



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:15 AM UTC

PDB ID : 6RVB / pdb_00006rvb
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

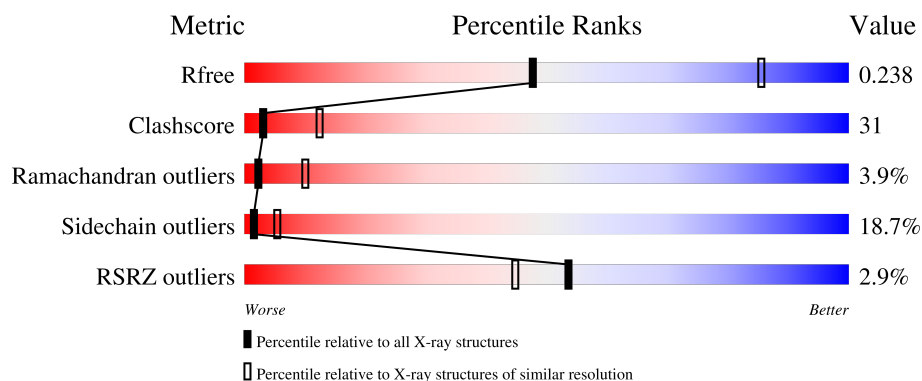
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	443	2% 52% 33% 10% 5%
1	B	443	3% 50% 30% 14% 5%
1	C	443	3% 52% 29% 13% 5%
1	D	443	4% 50% 32% 13% 5%

2 Entry composition ⓘ

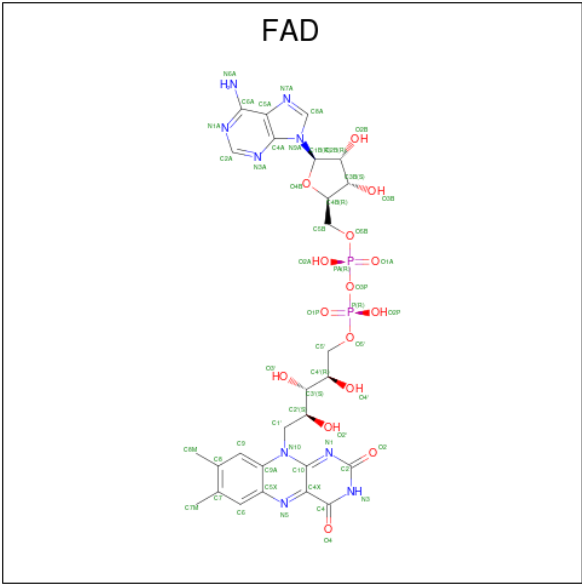
There are 5 unique types of molecules in this entry. The entry contains 14205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH oxidase.

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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



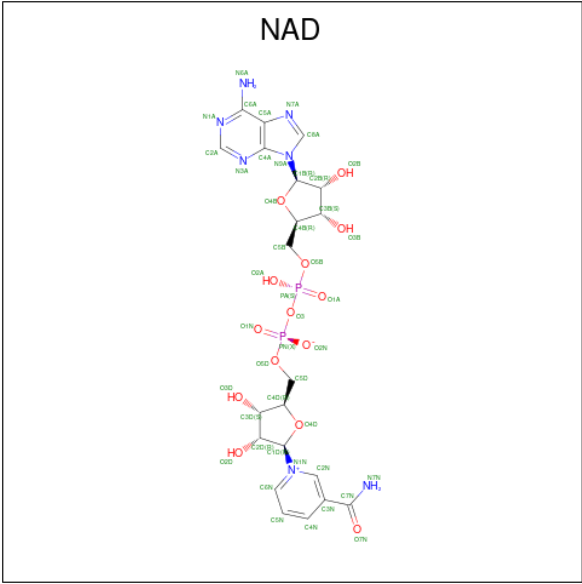
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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 (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

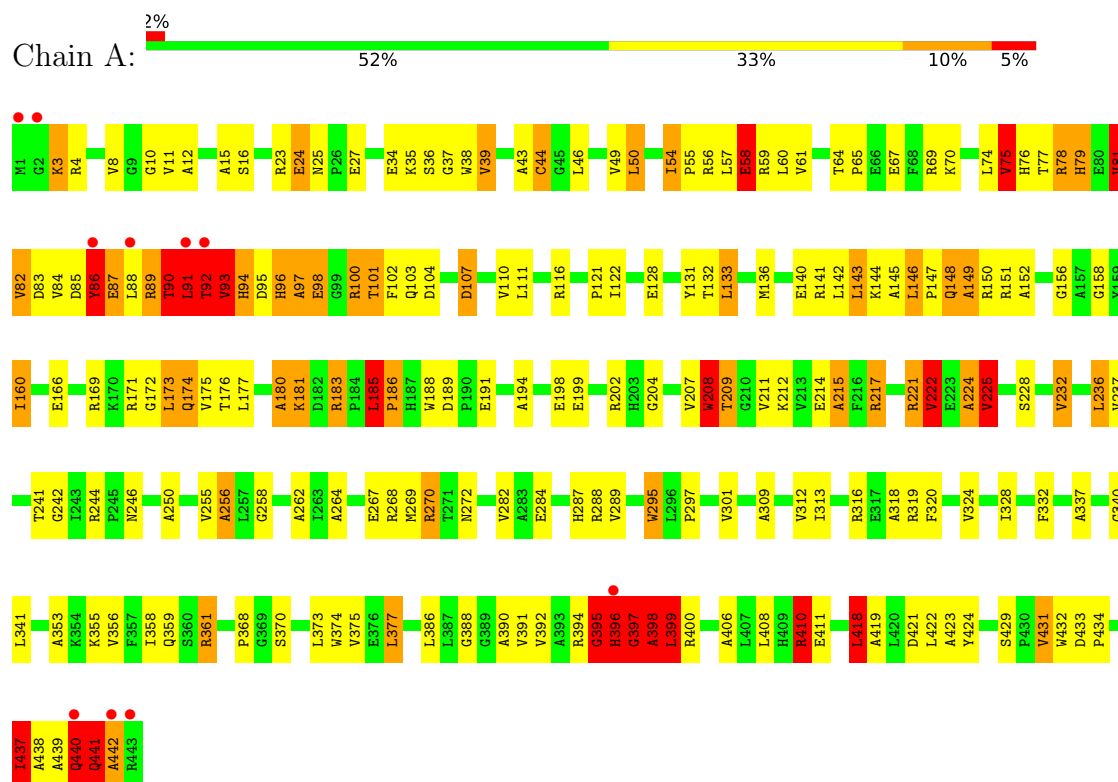
- Molecule 5 is water.

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		

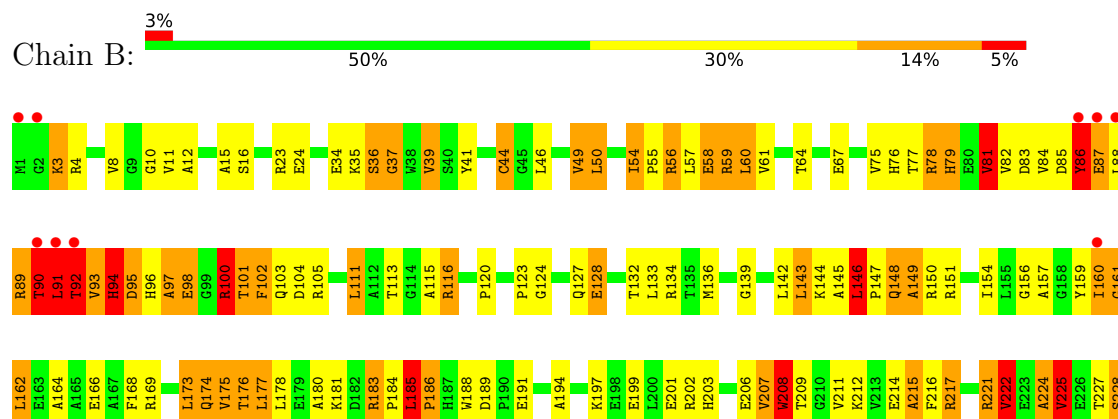
3 Residue-property plots [i](#)

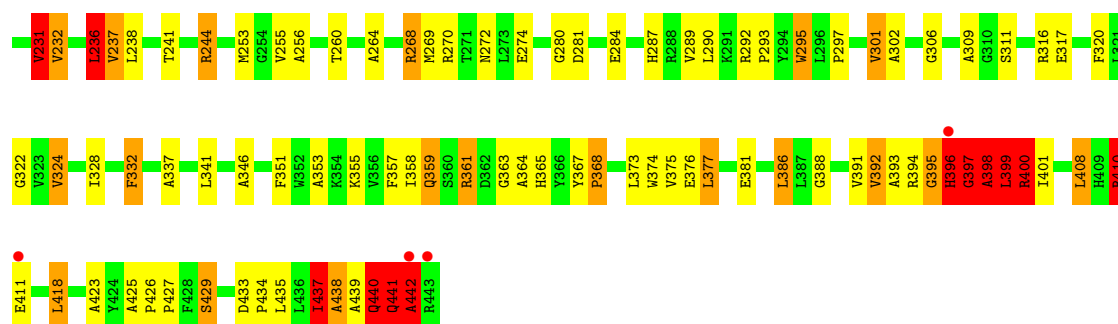
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: NADH oxidase

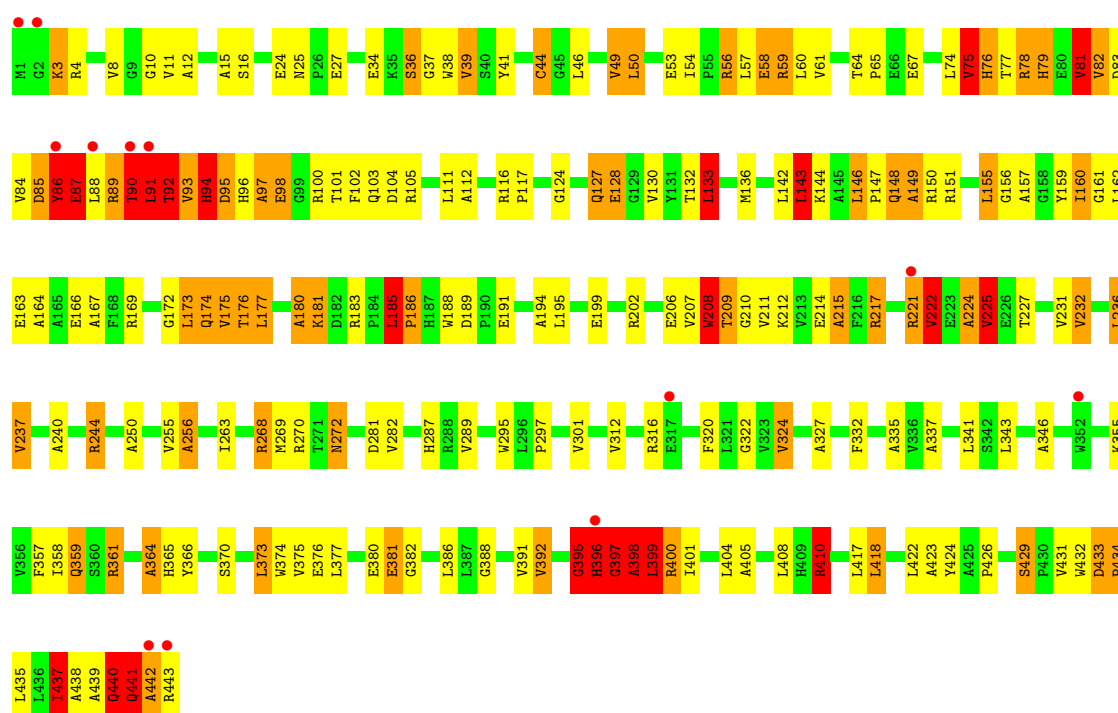


• Molecule 1: NADH oxidase

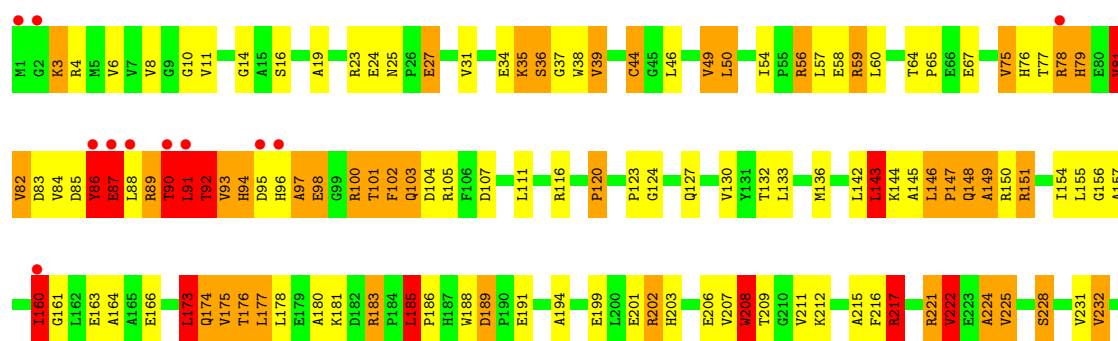


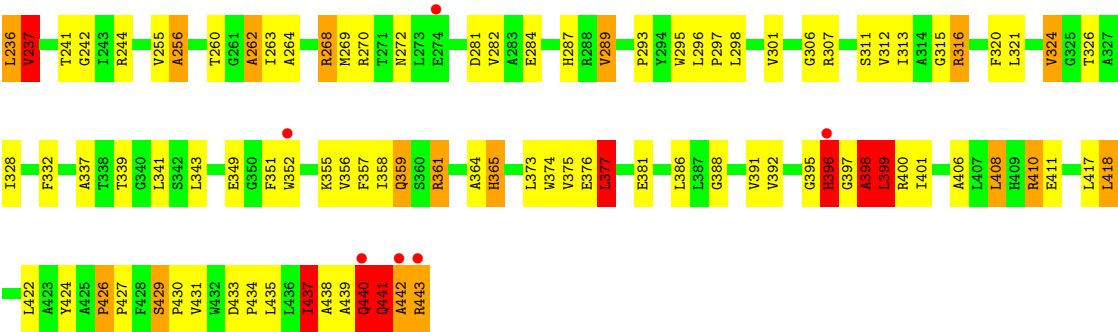


● Molecule 1: NADH oxidase



● 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) 99.9 (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 , 0.238	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 , 58.0	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, NAD, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.90	61/3451 (1.8%)	1.76	91/4686 (1.9%)
1	B	1.78	53/3451 (1.5%)	1.78	78/4686 (1.7%)
1	C	1.82	52/3450 (1.5%)	1.79	78/4683 (1.7%)
1	D	1.78	51/3449 (1.5%)	1.76	88/4683 (1.9%)
All	All	1.82	217/13801 (1.6%)	1.77	335/18738 (1.8%)

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 (217) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	440	GLN	C-O	13.48	1.41	1.24
1	D	396	HIS	C-O	13.17	1.41	1.24
1	B	440	GLN	C-O	12.00	1.39	1.24
1	C	194	ALA	CA-CB	-11.94	1.34	1.53
1	A	396	HIS	C-O	11.86	1.39	1.23
1	C	396	HIS	C-O	11.83	1.39	1.23
1	D	87	GLU	CA-C	11.67	1.67	1.53
1	A	440	GLN	C-O	11.55	1.38	1.24
1	D	440	GLN	C-O	11.12	1.38	1.24
1	B	87	GLU	CA-C	10.85	1.67	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	440	GLN	CD-NE2	10.58	1.55	1.33
1	A	440	GLN	CD-NE2	10.25	1.54	1.33
1	A	437	ILE	CA-CB	10.08	1.68	1.54
1	D	97	ALA	CA-CB	9.92	1.70	1.53
1	D	120	PRO	CA-C	9.86	1.58	1.52
1	A	225	VAL	CA-CB	9.83	1.67	1.54
1	B	194	ALA	CA-CB	-9.77	1.38	1.53
1	A	122	ILE	CA-CB	-9.59	1.47	1.54
1	D	194	ALA	CA-CB	-9.24	1.39	1.53
1	A	399	LEU	N-CA	9.13	1.57	1.46
1	A	87	GLU	CA-C	8.87	1.65	1.53
1	C	87	GLU	CA-C	8.81	1.66	1.53
1	B	438	ALA	CA-CB	-8.70	1.38	1.53
1	D	93	VAL	CA-CB	8.57	1.66	1.53
1	C	225	VAL	CA-CB	8.55	1.66	1.54
1	C	215	ALA	CA-CB	-8.50	1.36	1.53
1	A	97	ALA	N-CA	8.40	1.57	1.46
1	B	396	HIS	C-O	8.39	1.35	1.24
1	A	93	VAL	CA-CB	8.32	1.65	1.54
1	D	396	HIS	N-CA	8.26	1.55	1.46
1	B	440	GLN	CD-NE2	8.24	1.50	1.33
1	C	396	HIS	N-CA	8.23	1.56	1.46
1	A	256	ALA	CA-CB	-8.18	1.40	1.53
1	A	194	ALA	CA-CB	-8.10	1.40	1.53
1	B	437	ILE	CA-CB	8.05	1.64	1.54
1	C	160	ILE	CG1-CD1	8.04	1.83	1.51
1	D	324	VAL	CA-CB	-7.99	1.45	1.54
1	B	183	ARG	CA-C	-7.93	1.44	1.52
1	C	240	ALA	CA-CB	-7.93	1.38	1.53
1	C	97	ALA	CA-CB	7.93	1.66	1.53
1	D	398	ALA	CA-C	7.91	1.63	1.52
1	B	423	ALA	CA-CB	-7.91	1.42	1.53
1	A	396	HIS	N-CA	7.81	1.55	1.46
1	A	264	ALA	CA-CB	-7.70	1.41	1.53
1	A	225	VAL	N-CA	7.62	1.55	1.46
1	A	98	GLU	N-CA	7.61	1.56	1.46
1	C	423	ALA	CA-CB	-7.54	1.41	1.53
1	A	398	ALA	N-CA	7.54	1.55	1.46
1	C	441	GLN	CG-CD	7.51	1.70	1.52
1	D	316	ARG	C-O	-7.47	1.14	1.23
1	C	85	ASP	C-O	-7.46	1.13	1.23
1	B	97	ALA	N-CA	7.41	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	440	GLN	CD-NE2	7.41	1.48	1.33
1	D	97	ALA	N-CA	7.36	1.55	1.46
1	C	97	ALA	N-CA	7.35	1.55	1.46
1	B	160	ILE	CG1-CD1	7.31	1.80	1.51
1	C	224	ALA	CA-CB	-7.29	1.41	1.53
1	B	264	ALA	CA-CB	-7.23	1.42	1.53
1	D	398	ALA	N-CA	7.17	1.55	1.46
1	A	440	GLN	CA-CB	7.15	1.65	1.53
1	D	232	VAL	C-O	-7.14	1.15	1.24
1	A	398	ALA	CA-CB	-7.13	1.41	1.53
1	C	93	VAL	CA-C	7.13	1.62	1.52
1	D	19	ALA	CA-CB	-7.11	1.42	1.53
1	D	96	HIS	CA-C	7.05	1.60	1.52
1	C	324	VAL	CA-CB	-6.98	1.46	1.54
1	D	145	ALA	CA-CB	-6.98	1.42	1.53
1	D	441	GLN	CG-CD	6.96	1.69	1.52
1	A	92	THR	CA-CB	-6.94	1.41	1.53
1	A	441	GLN	CG-CD	6.92	1.69	1.52
1	A	406	ALA	CA-CB	-6.85	1.42	1.53
1	B	324	VAL	N-CA	-6.82	1.40	1.46
1	B	441	GLN	CG-CD	6.79	1.69	1.52
1	A	312	VAL	C-O	-6.79	1.16	1.24
1	C	256	ALA	CA-CB	-6.78	1.43	1.53
1	A	98	GLU	CG-CD	6.77	1.69	1.52
1	D	440	GLN	CD-OE1	6.76	1.36	1.23
1	D	364	ALA	CA-CB	-6.75	1.42	1.53
1	A	93	VAL	CA-C	6.71	1.61	1.52
1	C	324	VAL	CA-C	6.68	1.60	1.52
1	A	180	ALA	C-O	-6.67	1.16	1.24
1	C	112	ALA	CA-CB	-6.67	1.44	1.53
1	A	313	ILE	CA-CB	6.63	1.61	1.54
1	A	160	ILE	CG1-CD1	6.60	1.77	1.51
1	C	244	ARG	CA-C	6.58	1.58	1.52
1	B	207	VAL	CA-CB	6.58	1.62	1.53
1	C	398	ALA	CA-CB	-6.57	1.42	1.53
1	A	224	ALA	CA-CB	-6.56	1.42	1.53
1	C	93	VAL	CA-CB	6.55	1.62	1.54
1	A	262	ALA	CA-CB	-6.54	1.42	1.53
1	B	442	ALA	CA-CB	-6.51	1.42	1.53
1	D	160	ILE	CG1-CD1	6.50	1.77	1.51
1	A	202	ARG	C-O	-6.48	1.15	1.24
1	B	225	VAL	CA-CB	6.44	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	VAL	N-CA	6.42	1.54	1.46
1	B	396	HIS	N-CA	6.42	1.53	1.46
1	B	398	ALA	N-CA	6.42	1.54	1.46
1	B	302	ALA	CA-CB	-6.40	1.43	1.53
1	B	381	GLU	C-O	-6.38	1.16	1.24
1	B	317	GLU	C-O	-6.37	1.16	1.24
1	D	232	VAL	CA-CB	-6.33	1.47	1.53
1	B	222	VAL	CA-CB	6.28	1.62	1.54
1	D	228	SER	CA-C	6.28	1.61	1.52
1	B	425	ALA	CA-CB	-6.27	1.44	1.54
1	A	146	LEU	N-CA	-6.26	1.40	1.46
1	D	437	ILE	CA-CB	6.23	1.61	1.54
1	B	353	ALA	C-O	-6.21	1.16	1.23
1	C	167	ALA	CA-C	-6.18	1.45	1.52
1	C	398	ALA	N-CA	6.16	1.54	1.46
1	A	309	ALA	CA-CB	-6.14	1.43	1.53
1	B	93	VAL	CA-CB	6.11	1.62	1.54
1	C	85	ASP	CA-C	-6.11	1.46	1.53
1	D	81	VAL	CA-CB	6.10	1.61	1.54
1	A	423	ALA	CA-CB	-6.09	1.44	1.53
1	C	98	GLU	N-CA	6.08	1.54	1.46
1	D	203	HIS	CA-C	-6.08	1.44	1.52
1	C	180	ALA	CA-CB	-6.07	1.43	1.53
1	D	93	VAL	CA-C	6.06	1.59	1.52
1	B	393	ALA	CA-CB	-6.05	1.43	1.53
1	A	75	VAL	C-O	-6.03	1.17	1.24
1	D	381	GLU	C-O	6.02	1.31	1.24
1	B	398	ALA	CA-C	5.99	1.60	1.52
1	C	155	LEU	C-O	-5.99	1.16	1.24
1	D	82	VAL	CA-CB	-5.98	1.46	1.54
1	B	87	GLU	C-O	5.96	1.30	1.23
1	D	237	VAL	CA-CB	5.94	1.61	1.54
1	B	244	ARG	CA-C	5.93	1.58	1.52
1	C	440	GLN	CA-CB	5.91	1.63	1.53
1	D	440	GLN	CA-CB	5.88	1.63	1.53
1	B	60	LEU	CA-C	5.87	1.60	1.52
1	A	86	TYR	CB-CG	5.86	1.64	1.51
1	A	180	ALA	CA-CB	-5.86	1.43	1.53
1	D	256	ALA	CA-CB	-5.86	1.43	1.53
1	D	154	ILE	CA-CB	-5.83	1.47	1.54
1	C	337	ALA	CA-CB	-5.82	1.43	1.53
1	C	335	ALA	CA-CB	-5.81	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	ALA	CA-CB	5.79	1.63	1.53
1	B	92	THR	CA-CB	-5.79	1.43	1.53
1	A	295	TRP	C-O	-5.78	1.17	1.24
1	C	373	LEU	C-O	-5.78	1.17	1.23
1	B	368	PRO	CA-C	-5.77	1.47	1.52
1	C	91	LEU	C-O	5.75	1.31	1.24
1	A	198	GLU	C-O	-5.73	1.17	1.24
1	D	242	GLY	C-O	5.72	1.29	1.23
1	D	224	ALA	CA-CB	-5.71	1.43	1.53
1	A	399	LEU	CA-CB	5.71	1.63	1.53
1	C	250	ALA	CA-CB	-5.71	1.44	1.53
1	D	377	LEU	CA-C	5.70	1.59	1.52
1	C	15	ALA	C-O	-5.66	1.17	1.24
1	B	309	ALA	CA-CB	-5.62	1.44	1.53
1	C	117	PRO	C-O	-5.61	1.17	1.23
1	B	301	VAL	CB-CG1	-5.59	1.34	1.52
1	C	232	VAL	C-O	-5.57	1.17	1.24
1	D	163	GLU	CA-C	-5.56	1.45	1.52
1	A	353	ALA	C-O	-5.55	1.17	1.23
1	B	95	ASP	CA-C	5.55	1.59	1.52
1	C	327	ALA	CA-CB	-5.55	1.44	1.53
1	A	58	GLU	C-O	-5.54	1.16	1.24
1	C	86	TYR	CB-CG	5.54	1.63	1.51
1	C	405	ALA	CA-C	5.52	1.59	1.52
1	D	293	PRO	C-O	5.51	1.30	1.23
1	D	103	GLN	C-O	5.47	1.30	1.23
1	A	145	ALA	CA-CB	-5.47	1.44	1.53
1	A	250	ALA	CA-CB	-5.47	1.44	1.53
1	B	438	ALA	C-O	-5.45	1.17	1.24
1	D	406	ALA	CA-CB	-5.45	1.44	1.53
1	D	396	HIS	C-N	5.44	1.41	1.33
1	B	351	PHE	CA-C	-5.43	1.45	1.52
1	A	185	LEU	C-O	-5.43	1.21	1.23
1	A	421	ASP	CA-C	5.42	1.59	1.53
1	C	81	VAL	CA-CB	5.39	1.59	1.53
1	A	397	GLY	CA-C	5.37	1.59	1.51
1	C	441	GLN	CA-C	5.36	1.59	1.52
1	A	81	VAL	CA-CB	5.35	1.60	1.53
1	A	215	ALA	CA-CB	-5.34	1.44	1.53
1	B	346	ALA	C-O	-5.31	1.17	1.24
1	D	326	THR	CA-CB	-5.30	1.44	1.53
1	D	441	GLN	C-O	5.30	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	ALA	CA-CB	-5.29	1.44	1.53
1	D	441	GLN	CA-C	5.29	1.59	1.52
1	B	98	GLU	N-CA	5.28	1.53	1.46
1	B	295	TRP	C-O	-5.28	1.18	1.24
1	A	313	ILE	C-O	-5.28	1.18	1.24
1	C	364	ALA	CA-CB	-5.28	1.44	1.53
1	A	241	THR	CA-CB	5.26	1.60	1.53
1	C	96	HIS	CA-C	5.26	1.58	1.52
1	B	236	LEU	C-O	5.25	1.30	1.23
1	A	185	LEU	CA-C	-5.21	1.50	1.53
1	C	53	GLU	CA-C	5.20	1.59	1.52
1	A	431	VAL	CA-C	5.20	1.59	1.52
1	B	238	LEU	C-O	5.18	1.30	1.24
1	C	98	GLU	CA-C	5.18	1.59	1.52
1	A	96	HIS	CA-C	5.17	1.58	1.52
1	D	262	ALA	CA-CB	-5.17	1.44	1.53
1	A	43	ALA	CA-CB	-5.16	1.44	1.53
1	D	175	VAL	C-O	5.16	1.29	1.24
1	C	94	HIS	CA-C	-5.16	1.46	1.52
1	D	202	ARG	C-O	-5.16	1.17	1.24
1	B	399	LEU	N-CA	5.15	1.56	1.46
1	B	228	SER	CA-C	5.14	1.59	1.52
1	B	332	PHE	C-O	-5.13	1.20	1.24
1	B	392	VAL	CA-C	-5.13	1.46	1.52
1	D	264	ALA	CA-CB	-5.10	1.45	1.53
1	A	318	ALA	CA-CB	-5.10	1.45	1.53
1	B	86	TYR	CB-CG	5.10	1.62	1.51
1	A	181	LYS	C-O	-5.09	1.18	1.23
1	B	410	ARG	NE-CZ	5.09	1.38	1.33
1	B	324	VAL	C-O	-5.08	1.18	1.24
1	D	441	GLN	CA-CB	5.08	1.62	1.53
1	A	87	GLU	C-O	5.07	1.29	1.23
1	C	364	ALA	C-O	-5.06	1.17	1.24
1	C	95	ASP	CA-C	5.05	1.59	1.53
1	B	215	ALA	CA-CB	-5.04	1.43	1.53
1	D	14	GLY	C-O	-5.04	1.17	1.23
1	B	208	TRP	CG-CD1	5.04	1.49	1.36
1	A	270	ARG	CB-CG	5.02	1.67	1.52
1	B	162	LEU	C-O	-5.00	1.18	1.24

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396	HIS	O-C-N	14.32	140.67	122.19
1	A	185	LEU	CA-C-N	13.07	132.89	119.56
1	A	185	LEU	C-N-CA	13.07	132.89	119.56
1	B	397	GLY	N-CA-C	12.25	148.83	113.30
1	B	185	LEU	CA-C-N	11.93	132.40	119.28
1	B	185	LEU	C-N-CA	11.93	132.40	119.28
1	C	396	HIS	O-C-N	11.14	137.01	121.97
1	A	396	HIS	O-C-N	11.02	136.30	122.20
1	D	396	HIS	CA-C-N	10.50	142.00	121.41
1	D	396	HIS	C-N-CA	10.50	142.00	121.41
1	C	185	LEU	CA-C-N	10.41	130.74	119.28
1	C	185	LEU	C-N-CA	10.41	130.74	119.28
1	B	189	ASP	CA-C-N	-9.62	107.81	119.84
1	B	189	ASP	C-N-CA	-9.62	107.81	119.84
1	A	46	LEU	CA-C-N	-9.56	109.91	119.56
1	A	46	LEU	C-N-CA	-9.56	109.91	119.56
1	A	437	ILE	N-CA-C	-9.38	100.78	111.00
1	C	46	LEU	CA-C-N	-9.28	110.19	119.56
1	C	46	LEU	C-N-CA	-9.28	110.19	119.56
1	D	185	LEU	CA-C-N	9.12	128.86	119.56
1	D	185	LEU	C-N-CA	9.12	128.86	119.56
1	C	232	VAL	CA-C-N	-9.11	110.48	120.14
1	C	232	VAL	C-N-CA	-9.11	110.48	120.14
1	D	54	ILE	CA-C-N	9.08	131.19	119.84
1	D	54	ILE	C-N-CA	9.08	131.19	119.84
1	C	396	HIS	CA-C-N	9.03	139.12	121.41
1	C	396	HIS	C-N-CA	9.03	139.12	121.41
1	D	46	LEU	CA-C-N	-8.98	110.40	119.56
1	D	46	LEU	C-N-CA	-8.98	110.40	119.56
1	C	54	ILE	CA-C-N	8.94	131.01	119.84
1	C	54	ILE	C-N-CA	8.94	131.01	119.84
1	D	232	VAL	CA-C-N	-8.92	110.36	119.99
1	D	232	VAL	C-N-CA	-8.92	110.36	119.99
1	B	79	HIS	CA-C-N	-8.83	110.68	123.05
1	B	79	HIS	C-N-CA	-8.83	110.68	123.05
1	D	160	ILE	CA-C-N	-8.83	104.10	121.41
1	D	160	ILE	C-N-CA	-8.83	104.10	121.41
1	C	324	VAL	N-CA-CB	-8.70	101.98	112.33
1	A	54	ILE	CA-C-N	8.68	130.69	119.84
1	A	54	ILE	C-N-CA	8.68	130.69	119.84
1	B	160	ILE	CA-C-N	-8.64	104.47	121.41
1	B	160	ILE	C-N-CA	-8.64	104.47	121.41
1	B	35	LYS	N-CA-C	8.62	121.82	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	GLU	N-CA-C	-8.58	102.95	113.50
1	C	440	GLN	O-C-N	8.44	133.82	122.59
1	C	146	LEU	CA-C-N	-8.37	111.39	119.76
1	C	146	LEU	C-N-CA	-8.37	111.39	119.76
1	A	440	GLN	O-C-N	8.33	133.67	122.59
1	A	232	VAL	CA-C-N	-8.28	111.04	119.99
1	A	232	VAL	C-N-CA	-8.28	111.04	119.99
1	C	160	ILE	CA-C-N	-8.24	105.26	121.41
1	C	160	ILE	C-N-CA	-8.24	105.26	121.41
1	A	396	HIS	CA-C-N	8.09	137.27	121.41
1	A	396	HIS	C-N-CA	8.09	137.27	121.41
1	C	82	VAL	CB-CA-C	-8.03	100.33	111.65
1	D	206	GLU	CA-C-N	-7.99	112.25	123.11
1	D	206	GLU	C-N-CA	-7.99	112.25	123.11
1	B	90	THR	CA-C-N	7.98	136.07	121.70
1	B	90	THR	C-N-CA	7.98	136.07	121.70
1	B	363	GLY	N-CA-C	-7.97	99.20	111.00
1	B	274	GLU	N-CA-C	-7.97	98.49	110.28
1	D	437	ILE	N-CA-C	-7.96	103.05	110.53
1	C	206	GLU	CA-C-N	-7.92	112.83	123.12
1	C	206	GLU	C-N-CA	-7.92	112.83	123.12
1	D	160	ILE	N-CA-C	-7.89	99.41	109.58
1	C	10	GLY	CA-C-N	-7.78	110.14	121.65
1	C	10	GLY	C-N-CA	-7.78	110.14	121.65
1	A	422	LEU	N-CA-C	7.77	120.79	110.53
1	D	49	VAL	N-CA-C	-7.73	104.33	111.67
1	C	79	HIS	CA-C-N	-7.71	112.25	123.05
1	C	79	HIS	C-N-CA	-7.71	112.25	123.05
1	B	102	PHE	N-CA-C	7.67	119.81	108.14
1	A	160	ILE	CA-C-N	-7.64	106.43	121.41
1	A	160	ILE	C-N-CA	-7.64	106.43	121.41
1	D	440	GLN	O-C-N	7.62	132.73	122.59
1	D	87	GLU	N-CA-C	7.62	121.45	107.73
1	B	128	GLU	N-CA-C	7.55	120.98	111.69
1	C	208	TRP	CA-CB-CG	7.53	127.92	113.60
1	C	102	PHE	N-CA-C	7.41	119.39	108.14
1	C	395	GLY	CA-C-N	7.37	134.16	123.17
1	C	395	GLY	C-N-CA	7.37	134.16	123.17
1	B	224	ALA	N-CA-C	7.35	126.45	110.80
1	B	160	ILE	N-CA-C	-7.31	100.16	109.30
1	C	397	GLY	N-CA-C	7.27	130.42	113.18
1	B	54	ILE	CA-C-N	7.20	128.84	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ILE	C-N-CA	7.20	128.84	119.84
1	D	397	GLY	N-CA-C	7.19	130.22	113.18
1	A	399	LEU	N-CA-CB	7.17	122.61	110.49
1	D	395	GLY	CA-C-N	7.17	133.87	122.83
1	D	395	GLY	C-N-CA	7.17	133.87	122.83
1	A	183	ARG	CA-C-N	-7.14	112.96	120.03
1	A	183	ARG	C-N-CA	-7.14	112.96	120.03
1	B	324	VAL	N-CA-CB	-7.14	103.83	112.33
1	C	92	THR	CA-C-N	-7.10	110.32	120.69
1	C	92	THR	C-N-CA	-7.10	110.32	120.69
1	C	36	SER	CA-C-N	-7.10	107.50	121.41
1	C	36	SER	C-N-CA	-7.10	107.50	121.41
1	D	96	HIS	N-CA-CB	-7.10	99.58	110.65
1	D	36	SER	CA-C-N	-7.06	107.58	121.41
1	D	36	SER	C-N-CA	-7.06	107.58	121.41
1	A	395	GLY	CA-C-N	7.00	133.57	122.86
1	A	395	GLY	C-N-CA	7.00	133.57	122.86
1	A	102	PHE	N-CA-C	6.99	118.76	108.14
1	A	145	ALA	N-CA-C	6.90	118.80	111.28
1	D	437	ILE	CB-CA-C	6.90	121.06	112.02
1	D	437	ILE	N-CA-CB	6.89	119.39	110.57
1	B	440	GLN	O-C-N	6.89	131.75	122.59
1	C	96	HIS	N-CA-CB	-6.84	99.99	110.65
1	A	390	ALA	CA-C-N	-6.81	113.48	122.94
1	A	390	ALA	C-N-CA	-6.81	113.48	122.94
1	B	87	GLU	N-CA-C	6.79	121.13	107.41
1	D	351	PHE	CA-C-N	-6.78	110.40	122.32
1	D	351	PHE	C-N-CA	-6.78	110.40	122.32
1	D	189	ASP	CA-C-N	-6.75	113.25	120.47
1	D	189	ASP	C-N-CA	-6.75	113.25	120.47
1	B	231	VAL	CA-C-N	-6.75	117.73	122.59
1	B	231	VAL	C-N-CA	-6.75	117.73	122.59
1	C	160	ILE	N-CA-C	-6.72	100.90	109.30
1	A	10	GLY	CA-C-N	-6.67	111.77	121.65
1	A	10	GLY	C-N-CA	-6.67	111.77	121.65
1	B	324	VAL	CB-CA-C	6.65	117.80	110.62
1	A	90	THR	CA-C-N	6.62	133.61	121.70
1	A	90	THR	C-N-CA	6.62	133.61	121.70
1	B	232	VAL	CA-C-N	-6.59	112.87	119.99
1	B	232	VAL	C-N-CA	-6.59	112.87	119.99
1	A	160	ILE	O-C-N	-6.59	115.43	122.61
1	D	90	THR	CA-C-N	6.58	133.54	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	THR	C-N-CA	6.58	133.54	121.70
1	D	208	TRP	CA-CB-CG	6.57	126.09	113.60
1	D	224	ALA	N-CA-C	6.57	124.80	110.80
1	B	437	ILE	N-CA-CB	6.51	118.90	110.57
1	A	208	TRP	CA-CB-CG	6.50	125.96	113.60
1	C	49	VAL	N-CA-C	-6.49	106.23	111.81
1	A	225	VAL	N-CA-CB	6.49	121.94	111.23
1	B	185	LEU	O-C-N	6.48	124.51	121.53
1	A	224	ALA	N-CA-C	6.47	124.59	110.80
1	D	79	HIS	CA-C-N	-6.46	114.08	123.00
1	D	79	HIS	C-N-CA	-6.46	114.08	123.00
1	A	172	GLY	N-CA-C	6.45	123.92	115.40
1	B	46	LEU	CA-C-N	-6.45	113.05	119.56
1	B	46	LEU	C-N-CA	-6.45	113.05	119.56
1	A	96	HIS	CA-C-O	-6.44	113.41	120.24
1	D	160	ILE	O-C-N	-6.43	115.61	122.61
1	A	79	HIS	CA-C-N	-6.42	114.06	123.05
1	A	79	HIS	C-N-CA	-6.42	114.06	123.05
1	B	208	TRP	CA-CB-CG	6.40	125.75	113.60
1	D	232	VAL	N-CA-C	6.39	113.38	107.56
1	C	437	ILE	N-CA-C	-6.38	104.28	110.72
1	B	400	ARG	N-CA-C	-6.32	105.28	112.87
1	C	366	TYR	N-CA-C	6.31	120.44	112.87
1	D	201	GLU	N-CA-C	-6.31	103.71	111.40
1	A	437	ILE	N-CA-CB	6.29	121.06	110.56
1	C	437	ILE	N-CA-CB	6.27	119.99	110.58
1	C	322	GLY	N-CA-C	6.26	118.41	112.08
1	B	93	VAL	CB-CA-C	6.25	121.53	111.29
1	B	94	HIS	N-CA-C	-6.23	98.37	108.52
1	A	440	GLN	CA-C-N	6.22	133.42	121.54
1	A	440	GLN	C-N-CA	6.22	133.42	121.54
1	C	87	GLU	N-CA-C	6.22	119.53	107.71
1	A	441	GLN	CB-CG-CD	6.21	123.16	112.60
1	C	98	GLU	CA-CB-CG	-6.21	101.67	114.10
1	B	396	HIS	O-C-N	6.21	129.90	122.26
1	D	422	LEU	N-CA-C	6.20	118.04	110.41
1	B	206	GLU	CA-C-N	-6.19	114.83	123.13
1	B	206	GLU	C-N-CA	-6.19	114.83	123.13
1	D	321	LEU	N-CA-C	6.18	120.53	112.92
1	D	143	LEU	CA-C-N	6.18	128.56	120.28
1	D	143	LEU	C-N-CA	6.18	128.56	120.28
1	A	288	ARG	N-CA-C	6.15	120.05	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	HIS	N-CA-C	-6.15	98.49	108.52
1	D	96	HIS	CA-C-O	-6.14	113.73	120.30
1	A	75	VAL	N-CA-C	6.13	116.69	107.80
1	C	231	VAL	CA-C-N	-6.11	118.19	122.59
1	C	231	VAL	C-N-CA	-6.11	118.19	122.59
1	B	36	SER	CA-C-N	-6.11	109.43	121.41
1	B	36	SER	C-N-CA	-6.11	109.43	121.41
1	A	209	THR	N-CA-CB	-6.09	101.91	111.05
1	C	176	THR	CB-CA-C	6.08	120.84	109.71
1	B	60	LEU	CA-C-O	6.08	126.89	119.11
1	C	433	ASP	N-CA-C	6.07	117.35	109.64
1	A	410	ARG	O-C-N	-6.05	114.54	122.59
1	B	322	GLY	N-CA-C	6.02	119.41	111.70
1	B	49	VAL	N-CA-C	-6.00	105.97	111.67
1	A	96	HIS	N-CA-C	5.99	118.17	108.34
1	A	242	GLY	N-CA-C	5.99	117.64	111.95
1	A	397	GLY	N-CA-C	5.98	127.36	113.18
1	C	160	ILE	O-C-N	-5.97	116.17	122.67
1	C	95	ASP	N-CA-C	5.96	118.28	109.69
1	C	426	PRO	N-CA-C	5.96	117.97	110.70
1	C	422	LEU	N-CA-C	5.94	117.72	110.41
1	C	346	ALA	N-CA-C	-5.93	104.89	111.36
1	B	120	PRO	N-CA-C	-5.93	103.47	110.70
1	A	441	GLN	N-CA-C	-5.91	98.21	110.80
1	D	399	LEU	N-CA-CB	5.89	120.51	110.50
1	B	145	ALA	N-CA-C	5.87	117.67	111.28
1	C	224	ALA	N-CA-C	5.86	123.28	110.80
1	A	96	HIS	N-CA-CB	-5.85	101.59	110.77
1	A	98	GLU	CG-CD-OE1	5.82	131.79	118.40
1	B	437	ILE	CB-CA-C	5.82	119.64	112.02
1	A	133	LEU	CB-CA-C	-5.79	102.96	111.77
1	A	92	THR	CA-C-N	-5.79	111.55	121.97
1	A	92	THR	C-N-CA	-5.79	111.55	121.97
1	C	417	LEU	N-CA-C	-5.77	104.99	111.28
1	D	10	GLY	CA-C-N	-5.77	111.59	121.97
1	D	10	GLY	C-N-CA	-5.77	111.59	121.97
1	A	16	SER	CB-CA-C	-5.74	101.32	110.84
1	A	87	GLU	N-CA-C	5.74	118.99	107.41
1	C	225	VAL	N-CA-CB	5.73	120.69	111.23
1	A	186	PRO	CB-CA-C	-5.72	103.73	111.85
1	B	395	GLY	CA-C-N	5.72	131.76	122.67
1	B	395	GLY	C-N-CA	5.72	131.76	122.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLU	CA-CB-CG	-5.71	102.68	114.10
1	A	97	ALA	N-CA-CB	5.70	120.13	110.49
1	C	16	SER	CB-CA-C	-5.68	101.96	110.88
1	D	174	GLN	CA-C-N	-5.67	115.06	122.94
1	D	174	GLN	C-N-CA	-5.67	115.06	122.94
1	B	399	LEU	N-CA-CB	5.66	120.13	110.50
1	A	35	LYS	N-CA-C	5.65	119.79	113.01
1	C	186	PRO	CB-CA-C	-5.64	103.41	112.21
1	D	217	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	D	146	LEU	CA-C-N	-5.62	114.14	119.76
1	D	146	LEU	C-N-CA	-5.62	114.14	119.76
1	A	146	LEU	CA-C-N	-5.61	113.93	119.99
1	A	146	LEU	C-N-CA	-5.61	113.93	119.99
1	C	324	VAL	CB-CA-C	5.61	116.67	110.62
1	B	81	VAL	N-CA-CB	5.59	117.21	110.95
1	D	231	VAL	CA-C-N	-5.58	118.81	122.60
1	D	231	VAL	C-N-CA	-5.58	118.81	122.60
1	D	324	VAL	N-CA-CB	-5.55	104.18	112.67
1	D	92	THR	CA-C-N	-5.53	112.69	120.77
1	D	92	THR	C-N-CA	-5.53	112.69	120.77
1	D	35	LYS	N-CA-C	5.53	119.29	112.54
1	D	173	LEU	CA-C-N	-5.53	115.10	122.72
1	D	173	LEU	C-N-CA	-5.53	115.10	122.72
1	C	75	VAL	N-CA-C	5.51	115.89	108.17
1	C	195	LEU	N-CA-C	-5.51	105.38	111.71
1	B	92	THR	CA-C-N	-5.51	112.06	121.97
1	B	92	THR	C-N-CA	-5.51	112.06	121.97
1	C	91	LEU	N-CA-C	-5.50	99.08	110.80
1	A	437	ILE	CB-CA-C	5.49	119.60	112.24
1	B	176	THR	CB-CA-C	5.47	119.72	109.71
1	C	143	LEU	CA-C-N	5.47	127.55	120.44
1	C	143	LEU	C-N-CA	5.47	127.55	120.44
1	A	36	SER	CA-C-N	-5.47	110.69	121.41
1	A	36	SER	C-N-CA	-5.47	110.69	121.41
1	A	93	VAL	CB-CA-C	5.47	120.26	111.29
1	D	349	GLU	N-CA-C	5.46	119.57	113.01
1	B	143	LEU	CA-C-N	5.46	127.54	120.44
1	B	143	LEU	C-N-CA	5.46	127.54	120.44
1	B	410	ARG	CA-C-N	-5.46	112.04	120.88
1	B	410	ARG	C-N-CA	-5.46	112.04	120.88
1	B	186	PRO	CB-CA-C	-5.45	103.72	112.21
1	D	365	HIS	N-CA-CB	5.44	118.05	109.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	GLU	N-CA-C	-5.44	105.51	111.82
1	D	107	ASP	N-CA-C	-5.43	107.31	114.04
1	C	399	LEU	N-CA-CB	5.42	119.72	110.50
1	D	441	GLN	CA-CB-CG	5.42	124.94	114.10
1	C	172	GLY	N-CA-C	5.42	122.55	115.40
1	B	10	GLY	CA-C-N	-5.41	112.24	121.97
1	B	10	GLY	C-N-CA	-5.41	112.24	121.97
1	A	399	LEU	CD1-CG-CD2	-5.40	98.93	110.80
1	A	353	ALA	N-CA-C	5.39	118.85	110.17
1	D	176	THR	CB-CA-C	5.39	119.57	109.71
1	A	82	VAL	CB-CA-C	-5.37	102.48	111.29
1	B	146	LEU	CA-C-N	-5.37	114.39	119.76
1	B	146	LEU	C-N-CA	-5.37	114.39	119.76
1	B	183	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	D	82	VAL	CB-CA-C	-5.36	102.51	111.29
1	D	93	VAL	CB-CA-C	5.35	120.04	111.69
1	A	246	ASN	N-CA-C	5.34	117.89	109.39
1	D	426	PRO	N-CA-C	5.33	117.21	110.70
1	B	295	TRP	CA-C-N	-5.33	116.61	123.16
1	B	295	TRP	C-N-CA	-5.33	116.61	123.16
1	C	381	GLU	N-CA-C	5.32	116.76	111.07
1	D	289	VAL	N-CA-C	-5.32	106.50	111.45
1	D	256	ALA	N-CA-C	5.32	117.94	110.23
1	D	399	LEU	CD1-CG-CD2	-5.30	99.13	110.80
1	A	174	GLN	CB-CA-C	5.30	118.27	109.53
1	A	232	VAL	CA-C-O	5.29	122.27	119.15
1	A	418	LEU	N-CA-C	5.29	117.80	111.71
1	C	404	LEU	N-CA-C	-5.27	105.21	111.69
1	A	160	ILE	N-CA-C	-5.27	102.78	109.58
1	C	174	GLN	CA-C-N	-5.27	115.62	122.94
1	C	174	GLN	C-N-CA	-5.27	115.62	122.94
1	D	147	PRO	CA-C-O	-5.27	114.99	121.31
1	A	131	TYR	N-CA-C	5.26	117.41	109.41
1	B	174	GLN	CA-C-N	-5.25	115.69	122.99
1	B	174	GLN	C-N-CA	-5.25	115.69	122.99
1	B	207	VAL	CB-CA-C	5.25	117.81	110.99
1	D	98	GLU	CA-CB-CG	-5.24	103.61	114.10
1	A	224	ALA	CA-C-N	-5.24	112.54	121.97
1	A	224	ALA	C-N-CA	-5.24	112.54	121.97
1	C	93	VAL	CB-CA-C	5.24	119.98	111.71
1	A	81	VAL	N-CA-CB	5.23	116.62	110.82
1	B	225	VAL	N-CA-CB	5.23	119.86	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	ARG	N-CA-C	-5.20	106.08	112.90
1	D	102	PHE	N-CA-C	5.19	116.02	108.14
1	A	189	ASP	CA-C-N	-5.18	114.63	120.89
1	A	189	ASP	C-N-CA	-5.18	114.63	120.89
1	C	128	GLU	CA-C-N	-5.18	111.27	121.41
1	C	128	GLU	C-N-CA	-5.18	111.27	121.41
1	A	395	GLY	N-CA-C	5.15	125.39	113.18
1	B	160	ILE	CB-CA-C	5.14	118.99	111.33
1	D	307	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	D	120	PRO	CA-C-N	5.14	126.27	119.84
1	D	120	PRO	C-N-CA	5.14	126.27	119.84
1	B	96	HIS	N-CA-CB	-5.13	102.65	110.65
1	A	107	ASP	N-CA-C	-5.13	107.09	113.55
1	C	76	HIS	N-CA-C	5.11	116.94	108.20
1	B	441	GLN	CB-CG-CD	5.11	121.28	112.60
1	C	97	ALA	N-CA-CB	5.11	119.12	110.49
1	A	74	LEU	CA-C-N	-5.10	116.49	123.12
1	A	74	LEU	C-N-CA	-5.10	116.49	123.12
1	A	174	GLN	CA-C-N	-5.09	115.91	122.99
1	A	174	GLN	C-N-CA	-5.09	115.91	122.99
1	D	98	GLU	O-C-N	5.09	129.13	122.87
1	A	394	ARG	N-CA-C	-5.08	105.39	112.45
1	D	97	ALA	N-CA-CB	5.08	119.07	110.49
1	D	397	GLY	CA-C-N	5.08	131.24	121.54
1	D	397	GLY	C-N-CA	5.08	131.24	121.54
1	A	172	GLY	CA-C-O	-5.07	113.67	119.04
1	B	364	ALA	N-CA-C	5.07	117.44	110.35
1	B	100	ARG	N-CA-C	5.05	118.19	110.36
1	D	417	LEU	N-CA-C	-5.05	105.67	111.07
1	B	113	THR	N-CA-C	5.04	119.30	113.20
1	D	4	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	D	96	HIS	N-CA-C	5.04	116.62	108.41
1	A	368	PRO	CB-CA-C	-5.03	106.08	111.56
1	C	194	ALA	N-CA-C	5.03	116.45	111.07
1	D	98	GLU	CG-CD-OE1	5.03	129.96	118.40
1	C	133	LEU	CB-CA-C	-5.02	104.91	112.09
1	C	399	LEU	CD1-CG-CD2	-5.02	99.76	110.80
1	B	82	VAL	CB-CA-C	-5.02	103.06	111.29
1	A	110	VAL	CB-CA-C	-5.01	104.29	111.31
1	C	410	ARG	O-C-N	-5.01	115.93	122.59

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	Peptide,Mainchain
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	220	0
1	B	3379	0	3407	263	0
1	C	3378	0	3402	198	0
1	D	3377	0	3402	204	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	48	0	31	0	0
4	D	48	0	31	3	0
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	15	0
All	All	14205	0	13970	883	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 (883) 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:CD1	1:D:160:ILE:CG1	1.77	1.54
1:B:160:ILE:CD1	1:B:160:ILE:CG1	1.80	1.53
1:C:160:ILE:CD1	1:C:160:ILE:CG1	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:B:437:ILE:C	1:B:437:ILE:HD12	1.71	1.15
1:C:437:ILE:C	1:C:437:ILE:HD12	1.71	1.15
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:437:ILE:HD12	1:A:437:ILE:C	1.73	1.11
1:A:439:ALA:O	1:A:441:GLN:CB	1.98	1.11
1:D:149:ALA:HB1	1:D:150:ARG:HA	1.16	1.11
1:A:440:GLN:NE2	1:A:440:GLN:HA	1.63	1.10
1:C:439:ALA:O	1:C:441:GLN:HB2	0.94	1.10
1:B:85:ASP:O	1:B:92:THR:HG22	1.49	1.09
1:A:90:THR:HA	1:A:92:THR:HG23	1.09	1.08
1:B:396:HIS:N	1:B:397:GLY:HA2	1.67	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:85:ASP:C	1:B:92:THR:HG22	1.80	1.07
1:C:149:ALA:HB1	1:C:150:ARG:HA	1.28	1.07
1:D:440:GLN:HA	1:D:440:GLN:NE2	1.68	1.06
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:A:85:ASP:C	1:A:92:THR:HG22	1.82	1.03
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:D:437:ILE:HD12	1:D:437:ILE:C	1.86	1.01
1:A:440:GLN:HA	1:A:440:GLN:HE21	1.17	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:410:ARG:NH1	1:B:410:ARG:NH1	2.11	0.98
1:D:440:GLN:HA	1:D:440:GLN:HE21	1.24	0.98
1:A:90:THR:HA	1:A:92:THR:CG2	1.94	0.96
1:B:440:GLN:HA	1:B:440:GLN:NE2	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:B:91:LEU:C	5:B:602:HOH:O	2.12	0.91
1:D:149:ALA:HB1	1:D:150:ARG:CA	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ALA:CB	1:B:150:ARG:CA	2.50	0.89
1:A:85:ASP:O	1:A:92:THR:HG22	1.70	0.89
1:B:373:LEU:HD22	1:B:434:PRO:HG2	1.55	0.89
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:87:GLU:OE1	5:C:602:HOH:O	1.91	0.85
1:C:398:ALA:H	1:C:399:LEU:HB2	1.40	0.85
1:B:64:THR:OG1	1:B:67:GLU:HG3	1.76	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:B:437:ILE:C	1:B:437:ILE:CD1	2.53	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:B:236:LEU:C	1:B:236:LEU:HD12	2.06	0.80
1:A:64:THR:OG1	1:A:67:GLU:HG3	1.82	0.80
1:A:149:ALA:CB	1:A:150:ARG:CA	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:50:LEU:HD12	1:D:143:LEU:HD13	1.64	0.79
3:D:502:NAD:C4B	5:D:604:HOH:O	2.31	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:B:87:GLU:HA	1:B:88:LEU:C	2.08	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:87:GLU:HA	1:C:88:LEU:C	2.10	0.77
1:A:89:ARG:C	1:A:90:THR:O	2.27	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:HA	1:B:440:GLN:HE21	1.45	0.77
1:B:395:GLY:C	1:B:397:GLY:CA	2.58	0.76
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: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: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:B:395:GLY:C	1:B:397:GLY:HA2	2.11	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:O5B	3:A:502:NAD:O3B	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:A:92:THR:O	1:A:93:VAL:C	2.30	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:GLU:N	5:C:604:HOH:O	2.19	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:269:MET:HE3	1:D:320:PHE:HB3	1.71	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
1:C:224:ALA:O	1:C:232:VAL:O	2.06	0.72
1:D:236:LEU:HD12	1:D:236:LEU:C	2.14	0.72
1:B:256:ALA:H	1:B:272:ASN:HD21	1.37	0.72
1:B:439:ALA:C	1:B:441:GLN:HB2	2.08	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: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:91:LEU:HD13	1:B:103:GLN:OE1	1.89	0.71
1:B:116:ARG:NH1	1:B:244:ARG:HH11	1.88	0.71
1:D:87:GLU:HA	1:D:88:LEU:C	2.15	0.71
1:D:94:HIS:CD2	1:D:94:HIS:H	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:92:THR:O	1:C:93:VAL:C	2.31	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: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
1:C:269:MET:HE3	1:C:320:PHE:HB3	1.72	0.70
3:D:502:NAD:O5B	3:D:502:NAD:O3B	2.06	0.70
1:D:98:GLU:HA	1:D:98:GLU:OE2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:502:NAD:O3B	3:C:502:NAD:O5B	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:HD23	1:B:173:LEU:N	2.07	0.70
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
3:B:502:NAD:C4A	3:B:502:NAD:O2B	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:B:92:THR:O	1:B:93:VAL:C	2.35	0.69
3:B:502:NAD:O5B	3:B:502:NAD:O3B	2.00	0.69
1:C:64:THR:OG1	1:C:67:GLU:HG3	1.93	0.69
1:C:295:TRP:CE2	1:C:297:PRO:HG3	2.28	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:85:ASP:H	1:A:92:THR:HA	1.56	0.68
1:A:396:HIS:CE1	1:B:396:HIS:H	2.11	0.68
1:A:91:LEU:C	1:A:92:THR:HG23	2.19	0.68
1:B:149:ALA:HB3	1:B:150:ARG:HA	1.70	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:89:ARG:O	1:B:90:THR:O	2.11	0.67
1:B:270:ARG:HH11	1:B:270:ARG:HB2	1.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:O	1:B:149:ALA:O	2.12	0.67
1:D:358:ILE:C	1:D:358:ILE:HD12	2.20	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:34:GLU:HG2	1:B:39:VAL:HG23	1.76	0.66
1:B:221:ARG:O	1:B:222:VAL:HG12	1.95	0.66
1:C:185:LEU:N	1:C:186:PRO:HD3	2.10	0.66
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:C:94:HIS:N	1:C:94:HIS:CD2	2.64	0.66
1:B:91:LEU:C	1:B:92:THR:HG23	2.20	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:A:121:PRO:HG3	1:D:149:ALA:HB3	1.78	0.65
1:B:76:HIS:HB3	1:B:79:HIS:CE1	2.29	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:CD2	1:D:94:HIS:N	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:87:GLU:N	1:B:87:GLU:OE2	2.30	0.65
1:B:410:ARG:HG3	1:B:411:GLU:N	2.09	0.65
1:B:44:CYS:HA	2:B:501:FAD:C6	2.27	0.65
1:C:437:ILE:C	1:C:437:ILE:CD1	2.55	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:87:GLU:HA	1:A:88:LEU:C	2.22	0.64
1:A:34:GLU:HG2	1:A:39:VAL:HG23	1.79	0.64
1:A:149:ALA:HA	1:A:173:LEU:HD22	1.80	0.64
1:B:395:GLY:C	1:B:397:GLY:HA3	2.22	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:NE2	1:C:440:GLN:CA	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:A:437:ILE:C	1:A:437:ILE:CD1	2.59	0.63
1:C:94:HIS:CD2	1:C:94:HIS:H	2.16	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLU:N	1:D:87:GLU:OE2	2.30	0.63
1:C:272:ASN:H	1:C:272:ASN:ND2	1.93	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:91:LEU:O	1:B:92:THR:OG1	2.13	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:D:89:ARG:C	1:D:90:THR:O	2.41	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:A:440:GLN:C	1:A:441:GLN:O	2.41	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
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:236:LEU:C	1:C:236:LEU:HD12	2.24	0.62
1:B:440:GLN:C	1:B:441:GLN:O	2.42	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:HB2	1:A:270:ARG:NH1	2.16	0.61
1:C:87:GLU:OE2	1:C:87:GLU:N	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: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:411:GLU:OE1	1:A:411:GLU:HA	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:HH11	1:D:270:ARG:HB2	1.65	0.60
1:B:115:ALA:HB1	1:B:244:ARG:O	2.02	0.60
1:D:38:TRP:CE3	1:D:136:MET:HE2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HB3	1:D:224:ALA:HB3	1.82	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:HB2	1:C:270:ARG:HH11	1.66	0.59
1:D:161:GLY:H	1:D:164:ALA:H	1.48	0.59
1:A:358:ILE:HD12	1:A:358:ILE:C	2.28	0.59
1:B:185:LEU:N	1:B:186:PRO:HD3	2.16	0.59
1:A:272:ASN:H	1:A:272:ASN:HD22	1.47	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
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:A:89:ARG:O	1:A:90:THR:C	2.45	0.59
1:D:78:ARG:HB3	1:D:78:ARG:NH1	2.18	0.59
1:D:83:ASP:HB3	1:D:94:HIS:CD2	2.37	0.59
1:B:269:MET:HE3	1:B:320:PHE:HB3	1.85	0.58
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:439:ALA:C	1:A:441:GLN:HB2	2.13	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: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:B:197:LYS:NZ	5:B:607:HOH:O	2.37	0.58
1:B:94:HIS:HA	1:B:102:PHE:O	2.04	0.57
1:C:358:ILE:HD12	1:C:358:ILE:C	2.29	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:OD1	1:A:88:LEU:HD23	2.05	0.57
1:C:78:ARG:CZ	1:C:78:ARG:HB3	2.34	0.57
1:D:149:ALA:HA	1:D:173:LEU:HD22	1.85	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: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:A:121:PRO:CG	1:D:149:ALA:CB	2.84	0.56
1:C:270:ARG:NE	5:C:610:HOH:O	2.37	0.56
1:D:84:VAL:O	1:D:86:TYR:HD1	1.87	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:HH11	1:B:270:ARG:CB	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:97:ALA:O	1:A:98:GLU:OE1	2.24	0.56
1:A:359:GLN:HB2	1:A:374:TRP:CD1	2.41	0.56
1:B:395:GLY:O	1:B:397:GLY:HA3	2.06	0.56
1:B:85:ASP:OD1	1:B:88:LEU:HD23	2.06	0.55
1:B:437:ILE:O	1:B:441:GLN:HB3	2.07	0.55
1:D:398:ALA:N	1:D:399:LEU:CB	2.66	0.55
1:A:437:ILE:HD12	1:A:437:ILE:O	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:83:ASP:HB3	1:C:94:HIS:CD2	2.41	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: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:86:TYR:HD1	1:D:86:TYR:H	1.52	0.55
1:D:208:TRP:HB3	1:D:211:VAL:CG2	2.36	0.55
1:A:128:GLU:HG2	1:A:221:ARG:NH2	2.22	0.55
1:B:216:PHE:CD1	1:B:225:VAL:HG22	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:440:GLN:C	1:C:441:GLN:O	2.49	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:A:269:MET:HE3	1:A:320:PHE:HB3	1.89	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
1:A:121:PRO:CG	1:D:149:ALA:HB2	2.38	0.54
3:A:502:NAD:H51A	5:A:604:HOH:O	2.06	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:B:83:ASP:O	1:B:94:HIS:HD2	1.90	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:D:78:ARG:HB3	1:D:78:ARG:CZ	2.38	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: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:78:ARG:NH1	1:B:78:ARG:HB3	2.23	0.53
1:B:91:LEU:O	1:B:92:THR:HG23	2.07	0.53
1:B:151:ARG:HG2	1:B:174:GLN:NE2	2.15	0.53
1:C:433:ASP:O	1:C:434:PRO:C	2.51	0.53
1:A:95:ASP:OD1	1:A:95:ASP:C	2.42	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:HH11	1:C:270:ARG:CB	2.21	0.53
1:D:8:VAL:HG13	1:D:81:VAL:HG13	1.89	0.53
1:D:25:ASN:OD1	1:D:25:ASN:C	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:THR:O	1:D:93:VAL:C	2.49	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:A:39:VAL:HG11	1:A:75:VAL:HG21	1.91	0.52
1:A:25:ASN:OD1	1:A:25:ASN:C	2.51	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:90:THR:CA	1:B:92:THR:HG23	2.09	0.52
1:B:208:TRP:HB3	1:B:211:VAL:CG2	2.39	0.52
1:C:86:TYR:HD1	1:C:86:TYR:H	1.54	0.52
3:C:502:NAD:O2B	3:C:502:NAD:N3A	2.42	0.52
1:A:217:ARG:HB3	1:A:224:ALA:HB3	1.92	0.52
1:B:56:ARG:NH1	1:B:59:ARG:HD2	2.24	0.52
1:B:173:LEU:HD23	1:B:173:LEU:H	1.74	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:D:440:GLN:C	1:D:441:GLN:O	2.52	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:D:437:ILE:C	1:D:437:ILE:CD1	2.69	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:O2B	3:D:502:NAD:N3A	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:8:VAL:HG13	1:C:81:VAL:HG13	1.92	0.51
1:C:157:ALA:HB2	1:C:177:LEU:HD22	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:236:LEU:HD12	1:A:236:LEU:C	2.35	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:78:ARG:HB3	1:C:78:ARG:NH1	2.25	0.51
1:C:270:ARG:CB	1:C:270:ARG:NH1	2.74	0.51
2:C:501:FAD:O2'	2:C:501:FAD:H9	2.10	0.51
1:A:90:THR:CA	1:A:92:THR:HG23	2.05	0.51
1:A:270:ARG:NH1	1:A:270:ARG:CB	2.74	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:O	1:A:82:VAL:HG12	2.11	0.51
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:C:282:VAL:O	1:C:282:VAL:HG22	2.09	0.51
1:D:157:ALA:HB2	1:D:177:LEU:HD22	1.92	0.51
1:A:91:LEU:C	1:A:92:THR:CG2	2.81	0.51
1:C:44:CYS:HA	2:C:501:FAD:C6	2.41	0.51
1:C:166:GLU:HA	1:C:332:PHE:CZ	2.46	0.51
1:D:76:HIS:HB3	1:D:79:HIS:CE1	2.45	0.51
1:D:166:GLU:HA	1:D:332:PHE:CZ	2.46	0.51
1:B:244:ARG:NH2	5:B:611:HOH:O	2.44	0.50
1:D:272:ASN:HD22	1:D:272:ASN:H	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:25:ASN:OD1	1:C:27:GLU:HB2	2.12	0.50
1:C:116:ARG:HH12	1:C:244:ARG:HH11	1.59	0.50
1:C:437:ILE:HD12	1:C:437:ILE:O	2.10	0.50
1:D:352:TRP:CD1	5:D:612:HOH:O	2.65	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3:LYS:NZ	1:C:3:LYS:HB3	2.27	0.50
1:C:159:TYR:HB3	3:C:502:NAD:C4N	2.42	0.50
1:A:11:VAL:HG23	2:A:501:FAD:H4B	1.94	0.49
1:A:208:TRP:HB3	1:A:211:VAL:CG2	2.42	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:B:358:ILE:C	1:B:358:ILE:HD12	2.37	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:90:THR:HA	1:A:91:LEU:O	2.12	0.49
1:A:272:ASN:ND2	1:A:272:ASN:H	2.10	0.49
3:A:502:NAD:O2B	3:A:502:NAD:N3A	2.38	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:37:GLY:CA	1:C:77:THR:HB	2.35	0.49
1:C:224:ALA:O	1:C:225:VAL:CB	2.60	0.49
1:D:82:VAL:O	1:D:82:VAL:HG12	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:95:ASP:C	1:C:95:ASP:OD1	2.52	0.49
1:C:272:ASN:ND2	1:C:272:ASN:N	2.61	0.49
1:D:216:PHE:HD1	1:D:225:VAL:HG22	1.78	0.49
1:B:84:VAL:HG22	1:B:93:VAL:HG12	1.95	0.49
1:B:287:HIS:HD2	1:B:290:LEU:H	1.61	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:D:23:ARG:NH2	4:D:503:COA:O5A	2.46	0.49
1:D:160:ILE:HD11	3:D:502:NAD:O1N	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:148:GLN:O	1:B:149:ALA:C	2.55	0.48
1:B:399:LEU:C	1:B:401:ILE:N	2.69	0.48
1:A:437:ILE:O	1:A:441:GLN:HB3	2.13	0.48
1:B:97:ALA:O	1:B:98:GLU:OE1	2.30	0.48
1:B:440:GLN:NE2	5:B:612:HOH:O	2.47	0.48
1:B:441:GLN:C	1:B:442:ALA:O	2.56	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: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:38:TRP:CE3	1:A:136:MET:HE2	2.48	0.48
1:B:95:ASP:C	1:B:95:ASP:OD1	2.54	0.48
1:A:23:ARG:NH2	4:A:503:COA:O5A	2.47	0.48
1:B:270:ARG:HB2	1:B:270:ARG:NH1	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
1:D:263:ILE:HD12	1:D:282:VAL:HG22	1.95	0.48
1:C:24:GLU:CG	1:C:316:ARG:HG3	2.44	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:89:ARG:O	1:B:90:THR:C	2.57	0.47
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:37:GLY:CA	1:D:77:THR:HB	2.23	0.47
1:D:178:LEU:HD23	1:D:208:TRP:HB2	1.95	0.47
1:A:91:LEU:C	1:A:92:THR:OG1	2.51	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:B:287:HIS:CD2	1:B:289:VAL:H	2.30	0.47
1:C:380:GLU:HG2	5:C:604:HOH:O	2.13	0.47
1:D:65:PRO:HB3	1:D:75:VAL:HG22	1.97	0.47
1:D:180:ALA:H	3:D:502:NAD:C8A	2.28	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:A:3:LYS:NZ	1:A:3:LYS:HB3	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLY:CA	5:A:607:HOH:O	2.61	0.47
1:A:160:ILE:HG23	3:A:502:NAD:H6N	1.97	0.47
1:B:76:HIS:HB3	1:B:79:HIS:ND1	2.29	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:C:4:ARG:NH1	1:C:104:ASP:OD2	2.47	0.47
1:C:116:ARG:HH12	1:C:244:ARG:HD2	1.79	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:D:56:ARG:NH1	1:D:59:ARG:HD2	2.29	0.47
1:D:116:ARG:HH12	1:D:244:ARG:HH11	1.62	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:A:58:GLU:O	1:A:61:VAL:HG12	2.15	0.47
1:A:150:ARG:HH12	1:C:150:ARG:NH2	2.13	0.47
1:A:398:ALA:N	1:A:399:LEU:CB	2.68	0.47
1:A:441:GLN:C	1:A:442:ALA:O	2.58	0.47
1:B:154:ILE:HD11	1:B:168:PHE:CD2	2.50	0.47
1:B:224:ALA:O	1:B:225:VAL:CB	2.63	0.47
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:83:ASP:O	1:D:94:HIS:HD2	1.96	0.47
1:D:86:TYR:O	1:D:89:ARG:CA	2.63	0.47
1:D:95:ASP:OD1	1:D:95:ASP:C	2.58	0.47
1:A:37:GLY:HA2	1:A:77:THR:CB	2.26	0.47
1:B:411:GLU:OE1	1:B:411:GLU:HA	2.14	0.47
1:C:56:ARG:NH1	1:C:59:ARG:HH11	2.11	0.47
1:C:151:ARG:NH1	5:C:612:HOH:O	2.38	0.47
1:D:270:ARG:HH11	1:D:270:ARG:CB	2.27	0.47
1:A:65:PRO:HB3	1:A:75:VAL:HG22	1.96	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:C:58:GLU:O	1:C:61:VAL:HG12	2.15	0.47
1:C:437:ILE:O	1:C:441:GLN:HB3	2.14	0.47
1:D:89:ARG:O	1:D:90:THR:C	2.58	0.47
1:A:116:ARG:HH12	1:A:244:ARG:HH11	1.62	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:D:255:VAL:HA	1:D:272:ASN:HD21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:36:SER:O	1:D:37:GLY:C	2.54	0.46
1:B:408:LEU:HA	1:B:408:LEU:HD12	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:C:222:VAL:O	1:C:222:VAL:CG1	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:B:169:ARG:CD	1:B:175:VAL:HG13	2.46	0.46
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:A:148:GLN:O	1:A:149:ALA:C	2.59	0.46
1:B:85:ASP:H	1:B:92:THR:CB	2.28	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:C:128:GLU:HG2	1:C:221:ARG:NH2	2.31	0.46
1:A:97:ALA:O	1:A:98:GLU:CD	2.59	0.46
1:A:295:TRP:CZ2	1:A:297:PRO:HG3	2.51	0.46
1:B:433:ASP:O	1:B:434:PRO:C	2.57	0.46
1:C:136:MET:HE3	1:C:136:MET:HB3	1.85	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:D:148:GLN:O	1:D:149:ALA:C	2.60	0.45
1:A:191:GLU:OE2	1:A:355:LYS:HE3	2.16	0.45
1:B:89:ARG:C	1:B:90:THR:O	2.59	0.45
1:D:313:ILE:C	1:D:315:GLY:H	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	1:D:3:LYS:HB3	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:C:269:MET:HE3	1:C:320:PHE:CB	2.44	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: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: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:B:399:LEU:C	1:B:401:ILE:H	2.24	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:256:ALA:N	1:B:272:ASN:HD21	2.10	0.45
1:B:260:THR:HG23	1:B:284:GLU:OE1	2.17	0.45
1:C:156:GLY:CA	3:C:502:NAD:H2B	2.45	0.45
1:D:398:ALA:C	5:D:602:HOH:O	2.51	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:A:136:MET:HE3	1:A:136:MET:HB3	1.85	0.44
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:D:224:ALA:O	1:D:225:VAL:CB	2.65	0.44
1:A:410:ARG:HH11	1:A:410:ARG:HG2	1.81	0.44
1:D:295:TRP:CZ2	1:D:297:PRO:HG3	2.52	0.44
2:B:501:FAD:O2'	2:B:501:FAD:H9	2.18	0.44
1:B:50:LEU:HD12	1:B:50:LEU:HA	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:C:443:ARG:OXT	1:C:443:ARG:HG2	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD13	1:A:439:ALA:CB	2.46	0.44
1:B:91:LEU:C	1:B:92:THR:OG1	2.60	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:136:MET:HE3	1:B:136:MET:HB3	1.85	0.44
1:C:104:ASP:OD1	1:C:105:ARG:N	2.48	0.44
1:A:160:ILE:CD1	1:A:160:ILE:HG21	2.48	0.43
1:A:76:HIS:HB3	1:A:79:HIS:CE1	2.52	0.43
1:C:12:ALA:HB3	2:C:501:FAD:H5'2	1.99	0.43
1:C:361:ARG:HD3	1:C:365:HIS:HA	2.00	0.43
1:C:410:ARG:HG2	1:C:410:ARG:HH11	1.82	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: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
1:C:396:HIS:N	1:C:397:GLY:CA	2.78	0.43
2:A:501:FAD:H9	2:A:501:FAD:O2'	2.18	0.43
1:B:16:SER:CB	1:B:306:GLY:HA3	2.48	0.43
1:B:201:GLU:C	1:B:203:HIS:N	2.77	0.43
1:C:441:GLN:C	1:C:442:ALA:O	2.61	0.43
2:D:501:FAD:O2'	2:D:501:FAD:H9	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:D:352:TRP:NE1	5:D:612:HOH:O	2.50	0.43
1:A:69:ARG:O	1:A:70:LYS:C	2.58	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:B:12:ALA:HB3	2:B:501:FAD:O1P	2.19	0.43
1:B:23:ARG:HH22	4:B:503:COA:P2A	2.42	0.43
1:B:377:LEU:HD22	1:B:438:ALA:HB1	2.00	0.43
1:C:410:ARG:HG2	1:C:410:ARG:NH1	2.34	0.43
1:D:85:ASP:OD1	1:D:88:LEU:CD2	2.54	0.43
1:D:90:THR:OG1	1:D:91:LEU:O	2.18	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:CB	1:D:270:ARG:NH1	2.81	0.43
1:B:24:GLU:HG3	1:B:316:ARG:HG3	2.01	0.43
1:B:217:ARG:O	1:B:222:VAL:HA	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:ASP:O	1:A:86:TYR:O	2.38	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: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: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:B:159:TYR:HB3	3:B:502:NAD:C4N	2.49	0.42
1:B:280:GLY:HA3	2:B:501:FAD:O2P	2.20	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:A:258:GLY:HA3	1:A:284:GLU:CD	2.44	0.42
1:B:85:ASP:HB2	1:B:92:THR:HA	2.01	0.42
1:B:111:LEU:HD12	1:B:111:LEU:HA	1.84	0.42
1:D:90:THR:HA	1:D:91:LEU:O	2.20	0.42
1:D:343:LEU:HD22	1:D:355:LYS:HD3	2.01	0.42
1:A:96:HIS:C	1:A:96:HIS:CD2	2.98	0.42
1:A:160:ILE:CD1	1:A:160:ILE:CG2	2.96	0.42
1:B:57:LEU:HA	1:B:57:LEU:HD12	1.81	0.42
1:B:86:TYR:O	1:B:89:ARG:CA	2.67	0.42
1:C:36:SER:O	1:C:37:GLY:C	2.62	0.42
1:C:38:TRP:CE3	1:C:136:MET:HE2	2.54	0.42
1:C:281:ASP:OD2	2:C:501:FAD:H3'	2.20	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:65:PRO:HB3	1:C:75:VAL:HG22	2.02	0.42
1:C:270:ARG:HG2	5:C:607:HOH:O	2.19	0.42
1:D:281:ASP:OD2	2:D:501:FAD:H3'	2.20	0.42
1:A:183:ARG:NH1	1:A:188:TRP:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:424:TYR:CD1	1:C:431:VAL:HA	2.55	0.41
1:D:97:ALA:O	1:D:98:GLU:CD	2.63	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:134:ARG:NH2	1:B:281:ASP:OD2	2.53	0.41
1:B:231:VAL:O	1:B:231:VAL:HG12	2.19	0.41
1:D:127:GLN:NE2	1:D:216:PHE:O	2.53	0.41
1:B:396:HIS:H	1:B:397:GLY:HA2	1.67	0.41
1:D:50:LEU:HD12	1:D:50:LEU:HA	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:HD12	1:D:408:LEU:HA	1.84	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:A:169:ARG:HH11	1:A:169:ARG:HD2	1.72	0.41
1:B:201:GLU:O	1:B:203:HIS:N	2.53	0.41
1:C:130:VAL:HG13	1:C:237:VAL:HG22	2.03	0.41
1:D:88:LEU:O	1:D:89:ARG:CB	2.67	0.41
1:A:328:ILE:HG21	1:A:328:ILE:HD13	1.79	0.41
1:A:424:TYR:CD1	1:A:431:VAL:HA	2.56	0.41
1:B:83:ASP:C	1:B:94:HIS:HD2	2.28	0.41
1:C:82:VAL:O	1:C:82:VAL:HG12	2.19	0.41
1:C:89:ARG:C	1:C:90:THR:O	2.61	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:D:56:ARG:CZ	1:D:59:ARG:HH11	2.33	0.41
1:D:100:ARG:O	1:D:101:THR:HG22	2.21	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
1:B:36:SER:O	1:B:37:GLY:C	2.63	0.41
1:B:160:ILE:HG23	3:B:502:NAD:H6N	2.03	0.41
3:B:502:NAD:H2N	3:B:502:NAD:H2D	1.88	0.41
1:C:50:LEU:HD12	1:C:50:LEU:HA	1.64	0.41
1:C:209:THR:HG23	1:C:210:GLY:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ALA:CA	1:D:399:LEU:CB	2.99	0.41
1:D:433:ASP:O	1:D:434:PRO:C	2.62	0.41
1:A:140:GLU:O	1:A:141:ARG:C	2.61	0.41
1:A:418:LEU:HD12	1:A:418:LEU:HA	1.69	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:86:TYR:O	1:A:89:ARG:N	2.54	0.41
1:A:214:GLU:O	1:A:215:ALA:HB2	2.20	0.41
1:A:224:ALA:O	1:A:225:VAL:CB	2.67	0.41
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.74	0.41
1:C:221:ARG:O	1:C:222:VAL:CG1	2.68	0.41
1:C:439:ALA:O	1:C:441:GLN:CA	2.67	0.41
1:D:411:GLU:HA	1:D:411:GLU:OE1	2.21	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:44:CYS:HB3	2:C:501:FAD:C4X	2.51	0.40
1:C:133:LEU:HD23	1:C:133:LEU:HA	1.69	0.40
1:C:399:LEU:C	1:C:401:ILE:N	2.78	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
1:A:37:GLY:H	1:A:78:ARG:H	1.68	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: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%)	2	9
1	B	441/443 (100%)	392 (89%)	31 (7%)	18 (4%)	2	9
1	C	441/443 (100%)	390 (88%)	35 (8%)	16 (4%)	2	11
1	D	441/443 (100%)	388 (88%)	36 (8%)	17 (4%)	2	10
All	All	1764/1772 (100%)	1562 (88%)	133 (8%)	69 (4%)	2	10

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	280 (83%)	58 (17%)	2	7
1	B	338/338 (100%)	276 (82%)	62 (18%)	2	6
1	C	337/338 (100%)	273 (81%)	64 (19%)	1	5
1	D	337/338 (100%)	269 (80%)	68 (20%)	1	4
All	All	1350/1352 (100%)	1098 (81%)	252 (19%)	1	5

All (252) 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	58	GLU
1	A	59	ARG
1	A	60	LEU
1	A	75	VAL
1	A	78	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	81	VAL
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	111	LEU
1	A	132	THR
1	A	133	LEU
1	A	142	LEU
1	A	143	LEU
1	A	144	LYS
1	A	146	LEU
1	A	173	LEU
1	A	175	VAL
1	A	176	THR
1	A	177	LEU
1	A	181	LYS
1	A	185	LEU
1	A	199	GLU
1	A	207	VAL
1	A	208	TRP
1	A	209	THR
1	A	212	LYS
1	A	217	ARG
1	A	221	ARG
1	A	222	VAL
1	A	225	VAL
1	A	236	LEU
1	A	237	VAL
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	391	VAL
1	A	392	VAL
1	A	396	HIS
1	A	408	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	410	ARG
1	A	418	LEU
1	A	437	ILE
1	A	440	GLN
1	A	441	GLN
1	B	3	LYS
1	B	39	VAL
1	B	44	CYS
1	B	50	LEU
1	B	56	ARG
1	B	58	GLU
1	B	59	ARG
1	B	60	LEU
1	B	75	VAL
1	B	78	ARG
1	B	81	VAL
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	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
1	B	175	VAL
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	212	LYS
1	B	217	ARG
1	B	221	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	VAL
1	B	227	THR
1	B	231	VAL
1	B	236	LEU
1	B	237	VAL
1	B	268	ARG
1	B	301	VAL
1	B	311	SER
1	B	324	VAL
1	B	359	GLN
1	B	361	ARG
1	B	375	VAL
1	B	377	LEU
1	B	386	LEU
1	B	391	VAL
1	B	392	VAL
1	B	396	HIS
1	B	400	ARG
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	C	3	LYS
1	C	39	VAL
1	C	44	CYS
1	C	50	LEU
1	C	56	ARG
1	C	58	GLU
1	C	59	ARG
1	C	60	LEU
1	C	75	VAL
1	C	78	ARG
1	C	81	VAL
1	C	86	TYR
1	C	87	GLU
1	C	90	THR
1	C	91	LEU
1	C	94	HIS
1	C	100	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	101	THR
1	C	111	LEU
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	155	LEU
1	C	173	LEU
1	C	175	VAL
1	C	176	THR
1	C	177	LEU
1	C	181	LYS
1	C	185	LEU
1	C	199	GLU
1	C	207	VAL
1	C	208	TRP
1	C	209	THR
1	C	212	LYS
1	C	217	ARG
1	C	221	ARG
1	C	222	VAL
1	C	227	THR
1	C	236	LEU
1	C	237	VAL
1	C	268	ARG
1	C	272	ASN
1	C	301	VAL
1	C	324	VAL
1	C	359	GLN
1	C	361	ARG
1	C	375	VAL
1	C	377	LEU
1	C	386	LEU
1	C	391	VAL
1	C	392	VAL
1	C	396	HIS
1	C	400	ARG
1	C	408	LEU
1	C	410	ARG
1	C	418	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	429	SER
1	C	434	PRO
1	C	437	ILE
1	C	440	GLN
1	C	441	GLN
1	D	3	LYS
1	D	27	GLU
1	D	39	VAL
1	D	44	CYS
1	D	50	LEU
1	D	56	ARG
1	D	58	GLU
1	D	59	ARG
1	D	60	LEU
1	D	75	VAL
1	D	78	ARG
1	D	81	VAL
1	D	86	TYR
1	D	87	GLU
1	D	90	THR
1	D	91	LEU
1	D	94	HIS
1	D	100	ARG
1	D	101	THR
1	D	111	LEU
1	D	120	PRO
1	D	132	THR
1	D	133	LEU
1	D	142	LEU
1	D	143	LEU
1	D	144	LYS
1	D	146	LEU
1	D	151	ARG
1	D	155	LEU
1	D	160	ILE
1	D	173	LEU
1	D	175	VAL
1	D	176	THR
1	D	177	LEU
1	D	181	LYS
1	D	183	ARG
1	D	185	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	199	GLU
1	D	207	VAL
1	D	208	TRP
1	D	209	THR
1	D	212	LYS
1	D	217	ARG
1	D	221	ARG
1	D	222	VAL
1	D	236	LEU
1	D	237	VAL
1	D	241	THR
1	D	268	ARG
1	D	301	VAL
1	D	311	SER
1	D	324	VAL
1	D	359	GLN
1	D	361	ARG
1	D	375	VAL
1	D	377	LEU
1	D	386	LEU
1	D	391	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	272	ASN
1	A	287	HIS
1	A	359	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	396	HIS
1	A	440	GLN
1	B	96	HIS
1	B	174	GLN
1	B	187	HIS
1	B	272	ASN
1	B	287	HIS
1	B	396	HIS
1	B	440	GLN
1	C	94	HIS
1	C	103	GLN
1	C	174	GLN
1	C	272	ASN
1	C	287	HIS
1	C	359	GLN
1	C	409	HIS
1	C	440	GLN
1	D	94	HIS
1	D	96	HIS
1	D	103	GLN
1	D	174	GLN
1	D	187	HIS
1	D	251	GLN
1	D	272	ASN
1	D	287	HIS
1	D	409	HIS
1	D	440	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	D	501	-	58,58,58	2.42	19 (32%)	85,89,89	1.92	27 (31%)
4	COA	C	503	1	47,50,50	1.66	7 (14%)	69,75,75	2.43	25 (36%)
2	FAD	A	501	-	58,58,58	2.51	20 (34%)	85,89,89	1.87	21 (24%)
3	NAD	A	502	-	46,48,48	2.40	17 (36%)	64,73,73	3.80	32 (50%)
3	NAD	D	502	-	46,48,48	2.47	14 (30%)	64,73,73	3.84	32 (50%)
4	COA	A	503	1	47,50,50	1.59	7 (14%)	69,75,75	2.33	21 (30%)
3	NAD	B	502	-	46,48,48	2.42	13 (28%)	64,73,73	3.66	28 (43%)
4	COA	B	503	1	47,50,50	1.65	9 (19%)	69,75,75	2.27	22 (31%)
4	COA	D	503	1	47,50,50	1.73	7 (14%)	69,75,75	2.52	26 (37%)
2	FAD	B	501	-	58,58,58	2.57	20 (34%)	85,89,89	2.27	25 (29%)
2	FAD	C	501	-	58,58,58	2.26	20 (34%)	85,89,89	2.01	25 (29%)
3	NAD	C	502	-	46,48,48	2.40	12 (26%)	64,73,73	3.93	32 (50%)

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	D	501	-	-	8/34/50/50	0/6/6/6
4	COA	C	503	1	-	19/48/64/64	0/3/3/3
2	FAD	A	501	-	-	8/34/50/50	0/6/6/6
3	NAD	A	502	-	-	6/30/62/62	0/5/5/5
3	NAD	D	502	-	-	4/30/62/62	0/5/5/5
4	COA	A	503	1	-	17/48/64/64	0/3/3/3
3	NAD	B	502	-	-	5/30/62/62	0/5/5/5
4	COA	B	503	1	-	18/48/64/64	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	D	503	1	-	19/48/64/64	0/3/3/3
2	FAD	B	501	-	-	9/34/50/50	0/6/6/6
2	FAD	C	501	-	-	5/34/50/50	0/6/6/6
3	NAD	C	502	-	-	4/30/62/62	0/5/5/5

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAD	O7N-C7N	10.50	1.43	1.24
3	C	502	NAD	O7N-C7N	9.59	1.42	1.24
3	B	502	NAD	O7N-C7N	9.42	1.41	1.24
3	A	502	NAD	O7N-C7N	9.31	1.41	1.24
2	B	501	FAD	C9A-C5X	9.10	1.55	1.41
2	A	501	FAD	C9A-C5X	8.88	1.55	1.41
2	D	501	FAD	C9A-C5X	8.47	1.54	1.41
2	C	501	FAD	C9A-C5X	7.82	1.53	1.41
2	A	501	FAD	PA-O3P	7.73	1.67	1.59
2	D	501	FAD	C5A-C4A	7.10	1.51	1.39
2	A	501	FAD	C5A-C4A	6.77	1.51	1.39
4	B	503	COA	C5A-C4A	6.28	1.50	1.39
2	B	501	FAD	PA-O3P	6.19	1.66	1.59
2	B	501	FAD	C5A-C4A	5.87	1.49	1.39
2	D	501	FAD	PA-O3P	5.81	1.65	1.59
4	C	503	COA	C5A-C4A	5.72	1.49	1.39
4	D	503	COA	C5A-C4A	5.55	1.49	1.39
4	A	503	COA	C5A-C4A	5.51	1.48	1.39
2	C	501	FAD	C5A-C4A	5.23	1.48	1.39
2	B	501	FAD	C8-C7	5.22	1.53	1.40
2	B	501	FAD	P-O3P	5.10	1.65	1.59
2	C	501	FAD	PA-O3P	4.83	1.64	1.59
2	C	501	FAD	C8-C7	4.75	1.52	1.40
4	C	503	COA	P2A-O3A	4.72	1.64	1.59
3	D	502	NAD	C8A-N7A	4.63	1.40	1.31
4	D	503	COA	P2A-O3A	4.51	1.64	1.59
2	A	501	FAD	C8-C7	4.46	1.51	1.40
3	B	502	NAD	C2N-N1N	4.45	1.39	1.35
3	D	502	NAD	C8A-N9A	4.44	1.45	1.37
4	D	503	COA	C5A-C6A	4.35	1.53	1.41
4	A	503	COA	C5A-C6A	4.27	1.52	1.41
3	C	502	NAD	O4B-C1B	4.18	1.51	1.42
2	B	501	FAD	C9A-N10	4.18	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAD	C2N-N1N	4.17	1.39	1.35
4	D	503	COA	P1A-O3A	4.16	1.64	1.59
2	D	501	FAD	C8-C7	4.16	1.51	1.40
3	C	502	NAD	C2N-N1N	4.16	1.39	1.35
2	C	501	FAD	P-O3P	4.14	1.64	1.59
2	B	501	FAD	C4X-N5	4.13	1.39	1.30
3	B	502	NAD	C8A-N7A	4.10	1.39	1.31
3	C	502	NAD	C8A-N9A	4.07	1.44	1.37
3	C	502	NAD	C2A-N3A	4.06	1.41	1.33
3	D	502	NAD	C2A-N3A	4.05	1.41	1.33
3	D	502	NAD	C2N-N1N	4.04	1.39	1.35
2	C	501	FAD	C4X-N5	4.01	1.39	1.30
3	A	502	NAD	C2A-N1A	4.00	1.41	1.33
3	D	502	NAD	C2A-N1A	3.97	1.41	1.33
3	D	502	NAD	C5A-C6A	-3.90	1.30	1.41
3	B	502	NAD	C2A-N1A	3.86	1.40	1.33
3	C	502	NAD	C1B-N9A	3.83	1.56	1.46
2	D	501	FAD	C5A-C6A	3.80	1.51	1.41
2	D	501	FAD	C9A-N10	3.75	1.47	1.41
2	B	501	FAD	C5A-C6A	3.72	1.51	1.41
4	B	503	COA	P2A-O3A	3.69	1.63	1.59
2	D	501	FAD	C8A-N7A	3.68	1.38	1.31
2	A	501	FAD	C4X-N5	3.65	1.38	1.30
2	D	501	FAD	P-O3P	3.61	1.63	1.59
3	A	502	NAD	C8A-N7A	3.61	1.38	1.31
3	A	502	NAD	C2A-N3A	3.60	1.40	1.33
2	C	501	FAD	O4-C4	3.58	1.30	1.23
4	A	503	COA	P1A-O3A	3.57	1.63	1.59
4	C	503	COA	C5A-C6A	3.53	1.50	1.41
3	B	502	NAD	C8A-N9A	3.49	1.43	1.37
3	B	502	NAD	C5A-N7A	-3.47	1.32	1.39
3	B	502	NAD	C1B-N9A	3.46	1.55	1.46
3	C	502	NAD	C5A-N7A	-3.46	1.32	1.39
3	A	502	NAD	C5A-N7A	-3.42	1.32	1.39
3	B	502	NAD	C2A-N3A	3.38	1.39	1.33
2	C	501	FAD	C5A-C6A	3.37	1.50	1.41
3	B	502	NAD	O4B-C1B	3.34	1.49	1.42
3	C	502	NAD	C2A-N1A	3.30	1.39	1.33
2	A	501	FAD	PA-O1A	3.29	1.62	1.50
4	B	503	COA	C5A-C6A	3.27	1.50	1.41
2	D	501	FAD	C4X-N5	3.25	1.37	1.30
2	B	501	FAD	C4X-C10	3.21	1.53	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	PA-O1A	3.20	1.61	1.50
2	A	501	FAD	O4-C4	3.17	1.29	1.23
3	A	502	NAD	C3B-C4B	-3.08	1.45	1.53
2	B	501	FAD	O4-C4	3.06	1.29	1.23
2	B	501	FAD	C8A-N7A	3.06	1.37	1.31
2	A	501	FAD	C5A-C6A	3.05	1.49	1.41
4	B	503	COA	P1A-O3A	3.03	1.62	1.59
2	A	501	FAD	C2A-N1A	3.03	1.39	1.33
3	A	502	NAD	C8A-N9A	3.02	1.42	1.37
2	B	501	FAD	C10-N1	2.98	1.39	1.33
3	C	502	NAD	C8A-N7A	2.98	1.37	1.31
2	D	501	FAD	C6-C5X	2.98	1.44	1.40
4	C	503	COA	C8A-N7A	2.96	1.37	1.31
2	B	501	FAD	C6-C7	2.96	1.43	1.39
2	C	501	FAD	C9A-N10	2.94	1.46	1.41
2	A	501	FAD	P-O3P	2.94	1.62	1.59
4	C	503	COA	P1A-O3A	2.93	1.62	1.59
3	C	502	NAD	C5A-C6A	-2.92	1.32	1.41
4	B	503	COA	C2A-N3A	2.86	1.39	1.33
2	B	501	FAD	C10-N10	2.83	1.43	1.37
3	A	502	NAD	C5A-C6A	-2.79	1.33	1.41
2	C	501	FAD	C6-C7	2.78	1.43	1.39
4	C	503	COA	OAP-CAP	2.74	1.47	1.42
2	D	501	FAD	C10-N1	2.73	1.38	1.33
3	A	502	NAD	PA-O3	-2.69	1.56	1.59
4	B	503	COA	C4A-N3A	2.67	1.39	1.34
3	D	502	NAD	C5A-N7A	-2.66	1.34	1.39
4	A	503	COA	C6A-N6A	2.64	1.41	1.34
2	C	501	FAD	C8A-N7A	2.63	1.36	1.31
4	A	503	COA	C2A-N3A	2.62	1.38	1.33
3	B	502	NAD	PA-O3	-2.57	1.56	1.59
4	B	503	COA	C8A-N7A	2.55	1.36	1.31
2	A	501	FAD	C8A-N7A	2.54	1.36	1.31
3	A	502	NAD	PN-O3	2.53	1.62	1.59
2	D	501	FAD	O4-C4	2.52	1.28	1.23
4	D	503	COA	C2A-N3A	2.52	1.38	1.33
3	A	502	NAD	C2B-C1B	-2.51	1.45	1.53
2	A	501	FAD	C4X-C10	2.51	1.51	1.44
4	D	503	COA	C8A-N7A	2.47	1.36	1.31
2	D	501	FAD	C4X-C10	2.47	1.51	1.44
2	B	501	FAD	C4A-N3A	2.47	1.39	1.34
3	D	502	NAD	C1B-N9A	2.47	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	COA	C2A-N1A	2.46	1.38	1.33
3	B	502	NAD	C2N-C3N	2.45	1.42	1.39
2	D	501	FAD	O4B-C4B	-2.42	1.39	1.45
2	A	501	FAD	O4B-C1B	-2.42	1.36	1.42
3	C	502	NAD	C6A-N6A	-2.42	1.28	1.34
2	B	501	FAD	PA-O1A	2.41	1.59	1.50
2	A	501	FAD	C9A-N10	2.39	1.45	1.41
2	B	501	FAD	C6A-N6A	2.38	1.40	1.34
2	C	501	FAD	O4'-C4'	2.38	1.48	1.43
3	A	502	NAD	PA-O2A	-2.36	1.44	1.55
3	A	502	NAD	C6A-N6A	-2.36	1.28	1.34
2	A	501	FAD	C10-N10	2.36	1.42	1.37
4	C	503	COA	C2A-N1A	2.35	1.38	1.33
3	B	502	NAD	C5A-C6A	-2.33	1.34	1.41
3	D	502	NAD	C2N-C3N	2.32	1.42	1.39
2	D	501	FAD	O2-C2	2.30	1.28	1.24
3	A	502	NAD	O3B-C3B	-2.27	1.37	1.43
2	A	501	FAD	C2B-C3B	-2.26	1.47	1.53
2	C	501	FAD	O4B-C4B	-2.26	1.40	1.45
2	A	501	FAD	C2A-N3A	2.26	1.37	1.33
4	A	503	COA	C8A-N7A	2.23	1.36	1.31
3	D	502	NAD	O4B-C1B	2.23	1.47	1.42
3	B	502	NAD	C3N-C7N	2.22	1.53	1.50
2	D	501	FAD	O4'-C4'	2.21	1.48	1.43
2	C	501	FAD	C10-N1	2.21	1.37	1.33
2	B	501	FAD	O4'-C4'	2.16	1.47	1.43
2	A	501	FAD	C4A-N3A	2.15	1.38	1.34
3	D	502	NAD	C5A-C4A	2.15	1.42	1.39
3	D	502	NAD	C5B-C4B	2.15	1.58	1.51
2	C	501	FAD	O2-C2	2.14	1.28	1.24
4	B	503	COA	C6A-N1A	2.13	1.41	1.35
2	C	501	FAD	C5'-C4'	2.13	1.54	1.51
3	A	502	NAD	C1B-N9A	2.12	1.52	1.46
2	D	501	FAD	C10-N10	2.12	1.41	1.37
2	D	501	FAD	O4B-C1B	-2.11	1.37	1.42
4	A	503	COA	C6A-N1A	2.10	1.41	1.35
2	B	501	FAD	C2A-N1A	2.10	1.37	1.33
2	C	501	FAD	C5X-N5	-2.09	1.35	1.39
3	D	502	NAD	PN-O2N	-2.08	1.45	1.55
2	C	501	FAD	C4X-C4	2.06	1.52	1.44
2	A	501	FAD	C5'-C4'	2.06	1.54	1.51
2	C	501	FAD	C4X-C10	2.06	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAD	C4A-N3A	-2.05	1.30	1.34
3	C	502	NAD	PA-O2A	-2.04	1.45	1.55
2	B	501	FAD	C5'-C4'	2.03	1.54	1.51
2	A	501	FAD	O4'-C4'	2.03	1.47	1.43
4	D	503	COA	P3B-O3B	2.02	1.63	1.59
2	C	501	FAD	C2A-N3A	2.02	1.37	1.33

All (316) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAD	C2B-C1B-N9A	-16.01	73.53	113.30
3	A	502	NAD	C2B-C1B-N9A	-15.32	75.25	113.30
3	D	502	NAD	C2B-C1B-N9A	-15.18	75.59	113.30
3	B	502	NAD	C2B-C1B-N9A	-14.92	76.22	113.30
3	D	502	NAD	O4B-C1B-N9A	13.88	134.74	108.09
3	C	502	NAD	O4B-C1B-N9A	13.81	134.60	108.09
3	A	502	NAD	O4B-C1B-N9A	13.65	134.31	108.09
3	B	502	NAD	O4B-C1B-N9A	13.03	133.11	108.09
3	A	502	NAD	O4B-C4B-C5B	8.45	136.41	109.33
3	C	502	NAD	O4B-C4B-C5B	8.25	135.75	109.33
4	D	503	COA	C5A-C4A-N3A	-8.23	115.39	126.72
3	D	502	NAD	O4B-C4B-C5B	8.11	135.32	109.33
3	B	502	NAD	O4B-C4B-C5B	7.72	134.08	109.33
3	C	502	NAD	C4A-N9A-C8A	-7.66	97.69	105.74
4	A	503	COA	C5A-C4A-N3A	-7.36	116.59	126.72
4	C	503	COA	C5A-C4A-N3A	-7.25	116.73	126.72
4	D	503	COA	N3A-C4A-N9A	6.96	139.01	127.17
4	B	503	COA	C5A-C4A-N3A	-6.88	117.24	126.72
3	C	502	NAD	C4B-O4B-C1B	-6.84	94.36	109.47
2	B	501	FAD	C4'-C3'-C2'	-6.82	102.22	113.57
4	A	503	COA	C7P-C6P-C5P	-6.71	101.21	112.39
4	B	503	COA	N3A-C4A-N9A	6.65	138.48	127.17
4	C	503	COA	N3A-C4A-N9A	6.40	138.06	127.17
3	B	502	NAD	C4B-O4B-C1B	-6.39	95.35	109.47
3	B	502	NAD	C4A-N9A-C8A	-6.31	99.11	105.74
2	C	501	FAD	C5A-C4A-N3A	-6.26	118.09	126.72
3	D	502	NAD	C4A-N9A-C8A	-6.24	99.19	105.74
2	C	501	FAD	C4'-C3'-C2'	-6.22	103.21	113.57
3	C	502	NAD	C6N-N1N-C2N	-6.19	116.61	121.88
3	A	502	NAD	C4B-O4B-C1B	-6.18	95.83	109.47
4	C	503	COA	CEP-CBP-CAP	6.10	119.16	108.77
3	A	502	NAD	C6N-N1N-C2N	-6.02	116.76	121.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	COA	C7P-C6P-C5P	-5.94	102.50	112.39
4	C	503	COA	C3P-N4P-C5P	-5.91	111.82	122.82
4	A	503	COA	C3P-N4P-C5P	-5.86	111.92	122.82
3	D	502	NAD	C4B-O4B-C1B	-5.86	96.54	109.47
4	A	503	COA	N3A-C4A-N9A	5.63	136.74	127.17
3	B	502	NAD	C5A-C4A-N3A	-5.62	118.98	126.72
4	D	503	COA	C2A-N3A-C4A	5.50	125.25	111.83
2	B	501	FAD	N3A-C4A-N9A	5.47	136.47	127.17
2	B	501	FAD	C5A-C4A-N3A	-5.46	119.19	126.72
2	A	501	FAD	C4'-C3'-C2'	-5.46	104.49	113.57
2	B	501	FAD	O4B-C1B-N9A	5.33	118.33	108.09
2	D	501	FAD	C9A-C5X-N5	-5.32	116.81	122.45
3	C	502	NAD	C5A-C4A-N3A	-5.24	119.51	126.72
3	B	502	NAD	C6A-C5A-C4A	5.23	124.32	117.18
4	C	503	COA	C7P-N8P-C9P	-5.19	113.22	122.55
2	B	501	FAD	C4A-N9A-C8A	5.17	111.16	105.74
4	B	503	COA	C7P-C6P-C5P	-5.15	103.81	112.39
4	B	503	COA	C3P-N4P-C5P	-5.15	113.24	122.82
4	A	503	COA	C2A-N3A-C4A	5.03	124.11	111.83
3	C	502	NAD	C5A-C6A-N6A	-4.99	110.93	123.29
3	D	502	NAD	C6N-N1N-C2N	-4.97	117.65	121.88
3	A	502	NAD	C4A-N9A-C8A	-4.95	100.54	105.74
4	D	503	COA	C7P-N8P-C9P	-4.94	113.67	122.55
3	D	502	NAD	C5A-C6A-N6A	-4.89	111.19	123.29
2	C	501	FAD	N3A-C4A-N9A	4.84	135.40	127.17
2	B	501	FAD	C5X-C9A-N10	4.75	122.27	117.97
3	A	502	NAD	C5A-C4A-N3A	-4.73	120.20	126.72
2	D	501	FAD	C5A-C4A-N3A	-4.71	120.23	126.72
3	A	502	NAD	C5B-C4B-C3B	-4.70	98.29	115.21
4	A	503	COA	O4B-C1B-N9A	4.63	116.99	108.09
2	D	501	FAD	N3A-C4A-N9A	4.63	135.04	127.17
3	A	502	NAD	O2B-C2B-C3B	4.53	126.34	111.82
3	A	502	NAD	C5A-C6A-N6A	-4.50	112.15	123.29
3	D	502	NAD	C6A-C5A-N7A	-4.48	123.46	132.09
3	C	502	NAD	C5B-C4B-C3B	-4.39	99.41	115.21
4	D	503	COA	CEP-CBP-CAP	4.38	116.23	108.77
2	A	501	FAD	N3A-C4A-N9A	4.34	134.56	127.17
3	A	502	NAD	C6A-C5A-C4A	4.34	123.10	117.18
3	D	502	NAD	O2B-C2B-C1B	-4.32	95.22	110.10
3	B	502	NAD	O4B-C1B-C2B	-4.31	97.40	106.62
3	C	502	NAD	O3-PN-O1N	-4.29	97.81	110.70
2	D	501	FAD	C5X-C9A-N10	4.29	121.84	117.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	COA	C2A-N3A-C4A	4.28	122.28	111.83
4	C	503	COA	C7P-C6P-C5P	-4.27	105.27	112.39
2	A	501	FAD	C5A-C4A-N3A	-4.27	120.83	126.72
3	D	502	NAD	N6A-C6A-N1A	4.24	127.83	118.38
2	C	501	FAD	C5X-C9A-N10	4.22	121.78	117.97
3	A	502	NAD	N6A-C6A-N1A	4.21	127.76	118.38
4	B	503	COA	C7P-N8P-C9P	-4.20	115.00	122.55
4	B	503	COA	C2A-N3A-C4A	4.16	121.98	111.83
3	B	502	NAD	N3A-C2A-N1A	-4.15	122.30	128.58
3	D	502	NAD	O2N-PN-O3	4.13	118.43	107.27
3	A	502	NAD	O3B-C3B-C4B	-4.13	99.23	111.08
3	D	502	NAD	C4D-O4D-C1D	-4.12	106.16	109.92
3	B	502	NAD	C6A-C5A-N7A	-4.10	124.18	132.09
3	A	502	NAD	O2B-C2B-C1B	-4.08	96.05	110.10
2	D	501	FAD	C4'-C3'-C2'	-4.06	106.82	113.57
4	D	503	COA	C3P-N4P-C5P	-4.05	115.29	122.82
3	B	502	NAD	C6N-N1N-C2N	-4.03	118.45	121.88
2	A	501	FAD	C5X-C9A-N10	4.00	121.59	117.97
3	A	502	NAD	C6A-C5A-N7A	-3.97	124.44	132.09
2	C	501	FAD	C8M-C8-C9	-3.97	112.58	119.57
3	D	502	NAD	C5A-C4A-N3A	-3.93	121.30	126.72
3	C	502	NAD	C5A-C4A-N9A	3.91	110.07	105.81
2	C	501	FAD	C4A-C5A-N7A	-3.87	106.16	110.58
3	B	502	NAD	C5A-C4A-N9A	3.86	110.02	105.81
3	C	502	NAD	C5N-C4N-C3N	-3.86	116.57	120.36
4	A	503	COA	N3A-C2A-N1A	-3.85	122.76	128.58
4	B	503	COA	C4A-N9A-C8A	3.83	109.76	105.74
4	B	503	COA	N6A-C6A-N1A	3.81	126.87	118.38
4	B	503	COA	C5A-C6A-N6A	-3.77	113.94	123.29
3	D	502	NAD	C3B-C2B-C1B	3.76	108.57	101.46
3	C	502	NAD	O2B-C2B-C3B	3.75	123.83	111.82
4	A	503	COA	CDP-CBP-CAP	3.73	115.13	108.77
2	B	501	FAD	C5A-N7A-C8A	3.71	109.28	103.45
2	A	501	FAD	O2B-C2B-C3B	-3.67	100.05	111.82
3	D	502	NAD	O3-PN-O1N	-3.67	99.67	110.70
2	B	501	FAD	C4A-C5A-N7A	-3.65	106.40	110.58
3	A	502	NAD	O3-PN-O1N	-3.65	99.73	110.70
3	D	502	NAD	C5B-C4B-C3B	-3.65	102.08	115.21
4	C	503	COA	CDP-CBP-CCP	3.64	114.24	108.22
2	B	501	FAD	O4-C4-C4X	-3.63	116.94	126.53
2	A	501	FAD	O4-C4-C4X	-3.62	116.99	126.53
2	B	501	FAD	N9A-C8A-N7A	-3.61	108.81	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	COA	N3A-C2A-N1A	-3.59	123.14	128.58
2	D	501	FAD	C4A-N9A-C8A	3.59	109.51	105.74
3	D	502	NAD	C4A-C5A-N7A	3.59	114.68	110.58
3	C	502	NAD	C6A-C5A-N7A	-3.58	125.19	132.09
3	D	502	NAD	N3A-C2A-N1A	-3.58	123.16	128.58
4	D	503	COA	O3B-P3B-O7A	-3.58	96.58	109.33
3	B	502	NAD	O7N-C7N-C3N	3.55	123.94	119.60
4	D	503	COA	O9P-C9P-N8P	-3.54	115.48	122.98
2	A	501	FAD	C10-N1-C2	3.54	124.52	116.85
2	D	501	FAD	O3P-P-O1P	-3.53	100.08	110.70
2	C	501	FAD	C9A-C5X-N5	-3.52	118.72	122.45
3	B	502	NAD	C5B-C4B-C3B	-3.52	102.54	115.21
3	D	502	NAD	O2B-C2B-C3B	3.47	122.95	111.82
3	C	502	NAD	N6A-C6A-N1A	3.46	126.08	118.38
2	B	501	FAD	C2A-N3A-C4A	3.44	120.24	111.83
3	B	502	NAD	O3-PN-O1N	-3.44	100.35	110.70
2	A	501	FAD	C9A-N10-C10	-3.43	115.52	120.75
4	A	503	COA	CEP-CBP-CAP	3.42	114.60	108.77
3	C	502	NAD	O2N-PN-O3	3.41	116.49	107.27
4	A	503	COA	C7P-N8P-C9P	-3.40	116.43	122.55
3	D	502	NAD	C6A-C5A-C4A	3.40	121.82	117.18
2	B	501	FAD	N6A-C6A-N1A	3.40	125.95	118.38
3	B	502	NAD	N6A-C6A-N1A	3.40	125.94	118.38
2	C	501	FAD	C2A-N3A-C4A	3.36	120.05	111.83
3	B	502	NAD	O2N-PN-O3	3.34	116.31	107.27
2	A	501	FAD	O4B-C4B-C3B	3.34	111.78	105.15
4	D	503	COA	C6P-C5P-N4P	3.30	122.35	116.34
3	C	502	NAD	N9A-C8A-N7A	3.29	118.61	113.94
4	C	503	COA	C4A-N9A-C8A	3.26	109.16	105.74
2	C	501	FAD	C5A-N7A-C8A	3.26	108.57	103.45
4	D	503	COA	C4A-C5A-N7A	-3.23	106.89	110.58
2	B	501	FAD	C9A-N10-C10	-3.22	115.85	120.75
2	A	501	FAD	N6A-C6A-N1A	3.21	125.53	118.38
2	B	501	FAD	O4B-C4B-C3B	3.20	111.51	105.15
4	A	503	COA	O6A-CCP-CBP	-3.18	105.43	110.55
4	C	503	COA	C4A-C5A-N7A	-3.18	106.94	110.58
4	B	503	COA	CDP-CBP-CCP	3.17	113.46	108.22
2	A	501	FAD	C3B-C2B-C1B	3.16	107.44	101.46
4	D	503	COA	O6A-CCP-CBP	-3.16	105.47	110.55
3	D	502	NAD	O5D-PN-O1N	3.15	121.43	108.94
3	C	502	NAD	C6N-C5N-C4N	3.15	123.99	119.45
3	B	502	NAD	O2B-C2B-C3B	3.14	121.89	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAD	O2B-C2B-C1B	-3.12	99.35	110.10
3	A	502	NAD	O7N-C7N-N7N	-3.12	118.11	122.62
2	B	501	FAD	N3A-C2A-N1A	-3.12	123.86	128.58
3	D	502	NAD	C5N-C4N-C3N	-3.11	117.31	120.36
3	C	502	NAD	C6A-C5A-C4A	3.11	121.42	117.18
4	C	503	COA	O6A-CCP-CBP	-3.10	105.56	110.55
3	D	502	NAD	C1B-N9A-C8A	3.10	133.97	127.09
4	A	503	COA	O5P-C5P-N4P	-3.09	116.97	123.03
2	B	501	FAD	O4'-C4'-C5'	3.07	116.76	109.99
3	D	502	NAD	C5A-C4A-N9A	3.07	109.16	105.81
2	A	501	FAD	O4'-C4'-C3'	3.03	116.34	109.25
4	D	503	COA	C4A-N9A-C8A	3.01	108.90	105.74
3	D	502	NAD	O4D-C4D-C3D	2.99	111.08	105.15
4	D	503	COA	O5P-C5P-N4P	-2.98	117.18	123.03
3	B	502	NAD	O7N-C7N-N7N	-2.98	118.31	122.62
4	B	503	COA	O3B-P3B-O7A	-2.98	98.73	109.33
3	B	502	NAD	C3B-C2B-C1B	2.94	107.02	101.46
3	C	502	NAD	C5D-C4D-C3D	-2.91	104.73	115.21
2	D	501	FAD	O4B-C1B-N9A	2.91	113.67	108.09
2	D	501	FAD	O2B-C2B-C3B	-2.90	102.51	111.82
4	B	503	COA	N3A-C2A-N1A	-2.89	124.20	128.58
4	C	503	COA	CEP-CBP-CCP	-2.89	103.46	108.22
3	A	502	NAD	O7N-C7N-C3N	2.89	123.13	119.60
4	A	503	COA	C4A-C5A-N7A	-2.88	107.29	110.58
4	C	503	COA	C5A-N7A-C8A	2.87	107.96	103.45
3	D	502	NAD	C5A-N7A-C8A	-2.86	98.95	103.45
2	C	501	FAD	C10-N1-C2	2.86	123.04	116.85
3	A	502	NAD	C5A-C4A-N9A	2.85	108.92	105.81
3	A	502	NAD	O2N-PN-O3	2.83	114.93	107.27
2	B	501	FAD	C1'-N10-C9A	2.82	126.11	120.63
3	A	502	NAD	C3B-C2B-C1B	2.82	106.79	101.46
4	C	503	COA	CEP-CBP-CDP	-2.81	103.59	109.20
4	D	503	COA	CDP-CBP-CAP	2.77	113.49	108.77
2	D	501	FAD	O4-C4-C4X	-2.77	119.22	126.53
4	C	503	COA	N6A-C6A-N1A	2.76	124.53	118.38
4	B	503	COA	O2A-P1A-O3A	2.76	114.73	107.27
3	D	502	NAD	N9A-C8A-N7A	2.75	117.84	113.94
3	A	502	NAD	O4B-C1B-C2B	-2.75	100.73	106.62
2	A	501	FAD	C4X-C10-N1	-2.75	117.85	124.59
2	B	501	FAD	O2-C2-N1	-2.74	117.25	121.80
2	C	501	FAD	O4-C4-C4X	-2.73	119.32	126.53
4	C	503	COA	O3B-P3B-O7A	-2.72	99.63	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NAD	C2B-C3B-C4B	-2.71	97.37	102.61
4	D	503	COA	CAP-C9P-N8P	2.70	121.61	116.48
3	C	502	NAD	O7N-C7N-C3N	2.69	122.89	119.60
4	C	503	COA	O4B-C1B-N9A	2.69	113.25	108.09
3	B	502	NAD	C2A-N3A-C4A	2.69	118.39	111.83
4	D	503	COA	C5A-C6A-N6A	-2.68	116.66	123.29
2	A	501	FAD	O2P-P-O5'	2.67	119.69	107.57
4	B	503	COA	CEP-CBP-CCP	-2.67	103.82	108.22
3	A	502	NAD	C2D-C3D-C4D	-2.66	97.47	102.61
4	A	503	COA	C3B-C2B-C1B	2.65	105.73	99.89
4	D	503	COA	O4B-C1B-N9A	2.65	113.18	108.09
3	C	502	NAD	C2A-N1A-C6A	-2.65	114.38	118.73
2	B	501	FAD	O4-C4-N3	2.65	125.09	120.11
2	C	501	FAD	C4A-N9A-C8A	2.64	108.51	105.74
2	C	501	FAD	O4'-C4'-C5'	2.63	115.79	109.99
3	C	502	NAD	C3B-C2B-C1B	2.63	106.44	101.46
4	C	503	COA	C5A-C6A-N6A	-2.62	116.80	123.29
2	D	501	FAD	C4A-C5A-N7A	-2.61	107.59	110.58
4	B	503	COA	O4B-C1B-N9A	2.60	113.09	108.09
4	B	503	COA	C4A-C5A-N7A	-2.60	107.61	110.58
2	C	501	FAD	N9A-C8A-N7A	-2.57	110.29	113.94
3	B	502	NAD	C5A-C6A-N6A	-2.56	116.95	123.29
4	D	503	COA	O5A-P2A-O4A	2.56	124.34	112.44
2	C	501	FAD	C1'-N10-C9A	2.55	125.58	120.63
2	C	501	FAD	C2B-C1B-N9A	-2.54	106.99	113.30
2	A	501	FAD	O2P-P-O3P	-2.54	100.40	107.27
2	C	501	FAD	C9A-N10-C10	-2.54	116.88	120.75
4	D	503	COA	O2A-P1A-O3A	2.53	114.10	107.27
2	B	501	FAD	C9A-C5X-N5	-2.52	119.78	122.45
3	A	502	NAD	C6N-N1N-C1D	2.51	124.66	119.73
4	D	503	COA	O9A-P3B-O7A	2.51	120.60	110.83
2	C	501	FAD	C8M-C8-C7	2.51	125.88	120.76
3	B	502	NAD	C5D-C4D-C3D	-2.51	106.19	115.21
2	D	501	FAD	O2P-P-O1P	2.50	124.09	112.44
2	D	501	FAD	O4B-C4B-C5B	-2.50	101.33	109.33
3	C	502	NAD	N3A-C2A-N1A	-2.50	124.81	128.58
4	D	503	COA	C5A-N7A-C8A	2.49	107.36	103.45
3	D	502	NAD	O4B-C1B-C2B	-2.45	101.37	106.62
3	C	502	NAD	C4A-C5A-N7A	2.45	113.38	110.58
2	D	501	FAD	C3B-C2B-C1B	2.44	106.08	101.46
2	B	501	FAD	C2A-N1A-C6A	2.44	122.74	118.73
2	D	501	FAD	C2A-N3A-C4A	2.44	117.78	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NAD	O3B-C3B-C4B	-2.43	104.11	111.08
2	B	501	FAD	O2P-P-O3P	-2.43	100.71	107.27
2	C	501	FAD	O4B-C1B-N9A	2.42	112.73	108.09
2	D	501	FAD	N6A-C6A-N1A	2.42	123.76	118.38
3	D	502	NAD	C5D-C4D-C3D	-2.41	106.53	115.21
2	A	501	FAD	C4A-N9A-C8A	2.39	108.25	105.74
4	B	503	COA	O5A-P2A-O4A	2.38	123.54	112.44
4	A	503	COA	CAP-C9P-N8P	2.37	120.98	116.48
2	A	501	FAD	C4X-C10-N10	2.36	119.86	116.48
4	C	503	COA	N3A-C2A-N1A	-2.35	125.02	128.58
2	A	501	FAD	C5A-C6A-N6A	-2.35	117.46	123.29
3	A	502	NAD	C4D-O4D-C1D	-2.34	107.78	109.92
2	D	501	FAD	C10-N1-C2	2.33	121.88	116.85
3	A	502	NAD	O5D-PN-O1N	2.32	118.14	108.94
4	B	503	COA	C5A-N7A-C8A	2.32	107.10	103.45
4	A	503	COA	N6A-C6A-N1A	2.31	123.52	118.38
2	A	501	FAD	O4-C4-N3	2.31	124.45	120.11
3	C	502	NAD	O5D-C5D-C4D	2.30	116.82	108.99
3	B	502	NAD	C2B-C3B-C4B	-2.27	98.22	102.61
2	D	501	FAD	C5X-N5-C4X	2.27	121.75	118.09
4	A	503	COA	O2A-P1A-O3A	2.26	113.39	107.27
4	C	503	COA	N9A-C8A-N7A	-2.26	110.72	113.94
3	A	502	NAD	O5D-C5D-C4D	2.26	116.70	108.99
3	C	502	NAD	C1B-N9A-C8A	2.26	132.12	127.09
4	B	503	COA	C3B-C2B-C1B	2.26	104.86	99.89
3	B	502	NAD	N3A-C4A-N9A	2.25	130.99	127.17
3	A	502	NAD	C2A-N1A-C6A	-2.24	115.06	118.73
2	C	501	FAD	C3B-C2B-C1B	2.24	105.69	101.46
4	C	503	COA	O9P-C9P-N8P	-2.23	118.25	122.98
3	B	502	NAD	O5D-C5D-C4D	2.23	116.60	108.99
3	A	502	NAD	C5D-C4D-C3D	-2.23	107.18	115.21
4	B	503	COA	CDP-CBP-CAP	2.23	112.56	108.77
4	A	503	COA	O3B-P3B-O7A	-2.22	101.42	109.33
3	C	502	NAD	C5A-N7A-C8A	-2.20	100.00	103.45
4	A	503	COA	O5A-P2A-O3A	2.20	113.21	107.27
2	B	501	FAD	C2B-C1B-N9A	-2.18	107.89	113.30
4	A	503	COA	C6P-C5P-N4P	2.18	120.31	116.34
3	A	502	NAD	N3A-C4A-N9A	2.17	130.86	127.17
2	D	501	FAD	C9-C9A-C5X	-2.17	116.19	120.03
4	C	503	COA	CDP-CBP-CAP	2.17	112.46	108.77
4	A	503	COA	O2A-P1A-O1A	2.16	122.49	112.44
3	C	502	NAD	C5A-C6A-N1A	2.15	122.98	117.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	COA	O5B-P1A-O1A	-2.15	100.40	108.94
2	D	501	FAD	C8M-C8-C9	-2.15	115.79	119.57
2	C	501	FAD	C4-C4X-N5	2.13	121.14	118.21
3	B	502	NAD	O2A-PA-O5B	-2.12	97.95	107.57
2	D	501	FAD	O5B-PA-O1A	2.12	117.32	108.94
2	C	501	FAD	C4X-C4-N3	2.12	118.64	113.25
4	D	503	COA	O8A-P3B-O7A	2.11	119.08	110.83
3	A	502	NAD	O4D-C4D-C3D	2.09	109.31	105.15
2	D	501	FAD	C1'-N10-C9A	2.09	124.69	120.63
2	A	501	FAD	C4X-C4-N3	2.08	118.55	113.25
4	C	503	COA	O2A-P1A-O3A	2.08	112.88	107.27
2	D	501	FAD	O4'-C4'-C3'	2.07	114.10	109.25
2	D	501	FAD	C2B-C1B-N9A	-2.07	108.17	113.30
2	A	501	FAD	O2A-PA-O1A	2.06	122.05	112.44
4	C	503	COA	O9A-P3B-O7A	2.06	118.87	110.83
2	B	501	FAD	O5'-C5'-C4'	2.06	114.86	109.36
3	C	502	NAD	C2A-N3A-C4A	2.06	116.86	111.83
4	C	503	COA	P3B-O3B-C3B	2.06	128.93	123.43
3	D	502	NAD	C6N-C5N-C4N	2.06	122.42	119.45
2	C	501	FAD	C6A-C5A-N7A	2.06	136.06	132.09
2	C	501	FAD	O3P-PA-O1A	2.05	116.88	110.70
4	B	503	COA	CEP-CBP-CAP	2.05	112.27	108.77
3	B	502	NAD	C5N-C4N-C3N	-2.04	118.36	120.36
2	D	501	FAD	C6-C5X-C9A	2.04	121.85	119.05
4	B	503	COA	C1B-N9A-C8A	-2.04	122.58	127.09
3	C	502	NAD	O7N-C7N-N7N	-2.04	119.67	122.62
2	C	501	FAD	C4X-C10-N1	-2.04	119.60	124.59
2	D	501	FAD	C5A-N7A-C8A	2.03	106.65	103.45
3	A	502	NAD	C2B-C3B-C4B	-2.03	98.68	102.61
4	D	503	COA	N6A-C6A-N1A	2.03	122.90	118.38
2	B	501	FAD	O2P-P-O1P	2.03	121.88	112.44
2	D	501	FAD	C9A-N10-C10	-2.01	117.68	120.75

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C3'-C4'-C5'-O5'
2	A	501	FAD	C5'-O5'-P-O2P
2	B	501	FAD	C1'-C2'-C3'-C4'
2	B	501	FAD	C5'-O5'-P-O2P
2	C	501	FAD	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	FAD	C3'-C4'-C5'-O5'
3	A	502	NAD	C5D-O5D-PN-O3
3	A	502	NAD	C5D-O5D-PN-O2N
3	B	502	NAD	C5D-O5D-PN-O3
3	B	502	NAD	C5D-O5D-PN-O2N
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
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	B	503	COA	CCP-O6A-P2A-O3A
4	B	503	COA	CCP-O6A-P2A-O4A
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	C	503	COA	CCP-O6A-P2A-O3A
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
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
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	A	503	COA	C6P-C5P-N4P-C3P
4	D	503	COA	C6P-C5P-N4P-C3P
4	A	503	COA	O5P-C5P-N4P-C3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	503	COA	C6P-C5P-N4P-C3P
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	C	503	COA	C6P-C5P-N4P-C3P
4	B	503	COA	O5P-C5P-N4P-C3P
2	D	501	FAD	O4'-C4'-C5'-O5'
4	B	503	COA	C2B-C3B-O3B-P3B
4	D	503	COA	C2B-C3B-O3B-P3B
4	C	503	COA	O5P-C5P-N4P-C3P
2	A	501	FAD	O4B-C4B-C5B-O5B
3	A	502	NAD	O4D-C4D-C5D-O5D
4	A	503	COA	O4B-C4B-C5B-O5B
4	B	503	COA	O4B-C4B-C5B-O5B
2	B	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	D	503	COA	P1A-O3A-P2A-O4A
4	D	503	COA	C3B-O3B-P3B-O9A
2	B	501	FAD	C3B-C4B-C5B-O5B
3	D	502	NAD	O4D-C4D-C5D-O5D
4	A	503	COA	C3B-C4B-C5B-O5B
4	D	503	COA	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
4	C	503	COA	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	B	503	COA	P2A-O3A-P1A-O1A
4	D	503	COA	P2A-O3A-P1A-O1A
4	D	503	COA	P1A-O3A-P2A-O5A
2	D	501	FAD	C3B-C4B-C5B-O5B
2	D	501	FAD	C5'-O5'-P-O1P
3	A	502	NAD	C5B-O5B-PA-O1A
3	B	502	NAD	C5B-O5B-PA-O1A
3	C	502	NAD	C5B-O5B-PA-O1A
4	D	503	COA	C3B-C4B-C5B-O5B
4	A	503	COA	P1A-O3A-P2A-O5A
4	B	503	COA	P2A-O3A-P1A-O2A
4	B	503	COA	P1A-O3A-P2A-O5A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	503	COA	P2A-O3A-P1A-O1A
4	C	503	COA	P2A-O3A-P1A-O2A
4	C	503	COA	P1A-O3A-P2A-O5A
4	D	503	COA	P2A-O3A-P1A-O2A
4	C	503	COA	C3B-O3B-P3B-O9A
2	D	501	FAD	O4B-C4B-C5B-O5B
4	D	503	COA	C2P-C3P-N4P-C5P
4	B	503	COA	C3B-C4B-C5B-O5B
4	A	503	COA	C3B-O3B-P3B-O7A
2	C	501	FAD	P-O3P-PA-O2A
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	O2'-C2'-C3'-C4'
2	B	501	FAD	C1'-C2'-C3'-O3'
2	D	501	FAD	C1'-C2'-C3'-O3'
2	C	501	FAD	O4B-C4B-C5B-O5B
3	A	502	NAD	C3D-C4D-C5D-O5D
3	B	502	NAD	O4B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	P-O3P-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
3	A	502	NAD	O4B-C4B-C5B-O5B
4	A	503	COA	C3B-O3B-P3B-O8A
2	C	501	FAD	C3B-C4B-C5B-O5B
4	B	503	COA	C3B-O3B-P3B-O7A
4	C	503	COA	C3B-O3B-P3B-O7A
4	D	503	COA	C3B-O3B-P3B-O7A
4	C	503	COA	C3B-C4B-C5B-O5B
2	A	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	P-O3P-PA-O1A
4	B	503	COA	P1A-O3A-P2A-O4A

There are no ring outliers.

11 monomers are involved in 81 short contacts:

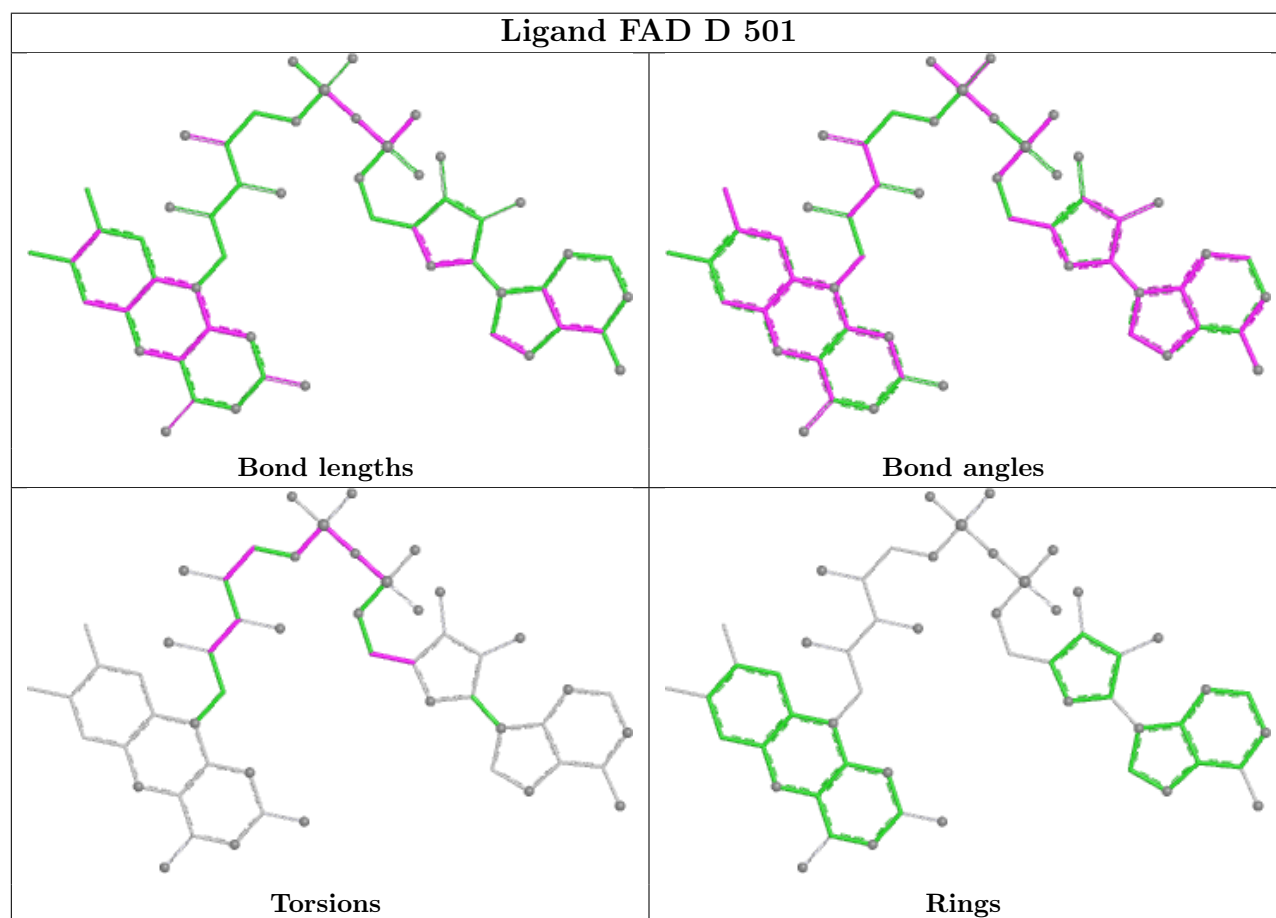
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FAD	6	0
2	A	501	FAD	7	0
3	A	502	NAD	11	0
3	D	502	NAD	12	0

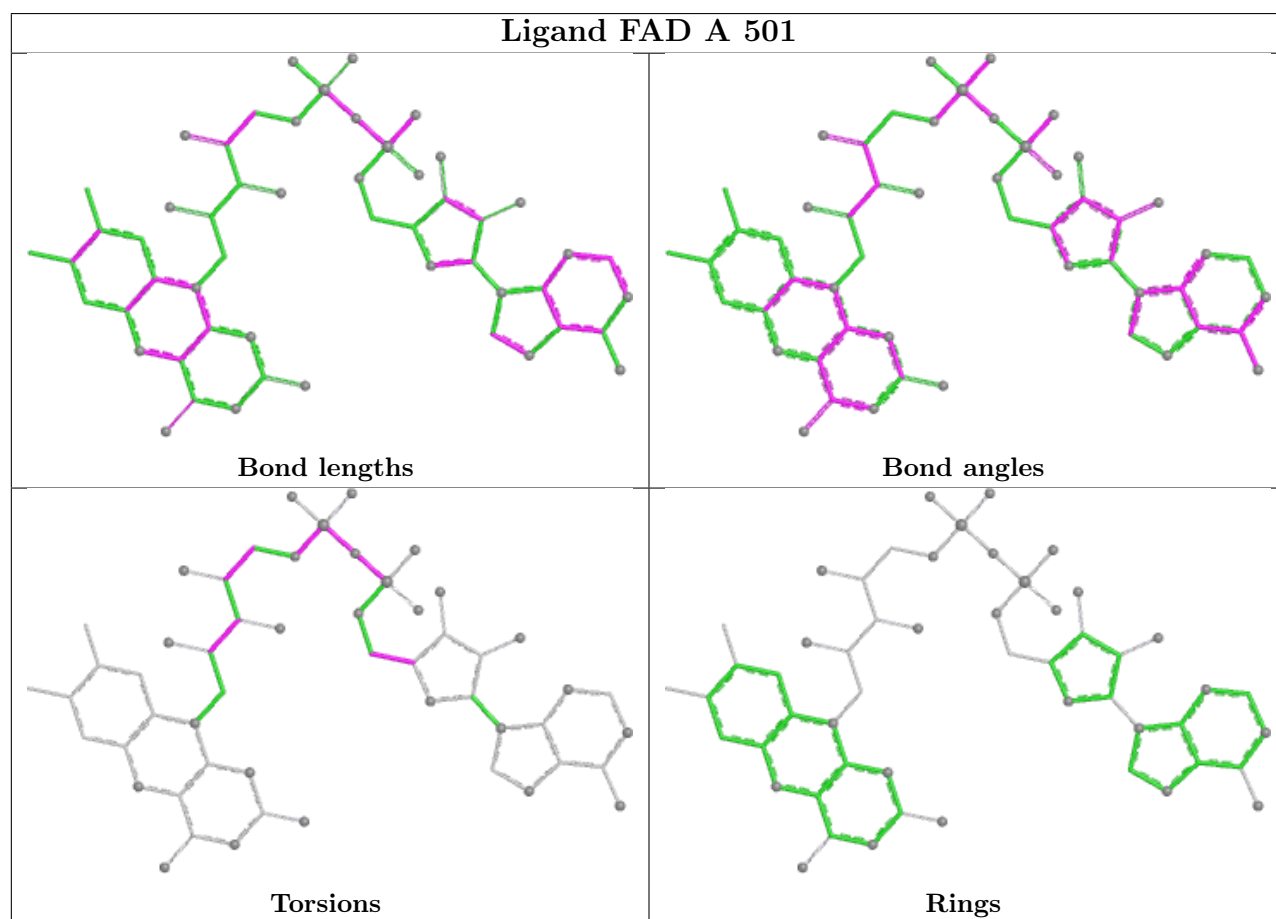
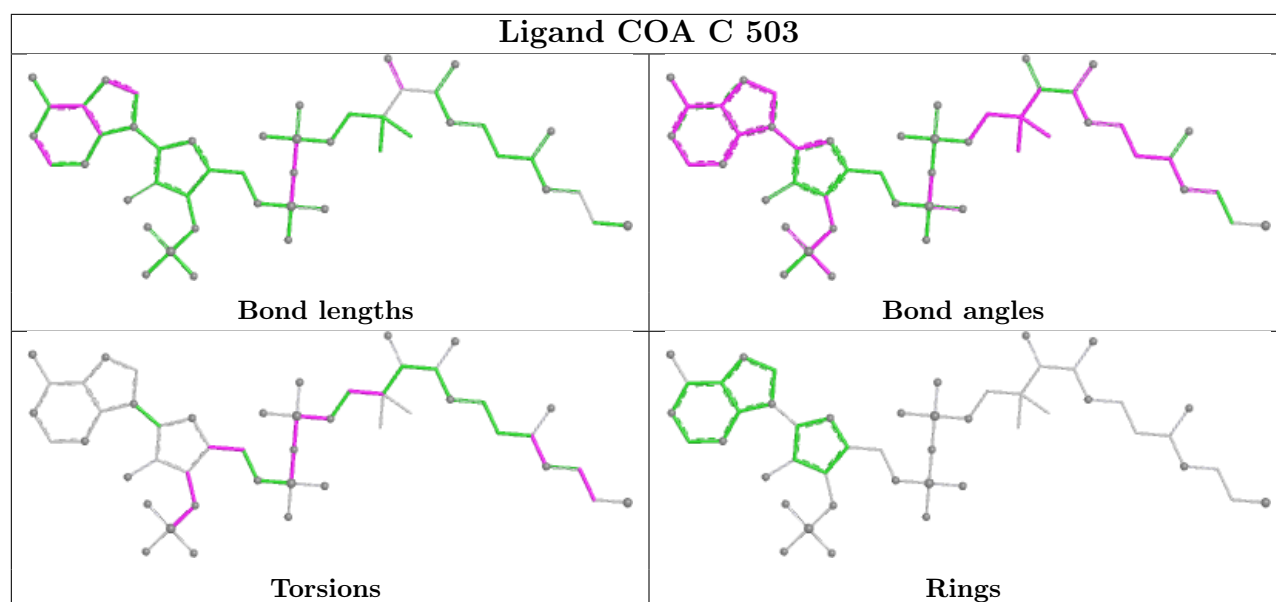
Continued on next page...

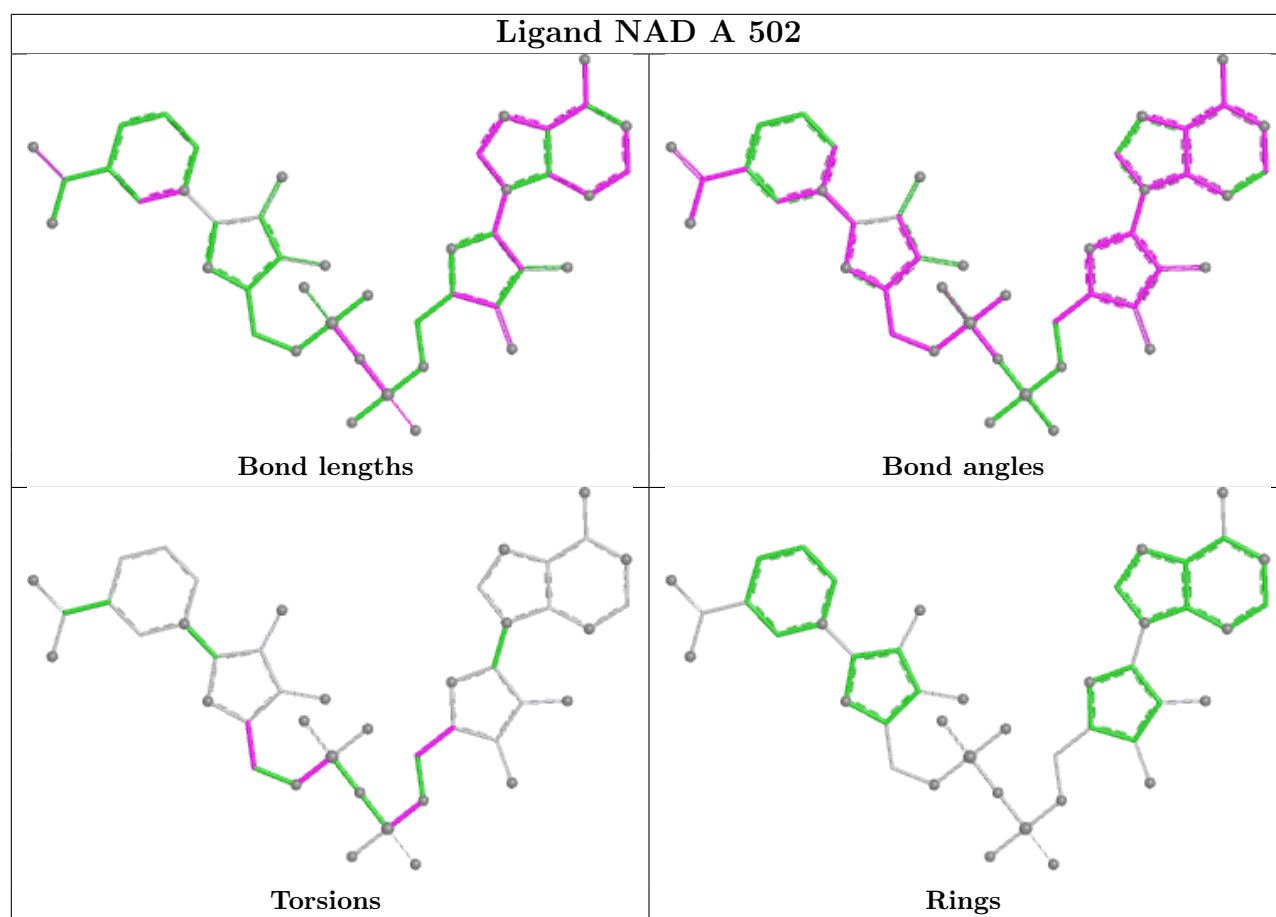
Continued from previous page...

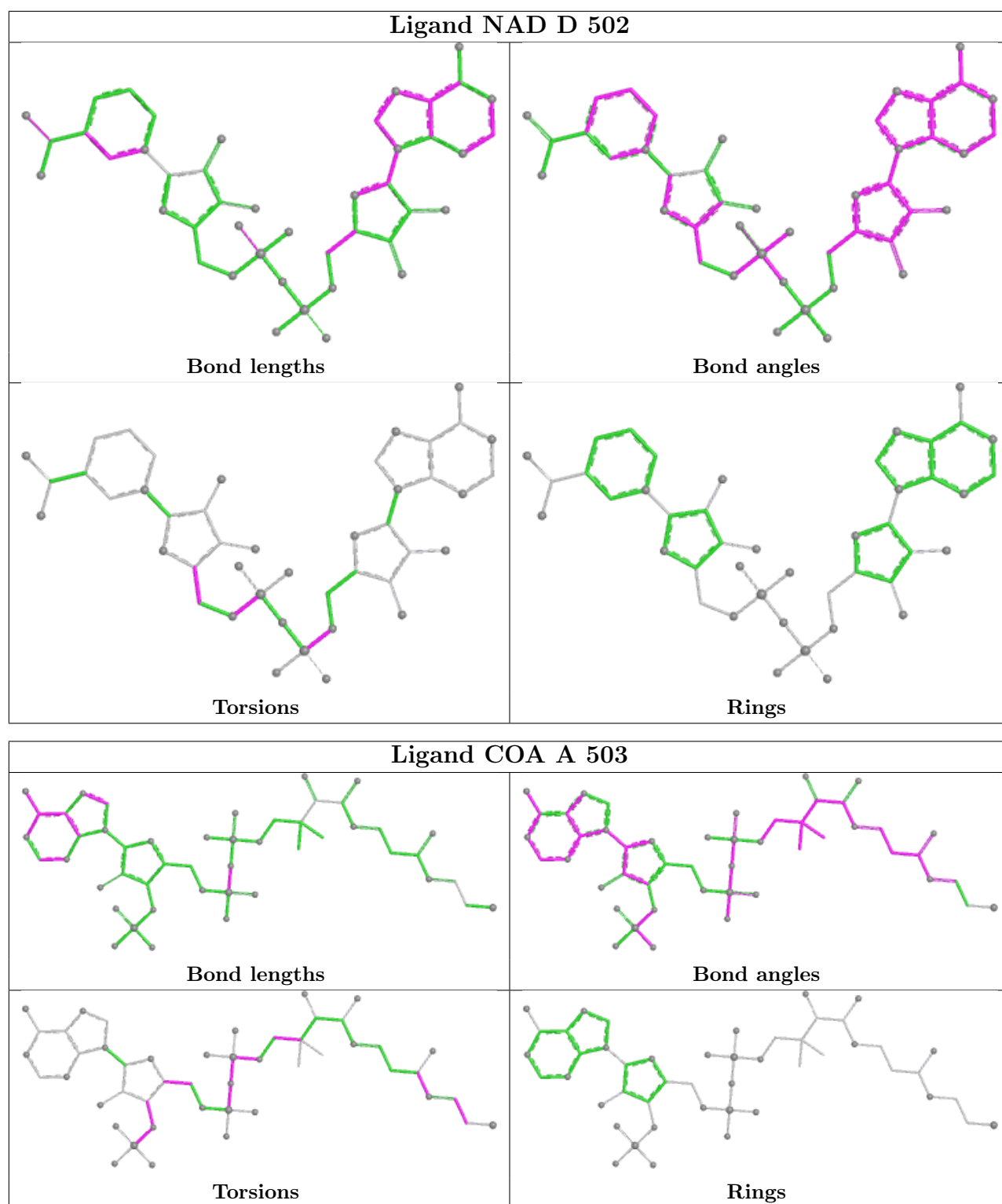
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	COA	3	0
3	B	502	NAD	10	0
4	B	503	COA	5	0
4	D	503	COA	3	0
2	B	501	FAD	11	0
2	C	501	FAD	7	0
3	C	502	NAD	9	0

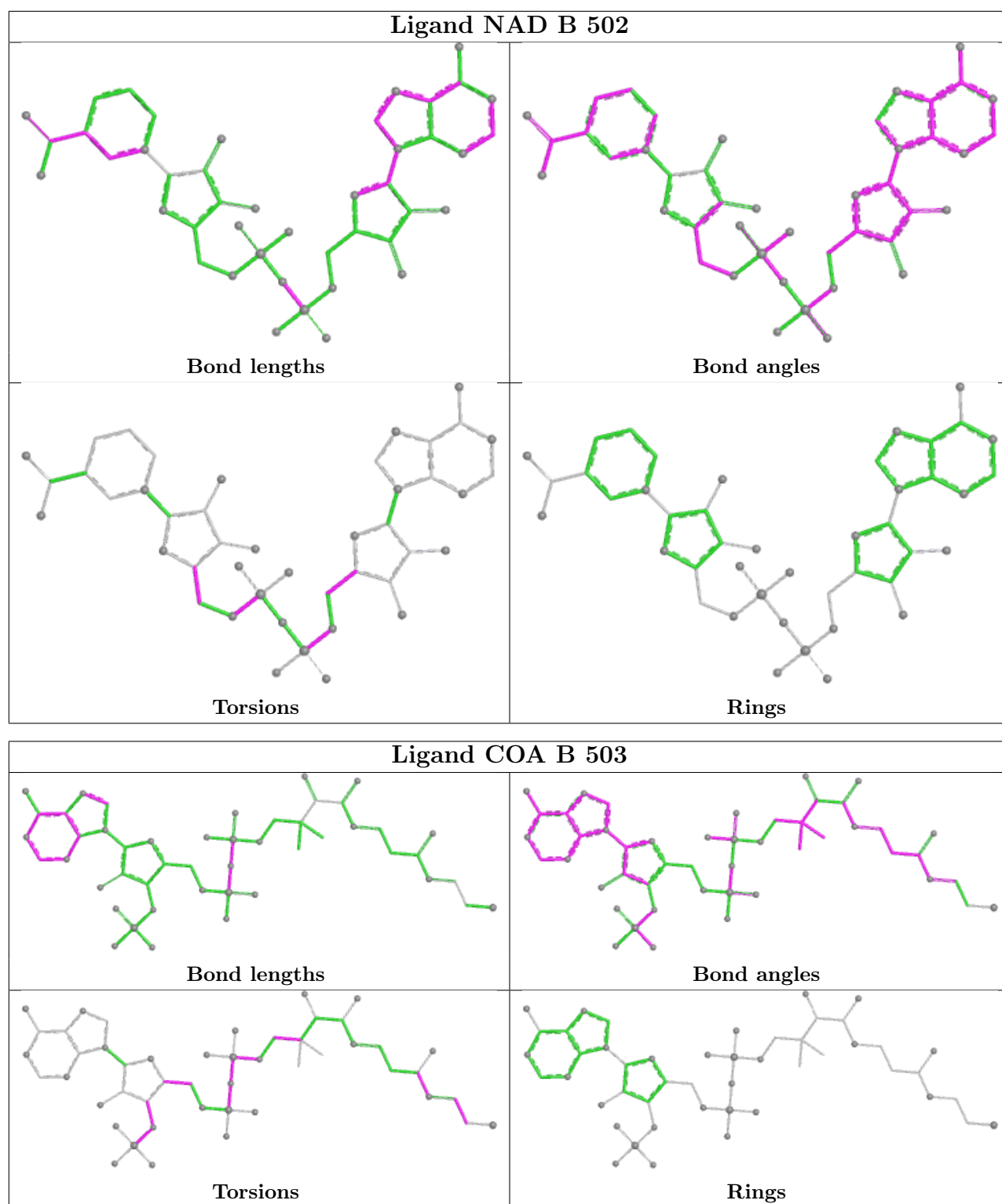
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

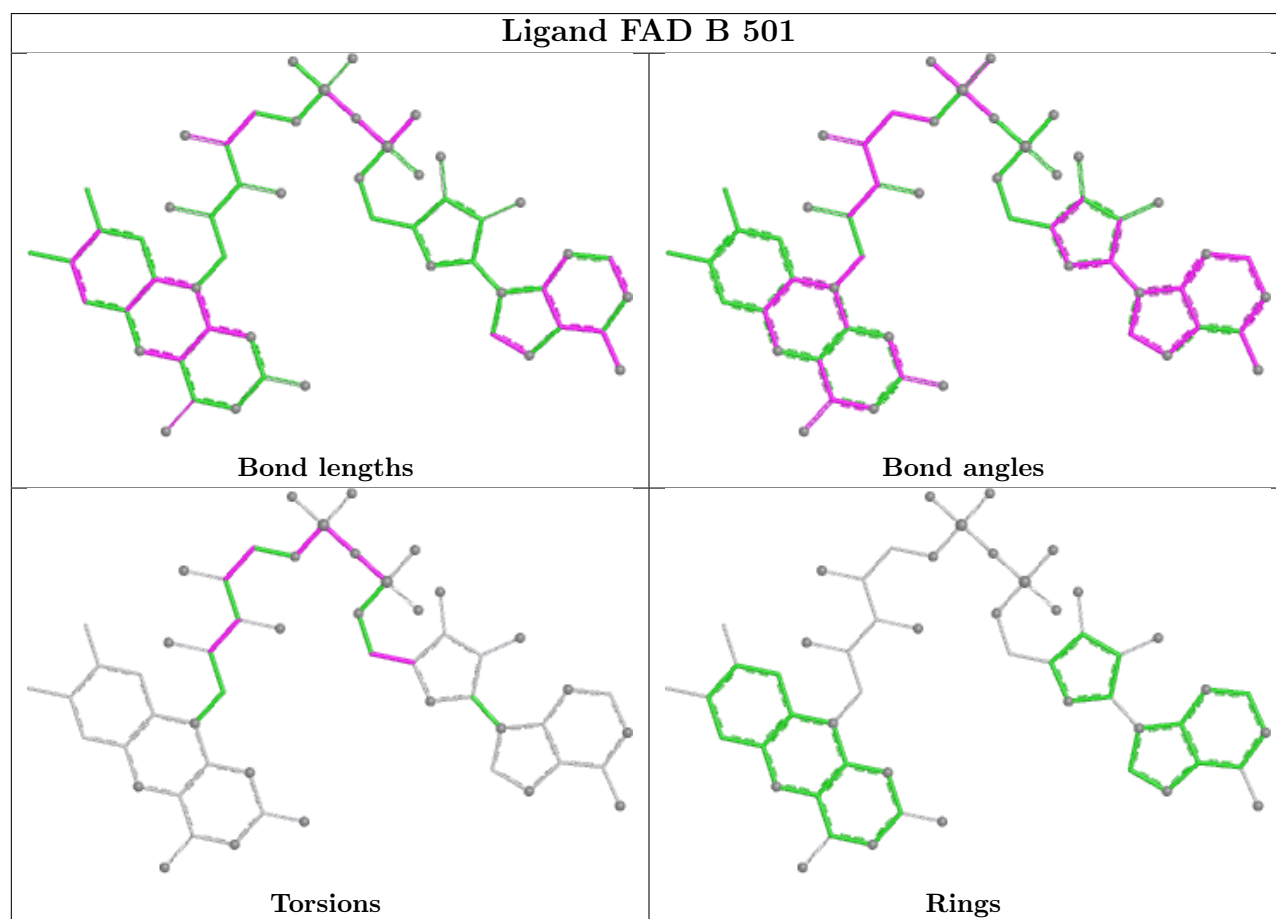
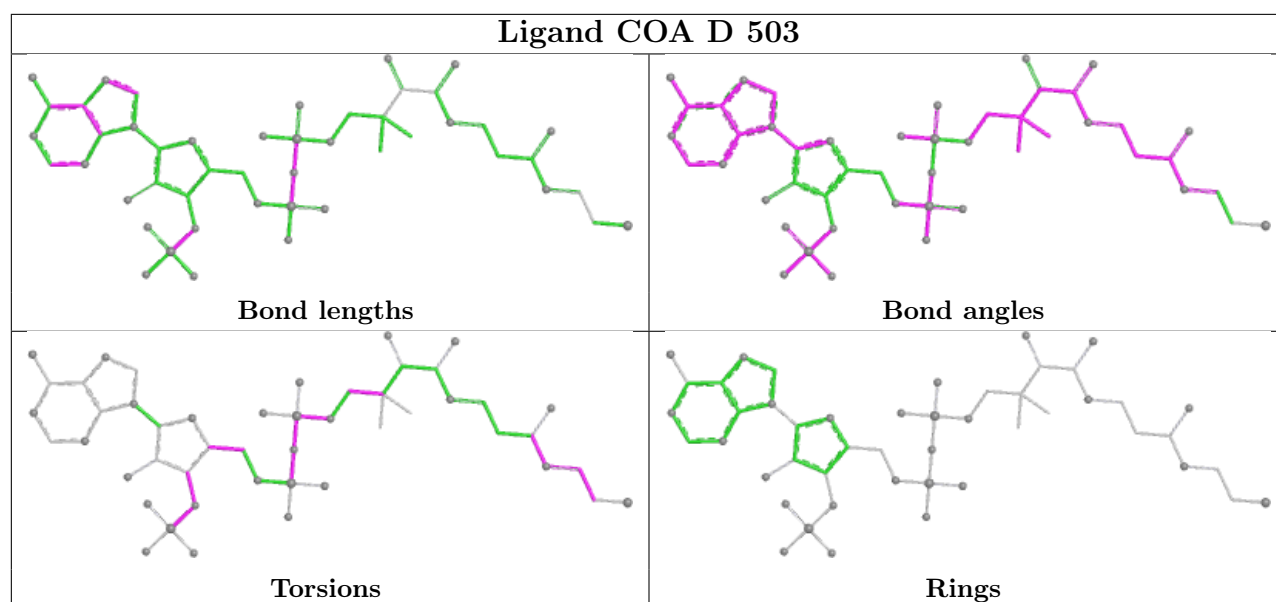


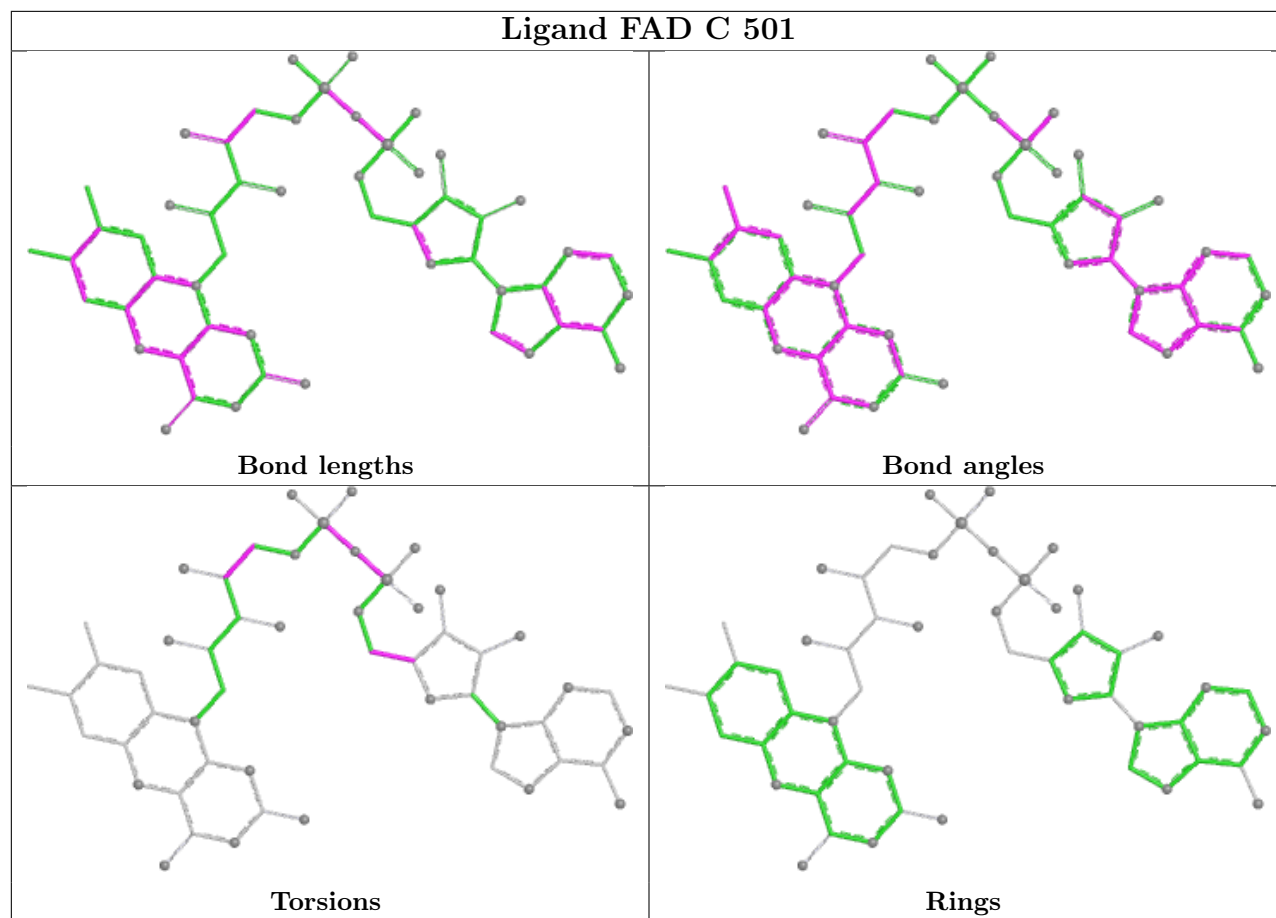


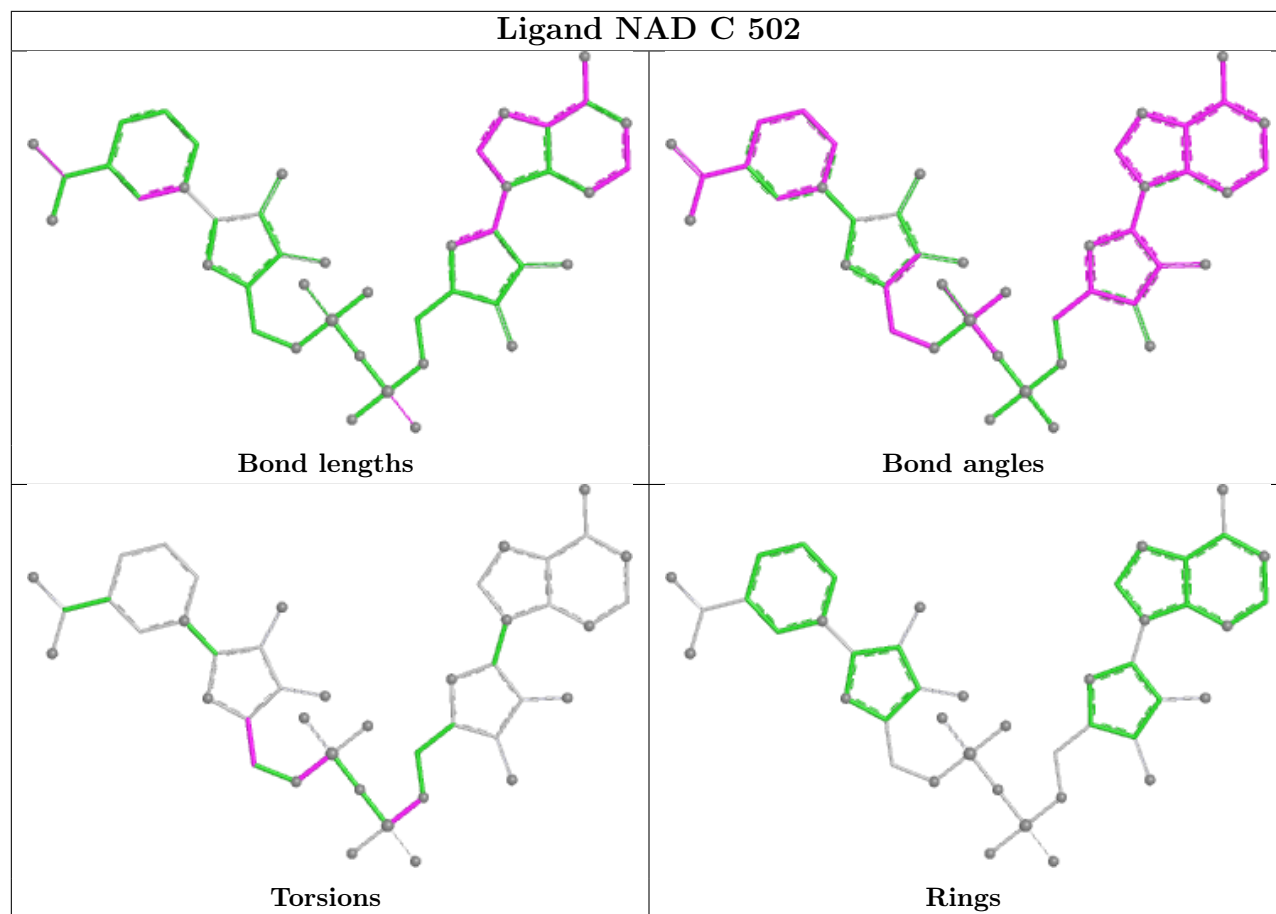












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.37	10 (2%) 61 52	30, 47, 75, 130	0
1	B	443/443 (100%)	-0.29	13 (2%) 53 45	31, 49, 77, 129	0
1	C	443/443 (100%)	-0.39	12 (2%) 56 47	31, 48, 76, 132	0
1	D	443/443 (100%)	-0.33	17 (3%) 44 36	29, 49, 78, 132	0
All	All	1772/1772 (100%)	-0.34	52 (2%) 53 45	29, 48, 77, 132	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.2
1	D	1	MET	6.2
1	C	1	MET	6.1
1	B	1	MET	5.3
1	A	88	LEU	5.2
1	A	86	TYR	5.0
1	C	88	LEU	4.8
1	A	2	GLY	4.4
1	D	443	ARG	4.3
1	B	88	LEU	4.2
1	D	442	ALA	4.2
1	A	443	ARG	4.1
1	C	86	TYR	4.1
1	A	91	LEU	4.0
1	B	86	TYR	3.9
1	A	442	ALA	3.9
1	D	2	GLY	3.7
1	B	443	ARG	3.5
1	B	91	LEU	3.3
1	C	91	LEU	3.2
1	C	443	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	442	ALA	3.1
1	C	317	GLU	3.1
1	B	2	GLY	3.0
1	D	88	LEU	3.0
1	A	396	HIS	3.0
1	D	274	GLU	2.8
1	A	92	THR	2.8
1	D	91	LEU	2.6
1	D	78	ARG	2.6
1	D	86	TYR	2.6
1	C	2	GLY	2.6
1	B	92	THR	2.6
1	B	87	GLU	2.5
1	B	160	ILE	2.4
1	A	440	GLN	2.3
1	D	396	HIS	2.3
1	B	396	HIS	2.3
1	D	87	GLU	2.2
1	D	96	HIS	2.2
1	C	352	TRP	2.2
1	D	352	TRP	2.2
1	B	411	GLU	2.2
1	C	442	ALA	2.2
1	D	95	ASP	2.2
1	C	90	THR	2.2
1	D	90	THR	2.2
1	D	160	ILE	2.1
1	B	90	THR	2.1
1	C	396	HIS	2.1
1	C	221	ARG	2.1
1	D	440	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

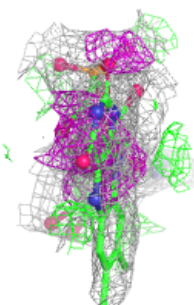
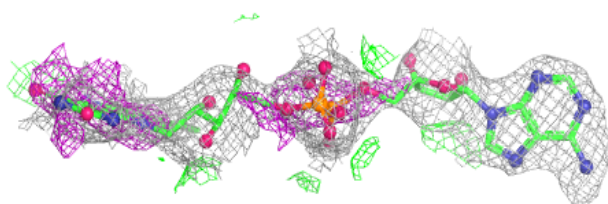
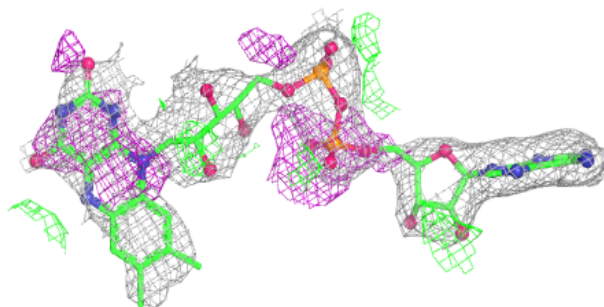
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	501	53/53	0.84	0.15	57,76,96,111	0
2	FAD	A	501	53/53	0.89	0.13	53,71,92,117	0
2	FAD	D	501	53/53	0.89	0.13	49,74,93,109	0
2	FAD	C	501	53/53	0.93	0.11	51,73,93,97	0
3	NAD	B	502	44/44	0.94	0.11	43,64,82,87	0
4	COA	A	503	48/48	0.94	0.10	54,72,85,110	0
4	COA	C	503	48/48	0.94	0.09	54,71,80,116	0
3	NAD	C	502	44/44	0.96	0.09	39,57,78,82	0
4	COA	B	503	48/48	0.96	0.08	54,70,80,103	0
3	NAD	D	502	44/44	0.96	0.09	45,62,79,82	0
4	COA	D	503	48/48	0.96	0.08	51,71,81,111	0
3	NAD	A	502	44/44	0.97	0.08	39,58,76,83	0

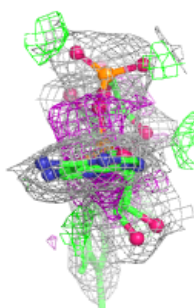
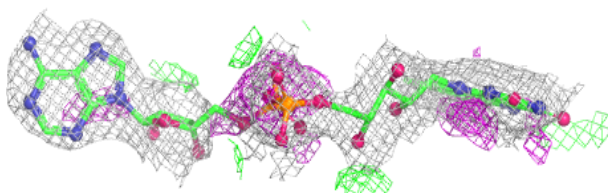
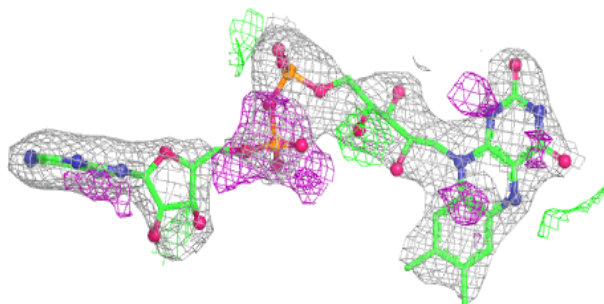
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 501:

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

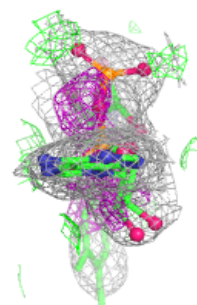
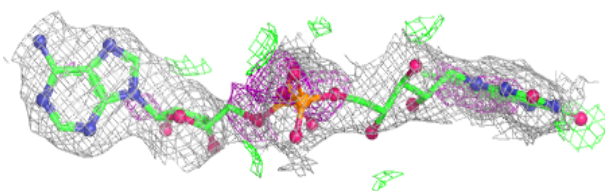
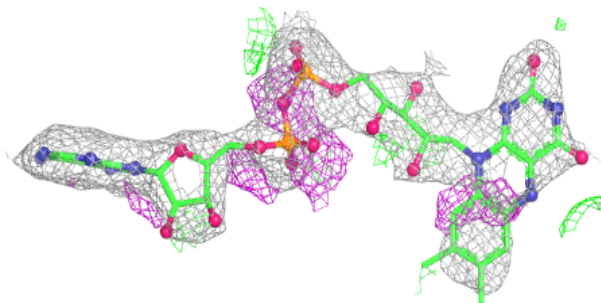
**Electron density around FAD A 501:**

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

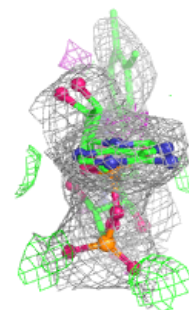
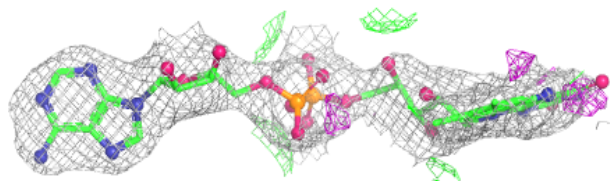
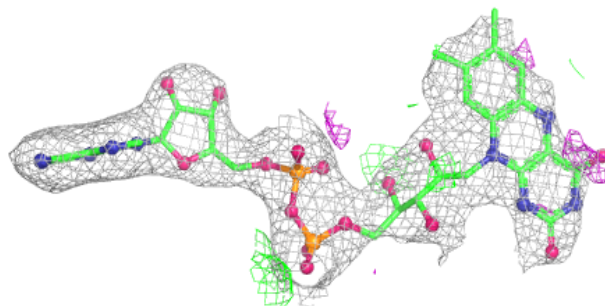


Electron density around FAD D 501:

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

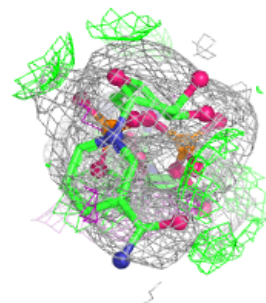
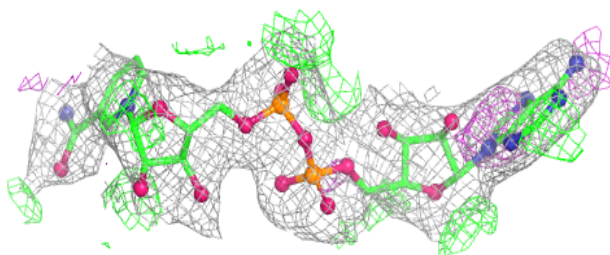
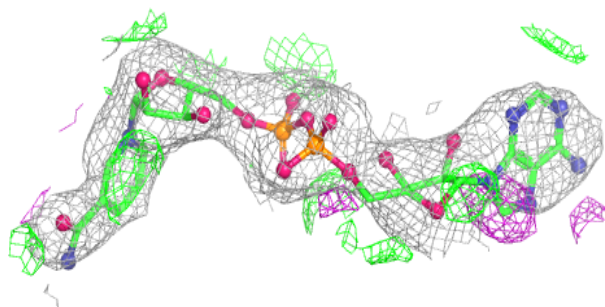
**Electron density around FAD C 501:**

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

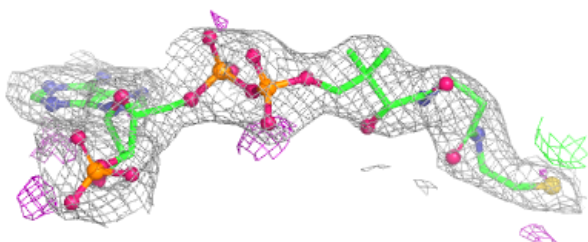
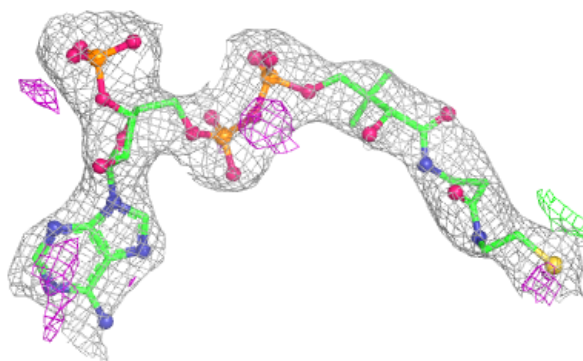


Electron density around NAD B 502:

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

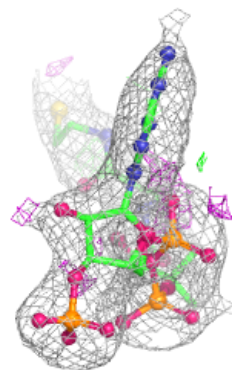
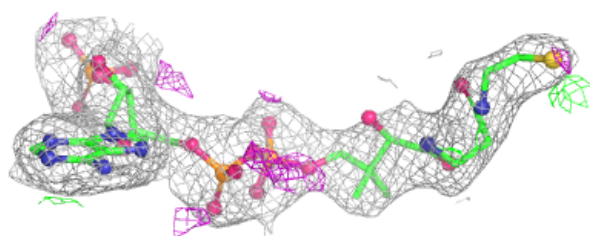
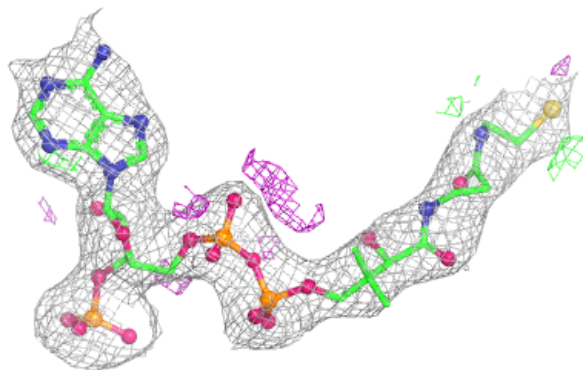
**Electron density around COA A 503:**

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

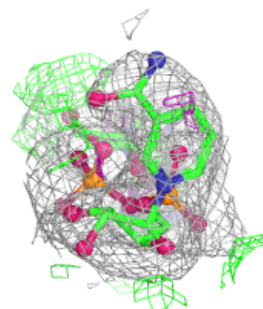
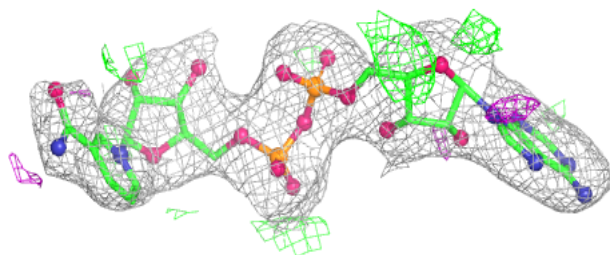
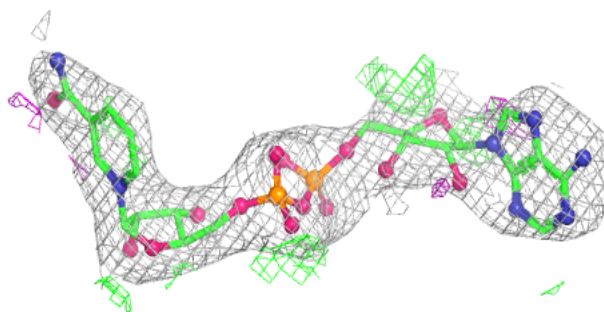


Electron density around COA C 503:

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

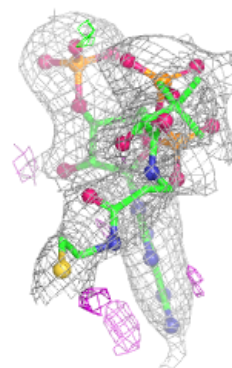
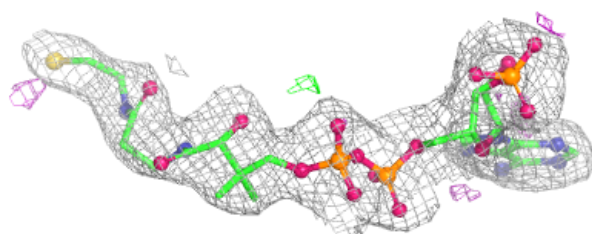
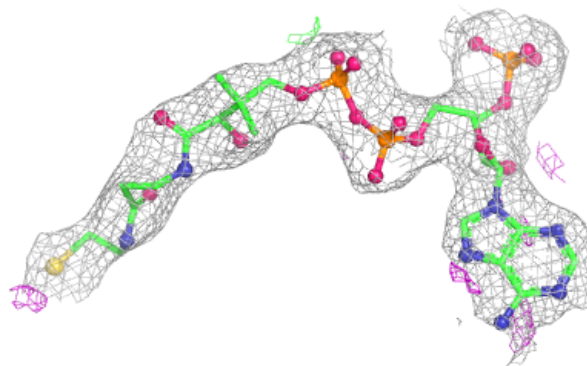
**Electron density around NAD C 502:**

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

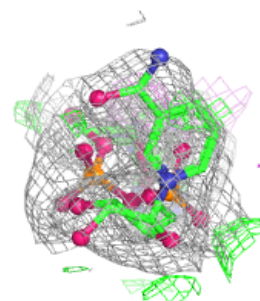
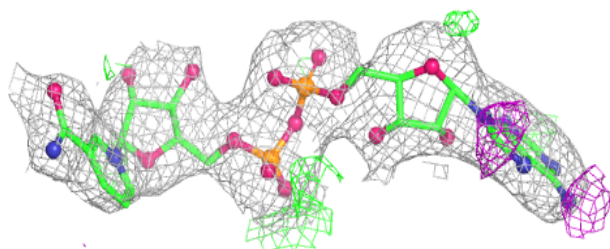
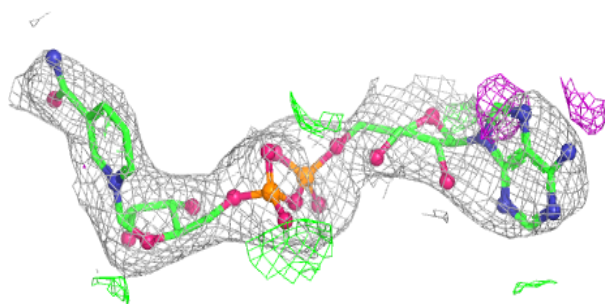


Electron density around COA B 503:

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

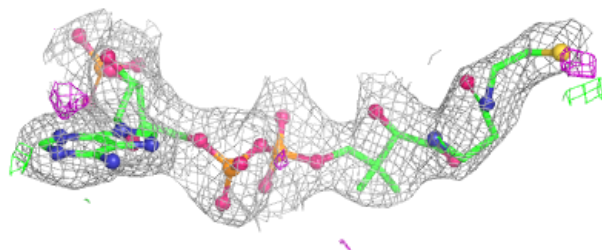
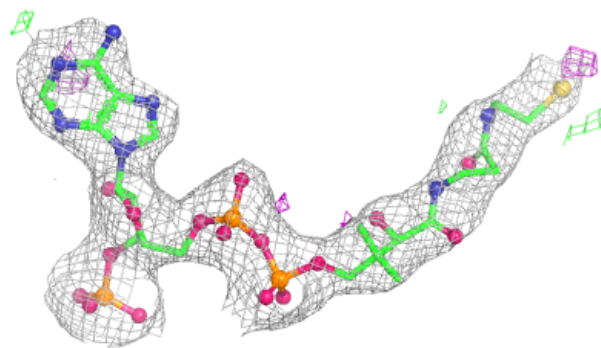
**Electron density around NAD D 502:**

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

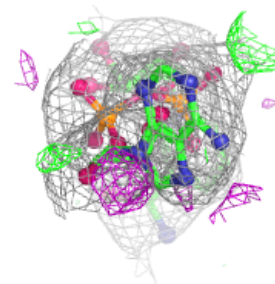
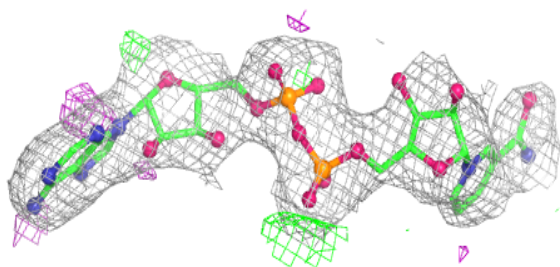
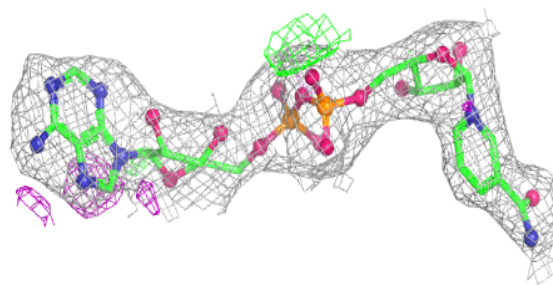


Electron density around COA D 503:

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

**Electron density around 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 ⓘ

There are no such residues in this entry.