



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:16 am BST

PDB ID : 2XLR  
Title : Joint-functions of protein residues and NADP(H) in oxygen-activation by flavin-containing monooxygenase: Asn78Asp mutant  
Authors : Orru, R.; Fraaije, M.W.; Mattevi, A.  
Deposited on : 2010-07-21  
Resolution : 2.55 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](mailto: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.

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

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

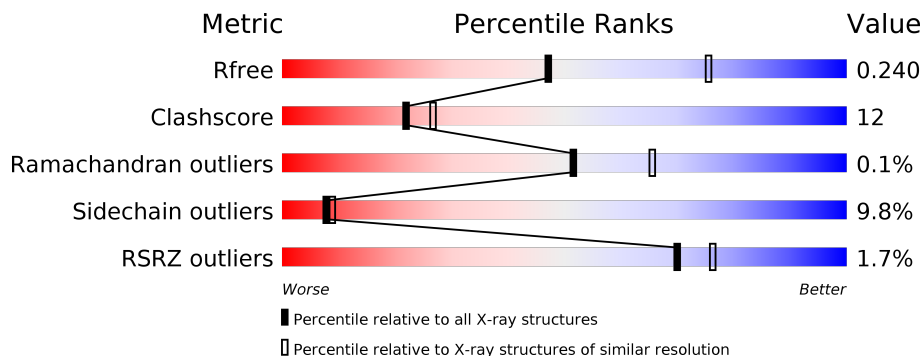
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	461	 3% 67% 23% 6% •
1	B	461	 77% 16% • •
1	C	461	 77% 16% • •
1	D	461	 3% 68% 23% 5% •

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 15348 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 FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	Total 3652	C 2341	N 605	O 685	S 21	0	0	0
1	B	447	Total 3661	C 2347	N 607	O 686	S 21	0	0	0
1	C	452	Total 3700	C 2373	N 612	O 694	S 21	0	0	0
1	D	447	Total 3658	C 2344	N 606	O 687	S 21	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

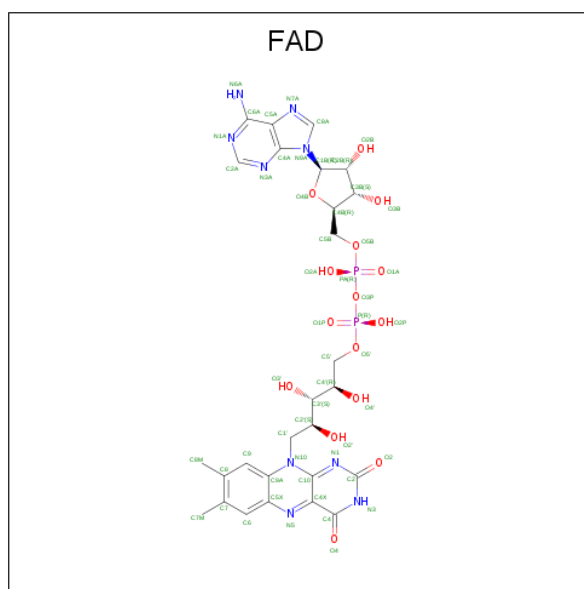
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q83XK4
A	2	ALA	-	expression tag	UNP Q83XK4
A	3	MET	-	expression tag	UNP Q83XK4
A	4	GLY	-	expression tag	UNP Q83XK4
A	5	SER	-	expression tag	UNP Q83XK4
A	78	ASP	ASN	engineered mutation	UNP Q83XK4
A	158	ALA	GLU	conflict	UNP Q83XK4
A	159	ALA	GLU	conflict	UNP Q83XK4
B	1	GLY	-	expression tag	UNP Q83XK4
B	2	ALA	-	expression tag	UNP Q83XK4
B	3	MET	-	expression tag	UNP Q83XK4
B	4	GLY	-	expression tag	UNP Q83XK4
B	5	SER	-	expression tag	UNP Q83XK4
B	78	ASP	ASN	engineered mutation	UNP Q83XK4
B	158	ALA	GLU	conflict	UNP Q83XK4
B	159	ALA	GLU	conflict	UNP Q83XK4
C	1	GLY	-	expression tag	UNP Q83XK4
C	2	ALA	-	expression tag	UNP Q83XK4
C	3	MET	-	expression tag	UNP Q83XK4
C	4	GLY	-	expression tag	UNP Q83XK4
C	5	SER	-	expression tag	UNP Q83XK4

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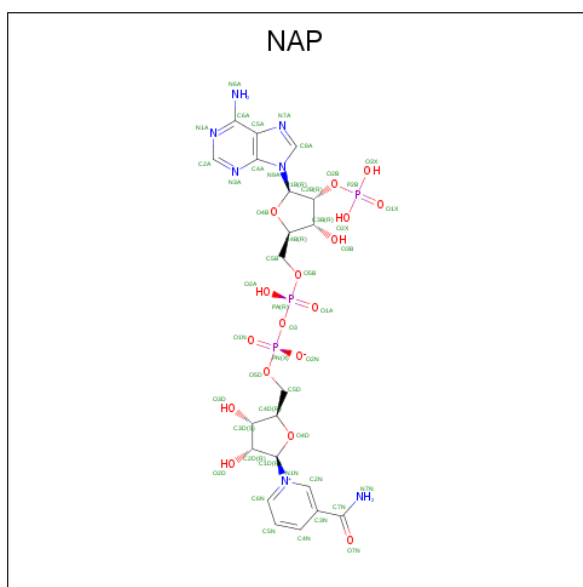
Chain	Residue	Modelled	Actual	Comment	Reference
C	78	ASP	ASN	engineered mutation	UNP Q83XK4
C	158	ALA	GLU	conflict	UNP Q83XK4
C	159	ALA	GLU	conflict	UNP Q83XK4
D	1	GLY	-	expression tag	UNP Q83XK4
D	2	ALA	-	expression tag	UNP Q83XK4
D	3	MET	-	expression tag	UNP Q83XK4
D	4	GLY	-	expression tag	UNP Q83XK4
D	5	SER	-	expression tag	UNP Q83XK4
D	78	ASP	ASN	engineered mutation	UNP Q83XK4
D	158	ALA	GLU	conflict	UNP Q83XK4
D	159	ALA	GLU	conflict	UNP Q83XK4

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	85	Total	O	0	0
			85	85		
4	C	91	Total	O	0	0
			91	91		
4	D	44	Total	O	0	0
			44	44		

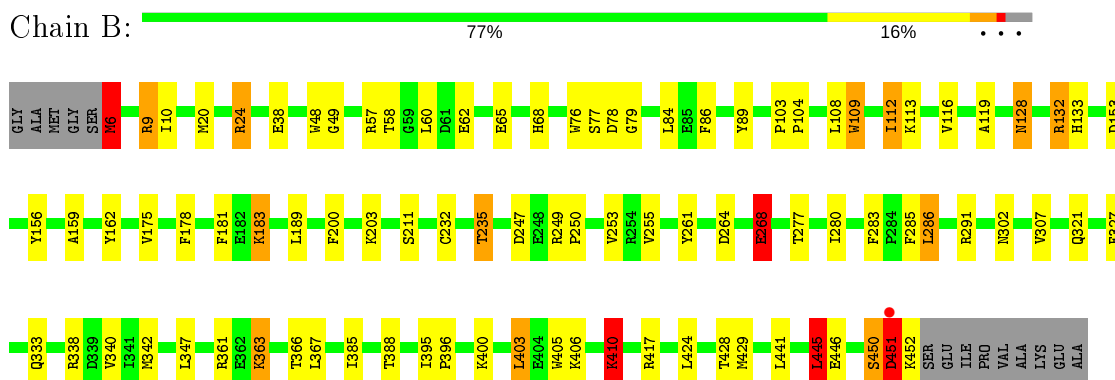
### 3 Residue-property plots [i](#)

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

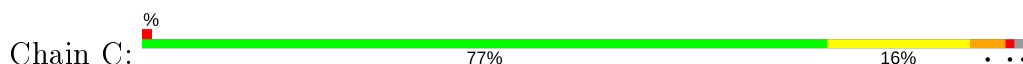
- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

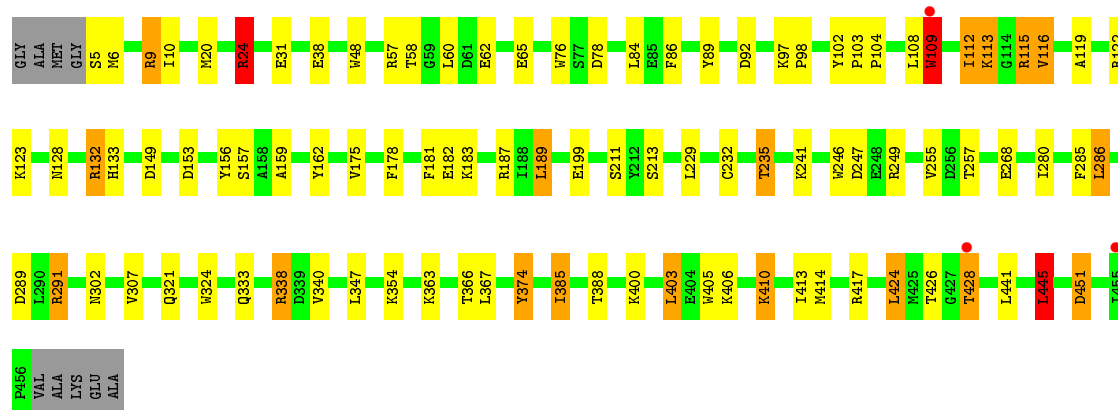


- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

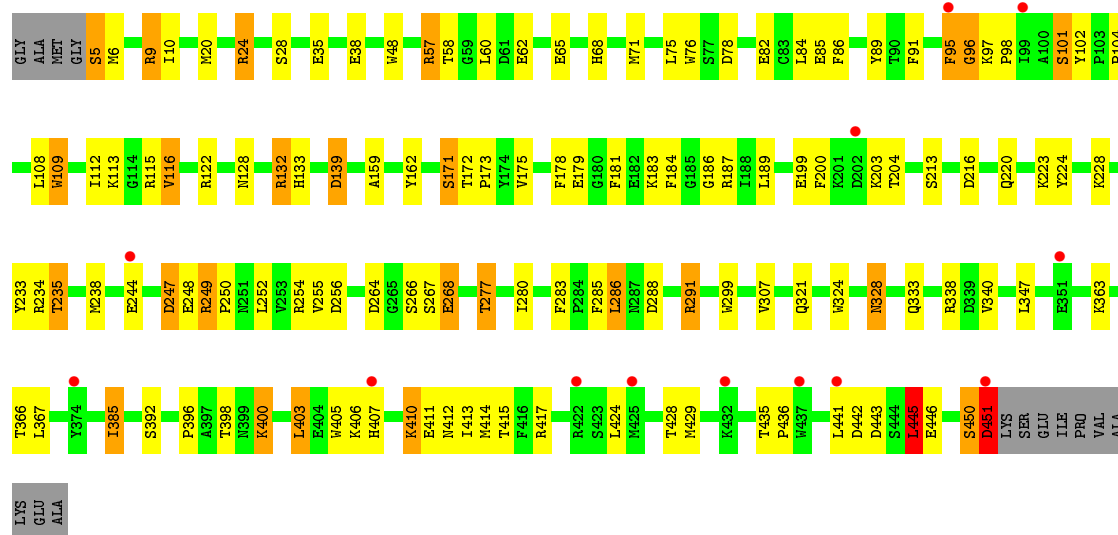


- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE





● Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.06Å 214.06Å 152.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.51 – 2.55 51.64 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.51-2.55) 99.9 (51.64-2.55)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.55Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.214 , 0.244 0.213 , 0.240	Depositor DCC
$R_{free}$ test set	6422 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.30	11/3765 (0.3%)	1.13	24/5112 (0.5%)
1	B	1.11	8/3774 (0.2%)	0.93	8/5123 (0.2%)
1	C	1.19	16/3815 (0.4%)	0.99	19/5180 (0.4%)
1	D	1.18	7/3771 (0.2%)	1.00	16/5120 (0.3%)
All	All	1.20	42/15125 (0.3%)	1.01	67/20535 (0.3%)

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

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	ASP	CB-CG	-26.44	0.96	1.51
1	C	109	TRP	CE3-CZ3	-19.23	1.05	1.38
1	C	451	ASP	CB-CG	-13.89	1.22	1.51
1	B	451	ASP	CB-CG	-12.51	1.25	1.51
1	A	451	ASP	CA-C	-11.92	1.22	1.52
1	C	109	TRP	CG-CD1	-11.77	1.20	1.36
1	C	109	TRP	CG-CD2	-11.69	1.23	1.43
1	A	268	GLU	CB-CG	-10.70	1.31	1.52
1	D	451	ASP	CB-CG	-10.57	1.29	1.51
1	A	451	ASP	CA-CB	-9.44	1.33	1.53
1	C	109	TRP	CD2-CE3	-9.30	1.26	1.40
1	A	6	MET	C-O	-9.00	1.06	1.23
1	C	109	TRP	CE2-CZ2	-7.26	1.27	1.39
1	C	374	TYR	CB-CG	-6.57	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	338	ARG	CB-CG	-6.42	1.35	1.52
1	C	182	GLU	CG-CD	6.42	1.61	1.51
1	D	109	TRP	CB-CG	-6.31	1.38	1.50
1	B	388	THR	C-O	6.12	1.34	1.23
1	A	109	TRP	CD2-CE3	-5.97	1.31	1.40
1	C	157	SER	CB-OG	-5.76	1.34	1.42
1	C	410	LYS	CD-CE	5.75	1.65	1.51
1	C	109	TRP	NE1-CE2	-5.74	1.30	1.37
1	A	446	GLU	CG-CD	5.67	1.60	1.51
1	D	244	GLU	CD-OE1	5.65	1.31	1.25
1	B	268	GLU	CB-CG	-5.58	1.41	1.52
1	C	213	SER	CB-OG	-5.50	1.35	1.42
1	C	31	GLU	CG-CD	5.49	1.60	1.51
1	A	109	TRP	CG-CD2	-5.46	1.34	1.43
1	D	109	TRP	CD2-CE3	-5.41	1.32	1.40
1	A	48	TRP	CG-CD1	5.41	1.44	1.36
1	D	410	LYS	CD-CE	5.28	1.64	1.51
1	C	451	ASP	CA-CB	-5.26	1.42	1.53
1	B	109	TRP	CG-CD1	-5.25	1.29	1.36
1	A	109	TRP	CB-CG	-5.25	1.40	1.50
1	A	74	TYR	CD2-CE2	5.24	1.47	1.39
1	B	109	TRP	CE3-CZ3	-5.17	1.29	1.38
1	C	156	TYR	CD2-CE2	5.09	1.47	1.39
1	B	109	TRP	CG-CD2	-5.08	1.35	1.43
1	D	199	GLU	CG-CD	5.08	1.59	1.51
1	D	299	TRP	CB-CG	-5.06	1.41	1.50
1	B	109	TRP	CD2-CE3	-5.02	1.32	1.40
1	B	156	TYR	CE2-CZ	5.01	1.45	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	ASP	CB-CG-OD1	-20.38	99.96	118.30
1	D	249	ARG	NE-CZ-NH2	18.22	129.41	120.30
1	A	451	ASP	CB-CA-C	-17.26	75.88	110.40
1	A	6	MET	CA-C-N	14.04	148.09	117.20
1	A	451	ASP	CB-CG-OD2	11.30	128.47	118.30
1	A	451	ASP	CA-C-O	-11.28	96.40	120.10
1	A	291	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	C	109	TRP	CD1-NE1-CE2	-9.66	100.30	109.00
1	C	109	TRP	CH2-CZ2-CE2	-9.52	107.88	117.40
1	D	249	ARG	NH1-CZ-NH2	-9.39	109.07	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	MET	C-N-CA	9.10	144.44	121.70
1	A	6	MET	CG-SD-CE	8.93	114.49	100.20
1	C	451	ASP	CB-CG-OD1	-8.89	110.30	118.30
1	C	109	TRP	CG-CD2-CE3	-8.86	125.92	133.90
1	A	6	MET	CA-C-O	-8.81	101.60	120.10
1	B	410	LYS	CD-CE-NZ	8.40	131.01	111.70
1	A	6	MET	O-C-N	-8.25	109.50	122.70
1	C	109	TRP	CG-CD1-NE1	7.98	118.08	110.10
1	C	451	ASP	CB-CG-OD2	7.87	125.38	118.30
1	B	6	MET	CG-SD-CE	7.63	112.41	100.20
1	A	451	ASP	N-CA-CB	7.35	123.83	110.60
1	B	132	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	6	MET	CG-SD-CE	7.30	111.88	100.20
1	D	95	PHE	CA-C-N	7.20	130.59	116.20
1	B	451	ASP	CB-CA-C	-6.98	96.44	110.40
1	C	6	MET	CG-SD-CE	6.62	110.79	100.20
1	A	149	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	149	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	115	ARG	NE-CZ-NH1	-6.43	117.09	120.30
1	D	445	LEU	CA-CB-CG	6.37	129.96	115.30
1	D	410	LYS	CD-CE-NZ	6.33	126.26	111.70
1	B	451	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	C	338	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	D	57	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	451	ASP	CB-CA-C	-6.03	98.33	110.40
1	C	132	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	122	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	445	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	291	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	132	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	354	LYS	CD-CE-NZ	5.74	124.90	111.70
1	C	109	TRP	CE2-CD2-CG	5.74	111.89	107.30
1	D	95	PHE	O-C-N	-5.74	113.45	123.20
1	A	403	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	C	109	TRP	CA-CB-CG	5.73	124.59	113.70
1	D	451	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	132	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	445	LEU	CA-CB-CG	5.63	128.25	115.30
1	D	291	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	403	LEU	N-CA-CB	-5.52	99.36	110.40
1	A	338	ARG	CG-CD-NE	-5.47	100.31	111.80
1	D	291	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	MET	CB-CA-C	-5.34	99.71	110.40
1	D	139	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	73	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	122	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	445	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	73	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	328	ASN	N-CA-CB	5.17	119.92	110.60
1	C	24	ARG	CB-CA-C	5.17	120.74	110.40
1	B	361	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	268	GLU	N-CA-CB	-5.13	101.37	110.60
1	A	139	ASP	CB-CG-OD1	5.11	122.89	118.30
1	C	338	ARG	N-CA-CB	5.09	119.76	110.60
1	A	338	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	291	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	C	338	ARG	CG-CD-NE	-5.03	101.23	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	SER	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	3652	0	3436	118	0
1	B	3661	0	3450	64	0
1	C	3700	0	3487	86	0
1	D	3658	0	3442	93	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	48	0	25	7	0
3	B	48	0	25	5	0
3	C	48	0	25	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	48	0	25	7	0
4	A	53	0	0	7	0
4	B	85	0	0	4	0
4	C	91	0	0	6	0
4	D	44	0	0	0	0
All	All	15348	0	14039	343	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 12.

All (343) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:TRP:CH2	1:C:113:LYS:HD3	1.24	1.64
1:C:109:TRP:CZ3	1:C:113:LYS:HD3	1.16	1.63
1:C:109:TRP:CH2	1:C:113:LYS:CD	2.01	1.40
1:C:109:TRP:CZ3	1:C:113:LYS:CD	2.03	1.39
1:A:204:THR:N	1:A:271:ASP:OD2	1.57	1.38
1:A:213:SER:O	1:A:217:ILE:CD1	1.85	1.25
1:A:271:ASP:CG	4:A:2027:HOH:O	1.74	1.23
1:B:451:ASP:N	1:B:451:ASP:OD1	1.65	1.20
1:A:213:SER:C	1:A:217:ILE:HD12	1.64	1.17
1:A:213:SER:O	1:A:217:ILE:HD12	0.89	1.05
1:A:213:SER:C	1:A:217:ILE:CD1	2.27	1.02
1:B:249:ARG:NH2	1:B:268:GLU:OE2	1.95	0.99
1:D:451:ASP:N	1:D:451:ASP:OD1	1.96	0.97
1:A:235:THR:CG2	3:A:501:NAP:O2X	2.16	0.94
1:A:235:THR:HG22	3:A:501:NAP:O2X	1.69	0.93
1:C:426:THR:HG1	1:C:428:THR:HG1	1.04	0.93
1:A:81:LYS:NZ	1:A:101:SER:HA	1.84	0.92
1:C:109:TRP:CE3	1:C:113:LYS:HE2	2.05	0.91
1:A:405:TRP:CZ3	1:A:406:LYS:HE2	2.05	0.90
1:B:405:TRP:CZ3	1:B:406:LYS:HE2	2.06	0.90
1:A:57:ARG:NH2	1:D:175:VAL:O	2.06	0.89
1:C:235:THR:CG2	3:C:501:NAP:O2X	2.21	0.89
1:D:235:THR:CG2	3:D:501:NAP:O2X	2.21	0.88
1:B:235:THR:CG2	3:B:501:NAP:O2X	2.23	0.87
1:C:109:TRP:HZ3	1:C:113:LYS:HD3	1.32	0.87
1:A:82:GLU:OE1	1:A:101:SER:OG	1.92	0.87
1:C:109:TRP:CZ3	1:C:113:LYS:CE	2.58	0.87
1:A:213:SER:HB3	1:A:217:ILE:HD11	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:TRP:CH2	1:C:113:LYS:HD2	2.10	0.82
1:A:408:HIS:ND1	1:A:419:HIS:CD2	2.49	0.81
1:A:271:ASP:OD1	4:A:2027:HOH:O	1.86	0.80
1:D:413:ILE:HG23	1:D:414:MET:HE2	1.64	0.80
1:A:213:SER:CB	1:A:217:ILE:HD11	2.12	0.80
1:C:388:THR:O	4:C:2078:HOH:O	2.00	0.79
1:C:249:ARG:NH2	1:C:268:GLU:OE2	2.16	0.79
1:D:405:TRP:CZ3	1:D:406:LYS:HE2	2.17	0.79
1:C:109:TRP:HH2	1:C:113:LYS:HD3	1.42	0.78
1:A:109:TRP:CE2	1:A:113:LYS:HD3	2.19	0.78
1:B:175:VAL:O	1:C:57:ARG:NH2	2.16	0.78
1:A:81:LYS:NZ	1:A:100:ALA:O	2.17	0.77
1:B:410:LYS:NZ	4:B:2070:HOH:O	2.17	0.77
1:A:390:TYR:O	4:A:2051:HOH:O	2.04	0.76
1:C:249:ARG:NH1	4:C:2052:HOH:O	2.00	0.76
1:A:81:LYS:HZ2	1:A:101:SER:HA	1.48	0.75
1:D:413:ILE:HG23	1:D:414:MET:CE	2.15	0.75
1:B:57:ARG:NH2	1:C:175:VAL:O	2.19	0.75
1:D:235:THR:HG23	3:D:501:NAP:O2X	1.85	0.75
1:A:175:VAL:O	1:D:57:ARG:NH2	2.20	0.75
1:D:65:GLU:OE2	1:D:132:ARG:NH2	2.18	0.74
1:B:235:THR:HG22	3:B:501:NAP:O2X	1.85	0.74
1:D:24:ARG:HD3	1:D:115:ARG:CZ	2.18	0.74
1:A:271:ASP:CB	4:A:2027:HOH:O	2.28	0.74
1:A:65:GLU:OE2	1:A:132:ARG:NH2	2.22	0.73
1:D:235:THR:HG22	3:D:501:NAP:O2X	1.89	0.73
1:A:81:LYS:HZ3	1:A:101:SER:HA	1.54	0.72
1:D:5:SER:HB3	1:D:35:GLU:CG	2.20	0.72
1:C:405:TRP:CZ3	1:C:406:LYS:HE2	2.25	0.71
1:C:235:THR:HG22	3:C:501:NAP:O2X	1.90	0.71
1:C:109:TRP:CZ3	1:C:113:LYS:HE2	2.23	0.71
1:A:28:SER:HB3	4:A:2004:HOH:O	1.92	0.70
1:D:412:ASN:ND2	1:D:415:THR:HG23	2.06	0.70
1:C:109:TRP:CD2	1:C:113:LYS:HE2	2.27	0.69
1:C:235:THR:HG23	3:C:501:NAP:O2X	1.93	0.69
1:A:213:SER:CA	1:A:217:ILE:HD11	2.23	0.69
1:D:321:GLN:NE2	1:D:321:GLN:H	1.91	0.69
1:C:321:GLN:NE2	1:C:321:GLN:H	1.90	0.69
1:C:363:LYS:O	1:C:366:THR:HB	1.93	0.69
1:D:97:LYS:HB2	1:D:98:PRO:HD2	1.75	0.69
1:A:363:LYS:O	1:A:366:THR:HB	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LEU:CD1	1:A:445:LEU:C	2.62	0.68
1:C:321:GLN:NE2	1:C:333:GLN:HE22	1.91	0.68
1:C:65:GLU:OE2	1:C:132:ARG:NH2	2.26	0.68
1:D:86:PHE:HB2	1:D:89:TYR:O	1.93	0.68
1:D:78:ASP:HA	1:D:417:ARG:HH21	1.57	0.68
1:C:109:TRP:HH2	1:C:113:LYS:CD	1.98	0.67
1:A:213:SER:HB3	1:A:217:ILE:CD1	2.25	0.67
1:A:426:THR:HG1	1:A:428:THR:HG1	0.68	0.67
1:C:10:ILE:HD12	1:C:162:TYR:HB2	1.76	0.66
1:A:81:LYS:NZ	1:A:100:ALA:C	2.48	0.66
1:D:10:ILE:HD12	1:D:162:TYR:HB2	1.77	0.66
1:B:363:LYS:O	1:B:366:THR:HB	1.96	0.66
1:A:78:ASP:HA	1:A:417:ARG:HH21	1.59	0.66
1:B:445:LEU:CD1	1:B:445:LEU:C	2.65	0.66
1:A:213:SER:CA	1:A:217:ILE:CD1	2.74	0.65
1:B:6:MET:CE	1:B:342:MET:HG2	2.26	0.65
1:A:249:ARG:NH2	1:A:268:GLU:OE2	2.29	0.65
1:A:108:LEU:O	1:A:112:ILE:HG23	1.96	0.65
1:A:216:ASP:O	1:A:220:GLN:HG2	1.97	0.65
1:D:445:LEU:CD1	1:D:445:LEU:C	2.66	0.64
1:A:445:LEU:HD12	1:A:445:LEU:C	2.19	0.62
1:B:235:THR:HG23	3:B:501:NAP:O2X	1.99	0.62
1:D:445:LEU:HD12	1:D:446:GLU:N	2.14	0.62
1:A:81:LYS:HZ2	1:A:100:ALA:C	2.02	0.62
1:D:68:HIS:O	1:D:171:SER:OG	2.16	0.62
1:A:97:LYS:HB2	1:A:98:PRO:HD2	1.79	0.61
1:D:20:MET:CE	1:D:116:VAL:HG21	2.30	0.61
1:B:321:GLN:H	1:B:321:GLN:NE2	1.98	0.61
1:B:133:HIS:HD2	1:C:133:HIS:CD2	2.18	0.61
1:D:97:LYS:HB2	1:D:98:PRO:CD	2.30	0.61
1:C:385:ILE:O	4:C:2078:HOH:O	2.16	0.61
1:C:445:LEU:C	1:C:445:LEU:CD1	2.69	0.60
1:C:426:THR:OG1	1:C:428:THR:OG1	1.96	0.60
1:C:86:PHE:HB2	1:C:89:TYR:O	2.01	0.60
1:A:321:GLN:NE2	1:A:321:GLN:H	1.99	0.60
1:D:249:ARG:NH2	1:D:268:GLU:OE2	2.35	0.60
1:D:435:THR:CG2	1:D:436:PRO:HD2	2.31	0.60
1:A:388:THR:O	4:A:2051:HOH:O	2.17	0.60
1:C:324:TRP:HE3	1:C:374:TYR:CZ	2.20	0.60
1:A:10:ILE:HD12	1:A:162:TYR:HB2	1.84	0.60
1:A:97:LYS:HB2	1:A:98:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLN:NE2	1:B:333:GLN:HE22	1.99	0.60
1:D:5:SER:HB3	1:D:35:GLU:HG3	1.84	0.60
1:D:321:GLN:NE2	1:D:333:GLN:HE22	2.00	0.59
1:A:321:GLN:NE2	1:A:333:GLN:HE22	2.00	0.59
1:A:285:PHE:HD1	1:A:286:LEU:HD13	1.67	0.59
1:A:223:LYS:HE2	1:A:224:TYR:CE1	2.37	0.59
1:B:133:HIS:HD2	1:C:133:HIS:HD2	1.49	0.59
1:C:9:ARG:NH1	1:C:159:ALA:O	2.36	0.59
1:C:109:TRP:CH2	1:C:113:LYS:CE	2.82	0.59
1:C:9:ARG:HG3	1:C:38:GLU:HB2	1.83	0.59
1:A:267:SER:O	1:A:268:GLU:HB2	2.01	0.59
1:A:253:VAL:HG22	1:A:261:TYR:O	2.02	0.58
1:A:86:PHE:HB2	1:A:89:TYR:O	2.03	0.58
1:B:128:ASN:ND2	4:B:2023:HOH:O	2.35	0.58
1:A:285:PHE:CD1	1:A:286:LEU:HD13	2.38	0.58
1:B:133:HIS:CD2	1:C:133:HIS:HD2	2.21	0.58
1:D:213:SER:OG	3:D:501:NAP:O2N	2.20	0.57
1:C:20:MET:CE	1:C:116:VAL:HG21	2.34	0.57
1:A:445:LEU:HD12	1:A:446:GLU:N	2.19	0.57
1:C:109:TRP:O	1:C:109:TRP:HE3	1.88	0.57
1:B:10:ILE:HD12	1:B:162:TYR:HB2	1.88	0.56
1:D:412:ASN:ND2	1:D:415:THR:CG2	2.68	0.56
1:D:109:TRP:CZ2	1:D:113:LYS:HD3	2.40	0.56
1:A:6:MET:CE	1:A:342:MET:HG2	2.35	0.56
1:B:9:ARG:NH1	1:B:159:ALA:O	2.38	0.56
1:B:445:LEU:C	1:B:445:LEU:HD12	2.24	0.56
1:B:133:HIS:CD2	1:C:133:HIS:CD2	2.93	0.56
1:B:77:SER:OG	1:B:79:GLY:O	2.23	0.56
1:B:9:ARG:HG3	1:B:38:GLU:HB2	1.88	0.56
1:C:20:MET:HE3	1:C:116:VAL:HG21	1.87	0.56
1:C:285:PHE:CD1	1:C:286:LEU:HD13	2.41	0.56
1:D:5:SER:HB3	1:D:35:GLU:HG2	1.86	0.55
1:D:71:MET:HG2	1:D:75:LEU:HD13	1.88	0.55
1:B:450:SER:C	1:B:451:ASP:OD1	2.43	0.55
1:D:285:PHE:CD1	1:D:286:LEU:HD13	2.41	0.55
1:C:102:TYR:HH	1:C:405:TRP:HD1	1.53	0.55
1:C:76:TRP:HA	1:C:104:PRO:HA	1.89	0.54
1:D:82:GLU:OE1	1:D:101:SER:OG	2.17	0.54
1:D:95:PHE:O	1:D:97:LYS:N	2.41	0.54
1:C:109:TRP:HE3	1:C:109:TRP:C	2.11	0.54
1:C:24:ARG:NH1	1:C:119:ALA:HB2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:NH1	3:D:501:NAP:N7A	2.56	0.54
1:A:57:ARG:HH21	1:D:175:VAL:HB	1.72	0.54
1:B:109:TRP:CD2	1:B:113:LYS:HE2	2.42	0.54
1:B:321:GLN:HE22	1:B:333:GLN:HE22	1.55	0.54
1:C:24:ARG:HD3	1:C:115:ARG:CZ	2.38	0.54
1:D:109:TRP:CD2	1:D:113:LYS:HE2	2.43	0.54
1:D:216:ASP:O	1:D:220:GLN:HG2	2.08	0.54
1:D:250:PRO:HG2	1:D:264:ASP:HB3	1.90	0.54
1:B:78:ASP:HA	1:B:417:ARG:HH21	1.74	0.53
1:B:65:GLU:OE2	1:B:132:ARG:NH2	2.41	0.53
1:D:9:ARG:NH1	1:D:159:ALA:O	2.42	0.53
1:B:76:TRP:HA	1:B:104:PRO:HA	1.90	0.53
1:B:6:MET:HE1	1:B:342:MET:HG2	1.91	0.53
1:D:20:MET:HE3	1:D:116:VAL:HG21	1.89	0.53
1:B:285:PHE:CD1	1:B:286:LEU:HD13	2.44	0.52
1:A:20:MET:CE	1:A:116:VAL:HG21	2.39	0.52
1:A:68:HIS:O	1:A:171:SER:OG	2.27	0.52
1:A:9:ARG:NH1	1:A:159:ALA:O	2.43	0.52
1:A:277:THR:HA	3:A:501:NAP:O4B	2.10	0.52
1:A:133:HIS:CD2	1:D:133:HIS:HD2	2.28	0.52
1:D:288:ASP:OD1	1:D:291:ARG:NH1	2.43	0.52
1:A:24:ARG:HH11	1:A:119:ALA:HB2	1.74	0.52
1:B:285:PHE:HD1	1:B:286:LEU:HD13	1.75	0.52
1:C:109:TRP:HE3	1:C:109:TRP:CA	2.23	0.52
1:A:76:TRP:HA	1:A:104:PRO:HA	1.93	0.51
1:C:24:ARG:HH11	1:C:119:ALA:HB2	1.75	0.51
1:A:133:HIS:CD2	1:D:133:HIS:CD2	2.98	0.51
1:B:445:LEU:HD12	1:B:446:GLU:N	2.25	0.51
1:D:184:PHE:HB2	1:D:255:VAL:CG1	2.41	0.51
1:A:234:ARG:NH1	3:A:501:NAP:N7A	2.58	0.51
1:A:235:THR:HG23	3:A:501:NAP:O2X	2.05	0.51
1:B:86:PHE:HB2	1:B:89:TYR:O	2.11	0.51
1:D:179:GLU:HB3	1:D:254:ARG:HB2	1.92	0.51
1:A:321:GLN:HE22	1:A:333:GLN:HE22	1.58	0.51
1:A:178:PHE:HB2	1:A:181:PHE:CZ	2.46	0.50
1:A:184:PHE:HB2	1:A:255:VAL:CG1	2.41	0.50
1:B:84:LEU:HD13	1:B:327:PHE:CD2	2.46	0.50
1:C:109:TRP:CE3	1:C:109:TRP:CA	2.94	0.50
1:C:413:ILE:HG23	1:C:414:MET:HE2	1.92	0.50
1:D:435:THR:HG23	1:D:436:PRO:HD2	1.92	0.50
1:D:277:THR:HG22	3:D:501:NAP:C4A	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:LEU:HD12	1:D:84:LEU:C	2.32	0.50
1:A:413:ILE:HG23	1:A:414:MET:CE	2.42	0.50
1:D:20:MET:HE2	1:D:116:VAL:HG21	1.93	0.50
1:A:435:THR:CG2	1:A:436:PRO:HD2	2.41	0.50
1:D:24:ARG:HD3	1:D:115:ARG:NH2	2.27	0.50
1:A:442:ASP:C	1:A:442:ASP:OD1	2.50	0.50
1:B:108:LEU:O	1:B:112:ILE:HG23	2.11	0.50
1:C:413:ILE:HG23	1:C:414:MET:CE	2.41	0.49
1:D:187:ARG:HD3	1:D:189:LEU:HD22	1.93	0.49
1:D:233:TYR:CD1	1:D:249:ARG:O	2.66	0.49
1:C:97:LYS:HB2	1:C:98:PRO:CD	2.42	0.49
1:D:363:LYS:O	1:D:366:THR:HB	2.12	0.49
1:D:400:LYS:N	1:D:400:LYS:HE3	2.28	0.49
1:B:175:VAL:HB	1:C:57:ARG:HH21	1.76	0.49
1:C:324:TRP:HB3	1:C:374:TYR:CE1	2.47	0.49
1:D:321:GLN:HE22	1:D:333:GLN:HE22	1.60	0.49
1:B:24:ARG:HH11	1:B:119:ALA:HB2	1.77	0.49
1:A:203:LYS:C	1:A:271:ASP:OD2	2.43	0.48
1:C:285:PHE:HD1	1:C:286:LEU:HD13	1.78	0.48
1:D:247:ASP:N	1:D:247:ASP:OD1	2.46	0.48
1:B:57:ARG:HH21	1:C:175:VAL:HB	1.78	0.48
1:B:395:ILE:N	1:B:396:PRO:CD	2.76	0.48
1:D:445:LEU:C	1:D:445:LEU:HD12	2.32	0.48
1:D:95:PHE:O	1:D:96:GLY:C	2.52	0.48
1:A:194:PHE:CE2	1:A:217:ILE:HG23	2.49	0.48
1:A:218:GLY:HA3	1:A:246:TRP:CH2	2.50	0.47
1:C:445:LEU:HD13	1:C:445:LEU:C	2.34	0.47
1:D:285:PHE:HD1	1:D:286:LEU:HD13	1.79	0.47
1:D:413:ILE:HG23	1:D:414:MET:HE3	1.94	0.47
1:A:133:HIS:HD2	1:D:133:HIS:CD2	2.31	0.47
1:A:234:ARG:NH2	3:A:501:NAP:O1X	2.48	0.47
1:D:9:ARG:HG3	1:D:38:GLU:HB2	1.95	0.47
1:A:256:ASP:C	1:A:256:ASP:OD1	2.53	0.47
1:A:217:ILE:HD13	1:A:276:CYS:SG	2.54	0.47
1:C:97:LYS:HB2	1:C:98:PRO:HD2	1.96	0.47
1:A:109:TRP:CZ2	1:A:113:LYS:HD3	2.49	0.47
1:B:84:LEU:C	1:B:84:LEU:HD12	2.34	0.47
1:D:109:TRP:CE2	1:D:113:LYS:HD3	2.50	0.47
1:B:20:MET:CE	1:B:116:VAL:HG21	2.44	0.47
1:D:277:THR:HA	3:D:501:NAP:O4B	2.14	0.47
1:D:76:TRP:HA	1:D:104:PRO:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:PRO:O	1:D:400:LYS:HE3	2.14	0.47
1:D:85:GLU:HB2	1:D:91:PHE:CE2	2.49	0.47
1:B:211:SER:HB3	3:B:501:NAP:O1N	2.15	0.47
1:A:442:ASP:OD1	1:A:443:ASP:N	2.47	0.47
1:A:408:HIS:ND1	1:A:419:HIS:HD2	2.11	0.46
1:B:232:CYS:HA	1:B:249:ARG:O	2.16	0.46
1:A:109:TRP:NE1	1:A:113:LYS:HD3	2.31	0.46
1:A:84:LEU:HD12	1:A:84:LEU:C	2.36	0.46
1:A:203:LYS:CA	1:A:271:ASP:OD2	2.64	0.46
1:A:426:THR:OG1	1:A:428:THR:OG1	1.89	0.46
1:A:175:VAL:HB	1:D:57:ARG:HH21	1.80	0.46
1:C:109:TRP:CZ3	1:C:113:LYS:CG	2.93	0.46
1:B:417:ARG:HB2	4:B:2072:HOH:O	2.15	0.46
1:D:223:LYS:HE2	1:D:224:TYR:CE1	2.50	0.46
1:C:109:TRP:CE3	1:C:113:LYS:CE	2.75	0.46
1:D:445:LEU:C	1:D:445:LEU:HD13	2.36	0.46
1:B:20:MET:HE3	1:B:116:VAL:HG21	1.98	0.45
1:A:204:THR:HA	1:A:228:LYS:O	2.16	0.45
1:A:253:VAL:CG2	1:A:261:TYR:O	2.64	0.45
1:D:178:PHE:HB2	1:D:181:PHE:CZ	2.50	0.45
1:A:288:ASP:OD1	1:A:291:ARG:NH1	2.49	0.45
1:A:247:ASP:OD1	1:A:247:ASP:N	2.50	0.45
1:D:252:LEU:HD11	1:D:255:VAL:HG23	1.98	0.45
1:D:238:MET:N	1:D:248:GLU:OE2	2.39	0.45
1:D:102:TYR:HH	1:D:405:TRP:HD1	1.64	0.45
1:A:84:LEU:HD13	1:A:327:PHE:CD2	2.51	0.45
1:C:232:CYS:HA	1:C:249:ARG:O	2.17	0.45
1:D:24:ARG:HD3	1:D:115:ARG:NE	2.32	0.45
1:D:442:ASP:OD1	1:D:443:ASP:N	2.50	0.45
1:C:78:ASP:HA	1:C:417:ARG:HH21	1.82	0.45
1:A:20:MET:HE2	1:A:116:VAL:HG21	1.98	0.44
1:B:235:THR:HG23	4:B:2044:HOH:O	2.17	0.44
1:A:179:GLU:HB3	1:A:254:ARG:HB2	1.99	0.44
1:A:408:HIS:CG	1:A:419:HIS:CD2	3.04	0.44
1:A:271:ASP:HB3	4:A:2027:HOH:O	2.05	0.44
1:B:452:LYS:HG3	1:B:452:LYS:O	2.16	0.44
1:C:187:ARG:HD3	1:C:189:LEU:HD22	1.99	0.44
1:D:324:TRP:N	1:D:324:TRP:CD1	2.84	0.44
1:D:200:PHE:HA	1:D:203:LYS:HD3	1.99	0.44
1:B:277:THR:HA	3:B:501:NAP:O4B	2.18	0.44
1:C:403:LEU:HD12	1:C:403:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:HA	1:A:367:LEU:HD22	1.99	0.44
1:B:178:PHE:HB2	1:B:181:PHE:CZ	2.52	0.43
1:A:178:PHE:HB2	1:A:181:PHE:CE1	2.53	0.43
1:D:256:ASP:OD1	1:D:256:ASP:C	2.57	0.43
1:B:291:ARG:NH2	1:C:153:ASP:OD1	2.52	0.43
1:A:100:ALA:CB	1:A:433:HIS:HB2	2.48	0.43
1:A:252:LEU:HD11	1:A:255:VAL:HG23	2.00	0.43
1:C:289:ASP:N	1:C:289:ASP:OD1	2.48	0.43
1:A:223:LYS:HG2	1:A:224:TYR:CD1	2.54	0.43
1:A:277:THR:HG22	3:A:501:NAP:C4A	2.48	0.43
1:D:172:THR:HA	1:D:173:PRO:HD3	1.84	0.43
1:B:153:ASP:OD1	1:C:291:ARG:NH2	2.52	0.43
1:C:417:ARG:HB2	4:C:2079:HOH:O	2.18	0.43
1:D:178:PHE:HB2	1:D:181:PHE:CE1	2.54	0.43
1:A:207:LEU:O	1:A:231:SER:HA	2.19	0.43
1:A:413:ILE:HG23	1:A:414:MET:HE2	2.00	0.43
1:C:108:LEU:O	1:C:112:ILE:HG23	2.17	0.43
1:A:35:GLU:OE1	1:C:354:LYS:HE3	2.19	0.43
1:D:435:THR:HG22	1:D:436:PRO:HD2	2.00	0.43
1:A:24:ARG:NH1	1:A:119:ALA:HB2	2.34	0.42
1:B:250:PRO:HG2	1:B:264:ASP:HB3	2.00	0.42
1:D:283:PHE:HB3	1:D:286:LEU:HD22	2.01	0.42
1:A:280:ILE:HG21	1:A:280:ILE:HD12	1.80	0.42
1:C:321:GLN:HE22	1:C:333:GLN:HE22	1.63	0.42
1:D:407:HIS:CE1	1:D:411:GLU:OE2	2.72	0.42
1:D:385:ILE:HD12	1:D:392:SER:HA	2.01	0.42
1:A:232:CYS:HA	1:A:249:ARG:O	2.20	0.42
1:A:71:MET:HG2	1:A:75:LEU:HD13	2.01	0.42
1:D:403:LEU:HA	1:D:403:LEU:HD12	1.77	0.42
1:C:123:LYS:NZ	4:C:2022:HOH:O	2.53	0.42
1:C:178:PHE:HB2	1:C:181:PHE:CZ	2.55	0.42
1:A:385:ILE:HD12	1:A:392:SER:HA	2.01	0.42
1:D:184:PHE:CE2	1:D:186:GLY:CA	3.03	0.42
1:A:324:TRP:CD1	1:A:324:TRP:N	2.88	0.41
1:B:283:PHE:HB3	1:B:286:LEU:HD22	2.01	0.41
1:C:229:LEU:O	1:C:246:TRP:HA	2.19	0.41
1:D:204:THR:HA	1:D:228:LYS:O	2.20	0.41
1:C:103:PRO:HA	1:C:104:PRO:HD3	1.91	0.41
1:C:109:TRP:HZ3	1:C:113:LYS:CD	2.03	0.41
1:D:108:LEU:HA	1:D:108:LEU:HD23	1.83	0.41
1:D:184:PHE:HB2	1:D:255:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ILE:CG2	1:D:414:MET:CE	2.93	0.41
1:A:22:GLN:HA	1:A:334:ALA:HB1	2.01	0.41
1:B:183:LYS:HE3	1:B:183:LYS:HB2	1.77	0.41
1:C:211:SER:HB3	3:C:501:NAP:O1N	2.20	0.41
1:A:134:VAL:HB	1:A:286:LEU:HD12	2.02	0.41
1:A:438:ILE:HG13	1:A:438:ILE:O	2.19	0.41
1:A:81:LYS:HZ2	1:A:101:SER:CA	2.28	0.41
1:B:103:PRO:HA	1:B:104:PRO:HD3	1.90	0.41
1:C:199:GLU:HG2	1:C:199:GLU:O	2.20	0.41
1:B:452:LYS:CG	1:B:452:LYS:O	2.69	0.41
1:A:200:PHE:HA	1:A:203:LYS:HD3	2.03	0.41
1:C:445:LEU:O	1:C:445:LEU:HD13	2.21	0.41
1:C:84:LEU:HD12	1:C:84:LEU:C	2.41	0.41
1:C:445:LEU:HD12	1:C:445:LEU:C	2.41	0.41
1:A:223:LYS:HG2	1:A:224:TYR:CE1	2.56	0.41
1:B:49:GLY:HA3	1:B:109:TRP:HE1	1.86	0.41
1:C:324:TRP:CE3	1:C:374:TYR:CZ	3.05	0.40
1:A:380:TYR:CZ	1:A:384:LEU:HD11	2.56	0.40
1:B:405:TRP:CH2	1:B:406:LYS:HE2	2.55	0.40
1:B:77:SER:HB2	1:B:108:LEU:HD11	2.03	0.40
1:A:20:MET:HE3	1:A:116:VAL:HG21	2.01	0.40
1:B:200:PHE:HA	1:B:203:LYS:HD3	2.02	0.40
1:B:68:HIS:CE1	2:B:500:FAD:H51A	2.56	0.40
1:C:424:LEU:N	4:C:2018:HOH:O	2.48	0.40
1:A:213:SER:CB	1:A:217:ILE:CD1	2.87	0.40
1:A:445:LEU:HD13	1:A:445:LEU:C	2.41	0.40
1:B:253:VAL:HG22	1:B:261:TYR:O	2.21	0.40
1:C:109:TRP:CE3	1:C:109:TRP:C	2.94	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	444/461 (96%)	426 (96%)	18 (4%)	0	100	100
1	B	445/461 (96%)	434 (98%)	11 (2%)	0	100	100
1	C	450/461 (98%)	438 (97%)	12 (3%)	0	100	100
1	D	445/461 (96%)	430 (97%)	13 (3%)	2 (0%)	34	46
All	All	1784/1844 (97%)	1728 (97%)	54 (3%)	2 (0%)	51	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	96	GLY
1	D	450	SER

### 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	386/397 (97%)	347 (90%)	39 (10%)	7	8
1	B	387/397 (98%)	352 (91%)	35 (9%)	9	11
1	C	392/397 (99%)	355 (91%)	37 (9%)	8	10
1	D	387/397 (98%)	346 (89%)	41 (11%)	6	7
All	All	1552/1588 (98%)	1400 (90%)	152 (10%)	8	9

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	24	ARG
1	A	28	SER
1	A	38	GLU
1	A	48	TRP
1	A	58	THR
1	A	60	LEU
1	A	62	GLU
1	A	82	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	112	ILE
1	A	113	LYS
1	A	116	VAL
1	A	128	ASN
1	A	171	SER
1	A	183	LYS
1	A	189	LEU
1	A	235	THR
1	A	241	LYS
1	A	247	ASP
1	A	253	VAL
1	A	267	SER
1	A	269	LYS
1	A	280	ILE
1	A	286	LEU
1	A	307	VAL
1	A	338	ARG
1	A	340	VAL
1	A	347	LEU
1	A	354	LYS
1	A	363	LYS
1	A	367	LEU
1	A	392	SER
1	A	400	LYS
1	A	410	LYS
1	A	424	LEU
1	A	428	THR
1	A	445	LEU
1	A	450	SER
1	A	451	ASP
1	B	6	MET
1	B	9	ARG
1	B	24	ARG
1	B	48	TRP
1	B	58	THR
1	B	60	LEU
1	B	62	GLU
1	B	112	ILE
1	B	128	ASN
1	B	183	LYS
1	B	189	LEU
1	B	235	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	247	ASP
1	B	255	VAL
1	B	268	GLU
1	B	280	ILE
1	B	286	LEU
1	B	302	ASN
1	B	307	VAL
1	B	338	ARG
1	B	340	VAL
1	B	347	LEU
1	B	363	LYS
1	B	367	LEU
1	B	385	ILE
1	B	400	LYS
1	B	403	LEU
1	B	410	LYS
1	B	424	LEU
1	B	428	THR
1	B	429	MET
1	B	441	LEU
1	B	445	LEU
1	B	450	SER
1	B	451	ASP
1	C	5	SER
1	C	9	ARG
1	C	24	ARG
1	C	48	TRP
1	C	58	THR
1	C	60	LEU
1	C	62	GLU
1	C	92	ASP
1	C	109	TRP
1	C	112	ILE
1	C	113	LYS
1	C	116	VAL
1	C	128	ASN
1	C	183	LYS
1	C	189	LEU
1	C	235	THR
1	C	241	LYS
1	C	247	ASP
1	C	255	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	257	THR
1	C	280	ILE
1	C	286	LEU
1	C	302	ASN
1	C	307	VAL
1	C	338	ARG
1	C	340	VAL
1	C	347	LEU
1	C	367	LEU
1	C	385	ILE
1	C	400	LYS
1	C	403	LEU
1	C	410	LYS
1	C	424	LEU
1	C	428	THR
1	C	441	LEU
1	C	445	LEU
1	C	451	ASP
1	D	5	SER
1	D	9	ARG
1	D	24	ARG
1	D	28	SER
1	D	48	TRP
1	D	58	THR
1	D	60	LEU
1	D	62	GLU
1	D	101	SER
1	D	112	ILE
1	D	116	VAL
1	D	128	ASN
1	D	139	ASP
1	D	171	SER
1	D	183	LYS
1	D	235	THR
1	D	247	ASP
1	D	266	SER
1	D	267	SER
1	D	268	GLU
1	D	277	THR
1	D	280	ILE
1	D	286	LEU
1	D	307	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	328	ASN
1	D	338	ARG
1	D	340	VAL
1	D	347	LEU
1	D	367	LEU
1	D	385	ILE
1	D	398	THR
1	D	400	LYS
1	D	403	LEU
1	D	410	LYS
1	D	424	LEU
1	D	428	THR
1	D	429	MET
1	D	441	LEU
1	D	445	LEU
1	D	450	SER
1	D	451	ASP

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	63	ASN
1	A	128	ASN
1	A	133	HIS
1	A	141	GLN
1	A	321	GLN
1	A	407	HIS
1	A	419	HIS
1	A	433	HIS
1	B	45	GLN
1	B	63	ASN
1	B	128	ASN
1	B	133	HIS
1	B	321	GLN
1	B	407	HIS
1	C	45	GLN
1	C	63	ASN
1	C	128	ASN
1	C	133	HIS
1	C	321	GLN
1	D	63	ASN
1	D	128	ASN

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Mol	Chain	Res	Type
1	D	133	HIS
1	D	321	GLN
1	D	407	HIS
1	D	412	ASN
1	D	433	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 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	501	-	45,52,52	1.75	10 (22%)	56,80,80	1.92	13 (23%)
3	NAP	A	501	-	45,52,52	1.54	8 (17%)	56,80,80	2.04	13 (23%)
2	FAD	A	500	-	51,58,58	1.44	7 (13%)	60,89,89	2.25	13 (21%)
3	NAP	C	501	-	45,52,52	1.43	7 (15%)	56,80,80	1.78	10 (17%)
2	FAD	C	500	-	51,58,58	1.57	8 (15%)	60,89,89	1.97	12 (20%)
3	NAP	B	501	-	45,52,52	1.48	8 (17%)	56,80,80	1.96	12 (21%)
2	FAD	D	500	-	51,58,58	1.56	6 (11%)	60,89,89	2.16	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	B	500	-	51,58,58	1.34	6 (11%)	60,89,89	1.94	16 (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	501	-	-	13/31/67/67	0/5/5/5
3	NAP	A	501	-	-	13/31/67/67	0/5/5/5
2	FAD	A	500	-	-	3/30/50/50	0/6/6/6
3	NAP	C	501	-	-	6/31/67/67	0/5/5/5
2	FAD	C	500	-	-	4/30/50/50	0/6/6/6
3	NAP	B	501	-	-	11/31/67/67	0/5/5/5
2	FAD	D	500	-	-	3/30/50/50	0/6/6/6
2	FAD	B	500	-	-	4/30/50/50	0/6/6/6

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	FAD	C10-N1	5.95	1.40	1.33
3	D	501	NAP	O4B-C1B	5.52	1.48	1.41
2	C	500	FAD	C4X-N5	4.87	1.40	1.33
2	D	500	FAD	C4X-N5	4.67	1.40	1.33
2	C	500	FAD	C2A-N3A	4.35	1.39	1.32
2	A	500	FAD	C10-N1	4.27	1.38	1.33
3	B	501	NAP	O4B-C1B	4.04	1.46	1.41
2	B	500	FAD	C4X-N5	3.98	1.39	1.33
2	B	500	FAD	C10-N1	3.91	1.38	1.33
3	D	501	NAP	P2B-O1X	3.86	1.63	1.50
3	C	501	NAP	O4D-C1D	3.74	1.46	1.41
3	A	501	NAP	O4D-C1D	3.71	1.46	1.41
2	B	500	FAD	C2A-N3A	3.70	1.38	1.32
3	A	501	NAP	P2B-O1X	3.58	1.62	1.50
3	D	501	NAP	C7N-N7N	3.53	1.39	1.33
3	B	501	NAP	C7N-N7N	3.52	1.39	1.33
3	C	501	NAP	P2B-O1X	3.45	1.61	1.50
3	C	501	NAP	P2B-O2B	3.41	1.65	1.59
3	D	501	NAP	O4D-C1D	3.30	1.45	1.41
3	A	501	NAP	C7N-N7N	3.27	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C10-N1	3.22	1.37	1.33
2	A	500	FAD	C4-N3	3.10	1.38	1.33
2	A	500	FAD	C4X-N5	3.10	1.37	1.33
3	B	501	NAP	O4D-C1D	3.01	1.45	1.41
3	B	501	NAP	P2B-O1X	2.93	1.60	1.50
2	A	500	FAD	C1'-N10	2.92	1.51	1.48
2	B	500	FAD	C2A-N1A	2.83	1.39	1.33
3	A	501	NAP	O4B-C1B	2.77	1.44	1.41
2	C	500	FAD	O2'-C2'	-2.76	1.37	1.43
3	A	501	NAP	P2B-O3X	2.74	1.65	1.54
2	D	500	FAD	C4-N3	2.73	1.37	1.33
2	D	500	FAD	C1'-N10	2.69	1.51	1.48
2	C	500	FAD	C2B-C1B	-2.66	1.49	1.53
3	C	501	NAP	C7N-N7N	2.66	1.38	1.33
3	D	501	NAP	C2N-C3N	2.64	1.43	1.39
3	A	501	NAP	C4N-C3N	2.63	1.43	1.39
3	B	501	NAP	P2B-O2B	2.56	1.64	1.59
2	C	500	FAD	C2A-N1A	2.56	1.38	1.33
3	D	501	NAP	P2B-O3X	2.54	1.64	1.54
3	D	501	NAP	C2A-N3A	2.53	1.36	1.32
3	C	501	NAP	O4B-C1B	2.52	1.44	1.41
3	D	501	NAP	C4N-C3N	2.51	1.43	1.39
2	B	500	FAD	P-O2P	-2.49	1.43	1.55
2	C	500	FAD	P-O2P	-2.49	1.43	1.55
2	D	500	FAD	C2A-N3A	2.48	1.36	1.32
3	B	501	NAP	C3B-C2B	2.48	1.58	1.52
3	A	501	NAP	C2N-N1N	2.48	1.38	1.35
2	A	500	FAD	C2A-N3A	2.45	1.36	1.32
3	D	501	NAP	C2N-N1N	2.42	1.37	1.35
2	A	500	FAD	C2B-C1B	-2.41	1.50	1.53
3	D	501	NAP	P2B-O2B	2.40	1.63	1.59
2	C	500	FAD	C6-C5X	-2.39	1.38	1.41
3	A	501	NAP	C2N-C3N	2.25	1.42	1.39
2	A	500	FAD	O4B-C4B	-2.24	1.40	1.45
2	D	500	FAD	C8A-N7A	2.20	1.38	1.34
3	B	501	NAP	C2N-C3N	2.20	1.42	1.39
3	B	501	NAP	C4N-C3N	2.13	1.42	1.39
3	C	501	NAP	C3N-C7N	-2.05	1.47	1.50
2	B	500	FAD	C5'-C4'	2.04	1.54	1.51
3	C	501	NAP	C2N-C3N	2.01	1.42	1.39

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C1'-N10-C9A	9.39	125.69	118.29
2	D	500	FAD	C1'-N10-C9A	8.45	124.94	118.29
2	B	500	FAD	C1'-N10-C9A	7.30	124.04	118.29
2	D	500	FAD	N3A-C2A-N1A	-7.05	117.66	128.68
2	A	500	FAD	C4-N3-C2	7.00	121.05	115.14
2	D	500	FAD	C4-N3-C2	6.84	120.92	115.14
2	C	500	FAD	C1'-N10-C9A	6.79	123.64	118.29
2	A	500	FAD	N3A-C2A-N1A	-6.69	118.22	128.68
2	C	500	FAD	C4-N3-C2	6.23	120.41	115.14
3	A	501	NAP	C3N-C7N-N7N	6.19	125.17	117.75
3	D	501	NAP	C3N-C7N-N7N	6.03	124.98	117.75
3	C	501	NAP	O5D-C5D-C4D	-5.63	89.61	108.99
2	B	500	FAD	C4-N3-C2	5.62	119.89	115.14
3	B	501	NAP	O5D-C5D-C4D	-5.49	90.10	108.99
2	B	500	FAD	N3A-C2A-N1A	-5.28	120.43	128.68
2	C	500	FAD	N3A-C2A-N1A	-5.25	120.47	128.68
3	A	501	NAP	N3A-C2A-N1A	-5.16	120.61	128.68
3	C	501	NAP	C3N-C7N-N7N	4.93	123.67	117.75
3	C	501	NAP	N3A-C2A-N1A	-4.90	121.02	128.68
3	A	501	NAP	O5B-C5B-C4B	-4.64	93.01	108.99
3	B	501	NAP	C3N-C7N-N7N	4.49	123.13	117.75
3	D	501	NAP	C3B-C2B-C1B	-4.41	94.60	102.89
3	B	501	NAP	N3A-C2A-N1A	-4.37	121.84	128.68
3	B	501	NAP	O3D-C3D-C4D	-4.29	98.65	111.05
3	D	501	NAP	O5B-C5B-C4B	-4.23	94.45	108.99
3	B	501	NAP	O5B-C5B-C4B	-4.20	94.52	108.99
2	B	500	FAD	C4X-N5-C5X	4.17	120.94	116.77
3	D	501	NAP	PN-O3-PA	-4.06	118.89	132.83
3	C	501	NAP	O5B-C5B-C4B	-4.04	95.10	108.99
3	A	501	NAP	O7N-C7N-C3N	-3.94	114.92	119.63
3	A	501	NAP	C3B-C2B-C1B	-3.84	95.67	102.89
3	D	501	NAP	N3A-C2A-N1A	-3.81	122.72	128.68
2	A	500	FAD	P-O3P-PA	-3.76	119.92	132.83
3	A	501	NAP	PN-O3-PA	-3.74	119.98	132.83
3	D	501	NAP	O7N-C7N-C3N	-3.74	115.16	119.63
2	C	500	FAD	C5X-C9A-N10	3.68	120.38	117.72
3	B	501	NAP	C3B-C2B-C1B	-3.67	96.00	102.89
3	B	501	NAP	PN-O3-PA	-3.62	120.40	132.83
2	C	500	FAD	O2'-C2'-C3'	-3.52	100.53	109.10
2	C	500	FAD	C4X-N5-C5X	3.49	120.26	116.77
2	B	500	FAD	C5X-C9A-N10	3.46	120.22	117.72
3	B	501	NAP	O7N-C7N-C3N	-3.39	115.57	119.63
2	D	500	FAD	C5X-C9A-N10	3.38	120.17	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	NAP	O5D-C5D-C4D	-3.38	97.36	108.99
3	C	501	NAP	C3B-C2B-C1B	-3.38	96.54	102.89
3	A	501	NAP	O2N-PN-O5D	-3.30	92.40	107.75
2	C	500	FAD	O2'-C2'-C1'	-3.23	101.82	109.59
2	C	500	FAD	P-O3P-PA	-3.21	121.80	132.83
3	C	501	NAP	O7N-C7N-C3N	-3.21	115.80	119.63
3	B	501	NAP	O2N-PN-O5D	-3.14	93.18	107.75
2	A	500	FAD	C4X-N5-C5X	3.12	119.89	116.77
3	D	501	NAP	O2N-PN-O5D	-3.10	93.36	107.75
3	A	501	NAP	O5D-C5D-C4D	-3.09	98.36	108.99
2	A	500	FAD	O2'-C2'-C1'	-2.91	102.58	109.59
2	A	500	FAD	C4A-C5A-N7A	-2.88	106.40	109.40
2	D	500	FAD	C4X-N5-C5X	2.85	119.62	116.77
2	A	500	FAD	C9A-N10-C10	-2.81	118.22	121.91
3	A	501	NAP	C2A-N1A-C6A	2.80	123.55	118.75
3	B	501	NAP	O3X-P2B-O1X	-2.75	99.90	110.68
3	C	501	NAP	PN-O3-PA	-2.75	123.40	132.83
2	C	500	FAD	C6-C5X-C9A	2.67	122.55	119.05
2	A	500	FAD	C1'-N10-C10	-2.64	116.05	118.41
3	D	501	NAP	O2B-C2B-C1B	-2.61	100.72	110.10
3	A	501	NAP	C3D-C2D-C1D	-2.52	97.18	100.98
2	D	500	FAD	C1'-N10-C10	-2.47	116.20	118.41
2	A	500	FAD	C5X-C9A-N10	2.46	119.50	117.72
3	A	501	NAP	C1B-N9A-C4A	-2.46	122.32	126.64
2	B	500	FAD	C10-C4X-N5	-2.45	119.56	121.26
3	A	501	NAP	O2B-C2B-C1B	-2.45	101.28	110.10
3	C	501	NAP	O2N-PN-O5D	-2.43	96.48	107.75
2	D	500	FAD	O2'-C2'-C3'	-2.41	103.25	109.10
2	D	500	FAD	C9A-N10-C10	-2.38	118.79	121.91
2	A	500	FAD	C4X-C4-N3	-2.37	120.19	123.43
3	D	501	NAP	O3D-C3D-C4D	-2.36	104.22	111.05
2	D	500	FAD	O2'-C2'-C1'	-2.33	103.97	109.59
3	D	501	NAP	O2D-C2D-C1D	-2.32	102.28	110.85
2	B	500	FAD	O2'-C2'-C1'	-2.28	104.11	109.59
2	C	500	FAD	C4-C4X-N5	2.27	121.20	118.60
2	D	500	FAD	C6-C5X-C9A	2.27	122.03	119.05
2	B	500	FAD	C4X-C4-N3	-2.27	120.33	123.43
2	B	500	FAD	C1'-N10-C10	-2.23	116.41	118.41
3	C	501	NAP	O3D-C3D-C2D	-2.22	104.63	111.82
2	B	500	FAD	C6-C5X-C9A	2.21	121.95	119.05
2	B	500	FAD	C1B-N9A-C4A	-2.21	122.76	126.64
2	C	500	FAD	C4X-C4-N3	-2.19	120.43	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	P-O3P-PA	-2.19	125.30	132.83
3	D	501	NAP	C4A-C5A-N7A	-2.19	107.12	109.40
2	D	500	FAD	P-O3P-PA	-2.16	125.41	132.83
2	A	500	FAD	O5'-C5'-C4'	-2.12	103.69	109.36
3	D	501	NAP	O2X-P2B-O2B	2.12	115.48	105.99
2	A	500	FAD	C4-C4X-N5	2.11	121.01	118.60
2	B	500	FAD	C9A-C5X-N5	-2.08	119.11	122.36
3	A	501	NAP	C4A-C5A-N7A	-2.08	107.24	109.40
2	B	500	FAD	O4B-C4B-C3B	2.07	109.22	105.11
2	D	500	FAD	C4-C4X-N5	2.06	120.95	118.60
3	C	501	NAP	C4A-C5A-N7A	-2.06	107.25	109.40
2	B	500	FAD	C3B-C2B-C1B	2.05	104.07	100.98
2	B	500	FAD	O2'-C2'-C3'	-2.05	104.11	109.10
3	B	501	NAP	O2D-C2D-C1D	-2.04	103.33	110.85
2	D	500	FAD	O5'-C5'-C4'	-2.03	103.95	109.36
3	B	501	NAP	C2A-N1A-C6A	2.01	122.20	118.75
2	C	500	FAD	C9A-N10-C10	-2.00	119.29	121.91

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	NAP	C5B-O5B-PA-O1A
3	D	501	NAP	C5B-O5B-PA-O2A
3	D	501	NAP	C3B-C4B-C5B-O5B
3	D	501	NAP	C5D-O5D-PN-O3
3	D	501	NAP	C5D-O5D-PN-O1N
3	D	501	NAP	C5D-O5D-PN-O2N
3	D	501	NAP	O4D-C4D-C5D-O5D
3	D	501	NAP	C3D-C4D-C5D-O5D
3	A	501	NAP	C5B-O5B-PA-O1A
3	A	501	NAP	C5B-O5B-PA-O2A
3	A	501	NAP	PN-O3-PA-O5B
3	A	501	NAP	O4B-C4B-C5B-O5B
3	A	501	NAP	C3B-C4B-C5B-O5B
3	A	501	NAP	C5D-O5D-PN-O3
3	A	501	NAP	C5D-O5D-PN-O2N
3	A	501	NAP	C3D-C4D-C5D-O5D
2	A	500	FAD	N10-C1'-C2'-O2'
2	A	500	FAD	N10-C1'-C2'-C3'
3	C	501	NAP	C2B-O2B-P2B-O3X
2	C	500	FAD	N10-C1'-C2'-O2'

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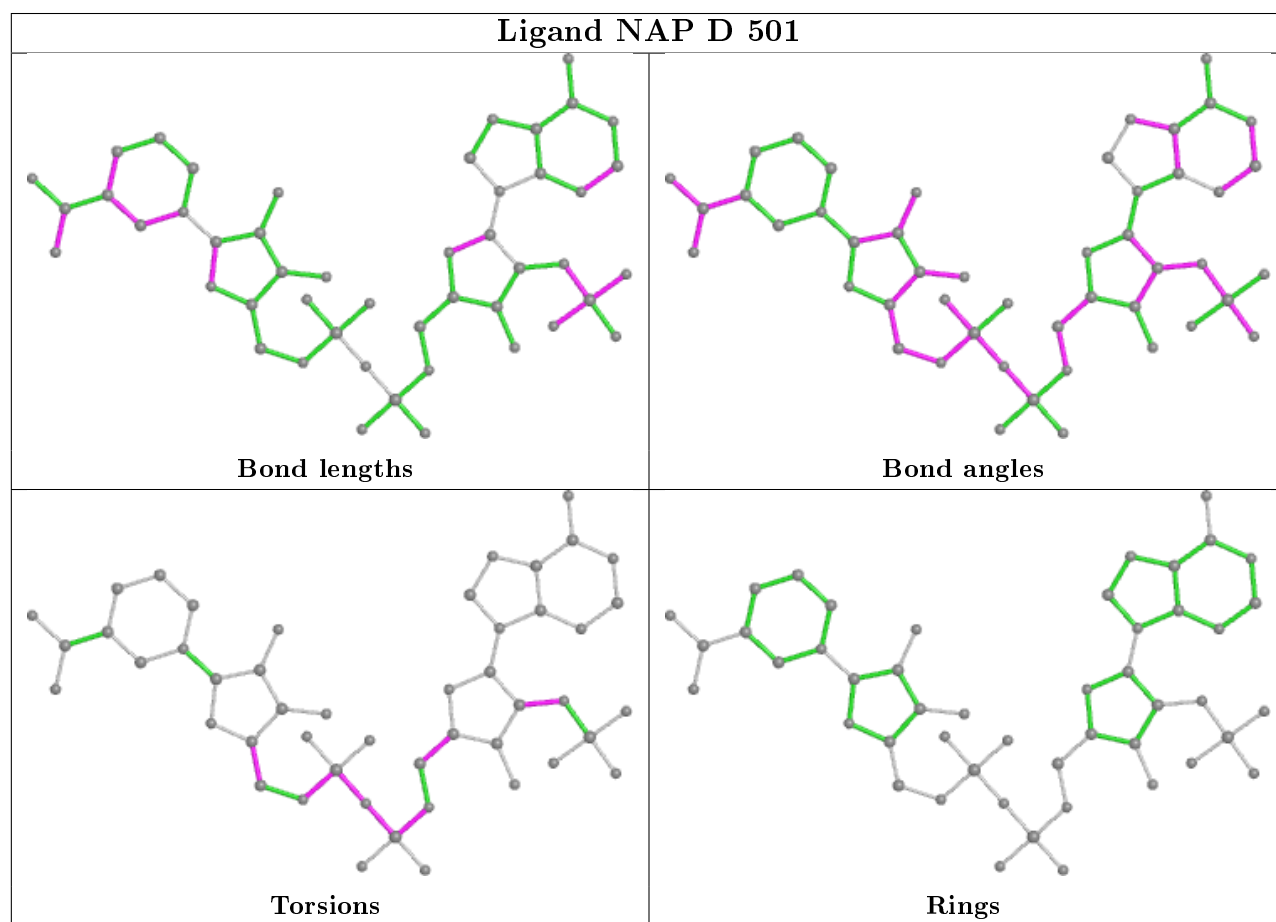
Mol	Chain	Res	Type	Atoms
2	C	500	FAD	N10-C1'-C2'-C3'
3	B	501	NAP	C5B-O5B-PA-O1A
3	B	501	NAP	C5B-O5B-PA-O2A
3	B	501	NAP	PN-O3-PA-O5B
3	B	501	NAP	C5D-O5D-PN-O3
3	B	501	NAP	C3D-C4D-C5D-O5D
2	D	500	FAD	N10-C1'-C2'-O2'
2	D	500	FAD	N10-C1'-C2'-C3'
2	B	500	FAD	N10-C1'-C2'-O2'
2	B	500	FAD	N10-C1'-C2'-C3'
3	D	501	NAP	O4B-C4B-C5B-O5B
3	C	501	NAP	O4B-C4B-C5B-O5B
3	C	501	NAP	C3D-C4D-C5D-O5D
3	B	501	NAP	O4B-C4B-C5B-O5B
3	B	501	NAP	C3B-C4B-C5B-O5B
3	A	501	NAP	O4D-C4D-C5D-O5D
3	B	501	NAP	O4D-C4D-C5D-O5D
3	A	501	NAP	C1B-C2B-O2B-P2B
3	D	501	NAP	C1B-C2B-O2B-P2B
3	D	501	NAP	PN-O3-PA-O5B
2	B	500	FAD	O4B-C4B-C5B-O5B
3	B	501	NAP	C5B-O5B-PA-O3
3	D	501	NAP	PA-O3-PN-O1N
3	A	501	NAP	PA-O3-PN-O1N
2	C	500	FAD	C2'-C3'-C4'-C5'
3	A	501	NAP	C5D-O5D-PN-O1N
3	B	501	NAP	C5D-O5D-PN-O2N
3	C	501	NAP	C3B-C4B-C5B-O5B
3	C	501	NAP	C1B-C2B-O2B-P2B
3	C	501	NAP	O4D-C4D-C5D-O5D
3	D	501	NAP	C5B-O5B-PA-O3
3	A	501	NAP	C5B-O5B-PA-O3
3	B	501	NAP	C2B-O2B-P2B-O3X
2	A	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	O4B-C4B-C5B-O5B
2	D	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	C2'-C3'-C4'-C5'

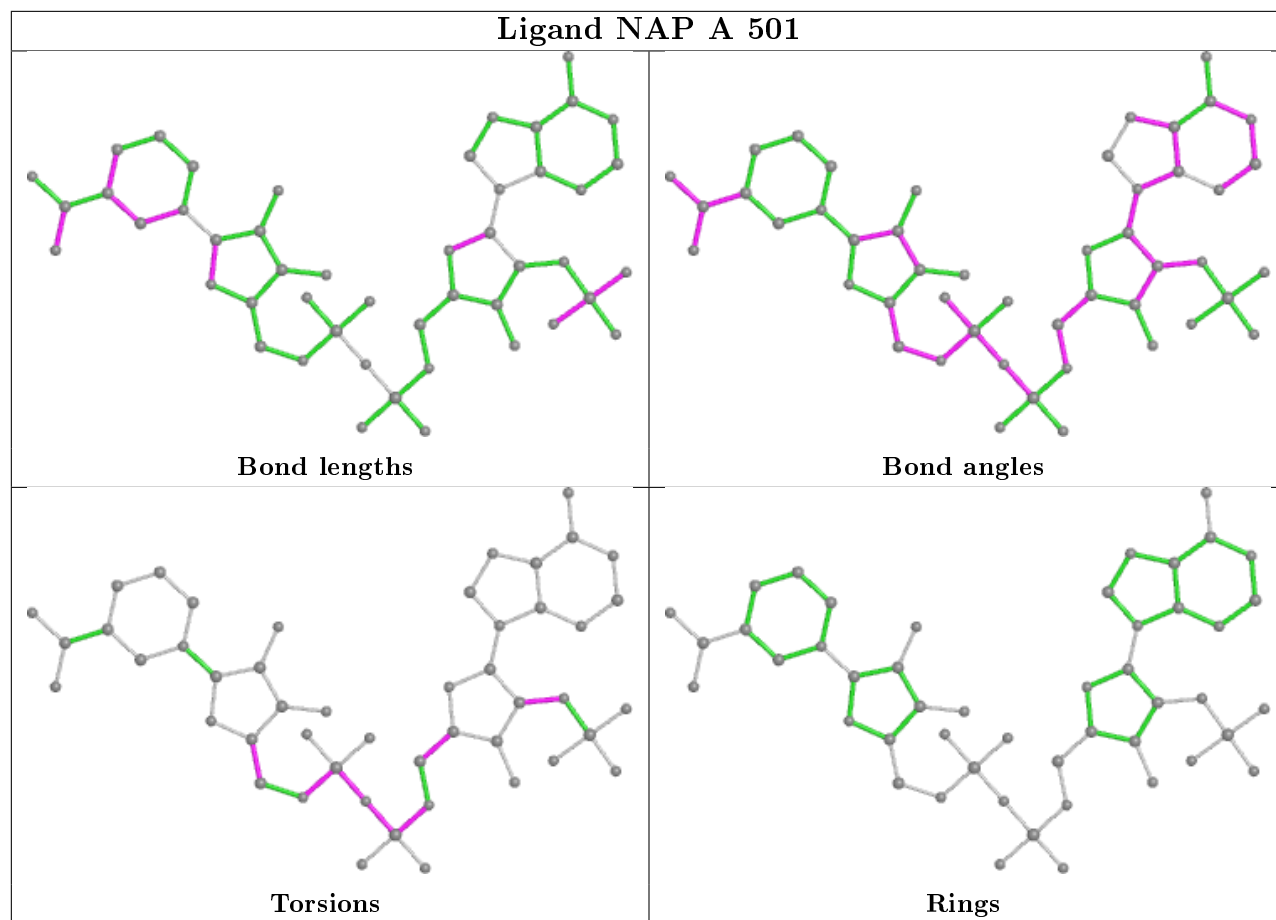
There are no ring outliers.

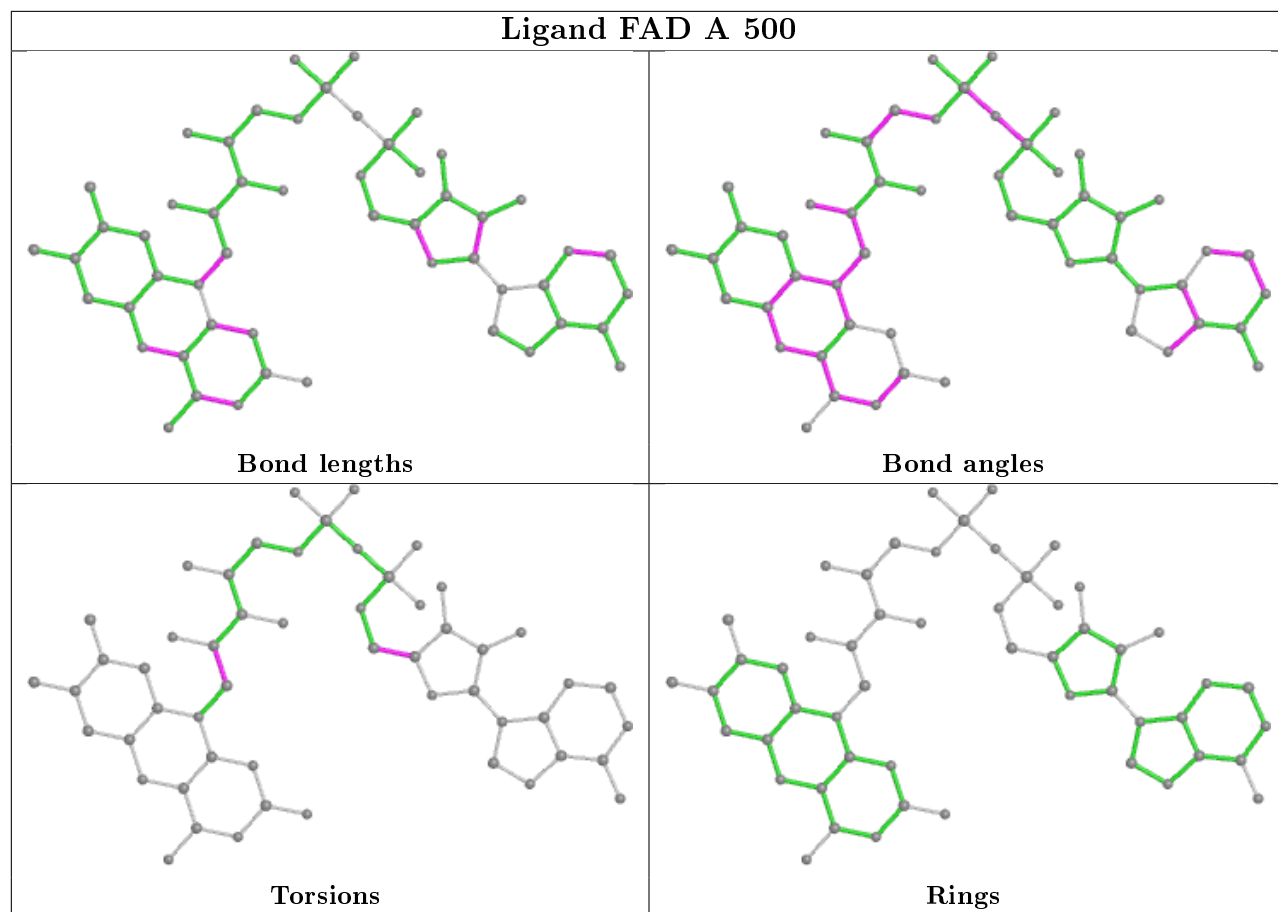
5 monomers are involved in 24 short contacts:

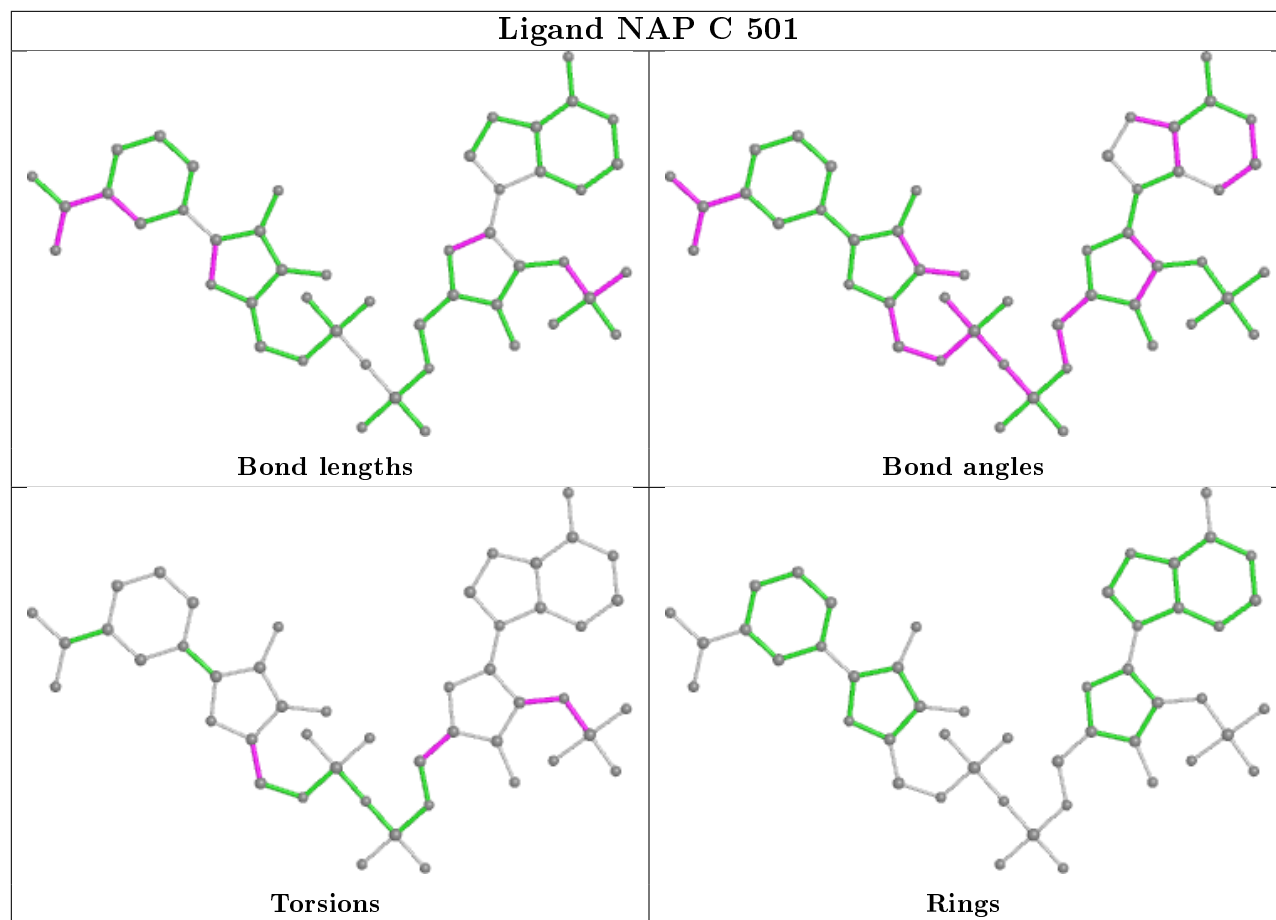
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	NAP	7	0
3	A	501	NAP	7	0
3	C	501	NAP	4	0
3	B	501	NAP	5	0
2	B	500	FAD	1	0

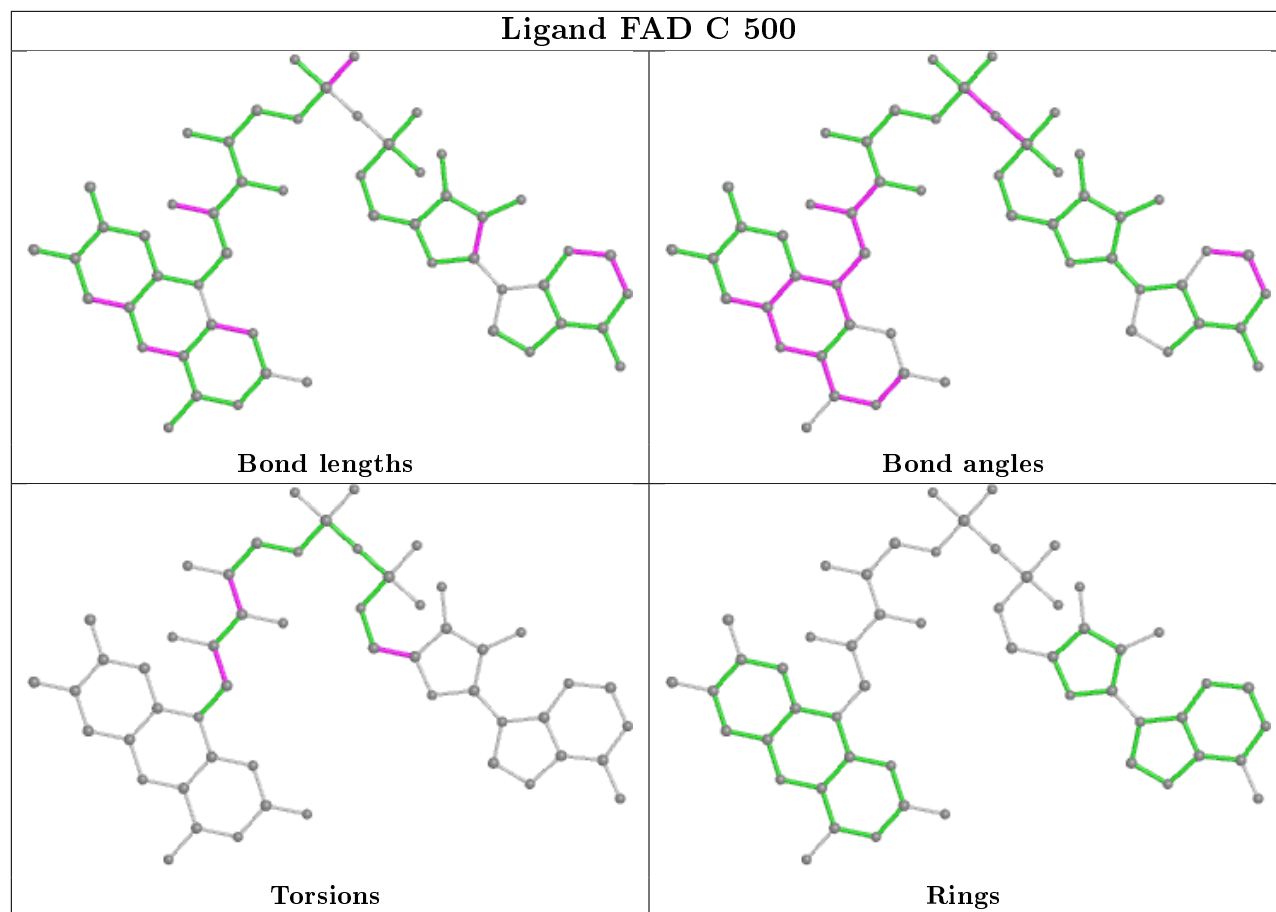
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

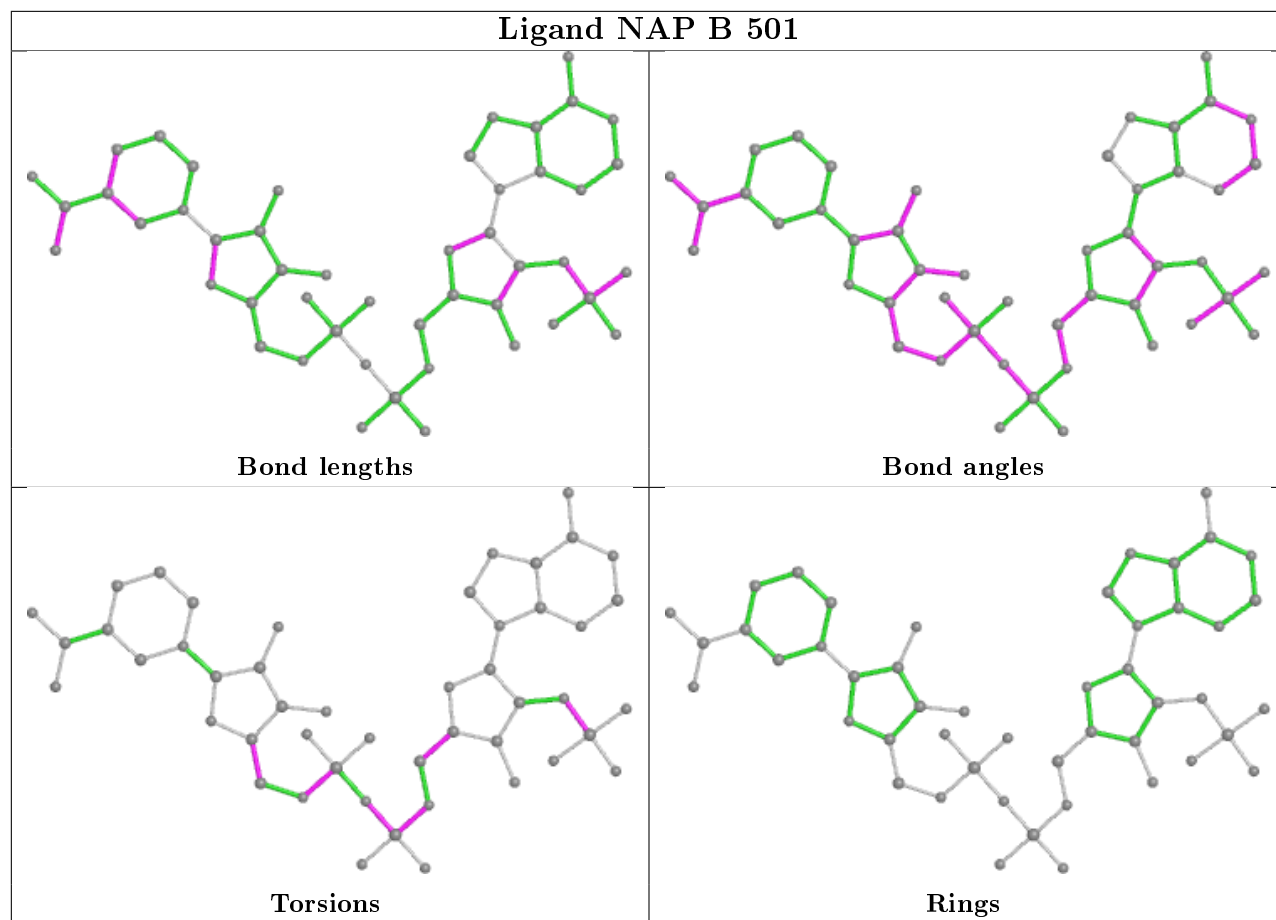


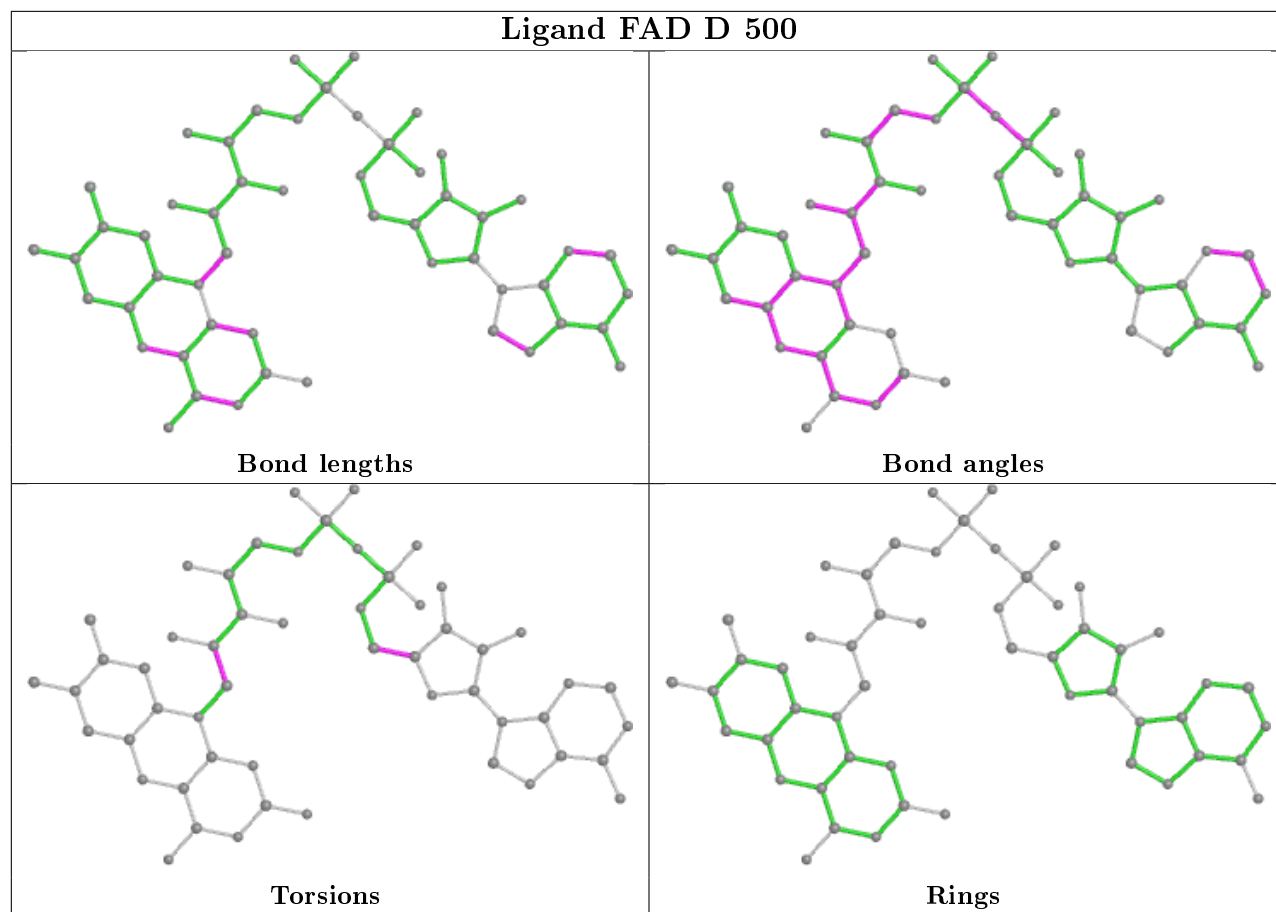




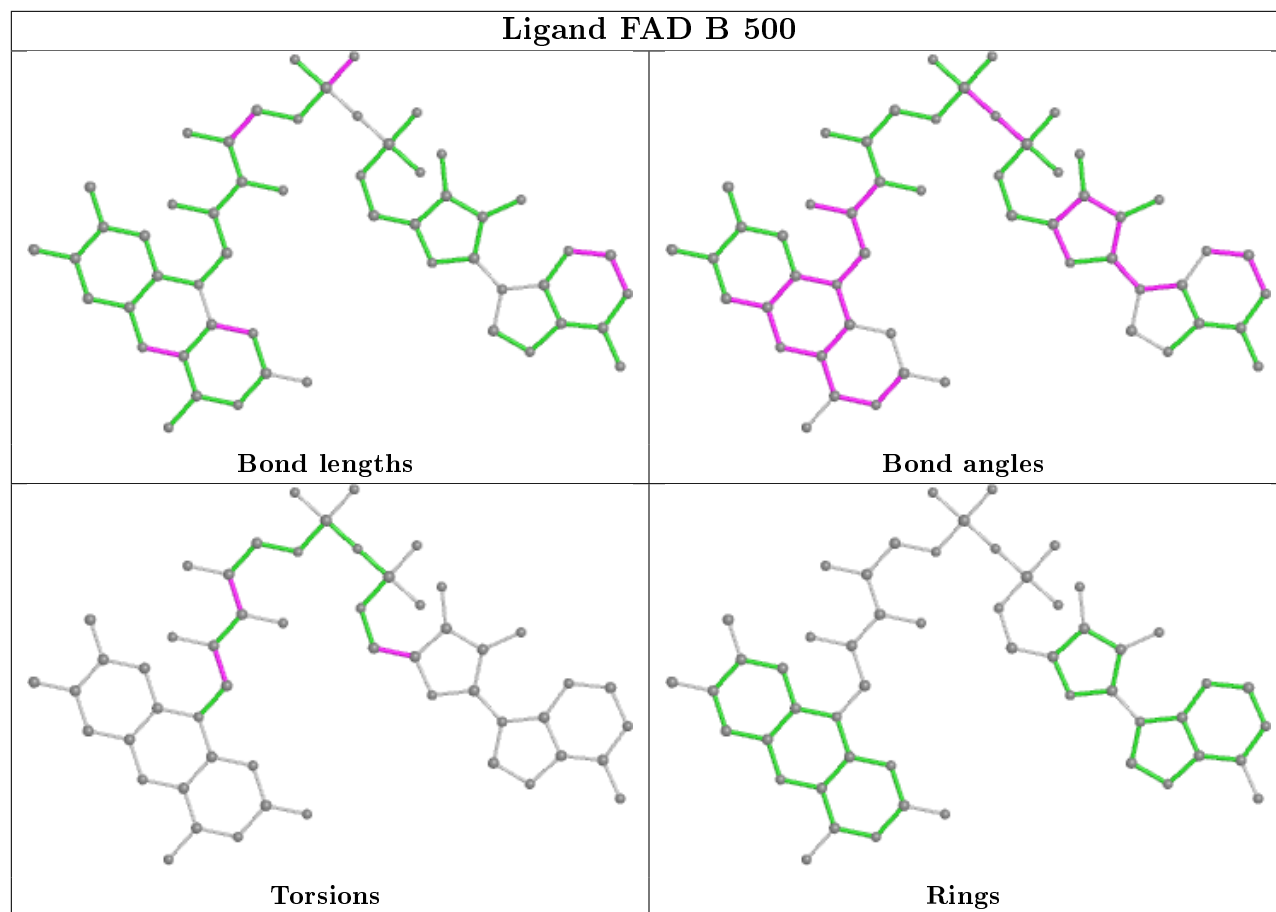












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	446/461 (96%)	-0.05	13 (2%) 51 59	25, 41, 60, 72	0
1	B	447/461 (96%)	-0.17	1 (0%) 95 97	25, 40, 60, 74	0
1	C	452/461 (98%)	-0.14	3 (0%) 87 90	24, 41, 60, 86	0
1	D	447/461 (96%)	-0.04	13 (2%) 51 59	25, 41, 60, 72	1 (0%)
All	All	1792/1844 (97%)	-0.10	30 (1%) 70 76	24, 41, 60, 86	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	GLU	3.9
1	A	451	ASP	3.4
1	C	455	ILE	3.2
1	D	202	ASP	3.1
1	B	451	ASP	2.9
1	A	450	SER	2.9
1	D	374	TYR	2.7
1	D	451	ASP	2.7
1	D	437	TRP	2.7
1	D	407	HIS	2.7
1	D	99	ILE	2.6
1	A	202	ASP	2.6
1	A	98	PRO	2.5
1	A	242	TRP	2.5
1	D	432	LYS	2.4
1	D	425	MET	2.4
1	A	244	GLU	2.4
1	A	419	HIS	2.3
1	A	272	ALA	2.3
1	C	109	TRP	2.3
1	D	422	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	434	HIS	2.2
1	C	428	THR	2.2
1	A	446	GLU	2.1
1	A	437	TRP	2.1
1	D	441	LEU	2.1
1	A	239	GLY	2.1
1	D	95	PHE	2.1
1	A	414	MET	2.0
1	D	351	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [\(i\)](#)

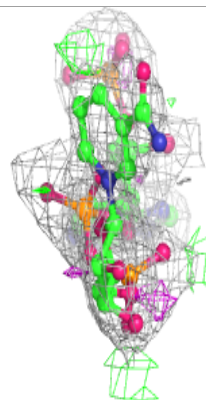
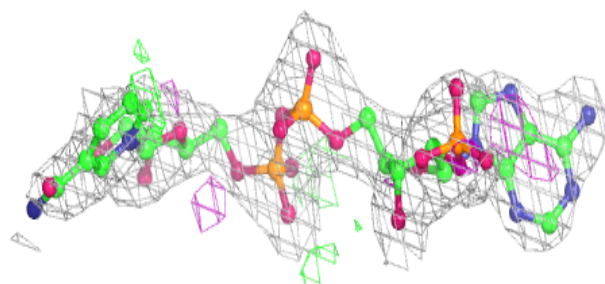
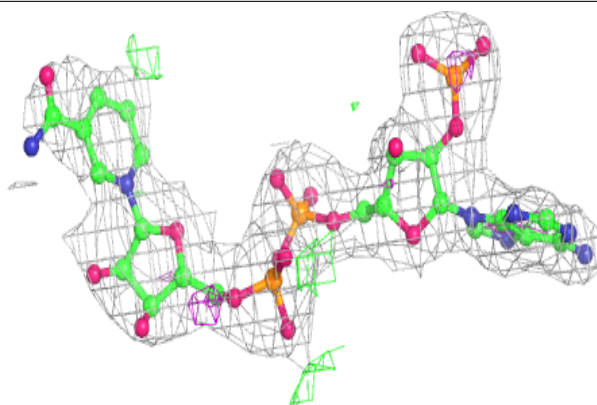
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	A	501	48/48	0.94	0.14	45,55,74,76	0
3	NAP	D	501	48/48	0.96	0.12	46,55,74,75	0
3	NAP	B	501	48/48	0.96	0.13	45,54,74,75	0
3	NAP	C	501	48/48	0.97	0.14	44,54,74,75	0
2	FAD	D	500	53/53	0.97	0.12	21,30,49,50	0
2	FAD	A	500	53/53	0.98	0.13	22,30,49,50	0
2	FAD	C	500	53/53	0.99	0.15	22,29,48,49	0
2	FAD	B	500	53/53	0.99	0.14	22,29,48,50	0

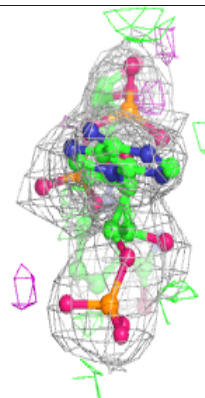
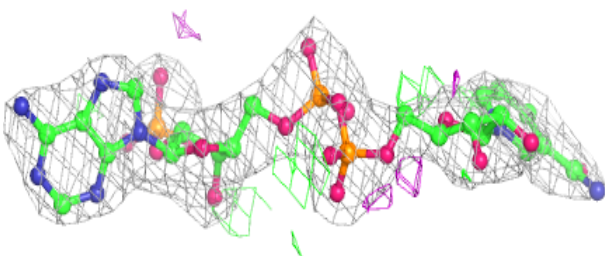
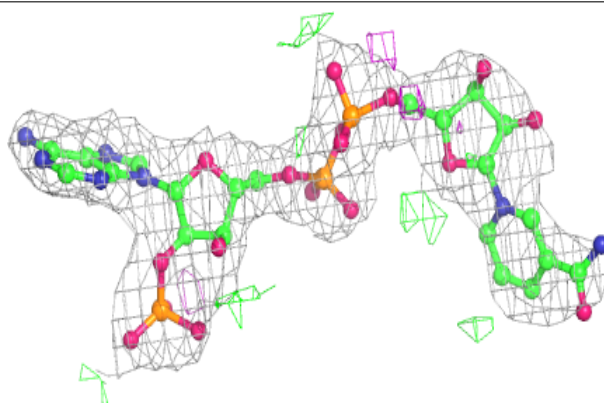
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

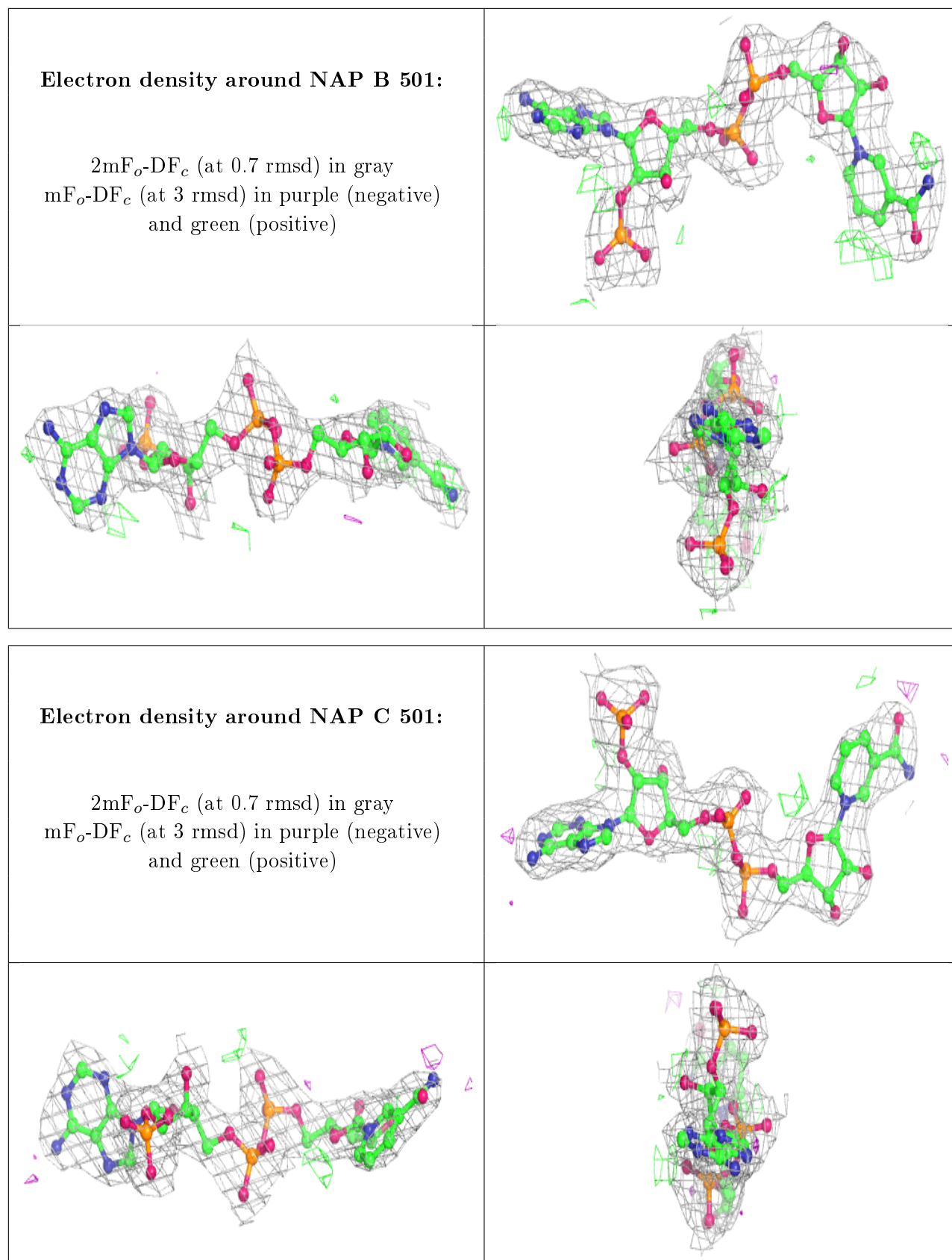
**Electron density around NAP A 501:**

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

**Electron density around NAP D 501:**

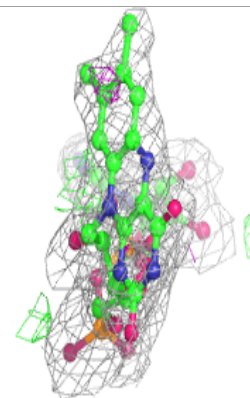
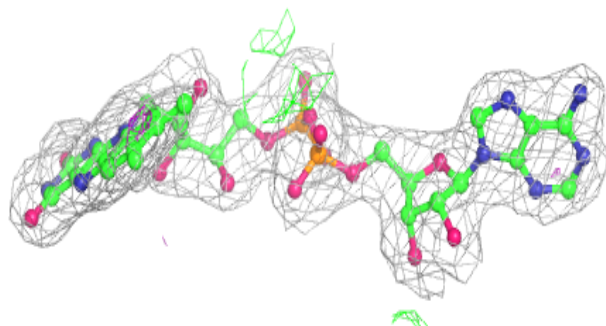
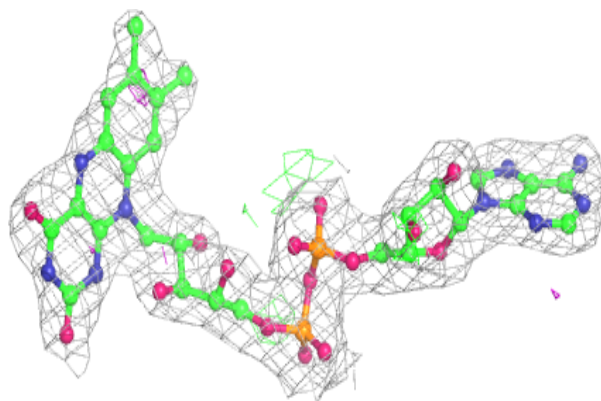
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



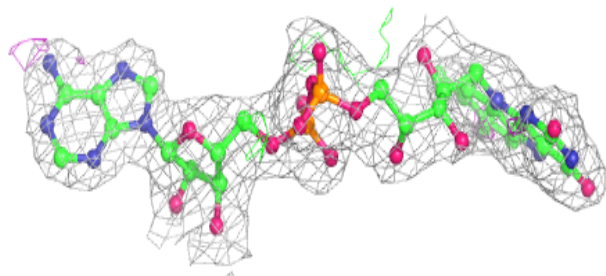
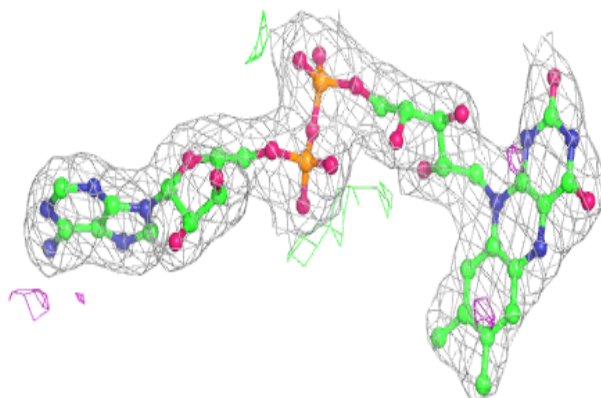


**Electron density around FAD D 500:**

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

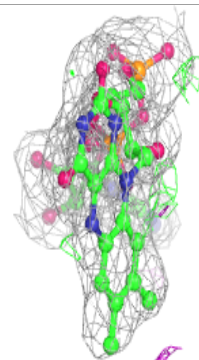
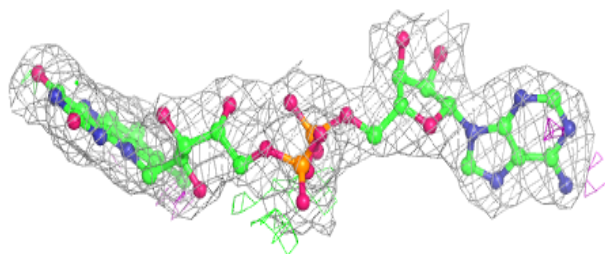
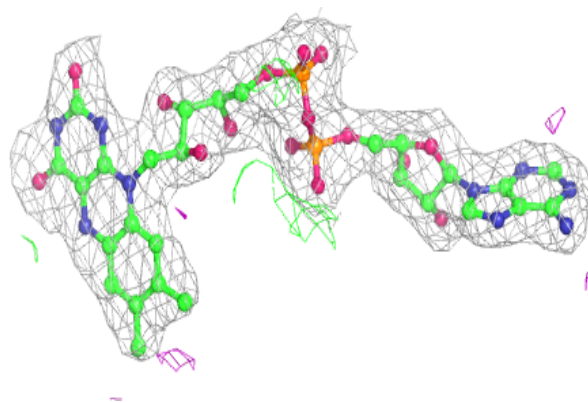
**Electron density around FAD A 500:**

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

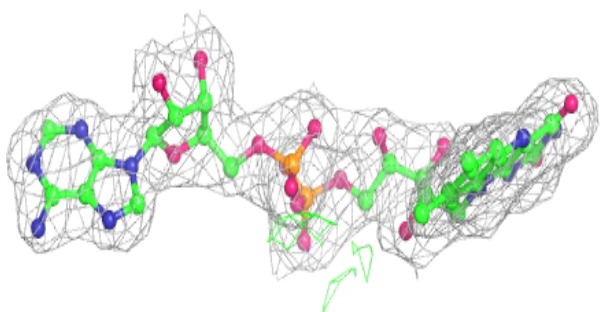
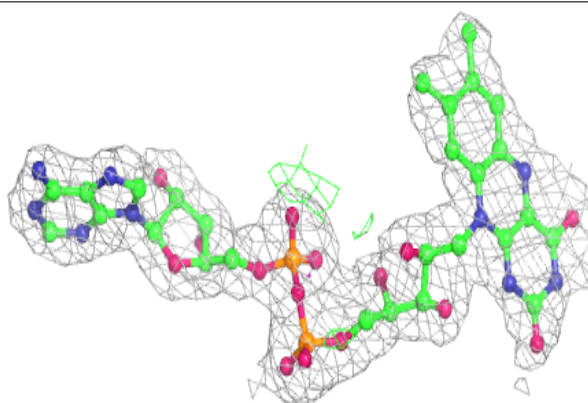


**Electron density around FAD C 500:**

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

**Electron density around FAD B 500:**

$2mF_o-DF_c$  (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.