



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 PM UTC

PDB ID : 2ONM / pdb_00002onm
Title : Human Mitochondrial Aldehyde Dehydrogenase Asian Variant, ALDH2*2, complexed with NAD+
Authors : Larson, H.N.; Hurley, T.D.
Deposited on : 2007-01-24
Resolution : 2.50 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

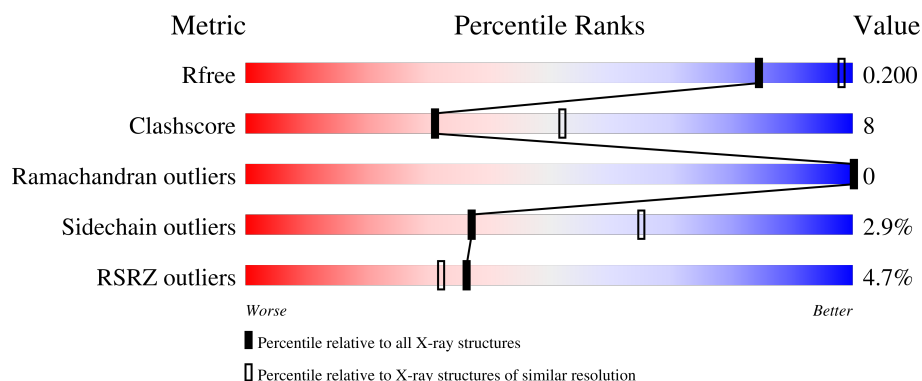
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	500	10% 77% 21% ..
1	B	500	% 80% 17% ..
1	C	500	3% 77% 20% ..
1	D	500	11% 77% 21% ..
1	E	500	% 79% 19% ..

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Mol	Chain	Length	Quality of chain
1	F	500	2% 79% 19% ..
1	G	500	% 78% 20% ..
1	H	500	77% 21% ..
1	I	500	2% 79% 19% ..
1	J	500	9% 74% 23% ..
1	K	500	4% 79% 19% ..
1	L	500	12% 77% 21% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 48124 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 Aldehyde dehydrogenase, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	I	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	J	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	K	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			
1	L	494	Total	C	N	O	S	0	0	0
			3798	2416	649	715	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	487	LYS	GLU	engineered mutation	UNP P05091
B	487	LYS	GLU	engineered mutation	UNP P05091
C	487	LYS	GLU	engineered mutation	UNP P05091
D	487	LYS	GLU	engineered mutation	UNP P05091
E	487	LYS	GLU	engineered mutation	UNP P05091

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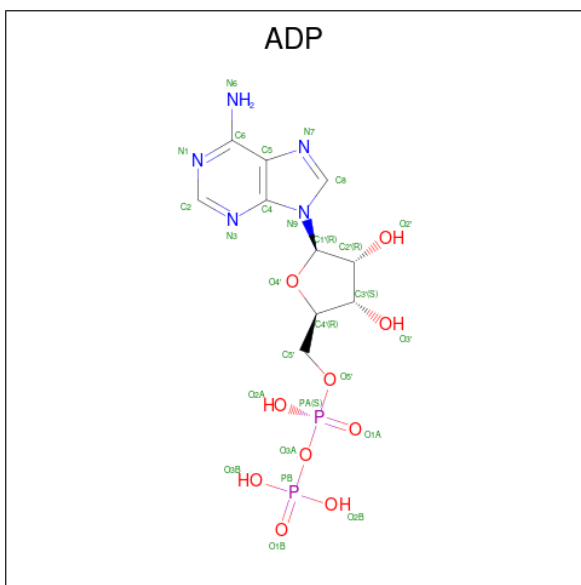
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Chain	Residue	Modelled	Actual	Comment	Reference
F	487	LYS	GLU	engineered mutation	UNP P05091
G	487	LYS	GLU	engineered mutation	UNP P05091
H	487	LYS	GLU	engineered mutation	UNP P05091
I	487	LYS	GLU	engineered mutation	UNP P05091
J	487	LYS	GLU	engineered mutation	UNP P05091
K	487	LYS	GLU	engineered mutation	UNP P05091
L	487	LYS	GLU	engineered mutation	UNP P05091

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	2	Total Na 2 2	0	0
2	C	2	Total Na 2 2	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	2	Total Na 2 2	0	0
2	G	2	Total Na 2 2	0	0
2	H	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0
2	K	2	Total Na 2 2	0	0
2	L	1	Total Na 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 54	C 20	N 10	O 20	P 4	0	1
3	D	1	Total 54	C 20	N 10	O 20	P 4	0	1
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



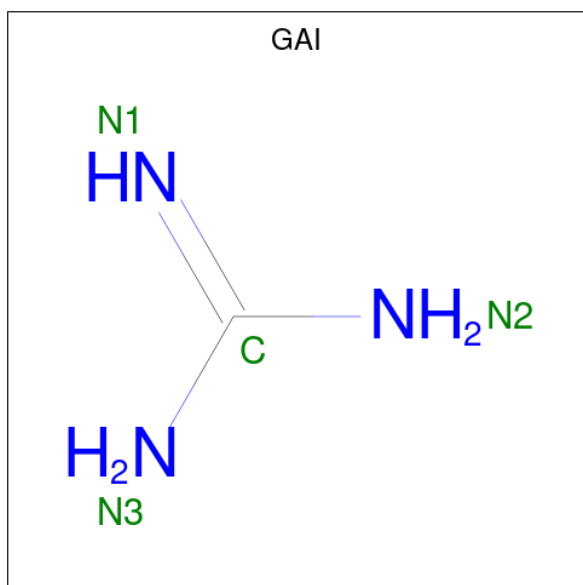
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

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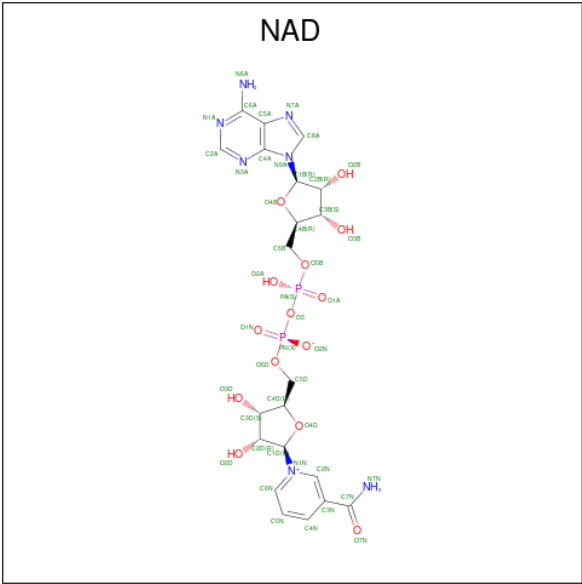
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GUANIDINE (CCD ID: GAI) (formula: CH₅N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 4 1 3	0	0
5	D	1	Total C N 4 1 3	0	0
5	E	1	Total C N 4 1 3	0	0
5	E	1	Total C N 4 1 3	0	0
5	G	1	Total C N 4 1 3	0	0
5	G	1	Total C N 4 1 3	0	0
5	H	1	Total C N 4 1 3	0	0
5	I	1	Total C N 4 1 3	0	0
5	J	1	Total C N 4 1 3	0	0

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
6	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
6	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

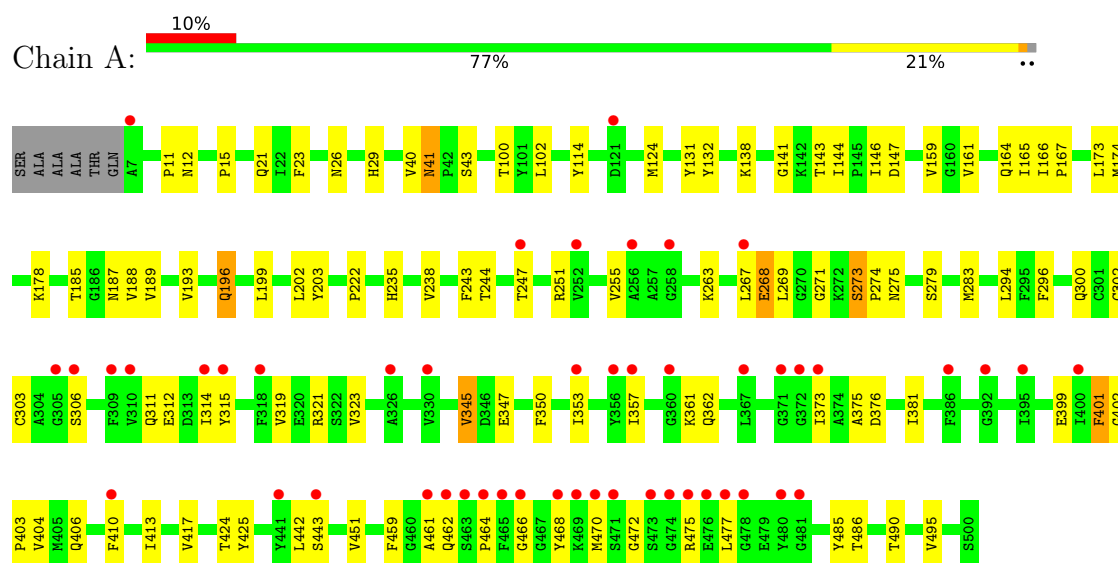
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	121	Total	O	0	0
			121	121		
7	B	223	Total	O	0	0
			223	223		
7	C	232	Total	O	0	0
			232	232		
7	D	133	Total	O	0	0
			133	133		
7	E	264	Total	O	0	0
			264	264		
7	F	251	Total	O	0	0
			251	251		
7	G	186	Total	O	0	0
			186	186		
7	H	185	Total	O	0	0
			185	185		
7	I	131	Total	O	0	0
			131	131		
7	J	63	Total	O	0	0
			63	63		
7	K	77	Total	O	0	0
			77	77		
7	L	66	Total	O	0	0
			66	66		

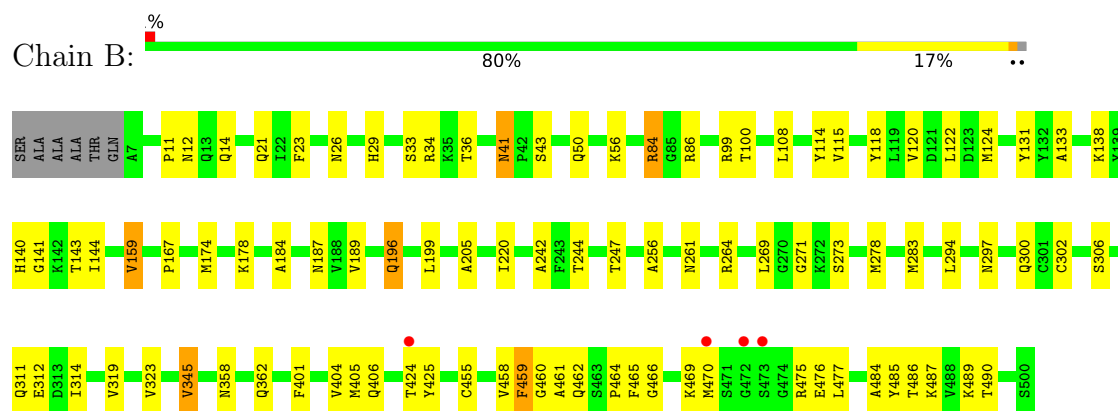
3 Residue-property plots [i](#)

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.

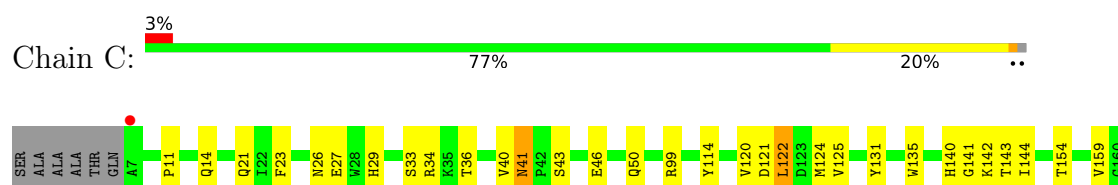
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

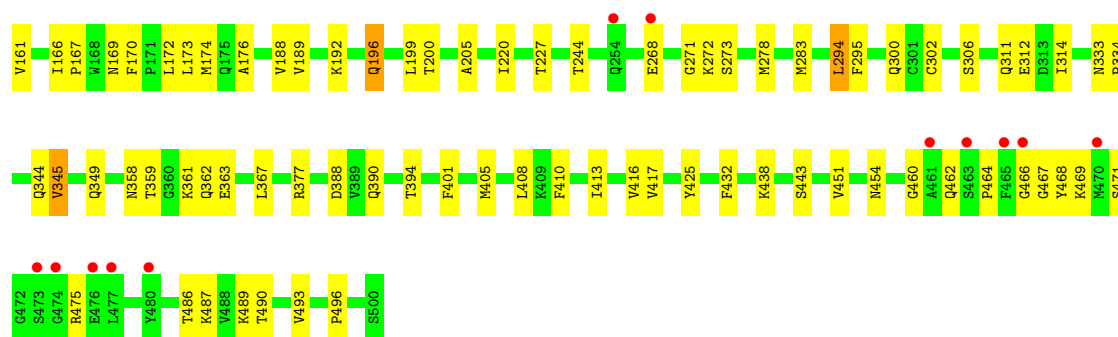


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

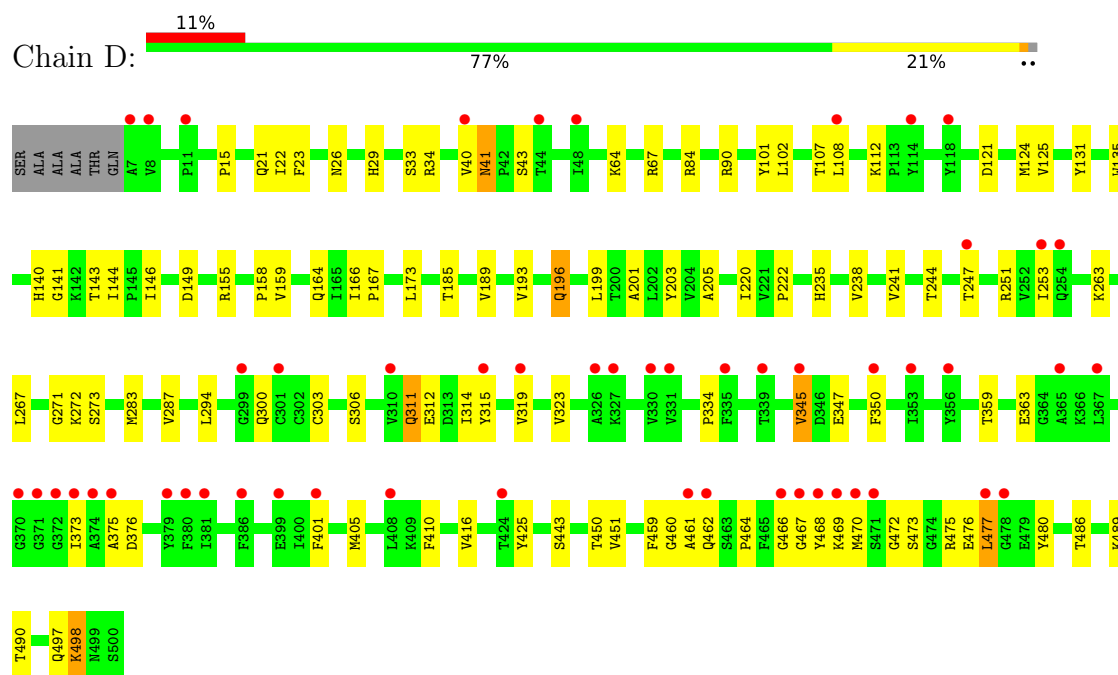


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

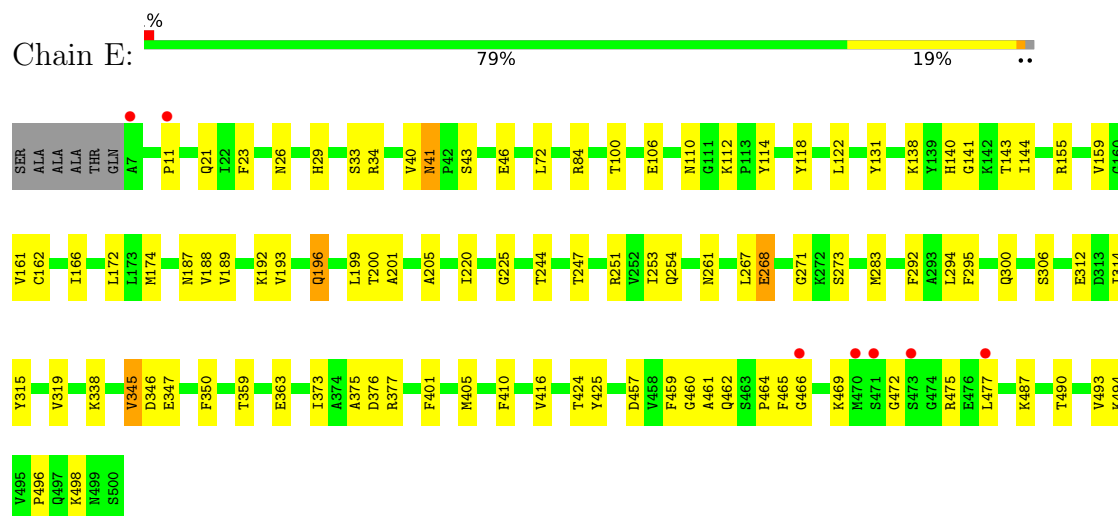




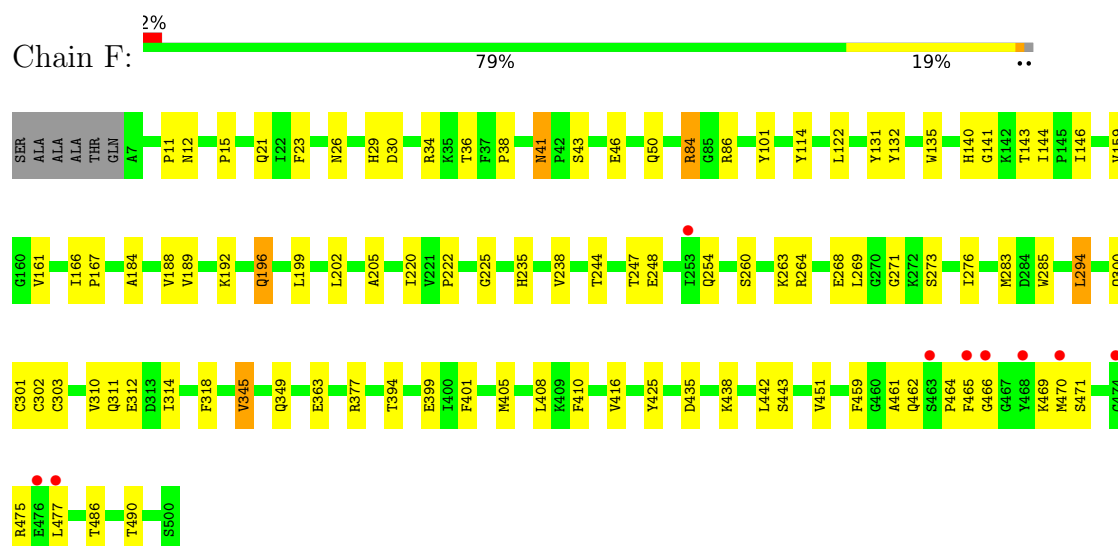
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



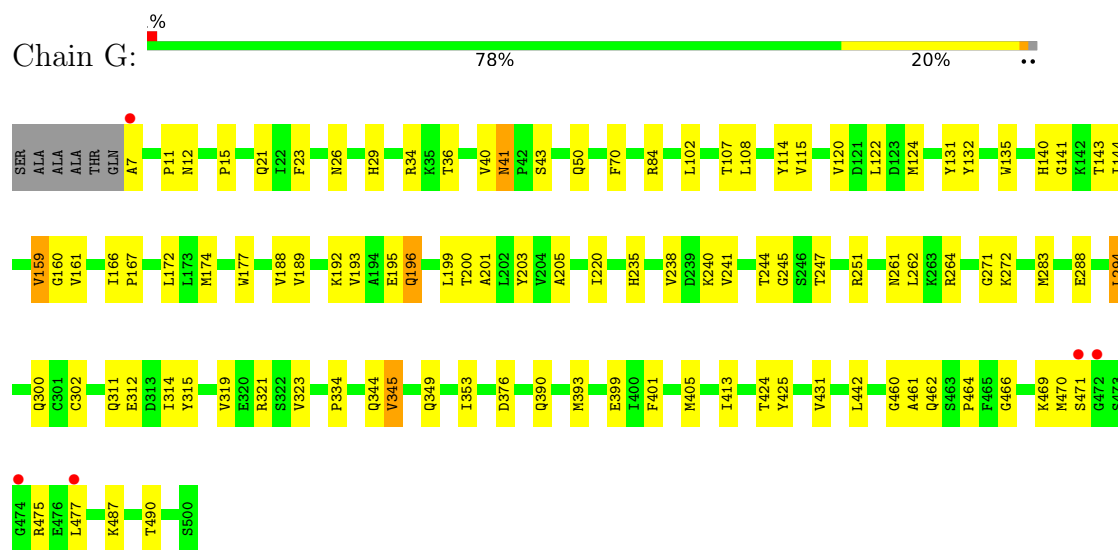
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



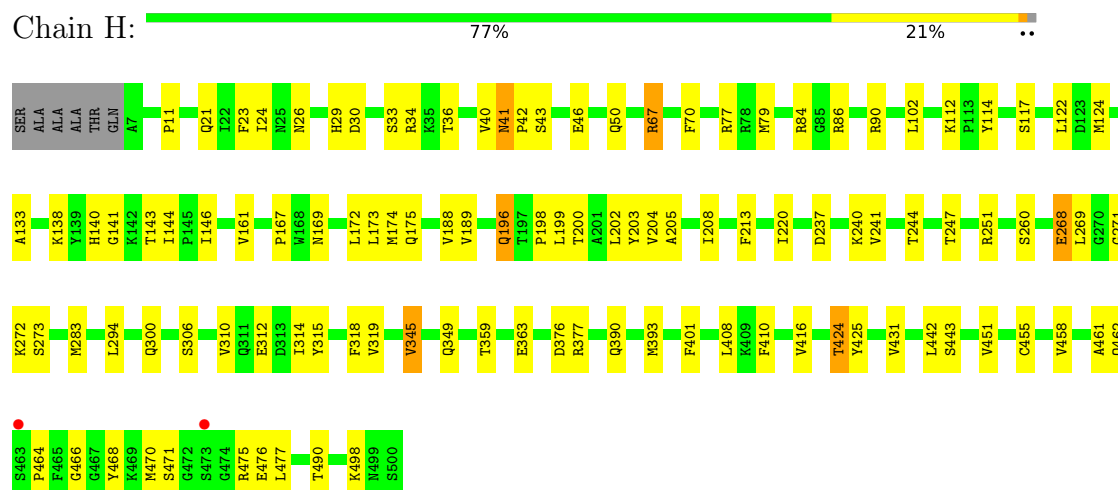
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



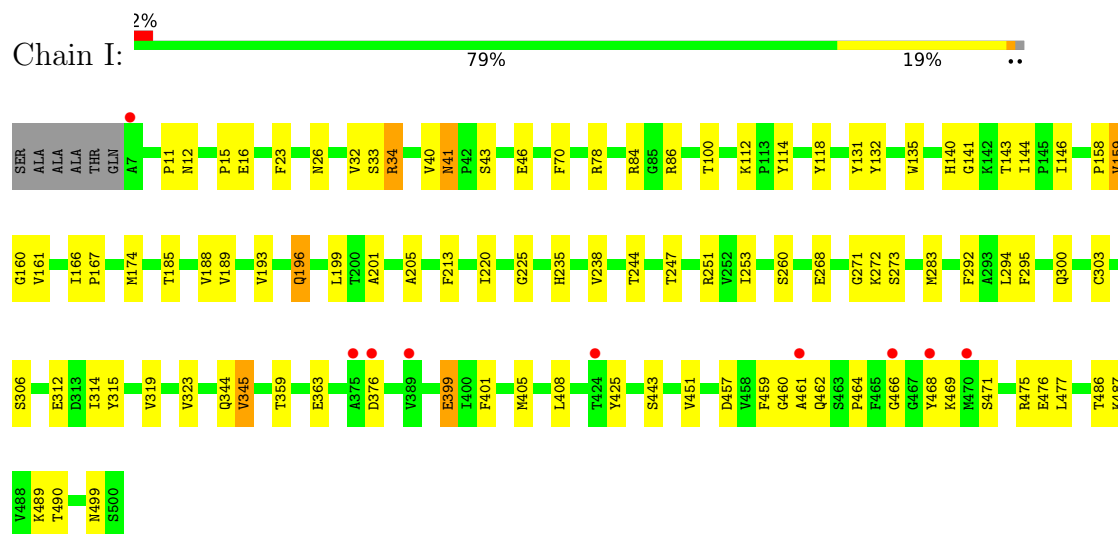
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



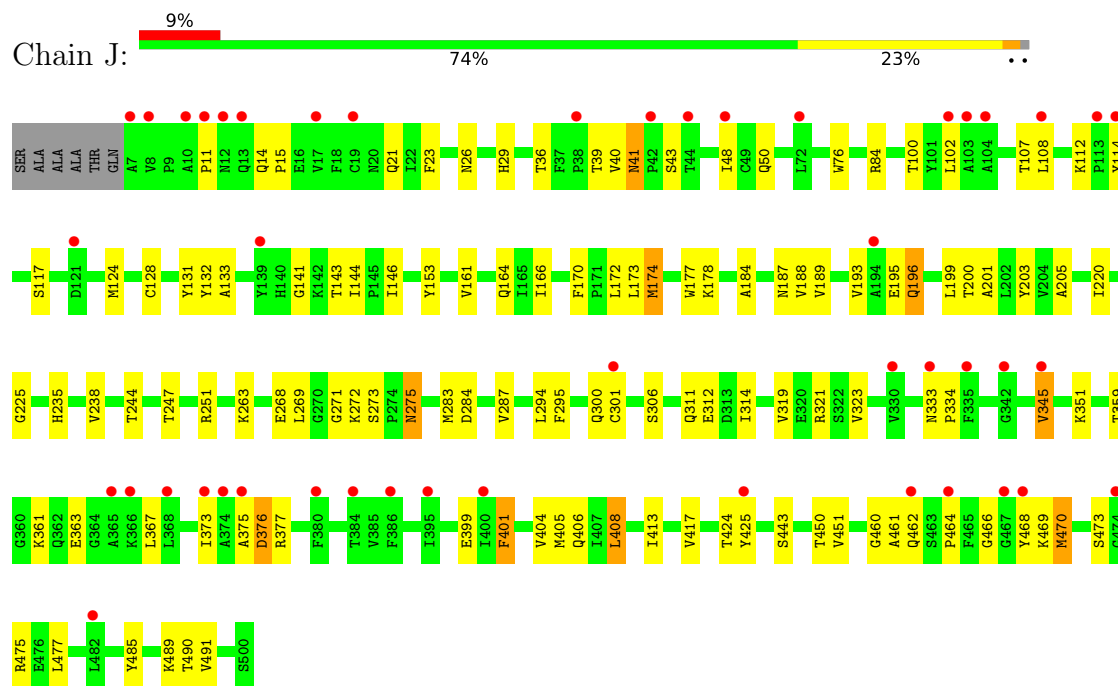
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



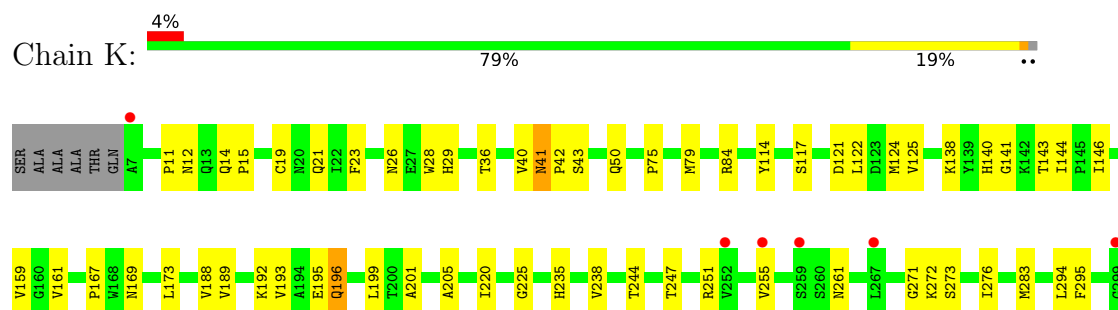
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

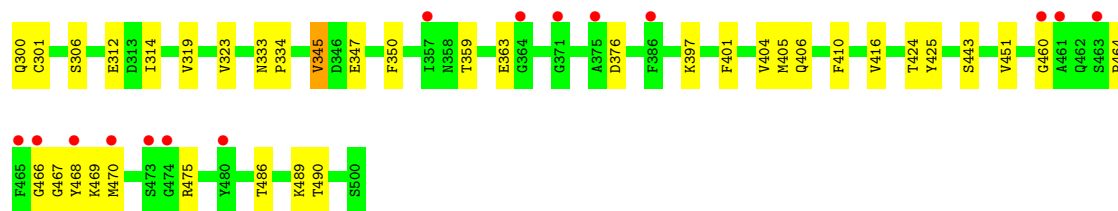


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

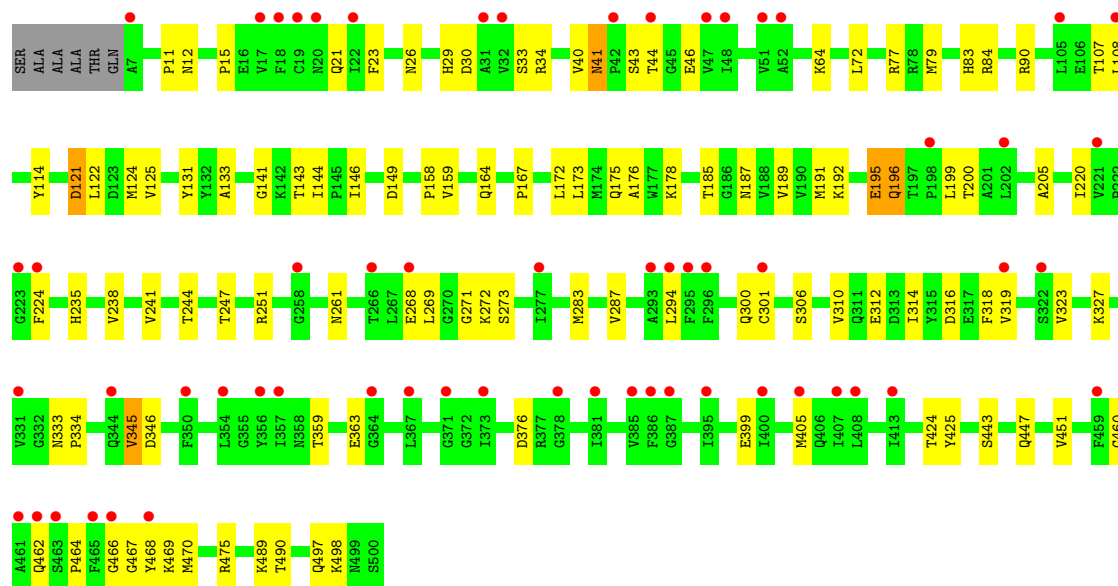
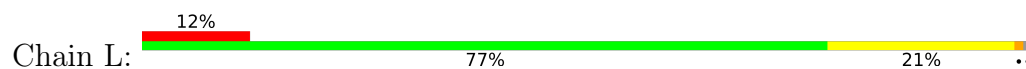


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor





- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.20Å 104.85Å 162.36Å 78.99° 82.14° 88.55°	Depositor
Resolution (Å)	44.01 – 2.50 44.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.01-2.50) 93.9 (44.01-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.271 0.250 , 0.200	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	48124	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: EDO, GAI, NA, NAD, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	1/3882 (0.0%)	0.97	9/5266 (0.2%)
1	B	0.63	0/3882	0.99	16/5266 (0.3%)
1	C	0.65	0/3882	0.99	17/5266 (0.3%)
1	D	0.56	0/3882	0.95	13/5266 (0.2%)
1	E	0.65	0/3882	0.99	14/5266 (0.3%)
1	F	0.69	0/3882	1.01	16/5266 (0.3%)
1	G	0.63	0/3882	0.96	13/5266 (0.2%)
1	H	0.62	1/3882 (0.0%)	0.97	16/5266 (0.3%)
1	I	0.56	0/3882	0.97	19/5266 (0.4%)
1	J	0.47	0/3882	0.95	13/5266 (0.2%)
1	K	0.47	0/3882	0.94	16/5266 (0.3%)
1	L	0.45	0/3882	0.94	14/5266 (0.3%)
All	All	0.58	2/46584 (0.0%)	0.97	176/63192 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	VAL	CA-CB	-5.36	1.50	1.55
1	H	79	MET	SD-CE	5.32	1.92	1.79

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	ILE	N-CA-C	8.88	117.57	107.89
1	F	199	LEU	N-CA-C	8.42	121.29	111.02
1	I	199	LEU	N-CA-C	8.33	121.18	111.02
1	B	144	ILE	N-CA-C	8.31	117.86	108.05
1	H	199	LEU	N-CA-C	8.30	120.02	110.97
1	G	144	ILE	N-CA-C	8.14	117.65	108.05
1	I	345	VAL	N-CA-C	7.91	119.64	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	199	LEU	N-CA-C	7.86	120.61	111.02
1	F	345	VAL	N-CA-C	7.85	118.63	110.62
1	L	141	GLY	N-CA-C	-7.80	101.88	112.57
1	C	199	LEU	N-CA-C	7.80	120.53	111.02
1	C	345	VAL	N-CA-C	7.70	119.40	110.62
1	C	273	SER	N-CA-C	7.65	118.98	109.57
1	F	144	ILE	N-CA-C	7.64	117.06	108.05
1	B	199	LEU	N-CA-C	7.62	120.32	111.02
1	E	199	LEU	N-CA-C	7.59	120.28	111.02
1	A	345	VAL	N-CA-C	7.52	118.26	110.36
1	A	199	LEU	N-CA-C	7.44	120.09	111.02
1	A	141	GLY	N-CA-C	-7.41	102.42	112.57
1	D	199	LEU	N-CA-C	7.39	120.03	111.02
1	E	312	GLU	N-CA-C	7.30	120.17	111.33
1	J	144	ILE	N-CA-C	7.29	116.65	108.05
1	L	199	LEU	N-CA-C	7.27	119.89	111.02
1	E	345	VAL	N-CA-C	7.25	117.97	110.36
1	G	141	GLY	N-CA-C	-7.22	102.68	112.57
1	L	144	ILE	N-CA-C	7.22	116.57	108.05
1	I	144	ILE	N-CA-C	7.18	116.52	108.05
1	H	144	ILE	N-CA-C	7.16	116.50	108.05
1	G	345	VAL	N-CA-C	7.12	118.74	110.62
1	K	144	ILE	N-CA-C	7.11	116.44	108.05
1	D	141	GLY	N-CA-C	-7.10	102.84	112.57
1	G	199	LEU	N-CA-C	7.10	118.71	110.97
1	K	345	VAL	N-CA-C	7.06	117.78	110.36
1	H	84	ARG	N-CA-C	-7.04	103.68	111.36
1	A	143	THR	N-CA-C	-7.04	97.04	108.52
1	I	189	VAL	N-CA-C	7.03	118.94	108.46
1	C	312	GLU	N-CA-C	7.03	119.83	111.33
1	A	144	ILE	N-CA-C	7.00	116.31	108.05
1	B	345	VAL	N-CA-C	6.98	118.58	110.62
1	D	345	VAL	N-CA-C	6.94	117.64	110.36
1	A	189	VAL	N-CA-C	6.92	118.45	108.48
1	L	345	VAL	N-CA-C	6.88	117.59	110.36
1	C	189	VAL	N-CA-C	6.87	118.70	108.46
1	J	345	VAL	N-CA-C	6.86	117.56	110.36
1	C	144	ILE	N-CA-C	6.79	116.06	108.05
1	H	141	GLY	N-CA-C	-6.72	103.36	112.57
1	H	345	VAL	N-CA-C	6.72	117.42	110.36
1	K	141	GLY	N-CA-C	-6.70	103.39	112.57
1	F	189	VAL	N-CA-C	6.68	118.42	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	143	THR	N-CA-C	-6.66	97.56	108.41
1	E	141	GLY	N-CA-C	-6.61	103.51	112.57
1	K	189	VAL	N-CA-C	6.61	118.31	108.46
1	J	199	LEU	N-CA-C	6.59	119.06	111.02
1	F	84	ARG	N-CA-C	-6.57	104.12	111.28
1	B	141	GLY	N-CA-C	-6.53	103.63	112.57
1	L	189	VAL	N-CA-C	6.48	117.81	108.48
1	D	143	THR	N-CA-C	-6.45	98.01	108.52
1	G	189	VAL	N-CA-C	6.44	118.06	108.46
1	A	273	SER	N-CA-C	6.41	118.81	109.71
1	E	143	THR	N-CA-C	-6.35	98.16	108.52
1	H	189	VAL	N-CA-C	6.34	117.91	108.46
1	C	272	LYS	N-CA-C	-6.33	102.84	110.44
1	J	312	GLU	N-CA-C	6.27	118.92	111.33
1	I	469	LYS	CB-CA-C	-6.25	109.35	116.54
1	G	312	GLU	N-CA-C	6.17	118.80	111.33
1	J	141	GLY	N-CA-C	-6.17	102.82	112.58
1	G	272	LYS	N-CA-C	-6.16	101.10	109.54
1	C	469	LYS	CB-CA-C	-6.15	109.47	116.54
1	E	189	VAL	N-CA-C	6.09	117.53	108.46
1	E	140	HIS	N-CA-C	6.04	118.51	110.53
1	E	40	VAL	N-CA-C	6.03	117.69	108.71
1	K	469	LYS	CB-CA-C	-6.01	109.62	116.54
1	H	40	VAL	N-CA-C	6.01	118.29	108.97
1	G	84	ARG	N-CA-C	-6.00	104.75	111.28
1	D	84	ARG	N-CA-C	-5.96	104.78	111.28
1	H	312	GLU	N-CA-C	5.92	118.49	111.33
1	K	312	GLU	N-CA-C	5.92	118.49	111.33
1	F	30	ASP	N-CA-C	-5.88	102.07	110.59
1	F	312	GLU	N-CA-C	5.88	118.44	111.33
1	B	143	THR	N-CA-C	-5.87	98.95	108.52
1	D	312	GLU	N-CA-C	5.86	118.42	111.33
1	E	144	ILE	N-CA-C	5.85	114.96	108.05
1	D	272	LYS	N-CA-C	-5.85	101.53	109.54
1	L	469	LYS	CB-CA-C	-5.83	109.84	116.54
1	H	273	SER	N-CA-C	5.81	117.96	109.71
1	G	40	VAL	N-CA-C	5.78	117.92	108.97
1	L	312	GLU	N-CA-C	5.76	118.30	111.33
1	A	312	GLU	N-CA-C	5.75	118.29	111.33
1	D	140	HIS	N-CA-C	5.75	118.61	110.50
1	G	143	THR	N-CA-C	-5.74	99.16	108.52
1	K	143	THR	N-CA-C	-5.74	99.16	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	143	THR	N-CA-C	-5.72	99.20	108.52
1	C	344	GLN	N-CA-C	-5.72	102.83	110.55
1	L	272	LYS	N-CA-C	-5.71	101.72	109.54
1	I	143	THR	N-CA-C	-5.68	99.26	108.52
1	L	40	VAL	N-CA-C	5.67	117.77	108.97
1	D	469	LYS	CB-CA-C	-5.67	110.02	116.54
1	J	273	SER	N-CA-C	5.66	117.75	109.71
1	I	213	PHE	CA-C-N	5.64	123.78	119.66
1	I	213	PHE	C-N-CA	5.64	123.78	119.66
1	I	40	VAL	N-CA-C	5.63	117.69	108.97
1	B	140	HIS	N-CA-C	5.61	118.41	110.50
1	I	312	GLU	N-CA-C	5.60	118.11	111.33
1	B	12	ASN	N-CA-C	-5.59	98.64	108.20
1	C	141	GLY	N-CA-C	-5.58	104.04	112.41
1	B	469	LYS	CB-CA-C	-5.58	110.13	116.54
1	E	469	LYS	CB-CA-C	-5.57	110.14	116.54
1	H	272	LYS	N-CA-C	-5.56	101.93	109.54
1	F	143	THR	N-CA-C	-5.55	98.31	108.02
1	A	40	VAL	N-CA-C	5.54	117.56	108.97
1	B	189	VAL	N-CA-C	5.52	117.86	108.86
1	F	471	SER	N-CA-C	-5.51	106.23	113.17
1	C	143	THR	N-CA-C	-5.51	98.24	107.99
1	I	84	ARG	N-CA-C	-5.48	105.31	111.28
1	I	295	PHE	N-CA-C	5.46	119.20	112.54
1	E	84	ARG	N-CA-C	-5.45	105.34	111.28
1	J	189	VAL	N-CA-C	5.43	117.72	108.86
1	K	295	PHE	N-CA-C	5.42	119.15	112.54
1	L	273	SER	N-CA-C	5.42	117.40	109.71
1	K	84	ARG	N-CA-C	-5.41	105.55	111.82
1	E	273	SER	N-CA-C	5.41	117.39	109.71
1	H	133	ALA	N-CA-C	-5.39	105.40	111.28
1	G	469	LYS	CB-CA-C	-5.39	110.34	116.54
1	I	344	GLN	N-CA-C	-5.38	103.28	110.55
1	J	40	VAL	N-CA-C	5.38	117.30	108.97
1	F	276	ILE	N-CA-C	5.37	116.10	107.73
1	C	295	PHE	N-CA-C	5.36	119.08	112.54
1	K	276	ILE	N-CA-C	5.36	116.43	108.23
1	L	84	ARG	N-CA-C	-5.35	105.56	111.71
1	C	471	SER	N-CA-C	-5.35	106.44	113.17
1	K	272	LYS	N-CA-C	-5.30	102.28	109.54
1	B	133	ALA	N-CA-C	-5.28	105.52	111.28
1	C	40	VAL	N-CA-C	5.27	117.14	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	273	SER	N-CA-C	5.26	117.18	109.71
1	L	143	THR	N-CA-C	-5.25	98.83	108.02
1	F	273	SER	N-CA-C	5.25	117.16	109.71
1	K	273	SER	N-CA-C	5.25	117.16	109.71
1	D	467	GLY	N-CA-C	5.24	118.79	111.14
1	D	40	VAL	N-CA-C	5.22	117.06	108.97
1	B	273	SER	N-CA-C	5.21	117.11	109.71
1	B	459	PHE	CA-C-N	-5.21	118.53	122.33
1	B	459	PHE	C-N-CA	-5.21	118.53	122.33
1	C	493	VAL	N-CA-C	5.20	115.80	108.36
1	G	471	SER	N-CA-C	-5.19	106.63	113.17
1	G	140	HIS	N-CA-C	5.19	117.38	110.53
1	B	312	GLU	N-CA-C	5.17	117.59	111.33
1	B	99	ARG	N-CA-C	5.16	116.59	111.07
1	H	30	ASP	N-CA-C	-5.15	102.89	110.52
1	K	140	HIS	N-CA-C	5.15	117.50	110.55
1	I	461	ALA	N-CA-C	-5.15	106.10	112.38
1	I	141	GLY	N-CA-C	-5.14	104.70	112.41
1	J	295	PHE	N-CA-C	5.13	118.80	112.54
1	F	141	GLY	N-CA-C	-5.12	104.73	112.41
1	H	461	ALA	N-CA-C	-5.12	106.14	112.38
1	J	133	ALA	N-CA-C	-5.12	105.70	111.28
1	K	40	VAL	N-CA-C	5.12	116.90	108.97
1	J	272	LYS	N-CA-C	-5.11	102.54	109.54
1	L	133	ALA	N-CA-C	-5.11	105.71	111.28
1	C	467	GLY	N-CA-C	5.11	118.59	111.14
1	I	273	SER	N-CA-C	5.10	116.95	109.71
1	E	295	PHE	N-CA-C	5.10	118.76	112.54
1	E	493	VAL	N-CA-C	5.10	115.31	108.17
1	F	469	LYS	CB-CA-C	-5.09	110.68	116.54
1	I	471	SER	N-CA-C	-5.09	106.75	113.17
1	C	140	HIS	N-CA-C	5.08	117.67	110.50
1	L	467	GLY	N-CA-C	5.07	118.55	111.14
1	H	471	SER	N-CA-C	-5.07	106.79	113.17
1	K	467	GLY	N-CA-C	5.07	118.54	111.14
1	B	84	ARG	N-CA-C	-5.07	105.76	111.28
1	I	140	HIS	N-CA-C	5.06	117.97	110.48
1	J	469	LYS	CB-CA-C	-5.05	110.74	116.54
1	H	140	HIS	N-CA-C	5.03	117.92	110.48
1	F	166	ILE	CA-C-N	5.02	126.36	120.98
1	F	166	ILE	C-N-CA	5.02	126.36	120.98
1	F	140	HIS	N-CA-C	5.01	117.90	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	272	LYS	N-CA-C	-5.00	100.35	109.56

There are no chirality outliers.

There are no planarity outliers.

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	3798	0	3752	84	0
1	B	3798	0	3752	61	0
1	C	3798	0	3752	68	0
1	D	3798	0	3752	68	0
1	E	3798	0	3752	70	0
1	F	3798	0	3752	58	0
1	G	3798	0	3752	67	0
1	H	3798	0	3752	60	0
1	I	3798	0	3752	76	0
1	J	3798	0	3752	78	0
1	K	3798	0	3752	52	0
1	L	3798	0	3752	68	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
3	A	54	0	24	3	0
3	D	54	0	24	1	0
3	E	27	0	12	2	0
3	I	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	27	0	12	1	0
3	K	27	0	12	1	0
3	L	27	0	12	0	0
4	A	4	0	6	0	0
4	B	12	0	18	2	0
4	C	8	0	12	1	0
4	D	8	0	12	2	0
4	E	12	0	18	1	0
4	F	16	0	24	2	0
4	G	8	0	12	1	0
4	H	12	0	18	1	0
4	I	8	0	12	2	0
4	K	4	0	6	0	0
4	L	8	0	12	0	0
5	A	4	0	4	0	0
5	D	4	0	5	0	0
5	E	8	0	10	0	0
5	G	8	0	10	0	0
5	H	4	0	5	0	0
5	I	4	0	5	0	0
5	J	4	0	5	0	0
6	B	44	0	26	5	0
6	C	44	0	26	1	0
6	F	44	0	26	2	0
6	G	44	0	26	3	0
6	H	44	0	26	2	0
7	A	121	0	0	1	0
7	B	223	0	0	5	0
7	C	232	0	0	11	0
7	D	133	0	0	2	0
7	E	264	0	0	3	0
7	F	251	0	0	6	0
7	G	186	0	0	6	0
7	H	185	0	0	1	0
7	I	131	0	0	1	0
7	J	63	0	0	1	0
7	K	77	0	0	2	0
7	L	66	0	0	1	0
All	All	48124	0	45456	748	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (748) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLN:HE21	1:C:196:GLN:H	1.03	1.01
1:J:196:GLN:H	1:J:196:GLN:HE21	1.08	0.98
1:C:46:GLU:HB2	4:C:803:EDO:H21	1.47	0.95
1:G:300:GLN:HE22	1:G:345:VAL:H	1.15	0.95
1:E:196:GLN:H	1:E:196:GLN:HE21	1.12	0.95
1:B:300:GLN:HE22	1:B:345:VAL:H	1.13	0.93
1:A:196:GLN:H	1:A:196:GLN:HE21	0.97	0.93
1:K:196:GLN:H	1:K:196:GLN:HE21	1.13	0.93
1:B:196:GLN:H	1:B:196:GLN:HE21	1.18	0.89
1:D:196:GLN:H	1:D:196:GLN:HE21	1.20	0.89
1:L:300:GLN:HE22	1:L:345:VAL:H	1.21	0.89
1:F:196:GLN:H	1:F:196:GLN:HE21	1.21	0.89
1:H:300:GLN:HE22	1:H:345:VAL:H	1.20	0.88
1:I:196:GLN:H	1:I:196:GLN:HE21	1.21	0.87
1:H:196:GLN:HE21	1:H:196:GLN:H	1.19	0.87
1:K:300:GLN:HE22	1:K:345:VAL:H	1.23	0.87
1:J:300:GLN:HE22	1:J:345:VAL:H	1.24	0.85
1:B:41:ASN:ND2	1:B:43:SER:H	1.76	0.84
1:I:300:GLN:HE22	1:I:345:VAL:H	1.25	0.83
1:E:300:GLN:HE22	1:E:345:VAL:H	1.24	0.82
1:D:300:GLN:HE22	1:D:345:VAL:H	1.26	0.81
1:A:196:GLN:HE21	1:A:196:GLN:N	1.76	0.81
1:B:41:ASN:C	1:B:41:ASN:HD22	1.87	0.81
1:F:300:GLN:HE22	1:F:345:VAL:H	1.27	0.81
1:E:338:LYS:HD2	1:I:34:ARG:HH21	1.45	0.80
1:C:300:GLN:HE22	1:C:345:VAL:H	1.30	0.80
1:A:300:GLN:HE22	1:A:345:VAL:H	1.29	0.78
1:E:41:ASN:C	1:E:41:ASN:HD22	1.91	0.78
1:L:294:LEU:HD12	1:L:306:SER:HA	1.66	0.78
1:C:196:GLN:HE21	1:C:196:GLN:N	1.82	0.76
1:J:196:GLN:H	1:J:196:GLN:NE2	1.83	0.76
1:H:41:ASN:C	1:H:41:ASN:HD22	1.94	0.76
1:G:41:ASN:C	1:G:41:ASN:HD22	1.94	0.75
1:C:41:ASN:C	1:C:41:ASN:HD22	1.94	0.75
1:C:196:GLN:H	1:C:196:GLN:NE2	1.83	0.75
1:D:294:LEU:HD12	1:D:306:SER:HA	1.67	0.75
1:E:41:ASN:ND2	1:E:43:SER:H	1.84	0.74
1:I:244:THR:HG23	1:I:268:GLU:HB2	1.69	0.74
1:F:399:GLU:HG3	7:F:1405:HOH:O	1.87	0.73
1:B:41:ASN:HD22	1:B:43:SER:H	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:GLU:HB2	4:H:808:EDO:H21	1.70	0.73
1:G:7:ALA:HB3	7:G:1365:HOH:O	1.87	0.73
1:D:283:MET:HE1	1:D:314:ILE:HB	1.71	0.72
1:L:205:ALA:HB2	1:L:220:ILE:HD12	1.70	0.72
1:I:46:GLU:HB2	4:I:809:EDO:H11	1.71	0.72
1:J:196:GLN:HE21	1:J:196:GLN:N	1.87	0.71
1:L:196:GLN:H	1:L:196:GLN:HE21	1.38	0.71
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.72	0.71
1:C:205:ALA:HB2	1:C:220:ILE:HD12	1.72	0.71
1:C:41:ASN:HD22	1:C:43:SER:H	1.39	0.71
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.73	0.71
1:D:41:ASN:HD22	1:D:43:SER:H	1.39	0.71
1:K:205:ALA:HB2	1:K:220:ILE:HD12	1.74	0.70
1:G:41:ASN:ND2	1:G:43:SER:H	1.90	0.70
1:A:283:MET:HE1	1:A:314:ILE:HB	1.73	0.70
1:I:359:THR:O	1:I:363:GLU:HG2	1.90	0.70
1:A:353:ILE:CD1	1:A:402:GLY:HA3	2.21	0.69
1:A:196:GLN:H	1:A:196:GLN:NE2	1.82	0.69
1:E:100:THR:HG21	1:I:16:GLU:OE1	1.91	0.69
1:G:196:GLN:H	1:G:196:GLN:HE21	1.40	0.69
1:D:41:ASN:HD22	1:D:41:ASN:C	2.00	0.69
1:C:41:ASN:ND2	1:C:43:SER:H	1.90	0.69
1:G:349:GLN:NE2	6:G:507:NAD:H52N	2.07	0.69
1:A:294:LEU:HD12	1:A:306:SER:HA	1.73	0.69
1:I:41:ASN:C	1:I:41:ASN:HD22	2.01	0.69
1:I:490:THR:OG1	1:J:464:PRO:HG2	1.94	0.68
1:F:461:ALA:HA	1:F:477:LEU:HD22	1.75	0.68
1:G:261:ASN:HA	1:H:470:MET:HE3	1.76	0.68
1:H:41:ASN:HD22	1:H:43:SER:H	1.41	0.68
1:A:41:ASN:C	1:A:41:ASN:HD22	2.01	0.68
1:L:359:THR:O	1:L:363:GLU:HG2	1.94	0.68
1:D:196:GLN:H	1:D:196:GLN:NE2	1.92	0.67
1:E:205:ALA:HB2	1:E:220:ILE:HD12	1.76	0.67
1:H:41:ASN:ND2	1:H:43:SER:H	1.92	0.67
1:K:283:MET:HE1	1:K:314:ILE:HB	1.76	0.67
1:A:166:ILE:HD11	1:A:193:VAL:HG12	1.76	0.67
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.75	0.67
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.76	0.67
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.30	0.67
1:A:41:ASN:HD22	1:A:43:SER:H	1.43	0.67
1:L:196:GLN:H	1:L:196:GLN:NE2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLN:HG2	7:C:2212:HOH:O	1.95	0.67
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.30	0.66
1:E:41:ASN:HD22	1:E:43:SER:H	1.42	0.66
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.77	0.66
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.77	0.66
1:J:443:SER:HA	1:J:451:VAL:HG11	1.78	0.66
1:B:196:GLN:H	1:B:196:GLN:NE2	1.91	0.66
1:D:166:ILE:HD11	1:D:193:VAL:HG12	1.77	0.66
1:J:36:THR:HB	1:J:50:GLN:HG3	1.77	0.66
1:D:41:ASN:ND2	1:D:43:SER:H	1.93	0.66
1:J:271:GLY:HA2	1:J:425:TYR:CG	2.31	0.65
1:D:155:ARG:HD2	4:D:704:EDO:O2	1.95	0.65
1:I:489:LYS:HB2	1:J:468:TYR:OH	1.96	0.65
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.79	0.65
1:K:196:GLN:HE21	1:K:196:GLN:N	1.91	0.65
1:C:311:GLN:HG2	7:C:1633:HOH:O	1.97	0.65
1:B:120:VAL:HG12	1:B:124:MET:HE2	1.78	0.64
1:K:41:ASN:C	1:K:41:ASN:HD22	2.06	0.64
1:D:443:SER:HA	1:D:451:VAL:HG11	1.80	0.64
1:F:41:ASN:C	1:F:41:ASN:HD22	2.05	0.64
1:K:36:THR:HB	1:K:50:GLN:HG3	1.78	0.64
1:B:461:ALA:HA	1:B:477:LEU:HD22	1.79	0.64
1:I:464:PRO:HG2	1:J:490:THR:OG1	1.97	0.64
1:A:350:PHE:O	1:A:353:ILE:HG22	1.96	0.64
1:K:294:LEU:HD12	1:K:306:SER:HA	1.79	0.64
1:A:41:ASN:ND2	1:A:43:SER:H	1.96	0.63
1:L:271:GLY:HA2	1:L:425:TYR:CG	2.32	0.63
1:A:102:LEU:HD21	1:A:203:TYR:HD2	1.62	0.63
1:G:271:GLY:HA2	1:G:425:TYR:CG	2.33	0.63
1:D:466:GLY:HA3	1:D:475:ARG:HD3	1.80	0.63
1:H:33:SER:O	1:H:34:ARG:HB2	1.99	0.63
1:G:41:ASN:HD22	1:G:43:SER:H	1.44	0.63
1:E:166:ILE:HD11	1:E:193:VAL:HG12	1.80	0.63
1:G:311:GLN:HG2	7:G:1725:HOH:O	1.99	0.63
1:A:353:ILE:HG21	1:A:381:ILE:CD1	2.28	0.63
1:B:271:GLY:HA2	1:B:425:TYR:CG	2.34	0.63
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.81	0.62
1:I:443:SER:HA	1:I:451:VAL:HG11	1.80	0.62
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.35	0.62
1:A:466:GLY:HA3	1:A:475:ARG:HD3	1.80	0.62
1:A:353:ILE:HD11	1:A:403:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:GLN:H	1:E:196:GLN:NE2	1.93	0.62
1:F:196:GLN:H	1:F:196:GLN:NE2	1.95	0.62
1:I:466:GLY:HA3	1:I:475:ARG:HD3	1.81	0.62
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.34	0.62
1:I:41:ASN:ND2	1:I:43:SER:H	1.97	0.61
1:J:172:LEU:HD21	1:J:200:THR:HB	1.81	0.61
1:I:23:PHE:CZ	1:I:26:ASN:HA	2.35	0.61
1:L:23:PHE:CZ	1:L:26:ASN:HA	2.35	0.61
1:I:146:ILE:HG13	1:J:460:GLY:HA3	1.83	0.61
1:J:23:PHE:CZ	1:J:26:ASN:HA	2.35	0.61
1:B:34:ARG:HG2	1:B:34:ARG:HH11	1.64	0.61
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.36	0.61
1:J:424:THR:HG22	1:J:470:MET:HB2	1.82	0.61
1:K:121:ASP:O	1:K:125:VAL:HG23	2.01	0.61
1:A:353:ILE:HD11	1:A:402:GLY:HA3	1.83	0.61
1:J:283:MET:HE1	1:J:314:ILE:HB	1.82	0.61
1:A:461:ALA:HA	1:A:477:LEU:HD22	1.82	0.61
1:H:294:LEU:HD12	1:H:306:SER:HA	1.81	0.61
1:H:349:GLN:NE2	6:H:508:NAD:H52N	2.16	0.61
1:G:283:MET:HE1	1:G:314:ILE:HB	1.82	0.61
1:I:34:ARG:NH1	1:I:34:ARG:HG3	2.16	0.61
1:B:36:THR:OG1	1:B:50:GLN:HG3	2.01	0.60
1:I:78:ARG:HH11	1:L:497:GLN:NE2	1.98	0.60
1:J:131:TYR:CE1	1:J:462:GLN:HG3	2.36	0.60
1:J:466:GLY:HA3	1:J:475:ARG:HD3	1.82	0.60
1:E:359:THR:O	1:E:363:GLU:HG2	2.01	0.60
1:B:131:TYR:CE1	1:B:462:GLN:HG3	2.37	0.60
1:J:275:ASN:C	1:J:275:ASN:HD22	2.07	0.60
1:C:125:VAL:HG13	1:C:176:ALA:HB2	1.83	0.60
1:E:159:VAL:HG12	1:E:187:ASN:OD1	2.02	0.60
1:C:496:PRO:HG2	7:C:2088:HOH:O	2.02	0.59
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.38	0.59
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.37	0.59
1:H:466:GLY:HA3	1:H:475:ARG:HD3	1.83	0.59
1:F:132:TYR:OH	1:F:477:LEU:HA	2.02	0.59
1:H:196:GLN:HE21	1:H:196:GLN:N	1.97	0.59
1:E:459:PHE:HE2	1:E:465:PHE:CE1	2.21	0.58
1:L:12:ASN:O	1:L:15:PRO:HD3	2.02	0.58
1:L:34:ARG:HG3	1:L:34:ARG:HH11	1.68	0.58
1:E:247:THR:O	1:E:251:ARG:HG3	2.03	0.58
1:K:319:VAL:O	1:K:323:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:CYS:HB3	6:B:502:NAD:N7N	2.18	0.58
1:G:166:ILE:HD11	1:G:193:VAL:HG12	1.85	0.58
1:J:102:LEU:HD21	1:J:203:TYR:HD2	1.68	0.58
1:K:247:THR:O	1:K:251:ARG:HG3	2.03	0.58
1:G:36:THR:HB	1:G:50:GLN:HG3	1.86	0.58
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.39	0.58
1:L:466:GLY:HA3	1:L:475:ARG:HD3	1.86	0.58
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.39	0.57
1:H:208:ILE:HG23	1:H:213:PHE:CD1	2.39	0.57
1:I:196:GLN:H	1:I:196:GLN:NE2	1.95	0.57
1:L:247:THR:O	1:L:251:ARG:HG3	2.05	0.57
1:L:443:SER:HA	1:L:451:VAL:HG11	1.86	0.57
1:C:172:LEU:HD21	1:C:200:THR:HB	1.86	0.57
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.87	0.57
1:E:261:ASN:HA	1:F:470:MET:HE2	1.86	0.57
1:I:271:GLY:HA2	1:I:425:TYR:CG	2.39	0.57
1:K:41:ASN:ND2	1:K:43:SER:H	2.01	0.57
1:I:46:GLU:HB2	4:I:809:EDO:C1	2.35	0.57
1:I:196:GLN:HE21	1:I:196:GLN:N	1.95	0.57
1:F:41:ASN:HD22	1:F:43:SER:H	1.51	0.57
1:I:247:THR:O	1:I:251:ARG:HG3	2.05	0.57
1:L:41:ASN:C	1:L:41:ASN:HD22	2.13	0.57
1:I:283:MET:HE1	1:I:314:ILE:HB	1.86	0.57
1:F:202:LEU:HD21	1:F:222:PRO:HG3	1.87	0.56
1:A:279:SER:HB3	1:A:311:GLN:HG2	1.88	0.56
1:C:36:THR:HB	1:C:50:GLN:HG3	1.87	0.56
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.05	0.56
1:C:377:ARG:NH1	7:C:2812:HOH:O	2.39	0.56
1:L:34:ARG:HG3	1:L:34:ARG:NH1	2.20	0.56
6:H:508:NAD:O5D	6:H:508:NAD:H6N	2.05	0.56
1:J:170:PHE:HB2	1:J:174:MET:HE2	1.87	0.56
1:C:21:GLN:HB3	1:C:29:HIS:O	2.06	0.56
1:G:41:ASN:C	1:G:41:ASN:ND2	2.64	0.56
1:I:225:GLY:HA3	3:I:509:ADP:C8	2.41	0.56
1:L:283:MET:HE1	1:L:314:ILE:HB	1.88	0.56
1:C:390:GLN:HB3	7:C:2182:HOH:O	2.05	0.56
1:E:155:ARG:HD2	4:E:705:EDO:O2	2.06	0.56
1:C:443:SER:HA	1:C:451:VAL:HG11	1.87	0.55
1:D:311:GLN:HG2	1:D:410:PHE:CZ	2.41	0.55
1:J:244:THR:HG23	1:J:268:GLU:HB2	1.88	0.55
1:C:359:THR:O	1:C:363:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:MET:HE2	1:C:244:THR:HG21	1.88	0.55
1:E:283:MET:HE1	1:E:314:ILE:HB	1.87	0.55
1:F:38:PRO:HD3	1:F:50:GLN:HE22	1.70	0.55
1:F:349:GLN:HG3	7:F:1196:HOH:O	2.06	0.55
1:I:460:GLY:HA3	1:J:146:ILE:HG13	1.87	0.55
1:A:443:SER:HA	1:A:451:VAL:HG11	1.88	0.55
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.42	0.55
1:G:461:ALA:HA	1:G:477:LEU:HD22	1.89	0.55
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.87	0.55
1:D:251:ARG:NH1	1:D:470:MET:HE1	2.21	0.55
1:L:33:SER:O	1:L:34:ARG:HB2	2.07	0.55
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.42	0.55
1:K:490:THR:OG1	1:L:464:PRO:HG2	2.07	0.55
1:A:413:ILE:O	1:A:417:VAL:HG23	2.07	0.54
1:I:131:TYR:CE1	1:I:462:GLN:HG3	2.42	0.54
1:B:34:ARG:HG2	1:B:34:ARG:NH1	2.20	0.54
1:D:21:GLN:HB3	1:D:29:HIS:O	2.07	0.54
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.89	0.54
1:B:108:LEU:HD11	4:B:802:EDO:H12	1.90	0.54
1:F:443:SER:HA	1:F:451:VAL:HG11	1.90	0.54
1:F:41:ASN:ND2	1:F:43:SER:H	2.05	0.54
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.43	0.54
1:L:41:ASN:ND2	1:L:43:SER:H	2.05	0.54
1:D:319:VAL:O	1:D:323:VAL:HG23	2.07	0.54
1:F:46:GLU:HB2	4:F:806:EDO:H21	1.89	0.54
1:L:44:THR:OG1	1:L:46:GLU:HG2	2.08	0.54
1:E:100:THR:HG22	1:E:118:TYR:HE1	1.73	0.54
1:J:311:GLN:HG2	7:J:1829:HOH:O	2.07	0.54
1:I:174:MET:HE2	1:I:244:THR:HG21	1.90	0.54
1:I:399:GLU:OE1	1:I:399:GLU:HA	2.06	0.54
1:L:319:VAL:O	1:L:323:VAL:HG23	2.08	0.54
1:E:21:GLN:HB3	1:E:29:HIS:O	2.08	0.53
1:I:12:ASN:O	1:I:15:PRO:HD3	2.08	0.53
1:B:294:LEU:HD22	1:B:405:MET:HB2	1.90	0.53
1:G:195:GLU:CD	1:G:195:GLU:H	2.16	0.53
1:H:172:LEU:HD21	1:H:200:THR:HB	1.90	0.53
1:B:302:CYS:HB3	6:B:502:NAD:C7N	2.38	0.53
1:G:247:THR:O	1:G:251:ARG:HG3	2.07	0.53
1:K:271:GLY:HA2	1:K:425:TYR:CG	2.44	0.53
1:C:120:VAL:HG12	1:C:124:MET:HE2	1.90	0.53
1:F:264:ARG:NH2	7:F:2163:HOH:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:443:SER:HA	1:K:451:VAL:HG11	1.91	0.53
1:J:294:LEU:HD12	1:J:306:SER:HA	1.90	0.53
1:D:196:GLN:HE21	1:D:196:GLN:N	1.99	0.53
1:G:132:TYR:OH	1:G:477:LEU:HA	2.08	0.53
1:E:338:LYS:CD	1:I:34:ARG:HH21	2.17	0.53
1:F:12:ASN:O	1:F:15:PRO:HD3	2.09	0.53
1:G:251:ARG:NH1	1:H:260:SER:O	2.41	0.53
1:H:21:GLN:HB3	1:H:29:HIS:O	2.09	0.53
1:I:294:LEU:HD12	1:I:306:SER:HA	1.91	0.53
1:J:187:ASN:ND2	1:J:485:TYR:HB3	2.23	0.53
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.09	0.52
1:E:338:LYS:HZ2	1:I:34:ARG:HE	1.55	0.52
1:E:460:GLY:HA3	1:F:146:ILE:HG13	1.91	0.52
1:H:167:PRO:HD3	1:H:244:THR:HB	1.89	0.52
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.44	0.52
1:J:76:TRP:CH2	1:J:84:ARG:HG2	2.44	0.52
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.73	0.52
1:J:41:ASN:C	1:J:41:ASN:HD22	2.16	0.52
1:D:167:PRO:HD3	1:D:244:THR:HB	1.90	0.52
1:L:235:HIS:HB3	1:L:238:VAL:HG23	1.91	0.52
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.45	0.52
1:I:41:ASN:HD22	1:I:43:SER:H	1.57	0.52
1:L:121:ASP:O	1:L:125:VAL:HG23	2.10	0.52
1:C:489:LYS:HB2	1:D:468:TYR:OH	2.09	0.52
1:E:196:GLN:HE21	1:E:196:GLN:N	1.94	0.52
1:H:67:ARG:HD2	1:H:237:ASP:OD2	2.10	0.52
1:I:70:PHE:CZ	1:I:160:GLY:HA2	2.44	0.52
1:C:302:CYS:SG	7:C:2137:HOH:O	2.59	0.52
1:H:41:ASN:HD21	1:H:43:SER:HB2	1.75	0.52
1:I:159:VAL:HA	1:I:487:LYS:HG3	1.90	0.52
1:A:12:ASN:O	1:A:15:PRO:HD3	2.10	0.52
1:A:146:ILE:HG13	1:B:460:GLY:HA3	1.91	0.52
1:D:253:ILE:HD11	3:D:504[B]:ADP:C2	2.44	0.52
1:E:271:GLY:HA2	1:E:425:TYR:CG	2.45	0.52
1:D:33:SER:O	1:D:34:ARG:HB2	2.10	0.52
1:E:464:PRO:HG2	1:F:490:THR:OG1	2.09	0.52
1:G:21:GLN:HB3	1:G:29:HIS:O	2.09	0.52
1:J:164:GLN:CD	1:J:178:LYS:HB3	2.35	0.52
1:J:247:THR:O	1:J:251:ARG:HG3	2.09	0.52
1:D:315:TYR:O	1:D:319:VAL:HG23	2.09	0.51
1:J:21:GLN:HB3	1:J:29:HIS:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:470:MET:HE3	1:L:261:ASN:HA	1.92	0.51
1:I:11:PRO:HB3	1:I:114:TYR:CZ	2.45	0.51
1:I:499:ASN:HA	1:L:77:ARG:O	2.10	0.51
1:K:23:PHE:CZ	1:K:26:ASN:HA	2.45	0.51
1:L:399:GLU:HA	1:L:399:GLU:OE1	2.10	0.51
1:A:470:MET:HE2	1:B:261:ASN:HA	1.92	0.51
1:J:294:LEU:HD22	1:J:405:MET:HB2	1.92	0.51
1:K:464:PRO:HG2	1:L:490:THR:OG1	2.10	0.51
1:B:196:GLN:HE21	1:B:196:GLN:N	1.97	0.51
1:E:193:VAL:HG11	1:E:201:ALA:CB	2.41	0.51
1:F:283:MET:HE1	1:F:314:ILE:HB	1.92	0.51
1:I:167:PRO:HD3	1:I:244:THR:HB	1.93	0.51
1:H:175:GLN:HE22	1:H:204:VAL:HB	1.76	0.51
1:K:41:ASN:HD22	1:K:43:SER:H	1.57	0.51
1:A:353:ILE:HD12	1:A:402:GLY:HA3	1.91	0.51
1:D:41:ASN:HD21	1:D:43:SER:HB2	1.76	0.51
1:G:399:GLU:HG3	7:G:1106:HOH:O	2.10	0.51
1:A:21:GLN:HB3	1:A:29:HIS:O	2.11	0.51
1:B:159:VAL:HA	1:B:487:LYS:HD3	1.93	0.51
1:C:349:GLN:HB3	7:C:1069:HOH:O	2.11	0.51
1:C:408:LEU:HD12	1:C:408:LEU:N	2.25	0.51
1:C:460:GLY:HA3	1:D:146:ILE:HG13	1.92	0.51
1:F:86:ARG:HD2	7:F:2867:HOH:O	2.10	0.51
1:I:34:ARG:HG3	1:I:34:ARG:HH11	1.75	0.51
1:J:41:ASN:ND2	1:J:43:SER:H	2.08	0.51
1:F:247:THR:HA	1:F:269:LEU:HD22	1.94	0.51
1:G:424:THR:HG22	1:G:470:MET:HB2	1.93	0.51
1:H:310:VAL:HG21	1:H:318:PHE:CD2	2.46	0.51
1:A:174:MET:HA	1:A:174:MET:HE2	1.93	0.50
1:A:187:ASN:ND2	1:A:485:TYR:HB3	2.26	0.50
1:A:283:MET:HG3	1:A:321:ARG:HH11	1.76	0.50
1:B:278:MET:HE3	7:B:1529:HOH:O	2.11	0.50
1:G:300:GLN:NE2	1:G:345:VAL:H	1.98	0.50
1:I:41:ASN:C	1:I:41:ASN:ND2	2.70	0.50
1:J:225:GLY:HA3	3:J:510:ADP:C8	2.47	0.50
1:J:283:MET:O	1:J:287:VAL:HG23	2.12	0.50
1:E:254:GLN:HE21	1:F:254:GLN:HE21	1.58	0.50
1:F:302:CYS:HB3	6:F:506:NAD:O7N	2.11	0.50
1:K:146:ILE:HG13	1:L:460:GLY:HA3	1.94	0.50
1:K:300:GLN:NE2	1:K:345:VAL:H	2.01	0.50
7:K:2020:HOH:O	1:L:447:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:GLN:HE21	1:F:196:GLN:N	2.00	0.50
1:H:196:GLN:H	1:H:196:GLN:NE2	2.00	0.50
1:H:283:MET:HE1	1:H:314:ILE:HB	1.94	0.50
1:J:404:VAL:HG12	1:J:406:GLN:OE1	2.11	0.50
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.47	0.50
1:B:100:THR:HG22	1:B:118:TYR:HE1	1.77	0.50
1:B:115:VAL:HG23	7:B:1146:HOH:O	2.12	0.50
1:H:174:MET:HA	1:H:174:MET:HE2	1.94	0.50
1:J:301:CYS:C	1:J:401:PHE:HE1	2.20	0.50
1:F:161:VAL:HA	1:F:188:VAL:HG23	1.93	0.50
1:B:84:ARG:NH1	1:B:184:ALA:O	2.44	0.49
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.47	0.49
1:I:235:HIS:HB3	1:I:238:VAL:HG23	1.94	0.49
1:I:268:GLU:OE2	1:I:476:GLU:HG3	2.12	0.49
1:A:124:MET:HE2	1:A:173:LEU:HD21	1.94	0.49
1:B:424:THR:HG22	1:B:470:MET:HB2	1.93	0.49
1:L:271:GLY:HA2	1:L:425:TYR:CD2	2.48	0.49
1:A:296:PHE:HA	7:A:2378:HOH:O	2.12	0.49
1:D:294:LEU:CD1	1:D:306:SER:HA	2.41	0.49
1:I:33:SER:O	1:I:34:ARG:CB	2.60	0.49
1:J:11:PRO:HB3	1:J:114:TYR:CE1	2.47	0.49
1:I:135:TRP:CE2	1:K:138:LYS:HD3	2.48	0.49
1:B:358:ASN:O	1:B:362:GLN:HG2	2.13	0.49
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.47	0.49
1:E:41:ASN:C	1:E:41:ASN:ND2	2.61	0.49
1:A:187:ASN:HD21	1:A:485:TYR:HB3	1.76	0.49
1:A:267:LEU:O	1:A:472:GLY:HA3	2.13	0.49
1:E:410:PHE:CD1	1:E:416:VAL:HB	2.48	0.49
1:I:78:ARG:NH1	1:L:497:GLN:HE21	2.09	0.49
1:A:132:TYR:OH	1:A:477:LEU:HA	2.13	0.49
1:A:353:ILE:CD1	1:A:403:PRO:HD2	2.41	0.49
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.93	0.49
1:D:149:ASP:HA	1:D:498:LYS:HB2	1.95	0.48
1:E:41:ASN:HD21	1:E:43:SER:HB2	1.78	0.48
1:J:107:THR:HG23	1:J:112:LYS:O	2.12	0.48
1:L:294:LEU:CD1	1:L:306:SER:HA	2.39	0.48
1:E:494:LYS:HE3	1:F:285:TRP:CZ2	2.48	0.48
1:I:132:TYR:OH	1:I:477:LEU:HA	2.12	0.48
1:K:235:HIS:HB3	1:K:238:VAL:HG23	1.95	0.48
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.94	0.48
1:C:468:TYR:OH	1:D:489:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:LEU:HD12	1:E:306:SER:HA	1.94	0.48
1:F:377:ARG:HB2	7:F:2647:HOH:O	2.14	0.48
1:I:294:LEU:HD13	1:I:405:MET:HA	1.94	0.48
1:K:11:PRO:HB3	1:K:114:TYR:CZ	2.47	0.48
1:F:459:PHE:HE2	1:F:465:PHE:CE1	2.32	0.48
1:I:468:TYR:OH	1:J:489:LYS:HB2	2.12	0.48
1:K:261:ASN:HA	1:L:470:MET:CE	2.44	0.48
1:D:247:THR:O	1:D:251:ARG:HG3	2.13	0.48
1:E:172:LEU:HD21	1:E:200:THR:HB	1.94	0.48
1:E:338:LYS:CD	1:I:34:ARG:NH2	2.75	0.48
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.49	0.48
1:G:12:ASN:O	1:G:15:PRO:HD3	2.14	0.48
1:A:271:GLY:HA2	1:A:425:TYR:CD2	2.49	0.48
1:C:36:THR:CB	1:C:50:GLN:HG3	2.43	0.48
1:C:121:ASP:O	1:C:125:VAL:HG23	2.14	0.48
1:G:159:VAL:HG23	1:G:264:ARG:NH1	2.28	0.48
1:G:390:GLN:HG2	1:G:393:MET:HE3	1.96	0.48
1:I:253:ILE:HD11	3:I:509:ADP:C2	2.49	0.48
1:J:193:VAL:HG11	1:J:201:ALA:CB	2.43	0.48
1:L:125:VAL:HG13	1:L:176:ALA:HB2	1.96	0.48
1:B:41:ASN:HD21	1:B:43:SER:HB2	1.78	0.48
1:A:319:VAL:O	1:A:323:VAL:HG23	2.14	0.47
1:J:319:VAL:O	1:J:323:VAL:HG23	2.14	0.47
1:J:408:LEU:N	1:J:408:LEU:HD12	2.28	0.47
1:B:294:LEU:HD12	1:B:306:SER:HA	1.96	0.47
1:A:275:ASN:C	1:A:275:ASN:HD22	2.21	0.47
1:J:271:GLY:O	1:J:399:GLU:OE2	2.31	0.47
1:K:489:LYS:HB2	1:L:468:TYR:OH	2.13	0.47
1:L:149:ASP:HA	1:L:498:LYS:HB2	1.97	0.47
1:B:300:GLN:HE22	1:B:345:VAL:N	1.96	0.47
1:C:131:TYR:CE1	1:C:462:GLN:HB3	2.49	0.47
1:G:464:PRO:HG2	1:H:490:THR:OG1	2.15	0.47
1:I:193:VAL:HG11	1:I:201:ALA:CB	2.45	0.47
1:D:238:VAL:O	1:D:263:LYS:HE3	2.13	0.47
1:F:301:CYS:HB2	7:F:2754:HOH:O	2.14	0.47
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.95	0.47
1:J:461:ALA:HA	1:J:477:LEU:HD22	1.96	0.47
1:A:247:THR:HG23	1:A:269:LEU:HD13	1.97	0.47
1:A:283:MET:CG	1:A:321:ARG:NH1	2.78	0.47
1:B:297:ASN:HA	7:B:1057:HOH:O	2.14	0.47
1:C:159:VAL:HA	1:C:487:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:CYS:HB3	6:C:503:NAD:O7N	2.13	0.47
1:F:435:ASP:HB3	1:F:438:LYS:HD2	1.97	0.47
1:G:41:ASN:HD21	1:G:43:SER:HB2	1.78	0.47
1:G:349:GLN:O	1:G:353:ILE:HG13	2.14	0.47
1:J:132:TYR:OH	1:J:477:LEU:HA	2.14	0.47
1:K:41:ASN:C	1:K:41:ASN:ND2	2.73	0.47
1:L:124:MET:HE2	1:L:173:LEU:HD21	1.96	0.47
1:G:302:CYS:HB3	6:G:507:NAD:O7N	2.14	0.47
1:G:413:ILE:HD11	1:G:442:LEU:HG	1.97	0.47
1:G:460:GLY:HA3	1:H:146:ILE:HG13	1.97	0.47
1:I:33:SER:O	1:I:34:ARG:HB2	2.15	0.47
1:I:100:THR:HG22	1:I:118:TYR:CE1	2.50	0.47
1:I:158:PRO:HG3	1:I:185:THR:O	2.15	0.47
1:I:300:GLN:NE2	1:I:345:VAL:H	2.02	0.47
1:J:161:VAL:HA	1:J:188:VAL:HG23	1.97	0.47
1:J:247:THR:HG23	1:J:269:LEU:HD13	1.96	0.47
1:A:41:ASN:C	1:A:41:ASN:ND2	2.72	0.47
1:A:244:THR:HG23	1:A:268:GLU:HB3	1.96	0.47
1:B:283:MET:HE1	1:B:314:ILE:HB	1.97	0.47
1:C:33:SER:O	1:C:34:ARG:CB	2.62	0.47
1:G:315:TYR:O	1:G:319:VAL:HG23	2.15	0.47
1:L:11:PRO:HB3	1:L:114:TYR:CZ	2.50	0.47
1:D:193:VAL:HG11	1:D:201:ALA:CB	2.44	0.47
1:E:161:VAL:HA	1:E:188:VAL:HG23	1.97	0.47
1:F:84:ARG:NH1	1:F:184:ALA:O	2.48	0.47
1:H:36:THR:OG1	1:H:50:GLN:NE2	2.43	0.46
1:B:167:PRO:HD3	1:B:244:THR:HB	1.96	0.46
1:C:283:MET:HE1	1:C:314:ILE:HB	1.97	0.46
1:E:496:PRO:HD2	7:E:2061:HOH:O	2.15	0.46
1:J:361:LYS:HD3	1:J:367:LEU:HD22	1.97	0.46
1:L:21:GLN:HB3	1:L:29:HIS:O	2.15	0.46
1:A:302:CYS:HA	1:A:401:PHE:CZ	2.50	0.46
1:B:302:CYS:CB	6:B:502:NAD:N7N	2.79	0.46
1:D:15:PRO:HD2	1:D:108:LEU:HD22	1.97	0.46
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.97	0.46
1:H:408:LEU:HD12	1:H:408:LEU:N	2.30	0.46
1:E:253:ILE:HD11	3:E:505:ADP:C2	2.50	0.46
1:E:292:PHE:HE1	1:E:457:ASP:HB2	1.79	0.46
1:G:235:HIS:HB3	1:G:238:VAL:HG23	1.97	0.46
1:G:431:VAL:HG21	1:G:442:LEU:HB3	1.97	0.46
1:I:260:SER:O	1:J:251:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:36:THR:CB	1:J:50:GLN:HG3	2.44	0.46
1:B:247:THR:HA	1:B:269:LEU:HD13	1.98	0.46
1:C:413:ILE:O	1:C:417:VAL:HG23	2.16	0.46
1:G:131:TYR:CE1	1:G:462:GLN:HB3	2.50	0.46
1:A:102:LEU:HD21	1:A:203:TYR:CD2	2.48	0.46
1:D:461:ALA:HA	1:D:477:LEU:CD1	2.46	0.46
1:J:187:ASN:HD21	1:J:485:TYR:HB3	1.80	0.46
1:G:344:GLN:HG3	1:G:353:ILE:HD12	1.98	0.46
1:J:170:PHE:O	1:J:174:MET:HB2	2.16	0.46
1:B:459:PHE:HE2	1:B:465:PHE:CE1	2.34	0.46
1:E:338:LYS:NZ	1:I:34:ARG:HE	2.13	0.46
1:G:159:VAL:HG23	1:G:264:ARG:HH11	1.80	0.46
1:A:161:VAL:HA	1:A:188:VAL:HG23	1.98	0.46
1:A:294:LEU:CD1	1:A:306:SER:HA	2.44	0.46
1:C:294:LEU:HD12	1:C:306:SER:HA	1.98	0.46
1:G:271:GLY:HA2	1:G:425:TYR:CD2	2.50	0.46
1:G:319:VAL:O	1:G:323:VAL:HG23	2.15	0.46
1:C:363:GLU:CD	1:C:394:THR:H	2.23	0.46
1:G:11:PRO:HB3	1:G:114:TYR:CE1	2.51	0.46
1:K:21:GLN:HB3	1:K:29:HIS:O	2.16	0.46
1:A:353:ILE:HG21	1:A:381:ILE:HD13	1.98	0.45
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.16	0.45
1:F:21:GLN:HB3	1:F:29:HIS:O	2.16	0.45
1:F:235:HIS:HB3	1:F:238:VAL:HG23	1.98	0.45
1:I:86:ARG:HD2	7:I:1738:HOH:O	2.16	0.45
1:J:235:HIS:HB3	1:J:238:VAL:HG23	1.98	0.45
1:A:283:MET:HG3	1:A:321:ARG:NH1	2.31	0.45
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.50	0.45
1:C:161:VAL:HA	1:C:188:VAL:HG23	1.99	0.45
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.16	0.45
1:E:159:VAL:HA	1:E:487:LYS:HG3	1.98	0.45
1:H:24:ILE:HB	1:H:29:HIS:CE1	2.51	0.45
1:H:390:GLN:HG3	1:H:393:MET:HE3	1.97	0.45
1:L:131:TYR:CE1	1:L:462:GLN:HB3	2.51	0.45
1:I:166:ILE:HD11	1:I:193:VAL:HG12	1.97	0.45
1:K:359:THR:O	1:K:363:GLU:HG3	2.16	0.45
1:L:310:VAL:HG21	1:L:318:PHE:CD2	2.51	0.45
1:E:33:SER:O	1:E:34:ARG:HB2	2.17	0.45
1:F:410:PHE:CD1	1:F:416:VAL:HB	2.51	0.45
1:G:172:LEU:HD21	1:G:200:THR:HB	1.98	0.45
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:225:GLY:HA3	3:K:511:ADP:C8	2.51	0.45
1:L:172:LEU:HD21	1:L:200:THR:HB	1.97	0.45
1:A:202:LEU:HD21	1:A:222:PRO:HG3	1.99	0.45
1:A:413:ILE:HD11	1:A:442:LEU:HG	1.99	0.45
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.52	0.45
1:G:36:THR:CB	1:G:50:GLN:HG3	2.45	0.45
1:G:107:THR:HG23	1:G:334:PRO:HB2	1.98	0.45
1:I:292:PHE:HE1	1:I:457:ASP:HB2	1.81	0.45
1:J:84:ARG:NH1	1:J:184:ALA:O	2.50	0.45
1:L:15:PRO:HG2	1:L:108:LEU:HD22	1.99	0.45
1:L:316:ASP:N	7:L:2214:HOH:O	2.49	0.45
1:B:178:LYS:HE3	1:B:242:ALA:HB1	1.97	0.45
1:L:247:THR:HA	1:L:269:LEU:HD13	1.98	0.45
1:B:264:ARG:NH1	1:B:484:ALA:O	2.50	0.45
1:E:338:LYS:HD2	1:I:34:ARG:NH2	2.21	0.45
1:K:12:ASN:O	1:K:15:PRO:HD3	2.17	0.45
1:A:353:ILE:O	1:A:357:ILE:HG13	2.16	0.45
1:A:399:GLU:CD	1:A:401:PHE:CE1	2.95	0.45
1:C:358:ASN:ND2	7:C:2390:HOH:O	2.48	0.45
1:E:100:THR:HG22	1:E:118:TYR:CE1	2.52	0.45
1:G:34:ARG:NH2	1:K:14:GLN:O	2.50	0.45
1:B:404:VAL:HG12	1:B:406:GLN:OE1	2.17	0.45
1:B:256:ALA:HB2	7:B:1412:HOH:O	2.17	0.44
1:D:347:GLU:O	1:D:350:PHE:HB3	2.17	0.44
1:D:359:THR:O	1:D:363:GLU:HG3	2.17	0.44
1:E:315:TYR:O	1:E:319:VAL:HG23	2.17	0.44
1:B:120:VAL:CG1	1:B:124:MET:HE2	2.46	0.44
1:C:294:LEU:HD22	1:C:405:MET:HB2	2.00	0.44
1:D:460:GLY:O	1:D:477:LEU:HD12	2.17	0.44
1:G:120:VAL:HG12	1:G:124:MET:HE2	1.98	0.44
1:H:86:ARG:HG3	7:H:1869:HOH:O	2.18	0.44
1:J:131:TYR:CZ	1:J:462:GLN:HA	2.52	0.44
1:F:36:THR:OG1	1:F:50:GLN:HG3	2.17	0.44
1:H:240:LYS:HG2	1:H:241:VAL:N	2.31	0.44
1:J:205:ALA:HB2	1:J:220:ILE:HD12	1.99	0.44
1:B:174:MET:HE2	1:B:174:MET:HA	2.00	0.44
1:B:302:CYS:CB	6:B:502:NAD:H72N	2.30	0.44
1:C:166:ILE:HD11	7:C:1483:HOH:O	2.17	0.44
1:C:278:MET:HE2	1:C:438:LYS:HD3	1.99	0.44
1:D:107:THR:HG23	1:D:112:LYS:O	2.17	0.44
1:B:167:PRO:HB2	6:B:502:NAD:H5N	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ILE:HG12	1:D:222:PRO:HD2	1.99	0.44
1:D:102:LEU:HD21	1:D:203:TYR:HD2	1.81	0.44
1:E:498:LYS:HB3	1:E:498:LYS:HE2	1.75	0.44
1:H:247:THR:O	1:H:251:ARG:HG3	2.17	0.44
1:J:124:MET:HE3	1:J:173:LEU:HD22	2.00	0.44
1:K:294:LEU:HD22	1:K:405:MET:HB2	1.99	0.44
1:A:243:PHE:CE1	3:A:501[A]:ADP:H5'1	2.53	0.44
1:A:468:TYR:OH	1:B:489:LYS:HB2	2.17	0.44
1:B:319:VAL:O	1:B:323:VAL:HG23	2.17	0.44
1:D:373:ILE:HG22	1:D:375:ALA:H	1.82	0.44
1:J:15:PRO:HD2	1:J:108:LEU:HD22	2.00	0.44
1:A:165:ILE:HG22	3:A:501[B]:ADP:H4'	2.00	0.44
1:A:315:TYR:O	1:A:319:VAL:HG23	2.17	0.44
1:F:167:PRO:HD3	1:F:244:THR:HB	2.00	0.44
1:H:359:THR:O	1:H:363:GLU:HG3	2.18	0.44
1:C:46:GLU:HG3	7:C:2480:HOH:O	2.17	0.44
1:G:159:VAL:CG2	1:G:264:ARG:HH11	2.31	0.44
1:G:167:PRO:HD3	1:G:244:THR:HB	1.99	0.44
1:I:100:THR:HG22	1:I:118:TYR:HE1	1.83	0.44
1:J:102:LEU:HD21	1:J:203:TYR:CD2	2.51	0.44
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.53	0.43
1:C:170:PHE:O	1:C:174:MET:HG2	2.17	0.43
1:D:158:PRO:HG3	1:D:185:THR:O	2.17	0.43
1:D:235:HIS:HB3	1:D:238:VAL:HG23	2.00	0.43
1:F:131:TYR:CE1	1:F:462:GLN:HG3	2.53	0.43
1:A:347:GLU:O	1:A:350:PHE:HB3	2.17	0.43
1:A:238:VAL:O	1:A:263:LYS:HE3	2.18	0.43
1:A:353:ILE:CG2	1:A:381:ILE:CD1	2.95	0.43
1:E:338:LYS:NZ	1:I:34:ARG:NE	2.66	0.43
1:L:283:MET:O	1:L:287:VAL:HG23	2.19	0.43
1:A:353:ILE:CG2	1:A:381:ILE:HD13	2.49	0.43
1:B:86:ARG:HD3	7:B:2785:HOH:O	2.19	0.43
1:D:294:LEU:HD13	1:D:405:MET:HA	2.00	0.43
1:F:36:THR:HB	1:F:50:GLN:HG3	2.00	0.43
1:C:361:LYS:HE2	1:C:367:LEU:HD22	2.01	0.43
1:D:101:TYR:CG	4:D:904:EDO:H11	2.54	0.43
1:D:267:LEU:O	1:D:472:GLY:HA3	2.18	0.43
1:H:169:ASN:OD1	1:H:169:ASN:N	2.49	0.43
1:B:21:GLN:HB3	1:B:29:HIS:O	2.19	0.43
1:G:102:LEU:HD21	1:G:203:TYR:HD2	1.82	0.43
1:K:251:ARG:O	1:K:255:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:345:VAL:HG13	1:L:346:ASP:N	2.34	0.43
1:E:244:THR:HG23	1:E:268:GLU:HB3	2.01	0.43
1:K:404:VAL:HG12	1:K:406:GLN:OE1	2.18	0.43
1:L:159:VAL:HG12	1:L:187:ASN:OD1	2.19	0.43
1:A:243:PHE:CZ	3:A:501[A]:ADP:H5'1	2.54	0.43
1:H:198:PRO:O	1:H:202:LEU:HG	2.19	0.43
1:J:238:VAL:O	1:J:263:LYS:HE3	2.18	0.43
1:A:302:CYS:HA	1:A:401:PHE:HZ	1.84	0.43
1:D:311:GLN:HG2	1:D:410:PHE:CE1	2.53	0.43
1:H:315:TYR:CE1	1:H:319:VAL:HG21	2.54	0.43
1:K:161:VAL:HA	1:K:188:VAL:HG23	2.00	0.43
1:A:273:SER:HA	1:A:274:PRO:HD2	1.95	0.43
1:E:461:ALA:HA	1:E:477:LEU:HD22	2.01	0.43
1:H:244:THR:HG23	1:H:268:GLU:HB3	2.01	0.43
1:I:78:ARG:NH1	1:L:497:GLN:NE2	2.62	0.43
1:L:167:PRO:HD3	1:L:244:THR:HB	2.00	0.43
1:A:185:THR:OG1	1:A:187:ASN:ND2	2.52	0.42
1:D:303:CYS:SG	1:D:459:PHE:HZ	2.42	0.42
1:H:455:CYS:SG	1:H:458:VAL:HG21	2.59	0.42
1:K:460:GLY:HA3	1:L:146:ILE:HG13	2.01	0.42
1:K:468:TYR:OH	1:L:489:LYS:HB2	2.18	0.42
1:D:41:ASN:C	1:D:41:ASN:ND2	2.71	0.42
1:D:461:ALA:HA	1:D:477:LEU:HD13	2.01	0.42
1:E:106:GLU:O	1:E:110:ASN:HB3	2.19	0.42
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.19	0.42
1:G:108:LEU:HD11	4:G:807:EDO:O1	2.19	0.42
1:C:462:GLN:CD	1:C:462:GLN:H	2.28	0.42
1:C:490:THR:O	1:D:450:THR:HA	2.19	0.42
1:E:294:LEU:HD13	1:E:405:MET:HA	2.01	0.42
1:F:36:THR:CB	1:F:50:GLN:HG3	2.49	0.42
1:F:135:TRP:CE2	1:H:138:LYS:HD3	2.54	0.42
1:I:408:LEU:N	1:I:408:LEU:HD12	2.33	0.42
1:J:275:ASN:C	1:J:275:ASN:ND2	2.77	0.42
1:K:36:THR:CB	1:K:50:GLN:HG3	2.47	0.42
1:L:195:GLU:HG2	1:L:224:PHE:HA	2.01	0.42
1:A:167:PRO:HD3	1:A:244:THR:O	2.20	0.42
1:C:41:ASN:HD21	1:C:43:SER:HB2	1.84	0.42
1:E:131:TYR:CE1	1:E:462:GLN:HG3	2.54	0.42
1:E:315:TYR:CE1	1:E:319:VAL:HG21	2.54	0.42
1:E:345:VAL:HG13	1:E:346:ASP:N	2.33	0.42
1:G:240:LYS:HG2	1:G:241:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:373:ILE:HG22	1:J:375:ALA:H	1.85	0.42
1:L:11:PRO:HB3	1:L:114:TYR:CE1	2.54	0.42
1:L:41:ASN:HD22	1:L:43:SER:H	1.68	0.42
1:C:142:LYS:HE2	1:D:480:TYR:CZ	2.55	0.42
1:D:476:GLU:O	1:D:477:LEU:HB2	2.19	0.42
1:G:487:LYS:HD3	1:H:468:TYR:CZ	2.54	0.42
1:H:462:GLN:CD	1:H:462:GLN:H	2.26	0.42
1:H:476:GLU:O	1:H:477:LEU:HB2	2.18	0.42
1:K:410:PHE:CD1	1:K:416:VAL:HB	2.55	0.42
1:L:158:PRO:HG3	1:L:185:THR:O	2.19	0.42
1:C:271:GLY:HA2	1:C:425:TYR:CD2	2.54	0.42
1:K:42:PRO:HB3	1:K:345:VAL:O	2.19	0.42
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.55	0.42
1:E:254:GLN:HE21	1:F:254:GLN:NE2	2.17	0.42
1:E:377:ARG:NH1	7:E:1554:HOH:O	2.51	0.42
1:A:167:PRO:HD3	1:A:244:THR:HB	2.00	0.42
1:B:476:GLU:O	1:B:477:LEU:HB2	2.20	0.42
1:C:99:ARG:HG3	1:C:122:LEU:HD22	2.01	0.42
1:J:41:ASN:HD22	1:J:43:SER:H	1.68	0.42
1:L:107:THR:HG23	1:L:334:PRO:HB2	2.01	0.42
1:A:303:CYS:SG	1:A:459:PHE:HZ	2.43	0.42
1:A:404:VAL:HG12	1:A:406:GLN:OE1	2.20	0.42
1:B:455:CYS:SG	1:B:458:VAL:HG21	2.59	0.42
1:D:283:MET:O	1:D:287:VAL:HG23	2.19	0.42
1:H:70:PHE:CD1	1:H:77:ARG:HD3	2.55	0.42
1:H:443:SER:HA	1:H:451:VAL:HG11	2.01	0.42
1:L:41:ASN:C	1:L:41:ASN:ND2	2.78	0.42
1:A:235:HIS:HB3	1:A:238:VAL:HG23	2.01	0.42
1:D:121:ASP:O	1:D:125:VAL:HG23	2.20	0.42
1:D:131:TYR:CE1	1:D:462:GLN:HB3	2.55	0.42
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.55	0.42
1:E:138:LYS:HE3	1:G:135:TRP:CD1	2.55	0.42
1:F:101:TYR:CG	4:F:906:EDO:H11	2.54	0.42
1:B:108:LEU:HD11	4:B:802:EDO:C1	2.50	0.41
1:D:164:GLN:OE1	1:D:189:VAL:HG11	2.20	0.41
1:D:410:PHE:CD1	1:D:416:VAL:HB	2.55	0.41
1:I:490:THR:O	1:J:450:THR:HA	2.20	0.41
1:K:75:PRO:O	1:K:79:MET:HB2	2.20	0.41
1:K:347:GLU:O	1:K:350:PHE:HB3	2.19	0.41
1:C:410:PHE:CD1	1:C:416:VAL:HB	2.55	0.41
1:I:319:VAL:O	1:I:323:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:490:THR:HG1	1:L:464:PRO:HG2	1.84	0.41
1:L:294:LEU:HD13	1:L:405:MET:HA	2.02	0.41
1:A:247:THR:HA	1:A:269:LEU:HD22	2.01	0.41
1:B:100:THR:HG22	1:B:118:TYR:CE1	2.55	0.41
1:C:169:ASN:OD1	1:C:169:ASN:N	2.52	0.41
1:D:64:LYS:HA	7:D:1478:HOH:O	2.21	0.41
1:E:225:GLY:HA3	3:E:505:ADP:C8	2.56	0.41
1:H:431:VAL:HG21	1:H:442:LEU:HB3	2.01	0.41
1:I:315:TYR:O	1:I:319:VAL:HG23	2.20	0.41
1:I:462:GLN:OE1	1:I:462:GLN:N	2.50	0.41
1:K:167:PRO:HD3	1:K:244:THR:HB	2.01	0.41
1:K:193:VAL:HG11	1:K:201:ALA:CB	2.50	0.41
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.79	0.41
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.56	0.41
1:C:154:THR:HA	1:C:489:LYS:O	2.20	0.41
1:C:167:PRO:HD3	1:C:244:THR:HB	2.02	0.41
1:G:201:ALA:HB2	7:G:1228:HOH:O	2.21	0.41
1:J:153:TYR:CZ	1:J:491:VAL:HB	2.56	0.41
1:J:301:CYS:O	1:J:401:PHE:HE1	2.03	0.41
1:L:175:GLN:HG3	1:L:191:MET:SD	2.60	0.41
1:E:347:GLU:O	1:E:350:PHE:HB3	2.20	0.41
1:G:262:LEU:HD13	1:H:269:LEU:HD11	2.01	0.41
1:J:11:PRO:HB3	1:J:114:TYR:CZ	2.56	0.41
1:J:284:ASP:OD1	1:J:321:ARG:NH1	2.53	0.41
1:K:124:MET:HE3	1:K:173:LEU:HD22	2.01	0.41
1:A:41:ASN:HD21	1:A:43:SER:HB2	1.85	0.41
1:E:174:MET:HE2	1:E:174:MET:HA	2.02	0.41
1:E:251:ARG:NH2	1:F:260:SER:O	2.53	0.41
1:H:161:VAL:HA	1:H:188:VAL:HG23	2.02	0.41
1:L:323:VAL:O	1:L:327:LYS:HG3	2.21	0.41
1:C:333:ASN:HA	1:C:334:PRO:HD2	1.92	0.41
1:D:124:MET:HE3	1:D:173:LEU:CD2	2.50	0.41
1:D:462:GLN:CD	1:D:462:GLN:H	2.28	0.41
1:F:363:GLU:CD	1:F:394:THR:H	2.28	0.41
1:I:205:ALA:HB2	1:I:220:ILE:HD12	2.02	0.41
1:K:333:ASN:HA	1:K:334:PRO:HD2	1.93	0.41
1:I:112:LYS:HB3	1:I:112:LYS:HE2	1.91	0.41
1:J:23:PHE:CE1	1:J:26:ASN:HA	2.55	0.41
1:J:39:THR:HG23	1:J:48:ILE:HB	2.01	0.41
1:J:359:THR:O	1:J:363:GLU:HG3	2.20	0.41
1:K:19:CYS:HB3	1:K:28:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:SER:O	1:B:34:ARG:HB2	2.21	0.41
1:B:187:ASN:HD21	1:B:485:TYR:HB3	1.86	0.41
1:C:358:ASN:O	1:C:362:GLN:HG2	2.21	0.41
1:D:107:THR:HG23	1:D:334:PRO:HB2	2.02	0.41
1:G:115:VAL:HG23	7:G:1190:HOH:O	2.20	0.41
1:G:321:ARG:NH1	7:G:1164:HOH:O	2.54	0.41
1:H:42:PRO:HB3	1:H:345:VAL:O	2.21	0.41
1:I:294:LEU:HD22	1:I:405:MET:HB2	2.02	0.41
1:L:333:ASN:HA	1:L:334:PRO:HD2	1.91	0.41
1:A:164:GLN:CD	1:A:178:LYS:HB3	2.46	0.41
1:A:373:ILE:HG22	1:A:375:ALA:H	1.85	0.41
1:C:432:PHE:HA	1:C:454:ASN:OD1	2.21	0.41
1:J:164:GLN:NE2	1:J:178:LYS:HB3	2.36	0.41
1:A:311:GLN:OE1	1:A:410:PHE:CE1	2.75	0.40
1:C:227:THR:HG21	7:C:1394:HOH:O	2.21	0.40
1:E:373:ILE:HG22	1:E:375:ALA:H	1.86	0.40
1:H:112:LYS:HB3	1:H:112:LYS:HE2	1.86	0.40
1:J:413:ILE:O	1:J:417:VAL:HG23	2.21	0.40
1:F:238:VAL:O	1:F:263:LYS:HE3	2.21	0.40
1:J:107:THR:HG23	1:J:334:PRO:HB2	2.03	0.40
1:K:464:PRO:HG2	1:L:490:THR:HG1	1.87	0.40
1:L:498:LYS:HB3	1:L:498:LYS:HE2	1.87	0.40
1:E:100:THR:HG23	7:E:1808:HOH:O	2.21	0.40
1:F:442:LEU:HD23	1:F:442:LEU:HA	1.96	0.40
1:G:245:GLY:HA2	6:G:507:NAD:C4N	2.51	0.40
1:H:67:ARG:HH11	1:H:237:ASP:CG	2.30	0.40
1:I:196:GLN:NE2	1:I:196:GLN:N	2.63	0.40
1:I:303:CYS:SG	1:I:459:PHE:HZ	2.43	0.40
1:J:128:CYS:SG	1:J:177:TRP:HD1	2.44	0.40
1:J:166:ILE:HD11	1:J:193:VAL:HG12	2.04	0.40
1:L:79:MET:SD	1:L:83:HIS:HD2	2.44	0.40
1:L:164:GLN:OE1	1:L:178:LYS:HB3	2.21	0.40
1:D:497:GLN:HB3	7:D:2272:HOH:O	2.21	0.40
1:E:112:LYS:HB3	1:E:112:LYS:HE2	1.77	0.40
1:E:159:VAL:CG1	1:E:162:CYS:SG	3.10	0.40
1:E:267:LEU:O	1:E:472:GLY:HA3	2.21	0.40
1:F:225:GLY:HA3	6:F:506:NAD:C8A	2.51	0.40
1:F:303:CYS:SG	1:F:459:PHE:HZ	2.44	0.40
1:H:424:THR:CG2	1:H:470:MET:SD	3.10	0.40
1:I:161:VAL:HA	1:I:188:VAL:HG23	2.03	0.40
1:J:333:ASN:HA	1:J:334:PRO:HD2	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:169:ASN:ND2	7:K:2893:HOH:O	2.54	0.40
1:K:466:GLY:HA3	1:K:475:ARG:HD3	2.03	0.40
1:A:146:ILE:HG12	1:A:147:ASP:N	2.37	0.40
1:A:251:ARG:O	1:A:255:VAL:HG23	2.20	0.40
1:D:112:LYS:HB3	1:D:112:LYS:HE2	1.92	0.40
1:F:310:VAL:HG21	1:F:318:PHE:CD2	2.57	0.40
1:F:408:LEU:HD12	1:F:408:LEU:N	2.36	0.40
1:G:70:PHE:CZ	1:G:160:GLY:HA2	2.56	0.40
1:G:174:MET:HE1	1:G:177:TRP:CZ3	2.56	0.40
1:H:410:PHE:CD1	1:H:416:VAL:HB	2.57	0.40
1:J:376:ASP:OD1	1:J:376:ASP:N	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/500 (98%)	469 (95%)	23 (5%)	0	100	100
1	B	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
1	C	492/500 (98%)	474 (96%)	18 (4%)	0	100	100
1	D	492/500 (98%)	470 (96%)	22 (4%)	0	100	100
1	E	492/500 (98%)	475 (96%)	17 (4%)	0	100	100
1	F	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	G	492/500 (98%)	474 (96%)	18 (4%)	0	100	100
1	H	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	I	492/500 (98%)	474 (96%)	18 (4%)	0	100	100
1	J	492/500 (98%)	469 (95%)	23 (5%)	0	100	100
1	K	492/500 (98%)	473 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	492/500 (98%)	471 (96%)	21 (4%)	0	100	100
All	All	5904/6000 (98%)	5675 (96%)	229 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	399/402 (99%)	388 (97%)	11 (3%)	38	66
1	B	399/402 (99%)	390 (98%)	9 (2%)	44	72
1	C	399/402 (99%)	389 (98%)	10 (2%)	42	69
1	D	399/402 (99%)	386 (97%)	13 (3%)	33	61
1	E	399/402 (99%)	389 (98%)	10 (2%)	42	69
1	F	399/402 (99%)	387 (97%)	12 (3%)	36	64
1	G	399/402 (99%)	390 (98%)	9 (2%)	44	72
1	H	399/402 (99%)	387 (97%)	12 (3%)	36	64
1	I	399/402 (99%)	390 (98%)	9 (2%)	44	72
1	J	399/402 (99%)	384 (96%)	15 (4%)	29	56
1	K	399/402 (99%)	386 (97%)	13 (3%)	33	61
1	L	399/402 (99%)	384 (96%)	15 (4%)	29	56
All	All	4788/4824 (99%)	4650 (97%)	138 (3%)	37	65

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	100	THR
1	A	159	VAL
1	A	196	GLN
1	A	268	GLU

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Mol	Chain	Res	Type
1	A	361	LYS
1	A	362	GLN
1	A	376	ASP
1	A	401	PHE
1	A	424	THR
1	A	486	THR
1	B	14	GLN
1	B	41	ASN
1	B	56	LYS
1	B	122	LEU
1	B	159	VAL
1	B	196	GLN
1	B	311	GLN
1	B	401	PHE
1	B	486	THR
1	C	27	GLU
1	C	41	ASN
1	C	122	LEU
1	C	192	LYS
1	C	196	GLN
1	C	268	GLU
1	C	294	LEU
1	C	388	ASP
1	C	401	PHE
1	C	486	THR
1	D	41	ASN
1	D	67	ARG
1	D	90	ARG
1	D	159	VAL
1	D	196	GLN
1	D	241	VAL
1	D	311	GLN
1	D	376	ASP
1	D	401	PHE
1	D	473	SER
1	D	477	LEU
1	D	486	THR
1	D	498	LYS
1	E	41	ASN
1	E	46	GLU
1	E	72	LEU
1	E	122	LEU

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Mol	Chain	Res	Type
1	E	192	LYS
1	E	196	GLN
1	E	268	GLU
1	E	376	ASP
1	E	401	PHE
1	E	424	THR
1	F	34	ARG
1	F	41	ASN
1	F	122	LEU
1	F	159	VAL
1	F	192	LYS
1	F	196	GLN
1	F	248	GLU
1	F	268	GLU
1	F	294	LEU
1	F	311	GLN
1	F	401	PHE
1	F	486	THR
1	G	41	ASN
1	G	122	LEU
1	G	159	VAL
1	G	192	LYS
1	G	196	GLN
1	G	288	GLU
1	G	294	LEU
1	G	376	ASP
1	G	401	PHE
1	H	41	ASN
1	H	67	ARG
1	H	90	ARG
1	H	117	SER
1	H	122	LEU
1	H	196	GLN
1	H	268	GLU
1	H	376	ASP
1	H	377	ARG
1	H	401	PHE
1	H	424	THR
1	H	498	LYS
1	I	32	VAL
1	I	34	ARG
1	I	41	ASN

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Mol	Chain	Res	Type
1	I	159	VAL
1	I	196	GLN
1	I	376	ASP
1	I	399	GLU
1	I	401	PHE
1	I	486	THR
1	J	14	GLN
1	J	41	ASN
1	J	100	THR
1	J	117	SER
1	J	174	MET
1	J	195	GLU
1	J	196	GLN
1	J	275	ASN
1	J	351	LYS
1	J	376	ASP
1	J	377	ARG
1	J	401	PHE
1	J	408	LEU
1	J	470	MET
1	J	473	SER
1	K	41	ASN
1	K	117	SER
1	K	122	LEU
1	K	159	VAL
1	K	192	LYS
1	K	195	GLU
1	K	196	GLN
1	K	301	CYS
1	K	376	ASP
1	K	397	LYS
1	K	401	PHE
1	K	424	THR
1	K	486	THR
1	L	30	ASP
1	L	41	ASN
1	L	64	LYS
1	L	72	LEU
1	L	90	ARG
1	L	121	ASP
1	L	122	LEU
1	L	192	LYS

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Mol	Chain	Res	Type
1	L	195	GLU
1	L	196	GLN
1	L	241	VAL
1	L	268	GLU
1	L	301	CYS
1	L	376	ASP
1	L	424	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	ASN
1	A	29	HIS
1	A	41	ASN
1	A	175	GLN
1	A	196	GLN
1	A	275	ASN
1	A	300	GLN
1	A	341	GLN
1	B	13	GLN
1	B	14	GLN
1	B	21	GLN
1	B	26	ASN
1	B	41	ASN
1	B	175	GLN
1	B	196	GLN
1	B	275	ASN
1	B	300	GLN
1	B	362	GLN
1	C	13	GLN
1	C	26	ASN
1	C	41	ASN
1	C	175	GLN
1	C	196	GLN
1	C	275	ASN
1	C	300	GLN
1	C	358	ASN
1	D	26	ASN
1	D	41	ASN
1	D	175	GLN
1	D	196	GLN

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Mol	Chain	Res	Type
1	D	275	ASN
1	D	289	GLN
1	D	300	GLN
1	D	358	ASN
1	D	462	GLN
1	E	13	GLN
1	E	26	ASN
1	E	29	HIS
1	E	41	ASN
1	E	196	GLN
1	E	254	GLN
1	E	275	ASN
1	E	300	GLN
1	F	26	ASN
1	F	41	ASN
1	F	50	GLN
1	F	175	GLN
1	F	196	GLN
1	F	254	GLN
1	F	275	ASN
1	F	300	GLN
1	F	362	GLN
1	G	26	ASN
1	G	41	ASN
1	G	175	GLN
1	G	196	GLN
1	G	254	GLN
1	G	275	ASN
1	G	300	GLN
1	H	13	GLN
1	H	26	ASN
1	H	29	HIS
1	H	41	ASN
1	H	50	GLN
1	H	175	GLN
1	H	196	GLN
1	H	275	ASN
1	H	300	GLN
1	H	349	GLN
1	H	440	ASN
1	I	13	GLN
1	I	26	ASN

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Mol	Chain	Res	Type
1	I	41	ASN
1	I	83	HIS
1	I	175	GLN
1	I	196	GLN
1	I	254	GLN
1	I	300	GLN
1	I	447	GLN
1	I	497	GLN
1	J	13	GLN
1	J	26	ASN
1	J	41	ASN
1	J	83	HIS
1	J	175	GLN
1	J	196	GLN
1	J	275	ASN
1	J	300	GLN
1	J	341	GLN
1	K	25	ASN
1	K	26	ASN
1	K	41	ASN
1	K	175	GLN
1	K	196	GLN
1	K	275	ASN
1	K	289	GLN
1	K	300	GLN
1	K	497	GLN
1	L	13	GLN
1	L	26	ASN
1	L	41	ASN
1	L	50	GLN
1	L	83	HIS
1	L	175	GLN
1	L	196	GLN
1	L	254	GLN
1	L	275	ASN
1	L	300	GLN
1	L	362	GLN
1	L	497	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 17 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	E	505	-	28,29,29	1.78	7 (25%)	43,45,45	1.67	10 (23%)
3	ADP	K	511	-	28,29,29	1.71	6 (21%)	43,45,45	1.55	7 (16%)
3	ADP	A	501[B]	-	28,29,29	1.62	6 (21%)	43,45,45	1.59	7 (16%)
4	EDO	E	905	-	3,3,3	0.12	0	2,2,2	0.59	0
5	GAI	I	910	-	3,3,3	1.26	1 (33%)	3,3,3	1.00	0
4	EDO	L	712	-	3,3,3	0.50	0	2,2,2	0.31	0
4	EDO	G	907	-	3,3,3	0.33	0	2,2,2	0.47	0
4	EDO	E	705	-	3,3,3	0.51	0	2,2,2	0.30	0
3	ADP	A	501[A]	-	28,29,29	1.77	5 (17%)	43,45,45	1.63	10 (23%)
6	NAD	F	506	-	46,48,48	2.76	10 (21%)	64,73,73	1.74	15 (23%)
5	GAI	J	611	-	3,3,3	1.18	0	3,3,3	1.18	0
4	EDO	C	803	-	3,3,3	0.41	0	2,2,2	0.36	0
3	ADP	J	510	-	28,29,29	2.07	5 (17%)	43,45,45	1.44	7 (16%)
4	EDO	F	806	-	3,3,3	0.40	0	2,2,2	0.37	0
4	EDO	K	911	-	3,3,3	0.57	0	2,2,2	0.30	0
4	EDO	H	708	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	F	706	-	3,3,3	0.39	0	2,2,2	0.43	0
5	GAI	G	5010	-	3,3,3	1.25	1 (33%)	3,3,3	1.16	0
4	EDO	E	805	-	3,3,3	0.58	0	2,2,2	0.23	0
4	EDO	H	908	-	3,3,3	0.38	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAD	C	503	-	46,48,48	2.22	9 (19%)	64,73,73	1.91	19 (29%)
3	ADP	D	504[B]	-	28,29,29	1.56	6 (21%)	43,45,45	1.45	9 (20%)
5	GAI	H	909	-	3,3,3	1.14	0	3,3,3	1.13	0
3	ADP	I	509	-	28,29,29	1.65	5 (17%)	43,45,45	1.71	9 (20%)
3	ADP	D	504[A]	-	28,29,29	1.79	6 (21%)	43,45,45	1.54	8 (18%)
4	EDO	D	904	-	3,3,3	0.38	0	2,2,2	0.40	0
4	EDO	D	704	-	3,3,3	0.55	0	2,2,2	0.33	0
4	EDO	H	808	-	3,3,3	0.62	0	2,2,2	0.26	0
4	EDO	F	707	-	3,3,3	0.72	0	2,2,2	0.18	0
4	EDO	I	909	-	3,3,3	0.35	0	2,2,2	0.41	0
5	GAI	A	902	-	3,3,3	1.09	0	3,3,3	1.19	0
5	GAI	D	905	-	3,3,3	1.30	1 (33%)	3,3,3	1.22	0
4	EDO	A	901	-	3,3,3	0.50	0	2,2,2	0.38	0
6	NAD	B	502	-	46,48,48	2.59	11 (23%)	64,73,73	1.75	17 (26%)
4	EDO	B	902	-	3,3,3	0.28	0	2,2,2	0.48	0
4	EDO	B	701	-	3,3,3	0.40	0	2,2,2	0.41	0
4	EDO	B	802	-	3,3,3	0.38	0	2,2,2	0.51	0
3	ADP	L	512	-	28,29,29	1.68	5 (17%)	43,45,45	1.62	10 (23%)
5	GAI	E	906	-	3,3,3	1.17	0	3,3,3	1.27	0
4	EDO	I	809	-	3,3,3	0.61	0	2,2,2	0.21	0
4	EDO	C	903	-	3,3,3	0.58	0	2,2,2	0.36	0
4	EDO	F	906	-	3,3,3	0.37	0	2,2,2	0.41	0
6	NAD	G	507	-	46,48,48	2.64	12 (26%)	64,73,73	1.52	12 (18%)
4	EDO	L	912	-	3,3,3	0.39	0	2,2,2	0.41	0
6	NAD	H	508	-	46,48,48	2.47	10 (21%)	64,73,73	1.70	16 (25%)
5	GAI	G	5009	-	3,3,3	1.12	0	3,3,3	1.11	0
5	GAI	E	907	-	3,3,3	1.30	1 (33%)	3,3,3	1.33	0
4	EDO	G	807	-	3,3,3	0.55	0	2,2,2	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	E	505	-	-	5/16/32/32	0/3/3/3
3	ADP	K	511	-	-	4/16/32/32	0/3/3/3
3	ADP	A	501[B]	-	-	3/16/32/32	0/3/3/3
4	EDO	E	905	-	-	0/1/1/1	-
4	EDO	L	712	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	G	907	-	-	0/1/1/1	-
4	EDO	E	705	-	-	0/1/1/1	-
3	ADP	A	501[A]	-	-	5/16/32/32	0/3/3/3
6	NAD	F	506	-	-	9/30/62/62	0/5/5/5
4	EDO	C	803	-	-	1/1/1/1	-
3	ADP	J	510	-	-	9/16/32/32	0/3/3/3
4	EDO	F	806	-	-	0/1/1/1	-
4	EDO	K	911	-	-	1/1/1/1	-
4	EDO	H	708	-	-	0/1/1/1	-
4	EDO	F	706	-	-	0/1/1/1	-
4	EDO	E	805	-	-	0/1/1/1	-
4	EDO	H	908	-	-	0/1/1/1	-
6	NAD	C	503	-	-	11/30/62/62	0/5/5/5
3	ADP	D	504[B]	-	-	6/16/32/32	0/3/3/3
3	ADP	I	509	-	-	6/16/32/32	0/3/3/3
3	ADP	D	504[A]	-	-	6/16/32/32	0/3/3/3
4	EDO	D	904	-	-	0/1/1/1	-
4	EDO	D	704	-	-	1/1/1/1	-
4	EDO	H	808	-	-	0/1/1/1	-
4	EDO	F	707	-	-	0/1/1/1	-
4	EDO	I	909	-	-	0/1/1/1	-
4	EDO	A	901	-	-	1/1/1/1	-
6	NAD	B	502	-	-	10/30/62/62	0/5/5/5
4	EDO	B	902	-	-	0/1/1/1	-
4	EDO	B	701	-	-	0/1/1/1	-
4	EDO	B	802	-	-	0/1/1/1	-
3	ADP	L	512	-	-	5/16/32/32	0/3/3/3
4	EDO	I	809	-	-	0/1/1/1	-
4	EDO	C	903	-	-	1/1/1/1	-
4	EDO	F	906	-	-	0/1/1/1	-
6	NAD	G	507	-	-	14/30/62/62	0/5/5/5
4	EDO	L	912	-	-	0/1/1/1	-
6	NAD	H	508	-	-	9/30/62/62	0/5/5/5
4	EDO	G	807	-	-	0/1/1/1	-

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	507	NAD	C3N-C7N	-12.10	1.32	1.50
6	H	508	NAD	C3N-C7N	-10.60	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	NAD	C3N-C7N	-10.24	1.35	1.50
6	F	506	NAD	PN-O3	9.94	1.70	1.59
6	F	506	NAD	C3N-C7N	-9.82	1.36	1.50
6	C	503	NAD	C3N-C7N	-9.55	1.36	1.50
6	B	502	NAD	PN-O3	8.36	1.68	1.59
3	J	510	ADP	PA-O3A	7.08	1.67	1.59
6	F	506	NAD	PA-O3	6.89	1.66	1.59
6	G	507	NAD	PN-O3	6.08	1.66	1.59
6	B	502	NAD	PA-O3	5.75	1.65	1.59
6	H	508	NAD	PN-O3	5.70	1.65	1.59
3	E	505	ADP	C8-N7	4.69	1.40	1.31
3	K	511	ADP	C8-N7	4.64	1.40	1.31
3	L	512	ADP	C8-N7	4.62	1.40	1.31
3	E	505	ADP	PA-O3A	4.58	1.64	1.59
3	A	501[A]	ADP	C8-N7	4.56	1.40	1.31
6	F	506	NAD	C8A-N7A	4.53	1.40	1.31
3	I	509	ADP	C8-N7	4.52	1.40	1.31
6	H	508	NAD	C8A-N7A	4.41	1.40	1.31
3	J	510	ADP	C8-N7	4.36	1.40	1.31
3	D	504[A]	ADP	C8-N7	4.30	1.39	1.31
6	C	503	NAD	PN-O3	4.27	1.64	1.59
6	G	507	NAD	PA-O3	4.25	1.64	1.59
6	C	503	NAD	C8A-N7A	4.23	1.39	1.31
6	H	508	NAD	O4D-C1D	4.22	1.46	1.40
3	D	504[A]	ADP	PB-O3B	4.22	1.70	1.54
3	A	501[B]	ADP	C8-N7	4.21	1.39	1.31
3	D	504[B]	ADP	C8-N7	4.16	1.39	1.31
6	G	507	NAD	C8A-N7A	4.15	1.39	1.31
6	C	503	NAD	C2A-N3A	4.04	1.41	1.33
6	G	507	NAD	C5N-C4N	-4.02	1.32	1.38
6	B	502	NAD	C8A-N7A	3.99	1.39	1.31
3	A	501[A]	ADP	C2-N1	3.92	1.40	1.33
6	H	508	NAD	C5N-C4N	-3.92	1.32	1.38
6	H	508	NAD	C4N-C3N	-3.91	1.33	1.39
6	C	503	NAD	C2A-N1A	3.70	1.40	1.33
3	D	504[A]	ADP	C2-N1	3.65	1.40	1.33
6	F	506	NAD	C2A-N3A	3.63	1.40	1.33
3	A	501[B]	ADP	C2-N1	3.62	1.40	1.33
6	C	503	NAD	O4D-C1D	3.61	1.45	1.40
3	A	501[A]	ADP	C2-N3	3.60	1.40	1.33
6	G	507	NAD	C4N-C3N	-3.58	1.34	1.39
3	I	509	ADP	C2-N1	3.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	507	NAD	C2A-N1A	3.49	1.40	1.33
6	F	506	NAD	O4D-C1D	3.47	1.45	1.40
6	G	507	NAD	O4D-C1D	3.46	1.45	1.40
6	B	502	NAD	C2A-N3A	3.45	1.40	1.33
3	J	510	ADP	C2-N1	3.45	1.40	1.33
3	K	511	ADP	PA-O3A	3.45	1.63	1.59
3	D	504[A]	ADP	C2-N3	3.44	1.40	1.33
3	L	512	ADP	C2-N1	3.40	1.40	1.33
6	H	508	NAD	C2N-N1N	-3.40	1.31	1.35
6	C	503	NAD	C4A-N3A	3.38	1.40	1.34
3	L	512	ADP	C2-N3	3.37	1.39	1.33
6	F	506	NAD	C5N-C4N	-3.37	1.33	1.38
6	B	502	NAD	C4N-C3N	-3.34	1.34	1.39
3	I	509	ADP	C2-N3	3.33	1.39	1.33
3	K	511	ADP	C2-N1	3.32	1.39	1.33
3	A	501[A]	ADP	C4-N3	3.28	1.40	1.34
3	A	501[B]	ADP	C2-N3	3.26	1.39	1.33
3	D	504[B]	ADP	C2-N1	3.24	1.39	1.33
3	J	510	ADP	C2-N3	3.23	1.39	1.33
6	F	506	NAD	C4N-C3N	-3.22	1.34	1.39
3	L	512	ADP	PA-O3A	3.17	1.62	1.59
6	B	502	NAD	C2A-N1A	3.15	1.39	1.33
3	K	511	ADP	C2-N3	3.15	1.39	1.33
3	D	504[B]	ADP	C2-N3	3.14	1.39	1.33
6	C	503	NAD	C5N-C4N	-3.11	1.33	1.38
3	E	505	ADP	C2-N1	3.11	1.39	1.33
3	I	509	ADP	PB-O3B	3.10	1.66	1.54
6	H	508	NAD	C2N-C3N	-2.99	1.34	1.39
6	B	502	NAD	O4D-C1D	2.98	1.44	1.40
6	G	507	NAD	C2A-N3A	2.96	1.39	1.33
3	E	505	ADP	PB-O3B	2.87	1.65	1.54
6	H	508	NAD	C2A-N1A	2.84	1.39	1.33
3	J	510	ADP	C4-N3	2.74	1.39	1.34
3	K	511	ADP	PB-O3B	2.73	1.65	1.54
6	C	503	NAD	C4N-C3N	-2.72	1.35	1.39
6	F	506	NAD	C2A-N1A	2.72	1.38	1.33
3	L	512	ADP	PB-O3B	2.71	1.64	1.54
6	F	506	NAD	C4A-N3A	2.68	1.39	1.34
6	B	502	NAD	C2N-N1N	-2.66	1.32	1.35
3	A	501[A]	ADP	PB-O3B	2.60	1.64	1.54
3	D	504[A]	ADP	C4-N3	2.58	1.39	1.34
3	A	501[B]	ADP	C4-N3	2.52	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504[B]	ADP	PB-O2B	-2.51	1.45	1.54
6	B	502	NAD	C2N-C3N	-2.47	1.35	1.39
3	D	504[A]	ADP	PA-O3A	2.43	1.62	1.59
3	E	505	ADP	C8-N9	2.41	1.41	1.37
6	B	502	NAD	C5N-C4N	-2.36	1.34	1.38
3	I	509	ADP	C4-N3	2.34	1.38	1.34
6	G	507	NAD	C4A-N3A	2.30	1.38	1.34
6	G	507	NAD	C2N-C3N	-2.29	1.35	1.39
6	G	507	NAD	C2N-N1N	-2.29	1.32	1.35
3	E	505	ADP	C2-N3	2.27	1.38	1.33
3	A	501[B]	ADP	PB-O2B	-2.22	1.46	1.54
6	H	508	NAD	C2A-N3A	2.18	1.37	1.33
5	I	910	GAI	C-N1	2.18	1.36	1.30
3	K	511	ADP	C4-N3	2.14	1.38	1.34
5	D	905	GAI	C-N1	2.14	1.36	1.30
3	D	504[B]	ADP	PA-O2A	-2.12	1.45	1.55
3	D	504[B]	ADP	C4-N3	2.08	1.38	1.34
5	G	5010	GAI	C-N1	2.03	1.35	1.30
3	E	505	ADP	C4-N3	2.03	1.38	1.34
3	A	501[B]	ADP	PA-O2A	-2.02	1.46	1.55
5	E	907	GAI	C-N1	2.00	1.35	1.30

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	512	ADP	C5-C4-N9	5.72	112.04	105.81
6	B	502	NAD	O4B-C1B-C2B	-5.53	94.77	106.62
3	I	509	ADP	O4'-C1'-C2'	-5.53	94.77	106.62
3	E	505	ADP	N3-C2-N1	-5.32	120.52	128.58
6	H	508	NAD	C5A-C4A-N9A	4.90	111.15	105.81
3	K	511	ADP	C2'-C3'-C4'	-4.83	93.28	102.61
3	A	501[A]	ADP	O4'-C1'-C2'	-4.72	96.51	106.62
6	C	503	NAD	O7N-C7N-N7N	-4.65	115.89	122.62
3	E	505	ADP	C5-C4-N9	4.59	110.81	105.81
3	A	501[B]	ADP	N3-C2-N1	-4.58	121.66	128.58
6	H	508	NAD	N3A-C2A-N1A	-4.57	121.66	128.58
6	F	506	NAD	C5A-C4A-N9A	4.56	110.78	105.81
3	D	504[A]	ADP	N3-C2-N1	-4.39	121.93	128.58
3	A	501[B]	ADP	C5-C4-N9	4.26	110.45	105.81
3	K	511	ADP	C5-C4-N9	4.19	110.38	105.81
3	I	509	ADP	C5-C4-N9	4.16	110.35	105.81
6	H	508	NAD	C6N-N1N-C2N	-4.08	118.41	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	507	NAD	C5A-C4A-N9A	4.08	110.26	105.81
6	C	503	NAD	O4D-C4D-C3D	-4.04	97.12	105.15
6	G	507	NAD	C2N-C3N-C4N	4.00	122.91	118.26
3	J	510	ADP	N3-C2-N1	-3.96	122.59	128.58
6	F	506	NAD	C2B-C3B-C4B	-3.95	94.97	102.61
6	C	503	NAD	C5A-C4A-N9A	3.95	110.12	105.81
6	B	502	NAD	C5A-C4A-N9A	3.93	110.10	105.81
6	C	503	NAD	C2B-C3B-C4B	-3.92	95.04	102.61
6	F	506	NAD	O4B-C4B-C3B	3.84	112.77	105.15
6	B	502	NAD	O4D-C4D-C3D	-3.77	97.67	105.15
6	C	503	NAD	N3A-C2A-N1A	-3.74	122.92	128.58
3	A	501[A]	ADP	N3-C2-N1	-3.67	123.03	128.58
6	H	508	NAD	O7N-C7N-N7N	-3.67	117.32	122.62
3	J	510	ADP	C5-C4-N9	3.64	109.78	105.81
6	G	507	NAD	N3A-C2A-N1A	-3.61	123.11	128.58
6	F	506	NAD	N3A-C2A-N1A	-3.60	123.14	128.58
3	D	504[B]	ADP	C5-C4-N9	3.45	109.57	105.81
3	L	512	ADP	C1'-N9-C8	3.44	134.74	127.09
3	L	512	ADP	N3-C2-N1	-3.43	123.38	128.58
3	K	511	ADP	N3-C2-N1	-3.41	123.42	128.58
6	H	508	NAD	C5A-C4A-N3A	-3.41	122.03	126.72
3	A	501[B]	ADP	C2'-C3'-C4'	-3.40	96.04	102.61
3	I	509	ADP	C3'-C2'-C1'	3.38	107.86	101.46
6	C	503	NAD	C4A-N9A-C8A	-3.37	102.19	105.74
6	B	502	NAD	O7N-C7N-C3N	3.33	123.67	119.60
6	C	503	NAD	O4B-C1B-C2B	-3.29	99.57	106.62
6	C	503	NAD	C3N-C7N-N7N	3.26	121.76	117.74
3	A	501[A]	ADP	C5-C4-N9	3.25	109.36	105.81
6	F	506	NAD	C3N-C7N-N7N	3.25	121.74	117.74
6	B	502	NAD	N3A-C2A-N1A	-3.25	123.66	128.58
3	D	504[A]	ADP	C5-C4-N9	3.17	109.26	105.81
3	D	504[B]	ADP	O4'-C1'-C2'	-3.12	99.95	106.62
3	I	509	ADP	C4-N9-C8	-3.10	102.49	105.74
3	I	509	ADP	N3-C2-N1	-3.08	123.92	128.58
6	B	502	NAD	C4A-N9A-C8A	-3.07	102.51	105.74
6	G	507	NAD	C6N-N1N-C2N	-3.05	119.28	121.88
3	A	501[B]	ADP	C4-N9-C8	-3.03	102.55	105.74
3	D	504[B]	ADP	N3-C2-N1	-3.02	124.02	128.58
6	G	507	NAD	C6N-C5N-C4N	-3.01	115.11	119.45
6	F	506	NAD	C5A-C4A-N3A	-3.01	122.57	126.72
6	B	502	NAD	C6A-C5A-C4A	2.99	121.26	117.18
6	F	506	NAD	C3B-C2B-C1B	2.99	107.11	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	506	NAD	O7N-C7N-N7N	-2.98	118.31	122.62
6	B	502	NAD	C6N-N1N-C1D	2.97	125.56	119.73
6	H	508	NAD	C4A-N9A-C8A	-2.97	102.62	105.74
6	C	503	NAD	C5A-C4A-N3A	-2.96	122.64	126.72
6	C	503	NAD	C6A-C5A-C4A	2.93	121.18	117.18
6	C	503	NAD	C6N-N1N-C2N	-2.93	119.38	121.88
3	E	505	ADP	O4'-C1'-C2'	-2.91	100.39	106.62
3	J	510	ADP	C2'-C3'-C4'	-2.89	97.02	102.61
6	C	503	NAD	O5B-C5B-C4B	2.88	118.79	108.99
6	F	506	NAD	O4B-C1B-C2B	-2.87	100.47	106.62
3	D	504[A]	ADP	O2A-PA-O3A	2.86	115.02	107.27
6	C	503	NAD	C5N-C4N-C3N	2.86	123.18	120.36
6	H	508	NAD	O7N-C7N-C3N	2.81	123.04	119.60
3	A	501[B]	ADP	C5-C4-N3	-2.77	122.89	126.72
3	L	512	ADP	C2'-C3'-C4'	-2.75	97.30	102.61
6	G	507	NAD	C2D-C3D-C4D	-2.73	97.34	102.61
3	A	501[A]	ADP	C2'-C3'-C4'	-2.72	97.34	102.61
6	B	502	NAD	C5A-C4A-N3A	-2.69	123.01	126.72
3	I	509	ADP	C6-C5-C4	2.69	120.84	117.18
3	I	509	ADP	C2'-C3'-C4'	-2.68	97.42	102.61
6	H	508	NAD	C6N-C5N-C4N	-2.68	115.59	119.45
3	E	505	ADP	C2'-C3'-C4'	-2.68	97.43	102.61
3	D	504[B]	ADP	C2'-C3'-C4'	-2.67	97.45	102.61
3	J	510	ADP	C4-N9-C8	-2.66	102.94	105.74
3	A	501[A]	ADP	O4'-C1'-N9	-2.66	102.97	108.09
6	F	506	NAD	C6A-C5A-C4A	2.66	120.81	117.18
3	E	505	ADP	C5-C4-N3	-2.65	123.06	126.72
3	J	510	ADP	C5-C4-N3	-2.65	123.06	126.72
6	H	508	NAD	O4B-C1B-C2B	-2.65	100.95	106.62
3	A	501[A]	ADP	C4'-O4'-C1'	-2.65	103.62	109.47
6	G	507	NAD	C6A-C5A-C4A	2.62	120.75	117.18
3	D	504[A]	ADP	C6-C5-C4	2.60	120.73	117.18
6	F	506	NAD	C4A-N9A-C8A	-2.60	103.01	105.74
6	B	502	NAD	O7N-C7N-N7N	-2.60	118.86	122.62
3	I	509	ADP	C5-C4-N3	-2.59	123.14	126.72
3	D	504[B]	ADP	O2A-PA-O3A	2.59	114.28	107.27
3	D	504[B]	ADP	C6-C5-C4	2.57	120.69	117.18
3	D	504[A]	ADP	O4'-C1'-C2'	-2.57	101.12	106.62
6	G	507	NAD	C5N-C6N-N1N	2.57	123.89	120.38
6	B	502	NAD	C2D-C3D-C4D	-2.56	97.66	102.61
3	A	501[B]	ADP	C6-C5-C4	2.55	120.66	117.18
3	J	510	ADP	C6-C5-C4	2.53	120.63	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	508	NAD	C2A-N3A-C4A	2.53	118.00	111.83
3	K	511	ADP	O5'-C5'-C4'	2.52	117.58	108.99
6	H	508	NAD	C2B-C3B-C4B	-2.51	97.75	102.61
6	C	503	NAD	C6N-C5N-C4N	-2.51	115.83	119.45
3	A	501[A]	ADP	C6-C5-C4	2.50	120.59	117.18
6	C	503	NAD	O5D-C5D-C4D	2.44	117.30	108.99
6	B	502	NAD	C6N-N1N-C2N	-2.43	119.81	121.88
3	E	505	ADP	O2B-PB-O3A	2.42	112.75	104.64
6	F	506	NAD	C5N-C4N-C3N	2.41	122.74	120.36
3	K	511	ADP	C6-C5-C4	2.41	120.47	117.18
6	F	506	NAD	O2N-PN-O3	2.40	113.77	107.27
3	E	505	ADP	C2-N3-C4	2.40	117.70	111.83
3	A	501[B]	ADP	O4'-C1'-C2'	-2.40	101.48	106.62
3	L	512	ADP	C6-C5-C4	2.38	120.43	117.18
3	D	504[A]	ADP	C2'-C3'-C4'	-2.37	98.02	102.61
6	G	507	NAD	C4N-C3N-C7N	-2.36	114.62	121.06
3	L	512	ADP	C4-N9-C8	-2.36	103.26	105.74
6	H	508	NAD	C6A-C5A-C4A	2.34	120.38	117.18
3	D	504[A]	ADP	C5-C4-N3	-2.34	123.50	126.72
3	E	505	ADP	C4-N9-C8	-2.33	103.29	105.74
6	B	502	NAD	C6A-C5A-N7A	-2.33	127.60	132.09
6	B	502	NAD	C2B-C3B-C4B	-2.32	98.12	102.61
6	F	506	NAD	C4D-O4D-C1D	-2.32	107.80	109.92
3	A	501[A]	ADP	C5-C4-N3	-2.31	123.54	126.72
6	G	507	NAD	C4A-N9A-C8A	-2.30	103.32	105.74
3	K	511	ADP	C4-N9-C8	-2.28	103.34	105.74
3	D	504[B]	ADP	C5-C4-N3	-2.28	123.58	126.72
6	B	502	NAD	C4A-N9A-C1B	2.27	131.95	126.63
6	C	503	NAD	O2A-PA-O3	2.26	113.39	107.27
3	L	512	ADP	N3-C4-N9	-2.26	123.33	127.17
3	A	501[A]	ADP	C3'-C2'-C1'	2.25	105.72	101.46
6	C	503	NAD	O7N-C7N-C3N	2.24	122.33	119.60
6	H	508	NAD	C6N-N1N-C1D	2.24	124.12	119.73
3	D	504[A]	ADP	C6-C5-N7	-2.22	127.80	132.09
6	B	502	NAD	C4D-O4D-C1D	-2.21	107.90	109.92
6	F	506	NAD	O2A-PA-O3	2.21	113.24	107.27
3	L	512	ADP	O2A-PA-O3A	2.19	113.19	107.27
6	C	503	NAD	C6A-C5A-N7A	-2.18	127.88	132.09
6	G	507	NAD	O2N-PN-O3	2.17	113.14	107.27
3	E	505	ADP	C6-C5-C4	2.17	120.14	117.18
3	K	511	ADP	O4'-C1'-C2'	-2.16	101.99	106.62
3	I	509	ADP	C6-C5-N7	-2.14	127.96	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	508	NAD	O5D-C5D-C4D	2.13	116.24	108.99
3	D	504[B]	ADP	C4-N9-C8	-2.11	103.53	105.74
3	D	504[B]	ADP	C6-C5-N7	-2.09	128.06	132.09
6	G	507	NAD	C5A-C4A-N3A	-2.09	123.84	126.72
3	A	501[A]	ADP	O2B-PB-O3A	2.06	111.55	104.64
6	C	503	NAD	O4B-C1B-N9A	2.06	112.05	108.09
3	J	510	ADP	C6-C5-N7	-2.04	128.15	132.09
6	H	508	NAD	C2N-C3N-C4N	2.04	120.63	118.26
6	B	502	NAD	C2N-N1N-C1D	-2.04	114.63	119.13
3	E	505	ADP	O2A-PA-O3A	2.04	112.79	107.27
6	H	508	NAD	C5N-C6N-N1N	2.04	123.17	120.38
3	L	512	ADP	C4-N9-C1'	-2.00	121.95	126.63
3	L	512	ADP	O2B-PB-O3A	2.00	111.35	104.64

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	504[A]	ADP	C5'-O5'-PA-O1A
3	D	504[A]	ADP	C5'-O5'-PA-O2A
3	D	504[A]	ADP	C5'-O5'-PA-O3A
3	D	504[B]	ADP	PA-O3A-PB-O2B
3	D	504[B]	ADP	PA-O3A-PB-O3B
3	E	505	ADP	PA-O3A-PB-O3B
3	I	509	ADP	PB-O3A-PA-O5'
3	I	509	ADP	C5'-O5'-PA-O2A
3	I	509	ADP	C5'-O5'-PA-O3A
3	J	510	ADP	C5'-O5'-PA-O1A
3	J	510	ADP	C5'-O5'-PA-O2A
3	J	510	ADP	C5'-O5'-PA-O3A
3	L	512	ADP	C5'-O5'-PA-O1A
3	L	512	ADP	O4'-C4'-C5'-O5'
6	B	502	NAD	C5B-O5B-PA-O1A
6	B	502	NAD	C5B-O5B-PA-O2A
6	B	502	NAD	C5B-O5B-PA-O3
6	B	502	NAD	O4D-C4D-C5D-O5D
6	C	503	NAD	C5B-O5B-PA-O1A
6	C	503	NAD	C5B-O5B-PA-O2A
6	C	503	NAD	C5B-O5B-PA-O3
6	F	506	NAD	C5B-O5B-PA-O1A
6	F	506	NAD	C5B-O5B-PA-O3
6	G	507	NAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
6	G	507	NAD	C5B-O5B-PA-O3
6	G	507	NAD	C5D-O5D-PN-O3
6	G	507	NAD	C5D-O5D-PN-O1N
6	G	507	NAD	C5D-O5D-PN-O2N
6	H	508	NAD	C5D-O5D-PN-O3
6	H	508	NAD	C5D-O5D-PN-O1N
6	H	508	NAD	C5D-O5D-PN-O2N
6	H	508	NAD	O4D-C4D-C5D-O5D
3	J	510	ADP	O4'-C4'-C5'-O5'
6	C	503	NAD	O4D-C4D-C5D-O5D
6	G	507	NAD	O4D-C4D-C5D-O5D
6	C	503	NAD	C2N-C3N-C7N-N7N
3	L	512	ADP	C3'-C4'-C5'-O5'
6	C	503	NAD	C4N-C3N-C7N-N7N
6	C	503	NAD	C2N-C3N-C7N-O7N
6	G	507	NAD	C3D-C4D-C5D-O5D
6	C	503	NAD	C4N-C3N-C7N-O7N
3	J	510	ADP	C3'-C4'-C5'-O5'
6	B	502	NAD	C3D-C4D-C5D-O5D
6	H	508	NAD	C3D-C4D-C5D-O5D
3	I	509	ADP	C4'-C5'-O5'-PA
4	C	903	EDO	O1-C1-C2-O2
3	A	501[B]	ADP	C2'-C1'-N9-C8
3	J	510	ADP	C2'-C1'-N9-C8
6	G	507	NAD	C2B-C1B-N9A-C8A
6	B	502	NAD	PN-O3-PA-O1A
3	A	501[A]	ADP	C4'-C5'-O5'-PA
6	B	502	NAD	C4D-C5D-O5D-PN
3	A	501[A]	ADP	C2'-C1'-N9-C8
3	D	504[A]	ADP	C2'-C1'-N9-C8
3	D	504[B]	ADP	C2'-C1'-N9-C8
3	E	505	ADP	C2'-C1'-N9-C8
3	I	509	ADP	C2'-C1'-N9-C8
3	K	511	ADP	C2'-C1'-N9-C8
3	L	512	ADP	C2'-C1'-N9-C8
6	B	502	NAD	C2B-C1B-N9A-C8A
6	C	503	NAD	C2B-C1B-N9A-C8A
6	F	506	NAD	C2B-C1B-N9A-C8A
6	H	508	NAD	C2B-C1B-N9A-C8A
3	K	511	ADP	PB-O3A-PA-O2A
6	H	508	NAD	C4D-C5D-O5D-PN
6	F	506	NAD	C5B-O5B-PA-O2A

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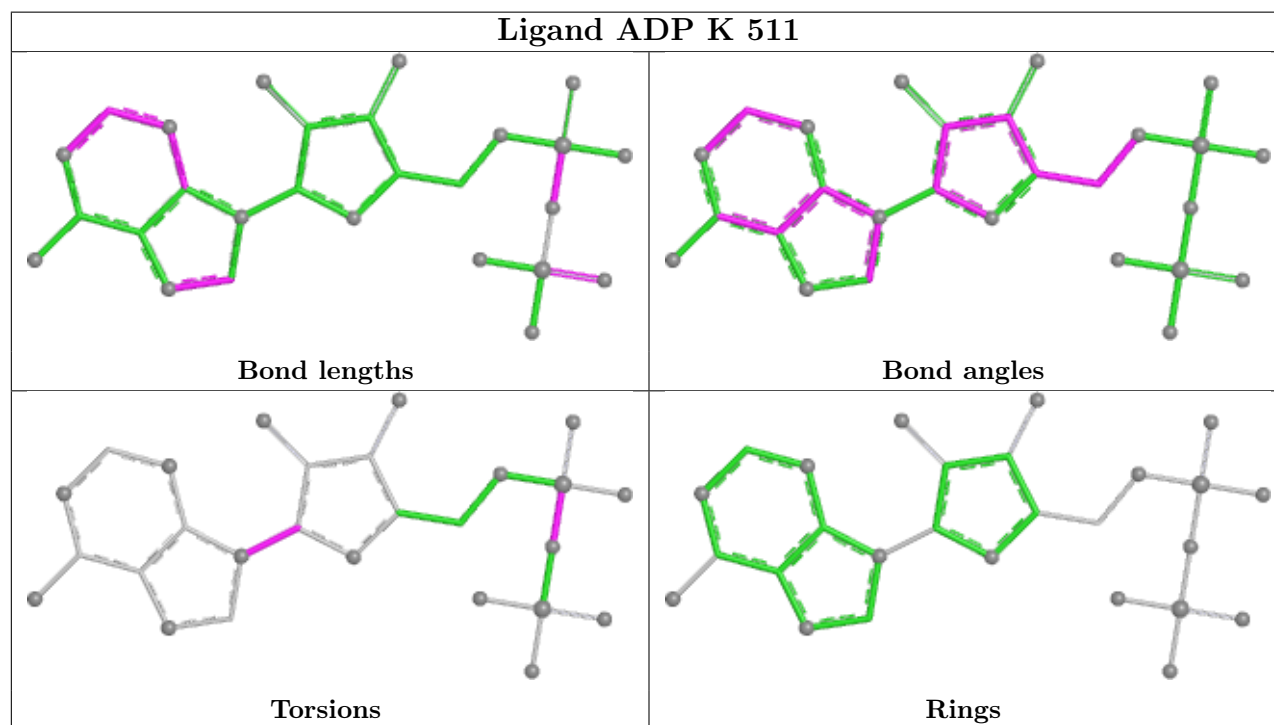
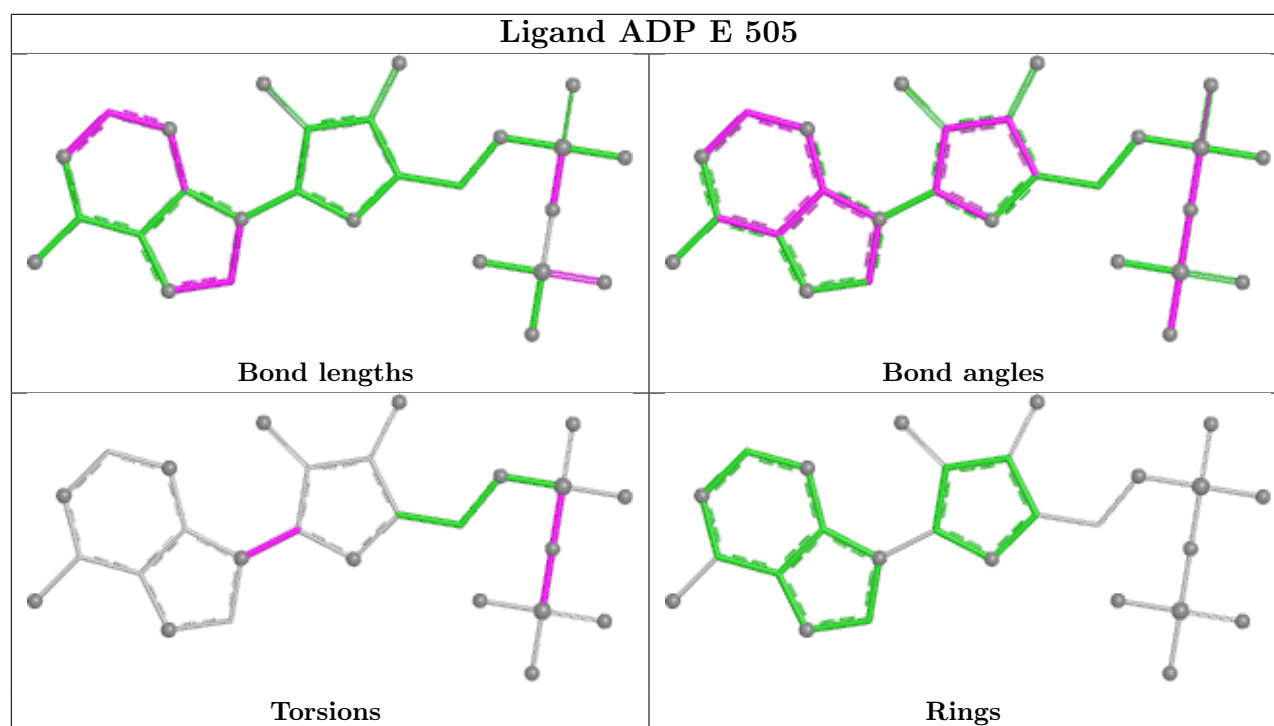
Mol	Chain	Res	Type	Atoms
6	G	507	NAD	C5B-O5B-PA-O2A
3	A	501[A]	ADP	PB-O3A-PA-O2A
3	D	504[B]	ADP	PB-O3A-PA-O2A
3	E	505	ADP	PB-O3A-PA-O2A
6	C	503	NAD	PN-O3-PA-O1A
6	G	507	NAD	PN-O3-PA-O2A
3	A	501[A]	ADP	C2'-C1'-N9-C4
3	A	501[B]	ADP	C2'-C1'-N9-C4
3	J	510	ADP	C2'-C1'-N9-C4
6	G	507	NAD	C2B-C1B-N9A-C4A
6	F	506	NAD	C4N-C3N-C7N-N7N
6	F	506	NAD	C4D-C5D-O5D-PN
6	G	507	NAD	C4D-C5D-O5D-PN
3	I	509	ADP	C2'-C1'-N9-C4
6	F	506	NAD	C2B-C1B-N9A-C4A
4	K	911	EDO	O1-C1-C2-O2
6	H	508	NAD	O4B-C4B-C5B-O5B
3	A	501[A]	ADP	PB-O3A-PA-O1A
3	E	505	ADP	PB-O3A-PA-O1A
6	H	508	NAD	PN-O3-PA-O1A
6	C	503	NAD	C4D-C5D-O5D-PN
6	G	507	NAD	O4B-C1B-N9A-C8A
3	D	504[A]	ADP	PA-O3A-PB-O3B
3	A	501[B]	ADP	O4'-C1'-N9-C8
3	J	510	ADP	O4'-C1'-N9-C8
3	K	511	ADP	O4'-C1'-N9-C8
4	D	704	EDO	O1-C1-C2-O2
3	D	504[B]	ADP	PB-O3A-PA-O1A
3	J	510	ADP	PB-O3A-PA-O2A
6	B	502	NAD	PN-O3-PA-O2A
6	G	507	NAD	PN-O3-PA-O1A
6	F	506	NAD	C4N-C3N-C7N-O7N
3	L	512	ADP	O4'-C1'-N9-C8
3	K	511	ADP	C2'-C1'-N9-C4
6	B	502	NAD	C2B-C1B-N9A-C4A
4	A	901	EDO	O1-C1-C2-O2
4	C	803	EDO	O1-C1-C2-O2
3	D	504[B]	ADP	O4'-C1'-N9-C8
3	E	505	ADP	O4'-C1'-N9-C8
3	D	504[A]	ADP	C4'-C5'-O5'-PA
6	F	506	NAD	C2N-C3N-C7N-N7N

There are no ring outliers.

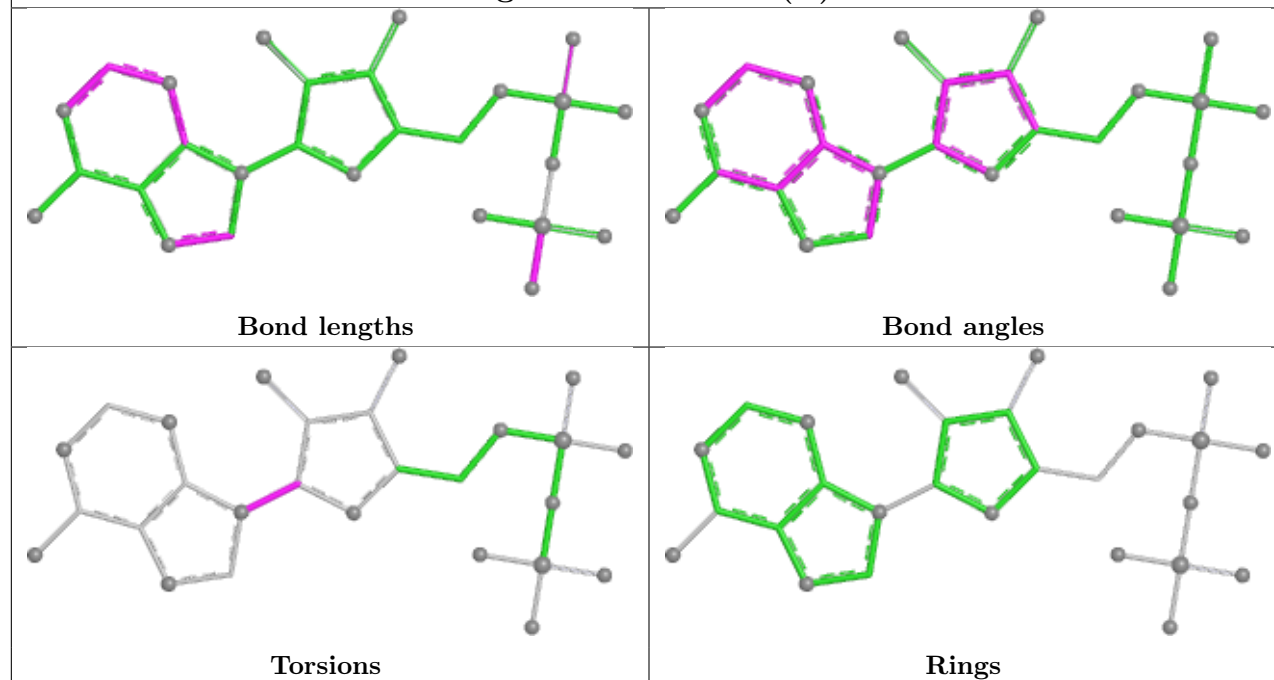
22 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	505	ADP	2	0
3	K	511	ADP	1	0
3	A	501[B]	ADP	1	0
4	E	705	EDO	1	0
3	A	501[A]	ADP	2	0
6	F	506	NAD	2	0
4	C	803	EDO	1	0
3	J	510	ADP	1	0
4	F	806	EDO	1	0
6	C	503	NAD	1	0
3	D	504[B]	ADP	1	0
3	I	509	ADP	2	0
4	D	904	EDO	1	0
4	D	704	EDO	1	0
4	H	808	EDO	1	0
6	B	502	NAD	5	0
4	B	802	EDO	2	0
4	I	809	EDO	2	0
4	F	906	EDO	1	0
6	G	507	NAD	3	0
6	H	508	NAD	2	0
4	G	807	EDO	1	0

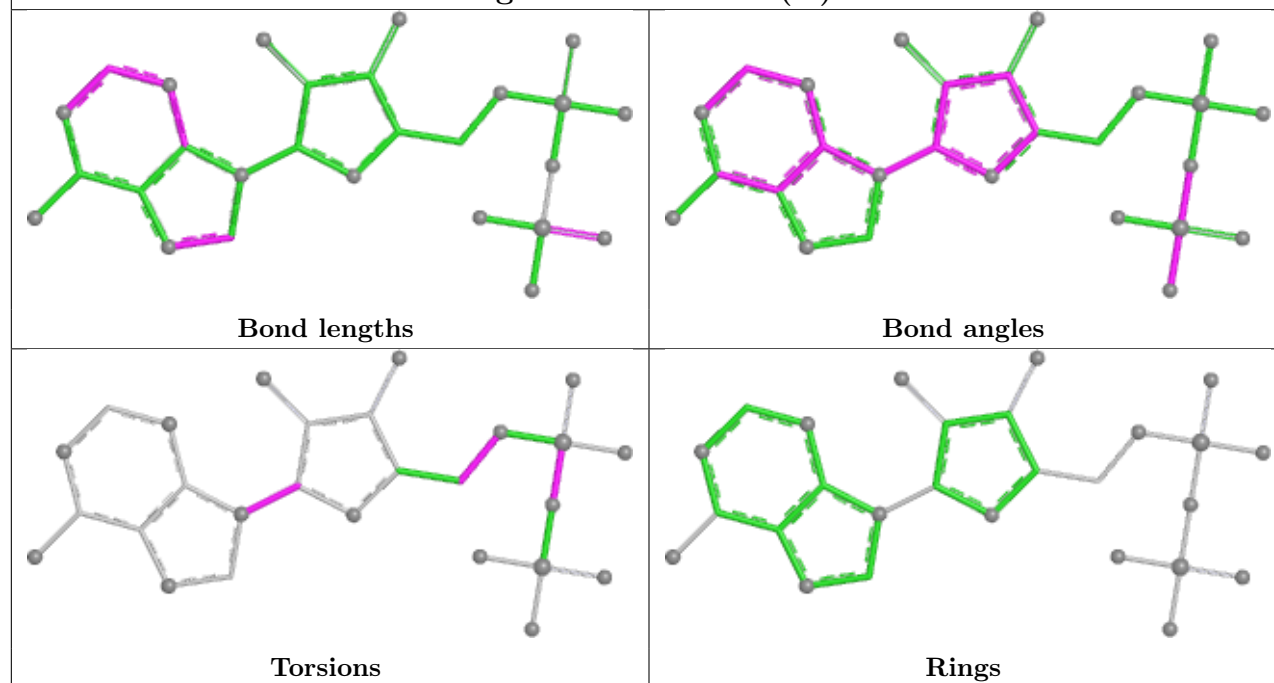
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

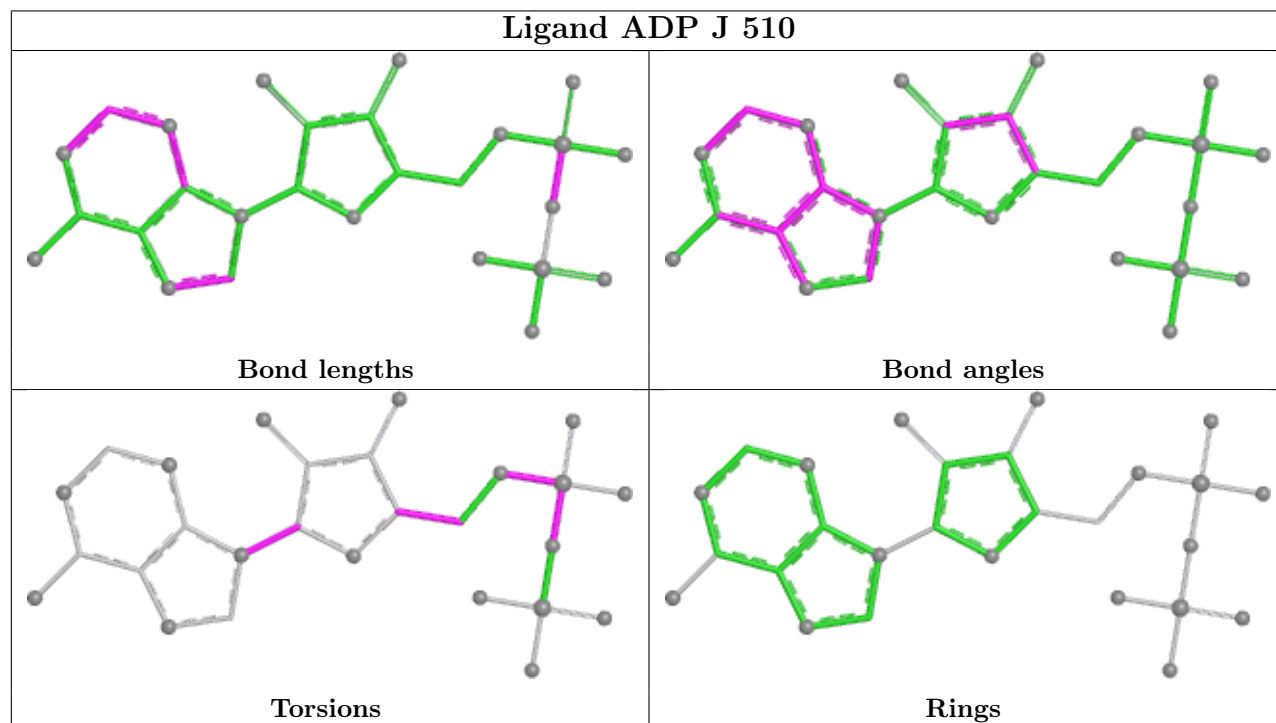
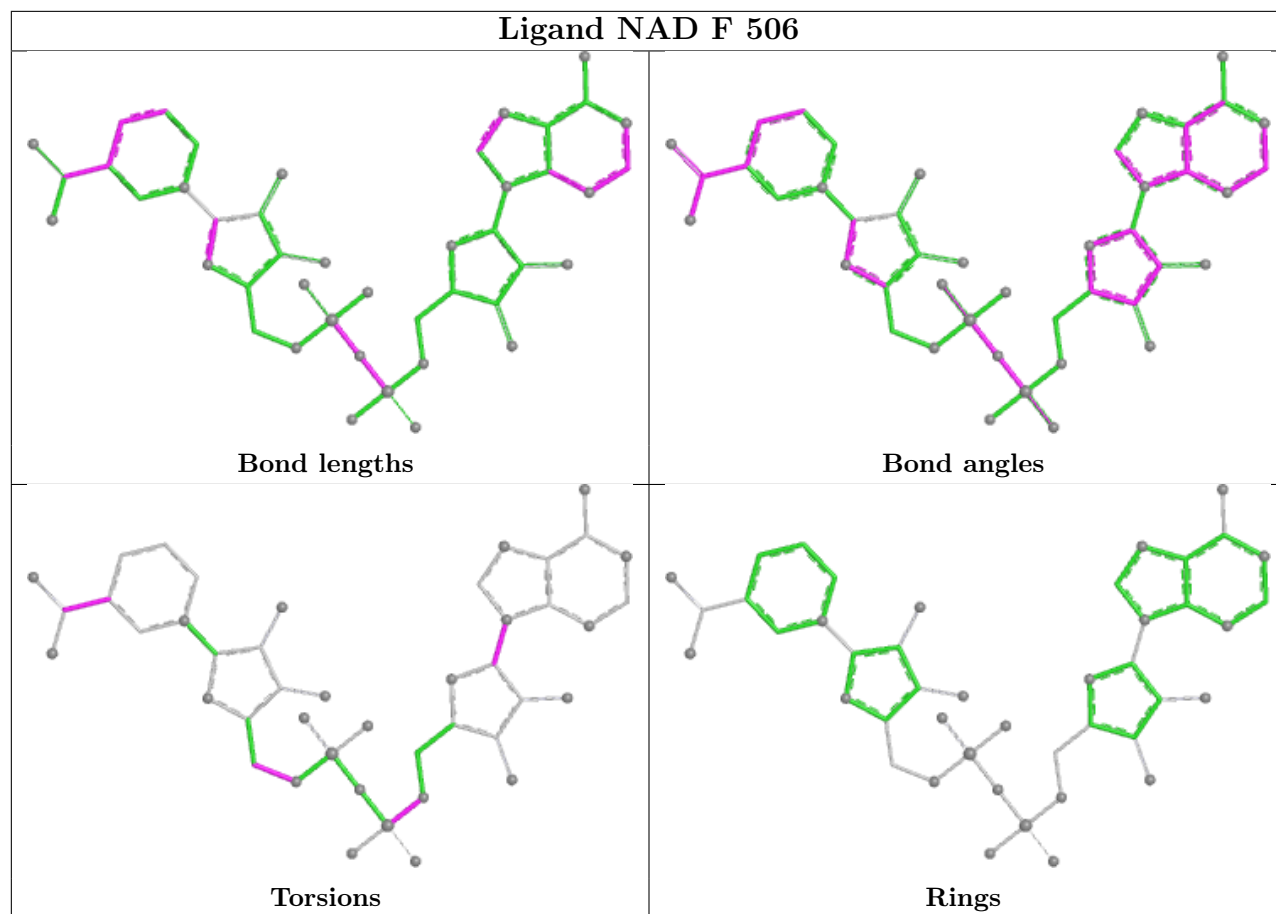


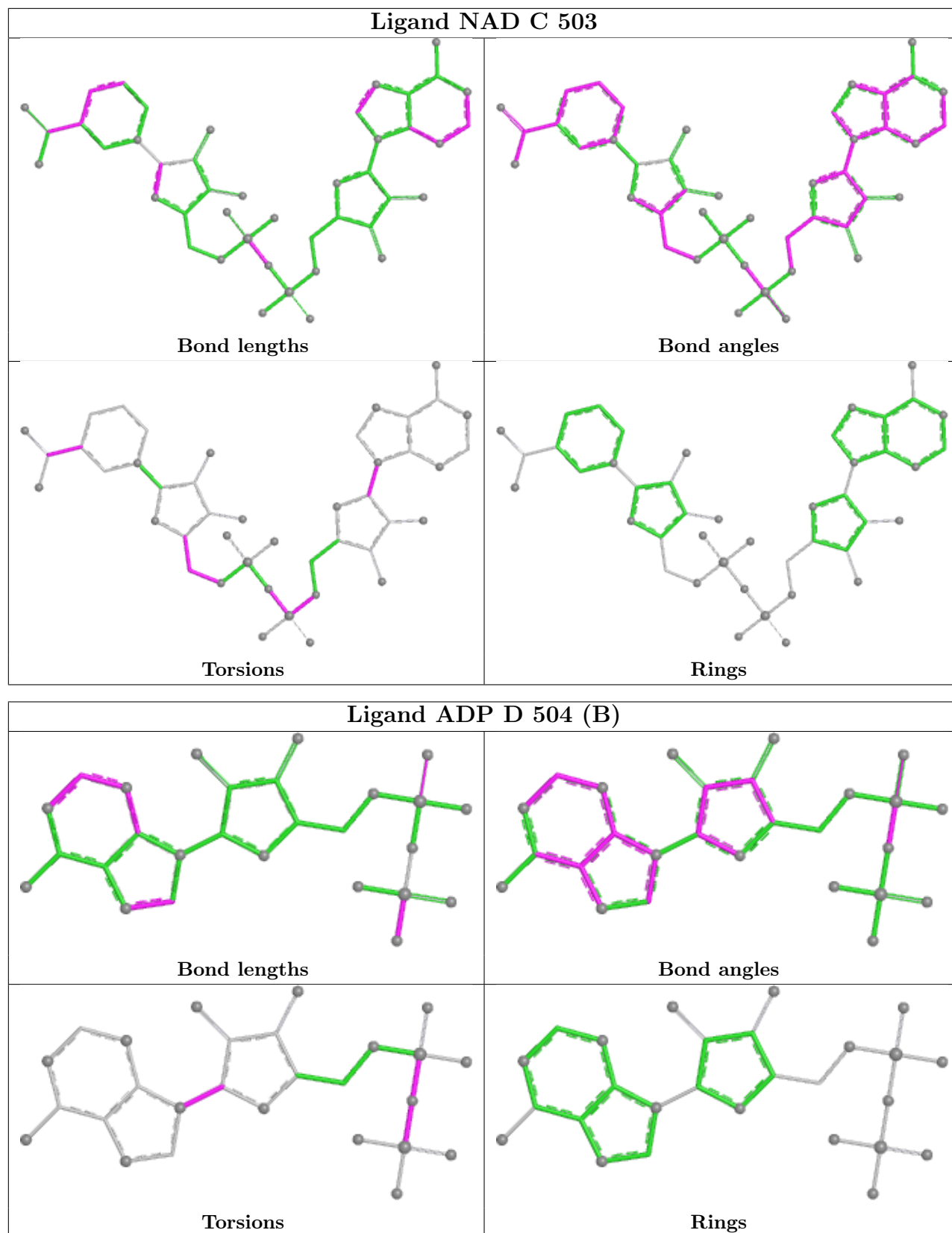
Ligand ADP A 501 (B)



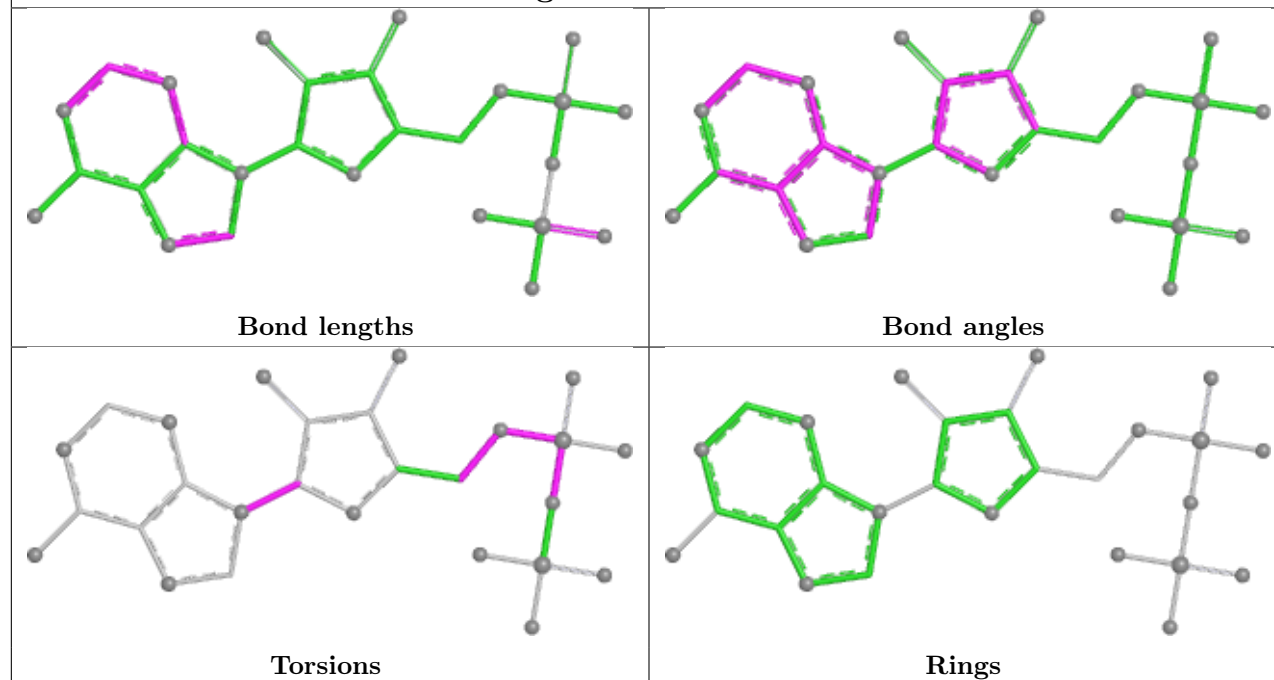
Ligand ADP A 501 (A)



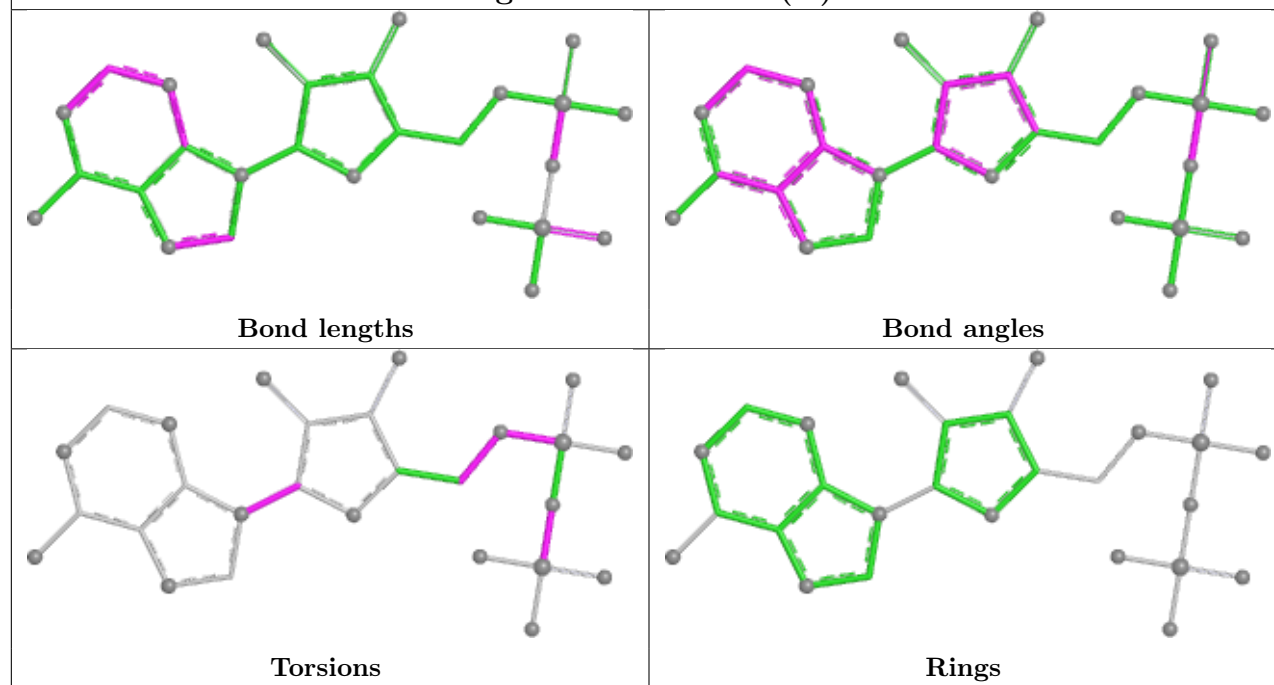


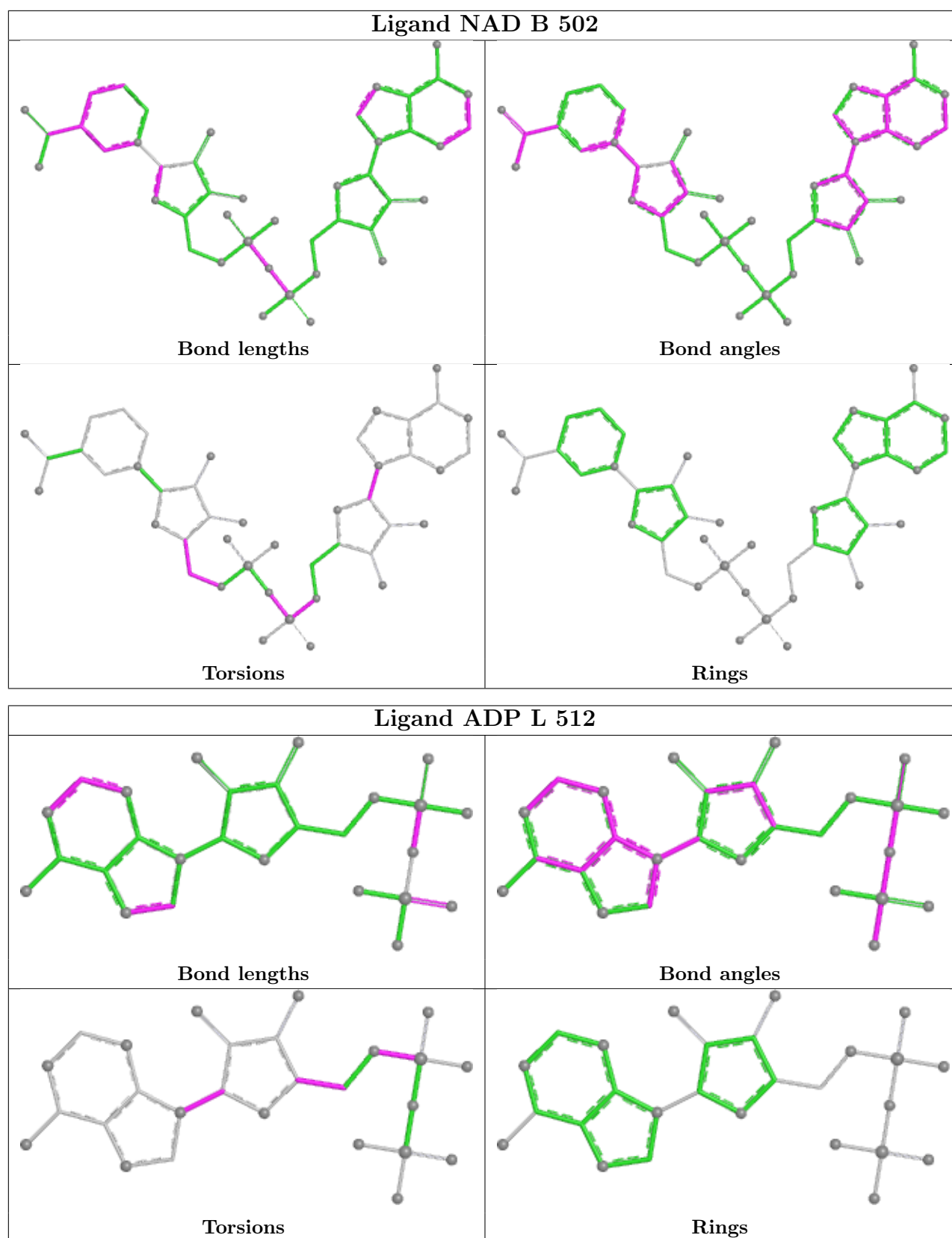


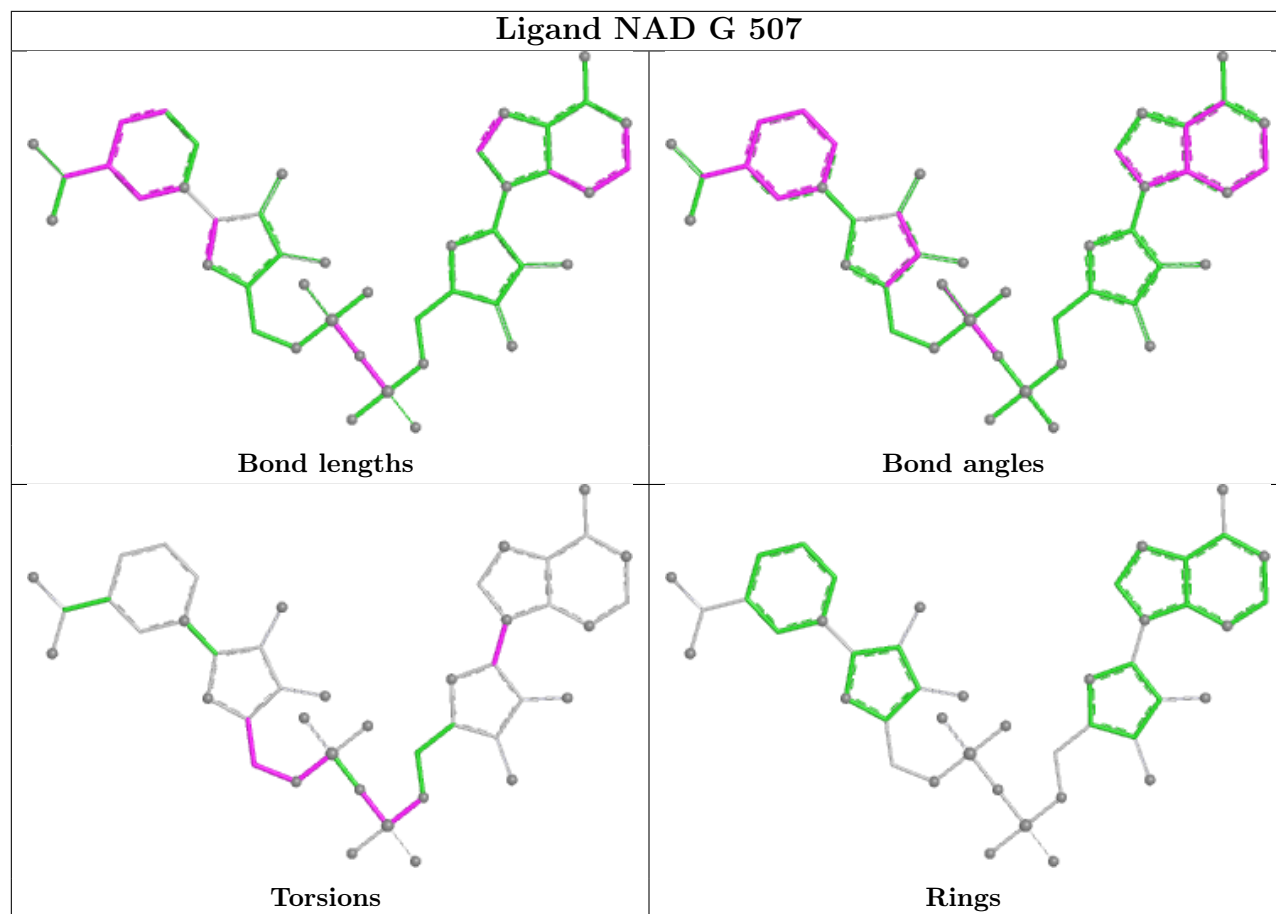
Ligand ADP I 509

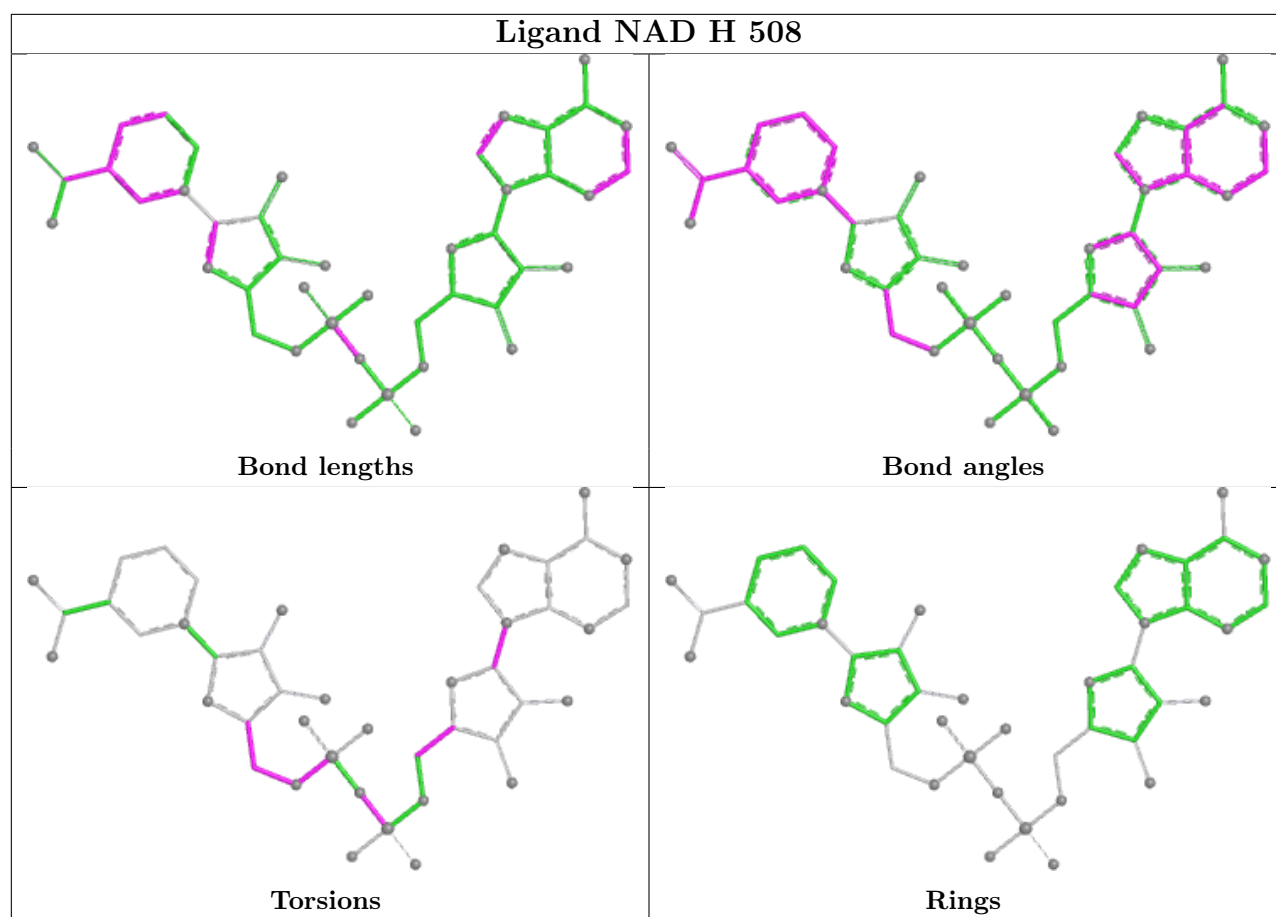


Ligand ADP D 504 (A)









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	494/500 (98%)	0.68	49 (9%) 13 11	21, 67, 104, 123	0
1	B	494/500 (98%)	-0.15	4 (0%) 82 80	24, 40, 78, 98	0
1	C	494/500 (98%)	-0.15	13 (2%) 57 52	23, 40, 72, 88	0
1	D	494/500 (98%)	0.79	53 (10%) 11 9	25, 68, 97, 118	0
1	E	494/500 (98%)	-0.21	7 (1%) 73 70	23, 41, 68, 96	0
1	F	494/500 (98%)	-0.19	9 (1%) 67 64	21, 37, 66, 94	0
1	G	494/500 (98%)	-0.02	5 (1%) 79 76	26, 46, 68, 98	0
1	H	494/500 (98%)	0.07	2 (0%) 88 86	24, 46, 77, 91	0
1	I	494/500 (98%)	0.36	9 (1%) 67 64	36, 58, 82, 105	0
1	J	494/500 (98%)	0.98	46 (9%) 14 12	44, 77, 104, 114	0
1	K	494/500 (98%)	0.69	21 (4%) 40 35	44, 71, 96, 115	0
1	L	494/500 (98%)	1.17	60 (12%) 8 7	47, 89, 115, 127	0
All	All	5928/6000 (98%)	0.34	278 (4%) 36 32	21, 55, 99, 127	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	365	ALA	5.3
1	A	477	LEU	4.8
1	L	378	GLY	4.2
1	J	7	ALA	4.2
1	A	468	TYR	4.1
1	L	461	ALA	4.1
1	K	463	SER	4.1
1	I	375	ALA	3.9
1	G	474	GLY	3.8
1	H	463	SER	3.6
1	A	367	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	356	TYR	3.5
1	K	386	PHE	3.5
1	A	371	GLY	3.5
1	L	223	GLY	3.4
1	L	463	SER	3.4
1	J	468	TYR	3.3
1	L	386	PHE	3.3
1	L	468	TYR	3.3
1	D	408	LEU	3.3
1	K	364	GLY	3.3
1	A	372	GLY	3.3
1	A	473	SER	3.2
1	D	424	THR	3.2
1	F	463	SER	3.2
1	A	395	ILE	3.2
1	A	463	SER	3.2
1	J	333	ASN	3.1
1	L	371	GLY	3.1
1	A	470	MET	3.1
1	A	474	GLY	3.1
1	D	326	ALA	3.1
1	A	461	ALA	3.0
1	L	42	PRO	3.0
1	A	258	GLY	3.0
1	L	7	ALA	3.0
1	L	408	LEU	3.0
1	D	310	VAL	3.0
1	L	405	MET	3.0
1	D	315	TYR	3.0
1	G	477	LEU	3.0
1	A	353	ILE	2.9
1	A	373	ILE	2.9
1	D	365	ALA	2.9
1	D	467	GLY	2.9
1	K	460	GLY	2.9
1	I	470	MET	2.9
1	D	40	VAL	2.9
1	L	32	VAL	2.9
1	J	108	LEU	2.9
1	L	354	LEU	2.9
1	F	477	LEU	2.9
1	L	108	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	462	GLN	2.9
1	D	466	GLY	2.9
1	J	8	VAL	2.8
1	J	335	PHE	2.8
1	L	295	PHE	2.8
1	D	468	TYR	2.8
1	A	465	PHE	2.8
1	J	114	TYR	2.8
1	E	11	PRO	2.8
1	A	357	ILE	2.7
1	A	469	LYS	2.7
1	F	465	PHE	2.7
1	J	11	PRO	2.7
1	L	356	TYR	2.7
1	A	305	GLY	2.7
1	A	267	LEU	2.7
1	D	367	LEU	2.7
1	K	7	ALA	2.7
1	A	252	VAL	2.7
1	J	102	LEU	2.7
1	L	367	LEU	2.7
1	C	477	LEU	2.6
1	A	471	SER	2.6
1	E	7	ALA	2.6
1	J	374	ALA	2.6
1	K	480	TYR	2.6
1	D	478	GLY	2.6
1	L	395	ILE	2.6
1	A	476	GLU	2.6
1	I	389	VAL	2.6
1	J	345	VAL	2.6
1	J	425	TYR	2.6
1	L	387	GLY	2.6
1	A	400	ILE	2.6
1	L	400	ILE	2.6
1	J	375	ALA	2.6
1	L	413	ILE	2.6
1	A	315	TYR	2.6
1	E	466	GLY	2.5
1	K	466	GLY	2.5
1	J	462	GLN	2.5
1	K	375	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	461	ALA	2.5
1	B	472	GLY	2.5
1	D	299	GLY	2.5
1	K	299	GLY	2.5
1	L	459	PHE	2.5
1	J	13	GLN	2.5
1	L	17	VAL	2.5
1	C	7	ALA	2.5
1	J	44	THR	2.5
1	J	400	ILE	2.5
1	L	294	LEU	2.5
1	L	301	CYS	2.5
1	A	464	PRO	2.5
1	K	474	GLY	2.5
1	D	335	PHE	2.5
1	L	350	PHE	2.4
1	D	319	VAL	2.4
1	A	256	ALA	2.4
1	D	374	ALA	2.4
1	J	10	ALA	2.4
1	J	104	ALA	2.4
1	A	478	GLY	2.4
1	L	381	ILE	2.4
1	D	477	LEU	2.4
1	K	465	PHE	2.4
1	D	470	MET	2.4
1	C	268	GLU	2.4
1	H	473	SER	2.4
1	D	301	CYS	2.4
1	D	381	ILE	2.4
1	F	253	ILE	2.4
1	L	357	ILE	2.4
1	A	475	ARG	2.4
1	J	17	VAL	2.4
1	D	471	SER	2.4
1	A	466	GLY	2.4
1	I	376	ASP	2.4
1	A	386	PHE	2.4
1	C	470	MET	2.4
1	E	470	MET	2.4
1	D	375	ALA	2.4
1	D	461	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	103	ALA	2.4
1	J	42	PRO	2.3
1	C	473	SER	2.3
1	E	473	SER	2.3
1	A	360	GLY	2.3
1	D	48	ILE	2.3
1	D	373	ILE	2.3
1	L	22	ILE	2.3
1	L	48	ILE	2.3
1	J	19	CYS	2.3
1	D	386	PHE	2.3
1	J	139	TYR	2.3
1	L	465	PHE	2.3
1	D	399	GLU	2.3
1	L	268	GLU	2.3
1	L	198	PRO	2.3
1	J	380	PHE	2.3
1	F	468	TYR	2.3
1	J	330	VAL	2.3
1	L	47	VAL	2.3
1	J	464	PRO	2.3
1	D	254	GLN	2.3
1	J	474	GLY	2.3
1	K	473	SER	2.3
1	D	353	ILE	2.3
1	J	48	ILE	2.3
1	D	11	PRO	2.3
1	L	364	GLY	2.3
1	C	463	SER	2.3
1	L	373	ILE	2.3
1	D	469	LYS	2.3
1	C	465	PHE	2.3
1	L	293	ALA	2.2
1	L	44	THR	2.2
1	C	474	GLY	2.2
1	B	470	MET	2.2
1	D	327	LYS	2.2
1	E	477	LEU	2.2
1	G	471	SER	2.2
1	J	368	LEU	2.2
1	A	309	PHE	2.2
1	J	386	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	18	PHE	2.2
1	L	224	PHE	2.2
1	D	330	VAL	2.2
1	L	52	ALA	2.2
1	J	342	GLY	2.2
1	L	105	LEU	2.2
1	L	296	PHE	2.2
1	D	8	VAL	2.2
1	D	345	VAL	2.2
1	D	7	ALA	2.2
1	I	461	ALA	2.2
1	L	20	ASN	2.2
1	A	247	THR	2.2
1	D	372	GLY	2.2
1	A	306	SER	2.2
1	A	443	SER	2.2
1	E	471	SER	2.2
1	D	401	PHE	2.2
1	F	470	MET	2.2
1	D	247	THR	2.2
1	C	466	GLY	2.2
1	D	371	GLY	2.2
1	L	466	GLY	2.2
1	D	253	ILE	2.2
1	J	373	ILE	2.2
1	J	121	ASP	2.2
1	J	113	PRO	2.2
1	A	310	VAL	2.1
1	A	326	ALA	2.1
1	L	31	ALA	2.1
1	D	370	GLY	2.1
1	J	384	THR	2.1
1	I	468	TYR	2.1
1	J	395	ILE	2.1
1	K	357	ILE	2.1
1	L	277	ILE	2.1
1	C	476	GLU	2.1
1	F	476	GLU	2.1
1	A	121	ASP	2.1
1	D	350	PHE	2.1
1	D	331	VAL	2.1
1	G	7	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	194	ALA	2.1
1	D	44	THR	2.1
1	D	114	TYR	2.1
1	D	379	TYR	2.1
1	A	330	VAL	2.1
1	A	462	GLN	2.1
1	C	254	GLN	2.1
1	D	462	GLN	2.1
1	K	255	VAL	2.1
1	L	221	VAL	2.1
1	L	331	VAL	2.1
1	D	339	THR	2.1
1	F	466	GLY	2.1
1	G	472	GLY	2.1
1	I	466	GLY	2.1
1	J	482	LEU	2.1
1	A	410	PHE	2.1
1	D	380	PHE	2.1
1	L	344	GLN	2.1
1	L	51	VAL	2.1
1	L	385	VAL	2.1
1	C	461	ALA	2.1
1	A	481	GLY	2.1
1	F	474	GLY	2.1
1	K	371	GLY	2.1
1	A	356	TYR	2.1
1	A	480	TYR	2.1
1	D	118	TYR	2.1
1	B	473	SER	2.1
1	L	19	CYS	2.1
1	A	318	PHE	2.0
1	K	252	VAL	2.0
1	A	7	ALA	2.0
1	J	12	ASN	2.0
1	J	72	LEU	2.0
1	K	267	LEU	2.0
1	A	314	ILE	2.0
1	B	424	THR	2.0
1	J	366	LYS	2.0
1	L	407	ILE	2.0
1	C	480	TYR	2.0
1	K	468	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	470	MET	2.0
1	L	322	SER	2.0
1	J	301	CYS	2.0
1	L	319	VAL	2.0
1	D	108	LEU	2.0
1	I	7	ALA	2.0
1	L	202	LEU	2.0
1	A	392	GLY	2.0
1	J	467	GLY	2.0
1	L	258	GLY	2.0
1	I	424	THR	2.0
1	L	266	THR	2.0
1	J	38	PRO	2.0
1	A	441	TYR	2.0
1	K	259	SER	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	D	504[A]	27/27	0.70	0.15	79,81,86,86	27
3	ADP	D	504[B]	27/27	0.70	0.15	89,91,96,96	27
4	EDO	I	809	4/4	0.74	0.21	81,82,82,82	0
2	NA	L	612	1/1	0.75	0.12	80,80,80,80	0
4	EDO	K	911	4/4	0.75	0.17	79,80,80,80	0
2	NA	C	603	1/1	0.77	0.12	54,54,54,54	0
3	ADP	A	501[A]	27/27	0.81	0.13	78,80,81,81	27
3	ADP	L	512	27/27	0.81	0.11	89,97,112,113	0

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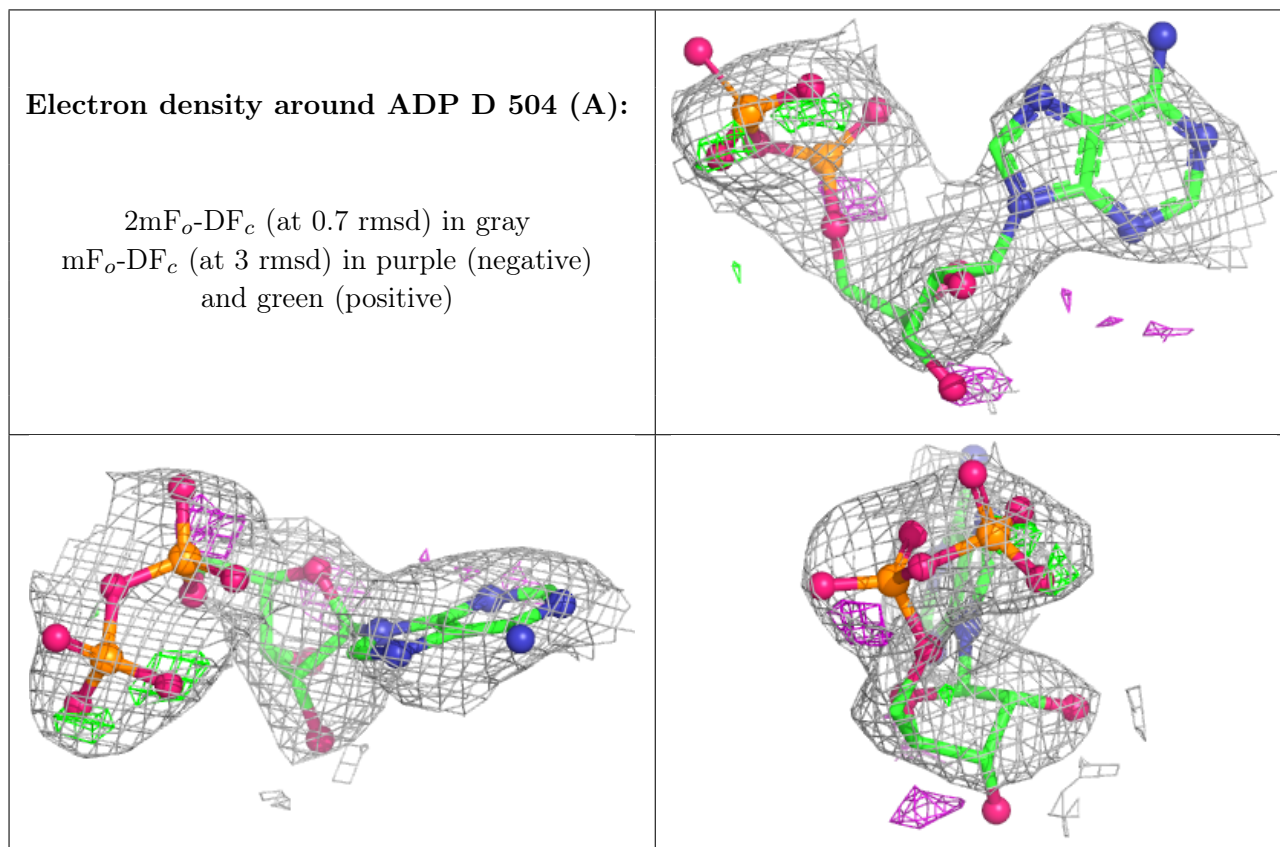
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	B	802	4/4	0.81	0.19	48,48,52,53	0
4	EDO	C	903	4/4	0.81	0.16	45,49,49,52	0
4	EDO	G	907	4/4	0.81	0.14	68,68,68,69	0
3	ADP	A	501[B]	27/27	0.81	0.13	91,93,93,93	27
2	NA	D	604	1/1	0.81	0.15	73,73,73,73	0
5	GAI	D	905	4/4	0.81	0.20	77,78,78,78	0
6	NAD	B	502	44/44	0.81	0.13	73,88,103,104	0
3	ADP	J	510	27/27	0.83	0.11	102,104,114,115	0
2	NA	A	601	1/1	0.84	0.11	82,82,82,82	0
2	NA	I	609	1/1	0.85	0.09	54,54,54,54	0
4	EDO	H	808	4/4	0.85	0.14	63,64,64,65	0
4	EDO	G	807	4/4	0.85	0.14	75,75,75,75	0
6	NAD	C	503	44/44	0.85	0.13	58,81,92,93	0
5	GAI	G	5010	4/4	0.86	0.12	47,47,49,49	0
4	EDO	H	908	4/4	0.86	0.20	79,79,79,80	0
5	GAI	E	907	4/4	0.86	0.15	47,48,49,49	0
3	ADP	I	509	27/27	0.87	0.10	79,81,94,95	0
5	GAI	H	909	4/4	0.87	0.21	95,95,95,95	0
5	GAI	E	906	4/4	0.87	0.23	51,54,55,55	0
4	EDO	L	912	4/4	0.87	0.10	68,69,70,72	0
6	NAD	G	507	44/44	0.87	0.12	61,77,91,92	0
4	EDO	E	805	4/4	0.88	0.19	83,83,85,85	0
5	GAI	I	910	4/4	0.88	0.18	94,94,94,95	0
4	EDO	F	706	4/4	0.88	0.20	74,76,79,80	0
4	EDO	L	712	4/4	0.88	0.14	70,72,73,73	0
6	NAD	F	506	44/44	0.88	0.11	38,68,81,84	0
4	EDO	A	901	4/4	0.88	0.12	75,75,76,77	0
6	NAD	H	508	44/44	0.88	0.12	49,81,89,90	0
5	GAI	J	611	4/4	0.89	0.10	64,66,66,66	0
3	ADP	K	511	27/27	0.89	0.09	94,99,105,106	0
4	EDO	F	906	4/4	0.89	0.10	63,63,65,65	0
4	EDO	E	905	4/4	0.90	0.13	51,52,53,58	0
5	GAI	A	902	4/4	0.90	0.12	63,64,64,65	0
2	NA	F	5007	1/1	0.90	0.16	54,54,54,54	0
4	EDO	C	803	4/4	0.90	0.09	49,53,53,55	0
4	EDO	I	909	4/4	0.90	0.14	62,62,63,64	0
2	NA	B	5003	1/1	0.90	0.08	55,55,55,55	0
2	NA	E	605	1/1	0.90	0.06	37,37,37,37	0
3	ADP	E	505	27/27	0.91	0.09	43,52,79,80	0
4	EDO	F	707	4/4	0.91	0.12	59,59,61,61	0
2	NA	J	610	1/1	0.91	0.11	75,75,75,75	0
4	EDO	B	902	4/4	0.92	0.17	63,63,65,65	0

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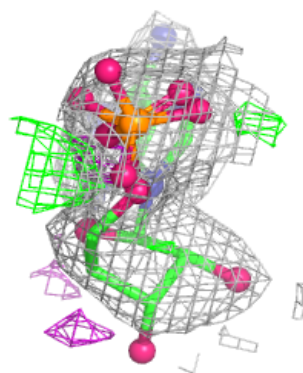
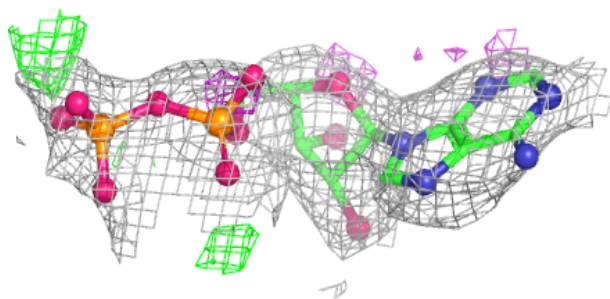
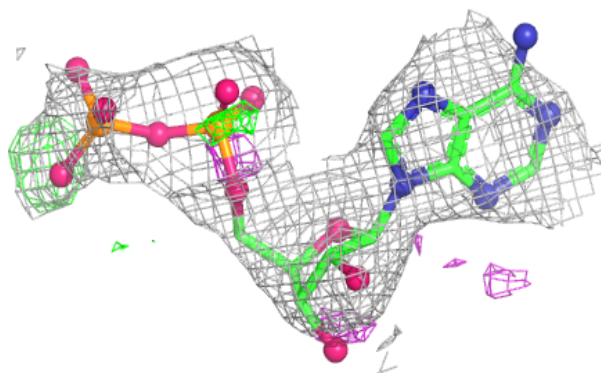
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GAI	G	5009	4/4	0.93	0.15	76,76,76,76	0
4	EDO	D	904	4/4	0.93	0.11	74,74,75,75	0
4	EDO	E	705	4/4	0.93	0.17	77,80,80,80	0
2	NA	K	5012	1/1	0.93	0.09	60,60,60,60	0
2	NA	G	607	1/1	0.93	0.07	46,46,46,46	0
4	EDO	F	806	4/4	0.94	0.10	53,54,54,58	0
2	NA	K	611	1/1	0.94	0.09	63,63,63,63	0
4	EDO	H	708	4/4	0.95	0.11	47,49,51,53	0
2	NA	C	5004	1/1	0.95	0.21	51,51,51,51	0
2	NA	F	606	1/1	0.96	0.04	32,32,32,32	0
4	EDO	B	701	4/4	0.96	0.13	67,67,67,68	0
2	NA	H	608	1/1	0.96	0.06	46,46,46,46	0
4	EDO	D	704	4/4	0.96	0.09	53,54,56,56	0
2	NA	G	5008	1/1	0.97	0.17	48,48,48,48	0
2	NA	B	602	1/1	0.97	0.06	40,40,40,40	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.



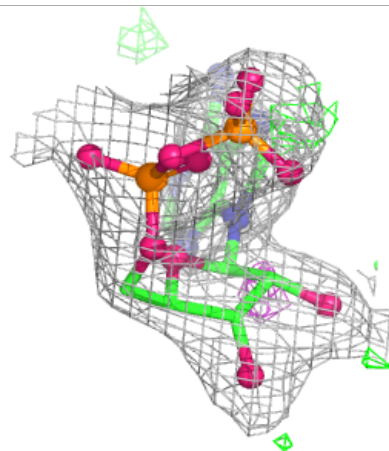
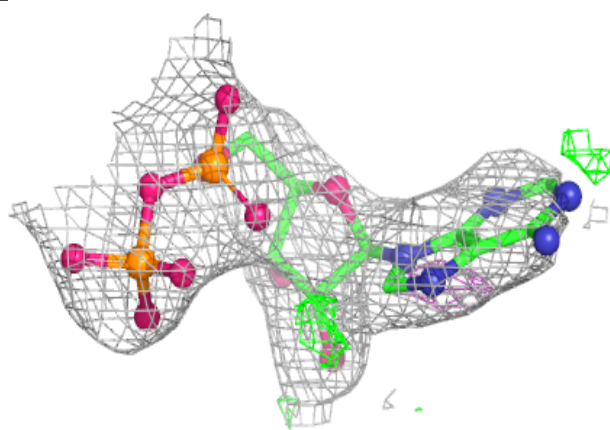
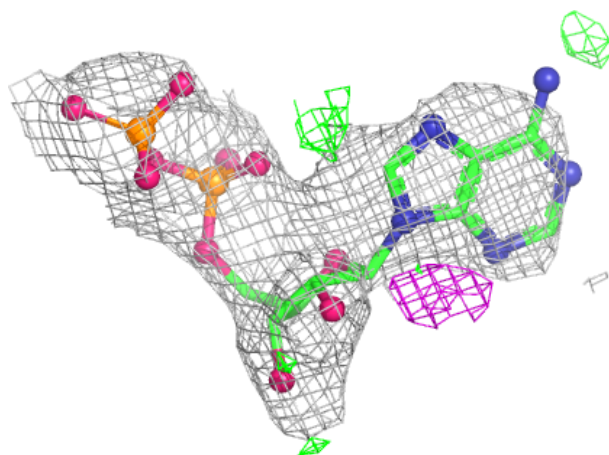
Electron density around ADP D 504 (B):

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



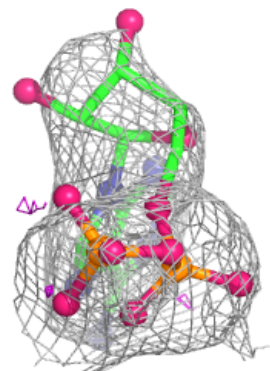
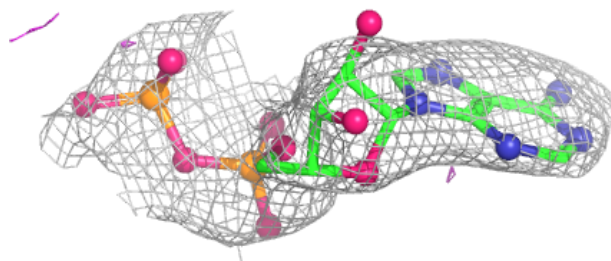
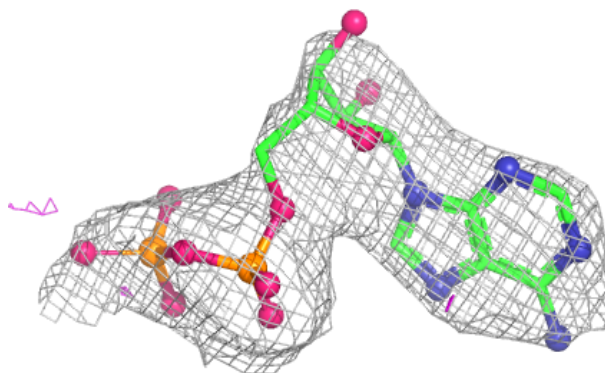
Electron density around ADP A 501 (A):

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



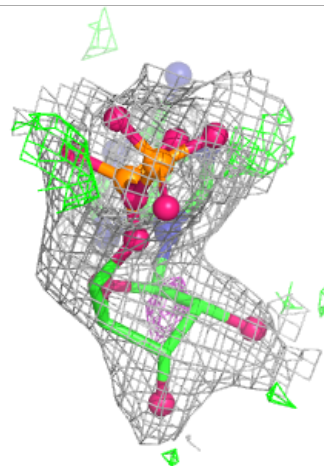
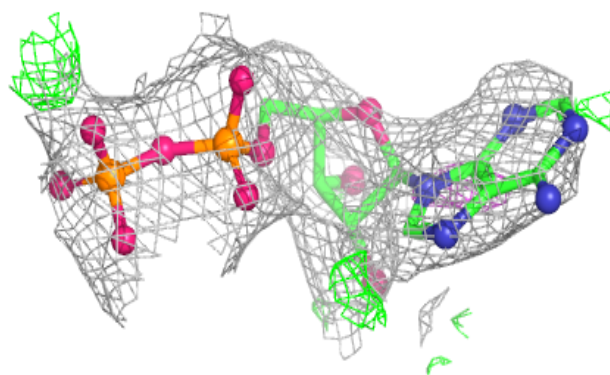
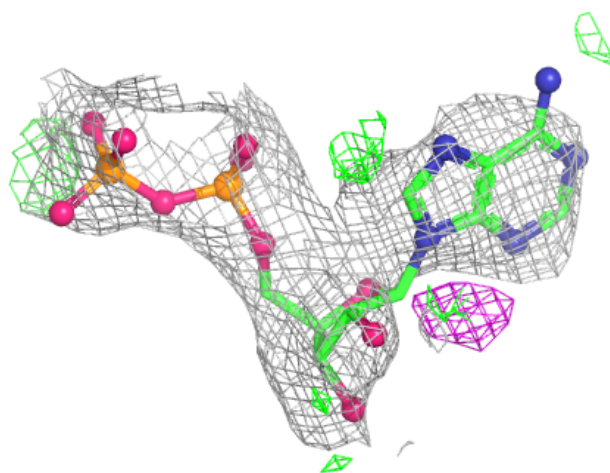
Electron density around ADP L 512:

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



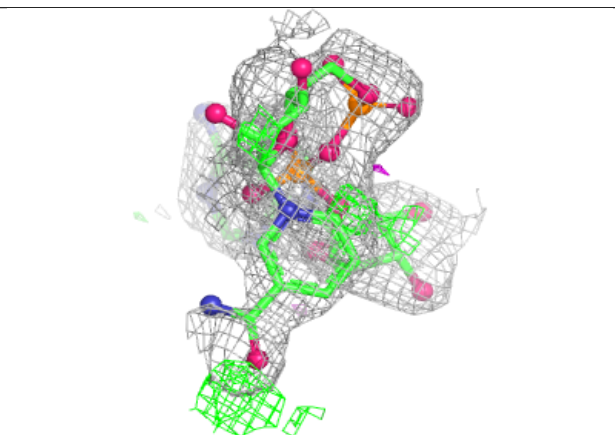
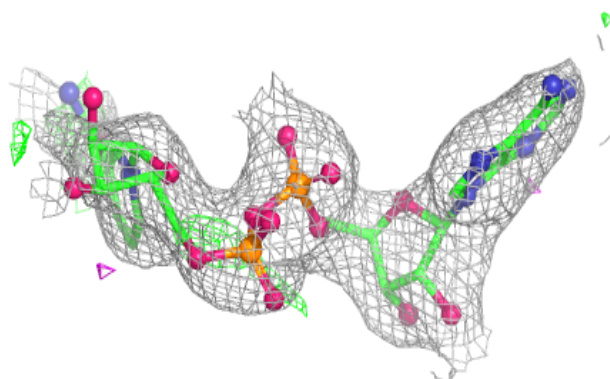
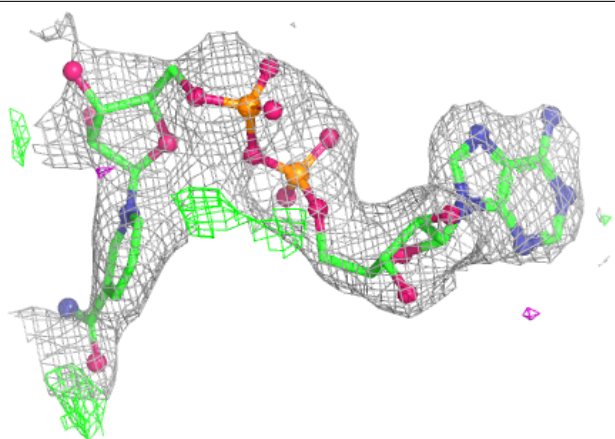
Electron density around ADP A 501 (B):

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

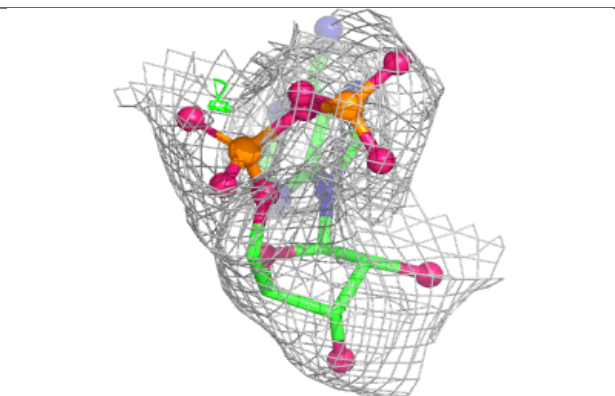
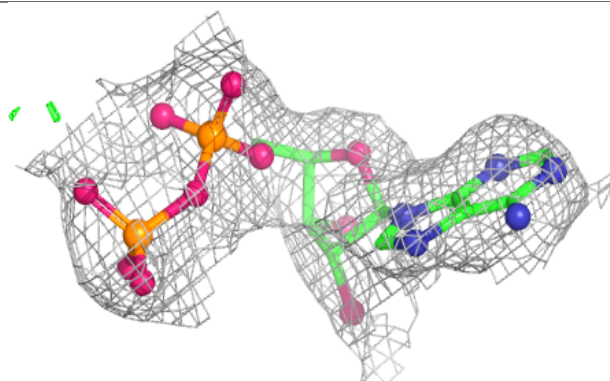
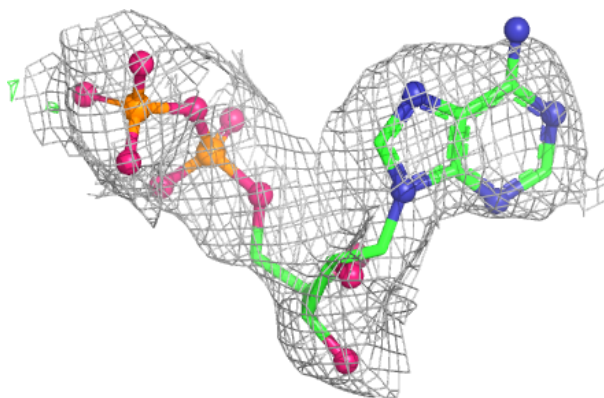


Electron density around NAD B 502:

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

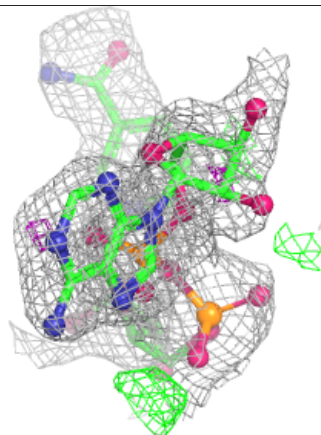
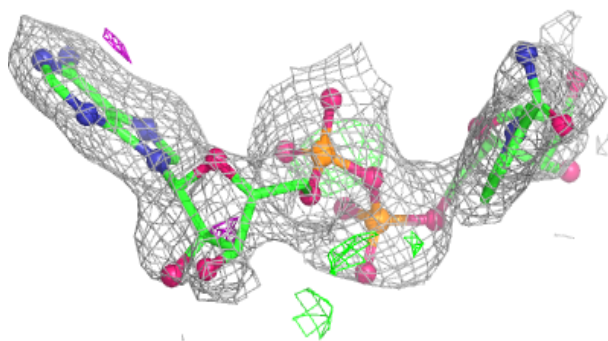
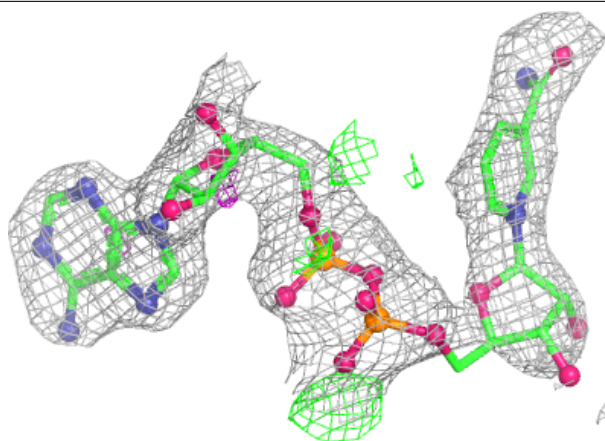
**Electron density around ADP J 510:**

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



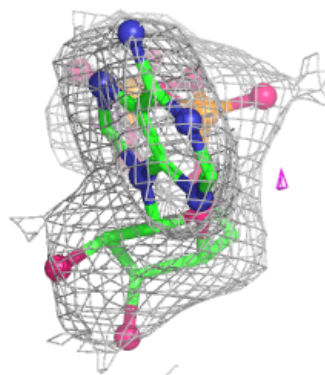
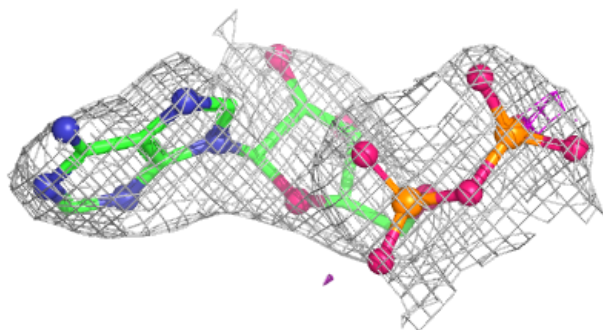
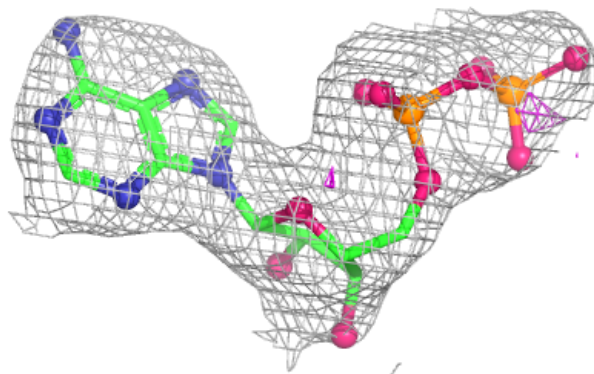
Electron density around NAD C 503:

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

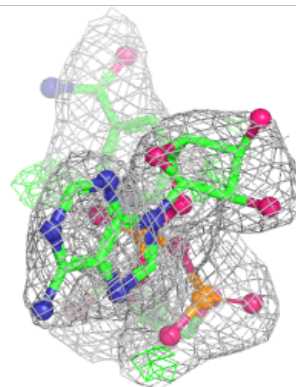
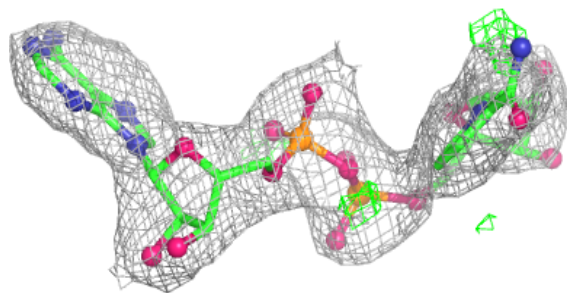
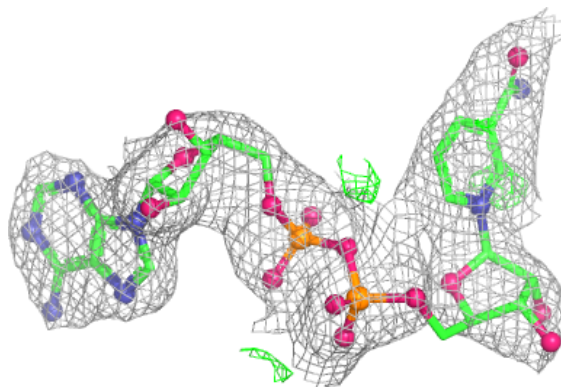


Electron density around ADP I 509:

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

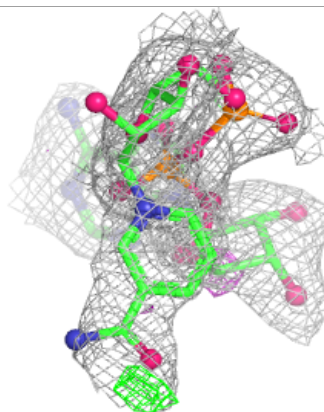
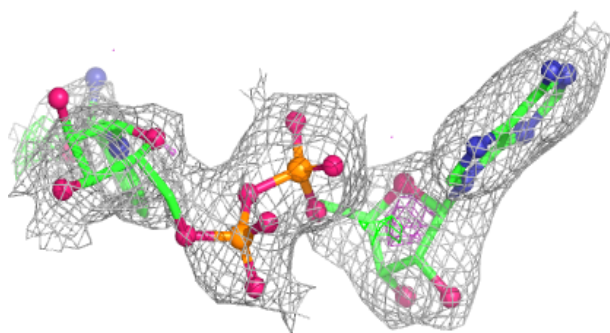
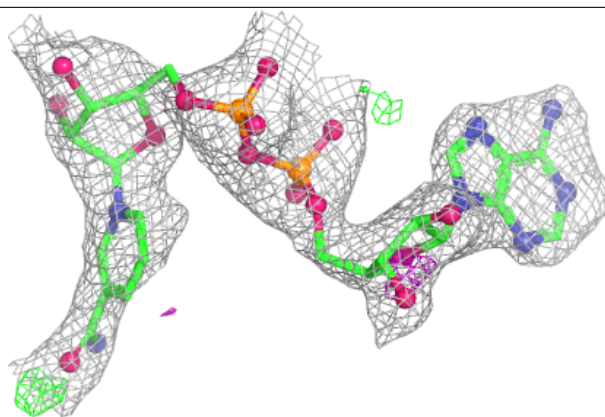
**Electron density around NAD G 507:**

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

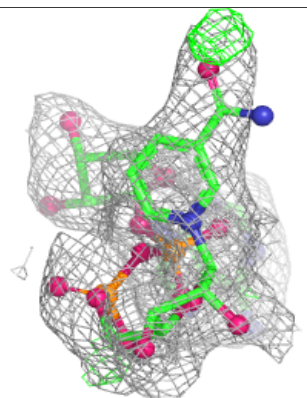
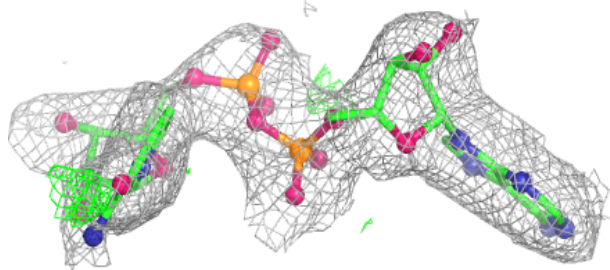
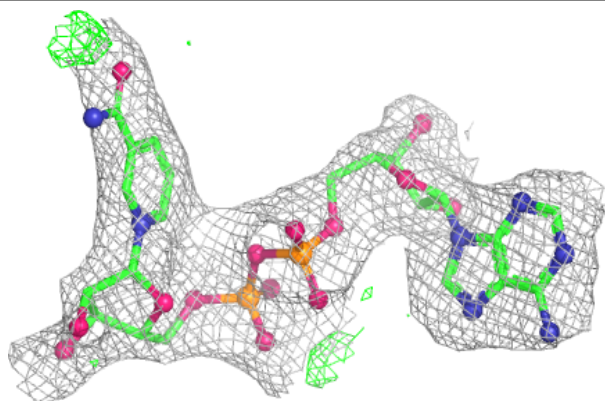


Electron density around NAD F 506:

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

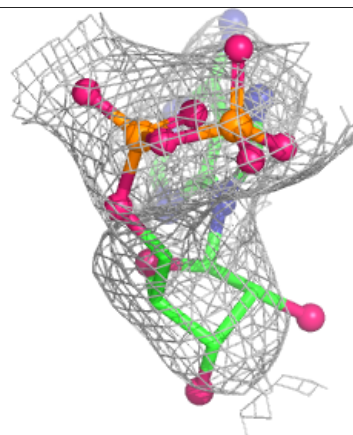
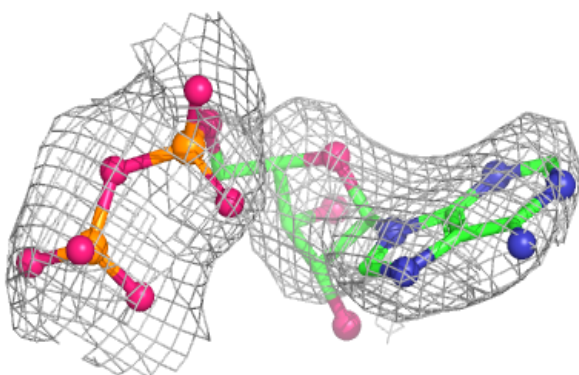
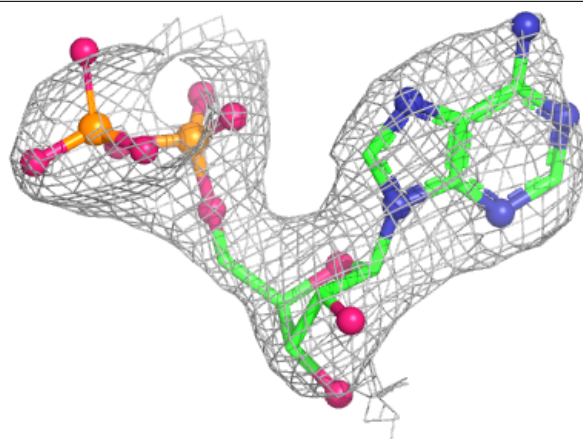
**Electron density around NAD H 508:**

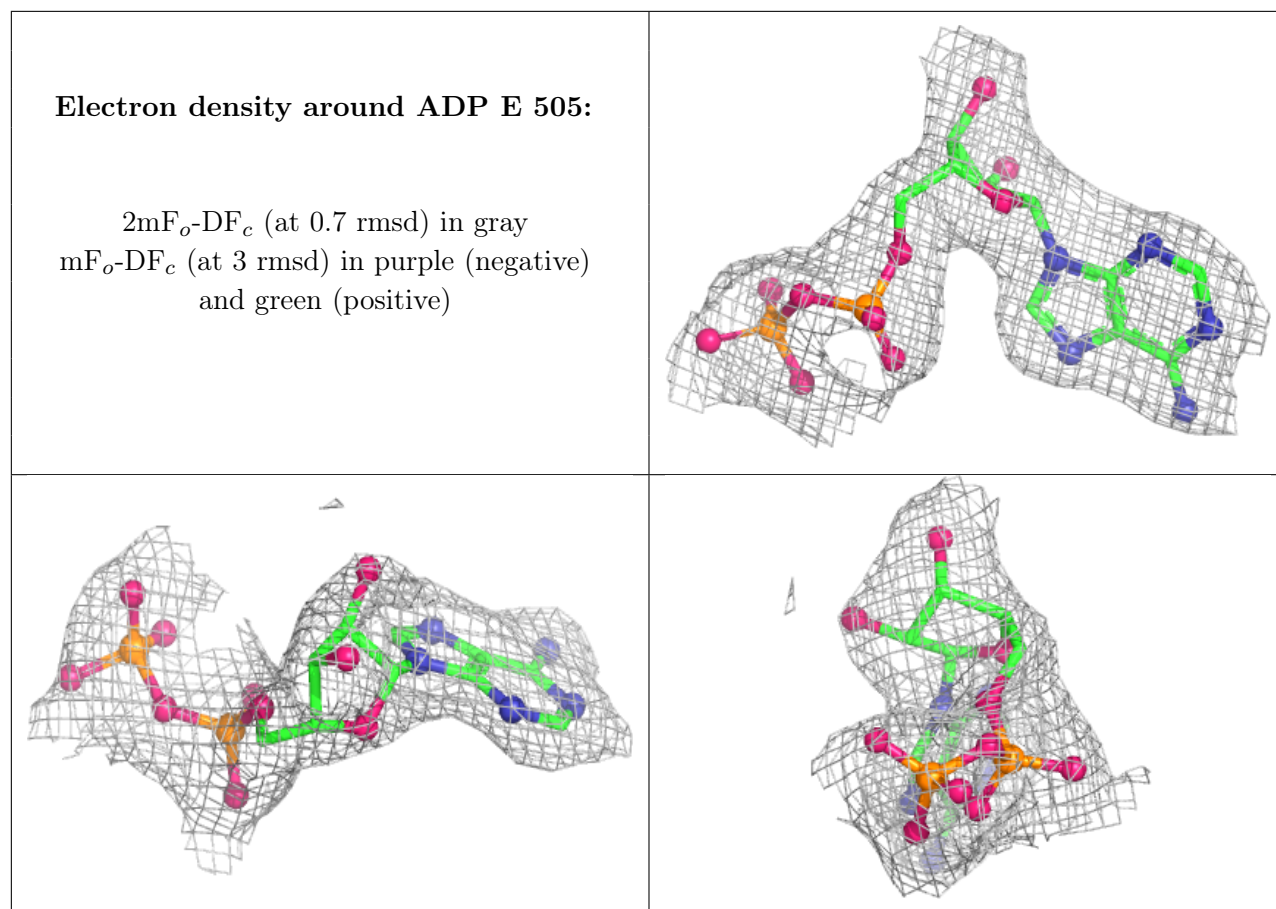
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP K 511:

$2mF_o-DF_c$ (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.