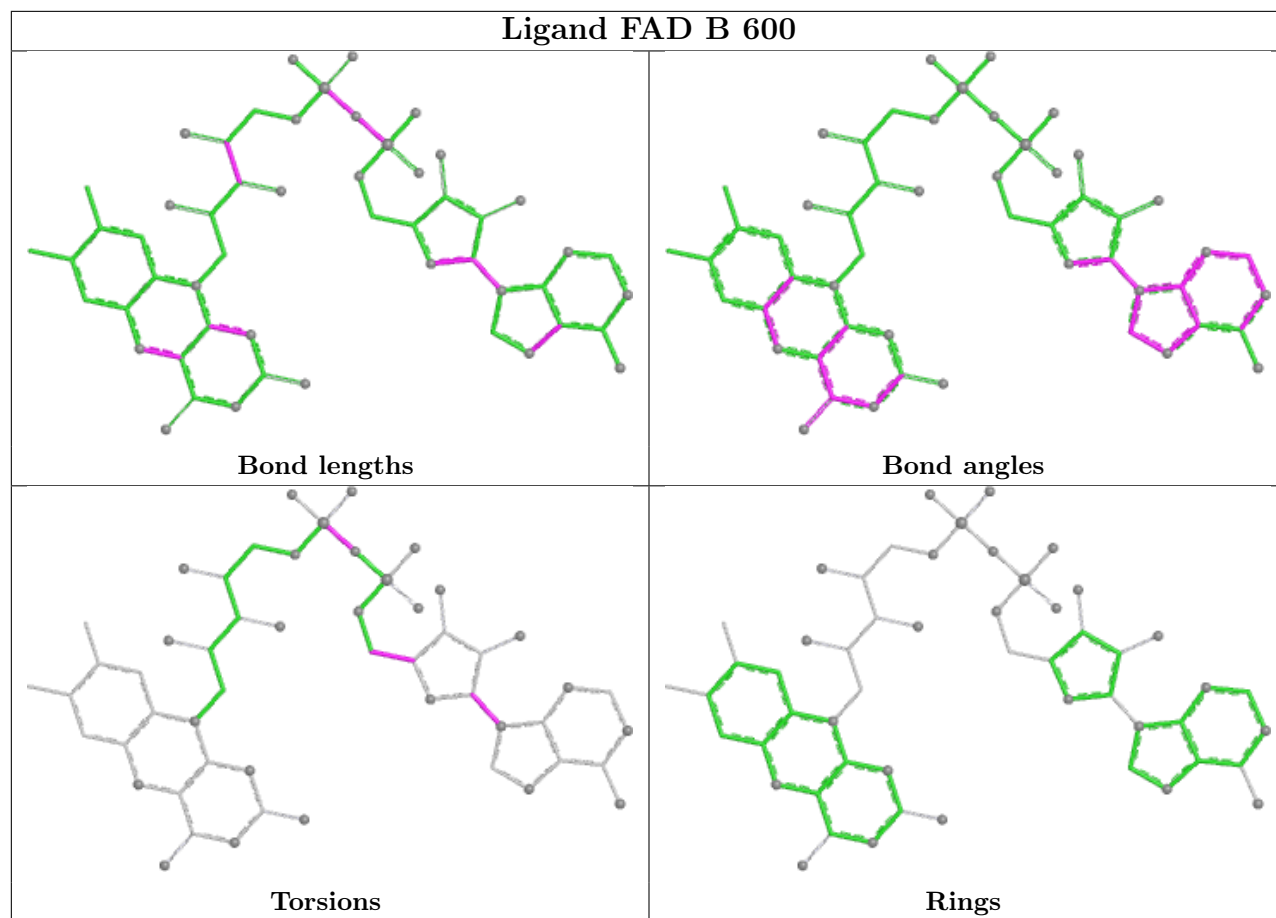
7 monomers are involved in 8 short contacts:

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

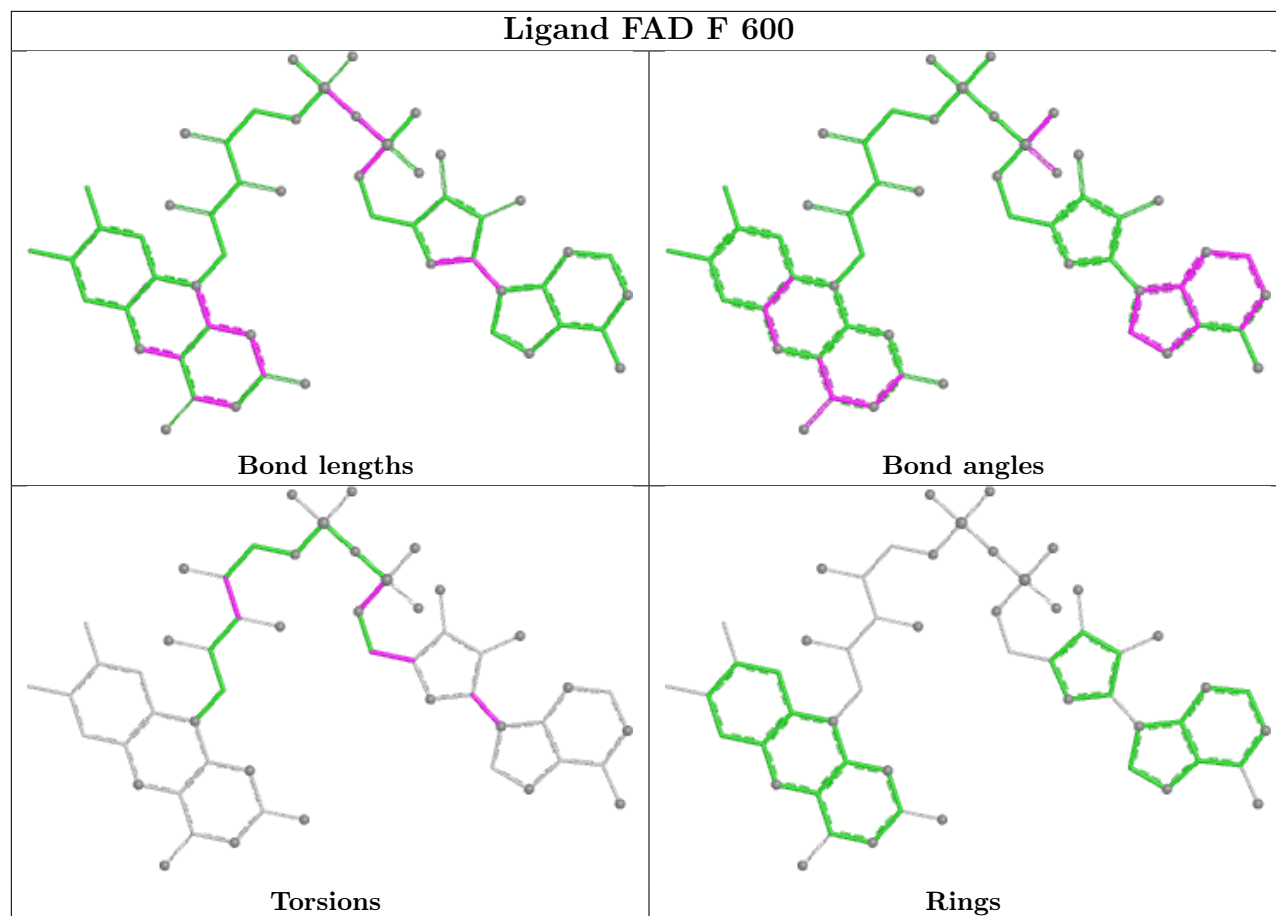
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

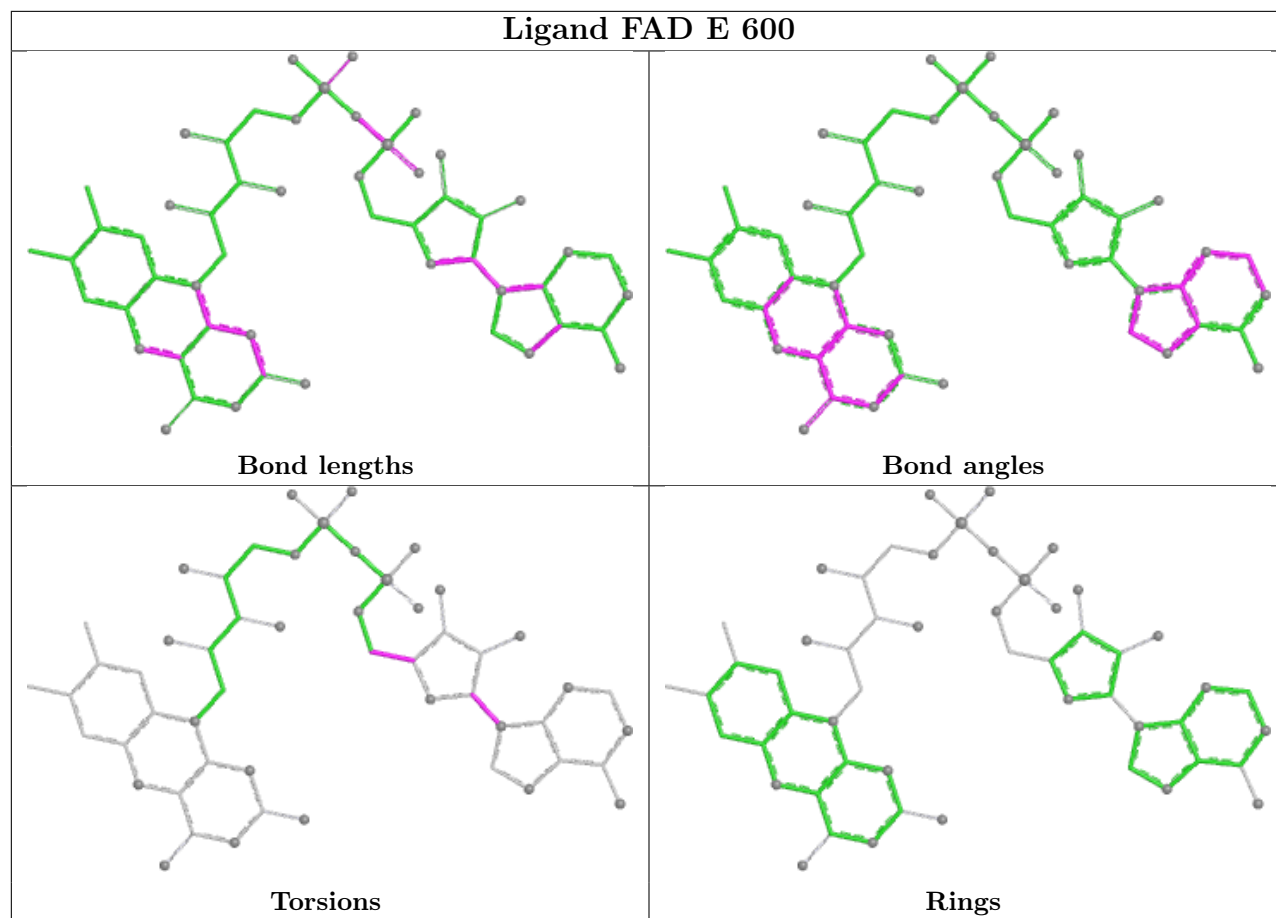




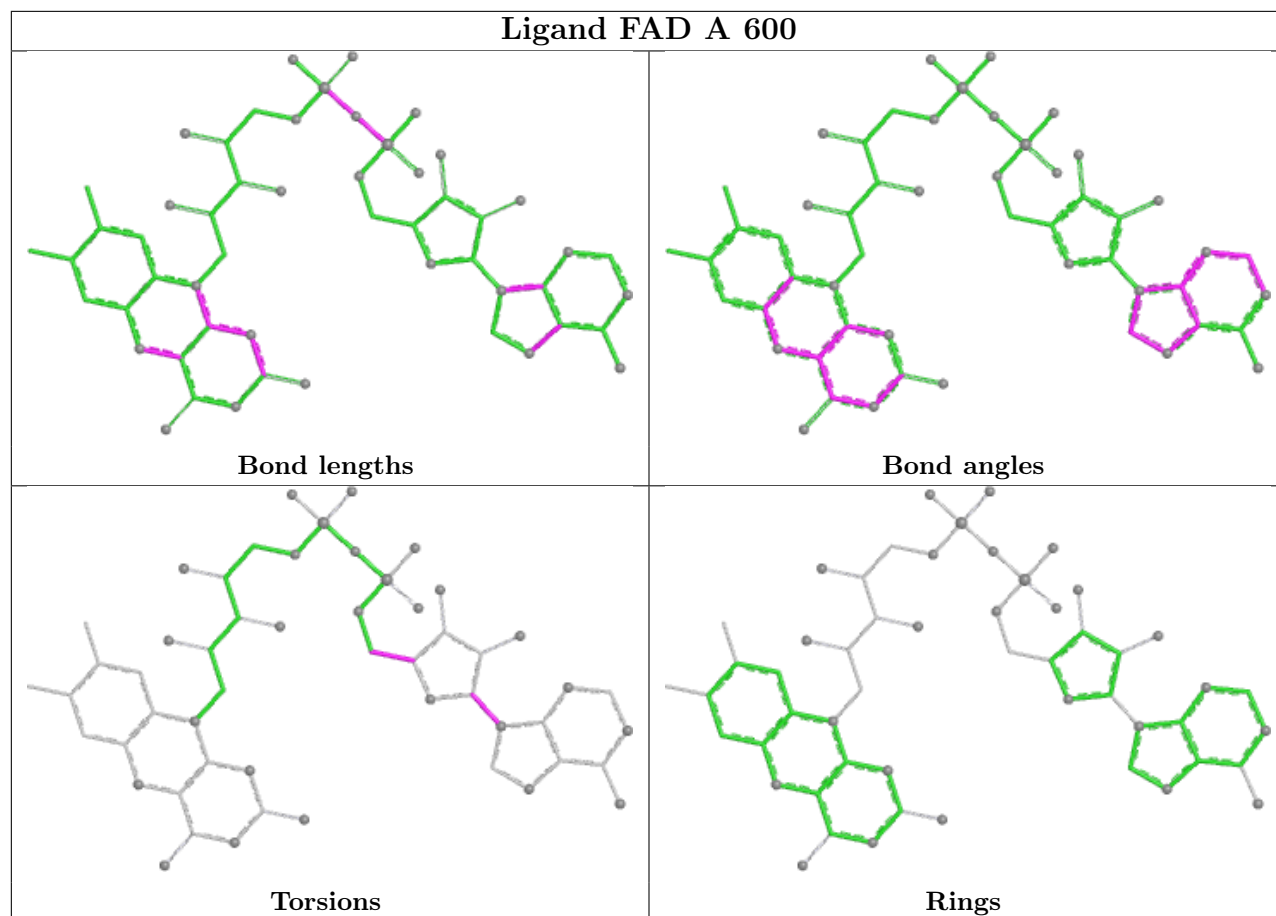


Ligand FAD F 600

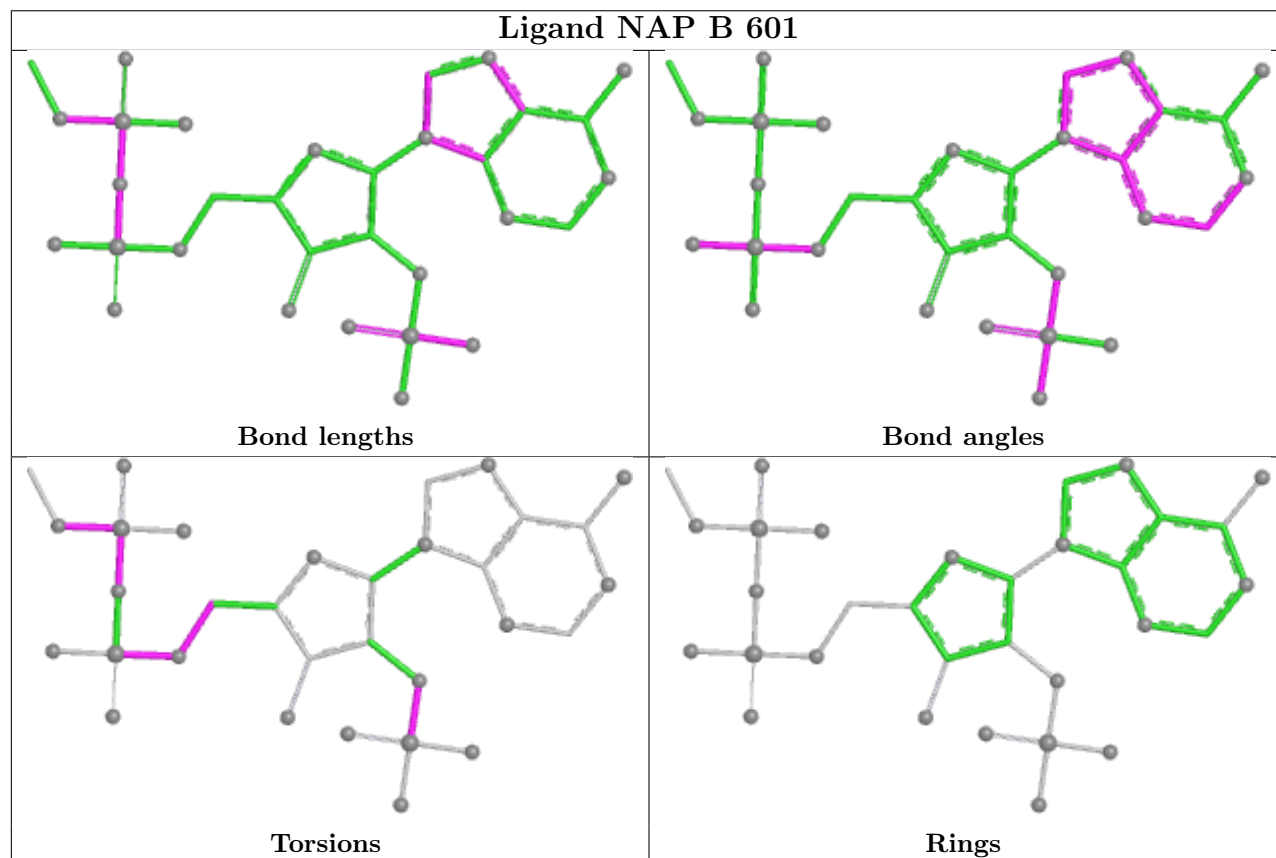


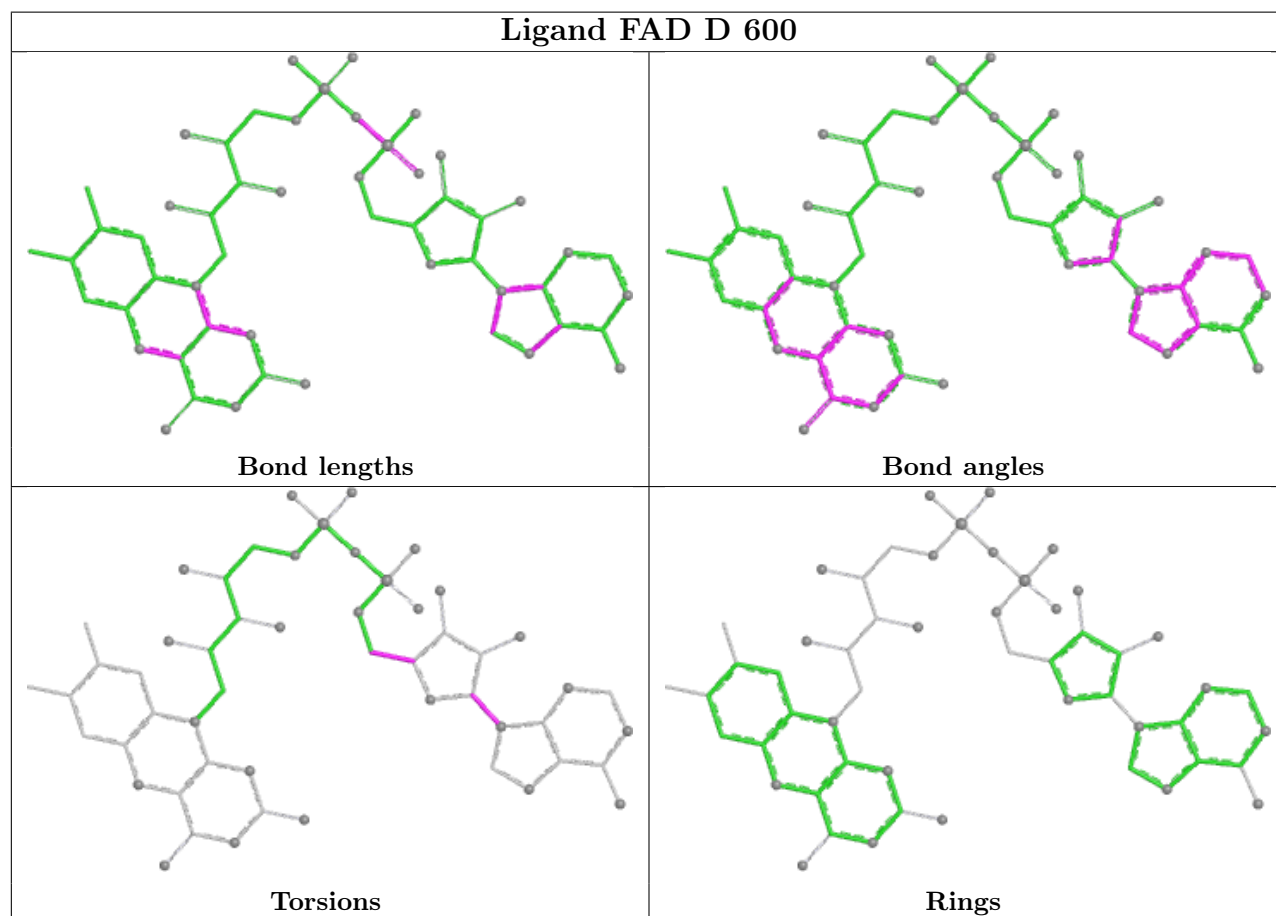
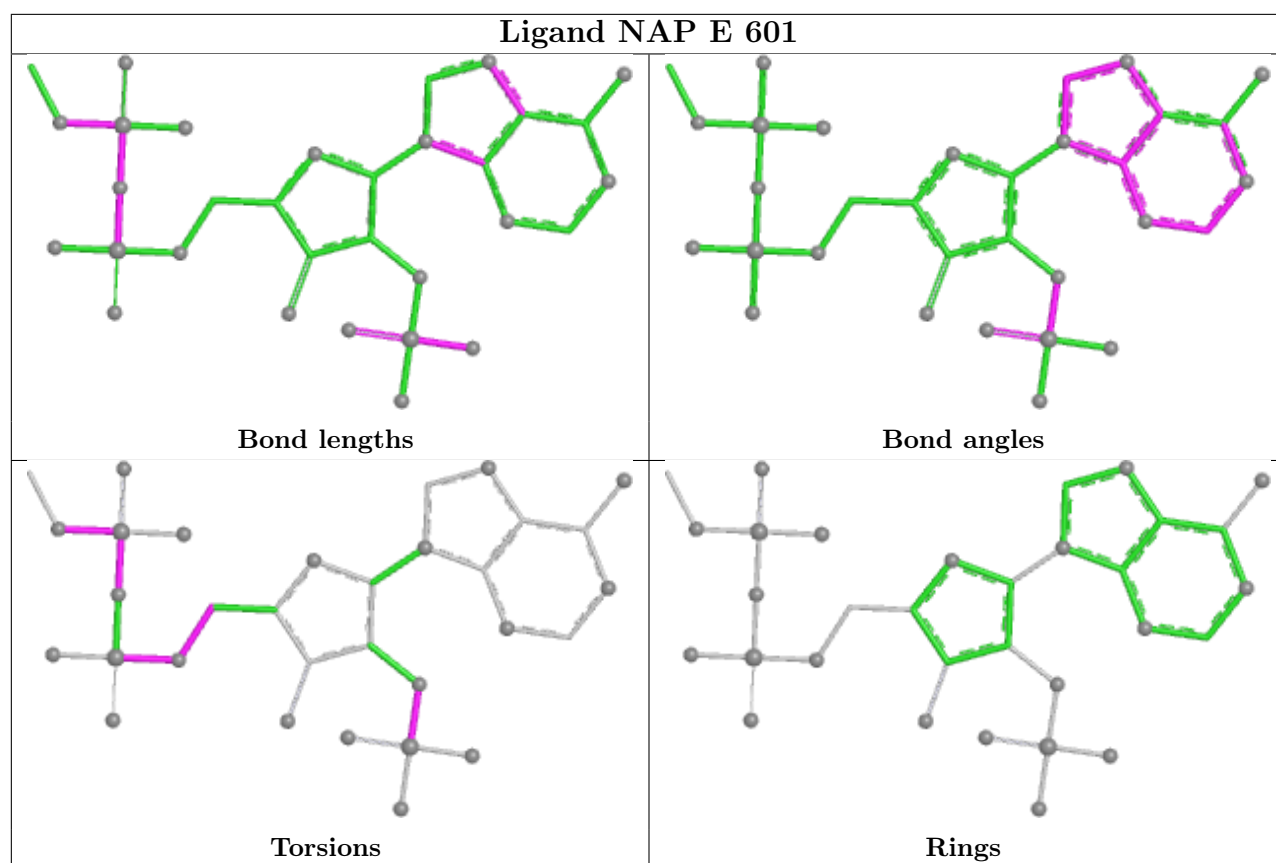


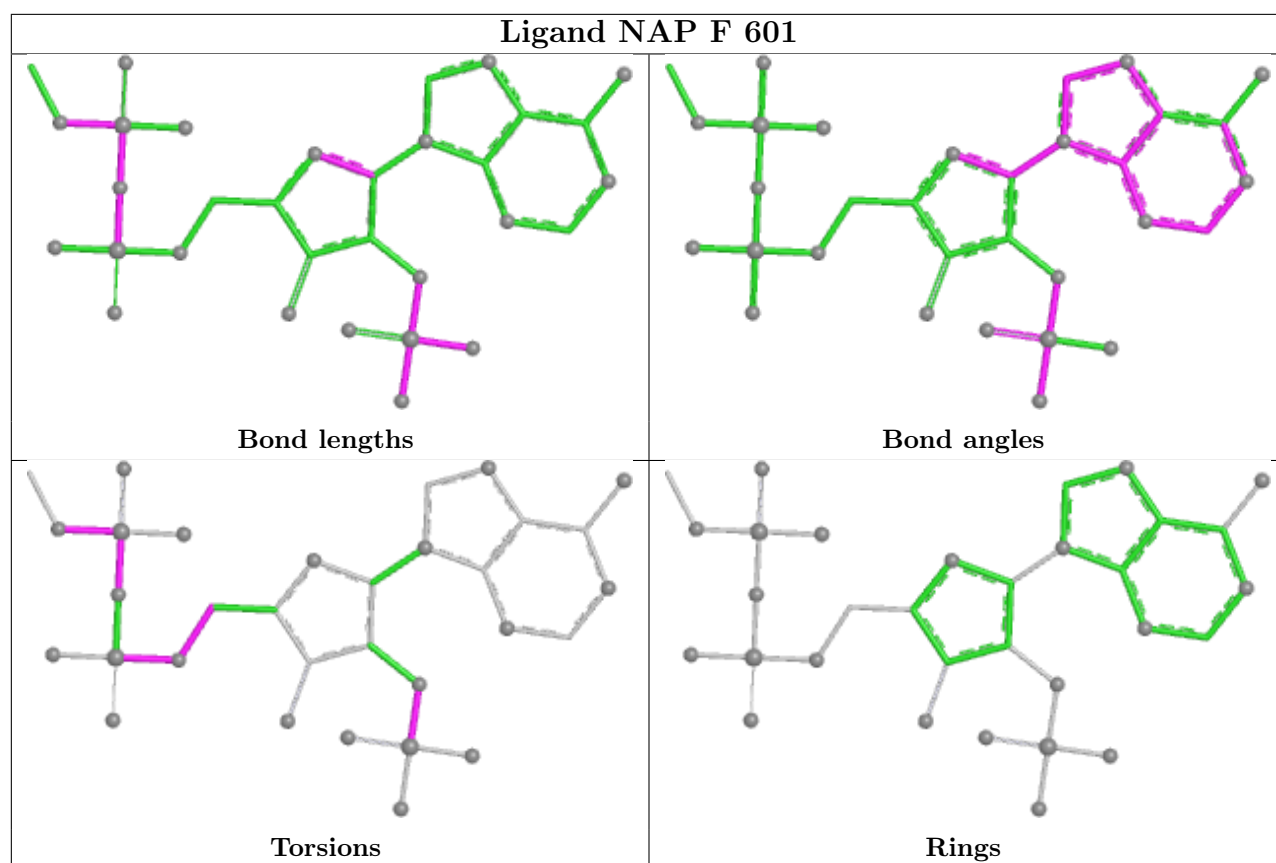
Ligand FAD A 600



Ligand NAP B 601







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	488/499 (97%)	0.07	3 (0%) 85 70	23, 55, 69, 96	0
1	B	489/499 (97%)	0.02	3 (0%) 85 70	23, 55, 69, 96	0
1	C	485/499 (97%)	0.34	13 (2%) 56 35	23, 55, 68, 96	0
1	D	490/499 (98%)	0.30	11 (2%) 62 41	23, 55, 68, 96	0
1	E	489/499 (97%)	0.27	10 (2%) 65 44	23, 55, 68, 96	0
1	F	488/499 (97%)	0.74	29 (5%) 28 15	23, 55, 69, 96	0
All	All	2929/2994 (97%)	0.29	69 (2%) 59 38	23, 55, 69, 96	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	130	ALA	5.1
1	F	306	GLY	3.9
1	B	197	GLY	3.8
1	A	132	GLY	3.5
1	A	497	CYS	3.3
1	F	143	THR	3.3
1	E	432	ASN	3.2
1	F	295	SER	3.2
1	F	132	GLY	3.1
1	D	497	CYS	3.0
1	E	497	CYS	3.0
1	F	297	THR	2.9
1	D	259	ILE	2.9
1	E	274	THR	2.9
1	B	494	GLN	2.9
1	F	307	VAL	2.9
1	F	499	GLY	2.9
1	C	132	GLY	2.8
1	D	489	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	497	CYS	2.7
1	F	335	ILE	2.7
1	F	278	GLU	2.7
1	C	494	GLN	2.6
1	F	253	PRO	2.6
1	E	398	ASN	2.6
1	F	324	THR	2.6
1	C	272	LYS	2.6
1	F	274	THR	2.5
1	D	496	GLY	2.5
1	F	152	TYR	2.5
1	D	332	ILE	2.5
1	D	415	SER	2.4
1	C	244	GLY	2.4
1	E	433	GLU	2.4
1	E	491	ASP	2.4
1	F	282	ASP	2.3
1	C	277	GLU	2.3
1	C	497	CYS	2.3
1	D	154	ALA	2.3
1	D	271	ALA	2.3
1	C	499	GLY	2.3
1	C	306	GLY	2.2
1	E	488	SER	2.2
1	D	433	GLU	2.2
1	D	360	GLY	2.2
1	E	260	GLU	2.2
1	F	144	ASN	2.2
1	F	19	GLY	2.2
1	F	280	ILE	2.1
1	F	316	ILE	2.1
1	F	11	TYR	2.1
1	E	494	GLN	2.1
1	F	137	PRO	2.1
1	A	395	GLY	2.1
1	C	264	PRO	2.1
1	E	400	GLU	2.1
1	F	219	MET	2.1
1	F	460	LEU	2.1
1	F	261	ALA	2.1
1	C	197	GLY	2.1
1	D	426	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	35	ASP	2.0
1	F	331	ALA	2.0
1	F	497	CYS	2.0
1	F	244	GLY	2.0
1	F	305	VAL	2.0
1	C	271	ALA	2.0
1	F	43	PHE	2.0
1	C	323	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

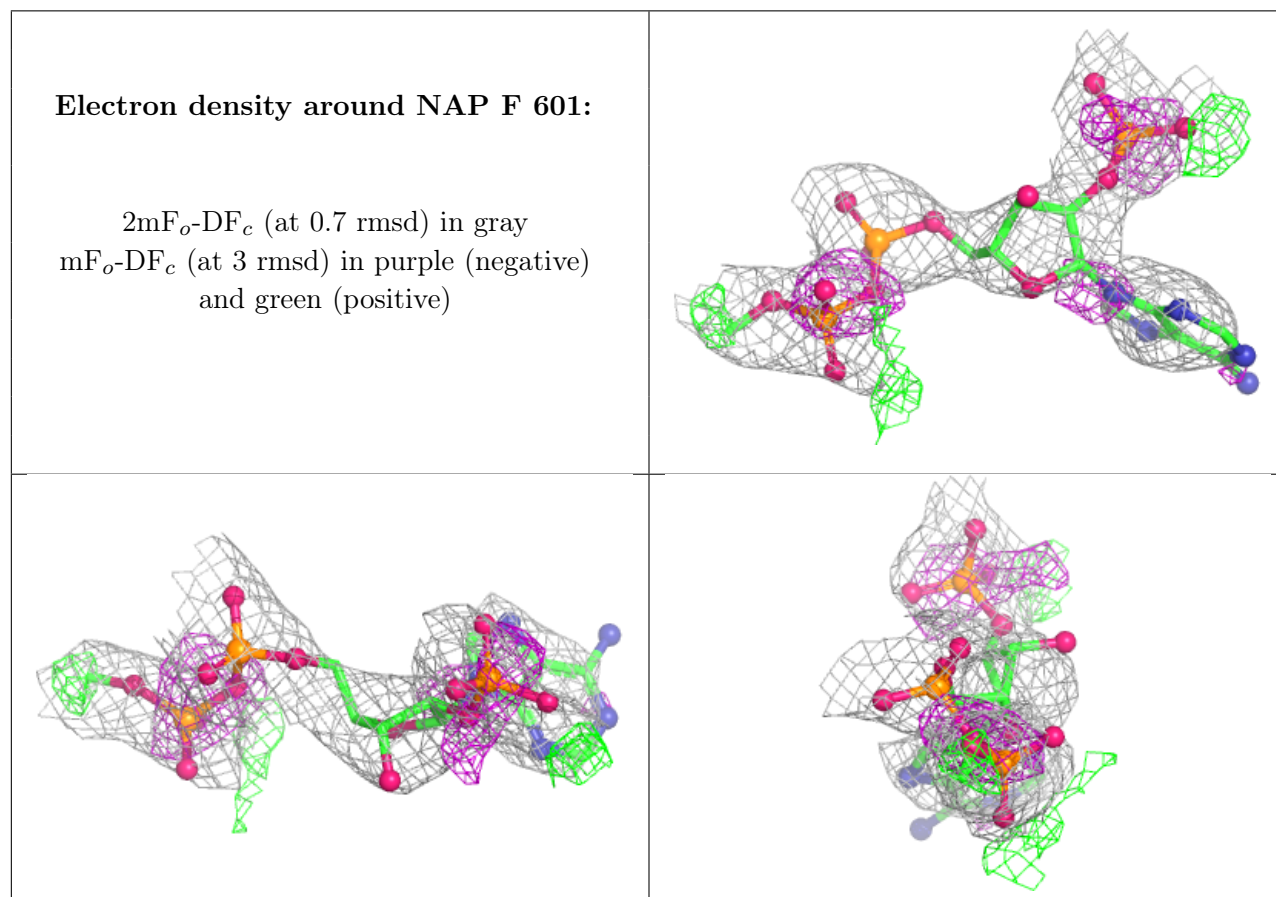
6.4 Ligands ⓘ

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	0.59	0.18	64,73,87,89	0
2	FAD	F	600	53/53	0.76	0.16	54,57,61,62	0
3	NAP	C	601	32/48	0.77	0.16	64,73,87,89	0
3	NAP	B	601	32/48	0.81	0.14	64,73,87,89	0
3	NAP	D	601	32/48	0.84	0.13	64,73,87,89	0
3	NAP	E	601	32/48	0.84	0.13	64,73,87,89	0
3	NAP	A	601	32/48	0.84	0.12	64,73,87,89	0
2	FAD	C	600	53/53	0.87	0.12	54,57,61,62	0
2	FAD	A	600	53/53	0.91	0.10	54,57,61,62	0
2	FAD	E	600	53/53	0.93	0.13	54,57,61,61	0
2	FAD	B	600	53/53	0.93	0.10	54,57,61,62	0
2	FAD	D	600	53/53	0.95	0.12	54,57,61,62	0

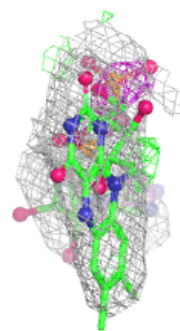
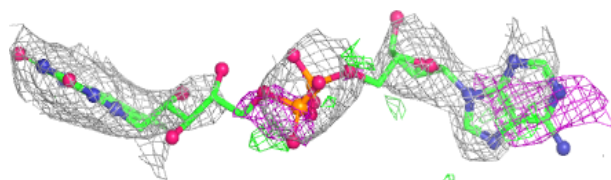
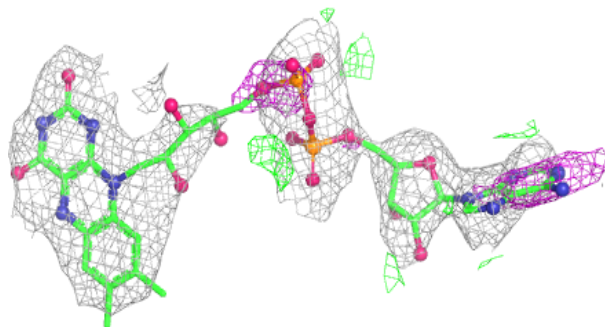
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

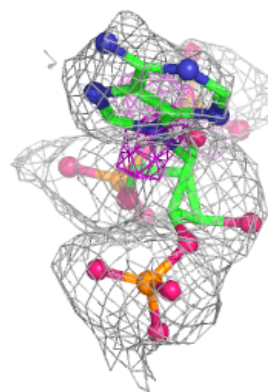
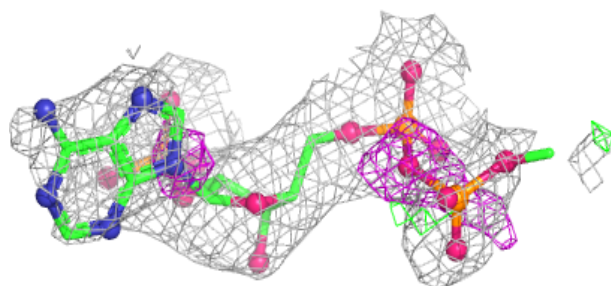
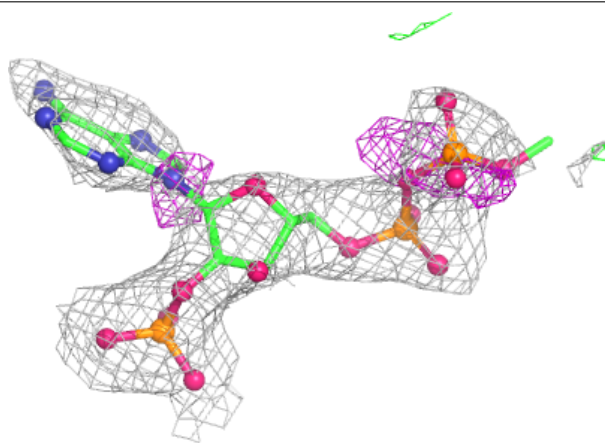


Electron density around FAD F 600:

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

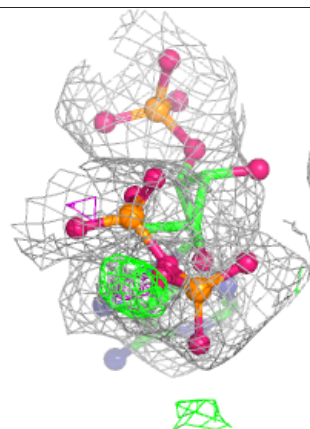
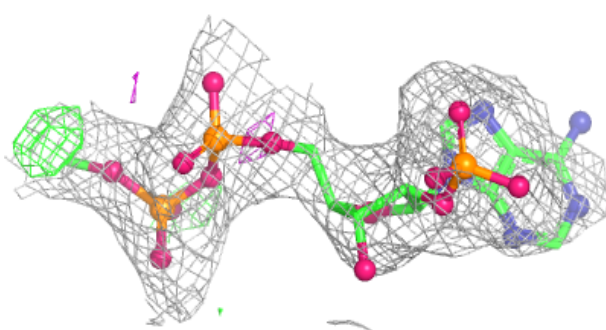
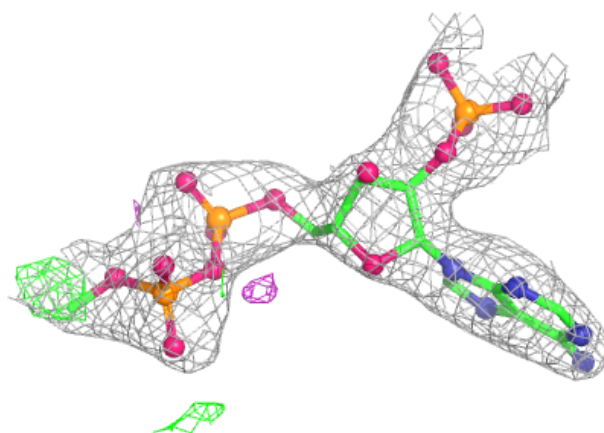
**Electron density around NAP C 601:**

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

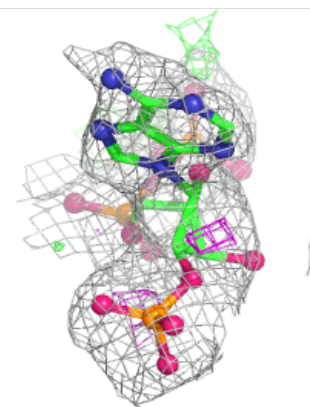
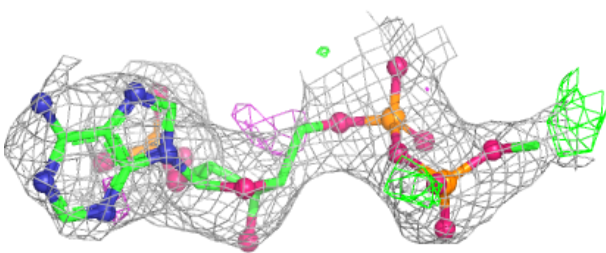
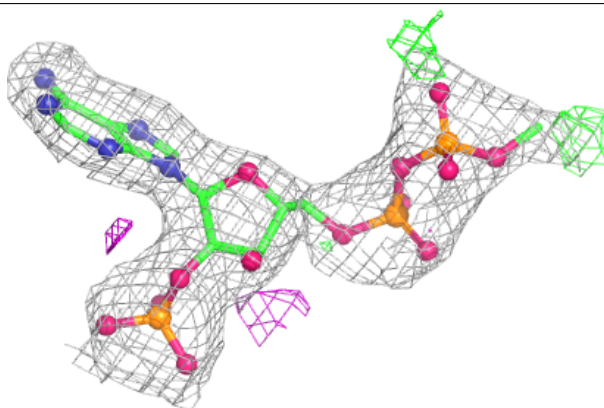


Electron density around NAP B 601:

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

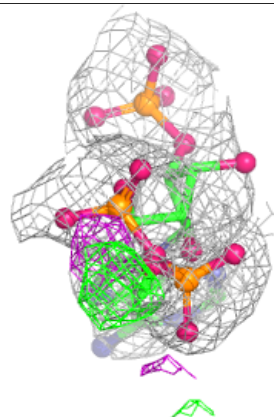
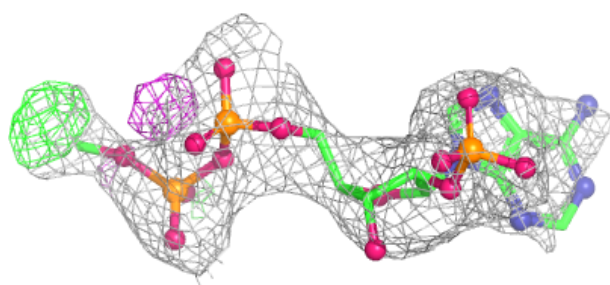
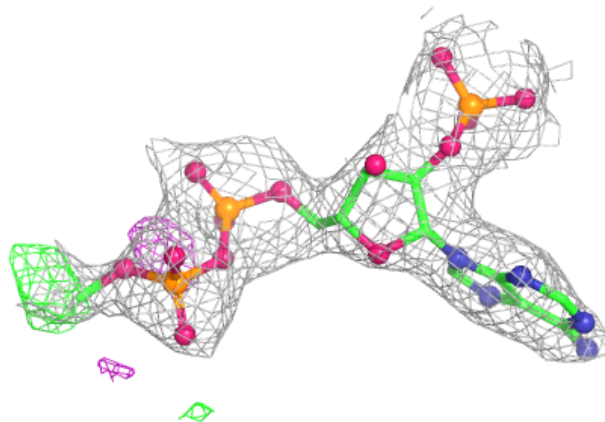
**Electron density around NAP D 601:**

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



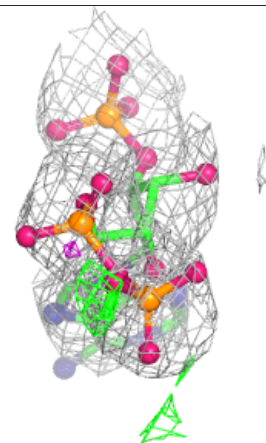
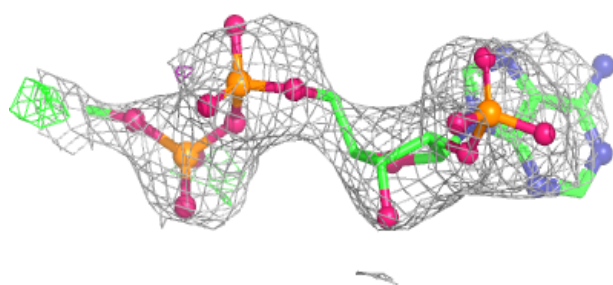
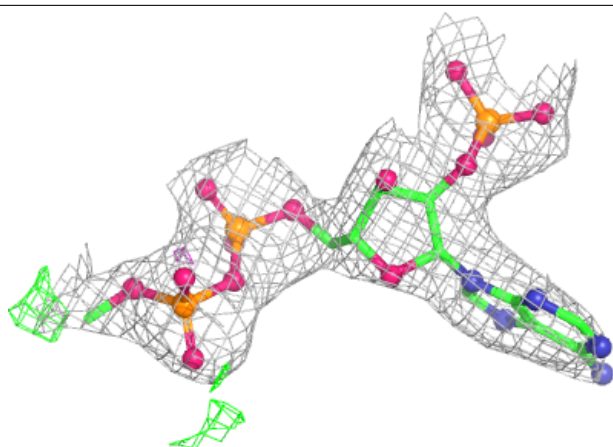
Electron density around NAP E 601:

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

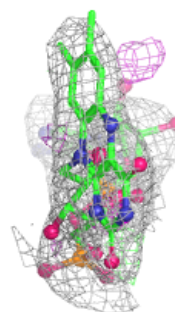
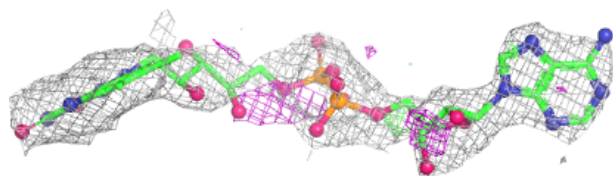
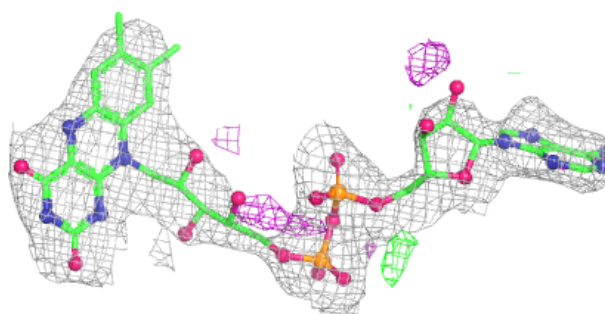


Electron density around NAP A 601:

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

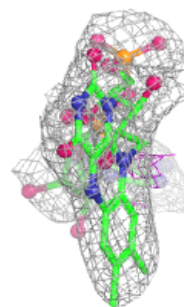
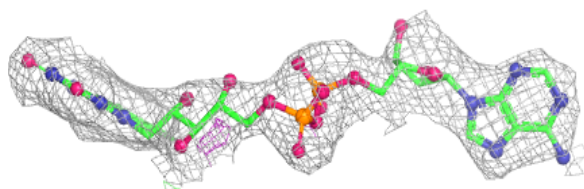
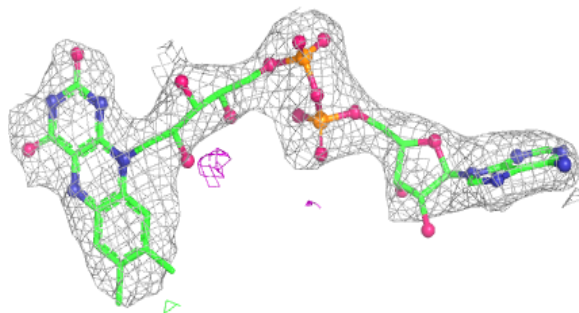
**Electron density around FAD C 600:**

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

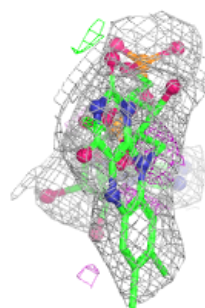
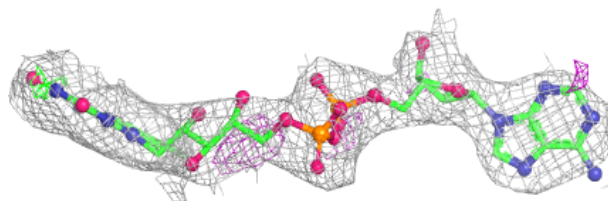
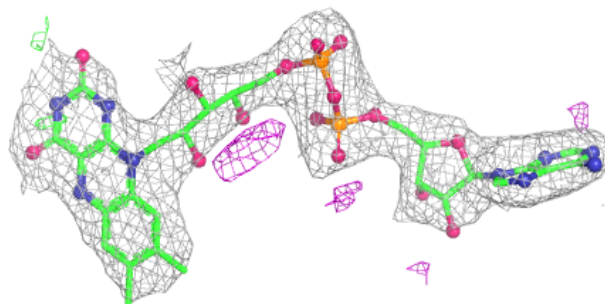


Electron density around FAD A 600:

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

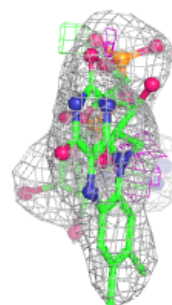
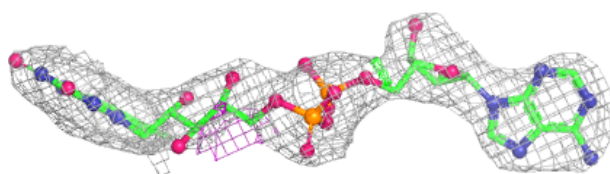
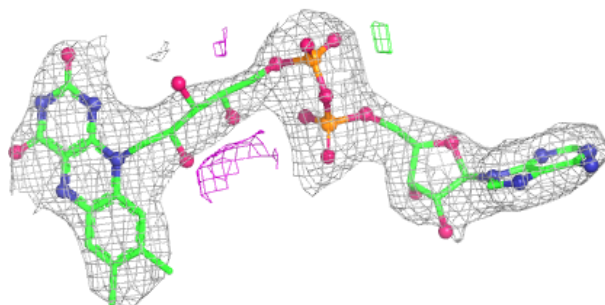
**Electron density around FAD E 600:**

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

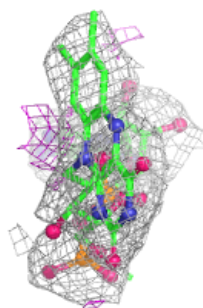
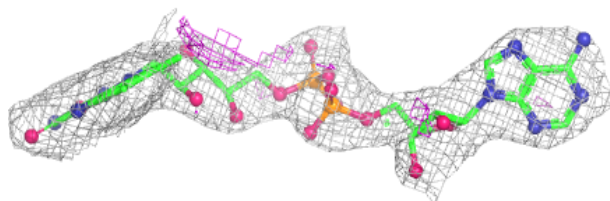
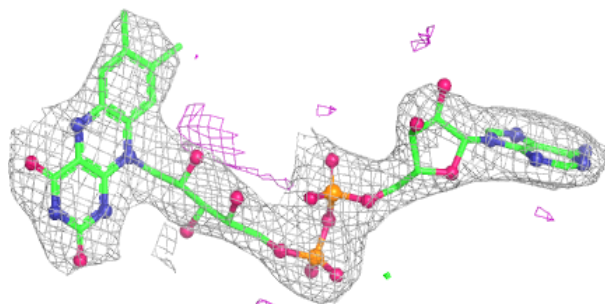


Electron density around FAD B 600:

$2mF_o-DF_c$ (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.