



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2019 – 11:24 AM EDT

PDB ID : 6RVB
Title : NADH-dependent Coenzyme A Disulfide Reductase soaked with NADH
Authors : Koepke, J.; Preu, J.
Deposited on : 2019-05-31
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

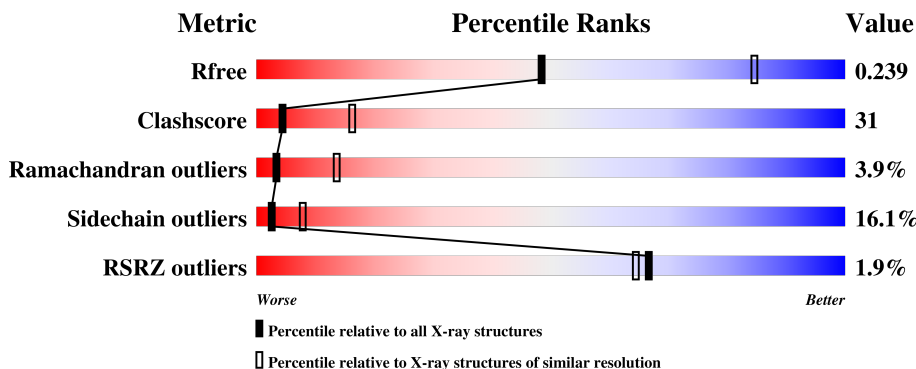
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

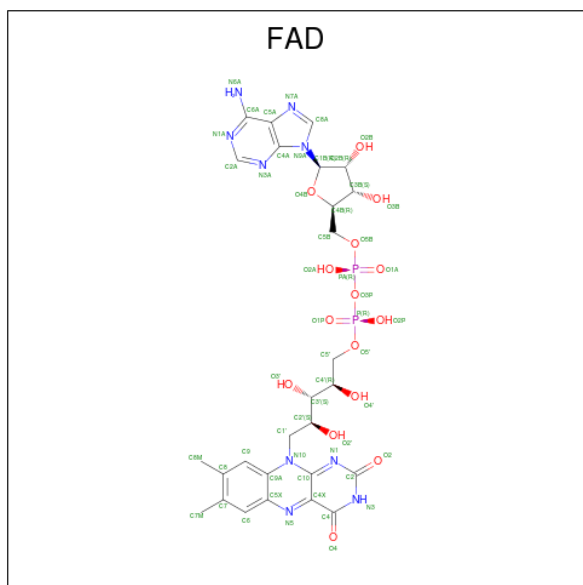
Mol	Chain	Length	Quality of chain
1	A	443	<div> <div>2%</div> <div>59% 28% 9% .</div> </div>
1	B	443	<div> <div>2%</div> <div>53% 32% 11% .</div> </div>
1	C	443	<div> <div>2%</div> <div>58% 27% 12% .</div> </div>
1	D	443	<div> <div>%</div> <div>56% 30% 12% .</div> </div>

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 NADH oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total 3379	C 2147	N 608	O 617	S 7	0	0	0
1	B	443	Total 3379	C 2147	N 608	O 617	S 7	0	0	0
1	C	443	Total 3378	C 2146	N 608	O 617	S 7	0	0	0
1	D	443	Total 3377	C 2146	N 608	O 616	S 7	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by author).



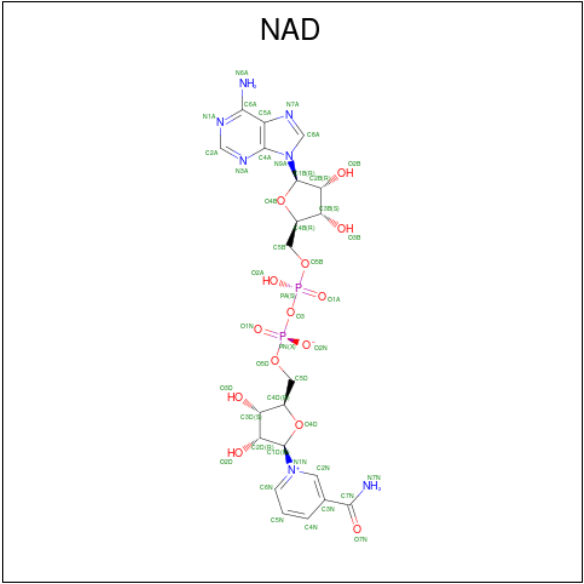
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

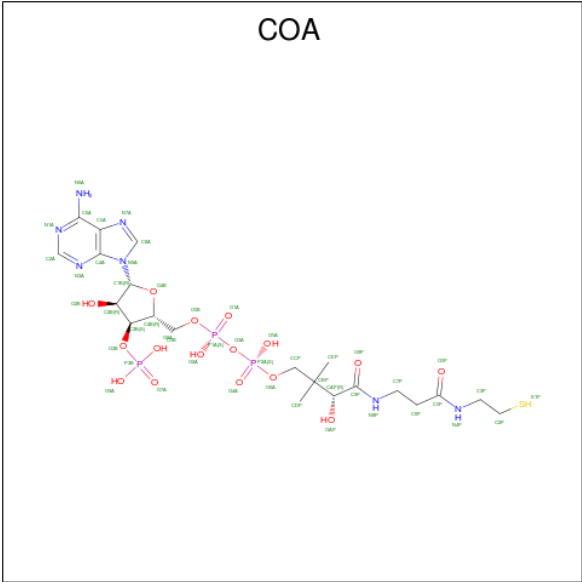
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
4	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
4	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
4	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

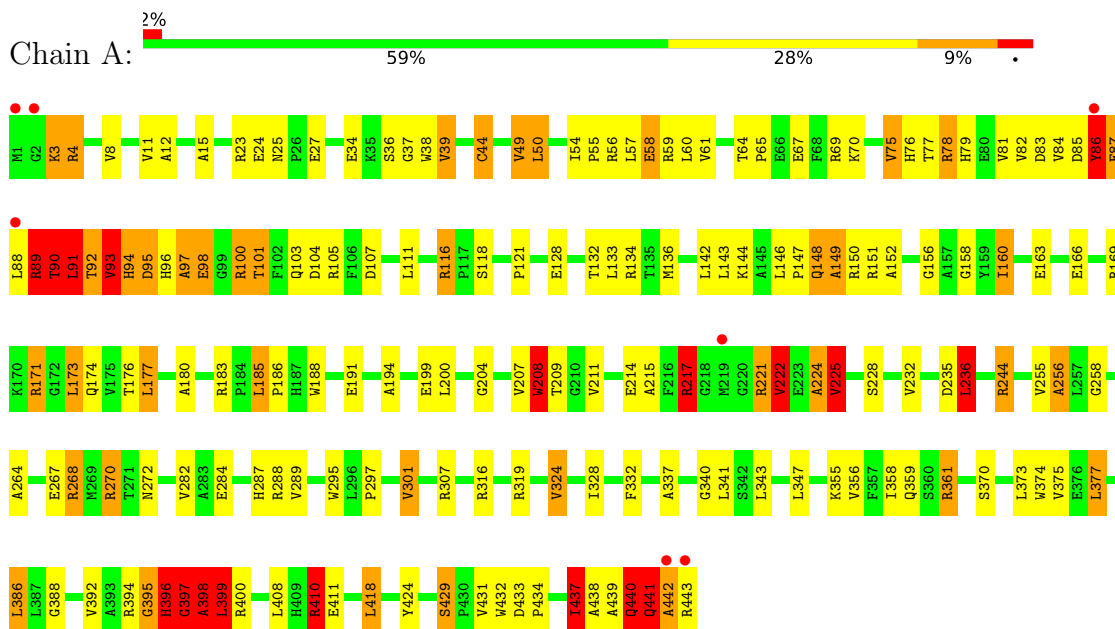
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	27	Total	O	0	0
			27	27		
5	C	27	Total	O	0	0
			27	27		
5	D	26	Total	O	0	0
			26	26		

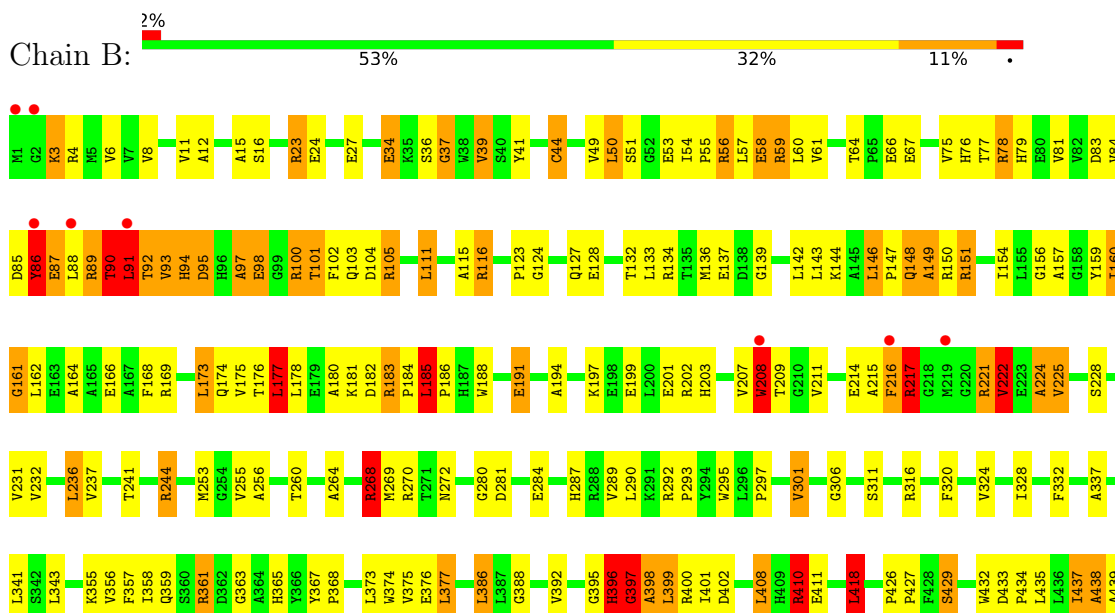
3 Residue-property plots

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: NADH oxidase

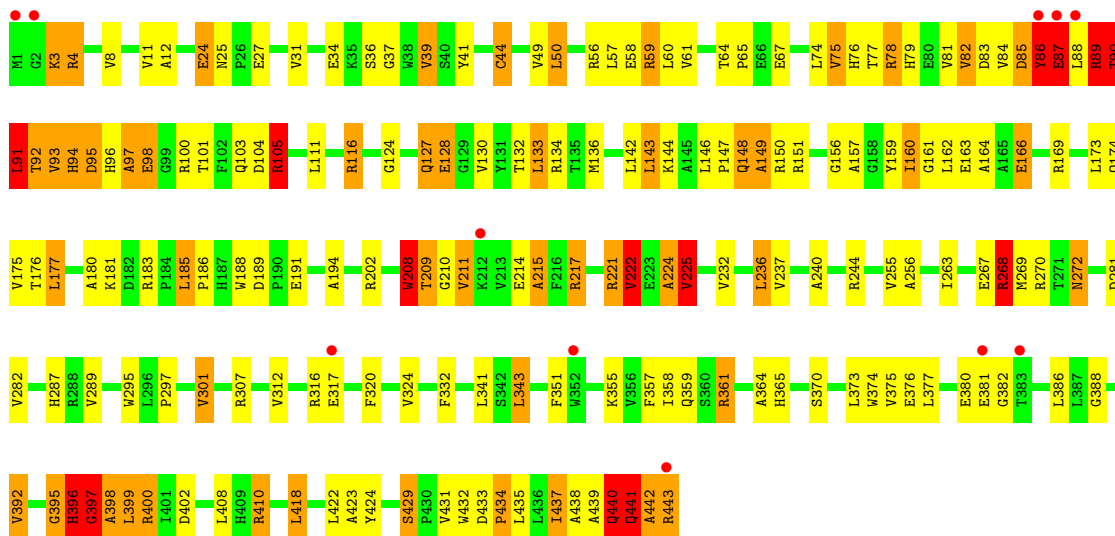


• Molecule 1: NADH oxidase

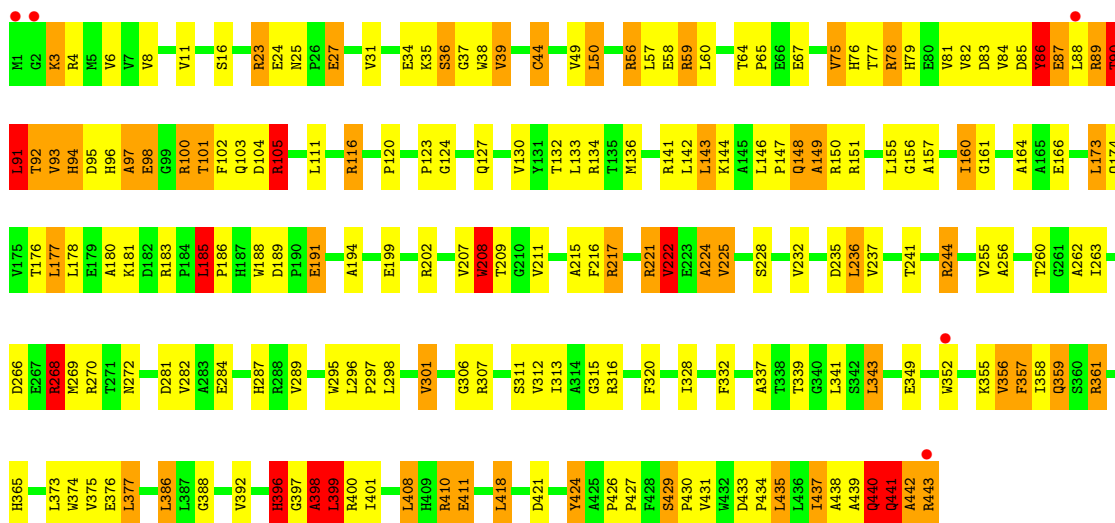




• Molecule 1: NADH oxidase



• Molecule 1: NADH oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	160.75Å 160.75Å 256.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 2.90 47.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.90-2.90) 100.0 (47.90-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.201 , 0.246 0.193 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14205	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: COA, FAD, NAD

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	1.55	36/3451 (1.0%)	1.39	37/4686 (0.8%)
1	B	1.50	28/3451 (0.8%)	1.38	31/4686 (0.7%)
1	C	1.48	32/3450 (0.9%)	1.37	29/4683 (0.6%)
1	D	1.49	25/3449 (0.7%)	1.38	36/4683 (0.8%)
All	All	1.51	121/13801 (0.9%)	1.38	133/18738 (0.7%)

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	6
1	B	0	4
1	C	0	6
1	D	0	3
All	All	0	19

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CG-CD	11.35	1.69	1.51
1	D	396	HIS	C-O	9.65	1.41	1.23
1	C	440	GLN	C-O	9.27	1.41	1.23
1	B	208	TRP	CG-CD1	9.14	1.49	1.36
1	D	440	GLN	CD-NE2	9.05	1.55	1.32
1	B	301	VAL	CB-CG1	-8.92	1.34	1.52
1	A	440	GLN	CD-NE2	8.77	1.54	1.32
1	C	396	HIS	C-O	8.65	1.39	1.23
1	A	86	TYR	CB-CG	8.60	1.64	1.51
1	C	441	GLN	CG-CD	8.60	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	ALA	CA-CB	8.46	1.70	1.52
1	C	194	ALA	CA-CB	-8.39	1.34	1.52
1	A	208	TRP	CG-CD1	8.35	1.48	1.36
1	A	396	HIS	C-O	8.34	1.39	1.23
1	B	98	GLU	CG-CD	8.29	1.64	1.51
1	B	440	GLN	C-O	8.29	1.39	1.23
1	C	86	TYR	CB-CG	8.13	1.63	1.51
1	B	98	GLU	CD-OE1	8.03	1.34	1.25
1	C	208	TRP	CG-CD1	8.02	1.48	1.36
1	D	441	GLN	CG-CD	8.00	1.69	1.51
1	A	440	GLN	C-O	7.99	1.38	1.23
1	A	441	GLN	CG-CD	7.96	1.69	1.51
1	D	208	TRP	CG-CD1	7.88	1.47	1.36
1	B	441	GLN	CG-CD	7.82	1.69	1.51
1	C	98	GLU	CG-CD	7.75	1.63	1.51
1	D	440	GLN	C-O	7.71	1.38	1.23
1	C	208	TRP	CB-CG	7.66	1.64	1.50
1	C	215	ALA	CA-CB	-7.55	1.36	1.52
1	D	98	GLU	CD-OE1	7.52	1.33	1.25
1	B	86	TYR	CB-CG	7.48	1.62	1.51
1	D	98	GLU	CG-CD	7.29	1.62	1.51
1	D	208	TRP	CB-CG	7.16	1.63	1.50
1	D	58	GLU	CG-CD	7.14	1.62	1.51
1	B	440	GLN	CD-NE2	7.08	1.50	1.32
1	B	208	TRP	CB-CG	7.07	1.62	1.50
1	A	58	GLU	CG-CD	7.00	1.62	1.51
1	A	86	TYR	CG-CD1	6.93	1.48	1.39
1	A	87	GLU	CD-OE2	6.93	1.33	1.25
1	C	97	ALA	CA-CB	6.87	1.66	1.52
1	B	194	ALA	CA-CB	-6.86	1.38	1.52
1	B	356	VAL	CB-CG2	-6.85	1.38	1.52
1	B	137	GLU	CG-CD	6.68	1.61	1.51
1	B	438	ALA	CA-CB	-6.54	1.38	1.52
1	C	240	ALA	CA-CB	-6.51	1.38	1.52
1	B	86	TYR	CD1-CE1	6.48	1.49	1.39
1	A	208	TRP	CB-CG	6.46	1.61	1.50
1	C	31	VAL	CB-CG2	-6.43	1.39	1.52
1	A	163	GLU	CD-OE1	6.40	1.32	1.25
1	D	194	ALA	CA-CB	-6.39	1.39	1.52
1	C	440	GLN	CD-NE2	6.38	1.48	1.32
1	D	87	GLU	CD-OE1	6.37	1.32	1.25
1	C	24	GLU	CD-OE2	6.36	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CB-CG	6.34	1.64	1.52
1	A	225	VAL	CA-CB	6.23	1.67	1.54
1	A	87	GLU	CD-OE1	6.20	1.32	1.25
1	B	396	HIS	C-O	6.15	1.35	1.23
1	A	49	VAL	CB-CG2	-6.09	1.40	1.52
1	D	424	TYR	CE2-CZ	6.02	1.46	1.38
1	C	93	VAL	CB-CG1	-5.99	1.40	1.52
1	C	301	VAL	CB-CG1	-5.93	1.40	1.52
1	D	86	TYR	CD1-CE1	5.92	1.48	1.39
1	A	93	VAL	CB-CG1	-5.92	1.40	1.52
1	B	432	TRP	CB-CG	-5.89	1.39	1.50
1	B	356	VAL	CB-CG1	-5.85	1.40	1.52
1	D	349	GLU	CD-OE1	5.85	1.32	1.25
1	C	267	GLU	CG-CD	5.84	1.60	1.51
1	B	216	PHE	CE2-CZ	5.82	1.48	1.37
1	A	399	LEU	N-CA	5.81	1.57	1.46
1	A	437	ILE	CA-CB	5.81	1.68	1.54
1	B	51	SER	CB-OG	5.79	1.49	1.42
1	C	24	GLU	CG-CD	5.78	1.60	1.51
1	C	86	TYR	CD1-CE1	5.78	1.48	1.39
1	C	93	VAL	CB-CG2	-5.78	1.40	1.52
1	B	191	GLU	CG-CD	5.73	1.60	1.51
1	C	86	TYR	CE1-CZ	5.72	1.46	1.38
1	D	357	PHE	CD1-CE1	5.70	1.50	1.39
1	B	87	GLU	CD-OE2	5.69	1.31	1.25
1	D	86	TYR	CB-CG	5.68	1.60	1.51
1	D	440	GLN	CD-OE1	5.66	1.36	1.24
1	A	98	GLU	CD-OE1	5.64	1.31	1.25
1	D	191	GLU	CD-OE2	5.63	1.31	1.25
1	D	301	VAL	CB-CG1	-5.62	1.41	1.52
1	B	87	GLU	CA-C	5.60	1.67	1.52
1	A	324	VAL	CB-CG2	-5.59	1.41	1.52
1	D	356	VAL	CB-CG2	-5.57	1.41	1.52
1	A	194	ALA	CA-CB	-5.55	1.40	1.52
1	A	270	ARG	CB-CG	5.54	1.67	1.52
1	A	256	ALA	CA-CB	-5.54	1.40	1.52
1	C	86	TYR	CG-CD1	5.51	1.46	1.39
1	D	93	VAL	CA-CB	5.49	1.66	1.54
1	A	244	ARG	CB-CG	5.48	1.67	1.52
1	A	270	ARG	CG-CD	5.46	1.65	1.51
1	D	87	GLU	CA-C	5.41	1.67	1.52
1	C	225	VAL	CA-CB	5.40	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	224	ALA	CA-CB	-5.38	1.41	1.52
1	A	264	ALA	CA-CB	-5.36	1.41	1.52
1	A	97	ALA	N-CA	5.34	1.57	1.46
1	C	351	PHE	CB-CG	-5.33	1.42	1.51
1	A	301	VAL	CB-CG1	-5.32	1.41	1.52
1	C	211	VAL	CB-CG2	-5.31	1.41	1.52
1	B	58	GLU	CG-CD	5.29	1.59	1.51
1	A	440	GLN	CA-CB	5.28	1.65	1.53
1	A	398	ALA	CA-CB	-5.25	1.41	1.52
1	A	93	VAL	CA-CB	5.25	1.65	1.54
1	C	317	GLU	CG-CD	5.24	1.59	1.51
1	D	411	GLU	CB-CG	5.22	1.62	1.52
1	B	53	GLU	CD-OE2	5.21	1.31	1.25
1	B	6	VAL	CB-CG2	-5.18	1.42	1.52
1	C	324	VAL	CB-CG2	-5.18	1.42	1.52
1	A	86	TYR	CE1-CZ	5.17	1.45	1.38
1	A	89	ARG	CB-CG	5.17	1.66	1.52
1	C	85	ASP	C-O	-5.16	1.13	1.23
1	C	87	GLU	CA-C	5.15	1.66	1.52
1	B	66	GLU	CG-CD	5.15	1.59	1.51
1	A	97	ALA	CA-CB	5.14	1.63	1.52
1	D	244	ARG	CG-CD	5.11	1.64	1.51
1	A	95	ASP	CB-CG	-5.09	1.41	1.51
1	C	423	ALA	CA-CB	-5.07	1.41	1.52
1	C	166	GLU	CG-CD	5.04	1.59	1.51
1	B	86	TYR	CG-CD1	5.03	1.45	1.39
1	B	264	ALA	CA-CB	-5.00	1.42	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	GLY	N-CA-C	14.29	148.83	113.10
1	D	268	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	D	396	HIS	CA-C-N	-10.42	95.36	116.20
1	D	396	HIS	O-C-N	10.28	140.67	123.20
1	C	396	HIS	CA-C-N	-9.77	96.66	116.20
1	B	410	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	A	396	HIS	CA-C-N	-9.48	97.23	116.20
1	D	396	HIS	C-N-CA	9.38	142.00	122.30
1	C	89	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	D	217	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	D	343	LEU	CB-CG-CD2	-8.70	96.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	ILE	C-N-CA	-8.67	104.10	122.30
1	B	402	ASP	CB-CG-OD2	8.62	126.05	118.30
1	B	160	ILE	C-N-CA	-8.49	104.47	122.30
1	C	343	LEU	CB-CG-CD2	-8.48	96.58	111.00
1	B	23	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	183	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	D	87	GLU	OE1-CD-OE2	8.20	133.14	123.30
1	B	87	GLU	OE1-CD-OE2	8.14	133.07	123.30
1	C	396	HIS	O-C-N	8.13	137.01	123.20
1	A	87	GLU	OE1-CD-OE2	8.12	133.05	123.30
1	C	160	ILE	C-N-CA	-8.12	105.26	122.30
1	B	23	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	C	396	HIS	C-N-CA	8.01	139.12	122.30
1	D	307	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	C	105	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	396	HIS	O-C-N	7.71	136.30	123.20
1	D	4	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	A	160	ILE	C-N-CA	-7.56	106.43	122.30
1	C	208	TRP	CA-CB-CG	7.48	127.92	113.70
1	C	4	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	A	217	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	A	268	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	134	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	185	LEU	CA-CB-CG	7.20	131.87	115.30
1	A	97	ALA	N-CA-CB	7.16	120.13	110.10
1	A	396	HIS	C-N-CA	7.13	137.27	122.30
1	A	95	ASP	CB-CG-OD1	-7.12	111.89	118.30
1	C	36	SER	C-N-CA	-7.05	107.50	122.30
1	D	36	SER	C-N-CA	-7.01	107.58	122.30
1	B	217	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	C	95	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	C	440	GLN	O-C-N	6.95	133.82	122.70
1	C	397	GLY	N-CA-C	6.93	130.42	113.10
1	D	105	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	268	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	343	LEU	CB-CG-CD2	-6.86	99.33	111.00
1	A	440	GLN	O-C-N	6.85	133.67	122.70
1	D	397	GLY	N-CA-C	6.85	130.22	113.10
1	C	307	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	A	270	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	98	GLU	CG-CD-OE1	6.75	131.79	118.30
1	C	91	LEU	CA-CB-CG	6.68	130.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	208	TRP	CA-CB-CG	6.52	126.09	113.70
1	C	93	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	D	268	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	208	TRP	CA-CB-CG	6.45	125.96	113.70
1	C	97	ALA	N-CA-CB	6.44	119.12	110.10
1	D	97	ALA	N-CA-CB	6.41	119.07	110.10
1	A	394	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	C	440	GLN	CA-C-N	-6.40	103.12	117.20
1	B	208	TRP	CA-CB-CG	6.34	125.75	113.70
1	A	236	LEU	CA-CB-CG	6.34	129.87	115.30
1	A	398	ALA	CB-CA-C	6.33	119.59	110.10
1	D	185	LEU	CA-CB-CG	6.30	129.79	115.30
1	D	235	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	D	23	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	D	440	GLN	O-C-N	6.27	132.73	122.70
1	A	177	LEU	CB-CG-CD1	-6.14	100.56	111.00
1	B	182	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	B	36	SER	C-N-CA	-6.13	109.43	122.30
1	D	96	HIS	N-CA-CB	-6.12	99.58	110.60
1	A	399	LEU	N-CA-CB	6.10	122.61	110.40
1	D	307	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	97	ALA	N-CA-CB	6.07	118.59	110.10
1	A	98	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	C	268	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	141	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	C	422	LEU	CB-CG-CD1	-5.95	100.88	111.00
1	C	96	HIS	N-CA-CB	-5.90	99.99	110.60
1	D	98	GLU	CG-CD-OE1	5.83	129.96	118.30
1	C	82	VAL	CB-CA-C	-5.83	100.33	111.40
1	A	91	LEU	CA-CB-CG	5.81	128.66	115.30
1	C	134	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	235	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	440	GLN	CA-C-N	-5.78	104.49	117.20
1	B	244	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	90	THR	C-N-CA	5.75	136.07	121.70
1	D	105	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	224	ALA	N-CA-C	5.72	126.45	111.00
1	A	397	GLY	N-CA-C	5.70	127.36	113.10
1	A	93	VAL	CG1-CB-CG2	-5.70	101.79	110.90
1	D	421	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	95	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	D	386	LEU	CB-CG-CD2	-5.66	101.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	GLN	O-C-N	5.66	131.75	122.70
1	A	4	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	386	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	363	GLY	N-CA-C	-5.56	99.20	113.10
1	A	386	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	36	SER	C-N-CA	-5.53	110.69	122.30
1	B	440	GLN	CA-C-N	-5.52	105.06	117.20
1	B	343	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	B	402	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	C	400	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	D	398	ALA	CB-CA-C	5.40	118.20	110.10
1	B	151	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	171	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	307	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	93	VAL	CB-CA-C	5.33	121.53	111.40
1	C	98	GLU	CA-CB-CG	-5.33	101.67	113.40
1	A	288	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	91	LEU	CB-CG-CD1	5.28	119.98	111.00
1	D	266	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	134	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	128	GLU	C-N-CA	-5.25	111.27	122.30
1	D	441	GLN	CA-CB-CG	5.25	124.94	113.40
1	D	435	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	D	143	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	89	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	224	ALA	N-CA-C	5.11	124.80	111.00
1	C	91	LEU	CA-C-N	-5.11	105.97	117.20
1	A	410	ARG	O-C-N	-5.10	114.54	122.70
1	C	402	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	91	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	34	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	200	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	D	399	LEU	N-CA-CB	5.05	120.51	110.40
1	A	347	LEU	CB-CG-CD2	5.05	119.59	111.00
1	A	224	ALA	N-CA-C	5.03	124.59	111.00
1	B	418	LEU	CB-CG-CD1	-5.03	102.46	111.00
1	B	177	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	A	96	HIS	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	HIS	Peptide
1	A	398	ALA	Peptide
1	A	399	LEU	Peptide
1	A	440	GLN	Peptide
1	A	91	LEU	Peptide
1	A	93	VAL	Peptide
1	B	161	GLY	Peptide
1	B	37	GLY	Peptide
1	B	440	GLN	Peptide
1	B	86	TYR	Peptide
1	C	127	GLN	Peptide
1	C	396	HIS	Mainchain,Peptide
1	C	440	GLN	Peptide
1	C	90	THR	Peptide
1	C	91	LEU	Peptide
1	D	396	HIS	Peptide
1	D	440	GLN	Peptide
1	D	91	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	3379	0	3407	215	0
1	B	3379	0	3407	257	0
1	C	3378	0	3402	191	0
1	D	3377	0	3402	201	0
2	A	53	0	31	7	0
2	B	53	0	31	11	0
2	C	53	0	31	7	0
2	D	53	0	31	6	0
3	A	44	0	26	11	0
3	B	44	0	26	10	0
3	C	44	0	26	9	0
3	D	44	0	26	12	0
4	A	48	0	31	3	0
4	B	48	0	31	5	0
4	C	48	0	31	0	0
4	D	48	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	32	0	0	10	1
5	B	27	0	0	17	1
5	C	27	0	0	17	0
5	D	26	0	0	13	0
All	All	14205	0	13970	862	1

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 31.

All (862) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:CD1	1:A:160:ILE:CG1	1.77	1.61
1:D:160:ILE:CG1	1:D:160:ILE:CD1	1.77	1.54
1:B:160:ILE:CD1	1:B:160:ILE:CG1	1.80	1.53
1:C:160:ILE:CG1	1:C:160:ILE:CD1	1.83	1.52
1:A:149:ALA:CB	1:A:150:ARG:HA	1.62	1.28
1:D:149:ALA:CB	1:D:150:ARG:HA	1.63	1.26
1:B:149:ALA:CB	1:B:150:ARG:HA	1.62	1.24
1:D:439:ALA:O	1:D:441:GLN:HB2	1.10	1.23
1:C:149:ALA:CB	1:C:150:ARG:HA	1.70	1.20
1:A:439:ALA:O	1:A:441:GLN:HB2	1.03	1.19
1:C:439:ALA:O	1:C:441:GLN:CB	1.89	1.18
1:B:37:GLY:HA2	1:B:77:THR:HB	1.25	1.18
1:B:439:ALA:O	1:B:441:GLN:CB	1.92	1.16
1:D:105:ARG:HD3	5:D:606:HOH:O	1.41	1.16
1:A:149:ALA:HB1	1:A:150:ARG:HA	1.16	1.13
1:B:439:ALA:O	1:B:441:GLN:HB2	0.96	1.12
1:D:37:GLY:HA2	1:D:77:THR:HB	1.32	1.11
1:A:439:ALA:O	1:A:441:GLN:CB	1.98	1.11
1:B:437:ILE:HD12	1:B:437:ILE:C	1.71	1.11
1:D:149:ALA:HB1	1:D:150:ARG:HA	1.16	1.11
1:A:440:GLN:HA	1:A:440:GLN:NE2	1.63	1.10
1:C:439:ALA:O	1:C:441:GLN:HB2	0.94	1.10
1:C:437:ILE:HD12	1:C:437:ILE:C	1.71	1.10
1:B:85:ASP:O	1:B:92:THR:HG22	1.49	1.09
1:B:396:HIS:N	1:B:397:GLY:HA2	1.67	1.08
1:A:90:THR:HA	1:A:92:THR:HG23	1.09	1.08
1:A:37:GLY:HA2	1:A:77:THR:HB	1.35	1.07
1:B:90:THR:HA	1:B:92:THR:HG23	1.13	1.07
1:C:149:ALA:HB1	1:C:150:ARG:HA	1.28	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:GLN:NE2	1:D:440:GLN:HA	1.68	1.06
1:A:437:ILE:HD12	1:A:437:ILE:C	1.73	1.05
1:B:149:ALA:HB1	1:B:150:ARG:HA	1.06	1.04
1:A:398:ALA:H	1:A:399:LEU:HB2	1.19	1.04
1:A:147:PRO:O	1:A:148:GLN:HB2	1.57	1.04
1:D:439:ALA:O	1:D:441:GLN:CB	2.04	1.03
1:C:443:ARG:NH2	5:C:603:HOH:O	1.91	1.03
1:D:398:ALA:H	1:D:399:LEU:HB2	1.23	1.02
1:A:440:GLN:HA	1:A:440:GLN:HE21	1.17	1.00
1:B:85:ASP:C	1:B:92:THR:HG22	1.80	1.00
1:B:92:THR:N	5:B:602:HOH:O	1.94	1.00
1:B:90:THR:HA	1:B:92:THR:CG2	1.90	0.99
1:A:85:ASP:C	1:A:92:THR:HG22	1.82	0.99
1:A:410:ARG:NH1	1:B:410:ARG:NH1	2.11	0.98
1:D:440:GLN:HE21	1:D:440:GLN:HA	1.24	0.98
1:A:90:THR:HA	1:A:92:THR:CG2	1.94	0.96
1:D:437:ILE:HD12	1:D:437:ILE:C	1.86	0.96
1:B:440:GLN:NE2	1:B:440:GLN:HA	1.79	0.95
1:B:91:LEU:O	5:B:601:HOH:O	1.84	0.95
1:B:256:ALA:H	1:B:272:ASN:ND2	1.65	0.95
1:C:147:PRO:O	1:C:148:GLN:HB2	1.66	0.95
1:B:398:ALA:H	1:B:399:LEU:HB2	1.32	0.94
1:D:85:ASP:OD1	1:D:88:LEU:HD23	1.67	0.94
1:A:89:ARG:O	1:A:90:THR:O	1.86	0.94
1:C:440:GLN:HA	1:C:440:GLN:HE21	1.32	0.93
1:B:151:ARG:HG2	1:B:174:GLN:HE21	1.34	0.93
1:D:443:ARG:NH1	5:D:601:HOH:O	1.94	0.93
1:A:150:ARG:NH1	5:A:601:HOH:O	2.02	0.92
1:C:440:GLN:HA	1:C:440:GLN:NE2	1.83	0.92
1:A:396:HIS:CG	1:B:396:HIS:CE1	2.58	0.91
1:D:147:PRO:O	1:D:148:GLN:HB2	1.70	0.91
1:D:149:ALA:HB1	1:D:150:ARG:CA	2.01	0.91
1:A:85:ASP:O	1:A:92:THR:HG22	1.70	0.91
1:A:396:HIS:CE1	1:B:396:HIS:CG	2.59	0.91
1:B:396:HIS:N	1:B:397:GLY:CA	2.33	0.90
1:A:410:ARG:HH11	1:B:410:ARG:NH1	1.70	0.90
1:D:256:ALA:H	1:D:272:ASN:ND2	1.69	0.90
3:A:502:NAD:C4A	3:A:502:NAD:O2B	2.14	0.89
3:C:502:NAD:O2B	3:C:502:NAD:C4A	2.14	0.89
1:B:149:ALA:CB	1:B:150:ARG:CA	2.50	0.89
1:B:373:LEU:HD22	1:B:434:PRO:HG2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ARG:O	5:C:601:HOH:O	1.90	0.89
1:A:149:ALA:HB3	1:A:150:ARG:HA	1.56	0.88
1:B:147:PRO:O	1:B:148:GLN:HB2	1.72	0.88
1:C:37:GLY:HA2	1:C:77:THR:HB	1.53	0.88
1:B:93:VAL:HG23	1:B:104:ASP:HB3	1.53	0.87
1:B:441:GLN:O	1:B:442:ALA:O	1.91	0.87
1:A:116:ARG:NH1	1:A:244:ARG:HD2	1.88	0.87
1:B:149:ALA:HB1	1:B:150:ARG:CA	1.99	0.87
1:C:149:ALA:HB3	1:C:150:ARG:HA	1.57	0.87
1:D:149:ALA:HB3	1:D:150:ARG:HA	1.56	0.87
1:D:116:ARG:NH1	1:D:244:ARG:HD2	1.89	0.87
1:A:396:HIS:CD2	1:B:396:HIS:NE2	2.43	0.86
1:A:410:ARG:NH1	1:B:410:ARG:HH11	1.69	0.86
1:D:93:VAL:HG23	1:D:104:ASP:HB3	1.57	0.86
1:C:398:ALA:H	1:C:399:LEU:HB2	1.40	0.85
1:C:87:GLU:OE1	5:C:602:HOH:O	1.91	0.85
1:B:64:THR:OG1	1:B:67:GLU:HG3	1.76	0.85
1:B:91:LEU:C	5:B:602:HOH:O	2.12	0.85
1:A:149:ALA:HB1	1:A:150:ARG:CA	2.05	0.85
1:D:400:ARG:HH12	1:D:429:SER:HB2	1.39	0.85
1:A:50:LEU:HD12	1:A:143:LEU:HD13	1.59	0.85
1:B:104:ASP:O	5:B:602:HOH:O	1.93	0.84
1:A:396:HIS:NE2	1:B:396:HIS:CD2	2.45	0.84
1:B:224:ALA:O	1:B:232:VAL:O	1.96	0.84
1:B:85:ASP:O	1:B:92:THR:CG2	2.25	0.83
1:D:64:THR:OG1	1:D:67:GLU:HG3	1.79	0.83
1:C:272:ASN:H	1:C:272:ASN:HD22	1.26	0.83
1:D:149:ALA:CB	1:D:150:ARG:CA	2.48	0.83
1:C:400:ARG:HH12	1:C:429:SER:HB2	1.45	0.82
1:A:396:HIS:CE1	1:B:396:HIS:CE1	2.69	0.81
1:C:440:GLN:HA	5:C:608:HOH:O	1.79	0.81
1:D:440:GLN:NE2	1:D:440:GLN:CA	2.44	0.81
1:B:85:ASP:H	1:B:92:THR:HA	1.46	0.81
1:A:149:ALA:CB	1:A:150:ARG:CA	2.49	0.80
1:A:64:THR:OG1	1:A:67:GLU:HG3	1.82	0.80
1:A:224:ALA:O	1:A:232:VAL:O	2.00	0.80
1:A:186:PRO:HG2	5:A:604:HOH:O	1.81	0.80
1:B:437:ILE:HD12	1:B:438:ALA:N	1.96	0.80
1:B:50:LEU:HD12	1:B:143:LEU:HD13	1.62	0.79
1:A:396:HIS:CE1	1:B:396:HIS:ND1	2.50	0.79
1:D:398:ALA:H	1:D:399:LEU:CB	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:GLN:O	1:C:442:ALA:O	2.01	0.79
1:A:398:ALA:H	1:A:399:LEU:CB	1.96	0.79
3:D:502:NAD:C4B	5:D:604:HOH:O	2.31	0.79
1:D:50:LEU:HD12	1:D:143:LEU:HD13	1.64	0.79
1:A:256:ALA:H	1:A:272:ASN:ND2	1.80	0.79
1:A:440:GLN:NE2	1:A:440:GLN:CA	2.43	0.78
1:C:270:ARG:NE	5:C:607:HOH:O	2.15	0.78
1:A:93:VAL:HG23	1:A:104:ASP:HB3	1.65	0.78
1:C:256:ALA:H	1:C:272:ASN:ND2	1.82	0.78
1:A:396:HIS:ND1	1:B:396:HIS:CE1	2.53	0.77
1:C:50:LEU:HD12	1:C:143:LEU:HD13	1.66	0.77
1:B:44:CYS:HA	2:B:501:FAD:C5X	2.14	0.77
1:C:418:LEU:HD13	1:C:439:ALA:HB3	1.66	0.77
1:C:149:ALA:HB1	1:C:150:ARG:CA	2.14	0.77
1:A:295:TRP:CE2	1:A:297:PRO:HG3	2.20	0.77
1:B:440:GLN:HE21	1:B:440:GLN:HA	1.45	0.77
1:A:121:PRO:HG3	1:D:149:ALA:CB	2.15	0.76
1:D:256:ALA:H	1:D:272:ASN:HD21	1.30	0.76
1:B:328:ILE:HG13	1:B:337:ALA:HB2	1.67	0.76
1:B:236:LEU:C	1:B:236:LEU:HD12	2.06	0.76
1:C:149:ALA:CB	1:C:150:ARG:CA	2.56	0.76
1:A:441:GLN:O	1:A:442:ALA:O	2.03	0.76
1:B:437:ILE:CD1	1:B:437:ILE:C	2.53	0.76
1:D:224:ALA:O	1:D:232:VAL:O	2.03	0.76
1:A:94:HIS:CD2	1:A:94:HIS:H	2.04	0.75
1:C:88:LEU:O	1:C:89:ARG:HB2	1.87	0.75
3:D:502:NAD:C4A	3:D:502:NAD:O2B	2.29	0.74
1:A:91:LEU:O	1:A:92:THR:HG23	1.87	0.74
1:C:34:GLU:HG2	1:C:39:VAL:HG23	1.68	0.74
1:C:270:ARG:CD	5:C:607:HOH:O	2.36	0.74
3:A:502:NAD:O3B	3:A:502:NAD:O5B	2.00	0.74
1:B:398:ALA:H	1:B:399:LEU:CB	2.01	0.74
1:D:398:ALA:O	5:D:602:HOH:O	2.06	0.74
1:C:381:GLU:N	5:C:604:HOH:O	2.19	0.73
1:B:87:GLU:HA	1:B:88:LEU:C	2.08	0.73
1:B:191:GLU:OE2	1:B:355:LYS:HE3	1.86	0.73
1:A:396:HIS:CD2	1:B:396:HIS:CE1	2.76	0.73
1:C:191:GLU:OE2	1:C:355:LYS:HE3	1.87	0.73
1:D:441:GLN:O	1:D:442:ALA:O	2.06	0.73
1:B:151:ARG:CG	1:B:174:GLN:HE21	2.02	0.73
1:A:94:HIS:CD2	1:A:94:HIS:N	2.57	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ALA:O	1:C:232:VAL:O	2.06	0.72
1:B:256:ALA:H	1:B:272:ASN:HD21	1.37	0.72
1:C:87:GLU:HA	1:C:88:LEU:C	2.10	0.72
1:D:44:CYS:HA	2:D:501:FAD:C5X	2.20	0.72
1:D:89:ARG:O	1:D:90:THR:O	2.08	0.72
1:A:151:ARG:HG2	1:A:174:GLN:HE21	1.54	0.72
1:A:89:ARG:C	1:A:90:THR:O	2.27	0.72
1:C:156:GLY:HA2	3:C:502:NAD:H2B	1.71	0.72
1:D:91:LEU:HD13	1:D:103:GLN:OE1	1.89	0.72
1:B:78:ARG:NH1	5:B:604:HOH:O	2.21	0.72
1:C:382:GLY:N	5:C:604:HOH:O	1.97	0.72
3:D:502:NAD:H51A	5:D:604:HOH:O	1.88	0.72
1:B:116:ARG:NH1	1:B:244:ARG:HH11	1.88	0.71
1:B:91:LEU:HD13	1:B:103:GLN:OE1	1.89	0.71
1:D:94:HIS:H	1:D:94:HIS:CD2	2.08	0.71
1:B:49:VAL:HG11	1:B:57:LEU:HD13	1.70	0.71
1:A:91:LEU:HD13	1:A:103:GLN:OE1	1.90	0.71
3:A:502:NAD:C4A	3:A:502:NAD:HO2A	2.00	0.71
1:C:151:ARG:HG2	1:C:174:GLN:HE21	1.55	0.71
1:C:440:GLN:NE2	5:C:608:HOH:O	2.23	0.71
1:B:123:PRO:HG2	1:B:215:ALA:HB2	1.72	0.71
1:B:395:GLY:C	1:B:397:GLY:CA	2.58	0.71
1:D:373:LEU:HD22	1:D:434:PRO:HG2	1.73	0.71
1:D:191:GLU:OE2	1:D:355:LYS:HE3	1.90	0.71
1:A:396:HIS:H	1:B:396:HIS:HE1	1.38	0.71
1:D:148:GLN:O	1:D:149:ALA:O	2.09	0.70
3:D:502:NAD:O5B	3:D:502:NAD:O3B	2.06	0.70
1:D:98:GLU:OE2	1:D:98:GLU:HA	1.89	0.70
1:B:359:GLN:HB2	1:B:374:TRP:CD1	2.26	0.70
1:A:91:LEU:O	1:A:92:THR:OG1	2.10	0.70
1:A:396:HIS:HE1	1:B:396:HIS:H	1.39	0.70
3:C:502:NAD:O5B	3:C:502:NAD:O3B	1.99	0.70
1:D:123:PRO:HG2	1:D:215:ALA:HB2	1.73	0.70
1:B:98:GLU:OE2	1:B:98:GLU:HA	1.91	0.70
1:C:116:ARG:NH1	1:C:244:ARG:HD2	2.06	0.70
1:A:396:HIS:H	1:B:396:HIS:CE1	2.10	0.70
1:C:163:GLU:OE1	5:C:605:HOH:O	2.08	0.70
1:B:173:LEU:N	1:B:173:LEU:HD23	2.07	0.70
1:B:395:GLY:C	1:B:397:GLY:HA2	2.11	0.69
1:A:396:HIS:NE2	1:B:396:HIS:NE2	2.39	0.69
1:D:130:VAL:O	5:D:603:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:502:NAD:O2B	3:B:502:NAD:C4A	2.35	0.69
1:B:116:ARG:NH1	1:B:244:ARG:HD2	2.07	0.69
1:B:295:TRP:CE2	1:B:297:PRO:HG3	2.27	0.69
1:D:24:GLU:HG2	1:D:316:ARG:HG3	1.75	0.69
3:D:502:NAD:C5B	5:D:604:HOH:O	2.41	0.69
1:A:92:THR:O	1:A:93:VAL:C	2.30	0.69
3:B:502:NAD:O3B	3:B:502:NAD:O5B	2.00	0.69
1:C:295:TRP:CE2	1:C:297:PRO:HG3	2.28	0.69
1:C:64:THR:OG1	1:C:67:GLU:HG3	1.93	0.69
1:B:386:LEU:O	5:B:603:HOH:O	2.11	0.69
1:B:440:GLN:HA	5:B:612:HOH:O	1.92	0.69
1:C:93:VAL:HG23	1:C:104:ASP:HB3	1.72	0.69
1:A:398:ALA:N	1:A:399:LEU:HB2	2.02	0.68
1:B:37:GLY:HA2	1:B:77:THR:CB	2.15	0.68
1:C:44:CYS:HA	2:C:501:FAD:C5X	2.23	0.68
1:A:396:HIS:CE1	1:B:396:HIS:H	2.11	0.68
1:A:85:ASP:H	1:A:92:THR:HA	1.56	0.68
1:B:149:ALA:HB3	1:B:150:ARG:HA	1.70	0.68
1:D:236:LEU:HD12	1:D:236:LEU:C	2.14	0.68
3:A:502:NAD:C4B	5:A:604:HOH:O	2.42	0.68
1:B:86:TYR:CE1	1:B:88:LEU:HD22	2.29	0.68
1:D:287:HIS:HD2	1:D:289:VAL:H	1.41	0.68
1:A:396:HIS:CE1	1:B:396:HIS:CD2	2.81	0.68
1:B:49:VAL:HG11	1:B:57:LEU:CD1	2.24	0.68
1:D:25:ASN:OD1	1:D:27:GLU:HB2	1.94	0.68
1:B:270:ARG:HH11	1:B:270:ARG:HB2	1.59	0.67
1:B:89:ARG:O	1:B:90:THR:O	2.11	0.67
1:C:92:THR:O	1:C:93:VAL:C	2.31	0.67
1:A:98:GLU:HA	1:A:98:GLU:OE2	1.95	0.67
1:D:398:ALA:CA	5:D:602:HOH:O	2.43	0.67
1:A:44:CYS:HA	2:A:501:FAD:C5X	2.25	0.67
1:B:440:GLN:NE2	1:B:440:GLN:CA	2.57	0.67
1:D:398:ALA:N	1:D:399:LEU:HB2	2.04	0.67
1:D:87:GLU:HA	1:D:88:LEU:C	2.15	0.67
1:B:148:GLN:O	1:B:149:ALA:O	2.12	0.67
1:D:268:ARG:HH12	1:D:270:ARG:HH22	1.41	0.67
1:A:255:VAL:HA	1:A:272:ASN:HD21	1.60	0.66
1:B:398:ALA:N	1:B:399:LEU:HB2	2.08	0.66
1:B:221:ARG:O	1:B:222:VAL:HG12	1.95	0.66
1:B:34:GLU:HG2	1:B:39:VAL:HG23	1.76	0.66
1:C:185:LEU:N	1:C:186:PRO:HD3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASP:OD1	1:C:88:LEU:HD23	1.96	0.66
1:C:91:LEU:HD13	1:C:103:GLN:OE1	1.95	0.66
1:B:91:LEU:O	1:B:92:THR:OG1	2.13	0.66
1:C:94:HIS:CD2	1:C:94:HIS:N	2.64	0.66
3:A:502:NAD:C5B	5:A:604:HOH:O	2.44	0.66
1:C:437:ILE:HD12	1:C:438:ALA:N	2.10	0.66
1:B:76:HIS:HB3	1:B:79:HIS:CE1	2.29	0.65
1:A:121:PRO:HG3	1:D:149:ALA:HB3	1.78	0.65
1:A:86:TYR:CE1	1:A:88:LEU:HD22	2.31	0.65
1:B:116:ARG:HH12	1:B:244:ARG:HH11	1.44	0.65
1:D:94:HIS:N	1:D:94:HIS:CD2	2.64	0.65
1:A:440:GLN:OE1	5:A:602:HOH:O	2.14	0.65
1:B:149:ALA:HA	1:B:173:LEU:HD22	1.78	0.65
1:B:410:ARG:HG3	1:B:411:GLU:N	2.09	0.65
1:B:87:GLU:OE2	1:B:87:GLU:N	2.30	0.65
1:B:44:CYS:HA	2:B:501:FAD:C6	2.27	0.65
1:A:156:GLY:HA2	3:A:502:NAD:H2B	1.77	0.65
1:A:270:ARG:HB2	1:A:270:ARG:HH11	1.62	0.65
1:B:156:GLY:HA2	3:B:502:NAD:H2B	1.78	0.65
1:C:395:GLY:HA3	1:C:397:GLY:O	1.97	0.64
1:B:85:ASP:H	1:B:92:THR:CA	2.09	0.64
1:A:34:GLU:HG2	1:A:39:VAL:HG23	1.79	0.64
1:B:92:THR:O	1:B:93:VAL:C	2.35	0.64
1:A:149:ALA:HA	1:A:173:LEU:HD22	1.80	0.64
1:C:272:ASN:H	1:C:272:ASN:ND2	1.93	0.64
1:D:85:ASP:H	1:D:92:THR:HA	1.62	0.64
1:C:287:HIS:HD2	1:C:289:VAL:H	1.46	0.64
1:C:440:GLN:CA	1:C:440:GLN:NE2	2.59	0.64
1:B:88:LEU:O	1:B:89:ARG:HB2	1.99	0.63
1:D:50:LEU:CD1	1:D:143:LEU:HD13	2.27	0.63
1:C:94:HIS:CD2	1:C:94:HIS:H	2.16	0.63
1:D:87:GLU:OE2	1:D:87:GLU:N	2.30	0.63
1:A:91:LEU:C	1:A:92:THR:HG23	2.19	0.63
1:D:34:GLU:HG2	1:D:39:VAL:HG23	1.81	0.63
1:A:88:LEU:O	1:A:89:ARG:HB2	1.99	0.63
1:B:166:GLU:HA	1:B:332:PHE:CZ	2.34	0.63
1:D:359:GLN:HB2	1:D:374:TRP:CD1	2.33	0.63
1:B:123:PRO:HG2	1:B:215:ALA:CB	2.28	0.62
1:A:116:ARG:HH12	1:A:244:ARG:HD2	1.62	0.62
1:D:151:ARG:HG2	1:D:174:GLN:HE21	1.64	0.62
1:A:208:TRP:HB3	1:A:211:VAL:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD13	1:A:439:ALA:HB3	1.80	0.62
1:C:98:GLU:OE2	1:C:98:GLU:HA	1.98	0.62
1:D:116:ARG:HH12	1:D:244:ARG:HD2	1.62	0.62
1:C:398:ALA:H	1:C:399:LEU:CB	2.11	0.62
1:A:87:GLU:OE2	1:A:87:GLU:N	2.33	0.62
1:B:3:LYS:HA	5:B:613:HOH:O	1.97	0.62
1:C:116:ARG:NH1	1:C:244:ARG:HH11	1.97	0.62
1:A:85:ASP:O	1:A:92:THR:CG2	2.46	0.61
1:A:270:ARG:NH1	1:A:270:ARG:HB2	2.16	0.61
1:C:87:GLU:N	1:C:87:GLU:OE2	2.33	0.61
1:B:83:ASP:HB3	1:B:94:HIS:CD2	2.35	0.61
1:C:49:VAL:HG11	1:C:57:LEU:HD13	1.81	0.61
1:D:358:ILE:HD12	1:D:358:ILE:C	2.20	0.61
1:A:398:ALA:HA	1:A:400:ARG:H	1.66	0.61
2:A:501:FAD:H2'	4:A:503:COA:S1P	2.40	0.61
1:C:373:LEU:HD22	1:C:434:PRO:HG2	1.81	0.61
1:A:437:ILE:CD1	1:A:437:ILE:C	2.59	0.61
1:B:91:LEU:C	1:B:92:THR:HG23	2.20	0.61
1:C:437:ILE:CD1	1:C:437:ILE:C	2.55	0.61
1:A:411:GLU:HA	1:A:411:GLU:OE1	2.01	0.61
1:C:24:GLU:HG2	1:C:316:ARG:HG3	1.82	0.61
1:D:328:ILE:HG13	1:D:337:ALA:HB2	1.81	0.61
1:A:396:HIS:N	1:B:396:HIS:HE1	1.99	0.61
1:C:85:ASP:H	1:C:92:THR:HA	1.64	0.61
1:B:255:VAL:HA	1:B:272:ASN:HD21	1.65	0.61
1:D:156:GLY:HA2	3:D:502:NAD:H2B	1.83	0.60
1:A:410:ARG:NH1	1:B:410:ARG:HH12	1.99	0.60
1:D:270:ARG:HB2	1:D:270:ARG:HH11	1.65	0.60
1:B:395:GLY:C	1:B:397:GLY:HA3	2.22	0.60
1:B:115:ALA:HB1	1:B:244:ARG:O	2.02	0.60
1:D:217:ARG:HB3	1:D:224:ALA:HB3	1.82	0.60
1:D:38:TRP:CE3	1:D:136:MET:HE2	2.37	0.60
1:B:400:ARG:HB3	1:B:435:LEU:HD11	1.82	0.60
1:A:49:VAL:HG11	1:A:57:LEU:HD13	1.83	0.59
1:C:270:ARG:HH11	1:C:270:ARG:HB2	1.66	0.59
1:D:161:GLY:H	1:D:164:ALA:H	1.48	0.59
1:B:185:LEU:N	1:B:186:PRO:HD3	2.16	0.59
1:A:272:ASN:HD22	1:A:272:ASN:H	1.47	0.59
1:A:87:GLU:HA	1:A:88:LEU:C	2.22	0.59
1:B:93:VAL:CG2	1:B:104:ASP:HB3	2.30	0.59
1:B:400:ARG:HH12	1:B:429:SER:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:H	1:A:92:THR:CA	2.15	0.59
1:A:91:LEU:O	1:A:92:THR:CG2	2.50	0.59
1:C:221:ARG:O	1:C:222:VAL:HG12	2.02	0.59
1:A:396:HIS:HE1	1:B:396:HIS:N	2.00	0.59
1:B:214:GLU:O	1:B:215:ALA:HB2	2.03	0.59
1:D:78:ARG:NH1	1:D:78:ARG:HB3	2.18	0.59
1:D:83:ASP:HB3	1:D:94:HIS:CD2	2.37	0.59
1:C:49:VAL:HG11	1:C:57:LEU:CD1	2.33	0.58
1:D:357:PHE:HD2	1:D:376:GLU:HB2	1.68	0.58
1:A:85:ASP:CB	1:A:92:THR:HA	2.34	0.58
1:A:185:LEU:N	1:A:186:PRO:HD3	2.17	0.58
1:B:44:CYS:HB3	2:B:501:FAD:C4X	2.34	0.58
1:B:78:ARG:CZ	1:B:78:ARG:HB3	2.34	0.58
1:C:50:LEU:CD1	1:C:143:LEU:HD13	2.34	0.58
1:C:149:ALA:HA	1:C:173:LEU:HD22	1.84	0.58
1:D:398:ALA:HB3	5:D:602:HOH:O	2.03	0.58
1:D:123:PRO:HG2	1:D:215:ALA:CB	2.34	0.58
1:D:89:ARG:C	1:D:90:THR:O	2.41	0.58
1:D:50:LEU:HD12	1:D:143:LEU:CD1	2.32	0.58
1:B:4:ARG:NH1	1:B:104:ASP:OD2	2.37	0.58
1:B:98:GLU:HB2	5:B:605:HOH:O	2.04	0.58
1:A:440:GLN:C	1:A:441:GLN:O	2.41	0.57
1:B:94:HIS:HA	1:B:102:PHE:O	2.04	0.57
1:C:236:LEU:HD12	1:C:236:LEU:C	2.24	0.57
1:D:116:ARG:NH1	1:D:244:ARG:HH11	2.01	0.57
1:D:44:CYS:HA	2:D:501:FAD:C6	2.35	0.57
1:A:287:HIS:HD2	1:A:289:VAL:H	1.53	0.57
1:B:440:GLN:C	1:B:441:GLN:O	2.42	0.57
1:D:85:ASP:CB	1:D:92:THR:HA	2.34	0.57
1:B:11:VAL:HG23	2:B:501:FAD:H4B	1.87	0.57
1:A:85:ASP:OD1	1:A:88:LEU:HD23	2.05	0.57
1:C:78:ARG:HB3	1:C:78:ARG:CZ	2.34	0.57
1:D:149:ALA:HA	1:D:173:LEU:HD22	1.85	0.57
1:A:95:ASP:OD1	1:A:95:ASP:C	2.42	0.57
1:B:58:GLU:O	1:B:61:VAL:HG12	2.05	0.57
1:D:93:VAL:CG2	1:D:104:ASP:HB3	2.34	0.57
1:D:90:THR:OG1	1:D:91:LEU:O	2.18	0.57
1:D:24:GLU:CG	1:D:316:ARG:HG3	2.35	0.56
1:B:85:ASP:CA	1:B:92:THR:HG22	2.35	0.56
1:C:400:ARG:HB3	1:C:435:LEU:HD11	1.87	0.56
1:C:270:ARG:NE	5:C:610:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:O	1:D:86:TYR:HD1	1.87	0.56
1:A:121:PRO:CG	1:D:149:ALA:CB	2.84	0.56
1:D:185:LEU:N	1:D:186:PRO:HD3	2.20	0.56
1:B:183:ARG:NH1	1:B:188:TRP:O	2.39	0.56
1:D:208:TRP:HB3	1:D:211:VAL:HG21	1.87	0.56
1:D:173:LEU:HD23	1:D:173:LEU:N	2.20	0.56
1:B:84:VAL:O	1:B:86:TYR:HD1	1.89	0.56
1:B:270:ARG:CB	1:B:270:ARG:HH11	2.19	0.56
1:B:270:ARG:CB	1:B:270:ARG:NH1	2.69	0.56
1:B:287:HIS:HD2	1:B:289:VAL:H	1.52	0.56
1:C:86:TYR:CE1	1:C:88:LEU:HD22	2.40	0.56
1:A:359:GLN:HB2	1:A:374:TRP:CD1	2.41	0.56
1:A:97:ALA:O	1:A:98:GLU:OE1	2.24	0.56
1:B:395:GLY:O	1:B:397:GLY:HA3	2.06	0.56
1:B:437:ILE:O	1:B:441:GLN:HB3	2.07	0.55
1:B:85:ASP:OD1	1:B:88:LEU:HD23	2.06	0.55
1:D:398:ALA:N	1:D:399:LEU:CB	2.66	0.55
1:A:437:ILE:O	1:A:437:ILE:HD12	2.06	0.55
1:B:8:VAL:HG13	1:B:81:VAL:HG13	1.87	0.55
1:B:85:ASP:N	1:B:92:THR:HA	2.18	0.55
1:D:418:LEU:HD13	1:D:439:ALA:HB3	1.87	0.55
1:B:85:ASP:CB	1:B:92:THR:HA	2.36	0.55
1:C:255:VAL:HA	1:C:272:ASN:HD21	1.70	0.55
1:C:418:LEU:HD13	1:C:439:ALA:CB	2.35	0.55
1:C:83:ASP:HB3	1:C:94:HIS:CD2	2.41	0.55
1:D:151:ARG:CG	1:D:174:GLN:HE21	2.20	0.55
1:C:214:GLU:O	1:C:215:ALA:HB2	2.06	0.55
1:D:343:LEU:HD22	1:D:355:LYS:HB3	1.88	0.55
1:D:208:TRP:HB3	1:D:211:VAL:CG2	2.36	0.55
1:D:86:TYR:HD1	1:D:86:TYR:H	1.52	0.55
1:A:128:GLU:HG2	1:A:221:ARG:NH2	2.22	0.55
1:A:358:ILE:HD12	1:A:358:ILE:C	2.28	0.55
1:B:216:PHE:CD1	1:B:225:VAL:HG22	2.42	0.55
1:C:256:ALA:H	1:C:272:ASN:HD21	1.51	0.55
1:C:400:ARG:HH12	1:C:429:SER:CB	2.16	0.55
1:D:88:LEU:O	1:D:89:ARG:HB2	2.07	0.55
1:B:183:ARG:HG3	1:B:184:PRO:O	2.07	0.55
1:C:381:GLU:CA	5:C:604:HOH:O	2.55	0.55
1:B:105:ARG:NH1	5:B:608:HOH:O	2.40	0.55
1:B:78:ARG:HD3	5:B:604:HOH:O	2.07	0.54
3:A:502:NAD:H51A	5:A:604:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:CG	1:D:149:ALA:HB2	2.38	0.54
1:B:287:HIS:CD2	1:B:290:LEU:H	2.25	0.54
1:D:398:ALA:HA	1:D:400:ARG:H	1.71	0.54
1:A:89:ARG:O	1:A:90:THR:C	2.45	0.54
1:B:208:TRP:HB3	1:B:211:VAL:HG21	1.89	0.54
1:B:236:LEU:HD12	1:B:237:VAL:N	2.21	0.54
1:B:83:ASP:O	1:B:94:HIS:HD2	1.90	0.54
1:D:78:ARG:CZ	1:D:78:ARG:HB3	2.38	0.54
1:B:197:LYS:NZ	5:B:607:HOH:O	2.37	0.54
1:C:84:VAL:O	1:C:86:TYR:HD1	1.90	0.54
1:A:437:ILE:HD12	1:A:438:ALA:N	2.18	0.54
1:B:295:TRP:CZ2	1:B:297:PRO:HG3	2.43	0.54
1:B:373:LEU:HD22	1:B:434:PRO:CG	2.35	0.54
1:B:91:LEU:O	1:B:92:THR:HG23	2.07	0.54
1:C:41:TYR:CE2	1:C:136:MET:HG2	2.43	0.54
1:A:92:THR:OG1	1:A:93:VAL:N	2.37	0.54
1:A:8:VAL:HG13	1:A:81:VAL:HG13	1.90	0.54
1:A:85:ASP:CA	1:A:92:THR:HG22	2.38	0.54
1:B:241:THR:HA	3:B:502:NAD:O2B	2.08	0.54
1:C:343:LEU:HD22	1:C:355:LYS:HB3	1.89	0.54
1:C:357:PHE:HD2	1:C:376:GLU:HB2	1.73	0.54
1:B:151:ARG:HG2	1:B:174:GLN:NE2	2.15	0.53
1:B:78:ARG:HB3	1:B:78:ARG:NH1	2.23	0.53
1:A:128:GLU:HG2	1:A:221:ARG:CZ	2.37	0.53
3:D:502:NAD:C4A	3:D:502:NAD:HO2A	2.20	0.53
1:C:270:ARG:CB	1:C:270:ARG:HH11	2.21	0.53
1:D:8:VAL:HG13	1:D:81:VAL:HG13	1.89	0.53
1:D:268:ARG:NH1	1:D:270:ARG:HH22	2.06	0.53
1:D:49:VAL:HG11	1:D:57:LEU:HD13	1.91	0.53
1:A:173:LEU:N	1:A:173:LEU:HD23	2.24	0.53
1:C:89:ARG:O	1:C:90:THR:O	2.27	0.53
1:A:148:GLN:O	1:A:149:ALA:O	2.27	0.53
1:D:11:VAL:HG23	2:D:501:FAD:H4B	1.91	0.53
1:D:256:ALA:N	1:D:272:ASN:HD21	2.03	0.53
1:B:124:GLY:O	1:B:127:GLN:HG3	2.08	0.53
1:C:148:GLN:O	1:C:149:ALA:O	2.26	0.53
1:D:426:PRO:HB2	1:D:427:PRO:HD3	1.91	0.53
1:A:12:ALA:HB3	2:A:501:FAD:H5'2	1.91	0.52
1:D:86:TYR:CE1	1:D:88:LEU:HD22	2.44	0.52
1:A:44:CYS:HA	2:A:501:FAD:C6	2.40	0.52
1:C:282:VAL:HG22	1:C:282:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HG11	1:A:75:VAL:HG21	1.91	0.52
1:C:358:ILE:HD12	1:C:358:ILE:C	2.29	0.52
1:A:396:HIS:CE1	1:B:395:GLY:HA2	2.45	0.52
1:A:400:ARG:HH12	1:A:429:SER:HB2	1.73	0.52
1:B:208:TRP:HB3	1:B:211:VAL:CG2	2.39	0.52
1:B:90:THR:CA	1:B:92:THR:HG23	2.09	0.52
3:C:502:NAD:N3A	3:C:502:NAD:O2B	2.42	0.52
1:C:86:TYR:H	1:C:86:TYR:HD1	1.54	0.52
1:A:217:ARG:HB3	1:A:224:ALA:HB3	1.92	0.52
1:B:173:LEU:HD23	1:B:173:LEU:H	1.74	0.52
1:B:56:ARG:NH1	1:B:59:ARG:HD2	2.24	0.52
1:C:56:ARG:NH1	1:C:59:ARG:HD2	2.24	0.52
1:D:85:ASP:H	1:D:92:THR:CA	2.22	0.52
1:B:292:ARG:HB2	1:B:293:PRO:HD2	1.92	0.52
1:C:50:LEU:HD12	1:C:143:LEU:CD1	2.39	0.52
1:A:151:ARG:CG	1:A:174:GLN:HE21	2.20	0.52
1:B:98:GLU:CB	5:B:605:HOH:O	2.57	0.52
1:C:88:LEU:O	1:C:89:ARG:CB	2.55	0.52
3:D:502:NAD:N3A	3:D:502:NAD:O2B	2.42	0.52
1:A:395:GLY:HA3	1:A:397:GLY:O	2.10	0.51
1:A:400:ARG:HH12	1:A:429:SER:CB	2.22	0.51
1:B:24:GLU:CG	1:B:316:ARG:HG3	2.40	0.51
3:D:502:NAD:O4B	5:D:604:HOH:O	2.18	0.51
1:A:149:ALA:HB3	1:A:150:ARG:CA	2.31	0.51
1:C:157:ALA:HB2	1:C:177:LEU:HD22	1.91	0.51
1:C:8:VAL:HG13	1:C:81:VAL:HG13	1.92	0.51
1:B:84:VAL:HG13	1:B:92:THR:HB	1.93	0.51
1:C:268:ARG:HG2	1:C:312:VAL:HG21	1.93	0.51
1:D:221:ARG:O	1:D:222:VAL:HG12	2.09	0.51
1:D:295:TRP:CE2	1:D:297:PRO:HG3	2.46	0.51
1:A:24:GLU:HG2	1:A:316:ARG:HG3	1.93	0.51
1:D:16:SER:HB2	1:D:306:GLY:HA3	1.93	0.51
1:A:373:LEU:HD22	1:A:434:PRO:HG2	1.92	0.51
1:C:270:ARG:NH1	1:C:270:ARG:CB	2.74	0.51
2:C:501:FAD:H9	2:C:501:FAD:O2'	2.10	0.51
1:C:78:ARG:NH1	1:C:78:ARG:HB3	2.25	0.51
1:A:270:ARG:NH1	1:A:270:ARG:CB	2.74	0.51
1:A:90:THR:CA	1:A:92:THR:HG23	2.05	0.51
1:B:94:HIS:CD2	1:B:94:HIS:H	2.27	0.51
1:D:56:ARG:NH1	1:D:59:ARG:HH11	2.09	0.51
1:A:82:VAL:HG12	1:A:82:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:HD11	3:B:502:NAD:O1N	2.11	0.51
1:B:357:PHE:HD2	1:B:376:GLU:HB2	1.74	0.51
1:D:157:ALA:HB2	1:D:177:LEU:HD22	1.92	0.51
1:C:166:GLU:HA	1:C:332:PHE:CZ	2.46	0.51
1:C:44:CYS:HA	2:C:501:FAD:C6	2.41	0.51
1:D:166:GLU:HA	1:D:332:PHE:CZ	2.46	0.51
1:D:76:HIS:HB3	1:D:79:HIS:CE1	2.45	0.51
1:B:244:ARG:NH2	5:B:611:HOH:O	2.44	0.50
1:D:272:ASN:H	1:D:272:ASN:HD22	1.58	0.50
1:A:267:GLU:OE2	1:A:319:ARG:HD3	2.10	0.50
1:B:146:LEU:HD12	1:B:173:LEU:HD11	1.92	0.50
1:A:91:LEU:O	1:A:92:THR:CB	2.60	0.50
1:B:50:LEU:HD12	1:B:143:LEU:CD1	2.36	0.50
1:C:76:HIS:HB3	1:C:79:HIS:CE1	2.46	0.50
1:B:105:ARG:HA	5:B:601:HOH:O	2.12	0.50
1:C:116:ARG:HH12	1:C:244:ARG:HH11	1.59	0.50
1:C:25:ASN:OD1	1:C:27:GLU:HB2	2.12	0.50
1:C:437:ILE:HD12	1:C:437:ILE:O	2.10	0.50
1:C:440:GLN:C	1:C:441:GLN:O	2.49	0.50
1:A:221:ARG:O	1:A:222:VAL:HG12	2.11	0.50
1:B:50:LEU:CD1	1:B:143:LEU:HD13	2.35	0.50
1:C:287:HIS:CD2	1:C:289:VAL:H	2.29	0.50
1:D:424:TYR:O	5:D:605:HOH:O	2.19	0.50
1:A:24:GLU:CG	1:A:316:ARG:HG3	2.41	0.50
1:B:94:HIS:CD2	1:B:94:HIS:N	2.79	0.50
1:D:341:LEU:O	1:D:388:GLY:HA3	2.11	0.50
1:A:116:ARG:NH1	1:A:244:ARG:HH11	2.09	0.50
1:A:395:GLY:HA2	1:B:396:HIS:CE1	2.47	0.50
1:D:97:ALA:O	1:D:98:GLU:OE1	2.30	0.50
1:A:166:GLU:HA	1:A:332:PHE:CZ	2.47	0.50
1:C:159:TYR:HB3	3:C:502:NAD:C4N	2.42	0.50
1:C:3:LYS:NZ	1:C:3:LYS:HB3	2.27	0.50
1:A:208:TRP:HB3	1:A:211:VAL:CG2	2.42	0.49
1:A:11:VAL:HG23	2:A:501:FAD:H4B	1.94	0.49
1:B:160:ILE:HG12	3:B:502:NAD:PN	2.51	0.49
1:D:85:ASP:O	1:D:86:TYR:O	2.30	0.49
1:D:149:ALA:HB3	1:D:150:ARG:CA	2.31	0.49
1:B:139:GLY:O	1:B:143:LEU:HB2	2.12	0.49
1:B:400:ARG:HH12	1:B:429:SER:CB	2.25	0.49
1:D:216:PHE:CD1	1:D:225:VAL:HG22	2.46	0.49
1:A:272:ASN:ND2	1:A:272:ASN:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:NAD:N3A	3:A:502:NAD:O2B	2.38	0.49
1:A:90:THR:HA	1:A:91:LEU:O	2.12	0.49
1:B:44:CYS:HB3	2:B:501:FAD:N5	2.27	0.49
1:C:97:ALA:O	1:C:98:GLU:OE1	2.29	0.49
1:D:400:ARG:HB3	1:D:435:LEU:HD11	1.94	0.49
1:B:86:TYR:HD1	1:B:86:TYR:H	1.57	0.49
1:C:208:TRP:HB3	1:C:211:VAL:CG2	2.43	0.49
1:C:224:ALA:O	1:C:225:VAL:CB	2.60	0.49
1:C:37:GLY:CA	1:C:77:THR:HB	2.35	0.49
1:D:82:VAL:HG12	1:D:82:VAL:O	2.13	0.49
1:A:171:ARG:NH2	5:A:605:HOH:O	2.32	0.49
2:B:501:FAD:H2'	4:B:503:COA:S1P	2.52	0.49
1:C:272:ASN:N	1:C:272:ASN:ND2	2.61	0.49
1:D:216:PHE:HD1	1:D:225:VAL:HG22	1.78	0.49
1:B:287:HIS:HD2	1:B:290:LEU:H	1.61	0.49
1:B:84:VAL:HG22	1:B:93:VAL:HG12	1.95	0.49
1:D:287:HIS:CD2	1:D:289:VAL:H	2.25	0.49
1:B:92:THR:OG1	1:B:93:VAL:N	2.46	0.49
1:C:433:ASP:O	1:C:434:PRO:C	2.51	0.49
1:D:160:ILE:HD11	3:D:502:NAD:O1N	2.13	0.49
1:D:23:ARG:NH2	4:D:503:COA:O5A	2.46	0.49
1:B:426:PRO:N	1:B:427:PRO:CD	2.76	0.49
1:C:224:ALA:O	1:C:225:VAL:HB	2.13	0.49
1:C:361:ARG:NH1	1:C:370:SER:OG	2.46	0.49
1:D:160:ILE:CD1	1:D:160:ILE:CG2	2.91	0.49
1:A:37:GLY:CA	1:A:77:THR:HB	2.26	0.48
1:D:25:ASN:C	1:D:25:ASN:OD1	2.52	0.48
1:A:437:ILE:O	1:A:441:GLN:HB3	2.13	0.48
1:B:269:MET:HE3	1:B:320:PHE:CD2	2.48	0.48
1:B:440:GLN:NE2	5:B:612:HOH:O	2.47	0.48
1:B:97:ALA:O	1:B:98:GLU:OE1	2.30	0.48
1:A:328:ILE:HG13	1:A:337:ALA:HB2	1.95	0.48
1:D:160:ILE:CD1	1:D:160:ILE:HG21	2.43	0.48
1:D:398:ALA:CB	5:D:602:HOH:O	2.61	0.48
1:D:92:THR:O	1:D:93:VAL:C	2.49	0.48
1:A:152:ALA:HA	1:A:236:LEU:O	2.14	0.48
1:B:418:LEU:HD13	1:B:439:ALA:HB3	1.94	0.48
1:A:23:ARG:NH2	4:A:503:COA:O5A	2.47	0.48
1:B:270:ARG:NH1	1:B:270:ARG:HB2	2.28	0.48
1:C:11:VAL:HG23	2:C:501:FAD:H4B	1.95	0.48
1:D:437:ILE:HD12	1:D:438:ALA:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ILE:HD12	1:D:282:VAL:HG22	1.95	0.48
1:D:437:ILE:CD1	1:D:437:ILE:C	2.69	0.48
1:C:24:GLU:CG	1:C:316:ARG:HG3	2.44	0.48
1:C:95:ASP:OD1	1:C:95:ASP:C	2.52	0.48
1:A:258:GLY:HA3	1:A:284:GLU:OE1	2.14	0.48
1:B:268:ARG:NH1	1:B:270:ARG:HH12	2.11	0.48
1:B:224:ALA:O	1:B:225:VAL:HB	2.14	0.47
1:A:282:VAL:O	1:A:282:VAL:HG22	2.15	0.47
1:A:396:HIS:NE2	1:B:396:HIS:CE1	2.81	0.47
1:C:202:ARG:NH1	5:C:614:HOH:O	2.47	0.47
1:C:263:ILE:HD12	1:C:282:VAL:HG22	1.96	0.47
1:D:178:LEU:HD23	1:D:208:TRP:HB2	1.95	0.47
1:D:37:GLY:CA	1:D:77:THR:HB	2.23	0.47
1:B:287:HIS:CD2	1:B:289:VAL:H	2.30	0.47
1:B:49:VAL:HG22	1:B:54:ILE:HB	1.95	0.47
1:B:86:TYR:HB3	1:B:253:MET:HB2	1.95	0.47
1:A:25:ASN:C	1:A:25:ASN:OD1	2.51	0.47
1:C:380:GLU:HG2	5:C:604:HOH:O	2.13	0.47
1:D:183:ARG:NH1	1:D:188:TRP:O	2.47	0.47
1:D:357:PHE:CD2	1:D:376:GLU:HB2	2.49	0.47
1:D:180:ALA:H	3:D:502:NAD:C8A	2.28	0.47
1:D:65:PRO:HB3	1:D:75:VAL:HG22	1.97	0.47
1:A:158:GLY:CA	5:A:607:HOH:O	2.61	0.47
1:A:3:LYS:HB3	1:A:3:LYS:NZ	2.29	0.47
1:A:160:ILE:HG23	3:A:502:NAD:H6N	1.97	0.47
1:B:440:GLN:CA	5:B:612:HOH:O	2.55	0.47
1:B:440:GLN:O	1:B:441:GLN:O	2.32	0.47
1:B:76:HIS:HB3	1:B:79:HIS:ND1	2.29	0.47
1:C:4:ARG:NH1	1:C:104:ASP:OD2	2.47	0.47
1:C:161:GLY:H	1:C:164:ALA:H	1.61	0.47
1:C:169:ARG:CD	1:C:175:VAL:HG13	2.44	0.47
1:C:116:ARG:HH12	1:C:244:ARG:HD2	1.79	0.47
1:D:116:ARG:HH12	1:D:244:ARG:HH11	1.62	0.47
1:D:56:ARG:NH1	1:D:59:ARG:HD2	2.29	0.47
1:A:180:ALA:H	3:A:502:NAD:C8A	2.27	0.47
1:B:128:GLU:HG2	1:B:221:ARG:NH2	2.30	0.47
1:C:359:GLN:HB2	1:C:374:TRP:CD1	2.50	0.47
1:D:440:GLN:C	1:D:441:GLN:O	2.52	0.47
1:A:398:ALA:N	1:A:399:LEU:CB	2.68	0.47
1:B:154:ILE:HD11	1:B:168:PHE:CD2	2.50	0.47
1:A:150:ARG:HH12	1:C:150:ARG:NH2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ALA:H	3:C:502:NAD:C8A	2.27	0.47
1:C:217:ARG:HB3	1:C:224:ALA:HB3	1.97	0.47
1:D:86:TYR:O	1:D:89:ARG:CA	2.63	0.47
1:A:58:GLU:O	1:A:61:VAL:HG12	2.15	0.47
1:B:224:ALA:O	1:B:225:VAL:CB	2.63	0.47
1:D:83:ASP:O	1:D:94:HIS:HD2	1.96	0.47
1:A:37:GLY:HA2	1:A:77:THR:CB	2.26	0.47
1:B:411:GLU:HA	1:B:411:GLU:OE1	2.14	0.47
1:C:151:ARG:NH1	5:C:612:HOH:O	2.38	0.47
1:C:56:ARG:NH1	1:C:59:ARG:HH11	2.11	0.47
1:D:270:ARG:HH11	1:D:270:ARG:CB	2.27	0.47
1:A:204:GLY:O	5:A:603:HOH:O	2.21	0.47
1:A:256:ALA:H	1:A:272:ASN:HD21	1.58	0.47
1:A:65:PRO:HB3	1:A:75:VAL:HG22	1.96	0.47
1:C:437:ILE:O	1:C:441:GLN:HB3	2.14	0.47
1:C:58:GLU:O	1:C:61:VAL:HG12	2.15	0.47
1:A:116:ARG:HH12	1:A:244:ARG:HH11	1.62	0.47
1:A:236:LEU:HD12	1:A:236:LEU:C	2.35	0.47
1:B:37:GLY:CA	1:B:77:THR:HB	2.18	0.47
1:D:160:ILE:HG12	3:D:502:NAD:O2N	2.15	0.47
1:A:432:TRP:HB3	1:A:437:ILE:HG22	1.97	0.46
1:C:269:MET:HE1	1:C:320:PHE:CD2	2.50	0.46
1:D:255:VAL:HA	1:D:272:ASN:HD21	1.80	0.46
1:D:269:MET:HE3	1:D:320:PHE:CD2	2.51	0.46
1:B:41:TYR:CE2	1:B:136:MET:HG2	2.50	0.46
1:C:160:ILE:HG23	3:C:502:NAD:H6N	1.97	0.46
1:D:6:VAL:HG22	1:D:31:VAL:CG1	2.45	0.46
1:B:408:LEU:HD12	1:B:408:LEU:HA	1.65	0.46
1:D:85:ASP:HB2	1:D:92:THR:HA	1.97	0.46
1:D:86:TYR:O	1:D:89:ARG:N	2.49	0.46
1:A:84:VAL:O	1:A:86:TYR:HD1	1.98	0.46
1:B:128:GLU:HG2	1:B:221:ARG:CZ	2.45	0.46
1:C:149:ALA:HB3	1:C:150:ARG:CA	2.35	0.46
1:C:221:ARG:O	1:C:222:VAL:CB	2.62	0.46
1:B:95:ASP:OD1	1:B:95:ASP:C	2.54	0.46
1:C:222:VAL:CG1	1:C:222:VAL:O	2.63	0.46
1:D:86:TYR:HB2	1:D:87:GLU:H	1.23	0.46
1:A:356:VAL:HG12	1:A:377:LEU:HB2	1.98	0.46
1:C:343:LEU:CD2	1:C:355:LYS:HD3	2.45	0.46
1:A:91:LEU:C	1:A:92:THR:CG2	2.81	0.46
1:B:169:ARG:CD	1:B:175:VAL:HG13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ALA:N	1:B:399:LEU:CB	2.74	0.46
1:C:124:GLY:O	1:C:127:GLN:HG3	2.16	0.46
2:D:501:FAD:H2'	4:D:503:COA:S1P	2.55	0.46
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.78	0.46
1:B:216:PHE:HD1	1:B:225:VAL:HG22	1.79	0.46
1:B:361:ARG:HD3	1:B:365:HIS:HA	1.97	0.46
1:B:85:ASP:H	1:B:92:THR:CB	2.28	0.46
1:C:128:GLU:HG2	1:C:221:ARG:NH2	2.31	0.46
1:A:295:TRP:CZ2	1:A:297:PRO:HG3	2.51	0.46
1:A:431:VAL:HG21	4:B:503:COA:H32	1.97	0.45
1:B:37:GLY:H	1:B:78:ARG:H	1.64	0.45
1:D:339:THR:HG22	1:D:401:ILE:HD11	1.97	0.45
1:B:341:LEU:O	1:B:388:GLY:HA3	2.16	0.45
1:C:56:ARG:CZ	1:C:59:ARG:HH11	2.29	0.45
1:D:124:GLY:O	1:D:127:GLN:HG3	2.16	0.45
1:A:191:GLU:OE2	1:A:355:LYS:HE3	2.16	0.45
1:B:399:LEU:C	1:B:401:ILE:N	2.69	0.45
1:A:49:VAL:HG11	1:A:57:LEU:CD1	2.45	0.45
1:B:12:ALA:HB3	2:B:501:FAD:H5'2	1.99	0.45
1:B:91:LEU:CD1	1:B:94:HIS:CE1	2.99	0.45
1:C:151:ARG:CG	1:C:174:GLN:HE21	2.25	0.45
1:C:208:TRP:HB3	1:C:211:VAL:HG21	1.98	0.45
1:D:3:LYS:HB3	1:D:3:LYS:NZ	2.32	0.45
1:B:180:ALA:H	3:B:502:NAD:C8A	2.29	0.45
1:C:183:ARG:NH1	1:C:188:TRP:O	2.49	0.45
1:D:356:VAL:HG12	1:D:377:LEU:HB2	1.97	0.45
1:D:418:LEU:HD13	1:D:439:ALA:CB	2.46	0.45
1:D:91:LEU:HB2	1:D:92:THR:H	1.28	0.45
1:D:94:HIS:HA	1:D:102:PHE:O	2.17	0.45
1:B:161:GLY:H	1:B:164:ALA:H	1.63	0.45
1:C:268:ARG:HH12	1:C:270:ARG:HH22	1.63	0.45
1:C:374:TRP:CE3	1:C:392:VAL:HG22	2.51	0.45
1:D:160:ILE:HG21	1:D:160:ILE:HD13	1.99	0.45
1:D:260:THR:HG23	1:D:284:GLU:OE1	2.17	0.45
1:A:3:LYS:HB2	1:A:107:ASP:OD2	2.17	0.45
1:A:83:ASP:O	1:A:94:HIS:HD2	1.99	0.45
1:D:91:LEU:O	1:D:92:THR:CB	2.64	0.45
1:A:396:HIS:ND1	1:B:396:HIS:ND1	2.64	0.45
1:B:260:THR:HG23	1:B:284:GLU:OE1	2.17	0.45
1:B:256:ALA:N	1:B:272:ASN:HD21	2.10	0.45
1:B:358:ILE:C	1:B:358:ILE:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLY:CA	3:C:502:NAD:H2B	2.45	0.45
1:A:341:LEU:O	1:A:388:GLY:HA3	2.17	0.45
1:A:361:ARG:NH1	1:A:370:SER:OG	2.50	0.45
1:B:272:ASN:HD22	1:B:272:ASN:H	1.64	0.45
1:C:443:ARG:HG2	1:C:443:ARG:OXT	2.17	0.45
1:D:224:ALA:O	1:D:225:VAL:CB	2.65	0.45
1:D:35:LYS:O	1:D:78:ARG:HA	2.18	0.44
1:A:340:GLY:HA3	1:A:388:GLY:HA2	1.98	0.44
1:A:410:ARG:HG2	1:A:410:ARG:HH11	1.81	0.44
1:D:295:TRP:CZ2	1:D:297:PRO:HG3	2.52	0.44
1:D:36:SER:O	1:D:37:GLY:C	2.54	0.44
2:B:501:FAD:H9	2:B:501:FAD:O2'	2.18	0.44
1:B:50:LEU:HA	1:B:50:LEU:HD12	1.70	0.44
1:C:341:LEU:O	1:C:388:GLY:HA3	2.18	0.44
1:C:432:TRP:HB3	1:C:437:ILE:HG22	1.99	0.44
1:D:262:ALA:HB3	1:D:284:GLU:HG2	1.99	0.44
1:D:400:ARG:NH1	1:D:433:ASP:OD2	2.49	0.44
1:A:418:LEU:HD13	1:A:439:ALA:CB	2.46	0.44
1:C:173:LEU:N	1:C:173:LEU:HD23	2.32	0.44
1:C:398:ALA:HA	1:C:400:ARG:H	1.82	0.44
1:B:148:GLN:O	1:B:149:ALA:C	2.55	0.44
1:C:104:ASP:OD1	1:C:105:ARG:N	2.48	0.44
1:A:160:ILE:HG21	1:A:160:ILE:CD1	2.48	0.43
1:A:76:HIS:HB3	1:A:79:HIS:CE1	2.52	0.43
1:C:361:ARG:HD3	1:C:365:HIS:HA	2.00	0.43
1:C:410:ARG:HH11	1:C:410:ARG:HG2	1.82	0.43
1:C:12:ALA:HB3	2:C:501:FAD:H5'2	1.99	0.43
1:D:37:GLY:HA2	1:D:77:THR:CB	2.24	0.43
1:B:292:ARG:HB2	1:B:293:PRO:CD	2.48	0.43
1:C:396:HIS:N	1:C:397:GLY:CA	2.78	0.43
1:C:61:VAL:O	1:C:61:VAL:HG13	2.19	0.43
1:C:83:ASP:O	1:C:94:HIS:HD2	2.01	0.43
2:A:501:FAD:O2'	2:A:501:FAD:H9	2.18	0.43
1:B:16:SER:CB	1:B:306:GLY:HA3	2.48	0.43
2:D:501:FAD:H9	2:D:501:FAD:O2'	2.18	0.43
1:B:367:TYR:CD1	1:B:368:PRO:HD2	2.54	0.43
1:C:128:GLU:HG2	1:C:221:ARG:CZ	2.48	0.43
1:A:88:LEU:O	1:A:89:ARG:CB	2.67	0.43
1:C:160:ILE:HG12	3:C:502:NAD:PN	2.59	0.43
1:D:352:TRP:NE1	5:D:612:HOH:O	2.50	0.43
1:B:12:ALA:HB3	2:B:501:FAD:O1P	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:HD22	1:B:438:ALA:HB1	2.00	0.43
1:B:23:ARG:HH22	4:B:503:COA:P2A	2.42	0.43
1:C:410:ARG:NH1	1:C:410:ARG:HG2	2.34	0.43
1:D:38:TRP:CD2	1:D:136:MET:HE2	2.54	0.43
1:D:85:ASP:OD1	1:D:88:LEU:CD2	2.54	0.43
1:A:38:TRP:CE3	1:A:136:MET:HE2	2.54	0.43
1:B:89:ARG:O	1:B:90:THR:C	2.57	0.43
1:D:437:ILE:O	1:D:441:GLN:HB3	2.19	0.43
1:A:54:ILE:HA	1:A:55:PRO:HD2	1.60	0.43
1:D:236:LEU:HD12	1:D:237:VAL:N	2.33	0.43
1:D:270:ARG:NH1	1:D:270:ARG:CB	2.81	0.43
1:A:91:LEU:C	1:A:92:THR:OG1	2.51	0.43
1:B:217:ARG:O	1:B:222:VAL:HA	2.19	0.43
1:B:24:GLU:HG3	1:B:316:ARG:HG3	2.01	0.43
1:D:161:GLY:N	1:D:164:ALA:H	2.15	0.43
1:A:100:ARG:O	1:A:101:THR:HG22	2.19	0.42
1:B:268:ARG:HH12	1:B:270:ARG:HH22	1.65	0.42
1:C:343:LEU:HD22	1:C:355:LYS:HD3	2.01	0.42
1:C:398:ALA:N	1:C:399:LEU:CB	2.81	0.42
1:A:160:ILE:CD1	1:A:160:ILE:CB	2.82	0.42
1:A:287:HIS:CD2	1:A:289:VAL:H	2.35	0.42
1:A:85:ASP:O	1:A:86:TYR:O	2.38	0.42
1:A:224:ALA:O	1:A:225:VAL:CB	2.67	0.42
1:A:44:CYS:HB3	2:A:501:FAD:C4X	2.49	0.42
1:B:16:SER:HB2	1:B:306:GLY:HA3	2.01	0.42
1:B:397:GLY:O	1:B:398:ALA:CB	2.67	0.42
1:C:74:LEU:HD23	1:C:74:LEU:HA	1.92	0.42
1:D:23:ARG:HH22	4:D:503:COA:P2A	2.42	0.42
1:A:441:GLN:C	1:A:442:ALA:O	2.58	0.42
1:A:8:VAL:HG13	1:A:81:VAL:CG1	2.49	0.42
1:B:4:ARG:HD3	1:B:105:ARG:O	2.20	0.42
1:C:180:ALA:O	1:C:210:GLY:HA2	2.19	0.42
1:D:424:TYR:CD1	1:D:431:VAL:HA	2.53	0.42
1:A:4:ARG:NH1	1:A:104:ASP:OD2	2.52	0.42
1:A:57:LEU:HG	1:A:136:MET:HE3	2.00	0.42
1:B:280:GLY:HA3	2:B:501:FAD:O2P	2.20	0.42
1:B:159:TYR:HB3	3:B:502:NAD:C4N	2.49	0.42
1:C:268:ARG:O	1:C:269:MET:HB2	2.20	0.42
1:D:272:ASN:ND2	1:D:272:ASN:H	2.16	0.42
1:D:296:LEU:HG	1:D:298:LEU:HD12	2.01	0.42
1:B:111:LEU:HD12	1:B:111:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:HIS:N	1:B:397:GLY:HA3	2.25	0.42
1:B:85:ASP:HB2	1:B:92:THR:HA	2.01	0.42
1:D:343:LEU:HD22	1:D:355:LYS:HD3	2.01	0.42
1:D:90:THR:HA	1:D:91:LEU:O	2.20	0.42
1:A:160:ILE:CD1	1:A:160:ILE:CG2	2.96	0.42
1:B:57:LEU:HD12	1:B:57:LEU:HA	1.81	0.42
1:B:86:TYR:O	1:B:89:ARG:CA	2.67	0.42
1:C:281:ASP:OD2	2:C:501:FAD:H3'	2.20	0.42
1:D:89:ARG:O	1:D:90:THR:C	2.58	0.42
1:A:160:ILE:HG12	3:A:502:NAD:PN	2.60	0.42
1:D:410:ARG:HG3	1:D:411:GLU:N	2.35	0.42
1:D:430:PRO:HD2	1:D:434:PRO:HD3	2.02	0.42
1:A:158:GLY:N	5:A:607:HOH:O	2.50	0.42
1:C:270:ARG:HG2	5:C:607:HOH:O	2.19	0.42
1:C:65:PRO:HB3	1:C:75:VAL:HG22	2.02	0.42
1:D:281:ASP:OD2	2:D:501:FAD:H3'	2.20	0.42
1:D:95:ASP:C	1:D:95:ASP:OD1	2.58	0.42
1:A:183:ARG:NH1	1:A:188:TRP:O	2.53	0.41
1:B:23:ARG:NH2	4:B:503:COA:O5A	2.53	0.41
1:B:24:GLU:HG2	1:B:316:ARG:HG3	2.00	0.41
1:B:97:ALA:HB1	1:B:98:GLU:H	1.52	0.41
1:C:424:TYR:CD1	1:C:431:VAL:HA	2.55	0.41
1:C:85:ASP:H	1:C:92:THR:CA	2.29	0.41
1:C:86:TYR:HB2	1:C:87:GLU:H	1.10	0.41
1:A:424:TYR:HD2	2:B:501:FAD:O2	2.03	0.41
1:B:15:ALA:HB1	4:B:503:COA:H142	2.02	0.41
1:B:231:VAL:HG12	1:B:231:VAL:O	2.19	0.41
1:B:134:ARG:NH2	1:B:281:ASP:OD2	2.53	0.41
1:D:127:GLN:NE2	1:D:216:PHE:O	2.53	0.41
1:D:88:LEU:O	1:D:89:ARG:CB	2.67	0.41
1:B:396:HIS:H	1:B:397:GLY:HA2	1.67	0.41
1:D:50:LEU:HA	1:D:50:LEU:HD12	1.58	0.41
1:A:94:HIS:H	1:A:94:HIS:HD2	1.64	0.41
1:B:178:LEU:HD23	1:B:208:TRP:HB2	2.02	0.41
1:B:221:ARG:O	1:B:221:ARG:HD3	2.20	0.41
1:C:85:ASP:CB	1:C:92:THR:HA	2.50	0.41
1:D:408:LEU:HA	1:D:408:LEU:HD12	1.84	0.41
1:A:169:ARG:HH11	1:A:169:ARG:HD2	1.72	0.41
1:A:15:ALA:HB1	4:A:503:COA:H142	2.02	0.41
1:A:86:TYR:O	1:A:89:ARG:CA	2.69	0.41
1:B:201:GLU:O	1:B:203:HIS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:VAL:HG13	1:C:237:VAL:HG22	2.03	0.41
1:A:328:ILE:HD13	1:A:328:ILE:HG21	1.79	0.41
1:A:424:TYR:CD1	1:A:431:VAL:HA	2.56	0.41
1:C:398:ALA:N	1:C:399:LEU:HB2	2.20	0.41
1:C:410:ARG:NH2	5:C:606:HOH:O	2.14	0.41
1:C:82:VAL:O	1:C:82:VAL:HG12	2.19	0.41
1:D:100:ARG:O	1:D:101:THR:HG22	2.21	0.41
1:D:56:ARG:CZ	1:D:59:ARG:HH11	2.33	0.41
1:A:148:GLN:O	1:A:149:ALA:C	2.59	0.41
1:A:85:ASP:H	1:A:92:THR:CB	2.33	0.41
1:A:85:ASP:N	1:A:92:THR:HA	2.29	0.41
3:B:502:NAD:H2D	3:B:502:NAD:H2N	1.88	0.41
1:B:160:ILE:HG23	3:B:502:NAD:H6N	2.03	0.41
1:C:209:THR:HG23	1:C:210:GLY:N	2.35	0.41
1:C:50:LEU:HD12	1:C:50:LEU:HA	1.64	0.41
1:D:398:ALA:CA	1:D:399:LEU:CB	2.99	0.41
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.69	0.41
1:A:97:ALA:O	1:A:98:GLU:CD	2.59	0.41
1:B:433:ASP:O	1:B:434:PRO:C	2.57	0.41
1:C:181:LYS:H	1:C:181:LYS:HG2	1.61	0.41
1:C:270:ARG:NH1	1:C:270:ARG:HB3	2.36	0.41
1:D:361:ARG:HD3	1:D:365:HIS:HA	2.02	0.41
1:A:64:THR:HG1	1:A:67:GLU:HG3	1.82	0.41
1:A:69:ARG:O	1:A:70:LYS:C	2.58	0.41
1:C:221:ARG:O	1:C:222:VAL:CG1	2.68	0.41
1:D:411:GLU:OE1	1:D:411:GLU:HA	2.21	0.41
1:A:214:GLU:O	1:A:215:ALA:HB2	2.20	0.41
1:A:86:TYR:O	1:A:89:ARG:N	2.54	0.41
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.74	0.41
1:C:439:ALA:O	1:C:441:GLN:CA	2.67	0.41
1:D:148:GLN:O	1:D:149:ALA:C	2.60	0.41
1:B:89:ARG:C	1:B:90:THR:O	2.59	0.41
1:A:410:ARG:HG3	1:A:411:GLU:N	2.36	0.40
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.70	0.40
1:C:295:TRP:CZ2	1:C:297:PRO:HG3	2.55	0.40
1:B:157:ALA:HB2	1:B:177:LEU:HD22	2.03	0.40
1:C:133:LEU:HD23	1:C:133:LEU:HA	1.69	0.40
1:C:44:CYS:HB3	2:C:501:FAD:C4X	2.51	0.40
1:D:268:ARG:HH22	1:D:270:ARG:NH2	2.20	0.40
1:D:268:ARG:O	1:D:269:MET:HB2	2.21	0.40
1:D:373:LEU:HD22	1:D:434:PRO:CG	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLY:H	1:A:78:ARG:H	1.68	0.40
1:B:399:LEU:C	1:B:401:ILE:H	2.24	0.40
1:A:410:ARG:HH12	1:B:410:ARG:NH1	2.08	0.40
1:B:91:LEU:O	1:B:92:THR:CG2	2.69	0.40
1:C:440:GLN:O	1:C:441:GLN:O	2.39	0.40
1:A:400:ARG:NH1	1:A:433:ASP:OD2	2.49	0.40
1:B:100:ARG:O	1:B:101:THR:HG22	2.21	0.40
1:C:169:ARG:HD3	1:C:175:VAL:HG13	2.03	0.40
1:D:268:ARG:CG	1:D:312:VAL:HG21	2.51	0.40
1:D:313:ILE:C	1:D:315:GLY:H	2.25	0.40
1:D:400:ARG:HH12	1:D:429:SER:CB	2.22	0.40
1:D:160:ILE:CD1	1:D:160:ILE:CB	2.81	0.40
1:D:418:LEU:HA	1:D:418:LEU:HD12	1.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:614:HOH:O	5:B:624:HOH:O[2_655]	2.01	0.19

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	441/443 (100%)	392 (89%)	31 (7%)	18 (4%)	3	12
1	B	441/443 (100%)	392 (89%)	31 (7%)	18 (4%)	3	12
1	C	441/443 (100%)	390 (88%)	35 (8%)	16 (4%)	4	16
1	D	441/443 (100%)	388 (88%)	36 (8%)	17 (4%)	3	13
All	All	1764/1772 (100%)	1562 (88%)	133 (8%)	69 (4%)	3	13

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	TYR
1	A	89	ARG
1	A	90	THR
1	A	91	LEU
1	A	92	THR
1	A	148	GLN
1	A	149	ALA
1	A	398	ALA
1	A	441	GLN
1	A	442	ALA
1	B	86	TYR
1	B	89	ARG
1	B	90	THR
1	B	91	LEU
1	B	92	THR
1	B	149	ALA
1	B	398	ALA
1	B	441	GLN
1	B	442	ALA
1	C	86	TYR
1	C	89	ARG
1	C	92	THR
1	C	149	ALA
1	C	398	ALA
1	C	441	GLN
1	C	442	ALA
1	D	86	TYR
1	D	90	THR
1	D	91	LEU
1	D	92	THR
1	D	149	ALA
1	D	398	ALA
1	D	441	GLN
1	D	442	ALA
1	A	222	VAL
1	A	399	LEU
1	B	148	GLN
1	B	202	ARG
1	B	228	SER
1	C	148	GLN
1	C	222	VAL
1	D	89	ARG
1	D	148	GLN

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Mol	Chain	Res	Type
1	D	222	VAL
1	D	399	LEU
1	A	228	SER
1	B	222	VAL
1	B	440	GLN
1	C	364	ALA
1	C	399	LEU
1	C	440	GLN
1	A	397	GLY
1	A	410	ARG
1	A	440	GLN
1	C	397	GLY
1	D	228	SER
1	D	440	GLN
1	A	225	VAL
1	B	225	VAL
1	C	189	ASP
1	C	225	VAL
1	C	395	GLY
1	D	202	ARG
1	D	225	VAL
1	B	55	PRO
1	B	399	LEU
1	D	189	ASP
1	B	397	GLY
1	A	395	GLY

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	338/338 (100%)	284 (84%)	54 (16%)	2	8
1	B	338/338 (100%)	283 (84%)	55 (16%)	2	7
1	C	337/338 (100%)	286 (85%)	51 (15%)	3	9
1	D	337/338 (100%)	280 (83%)	57 (17%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1350/1352 (100%)	1133 (84%)	217 (16%)	2 8

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	27	GLU
1	A	39	VAL
1	A	44	CYS
1	A	50	LEU
1	A	56	ARG
1	A	59	ARG
1	A	60	LEU
1	A	75	VAL
1	A	78	ARG
1	A	86	TYR
1	A	90	THR
1	A	91	LEU
1	A	94	HIS
1	A	100	ARG
1	A	101	THR
1	A	105	ARG
1	A	111	LEU
1	A	116	ARG
1	A	118	SER
1	A	132	THR
1	A	133	LEU
1	A	142	LEU
1	A	144	LYS
1	A	146	LEU
1	A	173	LEU
1	A	176	THR
1	A	177	LEU
1	A	185	LEU
1	A	199	GLU
1	A	207	VAL
1	A	208	TRP
1	A	209	THR
1	A	217	ARG
1	A	221	ARG
1	A	222	VAL
1	A	236	LEU

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Mol	Chain	Res	Type
1	A	268	ARG
1	A	301	VAL
1	A	324	VAL
1	A	361	ARG
1	A	375	VAL
1	A	377	LEU
1	A	386	LEU
1	A	392	VAL
1	A	396	HIS
1	A	408	LEU
1	A	410	ARG
1	A	418	LEU
1	A	429	SER
1	A	437	ILE
1	A	440	GLN
1	A	441	GLN
1	A	443	ARG
1	B	3	LYS
1	B	27	GLU
1	B	39	VAL
1	B	44	CYS
1	B	50	LEU
1	B	56	ARG
1	B	59	ARG
1	B	60	LEU
1	B	75	VAL
1	B	78	ARG
1	B	86	TYR
1	B	90	THR
1	B	91	LEU
1	B	94	HIS
1	B	100	ARG
1	B	101	THR
1	B	105	ARG
1	B	111	LEU
1	B	116	ARG
1	B	132	THR
1	B	133	LEU
1	B	142	LEU
1	B	144	LYS
1	B	146	LEU
1	B	173	LEU

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Mol	Chain	Res	Type
1	B	176	THR
1	B	177	LEU
1	B	181	LYS
1	B	185	LEU
1	B	199	GLU
1	B	207	VAL
1	B	208	TRP
1	B	209	THR
1	B	217	ARG
1	B	221	ARG
1	B	222	VAL
1	B	236	LEU
1	B	268	ARG
1	B	301	VAL
1	B	311	SER
1	B	324	VAL
1	B	361	ARG
1	B	375	VAL
1	B	377	LEU
1	B	386	LEU
1	B	392	VAL
1	B	396	HIS
1	B	408	LEU
1	B	410	ARG
1	B	418	LEU
1	B	429	SER
1	B	437	ILE
1	B	440	GLN
1	B	441	GLN
1	B	443	ARG
1	C	3	LYS
1	C	39	VAL
1	C	44	CYS
1	C	50	LEU
1	C	59	ARG
1	C	60	LEU
1	C	75	VAL
1	C	78	ARG
1	C	86	TYR
1	C	87	GLU
1	C	90	THR
1	C	91	LEU

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Mol	Chain	Res	Type
1	C	94	HIS
1	C	100	ARG
1	C	101	THR
1	C	105	ARG
1	C	111	LEU
1	C	116	ARG
1	C	132	THR
1	C	133	LEU
1	C	142	LEU
1	C	143	LEU
1	C	144	LYS
1	C	146	LEU
1	C	176	THR
1	C	177	LEU
1	C	185	LEU
1	C	208	TRP
1	C	209	THR
1	C	217	ARG
1	C	221	ARG
1	C	222	VAL
1	C	236	LEU
1	C	268	ARG
1	C	272	ASN
1	C	301	VAL
1	C	361	ARG
1	C	375	VAL
1	C	377	LEU
1	C	386	LEU
1	C	392	VAL
1	C	396	HIS
1	C	408	LEU
1	C	410	ARG
1	C	418	LEU
1	C	429	SER
1	C	434	PRO
1	C	437	ILE
1	C	440	GLN
1	C	441	GLN
1	C	443	ARG
1	D	3	LYS
1	D	27	GLU
1	D	39	VAL

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Mol	Chain	Res	Type
1	D	44	CYS
1	D	50	LEU
1	D	56	ARG
1	D	59	ARG
1	D	60	LEU
1	D	75	VAL
1	D	78	ARG
1	D	86	TYR
1	D	90	THR
1	D	91	LEU
1	D	94	HIS
1	D	100	ARG
1	D	101	THR
1	D	105	ARG
1	D	111	LEU
1	D	116	ARG
1	D	120	PRO
1	D	132	THR
1	D	133	LEU
1	D	142	LEU
1	D	144	LYS
1	D	146	LEU
1	D	155	LEU
1	D	173	LEU
1	D	176	THR
1	D	177	LEU
1	D	181	LYS
1	D	185	LEU
1	D	199	GLU
1	D	207	VAL
1	D	208	TRP
1	D	209	THR
1	D	221	ARG
1	D	222	VAL
1	D	236	LEU
1	D	241	THR
1	D	268	ARG
1	D	301	VAL
1	D	311	SER
1	D	359	GLN
1	D	361	ARG
1	D	375	VAL

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Mol	Chain	Res	Type
1	D	377	LEU
1	D	386	LEU
1	D	392	VAL
1	D	396	HIS
1	D	408	LEU
1	D	410	ARG
1	D	418	LEU
1	D	429	SER
1	D	437	ILE
1	D	440	GLN
1	D	441	GLN
1	D	443	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	96	HIS
1	A	103	GLN
1	A	174	GLN
1	A	203	HIS
1	A	272	ASN
1	A	287	HIS
1	A	396	HIS
1	A	440	GLN
1	A	441	GLN
1	B	96	HIS
1	B	174	GLN
1	B	272	ASN
1	B	287	HIS
1	B	396	HIS
1	B	440	GLN
1	B	441	GLN
1	C	96	HIS
1	C	174	GLN
1	C	272	ASN
1	C	287	HIS
1	C	440	GLN
1	D	94	HIS
1	D	96	HIS
1	D	103	GLN
1	D	174	GLN

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Mol	Chain	Res	Type
1	D	187	HIS
1	D	272	ASN
1	D	287	HIS
1	D	409	HIS
1	D	440	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	501	-	50,58,58	2.88	16 (32%)	58,89,89	2.62	15 (25%)
3	NAD	A	502	-	39,48,48	2.29	9 (23%)	44,73,73	3.21	18 (40%)
4	COA	A	503	1	40,50,50	1.25	4 (10%)	51,75,75	2.03	15 (29%)
2	FAD	B	501	-	50,58,58	3.21	16 (32%)	58,89,89	3.00	18 (31%)
3	NAD	B	502	-	39,48,48	2.38	8 (20%)	44,73,73	3.05	16 (36%)
4	COA	B	503	1	40,50,50	1.37	4 (10%)	51,75,75	1.93	13 (25%)
2	FAD	C	501	-	50,58,58	2.68	15 (30%)	58,89,89	2.71	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	C	502	-	39,48,48	2.47	6 (15%)	44,73,73	3.35	16 (36%)
4	COA	C	503	1	40,50,50	1.26	4 (10%)	51,75,75	2.13	17 (33%)
2	FAD	D	501	-	50,58,58	2.91	16 (32%)	58,89,89	2.72	20 (34%)
3	NAD	D	502	-	39,48,48	2.41	9 (23%)	44,73,73	3.18	17 (38%)
4	COA	D	503	1	40,50,50	1.31	4 (10%)	51,75,75	2.14	19 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	501	-	-	6/30/50/50	0/6/6/6
3	NAD	A	502	-	-	6/22/62/62	0/5/5/5
4	COA	A	503	1	-	17/44/64/64	0/3/3/3
2	FAD	B	501	-	-	7/30/50/50	0/6/6/6
3	NAD	B	502	-	-	5/22/62/62	0/5/5/5
4	COA	B	503	1	-	18/44/64/64	0/3/3/3
2	FAD	C	501	-	-	5/30/50/50	0/6/6/6
3	NAD	C	502	-	-	5/22/62/62	0/5/5/5
4	COA	C	503	1	-	19/44/64/64	0/3/3/3
2	FAD	D	501	-	-	7/30/50/50	0/6/6/6
3	NAD	D	502	-	-	6/22/62/62	0/5/5/5
4	COA	D	503	1	-	19/44/64/64	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C4X-C10	14.62	1.53	1.38
2	A	501	FAD	C4X-C10	12.57	1.51	1.38
2	D	501	FAD	C4X-C10	12.47	1.51	1.38
2	C	501	FAD	C4X-C10	11.27	1.50	1.38
3	D	502	NAD	O7N-C7N	10.04	1.43	1.24
3	C	502	NAD	O7N-C7N	9.17	1.42	1.24
3	B	502	NAD	O7N-C7N	9.01	1.41	1.24
3	A	502	NAD	O7N-C7N	8.90	1.41	1.24
3	C	502	NAD	O4B-C1B	7.46	1.51	1.41
2	B	501	FAD	C9A-N10	7.44	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C9A-N10	6.88	1.47	1.38
2	B	501	FAD	C9A-C5X	6.60	1.55	1.42
2	A	501	FAD	C9A-C5X	6.43	1.55	1.42
2	C	501	FAD	C4-C4X	6.12	1.52	1.41
2	D	501	FAD	C9A-C5X	6.10	1.54	1.42
3	B	502	NAD	O4B-C1B	6.07	1.49	1.41
2	C	501	FAD	C9A-N10	5.81	1.46	1.38
2	C	501	FAD	C9A-C5X	5.58	1.53	1.42
3	C	502	NAD	C2A-N3A	5.44	1.41	1.32
3	D	502	NAD	C2A-N3A	5.42	1.41	1.32
2	D	501	FAD	C4-C4X	5.31	1.50	1.41
2	B	501	FAD	C4-C4X	5.23	1.50	1.41
2	A	501	FAD	C9A-N10	5.08	1.45	1.38
2	B	501	FAD	C8-C7	5.05	1.53	1.40
2	A	501	FAD	C4-C4X	5.01	1.50	1.41
2	D	501	FAD	C5A-C4A	4.99	1.51	1.40
3	A	502	NAD	C2A-N3A	4.94	1.40	1.32
2	A	501	FAD	C5A-C4A	4.73	1.51	1.40
3	B	502	NAD	C2A-N3A	4.71	1.39	1.32
2	C	501	FAD	C8-C7	4.60	1.52	1.40
2	B	501	FAD	C10-N1	4.47	1.39	1.33
2	B	501	FAD	C4X-N5	4.37	1.39	1.33
4	B	503	COA	C5A-C4A	4.34	1.50	1.40
2	A	501	FAD	C8-C7	4.31	1.51	1.40
3	D	502	NAD	O4B-C1B	4.24	1.47	1.41
2	C	501	FAD	C4X-N5	4.19	1.39	1.33
4	B	503	COA	C2A-N3A	4.15	1.39	1.32
2	D	501	FAD	C10-N1	4.09	1.38	1.33
2	D	501	FAD	C8-C7	4.03	1.51	1.40
2	B	501	FAD	C5A-C4A	4.02	1.49	1.40
4	C	503	COA	C5A-C4A	3.90	1.49	1.40
4	A	503	COA	C2A-N3A	3.89	1.38	1.32
4	D	503	COA	C2A-N3A	3.79	1.38	1.32
3	A	502	NAD	C2A-N1A	3.77	1.41	1.33
2	B	501	FAD	C4-N3	3.77	1.39	1.33
4	D	503	COA	C5A-C4A	3.76	1.49	1.40
3	D	502	NAD	C2A-N1A	3.74	1.41	1.33
4	A	503	COA	C5A-C4A	3.73	1.48	1.40
2	A	501	FAD	C4X-N5	3.65	1.38	1.33
3	A	502	NAD	C4A-N3A	-3.65	1.30	1.35
3	B	502	NAD	C2A-N1A	3.64	1.40	1.33
2	C	501	FAD	C5A-C4A	3.51	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C2A-N3A	3.50	1.37	1.32
2	A	501	FAD	O4B-C1B	-3.46	1.36	1.41
3	D	502	NAD	C6A-C5A	-3.40	1.30	1.43
2	D	501	FAD	C4-N3	3.39	1.38	1.33
2	C	501	FAD	C10-N1	3.30	1.37	1.33
3	D	502	NAD	C8A-N7A	3.30	1.40	1.34
2	C	501	FAD	C2A-N3A	3.25	1.37	1.32
2	A	501	FAD	PA-O1A	3.16	1.62	1.50
3	C	502	NAD	C2A-N1A	3.11	1.39	1.33
2	A	501	FAD	C4-N3	3.08	1.38	1.33
2	D	501	FAD	C4X-N5	3.07	1.37	1.33
2	D	501	FAD	PA-O1A	3.07	1.61	1.50
3	A	502	NAD	C3B-C4B	-3.04	1.45	1.53
2	C	501	FAD	C4-N3	3.01	1.38	1.33
2	A	501	FAD	C10-N1	2.95	1.37	1.33
2	D	501	FAD	O4B-C1B	-2.94	1.37	1.41
2	B	501	FAD	C1'-N10	2.86	1.51	1.48
2	A	501	FAD	C2A-N1A	2.86	1.39	1.33
4	B	503	COA	C4A-N3A	2.77	1.39	1.35
3	C	502	NAD	C4A-N3A	-2.75	1.31	1.35
3	B	502	NAD	C8A-N7A	2.73	1.39	1.34
3	C	502	NAD	C6A-C5A	-2.69	1.32	1.43
4	C	503	COA	C2A-N3A	2.64	1.36	1.32
2	B	501	FAD	C2A-N3A	2.61	1.36	1.32
3	A	502	NAD	C6A-C5A	-2.60	1.33	1.43
4	C	503	COA	OAP-CAP	2.58	1.47	1.42
4	D	503	COA	C6A-C5A	2.56	1.53	1.43
4	A	503	COA	C6A-C5A	2.50	1.52	1.43
2	B	501	FAD	C4A-N3A	2.50	1.39	1.35
3	B	502	NAD	C2N-C3N	2.47	1.42	1.39
2	D	501	FAD	C2A-N3A	2.42	1.36	1.32
2	D	501	FAD	O4B-C4B	-2.41	1.39	1.45
2	A	501	FAD	C2B-C3B	-2.39	1.47	1.53
3	A	502	NAD	O3B-C3B	-2.39	1.37	1.43
3	D	502	NAD	C2N-C3N	2.34	1.42	1.39
4	A	503	COA	O4B-C1B	2.33	1.44	1.41
4	B	503	COA	C2A-N1A	2.33	1.38	1.33
2	C	501	FAD	O4'-C4'	2.32	1.48	1.43
2	C	501	FAD	O4-C4	2.31	1.30	1.24
2	B	501	FAD	PA-O1A	2.31	1.59	1.50
2	B	501	FAD	C6-C7	2.30	1.43	1.37
2	D	501	FAD	C8A-N7A	2.28	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NAD	C6A-C5A	-2.27	1.34	1.43
3	A	502	NAD	PA-O2A	-2.25	1.44	1.55
2	C	501	FAD	O4B-C4B	-2.24	1.40	1.45
4	C	503	COA	C2A-N1A	2.22	1.38	1.33
2	C	501	FAD	C6-C7	2.21	1.43	1.37
3	B	502	NAD	C3N-C7N	2.20	1.53	1.50
3	A	502	NAD	C8A-N7A	2.20	1.38	1.34
2	D	501	FAD	C6A-C5A	2.16	1.51	1.43
2	D	501	FAD	O4'-C4'	2.15	1.48	1.43
2	B	501	FAD	C6A-C5A	2.10	1.51	1.43
2	B	501	FAD	O4'-C4'	2.10	1.47	1.43
2	A	501	FAD	C4A-N3A	2.07	1.38	1.35
2	C	501	FAD	C5'-C4'	2.03	1.54	1.51
3	D	502	NAD	C5B-C4B	2.03	1.58	1.51
2	A	501	FAD	O3B-C3B	2.01	1.47	1.43
3	D	502	NAD	C4A-N3A	-2.01	1.32	1.35
4	D	503	COA	O4B-C1B	2.01	1.44	1.41

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAD	C4B-O4B-C1B	-14.84	94.36	109.83
3	B	502	NAD	C4B-O4B-C1B	-13.89	95.35	109.83
3	A	502	NAD	C4B-O4B-C1B	-13.43	95.83	109.83
3	D	502	NAD	C4B-O4B-C1B	-12.75	96.54	109.83
2	D	501	FAD	C4-N3-C2	11.15	124.55	115.14
2	B	501	FAD	C4-N3-C2	10.86	124.31	115.14
2	A	501	FAD	C4-N3-C2	10.69	124.17	115.14
2	C	501	FAD	C4-N3-C2	10.44	123.96	115.14
2	B	501	FAD	C1'-N10-C9A	8.96	126.11	118.31
2	C	501	FAD	C1'-N10-C9A	8.35	125.58	118.31
3	A	502	NAD	O4B-C4B-C5B	8.15	136.41	109.38
3	C	502	NAD	O4B-C4B-C5B	7.95	135.75	109.38
3	D	502	NAD	O4B-C4B-C5B	7.82	135.32	109.38
3	B	502	NAD	O4B-C4B-C5B	7.45	134.08	109.38
2	B	501	FAD	C4-C4X-C10	-7.36	114.52	119.95
2	D	501	FAD	C1'-N10-C9A	7.33	124.69	118.31
2	C	501	FAD	C4-C4X-C10	-6.86	114.88	119.95
4	A	503	COA	C7P-C6P-C5P	-6.70	101.21	112.36
2	A	501	FAD	C4-C4X-C10	-6.13	115.42	119.95
2	B	501	FAD	C10-C4X-N5	6.09	125.72	121.25
3	C	502	NAD	C5A-C6A-N6A	-6.02	110.93	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C5X-C9A-N10	5.96	122.27	117.71
4	C	503	COA	CEP-CBP-CAP	5.96	119.16	108.82
4	D	503	COA	C7P-C6P-C5P	-5.92	102.50	112.36
2	A	501	FAD	C1'-N10-C9A	5.88	123.43	118.31
3	D	502	NAD	C5A-C6A-N6A	-5.86	111.19	120.38
4	C	503	COA	C3P-N4P-C5P	-5.85	111.82	122.84
4	A	503	COA	C3P-N4P-C5P	-5.80	111.92	122.84
2	D	501	FAD	C5X-C9A-N10	5.41	121.84	117.71
2	C	501	FAD	C5X-C9A-N10	5.33	121.78	117.71
2	A	501	FAD	C10-C4X-N5	5.32	125.15	121.25
2	B	501	FAD	C4'-C3'-C2'	-5.30	102.22	113.40
3	A	502	NAD	C5A-C6A-N6A	-5.25	112.15	120.38
4	C	503	COA	C7P-N8P-C9P	-5.16	113.22	122.59
2	D	501	FAD	C4-C4X-C10	-5.15	116.15	119.95
4	B	503	COA	C7P-C6P-C5P	-5.13	103.81	112.36
4	B	503	COA	C3P-N4P-C5P	-5.10	113.24	122.84
2	A	501	FAD	C5X-C9A-N10	5.07	121.59	117.71
3	D	502	NAD	C4A-C5A-N7A	5.07	114.68	109.40
4	D	503	COA	C7P-N8P-C9P	-4.91	113.67	122.59
2	D	501	FAD	C4X-N5-C5X	4.85	121.75	116.77
2	C	501	FAD	C4'-C3'-C2'	-4.83	103.21	113.40
2	A	501	FAD	C9A-N10-C10	-4.80	115.52	121.77
2	B	501	FAD	C9A-N10-C10	-4.55	115.85	121.77
3	A	502	NAD	C5B-C4B-C3B	-4.50	98.29	115.21
3	A	502	NAD	O2B-C2B-C3B	4.48	126.34	111.80
3	D	502	NAD	N6A-C6A-N1A	4.46	127.83	118.57
3	A	502	NAD	N6A-C6A-N1A	4.43	127.76	118.57
3	C	502	NAD	C3N-C2N-N1N	4.42	124.90	120.40
4	D	503	COA	CEP-CBP-CAP	4.28	116.23	108.82
4	C	503	COA	C7P-C6P-C5P	-4.25	105.27	112.36
2	A	501	FAD	C4'-C3'-C2'	-4.23	104.49	113.40
3	C	502	NAD	C5B-C4B-C3B	-4.20	99.41	115.21
4	B	503	COA	C7P-N8P-C9P	-4.18	115.00	122.59
4	B	503	COA	C5A-C6A-N6A	-4.10	113.94	120.38
3	A	502	NAD	O3B-C3B-C4B	-4.10	99.23	111.07
2	D	501	FAD	C4X-C4-N3	-4.09	117.78	123.47
4	D	503	COA	C3P-N4P-C5P	-4.01	115.29	122.84
4	B	503	COA	N6A-C6A-N1A	4.00	126.87	118.57
2	D	501	FAD	C9A-C5X-N5	-3.99	116.81	122.34
3	B	502	NAD	N3A-C2A-N1A	-3.96	122.30	128.68
2	B	501	FAD	C4X-C4-N3	-3.95	117.97	123.47
3	C	502	NAD	C4A-C5A-N7A	3.82	113.38	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C9A-N10-C10	-3.76	116.88	121.77
3	C	502	NAD	O2B-C2B-C3B	3.71	123.83	111.80
2	C	501	FAD	C10-C4X-N5	3.71	123.97	121.25
2	D	501	FAD	C10-C4X-N5	3.69	123.96	121.25
4	C	503	COA	CDP-CBP-CCP	3.68	114.24	108.23
4	A	503	COA	N3A-C2A-N1A	-3.67	122.76	128.68
3	B	502	NAD	C3N-C2N-N1N	3.65	124.11	120.40
4	A	503	COA	CDP-CBP-CAP	3.64	115.13	108.82
2	A	501	FAD	O2B-C2B-C3B	-3.62	100.05	111.80
3	C	502	NAD	N6A-C6A-N1A	3.62	126.08	118.57
3	B	502	NAD	O7N-C7N-C3N	3.58	123.94	119.62
2	B	501	FAD	N6A-C6A-N1A	3.56	125.95	118.57
3	B	502	NAD	N6A-C6A-N1A	3.55	125.94	118.57
2	A	501	FAD	C4X-C4-N3	-3.53	118.55	123.47
3	D	502	NAD	C4D-O4D-C1D	-3.52	106.16	109.83
3	D	502	NAD	C5B-C4B-C3B	-3.49	102.08	115.21
4	D	503	COA	C6P-C5P-N4P	3.48	122.35	116.45
2	C	501	FAD	C4X-C4-N3	-3.47	118.64	123.47
3	D	502	NAD	O2B-C2B-C3B	3.44	122.95	111.80
4	D	503	COA	N3A-C2A-N1A	-3.44	123.14	128.68
4	D	503	COA	O9P-C9P-N8P	-3.43	115.48	122.98
3	D	502	NAD	N3A-C2A-N1A	-3.42	123.16	128.68
4	A	503	COA	C7P-N8P-C9P	-3.39	116.43	122.59
3	B	502	NAD	C5B-C4B-C3B	-3.37	102.54	115.21
2	A	501	FAD	O4B-C4B-C3B	3.36	111.78	105.14
2	A	501	FAD	N6A-C6A-N1A	3.36	125.53	118.57
4	A	503	COA	CEP-CBP-CAP	3.33	114.60	108.82
4	D	503	COA	O3B-P3B-O7A	-3.32	96.58	109.39
4	A	503	COA	O5P-C5P-N4P	-3.23	116.97	123.01
2	B	501	FAD	O4B-C4B-C3B	3.23	111.51	105.14
4	B	503	COA	CDP-CBP-CCP	3.21	113.46	108.23
2	C	501	FAD	C8M-C8-C9	-3.21	112.58	120.34
4	A	503	COA	O6A-CCP-CBP	-3.18	105.43	110.55
3	D	502	NAD	O5D-PN-O1N	3.16	121.43	109.07
4	D	503	COA	O6A-CCP-CBP	-3.16	105.47	110.55
3	A	502	NAD	O7N-C7N-N7N	-3.16	118.11	122.60
3	D	502	NAD	C3N-C2N-N1N	3.15	123.60	120.40
3	C	502	NAD	C5N-C4N-C3N	-3.14	116.57	120.34
2	D	501	FAD	C9A-N10-C10	-3.14	117.68	121.77
2	D	501	FAD	C4'-C3'-C2'	-3.12	106.82	113.40
4	D	503	COA	O5P-C5P-N4P	-3.12	117.18	123.01
2	C	501	FAD	C4A-C5A-N7A	-3.11	106.16	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAD	O2B-C2B-C3B	3.11	121.89	111.80
4	C	503	COA	O6A-CCP-CBP	-3.10	105.56	110.55
3	C	502	NAD	C6N-C5N-C4N	3.08	123.99	119.43
3	A	502	NAD	C3N-C2N-N1N	3.07	123.52	120.40
2	C	501	FAD	C4X-N5-C5X	3.06	119.92	116.77
3	B	502	NAD	O7N-C7N-N7N	-3.01	118.31	122.60
3	D	502	NAD	O4D-C4D-C3D	3.01	111.08	105.14
2	B	501	FAD	O4'-C4'-C5'	3.01	116.76	109.97
2	B	501	FAD	N3A-C2A-N1A	-2.99	123.86	128.68
2	A	501	FAD	O4'-C4'-C3'	2.96	116.34	109.11
2	B	501	FAD	C4B-O4B-C1B	-2.94	106.77	109.83
4	C	503	COA	CEP-CBP-CCP	-2.93	103.46	108.23
3	A	502	NAD	C4A-C5A-N7A	2.92	112.44	109.40
3	A	502	NAD	O7N-C7N-C3N	2.90	123.13	119.62
2	B	501	FAD	C4A-C5A-N7A	-2.87	106.40	109.40
4	C	503	COA	N6A-C6A-N1A	2.87	124.53	118.57
2	D	501	FAD	O2B-C2B-C3B	-2.87	102.51	111.80
3	C	502	NAD	C5D-C4D-C3D	-2.78	104.73	115.21
4	B	503	COA	N3A-C2A-N1A	-2.78	124.20	128.68
4	B	503	COA	O3B-P3B-O7A	-2.76	98.73	109.39
2	A	501	FAD	C4B-O4B-C1B	-2.73	106.98	109.83
3	D	502	NAD	C2B-C3B-C4B	-2.73	97.37	102.60
4	C	503	COA	CEP-CBP-CDP	-2.71	103.59	109.16
4	B	503	COA	CEP-CBP-CCP	-2.71	103.82	108.23
3	C	502	NAD	O7N-C7N-C3N	2.70	122.89	119.62
4	D	503	COA	CDP-CBP-CAP	2.69	113.49	108.82
3	A	502	NAD	C2D-C3D-C4D	-2.68	97.47	102.60
4	A	503	COA	C3B-C2B-C1B	2.64	105.73	99.89
2	C	501	FAD	C9A-C5X-N5	-2.61	118.72	122.34
2	C	501	FAD	O4'-C4'-C5'	2.58	115.79	109.97
2	A	501	FAD	O2P-P-O5'	2.57	119.69	107.75
4	D	503	COA	O9A-P3B-O7A	2.55	120.60	110.53
3	C	502	NAD	C2A-N1A-C6A	-2.53	114.38	118.77
3	D	502	NAD	C5N-C4N-C3N	-2.53	117.31	120.34
4	C	503	COA	O3B-P3B-O7A	-2.53	99.63	109.39
4	D	503	COA	CAP-C9P-N8P	2.53	121.61	116.58
2	A	501	FAD	C1'-N10-C10	2.52	120.93	118.46
2	D	501	FAD	N6A-C6A-N1A	2.50	123.76	118.57
2	C	501	FAD	C8M-C8-C7	2.46	125.88	120.72
2	D	501	FAD	O4B-C4B-C5B	-2.43	101.33	109.38
4	D	503	COA	O5A-P2A-O4A	2.42	124.34	112.21
3	D	502	NAD	O3B-C3B-C4B	-2.41	104.11	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	COA	C4A-C5A-N7A	-2.41	106.89	109.40
3	C	502	NAD	N3A-C2A-N1A	-2.40	124.81	128.68
3	B	502	NAD	C5D-C4D-C3D	-2.40	106.19	115.21
4	A	503	COA	N6A-C6A-N1A	2.39	123.52	118.57
4	D	503	COA	C5A-C6A-N6A	-2.37	116.66	120.38
2	D	501	FAD	O2P-P-O1P	2.37	124.09	112.21
4	C	503	COA	C4A-C5A-N7A	-2.36	106.94	109.40
3	B	502	NAD	C1B-N9A-C4A	2.34	130.69	126.64
3	A	502	NAD	O5D-PN-O1N	2.32	118.14	109.07
2	C	501	FAD	C4-C4X-N5	2.31	121.14	118.59
3	D	502	NAD	C5D-C4D-C3D	-2.31	106.53	115.21
2	D	501	FAD	C4X-C10-N10	-2.30	117.94	120.30
2	B	501	FAD	C2A-N1A-C6A	2.29	122.74	118.77
3	B	502	NAD	C2B-C3B-C4B	-2.29	98.22	102.60
4	C	503	COA	C5A-C6A-N6A	-2.28	116.80	120.38
4	A	503	COA	C6P-C5P-N4P	2.28	120.31	116.45
3	C	502	NAD	O5D-C5D-C4D	2.27	116.82	108.99
4	C	503	COA	N3A-C2A-N1A	-2.27	125.02	128.68
4	B	503	COA	O5A-P2A-O4A	2.26	123.54	112.21
4	B	503	COA	C3B-C2B-C1B	2.24	104.86	99.89
3	A	502	NAD	O5D-C5D-C4D	2.24	116.70	108.99
4	D	503	COA	O5B-P1A-O1A	-2.22	100.40	109.07
4	A	503	COA	CAP-C9P-N8P	2.21	120.98	116.58
3	B	502	NAD	O5D-C5D-C4D	2.21	116.60	108.99
3	B	502	NAD	C5A-C6A-N6A	-2.19	116.95	120.38
2	D	501	FAD	C9-C9A-C5X	-2.18	116.19	119.80
4	D	503	COA	O8A-P3B-O7A	2.17	119.08	110.53
4	C	503	COA	O9P-C9P-N8P	-2.16	118.25	122.98
2	B	501	FAD	O2'-C2'-C1'	2.16	114.77	109.53
4	B	503	COA	CDP-CBP-CAP	2.16	112.56	108.82
2	D	501	FAD	C6-C5X-N5	2.16	121.34	118.97
2	D	501	FAD	C6-C5X-C9A	2.15	121.85	119.06
3	A	502	NAD	C2A-N1A-C6A	-2.14	115.06	118.77
3	A	502	NAD	C5D-C4D-C3D	-2.13	107.18	115.21
4	C	503	COA	O9A-P3B-O7A	2.11	118.87	110.53
2	D	501	FAD	O5B-PA-O1A	2.11	117.32	109.07
3	A	502	NAD	O4D-C4D-C3D	2.11	109.31	105.14
3	B	502	NAD	O2A-PA-O5B	-2.11	97.95	107.75
4	C	503	COA	CDP-CBP-CAP	2.10	112.46	108.82
4	D	503	COA	N6A-C6A-N1A	2.09	122.90	118.57
4	A	503	COA	O3B-P3B-O7A	-2.06	101.42	109.39
2	B	501	FAD	O5'-C5'-C4'	2.06	114.86	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAD	O7N-C7N-N7N	-2.06	119.67	122.60
4	B	503	COA	O5B-P1A-O1A	-2.05	101.04	109.07
4	A	503	COA	O2A-P1A-O1A	2.05	122.49	112.21
4	C	503	COA	O8A-P3B-O7A	2.05	118.61	110.53
3	A	502	NAD	C2B-C3B-C4B	-2.05	98.68	102.60
2	D	501	FAD	O4'-C4'-C3'	2.04	114.10	109.11
2	B	501	FAD	C5A-C6A-N1A	-2.03	115.53	120.31
4	A	503	COA	C4A-C5A-N7A	-2.02	107.29	109.40
3	D	502	NAD	C6N-C5N-C4N	2.02	122.42	119.43
3	B	502	NAD	O4D-C4D-C3D	2.02	109.12	105.14

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3'-C4'-C5'-O5'
2	C	501	FAD	C3'-C4'-C5'-O5'
4	B	503	COA	C3B-O3B-P3B-O7A
4	B	503	COA	CCP-O6A-P2A-O3A
4	B	503	COA	CCP-O6A-P2A-O5A
4	B	503	COA	CDP-CBP-CCP-O6A
4	B	503	COA	CEP-CBP-CCP-O6A
4	B	503	COA	CAP-CBP-CCP-O6A
4	B	503	COA	S1P-C2P-C3P-N4P
4	D	503	COA	C3B-O3B-P3B-O7A
4	D	503	COA	C3B-O3B-P3B-O9A
4	D	503	COA	CCP-O6A-P2A-O3A
4	D	503	COA	CCP-O6A-P2A-O5A
4	D	503	COA	CDP-CBP-CCP-O6A
4	D	503	COA	CEP-CBP-CCP-O6A
4	D	503	COA	CAP-CBP-CCP-O6A
4	D	503	COA	S1P-C2P-C3P-N4P
3	C	502	NAD	C5D-O5D-PN-O3
3	C	502	NAD	C5D-O5D-PN-O2N
3	D	502	NAD	C5B-O5B-PA-O1A
3	D	502	NAD	C5D-O5D-PN-O3
3	D	502	NAD	C5D-O5D-PN-O2N
3	A	502	NAD	C5D-O5D-PN-O2N
3	A	502	NAD	O4D-C4D-C5D-O5D
3	B	502	NAD	C5D-O5D-PN-O3
3	B	502	NAD	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
4	A	503	COA	C3B-O3B-P3B-O7A
4	A	503	COA	CCP-O6A-P2A-O3A
4	A	503	COA	CCP-O6A-P2A-O5A
4	A	503	COA	CDP-CBP-CCP-O6A
4	A	503	COA	CEP-CBP-CCP-O6A
4	A	503	COA	CAP-CBP-CCP-O6A
4	A	503	COA	S1P-C2P-C3P-N4P
4	C	503	COA	C3B-O3B-P3B-O7A
4	C	503	COA	CCP-O6A-P2A-O4A
4	C	503	COA	CCP-O6A-P2A-O5A
4	C	503	COA	CDP-CBP-CCP-O6A
4	C	503	COA	CEP-CBP-CCP-O6A
4	C	503	COA	CAP-CBP-CCP-O6A
4	C	503	COA	S1P-C2P-C3P-N4P
2	D	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	O4B-C4B-C5B-O5B
3	C	502	NAD	O4D-C4D-C5D-O5D
3	B	502	NAD	O4D-C4D-C5D-O5D
4	B	503	COA	C4B-C3B-O3B-P3B
4	D	503	COA	C4B-C3B-O3B-P3B
4	D	503	COA	O5P-C5P-N4P-C3P
4	D	503	COA	C6P-C5P-N4P-C3P
4	A	503	COA	C6P-C5P-N4P-C3P
4	A	503	COA	O5P-C5P-N4P-C3P
3	D	502	NAD	O4D-C4D-C5D-O5D
4	A	503	COA	C2B-C3B-O3B-P3B
4	A	503	COA	C4B-C3B-O3B-P3B
4	C	503	COA	C2B-C3B-O3B-P3B
4	C	503	COA	C4B-C3B-O3B-P3B
4	B	503	COA	O5P-C5P-N4P-C3P
4	B	503	COA	C6P-C5P-N4P-C3P
2	B	501	FAD	C3B-C4B-C5B-O5B
4	A	503	COA	C3B-C4B-C5B-O5B
4	C	503	COA	C6P-C5P-N4P-C3P
4	C	503	COA	O5P-C5P-N4P-C3P
4	B	503	COA	C2B-C3B-O3B-P3B
4	D	503	COA	C2B-C3B-O3B-P3B
2	D	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	C3B-C4B-C5B-O5B
4	B	503	COA	O4B-C4B-C5B-O5B
4	A	503	COA	O4B-C4B-C5B-O5B
2	B	501	FAD	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	D	503	COA	P1A-O3A-P2A-O4A
2	B	501	FAD	C1'-C2'-C3'-C4'
2	D	501	FAD	C3B-C4B-C5B-O5B
4	D	503	COA	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
4	D	503	COA	C3B-C4B-C5B-O5B
4	C	503	COA	O4B-C4B-C5B-O5B
4	B	503	COA	C3B-O3B-P3B-O9A
4	C	503	COA	C3B-O3B-P3B-O9A
3	A	502	NAD	C5D-O5D-PN-O3
2	B	501	FAD	C5'-O5'-P-O2P
2	A	501	FAD	C5'-O5'-P-O2P
4	B	503	COA	P2A-O3A-P1A-O1A
4	B	503	COA	CCP-O6A-P2A-O4A
4	D	503	COA	P2A-O3A-P1A-O1A
4	D	503	COA	P1A-O3A-P2A-O5A
2	C	501	FAD	O4B-C4B-C5B-O5B
4	B	503	COA	C3B-C4B-C5B-O5B
3	B	502	NAD	O4B-C4B-C5B-O5B
4	B	503	COA	P2A-O3A-P1A-O2A
4	B	503	COA	P1A-O3A-P2A-O5A
4	D	503	COA	P2A-O3A-P1A-O2A
4	A	503	COA	P1A-O3A-P2A-O5A
4	C	503	COA	P2A-O3A-P1A-O1A
4	C	503	COA	P2A-O3A-P1A-O2A
4	C	503	COA	P1A-O3A-P2A-O5A
3	A	502	NAD	O4B-C4B-C5B-O5B
4	D	503	COA	C2P-C3P-N4P-C5P
2	C	501	FAD	C3B-C4B-C5B-O5B
4	C	503	COA	C3B-C4B-C5B-O5B
2	C	501	FAD	P-O3P-PA-O2A
2	A	501	FAD	PA-O3P-P-O5'
3	C	502	NAD	O4B-C4B-C5B-O5B
3	D	502	NAD	O4B-C4B-C5B-O5B
3	A	502	NAD	C3D-C4D-C5D-O5D
4	A	503	COA	C3B-O3B-P3B-O8A
3	D	502	NAD	C5B-O5B-PA-O3
4	C	503	COA	CCP-O6A-P2A-O3A
2	A	501	FAD	P-O3P-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	502	NAD	C5B-O5B-PA-O1A
3	A	502	NAD	C5B-O5B-PA-O1A
3	B	502	NAD	C5B-O5B-PA-O1A
4	A	503	COA	P2A-O3A-P1A-O2A
4	A	503	COA	P1A-O3A-P2A-O4A
4	C	503	COA	P1A-O3A-P2A-O4A
2	D	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	O2'-C2'-C3'-C4'

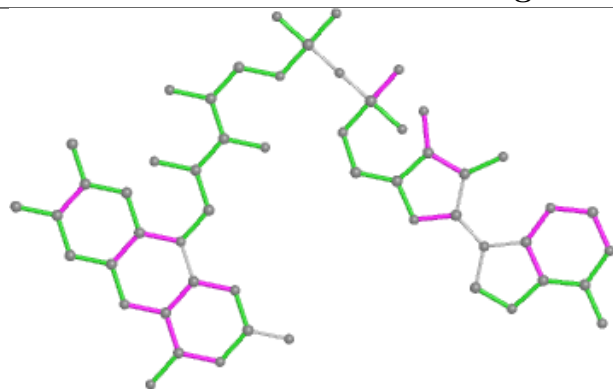
There are no ring outliers.

11 monomers are involved in 81 short contacts:

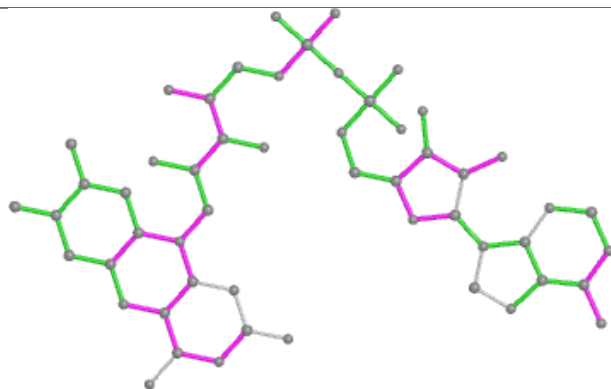
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	7	0
3	A	502	NAD	11	0
4	A	503	COA	3	0
2	B	501	FAD	11	0
3	B	502	NAD	10	0
4	B	503	COA	5	0
2	C	501	FAD	7	0
3	C	502	NAD	9	0
2	D	501	FAD	6	0
3	D	502	NAD	12	0
4	D	503	COA	3	0

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

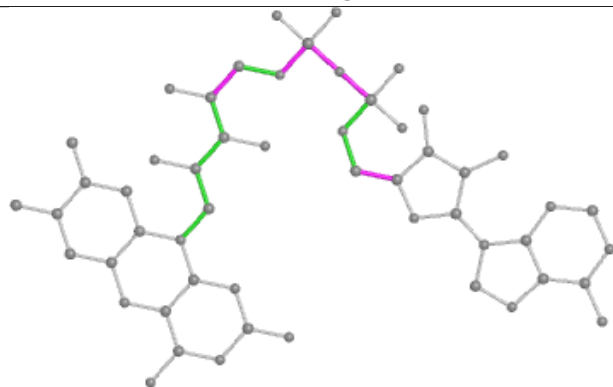
Ligand FAD A 501



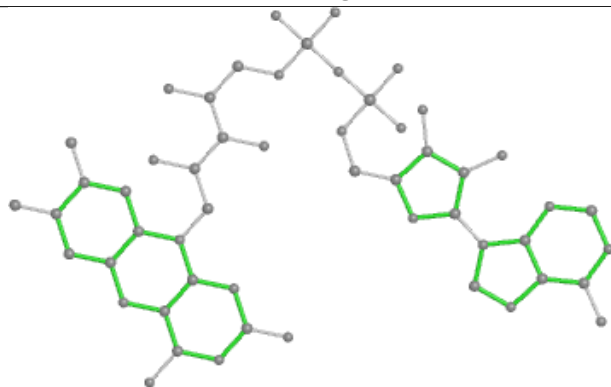
Bond lengths



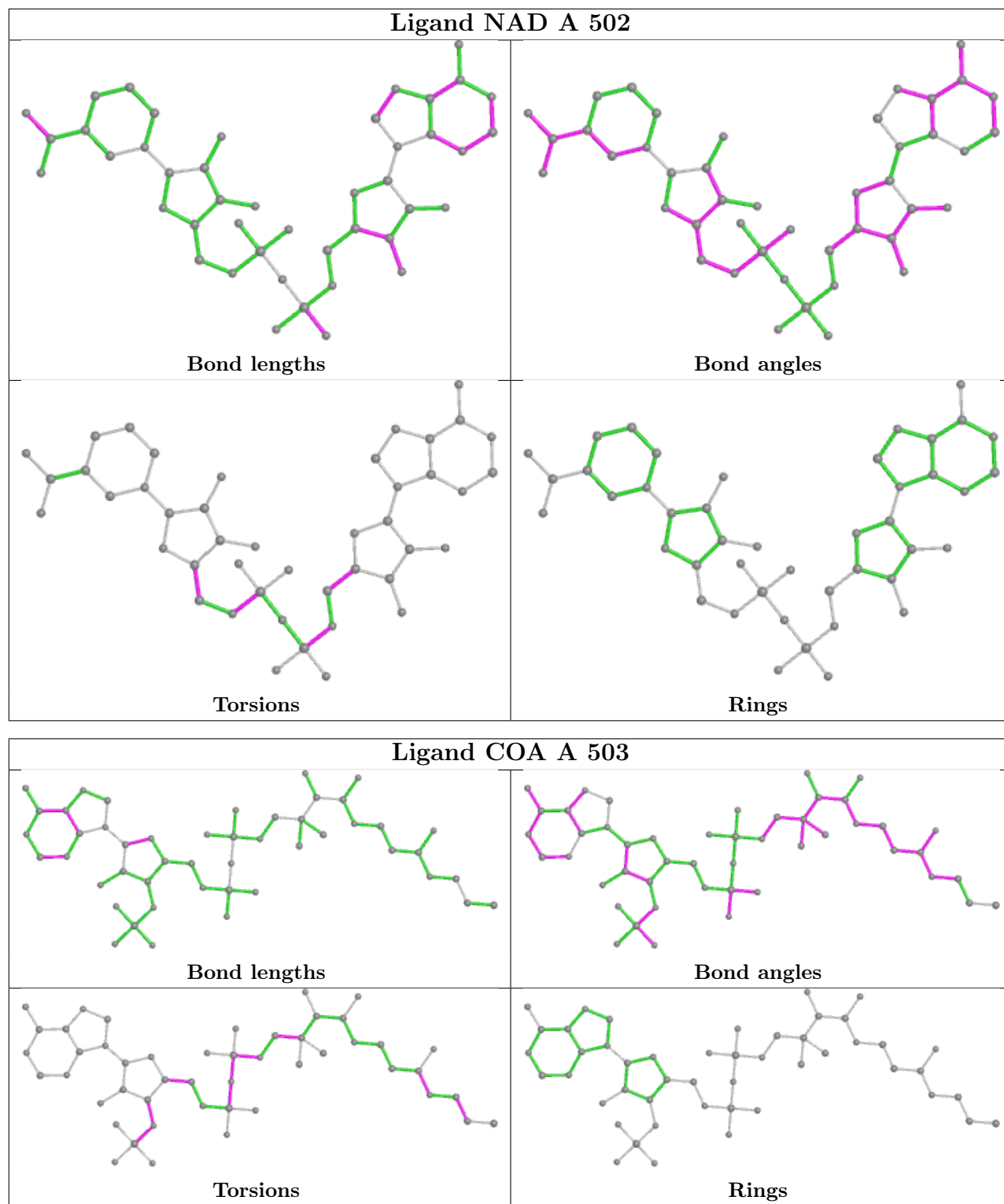
Bond angles

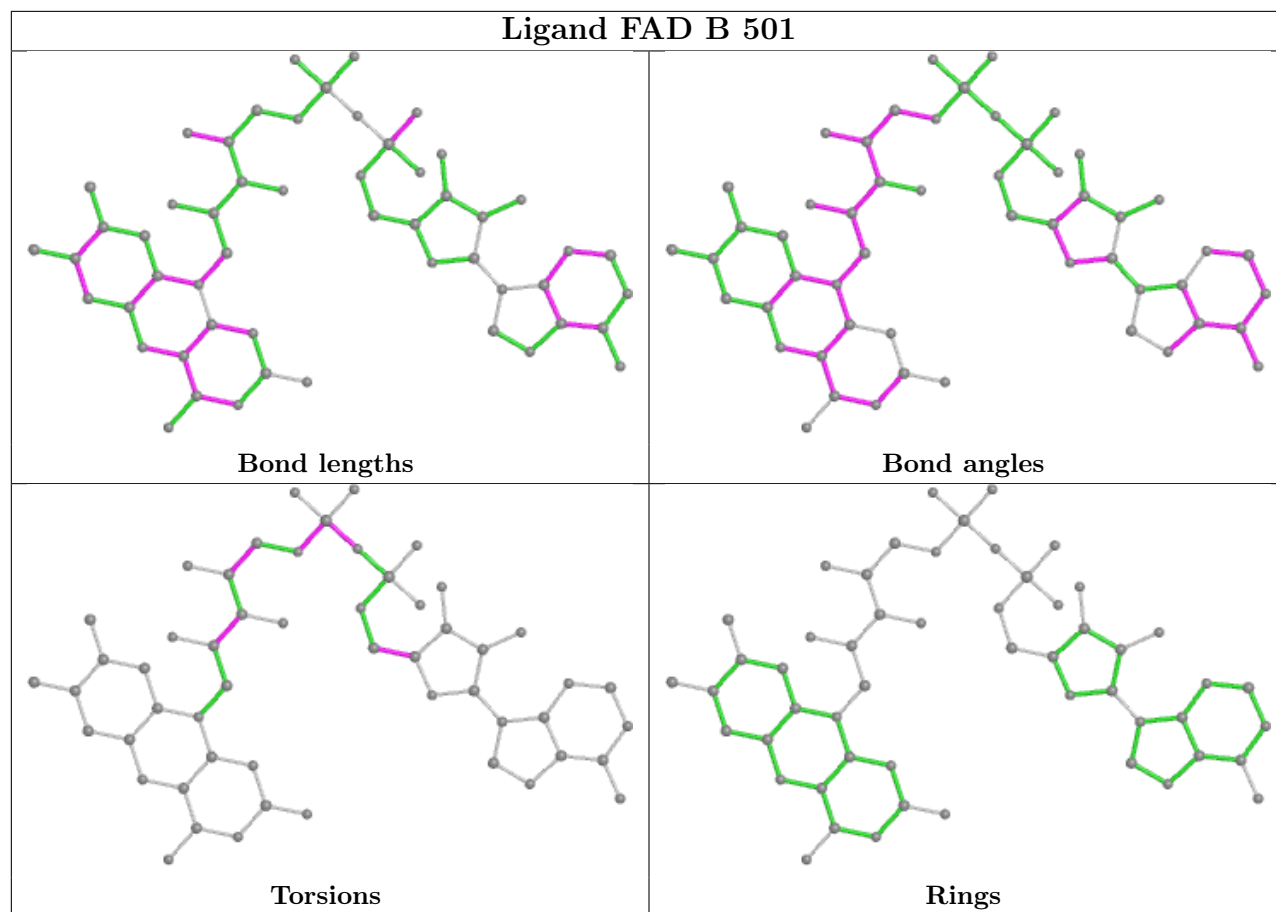


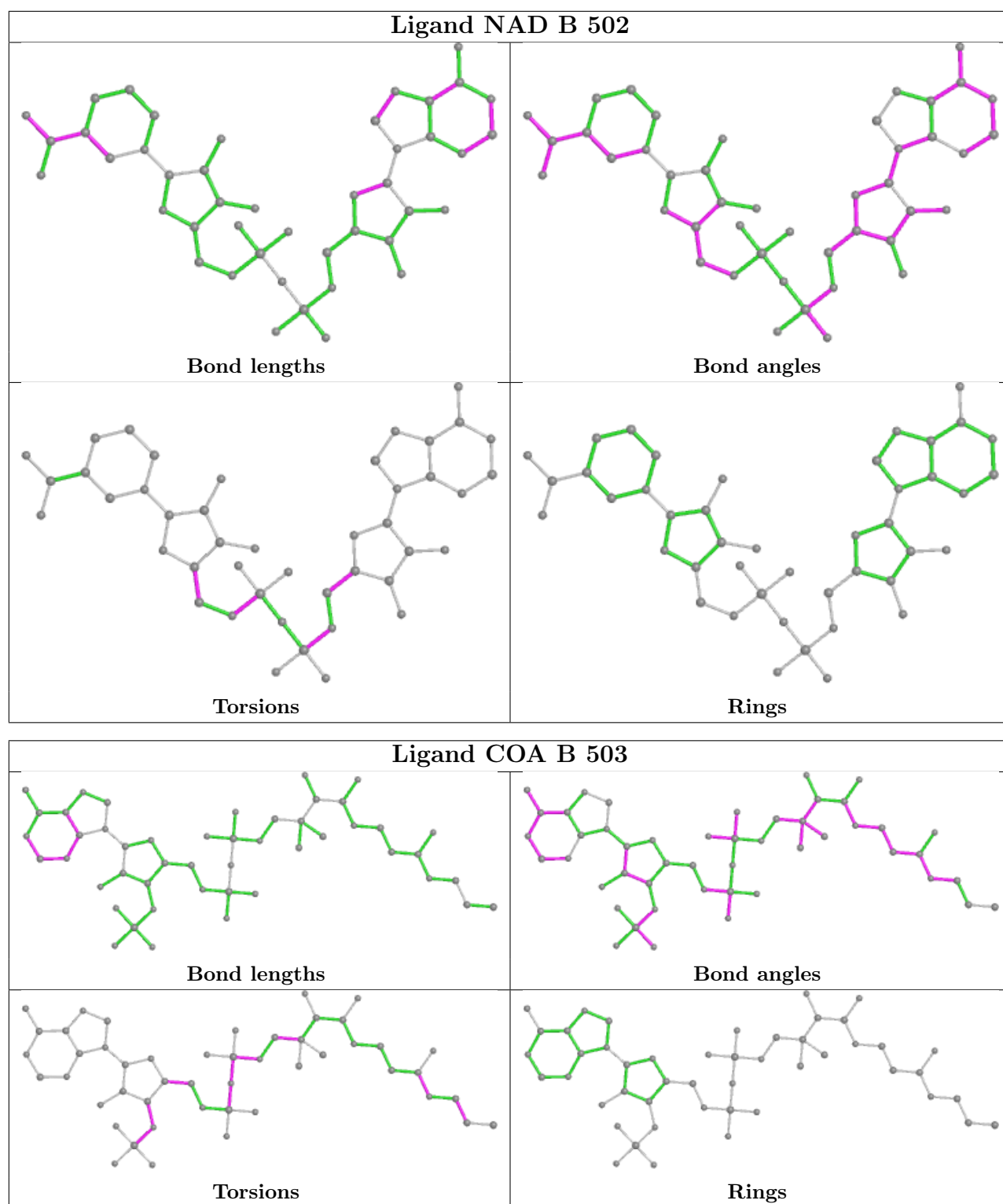
Torsions

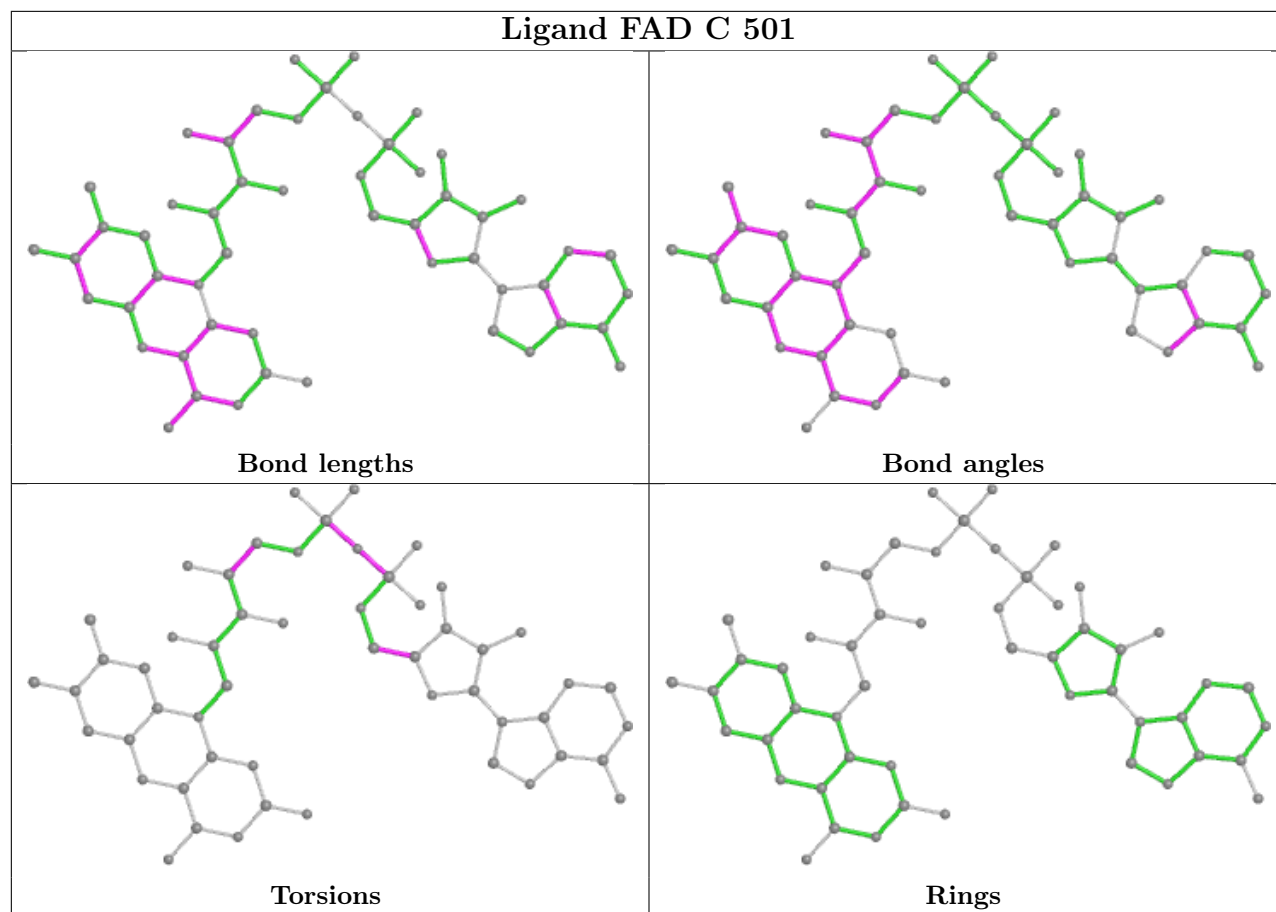


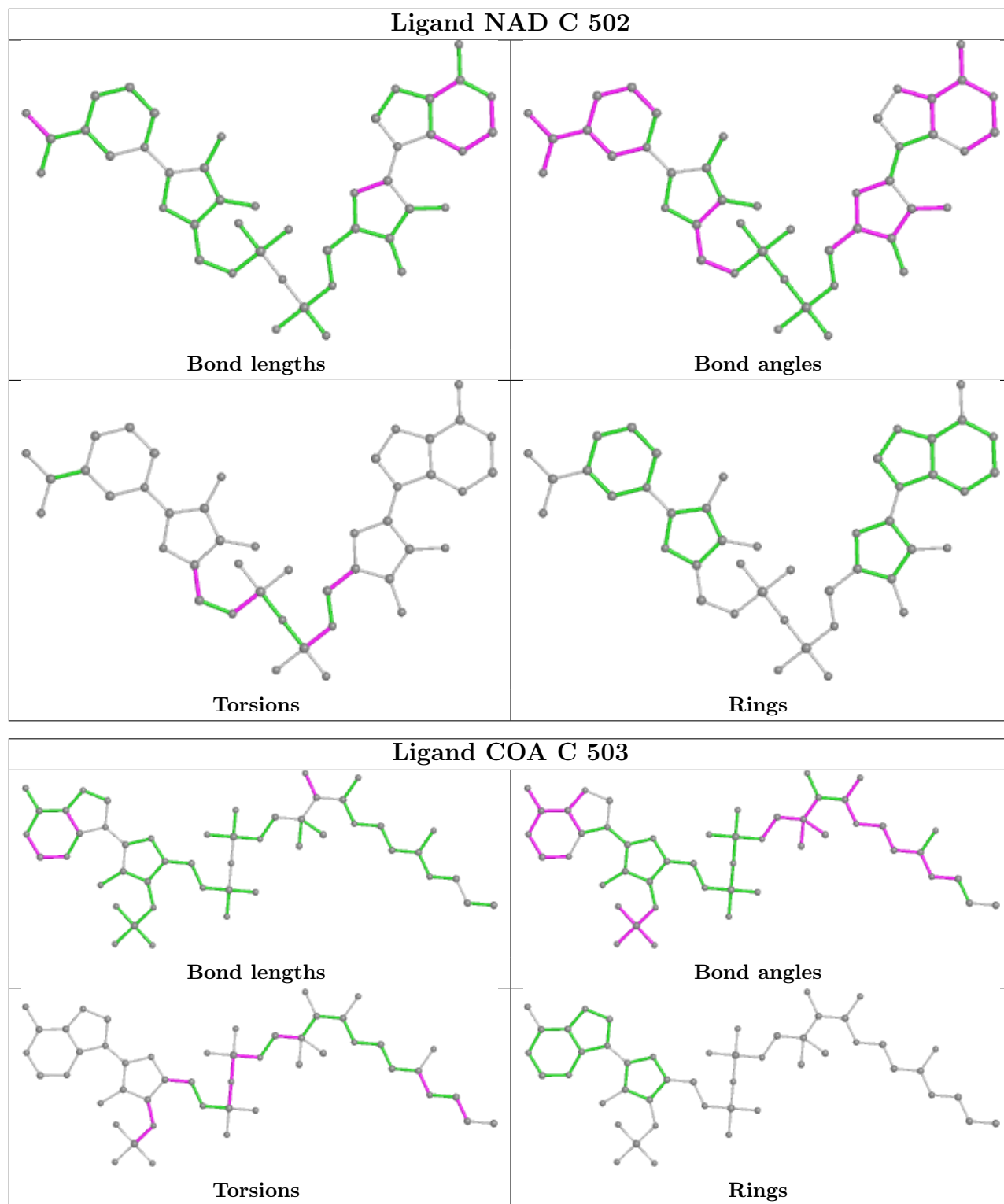
Rings

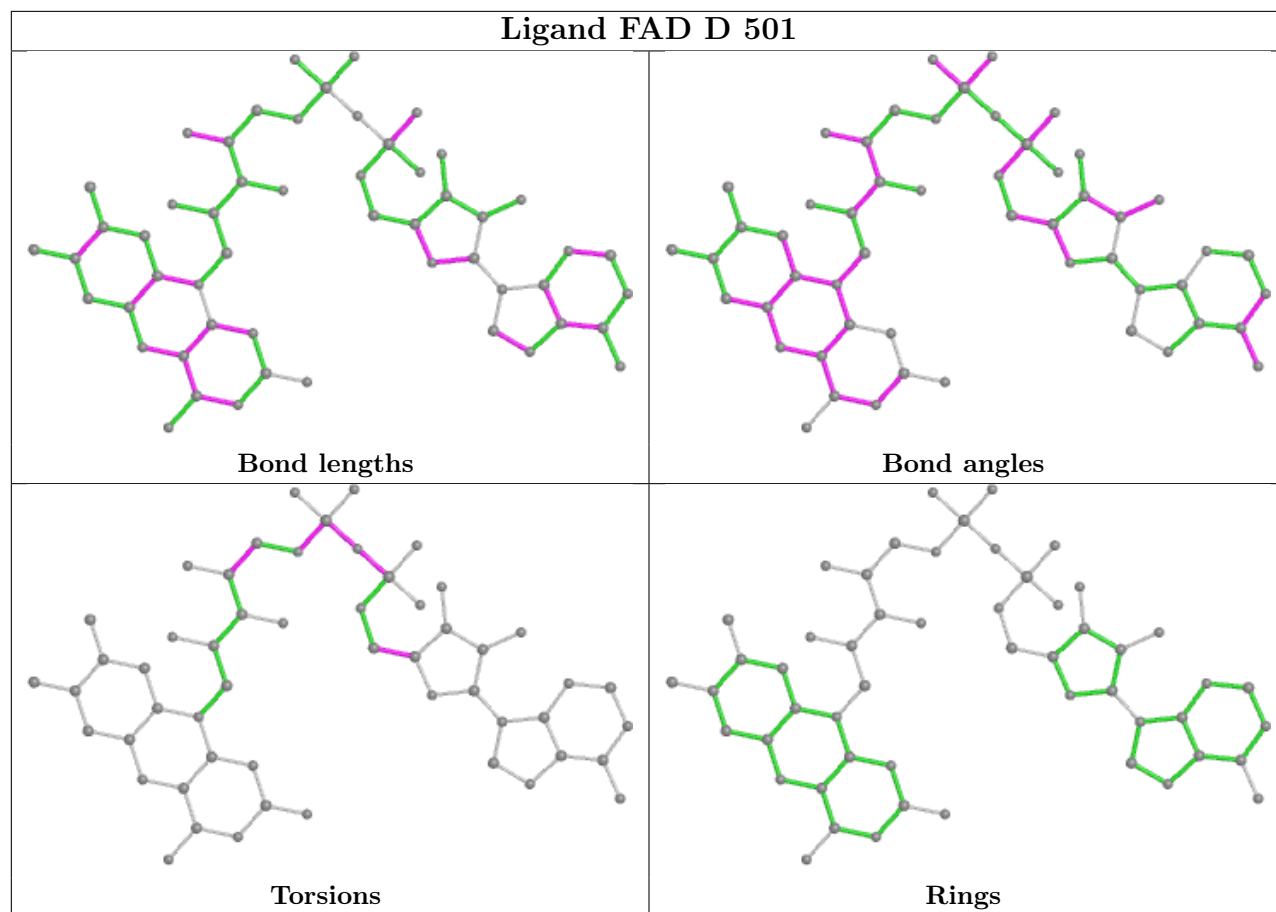


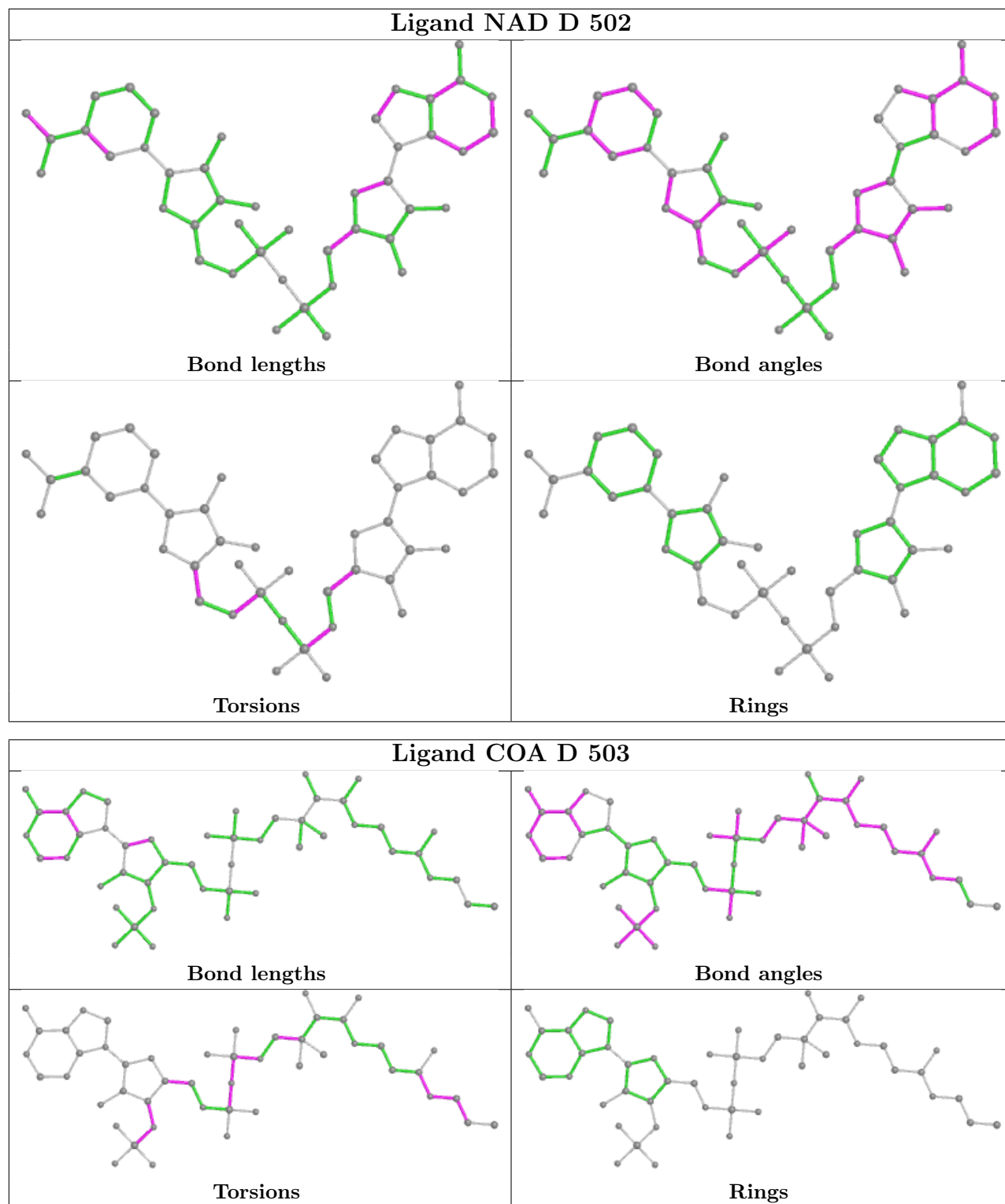












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	443/443 (100%)	-0.21	7 (1%) 72 71	30, 47, 75, 130	0
1	B	443/443 (100%)	-0.06	10 (2%) 60 58	31, 49, 77, 129	0
1	C	443/443 (100%)	-0.16	11 (2%) 57 54	31, 48, 76, 132	0
1	D	443/443 (100%)	-0.18	5 (1%) 80 80	29, 49, 78, 132	0
All	All	1772/1772 (100%)	-0.15	33 (1%) 66 64	29, 48, 77, 132	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	10.5
1	B	443	ARG	8.5
1	B	1	MET	8.5
1	A	1	MET	8.2
1	C	1	MET	7.7
1	C	2	GLY	5.8
1	B	2	GLY	5.7
1	A	86	TYR	5.3
1	C	443	ARG	5.2
1	A	88	LEU	4.9
1	D	2	GLY	4.7
1	A	2	GLY	4.4
1	B	86	TYR	4.2
1	D	443	ARG	4.1
1	A	443	ARG	3.8
1	C	86	TYR	3.4
1	D	352	TRP	3.3
1	C	352	TRP	3.1
1	B	442	ALA	3.1
1	B	88	LEU	3.1
1	B	208	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	88	LEU	2.8
1	C	88	LEU	2.7
1	A	219	MET	2.7
1	A	442	ALA	2.6
1	B	219	MET	2.5
1	B	216	PHE	2.5
1	C	383	THR	2.5
1	B	91	LEU	2.4
1	C	381	GLU	2.3
1	C	87	GLU	2.2
1	C	317	GLU	2.2
1	C	212	LYS	2.1

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, 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.

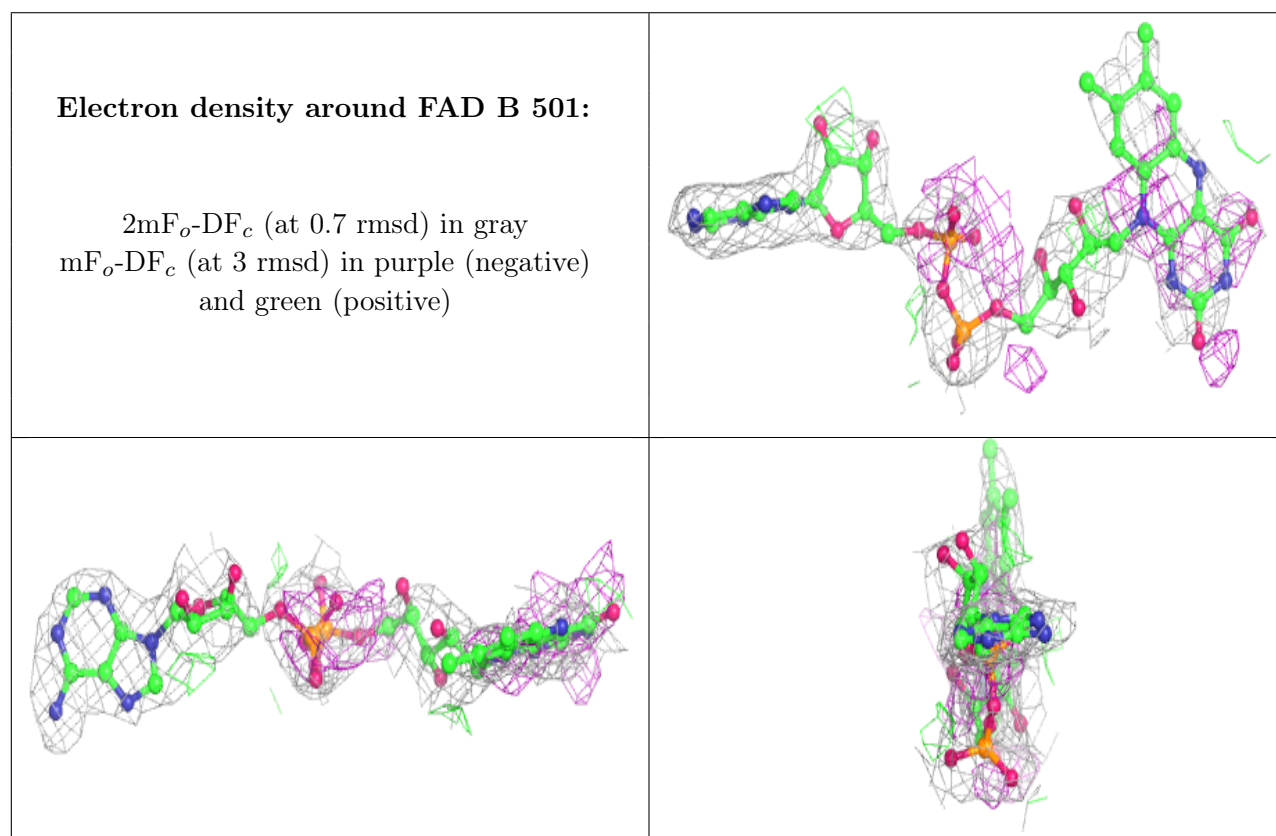
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	501	53/53	0.92	0.26	57,76,96,111	0
2	FAD	D	501	53/53	0.92	0.20	49,74,93,109	0
3	NAD	B	502	44/44	0.93	0.20	43,64,82,87	0
2	FAD	A	501	53/53	0.94	0.24	53,71,92,117	0
3	NAD	D	502	44/44	0.94	0.18	45,62,79,82	0
4	COA	D	503	48/48	0.95	0.17	51,71,81,111	0
4	COA	A	503	48/48	0.95	0.23	54,72,85,110	0
4	COA	C	503	48/48	0.95	0.15	54,71,80,116	0
2	FAD	C	501	53/53	0.95	0.19	51,73,93,97	0
4	COA	B	503	48/48	0.96	0.16	54,70,80,103	0
3	NAD	A	502	44/44	0.96	0.17	39,58,76,83	0

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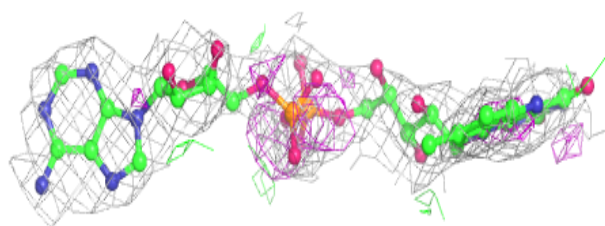
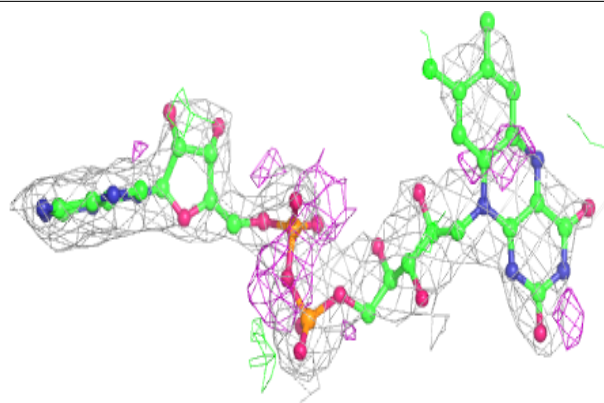
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAD	C	502	44/44	0.96	0.17	39,57,78,82	0

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.

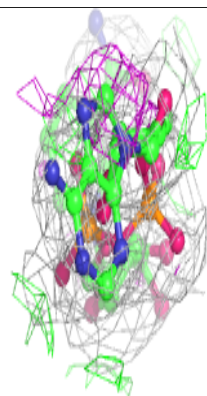
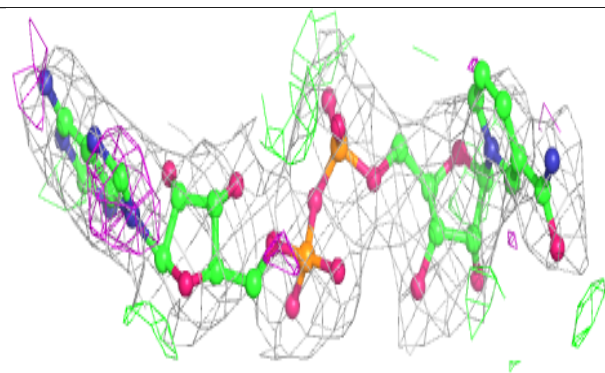
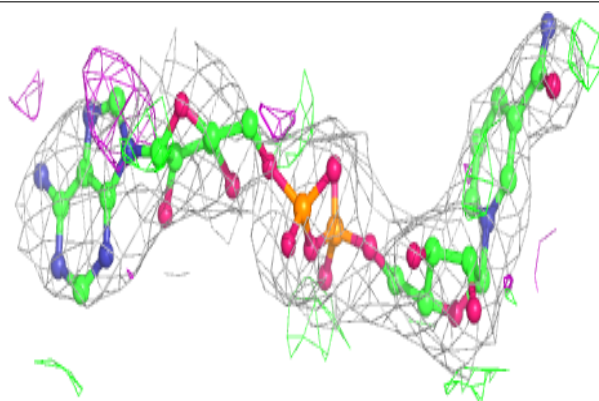


Electron density around FAD D 501:

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

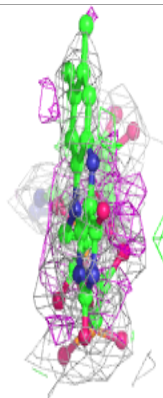
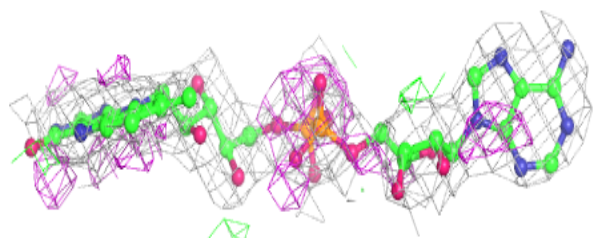
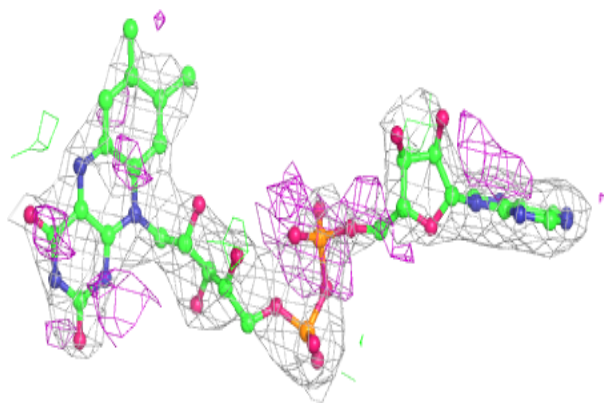
**Electron density around NAD B 502:**

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

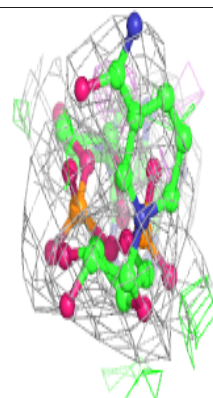
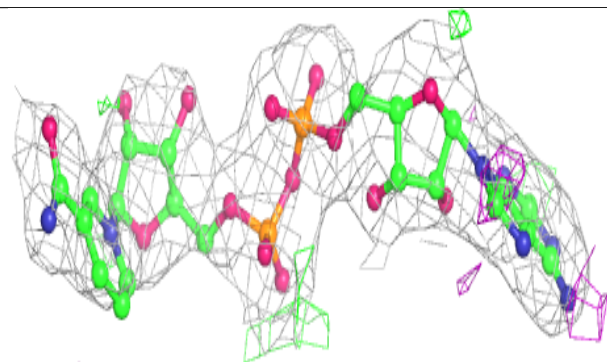
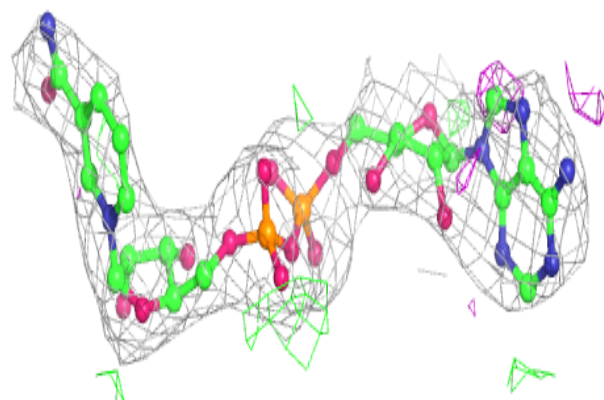


Electron density around FAD A 501:

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

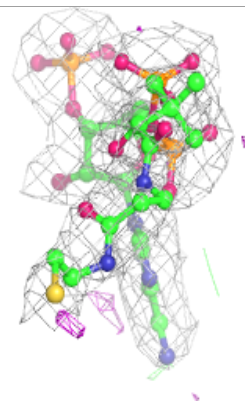
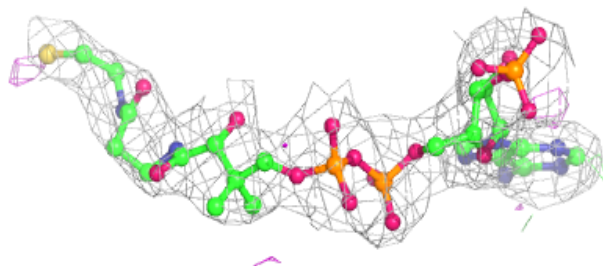
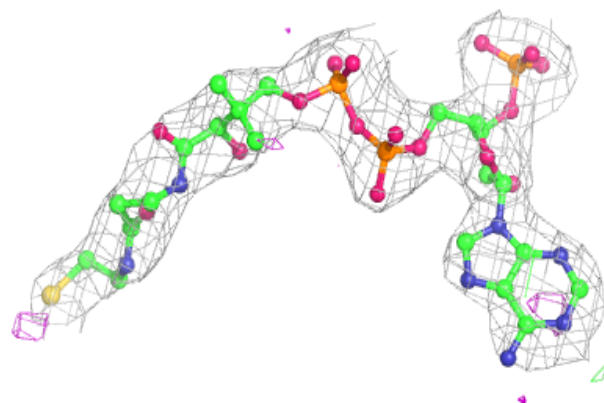
**Electron density around NAD D 502:**

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

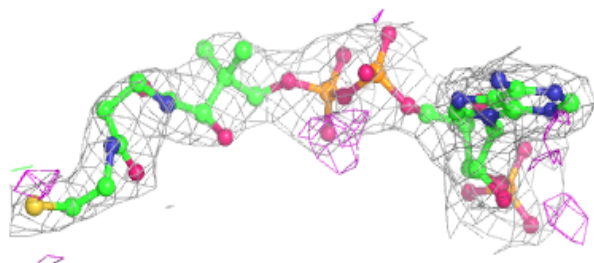
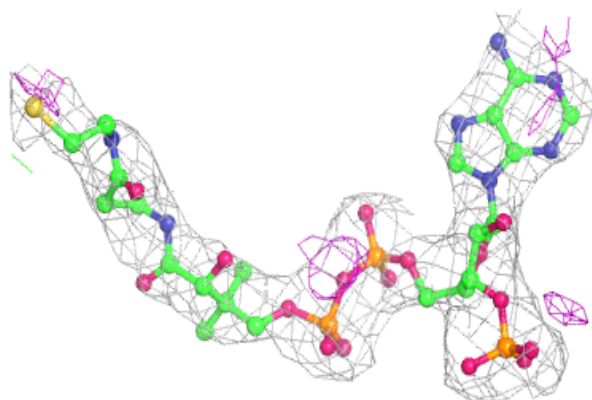


Electron density around COA D 503:

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

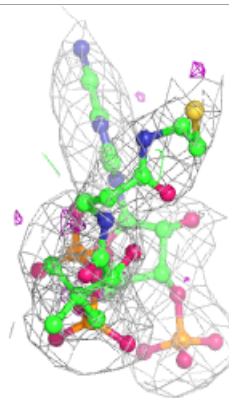
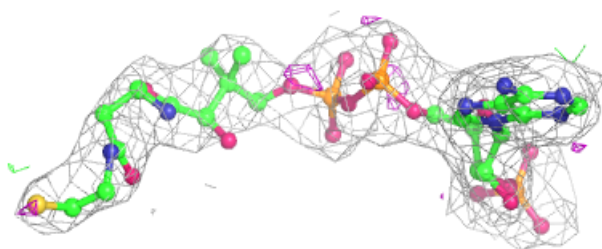
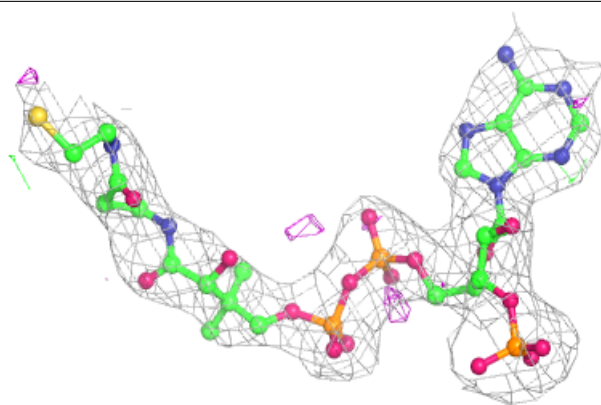
**Electron density around COA A 503:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

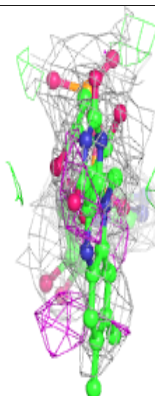
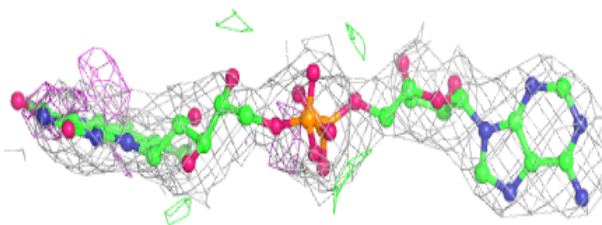
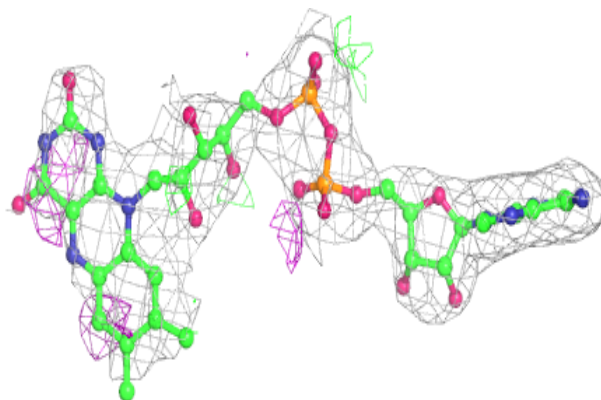


Electron density around COA C 503:

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

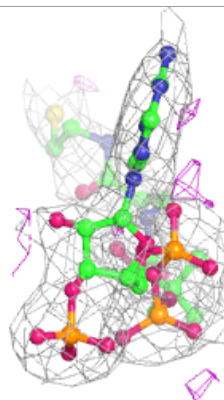
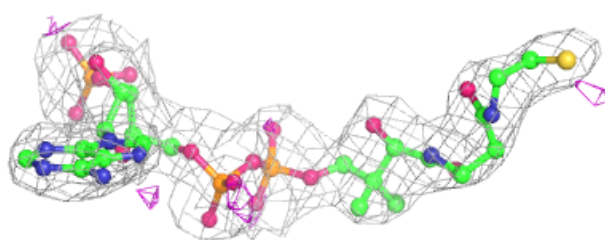
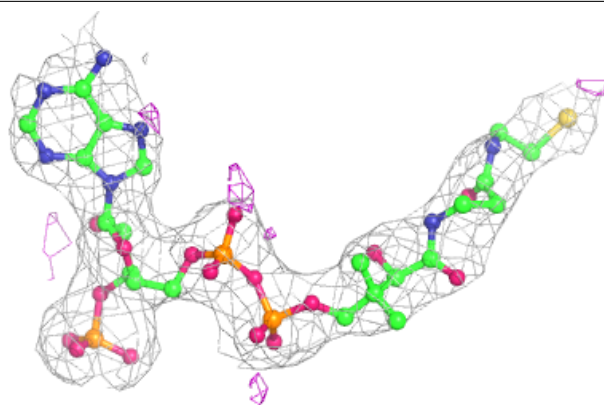
**Electron density around FAD C 501:**

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

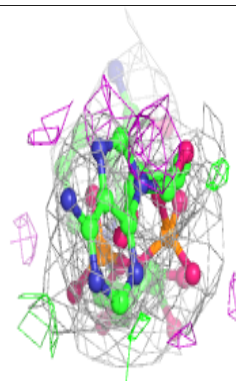
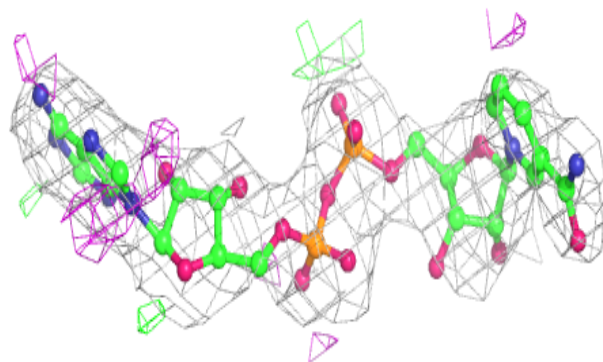
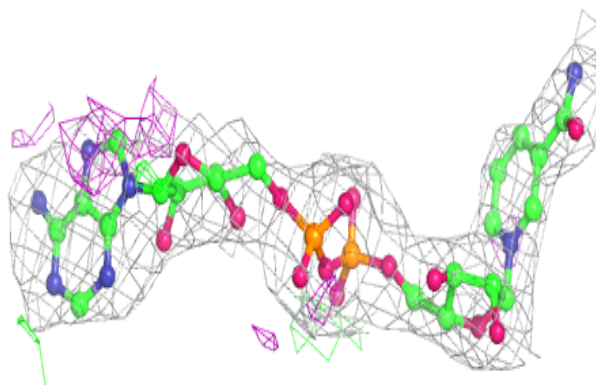


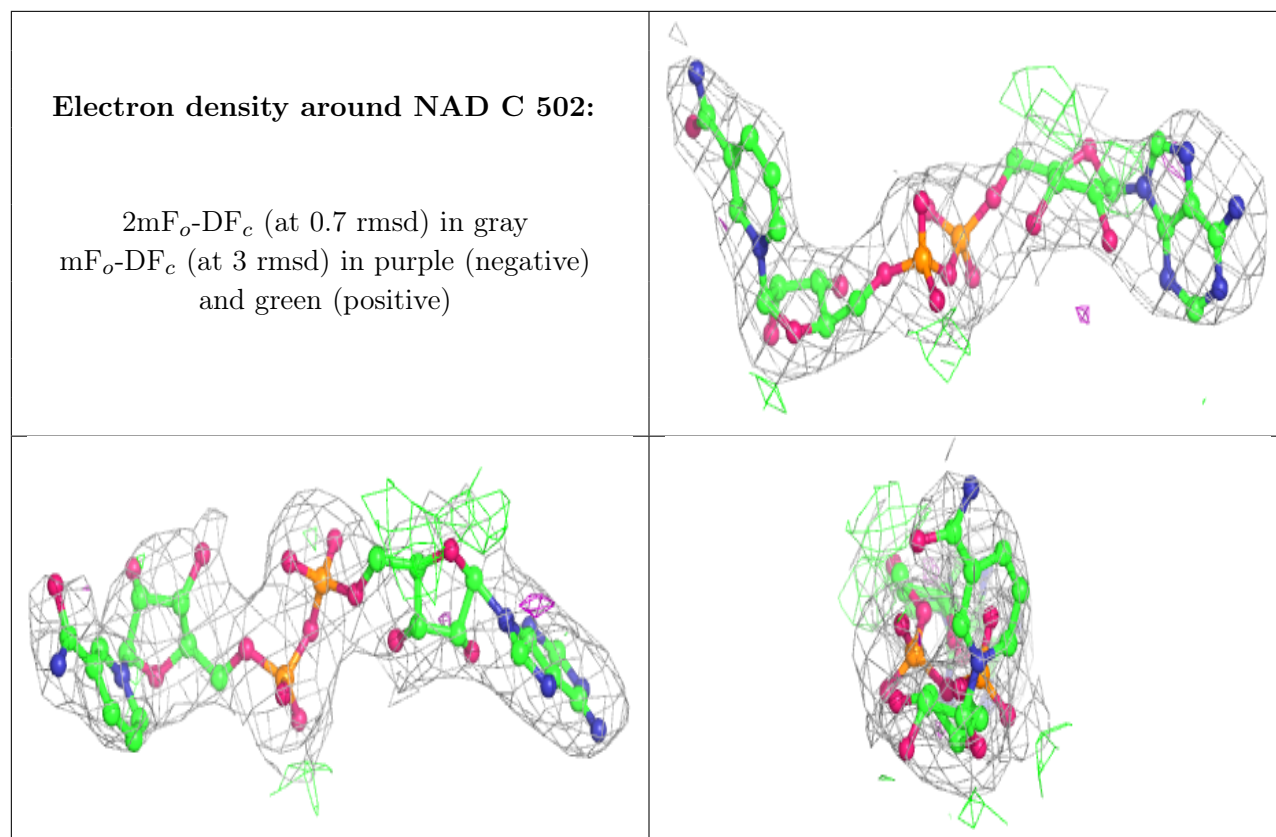
Electron density around COA B 503:

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

**Electron density around NAD A 502:**

$2mF_o-DF_c$ (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.