Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 03:57 PM EDT

PDB ID	:	2ONM
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 (i) 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 (i)) were used in the production of this report:

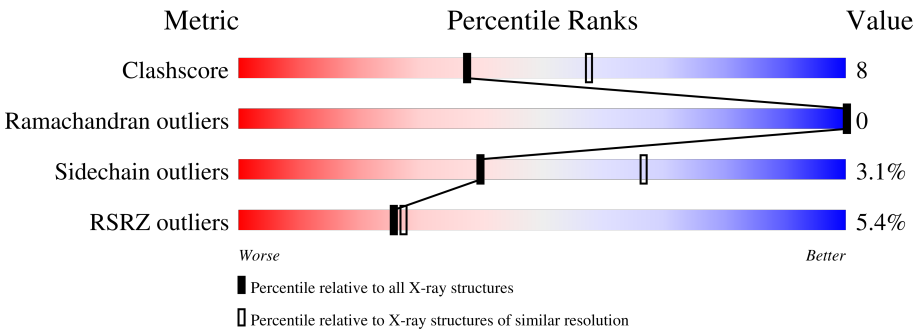
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	11%, 80%, 18%, ••
1	B	500	%, 84%, 14%, ••
1	C	500	82%, 16%, ••
1	D	500	8%, 80%, 18%, ••
1	E	500	82%, 16%, ••
1	F	500	%, 82%, 16%, ••

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Mol	Chain	Length	Quality of chain
1	G	500	%, 82%, 16%
1	H	500	2%, 80%, 17%
1	I	500	4%, 83%, 15%
1	J	500	8%, 77%, 20%
1	K	500	8%, 84%, 14%
1	L	500	20%, 80%, 18%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	494	3798	2416	649	715	18	0	0	0
1	B	494	3798	2416	649	715	18	0	0	0
1	C	494	3798	2416	649	715	18	0	0	0
1	D	494	3798	2416	649	715	18	0	0	0
1	E	494	3798	2416	649	715	18	0	0	0
1	F	494	3798	2416	649	715	18	0	0	0
1	G	494	3798	2416	649	715	18	0	0	0
1	H	494	3798	2416	649	715	18	0	0	0
1	I	494	3798	2416	649	715	18	0	0	0
1	J	494	3798	2416	649	715	18	0	0	0
1	K	494	3798	2416	649	715	18	0	0	0
1	L	494	3798	2416	649	715	18	0	0	0

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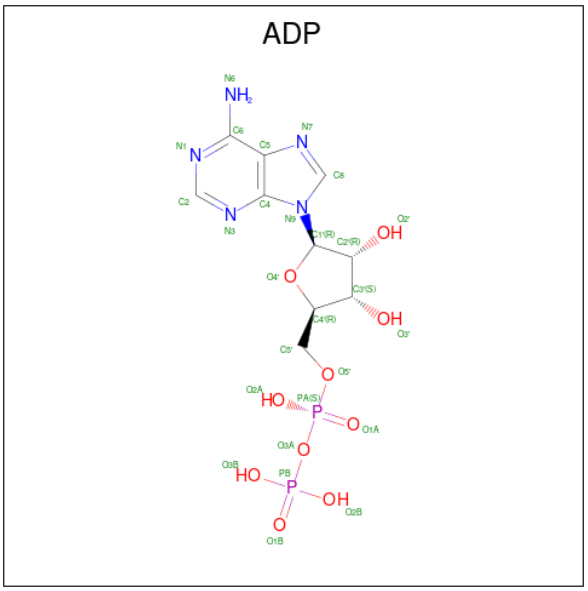
Chain	Residue	Modelled	Actual	Comment	Reference
F	487	LYS	GLU	engineered mutation	UNP P05091
G	487	LYS	GLU	engineered mutation	UNP P05091
H	487	LYS	GLU	engineered mutation	UNP P05091
I	487	LYS	GLU	engineered mutation	UNP P05091
J	487	LYS	GLU	engineered mutation	UNP P05091
K	487	LYS	GLU	engineered mutation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

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

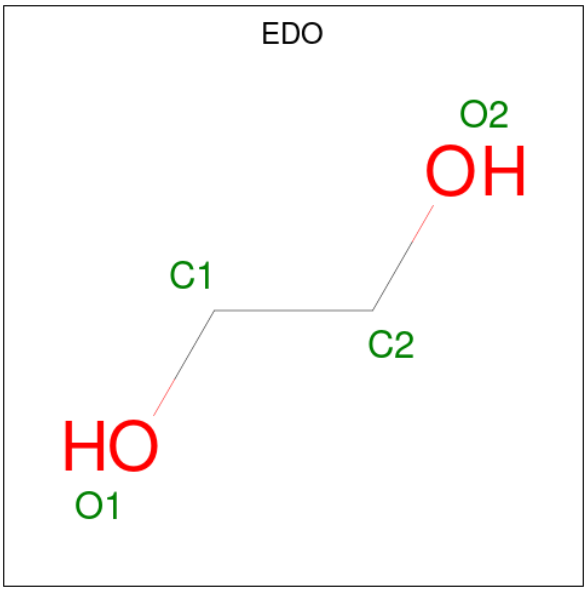
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	2	2	2	0	0
2	G	2	2	2	0	0
2	H	1	1	1	0	0
2	I	1	1	1	0	0
2	J	1	1	1	0	0
2	K	2	2	2	0	0
2	L	1	1	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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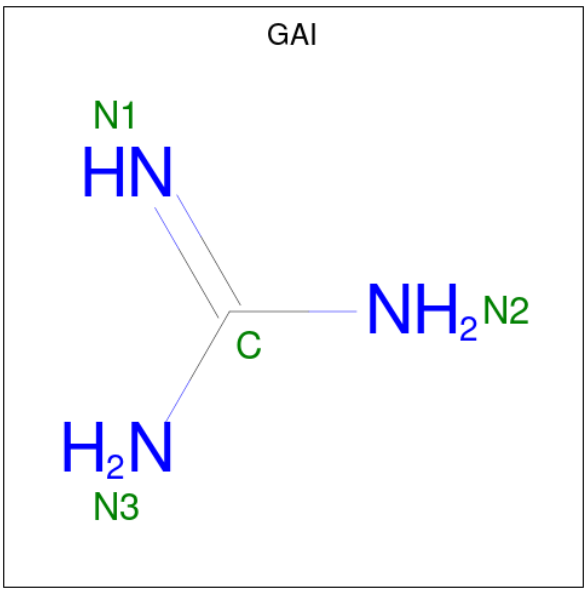
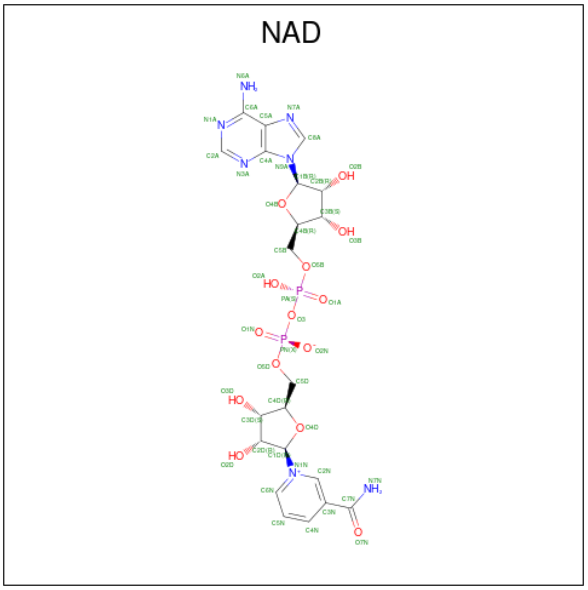
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	F	1	4	2	2		0	0
4	G	1	4	2	2		0	0
4	G	1	4	2	2		0	0
4	H	1	4	2	2		0	0
4	H	1	4	2	2		0	0
4	H	1	4	2	2		0	0
4	I	1	4	2	2		0	0
4	I	1	4	2	2		0	0
4	K	1	4	2	2		0	0
4	L	1	4	2	2		0	0
4	L	1	4	2	2		0	0

- Molecule 5 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



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

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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

- Molecule 7 is water.

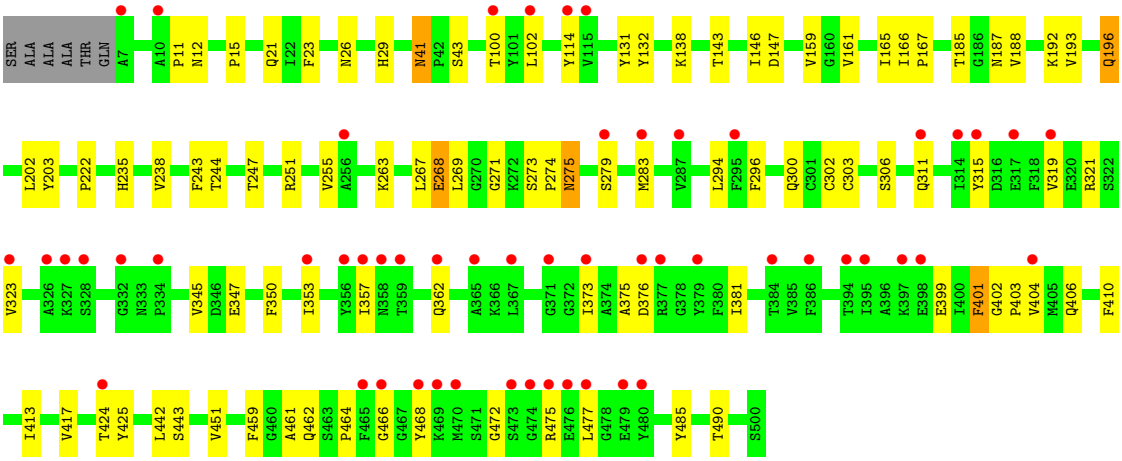
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	121	121	121	0	0
			Total	O		
7	B	223	223	223	0	0
			Total	O		
7	C	232	232	232	0	0
			Total	O		
7	D	133	133	133	0	0
			Total	O		
7	E	264	264	264	0	0
			Total	O		
7	F	251	251	251	0	0
			Total	O		
7	G	186	186	186	0	0
			Total	O		
7	H	185	185	185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

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.

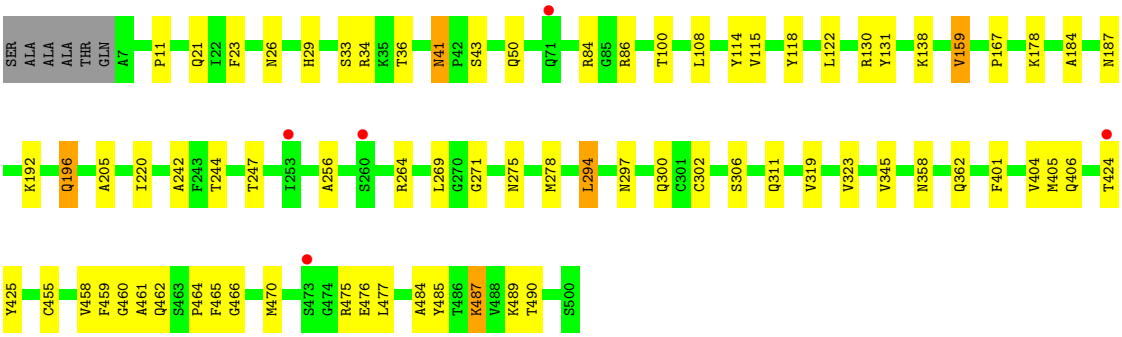
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain A:



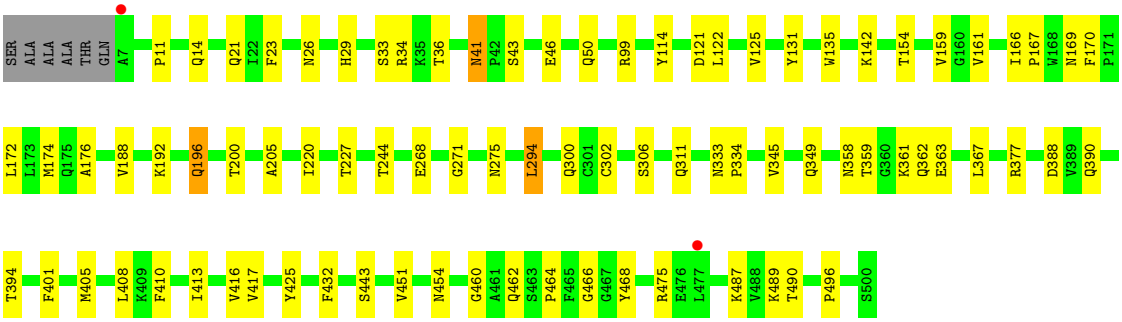
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain B:



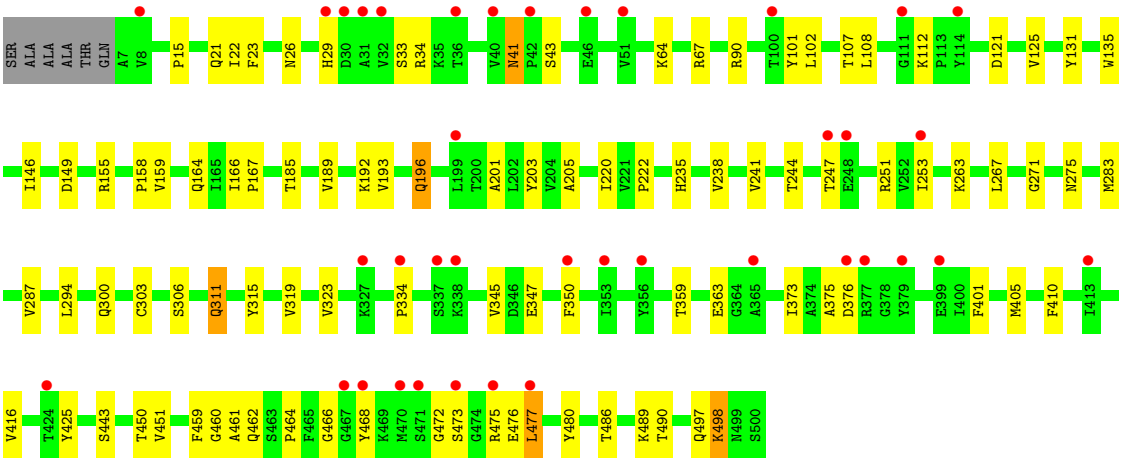
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain C:



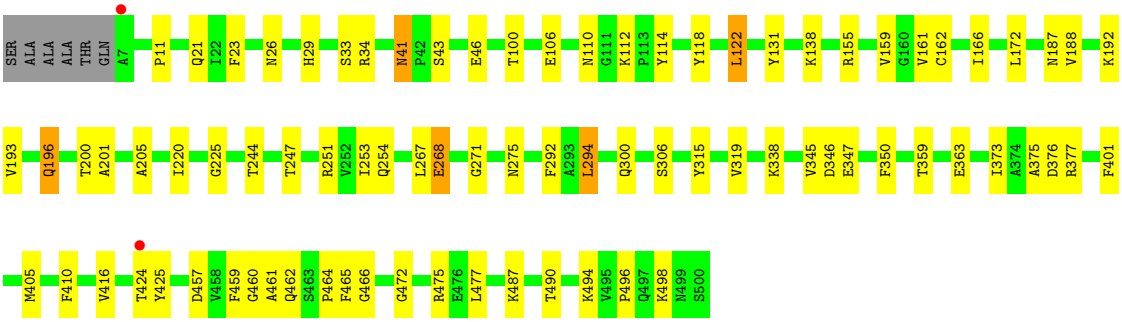
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain D:



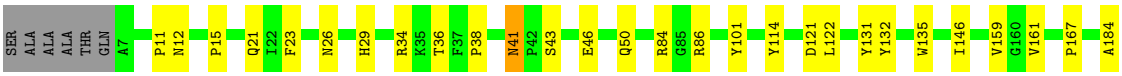
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

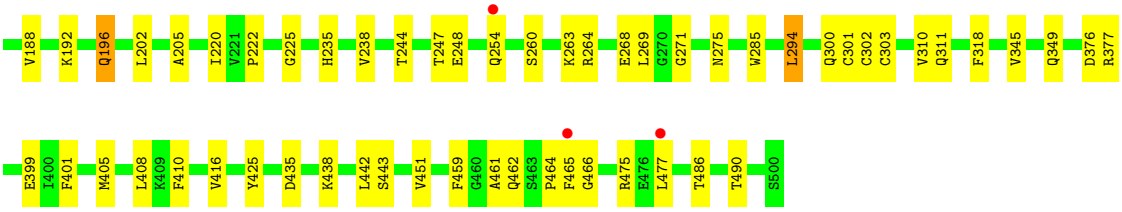
Chain E:



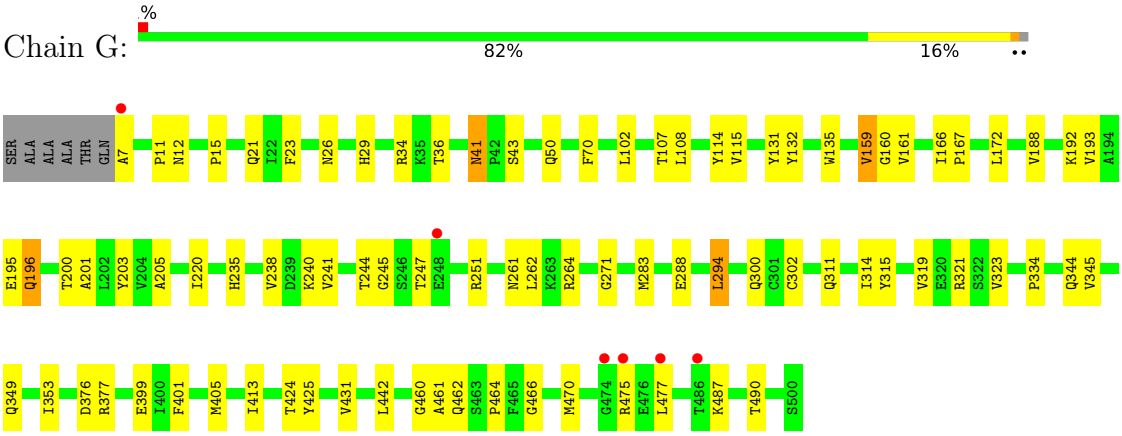
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain F:

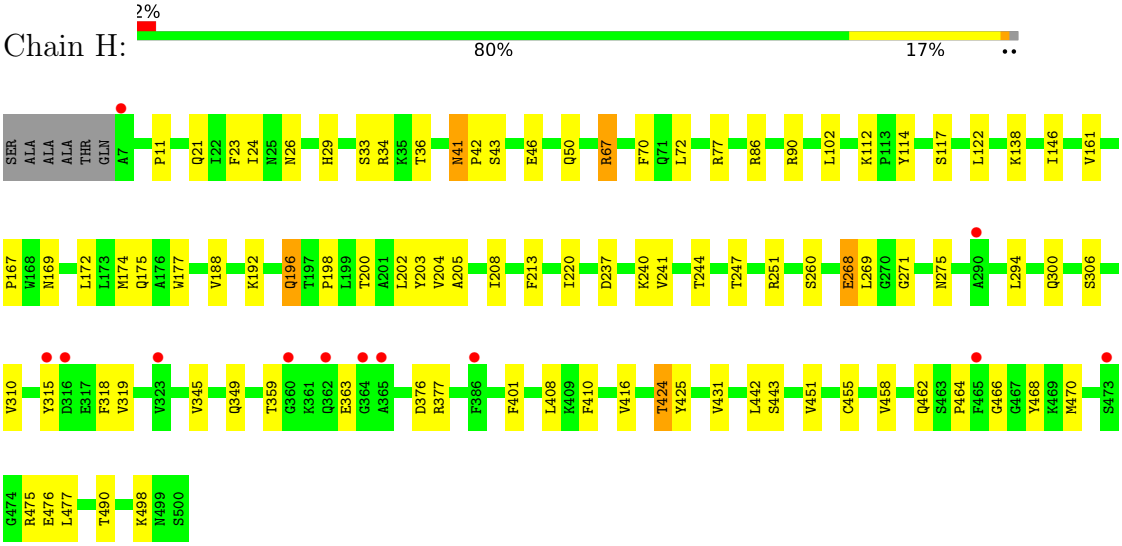




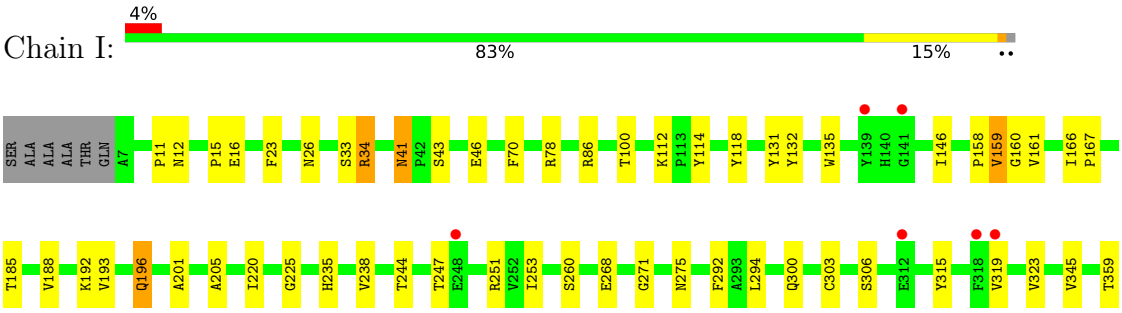
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



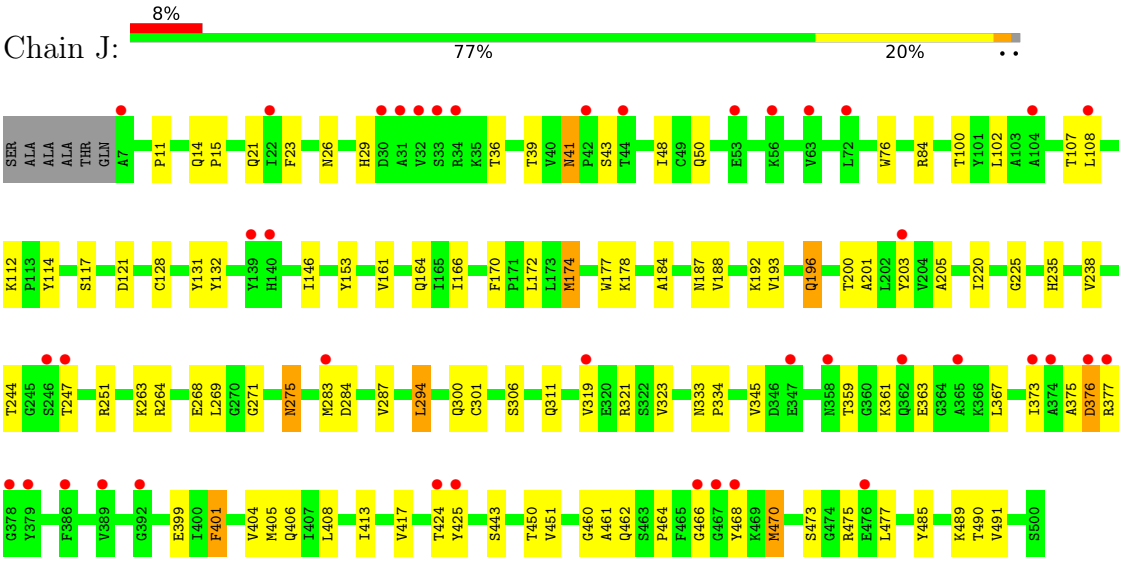
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



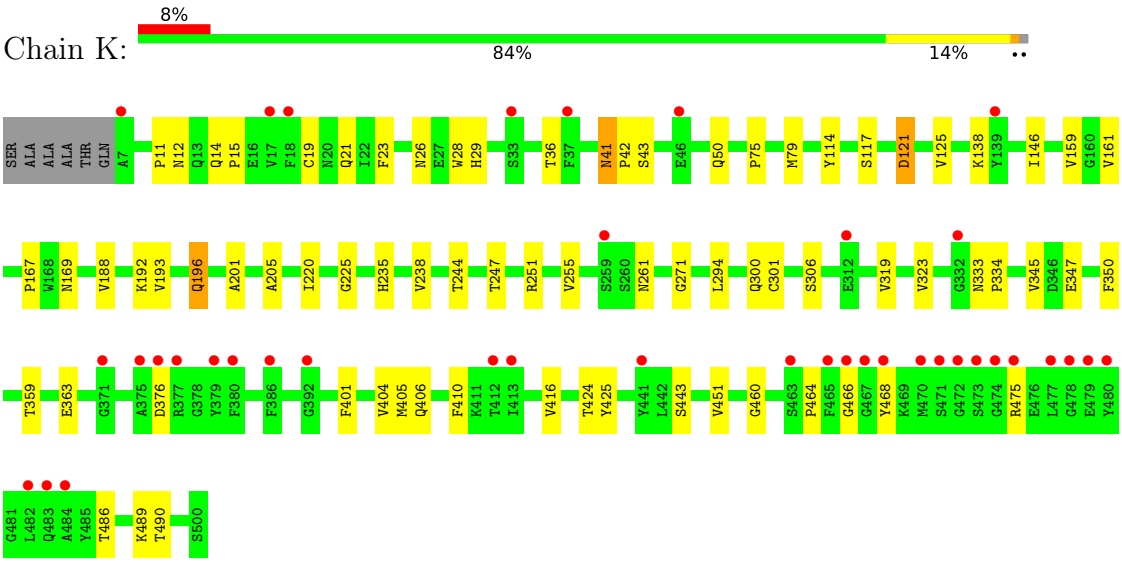
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



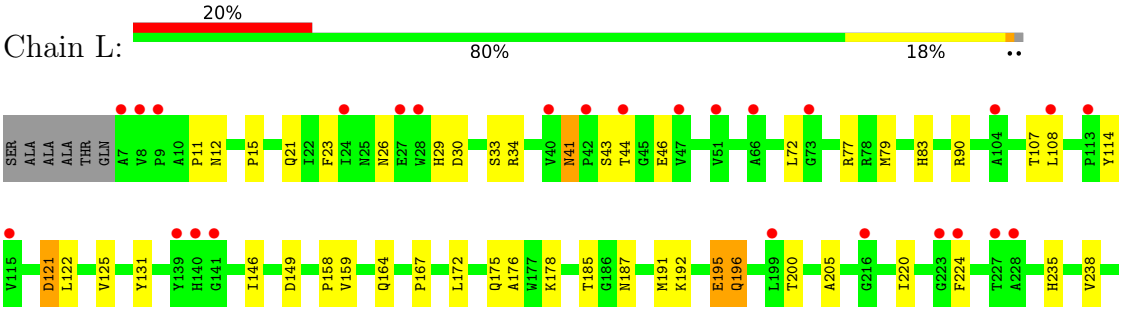
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

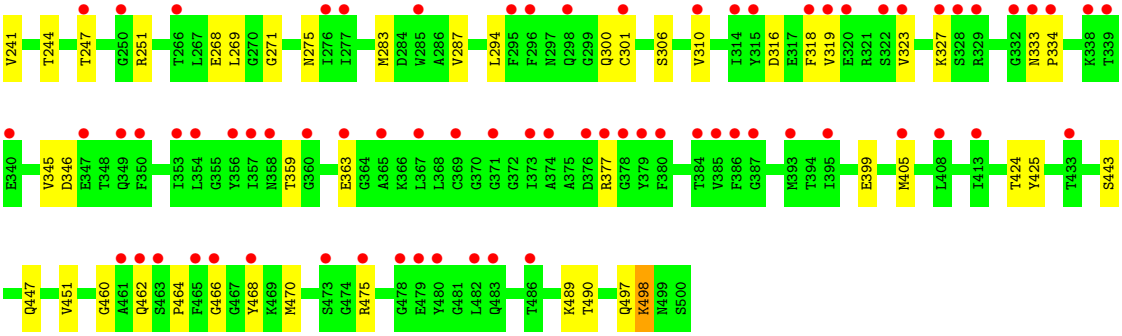


• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor




V241 T244 T247 G250 R251 T266 L267 E268 L269 G270 G271 N275 I276 I277 M283 D284 W285 A286 V287 L294 F295 F296 N297 Q298 G299 Q300 C301 S306 V310 I314 Y315 D316 E317 F318 V319 E320 R321 S322 V323 K327 S328 R329 G332 N333 P334 K338 T339
E340 V345 D346 E347 T348 Q349 F350 I353 L354 G355 Y356 I357 N358 T359 G360 E363 G364 A365 K366 L367 L368 C369 G370 G371 G372 I373 A374 A375 D376 R377 G378 Y379 F380 T384 V385 F386 G387 M393 T394 I395 E399 M405 L408 I413 T424 Y425 T433 S443
Q447 V451 G460 A461 Q462 S463 P464 F465 G466 G467 Y468 K469 M470 S473 G474 R475 G478 E479 Y480 G481 L482 Q483 T486 K489 T490 Q497 K498 M499 S500

4 Data and refinement statistics (i)

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 48.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.01-2.50) 93.9 (48.95-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.271 0.223 , (Not available)	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)	0.31 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, NA, ADP, GAI, EDO

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	0.46	0/3882	0.61	1/5266 (0.0%)
1	B	0.52	0/3882	0.67	1/5266 (0.0%)
1	C	0.53	0/3882	0.67	0/5266
1	D	0.47	0/3882	0.62	0/5266
1	E	0.55	0/3882	0.67	1/5266 (0.0%)
1	F	0.56	0/3882	0.68	0/5266
1	G	0.52	0/3882	0.65	0/5266
1	H	0.51	0/3882	0.64	0/5266
1	I	0.47	0/3882	0.63	0/5266
1	J	0.40	0/3882	0.61	1/5266 (0.0%)
1	K	0.40	0/3882	0.59	0/5266
1	L	0.38	0/3882	0.59	0/5266
All	All	0.48	0/46584	0.64	4/63192 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	264	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	E	122	LEU	CA-CB-CG	-5.51	102.63	115.30
1	A	143	THR	N-CA-C	-5.17	97.04	111.00
1	B	130	ARG	NE-CZ-NH1	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3752	78	0
1	B	3798	0	3752	57	0
1	C	3798	0	3752	63	0
1	D	3798	0	3752	63	0
1	E	3798	0	3752	67	0
1	F	3798	0	3752	55	0
1	G	3798	0	3752	64	0
1	H	3798	0	3752	56	0
1	I	3798	0	3752	74	0
1	J	3798	0	3752	75	0
1	K	3798	0	3752	46	0
1	L	3798	0	3752	62	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	702	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 (702) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:41:ASN:C	1:B:41:ASN:HD22	1.87	0.76
1:J:196:GLN:H	1:J:196:GLN:NE2	1.83	0.76
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
1:E:41:ASN:C	1:E:41:ASN:HD22	1.91	0.73
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:ASN:C	1:H:41:ASN:HD22	1.94	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:G:41:ASN:C	1:G:41:ASN:HD22	1.94	0.71
1:C:41:ASN:HD22	1:C:41:ASN:C	1.94	0.70
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: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: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: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:H:41:ASN:HD22	1:H:43:SER:H	1.41	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:41:ASN:HD22	1:D:41:ASN:C	2.00	0.65
1:C:311:GLN:HG2	7:C:1633:HOH:O	1.97	0.65
1:D:443:SER:HA	1:D:451:VAL:HG11	1.80	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:41:ASN:C	1:I:41:ASN:HD22	2.01	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:A:41:ASN:HD22	1:A:41:ASN:C	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:F:41:ASN:C	1:F:41:ASN:HD22	2.05	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
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:K:41:ASN:C	1:K:41:ASN:HD22	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.87	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: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:C:21:GLN:HB3	1:C:29:HIS:O	2.06	0.56
1:I:225:GLY:HA3	3:I:509:ADP:C8	2.41	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:J:275:ASN:C	1:J:275:ASN:HD22	2.07	0.55
1:C:359:THR:O	1:C:363:GLU:HG3	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:264:ARG:NH2	7:F:2163:HOH:O	2.40	0.53
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: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: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:41:ASN:C	1:L:41:ASN:HD22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:41:ASN:ND2	1:B:41:ASN:C	2.59	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: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
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:E:338:LYS:HZ2	1:I:34:ARG:HE	1.56	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:B:278:MET:HE3	7:B:1529:HOH:O	2.11	0.51
1:E:41:ASN:ND2	1:E:41:ASN:C	2.61	0.51
1:E:193:VAL:HG11	1:E:201:ALA:CB	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:300:GLN:NE2	1:G:345:VAL:H	1.98	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
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: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: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: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: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:G:283:MET:HE3	1:G:314:ILE:HB	1.95	0.49
1:D:149:ASP:HA	1:D:498:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:195:GLU:CD	1:G:195:GLU:H	2.16	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:468:TYR:OH	1:D:489:LYS:HB2	2.13	0.48
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:J:41:ASN:C	1:J:41:ASN:HD22	2.16	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: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:G:41:ASN:C	1:G:41:ASN:ND2	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:164:GLN:CD	1:J:178:LYS:HB3	2.35	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:244:THR:HG23	1:A:268:GLU:HB3	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:301:CYS:C	1:J:401:PHE:HE1	2.20	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: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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:41:ASN:C	1:C:41:ASN:ND2	2.66	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:I:490:THR:HG1	1:J:464:PRO:HG2	1.81	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
1:L:345:VAL:HG13	1:L:346:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:275:ASN:C	1:A:275:ASN:HD22	2.21	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: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: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:G:261:ASN:HA	1:H:470:MET:HE2	2.01	0.42
1:I:408:LEU:N	1:I:408:LEU:HD12	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:41:ASN:C	1:H:41:ASN:ND2	2.66	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:41:ASN:HD21	1:A:43:SER:HB2	1.85	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: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:C:363:GLU:CD	1:C:394:THR:H	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:333:ASN:HA	1:L:334:PRO:HD2	1.91	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: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: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:A:399:GLU:CD	1:A:401:PHE:CE1	2.95	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
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:H:174:MET:HE2	1:H:177:TRP:CE3	2.56	0.40
1:H:410:PHE:CD1	1:H:416:VAL:HB	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/402 (99%)	388 (97%)	11 (3%)	43	70
1	B	399/402 (99%)	389 (98%)	10 (2%)	47	73
1	C	399/402 (99%)	391 (98%)	8 (2%)	55	79
1	D	399/402 (99%)	384 (96%)	15 (4%)	33	58
1	E	399/402 (99%)	388 (97%)	11 (3%)	43	70
1	F	399/402 (99%)	384 (96%)	15 (4%)	33	58
1	G	399/402 (99%)	390 (98%)	9 (2%)	50	76
1	H	399/402 (99%)	383 (96%)	16 (4%)	31	56
1	I	399/402 (99%)	389 (98%)	10 (2%)	47	73
1	J	399/402 (99%)	384 (96%)	15 (4%)	33	58
1	K	399/402 (99%)	388 (97%)	11 (3%)	43	70
1	L	399/402 (99%)	383 (96%)	16 (4%)	31	56
All	All	4788/4824 (99%)	4641 (97%)	147 (3%)	40	67

All (147) 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	192	LYS
1	A	196	GLN
1	A	268	GLU
1	A	275	ASN
1	A	362	GLN
1	A	376	ASP
1	A	401	PHE
1	A	424	THR
1	B	41	ASN
1	B	122	LEU
1	B	159	VAL
1	B	192	LYS
1	B	196	GLN
1	B	275	ASN
1	B	294	LEU

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Mol	Chain	Res	Type
1	B	311	GLN
1	B	401	PHE
1	B	487	LYS
1	C	41	ASN
1	C	192	LYS
1	C	196	GLN
1	C	268	GLU
1	C	275	ASN
1	C	294	LEU
1	C	388	ASP
1	C	401	PHE
1	D	41	ASN
1	D	67	ARG
1	D	90	ARG
1	D	159	VAL
1	D	192	LYS
1	D	196	GLN
1	D	241	VAL
1	D	275	ASN
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	122	LEU
1	E	192	LYS
1	E	196	GLN
1	E	268	GLU
1	E	275	ASN
1	E	294	LEU
1	E	376	ASP
1	E	401	PHE
1	E	424	THR
1	F	34	ARG
1	F	41	ASN
1	F	121	ASP
1	F	122	LEU
1	F	159	VAL

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Mol	Chain	Res	Type
1	F	192	LYS
1	F	196	GLN
1	F	248	GLU
1	F	268	GLU
1	F	275	ASN
1	F	294	LEU
1	F	311	GLN
1	F	376	ASP
1	F	401	PHE
1	F	486	THR
1	G	41	ASN
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	377	ARG
1	G	401	PHE
1	H	41	ASN
1	H	67	ARG
1	H	72	LEU
1	H	90	ARG
1	H	117	SER
1	H	122	LEU
1	H	192	LYS
1	H	196	GLN
1	H	268	GLU
1	H	275	ASN
1	H	376	ASP
1	H	377	ARG
1	H	401	PHE
1	H	424	THR
1	H	462	GLN
1	H	498	LYS
1	I	34	ARG
1	I	41	ASN
1	I	159	VAL
1	I	192	LYS
1	I	196	GLN
1	I	275	ASN
1	I	376	ASP

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Mol	Chain	Res	Type
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	121	ASP
1	J	174	MET
1	J	192	LYS
1	J	196	GLN
1	J	275	ASN
1	J	294	LEU
1	J	376	ASP
1	J	377	ARG
1	J	401	PHE
1	J	470	MET
1	J	473	SER
1	K	41	ASN
1	K	117	SER
1	K	121	ASP
1	K	159	VAL
1	K	192	LYS
1	K	196	GLN
1	K	301	CYS
1	K	376	ASP
1	K	401	PHE
1	K	424	THR
1	K	486	THR
1	L	30	ASP
1	L	41	ASN
1	L	72	LEU
1	L	90	ARG
1	L	121	ASP
1	L	122	LEU
1	L	192	LYS
1	L	195	GLU
1	L	196	GLN
1	L	241	VAL
1	L	268	GLU
1	L	275	ASN
1	L	301	CYS

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Mol	Chain	Res	Type
1	L	377	ARG
1	L	424	THR
1	L	498	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) 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	83	HIS
1	A	175	GLN
1	A	196	GLN
1	A	275	ASN
1	A	300	GLN
1	B	13	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	349	GLN
1	B	362	GLN
1	C	13	GLN
1	C	26	ASN
1	C	41	ASN
1	C	50	GLN
1	C	83	HIS
1	C	175	GLN
1	C	196	GLN
1	C	275	ASN
1	C	300	GLN
1	D	26	ASN
1	D	41	ASN
1	D	71	GLN
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	300	GLN
1	D	440	ASN

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Mol	Chain	Res	Type
1	E	13	GLN
1	E	26	ASN
1	E	41	ASN
1	E	175	GLN
1	E	196	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	13	GLN
1	G	26	ASN
1	G	41	ASN
1	G	83	HIS
1	G	175	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	G	349	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	26	ASN
1	I	41	ASN
1	I	83	HIS
1	I	175	GLN
1	I	196	GLN
1	I	254	GLN
1	I	275	ASN

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Mol	Chain	Res	Type
1	I	300	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	349	GLN
1	K	26	ASN
1	K	41	ASN
1	K	83	HIS
1	K	175	GLN
1	K	196	GLN
1	K	275	ASN
1	K	300	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	275	ASN
1	L	300	GLN
1	L	497	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
4	EDO	I	909	-	3,3,3	0.39	0	2,2,2	0.37	0
5	GAI	G	5009	-	3,3,3	1.37	1 (33%)	3,3,3	1.11	0
5	GAI	E	906	-	3,3,3	1.39	1 (33%)	3,3,3	1.26	0
4	EDO	C	803	-	3,3,3	0.45	0	2,2,2	0.31	0
5	GAI	E	907	-	3,3,3	1.55	1 (33%)	3,3,3	1.32	0
4	EDO	B	701	-	3,3,3	0.43	0	2,2,2	0.37	0
3	ADP	L	512	-	24,29,29	1.68	4 (16%)	29,45,45	1.49	6 (20%)
5	GAI	G	5010	-	3,3,3	1.52	1 (33%)	3,3,3	1.16	0
4	EDO	F	806	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	G	807	-	3,3,3	0.60	0	2,2,2	0.20	0
4	EDO	E	905	-	3,3,3	0.13	0	2,2,2	0.56	0
4	EDO	H	708	-	3,3,3	0.46	0	2,2,2	0.29	0
4	EDO	E	805	-	3,3,3	0.64	0	2,2,2	0.18	0
4	EDO	L	912	-	3,3,3	0.43	0	2,2,2	0.36	0
3	ADP	K	511	-	24,29,29	1.67	5 (20%)	29,45,45	1.62	5 (17%)
4	EDO	D	904	-	3,3,3	0.41	0	2,2,2	0.36	0
4	EDO	C	903	-	3,3,3	0.63	0	2,2,2	0.33	0
3	ADP	D	504[A]	-	24,29,29	1.85	5 (20%)	29,45,45	1.68	4 (13%)
3	ADP	J	510	-	24,29,29	1.69	4 (16%)	29,45,45	1.35	3 (10%)
4	EDO	H	808	-	3,3,3	0.67	0	2,2,2	0.21	0
4	EDO	I	809	-	3,3,3	0.67	0	2,2,2	0.15	0
4	EDO	G	907	-	3,3,3	0.36	0	2,2,2	0.44	0
6	NAD	H	508	-	42,48,48	2.36	10 (23%)	50,73,73	1.69	10 (20%)
6	NAD	B	502	-	42,48,48	2.16	8 (19%)	50,73,73	1.90	11 (22%)
6	NAD	G	507	-	42,48,48	2.45	10 (23%)	50,73,73	1.54	10 (20%)
5	GAI	A	902	-	3,3,3	1.36	1 (33%)	3,3,3	1.18	0
5	GAI	J	611	-	3,3,3	1.39	1 (33%)	3,3,3	1.18	0
4	EDO	B	902	-	3,3,3	0.30	0	2,2,2	0.44	0
5	GAI	I	910	-	3,3,3	1.53	1 (33%)	3,3,3	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GAI	D	905	-	3,3,3	1.56	1 (33%)	3,3,3	1.22	0
4	EDO	L	712	-	3,3,3	0.55	0	2,2,2	0.26	0
3	ADP	E	505	-	24,29,29	1.53	4 (16%)	29,45,45	1.78	6 (20%)
6	NAD	C	503	-	42,48,48	2.21	8 (19%)	50,73,73	1.96	15 (30%)
4	EDO	F	707	-	3,3,3	0.77	0	2,2,2	0.13	0
3	ADP	A	501[A]	-	24,29,29	1.90	5 (20%)	29,45,45	1.97	6 (20%)
3	ADP	D	504[B]	-	24,29,29	1.65	5 (20%)	29,45,45	1.49	3 (10%)
4	EDO	K	911	-	3,3,3	0.61	0	2,2,2	0.26	0
4	EDO	F	906	-	3,3,3	0.40	0	2,2,2	0.37	0
3	ADP	I	509	-	24,29,29	1.76	5 (20%)	29,45,45	2.19	5 (17%)
4	EDO	B	802	-	3,3,3	0.41	0	2,2,2	0.47	0
6	NAD	F	506	-	42,48,48	2.20	9 (21%)	50,73,73	1.77	9 (18%)
4	EDO	D	704	-	3,3,3	0.60	0	2,2,2	0.28	0
5	GAI	H	909	-	3,3,3	1.38	1 (33%)	3,3,3	1.13	0
4	EDO	F	706	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	E	705	-	3,3,3	0.56	0	2,2,2	0.25	0
4	EDO	H	908	-	3,3,3	0.42	0	2,2,2	0.37	0
4	EDO	A	901	-	3,3,3	0.54	0	2,2,2	0.34	0
3	ADP	A	501[B]	-	24,29,29	1.71	5 (20%)	29,45,45	1.53	3 (10%)

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
4	EDO	I	909	-	-	0/1/1/1	-
4	EDO	C	803	-	-	1/1/1/1	-
4	EDO	B	701	-	-	0/1/1/1	-
3	ADP	L	512	-	-	4/12/32/32	0/3/3/3
4	EDO	F	806	-	-	0/1/1/1	-
4	EDO	G	807	-	-	0/1/1/1	-
4	EDO	E	905	-	-	0/1/1/1	-
4	EDO	H	708	-	-	0/1/1/1	-
4	EDO	E	805	-	-	0/1/1/1	-
4	EDO	L	912	-	-	0/1/1/1	-
3	ADP	K	511	-	-	1/12/32/32	0/3/3/3
4	EDO	D	904	-	-	0/1/1/1	-
4	EDO	C	903	-	-	1/1/1/1	-
3	ADP	D	504[A]	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	J	510	-	-	6/12/32/32	0/3/3/3
4	EDO	H	808	-	-	0/1/1/1	-
4	EDO	I	809	-	-	0/1/1/1	-
4	EDO	G	907	-	-	0/1/1/1	-
6	NAD	H	508	-	-	9/26/62/62	0/5/5/5
6	NAD	B	502	-	-	9/26/62/62	0/5/5/5
6	NAD	G	507	-	-	11/26/62/62	0/5/5/5
4	EDO	B	902	-	-	0/1/1/1	-
4	EDO	L	712	-	-	0/1/1/1	-
3	ADP	E	505	-	-	3/12/32/32	0/3/3/3
6	NAD	C	503	-	-	10/26/62/62	0/5/5/5
4	EDO	F	707	-	-	0/1/1/1	-
3	ADP	A	501[A]	-	-	3/12/32/32	0/3/3/3
3	ADP	D	504[B]	-	-	4/12/32/32	0/3/3/3
4	EDO	K	911	-	-	1/1/1/1	-
4	EDO	F	906	-	-	0/1/1/1	-
3	ADP	I	509	-	-	4/12/32/32	0/3/3/3
4	EDO	B	802	-	-	0/1/1/1	-
6	NAD	F	506	-	-	6/26/62/62	0/5/5/5
4	EDO	D	704	-	-	1/1/1/1	-
4	EDO	F	706	-	-	0/1/1/1	-
4	EDO	E	705	-	-	0/1/1/1	-
4	EDO	H	908	-	-	0/1/1/1	-
4	EDO	A	901	-	-	1/1/1/1	-
3	ADP	A	501[B]	-	-	0/12/32/32	0/3/3/3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	507	NAD	C3N-C7N	-11.97	1.32	1.50
6	H	508	NAD	C3N-C7N	-10.50	1.34	1.50
6	B	502	NAD	C3N-C7N	-10.14	1.35	1.50
6	F	506	NAD	C3N-C7N	-9.72	1.36	1.50
6	C	503	NAD	C3N-C7N	-9.45	1.36	1.50
6	C	503	NAD	C2A-N3A	5.58	1.41	1.32
6	F	506	NAD	C2A-N3A	5.14	1.40	1.32
3	A	501[A]	ADP	C2-N3	5.10	1.40	1.32
6	B	502	NAD	C2A-N3A	4.94	1.40	1.32
3	D	504[A]	ADP	C2-N3	4.93	1.40	1.32
3	L	512	ADP	C2-N3	4.85	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	509	ADP	C2-N3	4.81	1.39	1.32
3	A	501[B]	ADP	C2-N3	4.73	1.39	1.32
3	J	510	ADP	C2-N3	4.70	1.39	1.32
3	K	511	ADP	C2-N3	4.61	1.39	1.32
3	D	504[B]	ADP	C2-N3	4.60	1.39	1.32
6	G	507	NAD	C2A-N3A	4.40	1.39	1.32
3	D	504[A]	ADP	PB-O3B	4.05	1.70	1.54
6	H	508	NAD	O4D-C1D	3.83	1.46	1.41
3	A	501[A]	ADP	C2-N1	3.75	1.40	1.33
6	C	503	NAD	C4A-N3A	3.68	1.40	1.35
3	E	505	ADP	C2-N3	3.64	1.38	1.32
6	C	503	NAD	C2A-N1A	3.55	1.40	1.33
3	A	501[A]	ADP	C4-N3	3.55	1.40	1.35
6	H	508	NAD	C2A-N3A	3.55	1.37	1.32
3	D	504[A]	ADP	C2-N1	3.50	1.40	1.33
3	A	501[B]	ADP	C2-N1	3.47	1.40	1.33
6	H	508	NAD	C4N-C3N	-3.39	1.33	1.39
3	E	505	ADP	C8-N7	3.36	1.40	1.34
3	I	509	ADP	C2-N1	3.36	1.40	1.33
6	G	507	NAD	C2A-N1A	3.35	1.40	1.33
3	K	511	ADP	C8-N7	3.31	1.40	1.34
3	J	510	ADP	C2-N1	3.31	1.40	1.33
3	L	512	ADP	C8-N7	3.28	1.40	1.34
6	G	507	NAD	C5N-C4N	-3.28	1.32	1.38
3	L	512	ADP	C2-N1	3.27	1.40	1.33
6	C	503	NAD	O4D-C1D	3.26	1.45	1.41
3	A	501[A]	ADP	C8-N7	3.23	1.40	1.34
6	F	506	NAD	C8A-N7A	3.19	1.40	1.34
6	H	508	NAD	C5N-C4N	-3.19	1.32	1.38
3	K	511	ADP	C2-N1	3.18	1.39	1.33
3	I	509	ADP	C8-N7	3.18	1.40	1.34
6	F	506	NAD	O4D-C1D	3.13	1.45	1.41
6	G	507	NAD	O4D-C1D	3.12	1.45	1.41
3	D	504[B]	ADP	C2-N1	3.11	1.39	1.33
6	G	507	NAD	C4N-C3N	-3.10	1.34	1.39
6	H	508	NAD	C2N-C3N	-3.06	1.34	1.39
6	H	508	NAD	C8A-N7A	3.06	1.40	1.34
6	H	508	NAD	C2N-N1N	-3.04	1.31	1.35
6	B	502	NAD	C2A-N1A	3.02	1.39	1.33
3	J	510	ADP	C8-N7	3.00	1.40	1.34
3	E	505	ADP	C2-N1	2.98	1.39	1.33
3	I	509	ADP	PB-O3B	2.98	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504[A]	ADP	C8-N7	2.94	1.39	1.34
6	B	502	NAD	C4N-C3N	-2.88	1.34	1.39
6	C	503	NAD	C8A-N7A	2.87	1.39	1.34
3	A	501[B]	ADP	C8-N7	2.85	1.39	1.34
3	J	510	ADP	C4-N3	2.82	1.39	1.35
3	D	504[B]	ADP	C8-N7	2.80	1.39	1.34
6	H	508	NAD	O4B-C1B	2.80	1.45	1.41
6	F	506	NAD	C4N-C3N	-2.78	1.34	1.39
6	G	507	NAD	C8A-N7A	2.78	1.39	1.34
3	E	505	ADP	PB-O3B	2.76	1.65	1.54
6	F	506	NAD	C5N-C4N	-2.74	1.33	1.38
6	F	506	NAD	C4A-N3A	2.73	1.39	1.35
6	F	506	NAD	O4B-C1B	2.73	1.44	1.41
6	H	508	NAD	C2A-N1A	2.73	1.39	1.33
6	B	502	NAD	O4D-C1D	2.67	1.44	1.41
3	K	511	ADP	PB-O3B	2.63	1.65	1.54
5	I	910	GAI	C-N1	2.62	1.36	1.30
6	F	506	NAD	C2A-N1A	2.61	1.38	1.33
6	B	502	NAD	C8A-N7A	2.61	1.39	1.34
3	D	504[A]	ADP	C4-N3	2.60	1.39	1.35
3	L	512	ADP	PB-O3B	2.60	1.64	1.54
5	D	905	GAI	C-N1	2.57	1.36	1.30
6	C	503	NAD	C5N-C4N	-2.54	1.33	1.38
6	B	502	NAD	C2N-C3N	-2.53	1.35	1.39
3	A	501[B]	ADP	C4-N3	2.52	1.39	1.35
3	A	501[A]	ADP	PB-O3B	2.49	1.64	1.54
5	G	5010	GAI	C-N1	2.43	1.35	1.30
3	D	504[B]	ADP	PB-O2B	-2.43	1.45	1.54
5	E	907	GAI	C-N1	2.40	1.35	1.30
6	B	502	NAD	C2N-N1N	-2.37	1.32	1.35
5	J	611	GAI	C-N1	2.35	1.35	1.30
6	G	507	NAD	C2N-C3N	-2.35	1.35	1.39
6	C	503	NAD	C4N-C3N	-2.34	1.35	1.39
5	H	909	GAI	C-N1	2.33	1.35	1.30
5	G	5009	GAI	C-N1	2.31	1.35	1.30
5	E	906	GAI	C-N1	2.31	1.35	1.30
3	I	509	ADP	C4-N3	2.28	1.38	1.35
6	G	507	NAD	C4A-N3A	2.22	1.38	1.35
3	A	501[B]	ADP	PB-O2B	-2.15	1.46	1.54
5	A	902	GAI	C-N1	2.15	1.35	1.30
3	D	504[B]	ADP	PA-O2A	-2.08	1.45	1.55
6	G	507	NAD	C2N-N1N	-2.04	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	511	ADP	C4-N3	2.01	1.38	1.35

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	502	NAD	O4B-C1B-C2B	-8.32	94.77	106.93
3	I	509	ADP	O4'-C1'-C2'	-8.32	94.77	106.93
3	A	501[A]	ADP	O4'-C1'-C2'	-7.13	96.51	106.93
3	E	505	ADP	N3-C2-N1	-5.22	120.52	128.68
6	C	503	NAD	O4B-C1B-C2B	-5.03	99.57	106.93
3	K	511	ADP	C2'-C3'-C4'	-4.82	93.28	102.64
3	D	504[B]	ADP	O4'-C1'-C2'	-4.78	99.95	106.93
6	C	503	NAD	O7N-C7N-N7N	-4.71	115.89	122.58
3	I	509	ADP	C3'-C2'-C1'	4.57	107.86	100.98
3	A	501[B]	ADP	N3-C2-N1	-4.49	121.66	128.68
6	H	508	NAD	N3A-C2A-N1A	-4.49	121.66	128.68
3	E	505	ADP	O4'-C1'-C2'	-4.47	100.39	106.93
6	F	506	NAD	O4B-C1B-C2B	-4.41	100.47	106.93
3	D	504[A]	ADP	N3-C2-N1	-4.32	121.93	128.68
6	H	508	NAD	PN-O3-PA	-4.31	118.04	132.83
6	G	507	NAD	C2N-C3N-C4N	4.10	122.91	118.26
6	H	508	NAD	O4B-C1B-C2B	-4.09	100.95	106.93
6	F	506	NAD	C3B-C2B-C1B	4.07	107.11	100.98
6	C	503	NAD	O4D-C4D-C3D	-4.04	97.12	105.11
3	D	504[A]	ADP	O4'-C1'-C2'	-3.98	101.12	106.93
6	F	506	NAD	C2B-C3B-C4B	-3.95	94.97	102.64
6	C	503	NAD	C2B-C3B-C4B	-3.91	95.04	102.64
6	H	508	NAD	C6N-N1N-C2N	-3.91	118.41	121.97
3	J	510	ADP	N3-C2-N1	-3.90	122.59	128.68
3	I	509	ADP	PA-O3A-PB	-3.88	119.50	132.83
6	F	506	NAD	O4B-C4B-C3B	3.87	112.77	105.11
3	D	504[A]	ADP	PA-O3A-PB	-3.81	119.76	132.83
3	A	501[A]	ADP	PA-O3A-PB	-3.77	119.91	132.83
6	B	502	NAD	O4D-C4D-C3D	-3.76	97.67	105.11
3	A	501[B]	ADP	O4'-C1'-C2'	-3.73	101.48	106.93
6	H	508	NAD	O7N-C7N-N7N	-3.70	117.32	122.58
3	L	512	ADP	PA-O3A-PB	-3.69	120.16	132.83
6	C	503	NAD	N3A-C2A-N1A	-3.68	122.92	128.68
3	A	501[A]	ADP	N3-C2-N1	-3.61	123.03	128.68
6	G	507	NAD	N3A-C2A-N1A	-3.56	123.11	128.68
6	F	506	NAD	N3A-C2A-N1A	-3.54	123.14	128.68
3	A	501[B]	ADP	C2'-C3'-C4'	-3.40	96.04	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	512	ADP	N3-C2-N1	-3.39	123.38	128.68
3	K	511	ADP	O4'-C1'-C2'	-3.38	101.99	106.93
6	B	502	NAD	O7N-C7N-C3N	3.38	123.67	119.63
3	K	511	ADP	N3-C2-N1	-3.36	123.42	128.68
6	C	503	NAD	C3N-C7N-N7N	3.34	121.76	117.75
6	F	506	NAD	C3N-C7N-N7N	3.33	121.74	117.75
6	B	502	NAD	N3A-C2A-N1A	-3.21	123.66	128.68
3	A	501[A]	ADP	C3'-C2'-C1'	3.15	105.72	100.98
3	E	505	ADP	PA-O3A-PB	-3.13	122.08	132.83
6	G	507	NAD	C3N-C2N-N1N	-3.11	117.39	120.43
3	I	509	ADP	N3-C2-N1	-3.04	123.92	128.68
6	B	502	NAD	C1B-N9A-C4A	3.02	131.95	126.64
6	F	506	NAD	O7N-C7N-N7N	-3.00	118.31	122.58
3	K	511	ADP	PA-O3A-PB	-2.99	122.56	132.83
3	D	504[B]	ADP	N3-C2-N1	-2.98	124.02	128.68
6	G	507	NAD	C6N-C5N-C4N	-2.98	115.11	119.44
6	G	507	NAD	C6N-N1N-C2N	-2.95	119.28	121.97
3	J	510	ADP	C2'-C3'-C4'	-2.90	97.02	102.64
3	J	510	ADP	O4'-C1'-C2'	-2.87	102.73	106.93
6	C	503	NAD	O5B-C5B-C4B	2.85	118.79	108.99
6	H	508	NAD	O7N-C7N-C3N	2.84	123.04	119.63
6	C	503	NAD	C6N-N1N-C2N	-2.84	119.38	121.97
6	G	507	NAD	PN-O3-PA	-2.76	123.34	132.83
3	L	512	ADP	C2'-C3'-C4'	-2.75	97.30	102.64
6	G	507	NAD	C2D-C3D-C4D	-2.73	97.34	102.64
3	A	501[A]	ADP	C2'-C3'-C4'	-2.73	97.34	102.64
3	I	509	ADP	C2'-C3'-C4'	-2.69	97.42	102.64
3	E	505	ADP	C2'-C3'-C4'	-2.68	97.43	102.64
3	D	504[B]	ADP	C2'-C3'-C4'	-2.67	97.45	102.64
3	L	512	ADP	C1'-N9-C4	-2.67	121.95	126.64
6	H	508	NAD	C6N-C5N-C4N	-2.65	115.59	119.44
6	B	502	NAD	C3B-C2B-C1B	2.65	104.97	100.98
6	B	502	NAD	O7N-C7N-N7N	-2.61	118.86	122.58
3	L	512	ADP	C5-C6-N6	2.59	124.29	120.35
3	E	505	ADP	C5-C6-N6	2.57	124.26	120.35
6	B	502	NAD	C2D-C3D-C4D	-2.56	97.66	102.64
6	H	508	NAD	C2B-C3B-C4B	-2.52	97.75	102.64
6	G	507	NAD	O4B-C1B-C2B	-2.51	103.25	106.93
3	K	511	ADP	O5'-C5'-C4'	2.49	117.58	108.99
6	C	503	NAD	C6N-C5N-C4N	-2.48	115.83	119.44
6	C	503	NAD	PN-O3-PA	-2.45	124.43	132.83
6	G	507	NAD	C5N-C6N-N1N	2.43	123.89	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	506	NAD	PN-O3-PA	-2.43	124.49	132.83
3	E	505	ADP	O2B-PB-O3A	2.42	112.75	104.64
6	C	503	NAD	O5D-C5D-C4D	2.41	117.30	108.99
6	G	507	NAD	C4N-C3N-C7N	-2.40	114.62	121.04
6	C	503	NAD	C5N-C4N-C3N	2.39	123.18	120.34
3	D	504[A]	ADP	C2'-C3'-C4'	-2.38	98.02	102.64
6	B	502	NAD	C6N-N1N-C2N	-2.37	119.81	121.97
6	B	502	NAD	C2B-C3B-C4B	-2.33	98.12	102.64
6	C	503	NAD	O7N-C7N-C3N	2.26	122.33	119.63
6	C	503	NAD	C3B-C2B-C1B	2.17	104.24	100.98
6	H	508	NAD	O5D-C5D-C4D	2.10	116.24	108.99
6	H	508	NAD	C2N-C3N-C4N	2.10	120.63	118.26
3	A	501[A]	ADP	O2B-PB-O3A	2.06	111.55	104.64
6	B	502	NAD	C2N-N1N-C1D	-2.02	114.63	119.14
6	F	506	NAD	C5N-C4N-C3N	2.02	122.74	120.34
6	C	503	NAD	O4D-C1D-C2D	-2.01	103.99	106.93
3	L	512	ADP	O2B-PB-O3A	2.00	111.35	104.64

There are no chirality outliers.

All (80) 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[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	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	O4D-C4D-C5D-O5D
6	C	503	NAD	C5B-O5B-PA-O1A
6	C	503	NAD	C5B-O5B-PA-O2A
6	F	506	NAD	C5B-O5B-PA-O1A
6	G	507	NAD	C5B-O5B-PA-O1A
6	G	507	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
6	G	507	NAD	C5D-O5D-PN-O2N
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'
3	L	512	ADP	C3'-C4'-C5'-O5'
6	C	503	NAD	O4D-C4D-C5D-O5D
6	G	507	NAD	O4D-C4D-C5D-O5D
6	G	507	NAD	C3D-C4D-C5D-O5D
3	J	510	ADP	C3'-C4'-C5'-O5'
6	B	502	NAD	C3D-C4D-C5D-O5D
6	H	508	NAD	C3D-C4D-C5D-O5D
6	C	503	NAD	C2N-C3N-C7N-N7N
6	C	503	NAD	C4N-C3N-C7N-N7N
6	C	503	NAD	C4N-C3N-C7N-O7N
6	C	503	NAD	C2N-C3N-C7N-O7N
4	C	903	EDO	O1-C1-C2-O2
3	I	509	ADP	C4'-C5'-O5'-PA
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
6	H	508	NAD	C4D-C5D-O5D-PN
3	J	510	ADP	C5'-O5'-PA-O3A
3	L	512	ADP	C5'-O5'-PA-O3A
6	G	507	NAD	C5B-O5B-PA-O3
3	K	511	ADP	PB-O3A-PA-O2A
6	F	506	NAD	C5B-O5B-PA-O2A
6	G	507	NAD	C5B-O5B-PA-O2A
6	G	507	NAD	C4D-C5D-O5D-PN
6	F	506	NAD	C4D-C5D-O5D-PN
4	K	911	EDO	O1-C1-C2-O2
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
6	C	503	NAD	C4D-C5D-O5D-PN
6	F	506	NAD	C4N-C3N-C7N-N7N
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	H	508	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	A	901	EDO	O1-C1-C2-O2
4	C	803	EDO	O1-C1-C2-O2
3	D	504[A]	ADP	PA-O3A-PB-O3B
6	F	506	NAD	C4N-C3N-C7N-O7N
3	D	504[A]	ADP	C5'-O5'-PA-O3A
6	B	502	NAD	C5B-O5B-PA-O3
6	C	503	NAD	C5B-O5B-PA-O3
6	F	506	NAD	C5B-O5B-PA-O3
6	G	507	NAD	C5D-O5D-PN-O3
6	H	508	NAD	C5D-O5D-PN-O3
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	B	502	NAD	C5D-O5D-PN-O2N
6	H	508	NAD	C3B-C4B-C5B-O5B
4	D	704	EDO	O1-C1-C2-O2
3	D	504[A]	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

22 monomers are involved in 35 short contacts:

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

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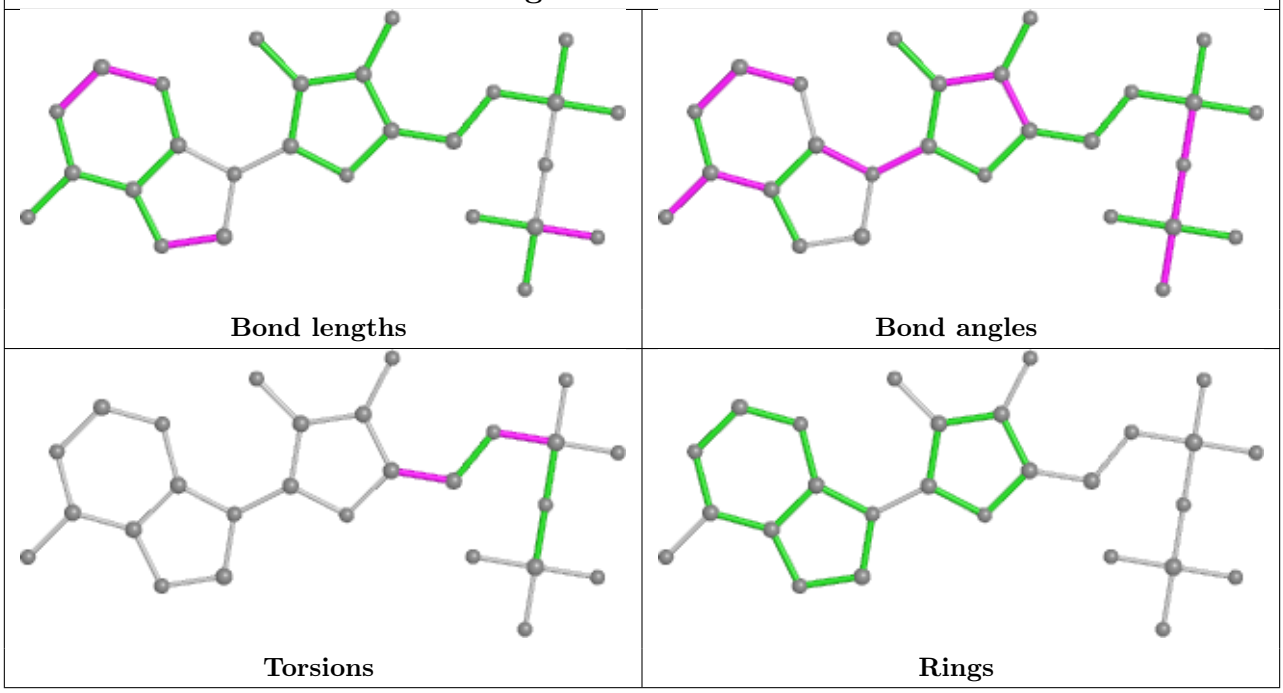
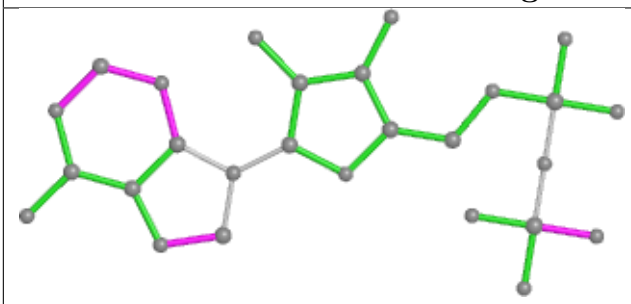
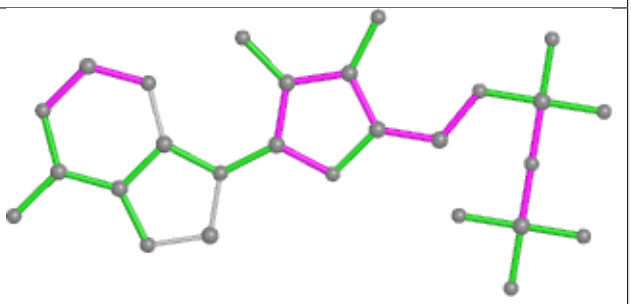
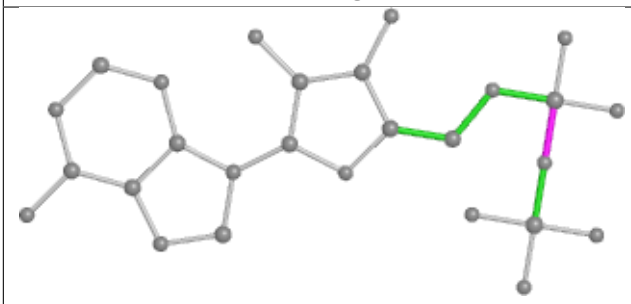
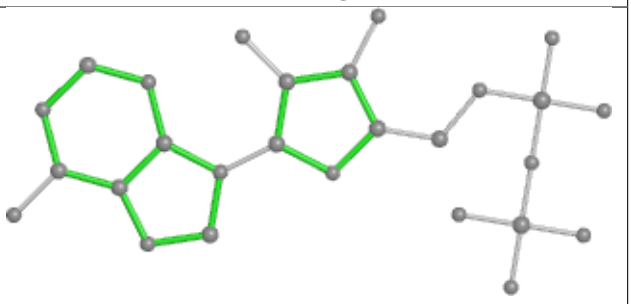
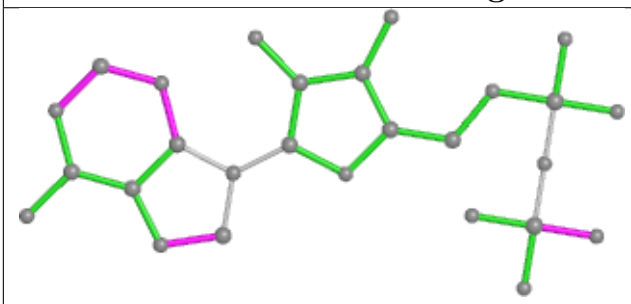
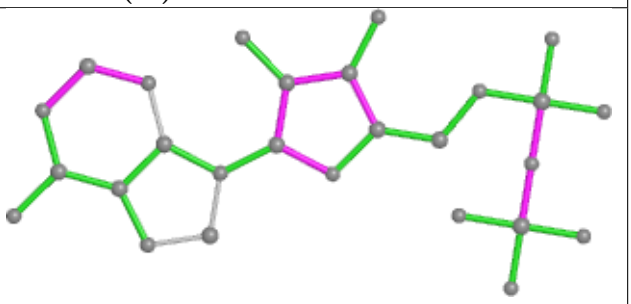
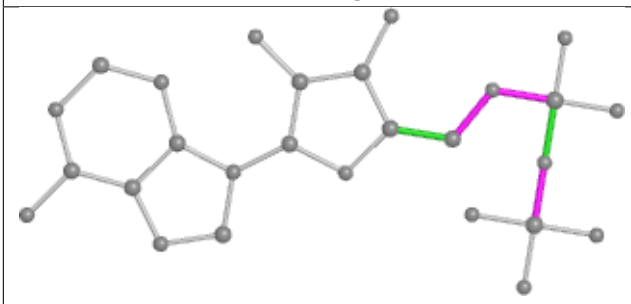
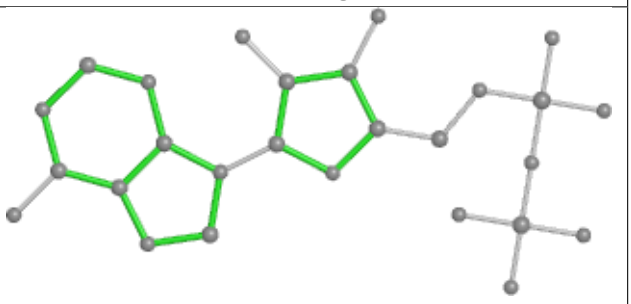
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	704	EDO	1	0
4	E	705	EDO	1	0
3	A	501[B]	ADP	1	0

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 then 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.

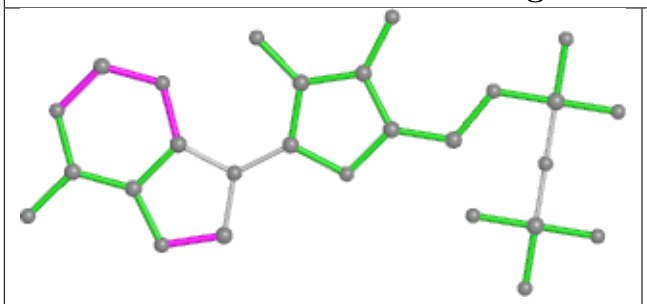
Ligand ADP L 512



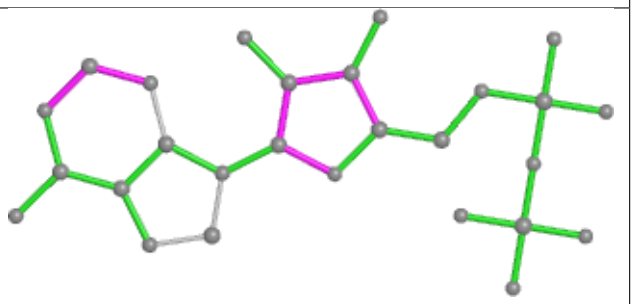
Ligand ADP K 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 504 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

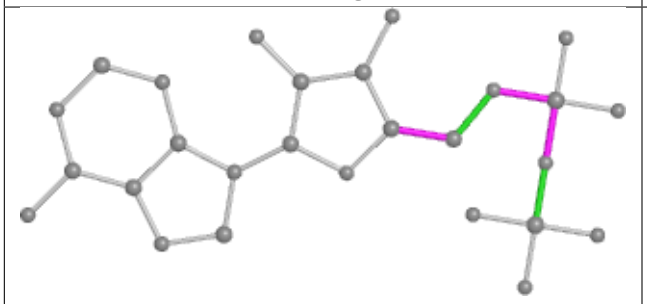
Ligand ADP J 510



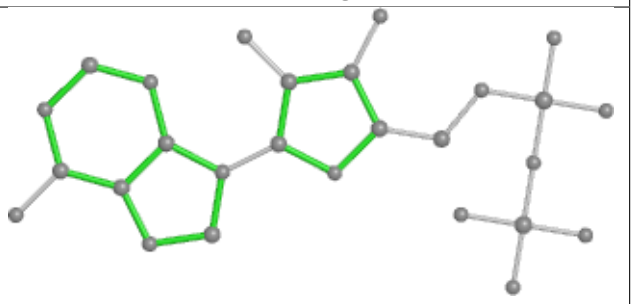
Bond lengths



Bond angles

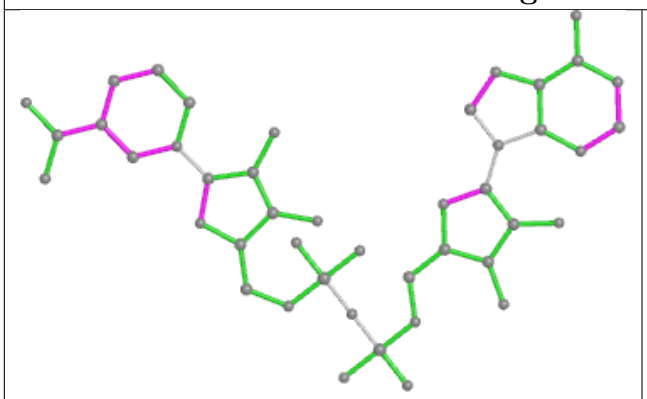


Torsions

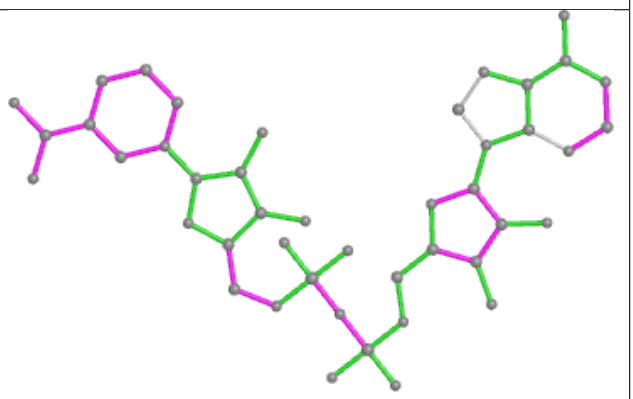


Rings

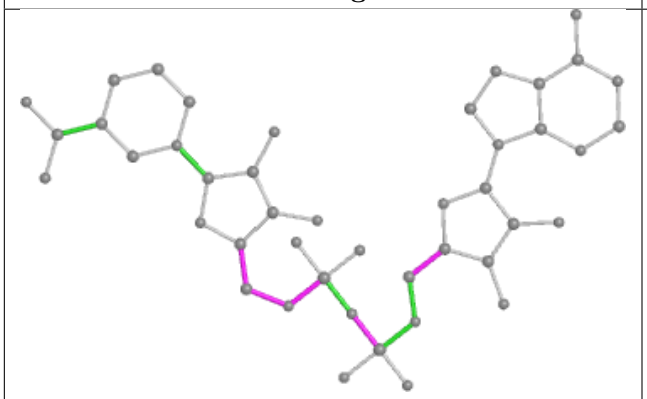
Ligand NAD H 508



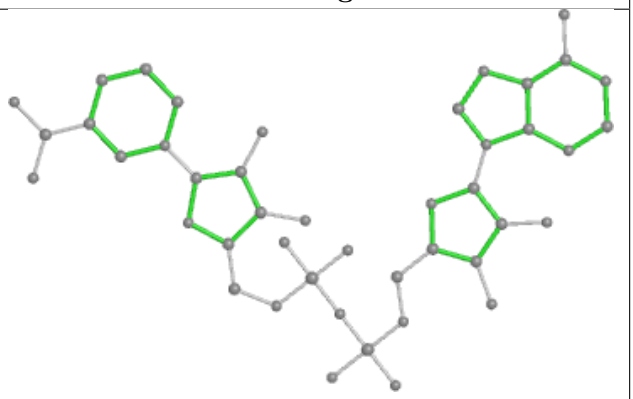
Bond lengths



Bond angles

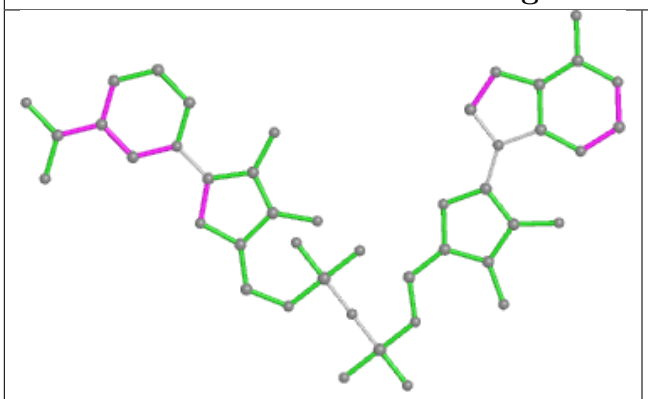


Torsions

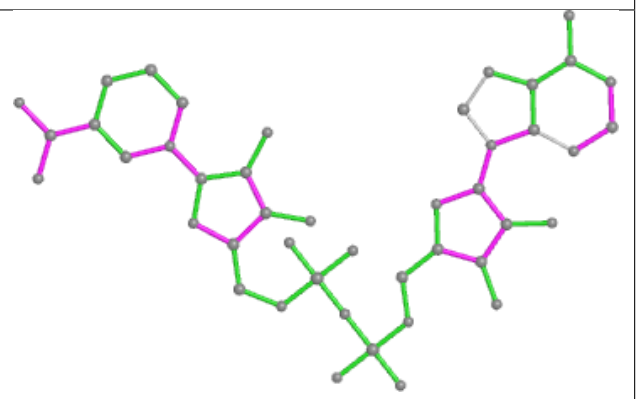


Rings

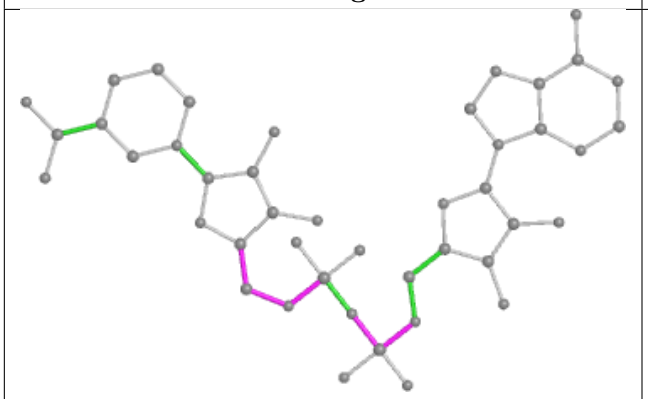
Ligand NAD B 502



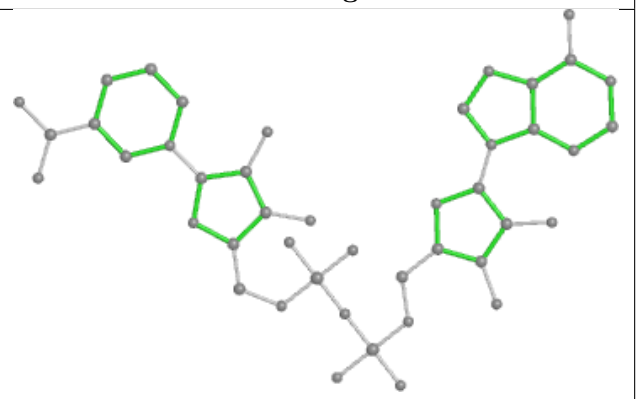
Bond lengths



Bond angles

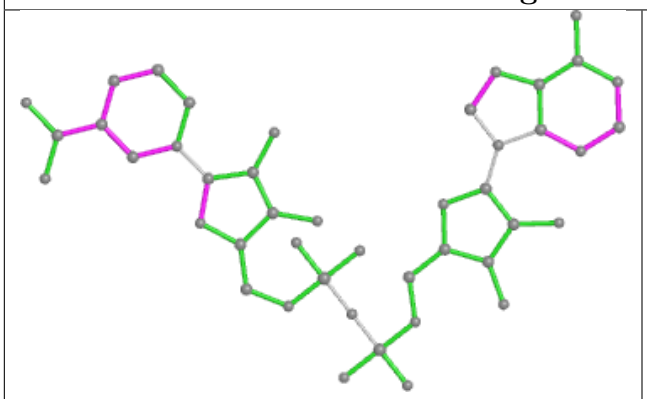


Torsions



Rings

Ligand NAD G 507



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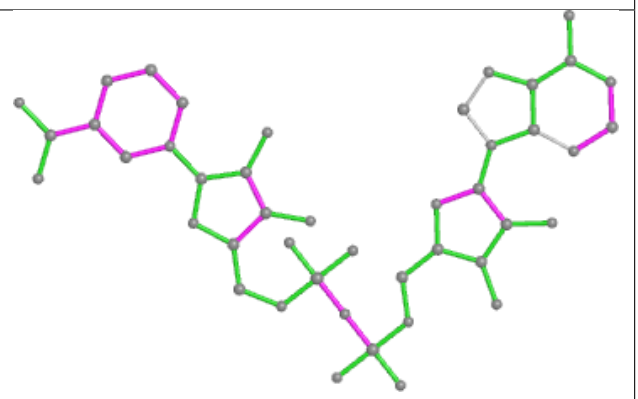
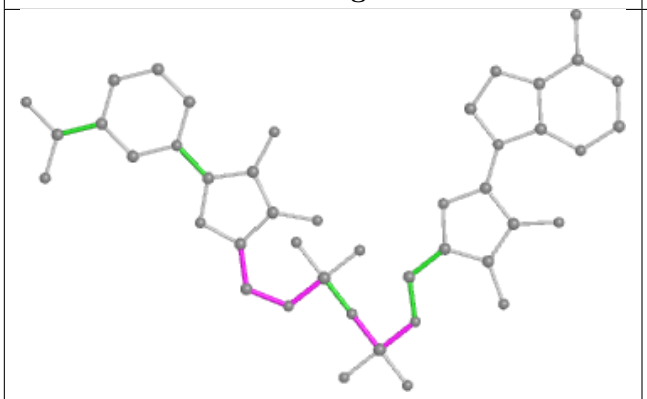
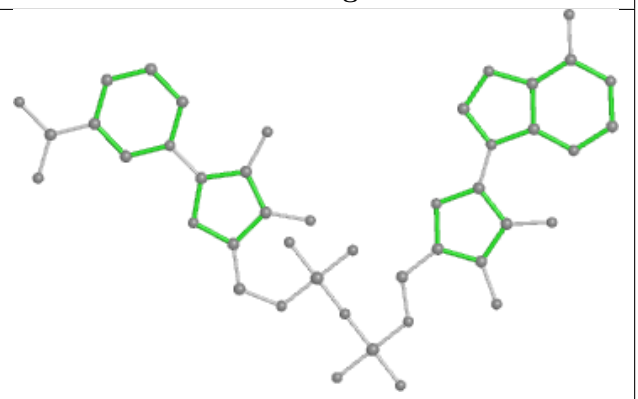


Bond angles

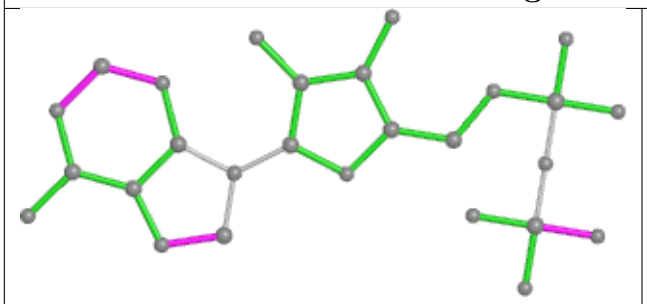


Torsions

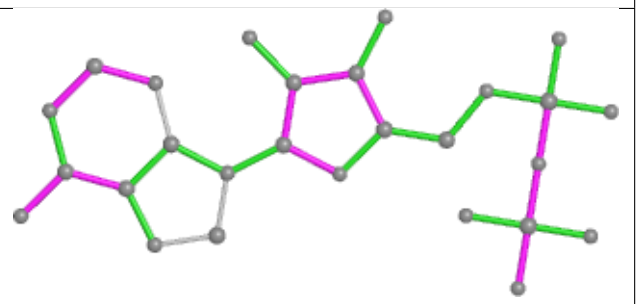


Rings

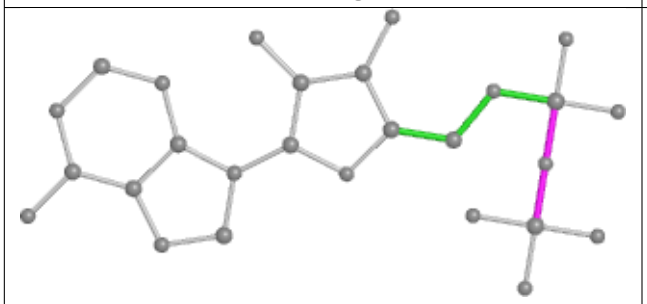
Ligand ADP E 505



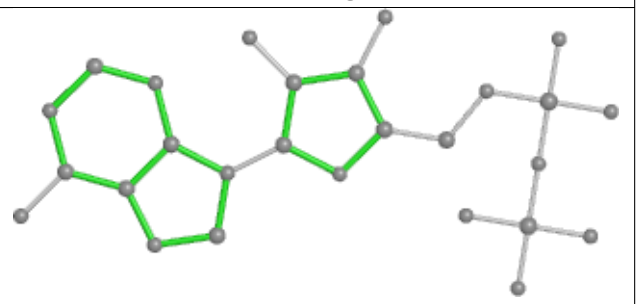
Bond lengths



Bond angles

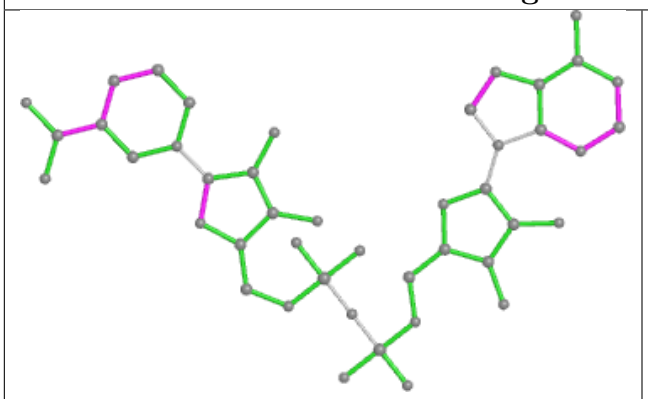


Torsions

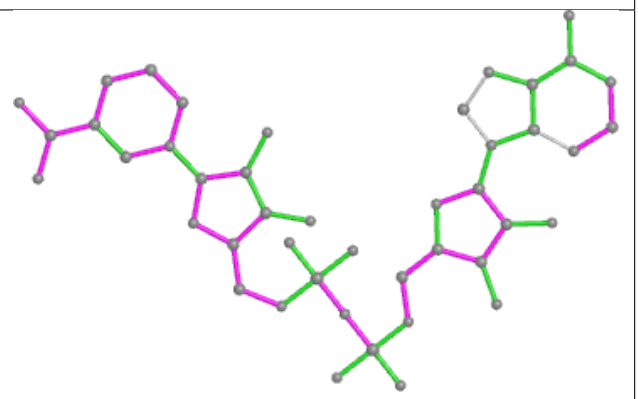


Rings

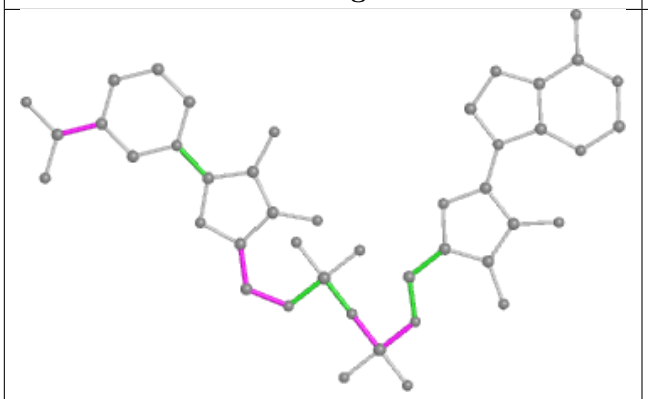
Ligand NAD C 503



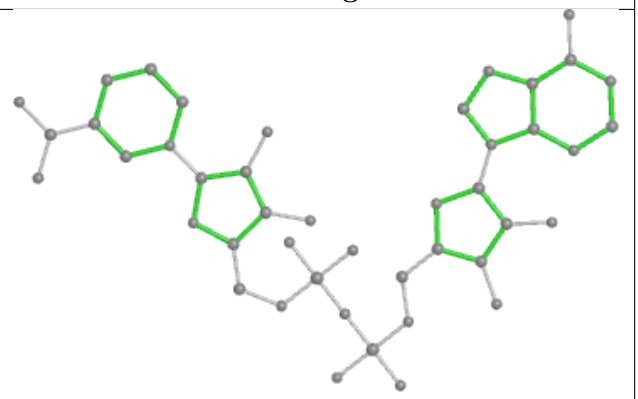
Bond lengths



Bond angles

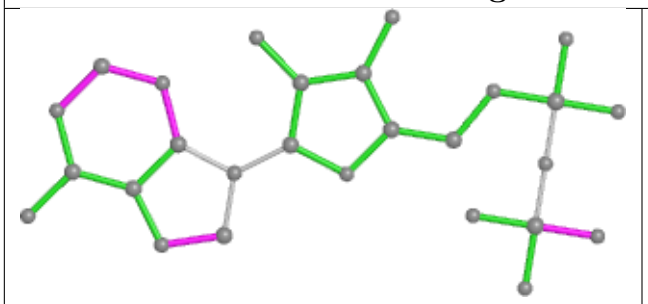


Torsions

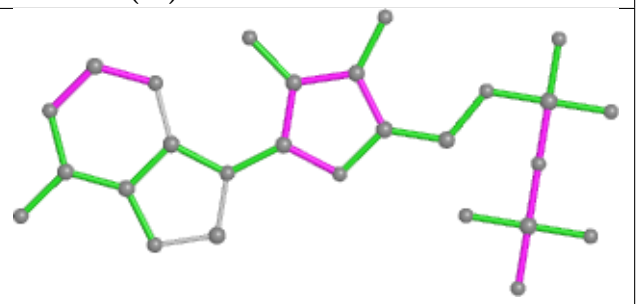


Rings

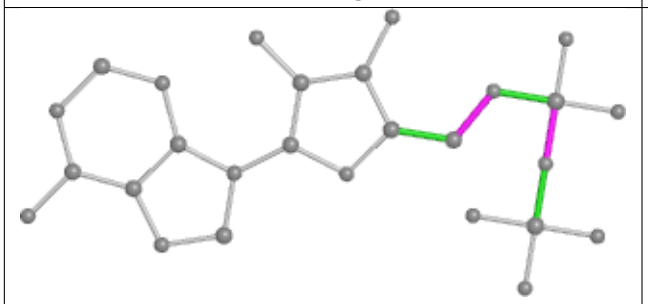
Ligand ADP A 501 (A)



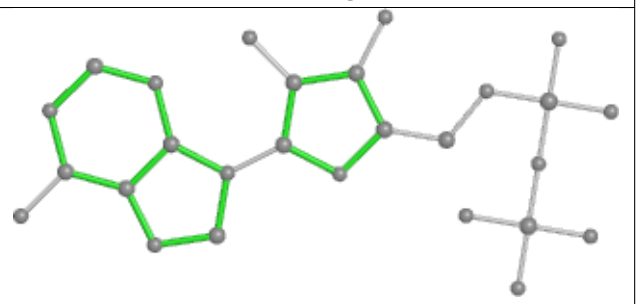
Bond lengths



Bond angles

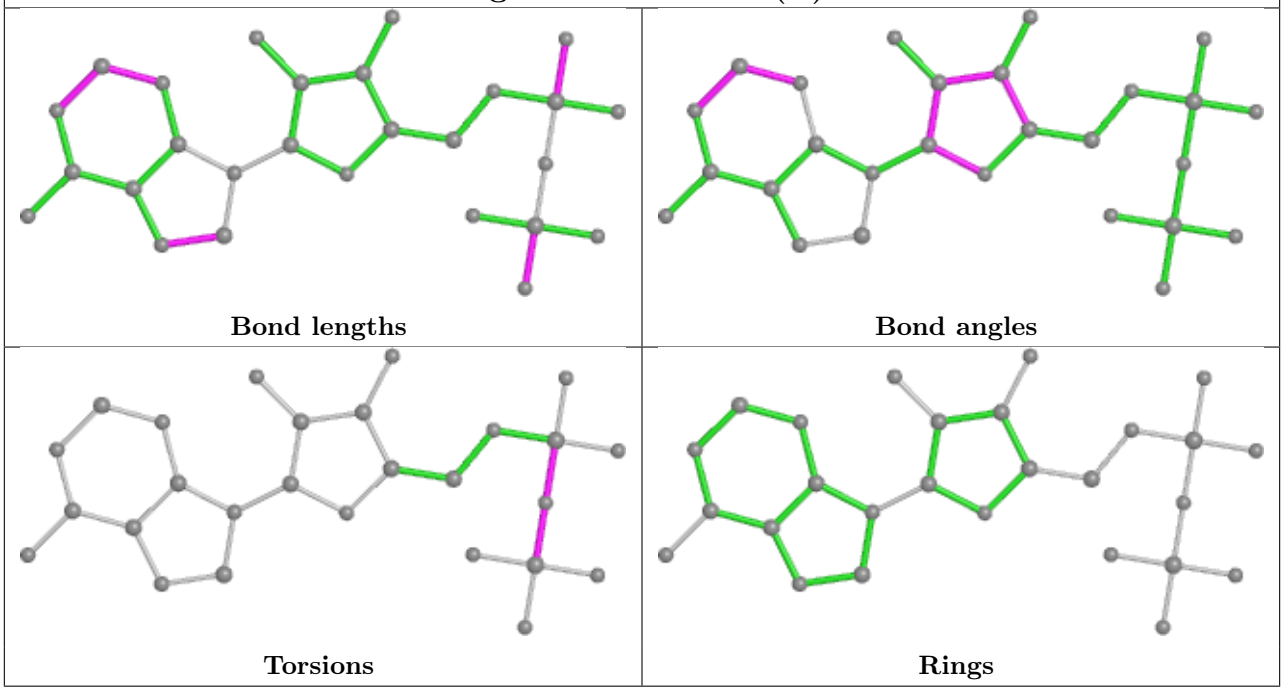


Torsions

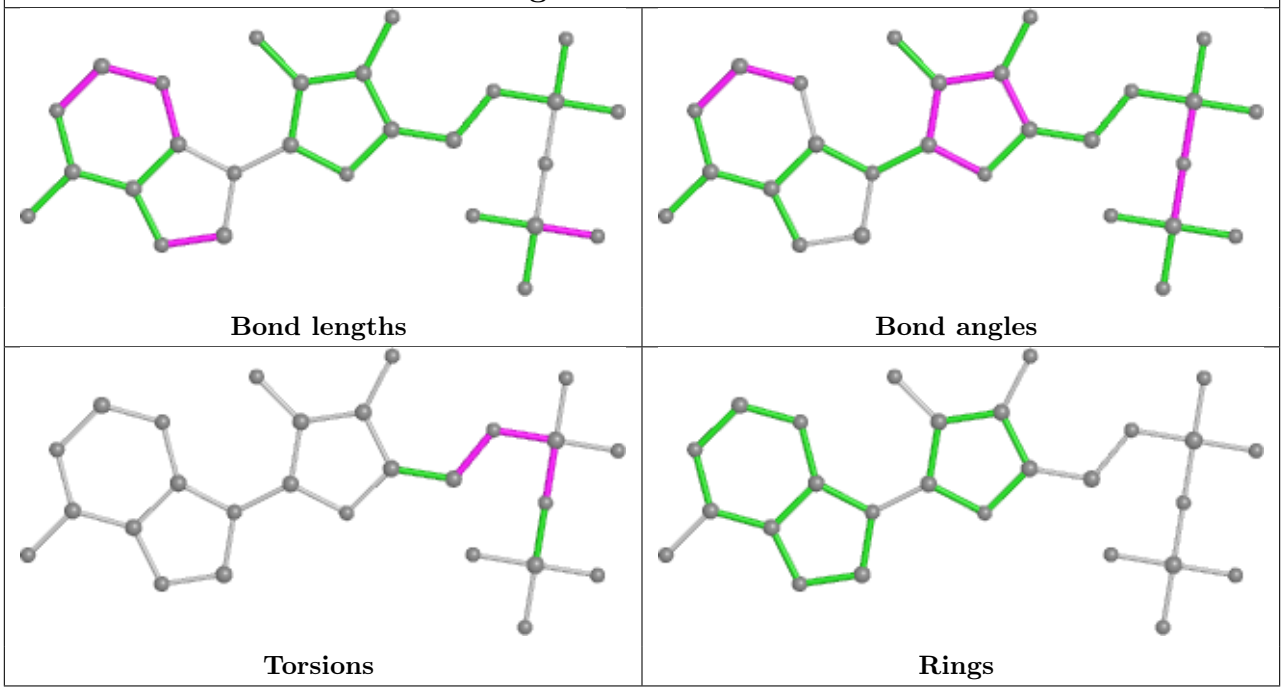


Rings

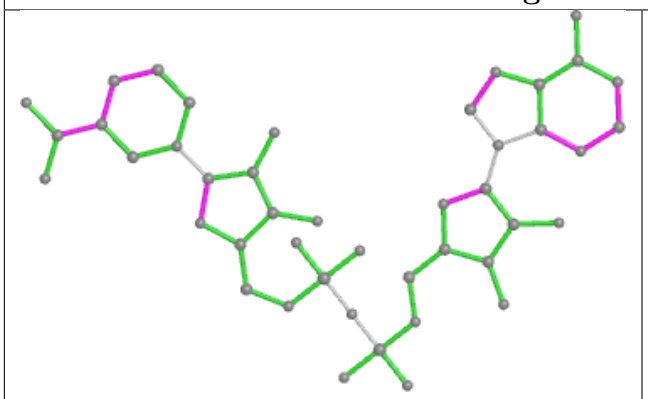
Ligand ADP D 504 (B)



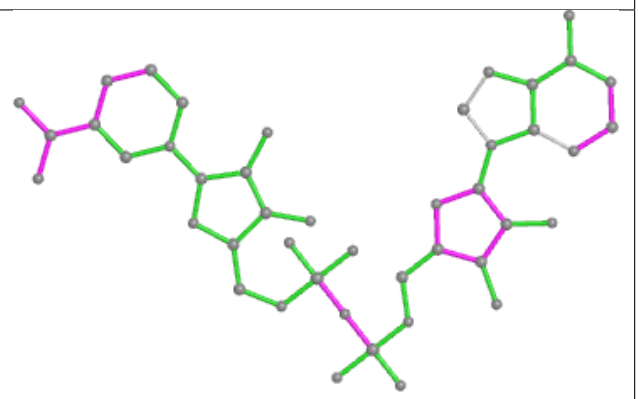
Ligand ADP I 509



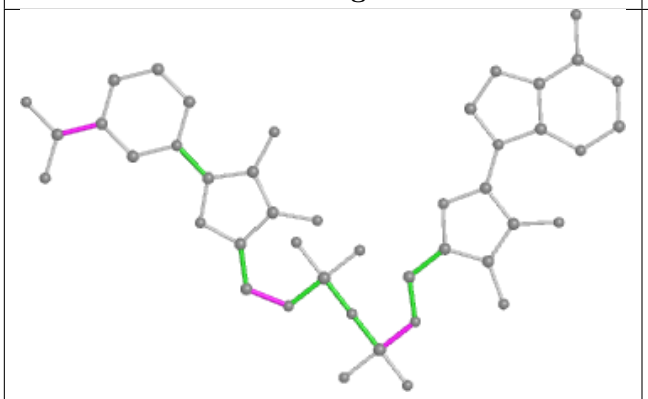
Ligand NAD F 506



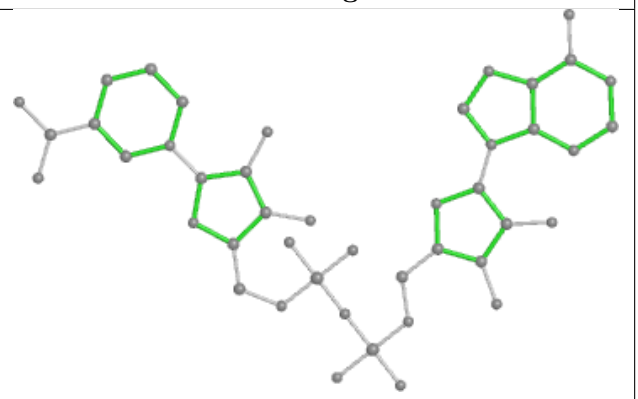
Bond lengths



Bond angles

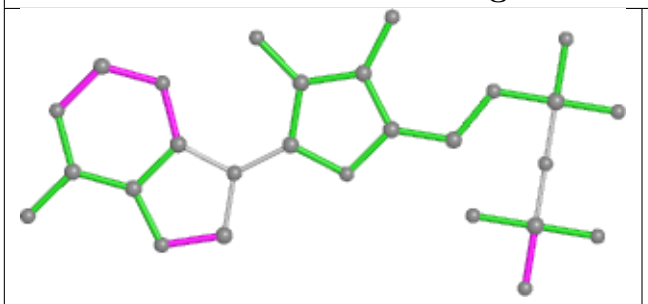


Torsions

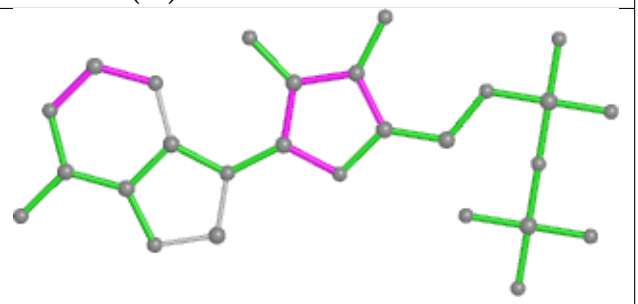


Rings

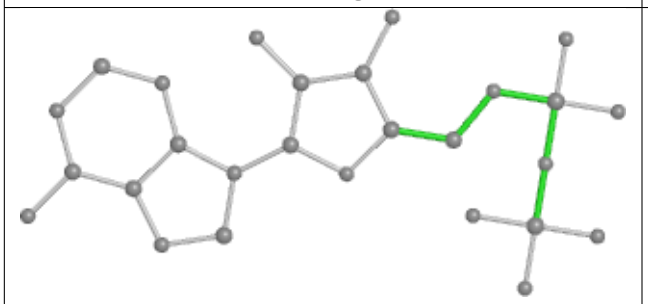
Ligand ADP A 501 (B)



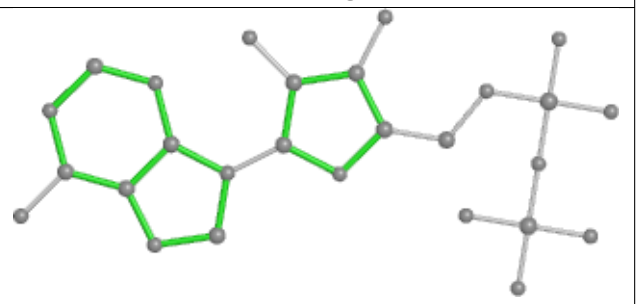
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.71	55 (11%)	5	5	21, 67, 104, 123	0
1	B	494/500 (98%)	-0.15	5 (1%)	82	84	24, 40, 78, 98	0
1	C	494/500 (98%)	-0.12	2 (0%)	92	93	23, 40, 72, 88	0
1	D	494/500 (98%)	0.60	38 (7%)	13	13	25, 68, 97, 118	0
1	E	494/500 (98%)	-0.17	2 (0%)	92	93	23, 41, 68, 96	0
1	F	494/500 (98%)	-0.09	3 (0%)	89	90	21, 37, 66, 94	0
1	G	494/500 (98%)	0.08	6 (1%)	79	80	26, 46, 68, 98	0
1	H	494/500 (98%)	0.11	12 (2%)	59	62	24, 46, 77, 91	0
1	I	494/500 (98%)	0.37	20 (4%)	38	41	36, 58, 82, 105	0
1	J	494/500 (98%)	0.77	41 (8%)	11	11	44, 77, 104, 114	0
1	K	494/500 (98%)	0.57	39 (7%)	12	12	44, 71, 96, 115	0
1	L	494/500 (98%)	1.15	98 (19%)	1	1	47, 89, 115, 127	0
All	All	5928/6000 (98%)	0.32	321 (5%)	25	27	21, 55, 99, 127	0

All (321) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	378	GLY	7.2
1	L	369	CYS	5.9
1	L	223	GLY	5.4
1	L	386	PHE	5.0
1	G	474	GLY	5.0
1	D	424	THR	5.0
1	L	295	PHE	4.9
1	A	362	GLN	4.9
1	A	371	GLY	4.8
1	K	475	ARG	4.7
1	L	373	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	K	377	ARG	4.7
1	J	365	ALA	4.5
1	L	333	ASN	4.5
1	A	473	SER	4.4
1	A	470	MET	4.4
1	A	477	LEU	4.3
1	D	327	LYS	4.3
1	A	353	ILE	4.3
1	K	376	ASP	4.2
1	L	332	GLY	4.2
1	L	360	GLY	4.2
1	D	356	TYR	4.2
1	A	315	TYR	4.2
1	J	108	LEU	4.1
1	L	356	TYR	4.1
1	K	474	GLY	4.1
1	E	7	ALA	4.0
1	L	350	PHE	4.0
1	J	7	ALA	4.0
1	L	357	ILE	3.9
1	L	285	TRP	3.9
1	D	470	MET	3.9
1	K	371	GLY	3.9
1	A	468	TYR	3.9
1	L	318	PHE	3.9
1	L	380	PHE	3.9
1	D	376	ASP	3.9
1	L	327	LYS	3.8
1	L	354	LEU	3.8
1	L	482	LEU	3.8
1	L	387	GLY	3.8
1	J	362	GLN	3.8
1	L	478	GLY	3.8
1	G	7	ALA	3.8
1	A	424	THR	3.7
1	K	473	SER	3.7
1	L	322	SER	3.7
1	L	377	ARG	3.7
1	K	470	MET	3.7
1	A	475	ARG	3.7
1	A	394	THR	3.6
1	L	358	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	310	VAL	3.6
1	A	358	ASN	3.5
1	L	108	LEU	3.5
1	K	413	ILE	3.5
1	A	334	PRO	3.5
1	L	480	TYR	3.4
1	I	408	LEU	3.4
1	I	319	VAL	3.4
1	A	474	GLY	3.4
1	K	463	SER	3.3
1	A	7	ALA	3.3
1	A	367	LEU	3.3
1	J	425	TYR	3.3
1	A	377	ARG	3.3
1	L	468	TYR	3.3
1	A	356	TYR	3.2
1	A	376	ASP	3.2
1	L	340	GLU	3.2
1	K	380	PHE	3.2
1	L	479	GLU	3.2
1	A	404	VAL	3.2
1	J	42	PRO	3.2
1	K	471	SER	3.1
1	J	139	TYR	3.1
1	K	379	TYR	3.1
1	J	378	GLY	3.1
1	L	314	ILE	3.1
1	D	29	HIS	3.1
1	A	319	VAL	3.1
1	D	247	THR	3.1
1	I	389	VAL	3.1
1	H	386	PHE	3.1
1	A	10	ALA	3.1
1	A	365	ALA	3.1
1	H	364	GLY	3.1
1	I	480	TYR	3.1
1	L	9	PRO	3.1
1	D	32	VAL	3.1
1	D	350	PHE	3.1
1	J	468	TYR	3.1
1	L	475	ARG	3.1
1	H	365	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	104	ALA	3.0
1	K	468	TYR	3.0
1	H	362	GLN	3.0
1	L	408	LEU	3.0
1	L	353	ILE	3.0
1	K	466	GLY	3.0
1	L	349	GLN	3.0
1	L	347	GLU	3.0
1	A	469	LYS	3.0
1	D	353	ILE	2.9
1	A	373	ILE	2.9
1	A	279	SER	2.9
1	J	247	THR	2.9
1	L	367	LEU	2.9
1	L	376	ASP	2.9
1	A	386	PHE	2.9
1	A	395	ILE	2.9
1	D	31	ALA	2.9
1	K	139	TYR	2.9
1	J	22	ILE	2.9
1	K	472	GLY	2.9
1	I	139	TYR	2.9
1	J	476	GLU	2.8
1	D	475	ARG	2.8
1	K	375	ALA	2.8
1	L	28	TRP	2.8
1	L	216	GLY	2.8
1	H	290	ALA	2.8
1	F	477	LEU	2.8
1	H	7	ALA	2.8
1	G	477	LEU	2.8
1	J	373	ILE	2.8
1	J	30	ASP	2.8
1	K	467	GLY	2.8
1	K	465	PHE	2.8
1	K	17	VAL	2.8
1	A	326	ALA	2.8
1	K	484	ALA	2.8
1	L	139	TYR	2.7
1	D	365	ALA	2.7
1	L	8	VAL	2.7
1	L	329	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	253	ILE	2.7
1	I	470	MET	2.7
1	L	115	VAL	2.7
1	L	465	PHE	2.7
1	K	46	GLU	2.7
1	L	113	PRO	2.7
1	J	376	ASP	2.7
1	A	287	VAL	2.7
1	L	385	VAL	2.7
1	A	398	GLU	2.7
1	L	27	GLU	2.6
1	L	301	CYS	2.6
1	A	295	PHE	2.6
1	J	392	GLY	2.6
1	D	468	TYR	2.6
1	J	44	THR	2.6
1	K	7	ALA	2.6
1	L	463	SER	2.6
1	J	32	VAL	2.6
1	I	486	THR	2.6
1	J	31	ALA	2.6
1	D	471	SER	2.6
1	J	374	ALA	2.6
1	L	461	ALA	2.6
1	L	462	GLN	2.6
1	L	413	ILE	2.6
1	L	363	GLU	2.6
1	J	347	GLU	2.6
1	L	466	GLY	2.6
1	A	100	THR	2.5
1	E	424	THR	2.5
1	A	327	LYS	2.5
1	A	397	LYS	2.5
1	D	334	PRO	2.5
1	J	33	SER	2.5
1	J	203	TYR	2.5
1	L	365	ALA	2.5
1	D	379	TYR	2.5
1	G	486	THR	2.5
1	L	47	VAL	2.5
1	L	319	VAL	2.5
1	L	7	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	323	VAL	2.5
1	D	399	GLU	2.5
1	L	486	THR	2.5
1	A	379	TYR	2.5
1	D	199	LEU	2.5
1	I	141	GLY	2.5
1	J	53	GLU	2.5
1	L	339	THR	2.5
1	K	478	GLY	2.5
1	A	323	VAL	2.5
1	A	480	TYR	2.5
1	L	40	VAL	2.5
1	A	256	ALA	2.5
1	L	66	ALA	2.5
1	D	8	VAL	2.4
1	A	465	PHE	2.4
1	J	386	PHE	2.4
1	H	360	GLY	2.4
1	G	475	ARG	2.4
1	L	338	LYS	2.4
1	A	357	ILE	2.4
1	B	253	ILE	2.4
1	I	479	GLU	2.4
1	I	411	LYS	2.4
1	K	332	GLY	2.4
1	L	473	SER	2.4
1	A	114	TYR	2.4
1	J	56	LYS	2.4
1	J	63	VAL	2.4
1	A	332	GLY	2.4
1	I	318	PHE	2.4
1	D	100	THR	2.4
1	B	473	SER	2.4
1	D	51	VAL	2.4
1	K	479	GLU	2.4
1	L	42	PRO	2.4
1	L	393	MET	2.4
1	I	474	GLY	2.4
1	L	104	ALA	2.4
1	L	384	THR	2.4
1	L	296	PHE	2.3
1	L	266	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	141	GLY	2.3
1	J	283	MET	2.3
1	H	473	SER	2.3
1	C	477	LEU	2.3
1	J	377	ARG	2.3
1	D	40	VAL	2.3
1	L	405	MET	2.3
1	D	337	SER	2.3
1	K	259	SER	2.3
1	L	328	SER	2.3
1	D	477	LEU	2.3
1	I	482	LEU	2.3
1	A	317	GLU	2.3
1	K	386	PHE	2.3
1	D	377	ARG	2.3
1	J	389	VAL	2.3
1	I	388	ASP	2.3
1	J	72	LEU	2.3
1	J	379	TYR	2.3
1	K	312	GLU	2.3
1	L	315	TYR	2.3
1	H	316	ASP	2.2
1	D	413	ILE	2.2
1	L	320	GLU	2.2
1	I	477	LEU	2.2
1	B	71	GLN	2.2
1	F	254	GLN	2.2
1	J	467	GLY	2.2
1	L	73	GLY	2.2
1	D	46	GLU	2.2
1	B	260	SER	2.2
1	A	314	ILE	2.2
1	L	395	ILE	2.2
1	A	328	SER	2.2
1	H	323	VAL	2.2
1	L	374	ALA	2.2
1	A	102	LEU	2.2
1	J	358	ASN	2.2
1	A	466	GLY	2.2
1	J	319	VAL	2.2
1	D	36	THR	2.2
1	K	392	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	476	GLU	2.2
1	C	7	ALA	2.2
1	L	228	ALA	2.2
1	L	433	THR	2.2
1	I	478	GLY	2.2
1	K	477	LEU	2.2
1	D	473	SER	2.2
1	L	379	TYR	2.1
1	A	479	GLU	2.1
1	D	42	PRO	2.1
1	K	441	TYR	2.1
1	D	111	GLY	2.1
1	I	312	GLU	2.1
1	L	250	GLY	2.1
1	L	371	GLY	2.1
1	K	412	THR	2.1
1	J	246	SER	2.1
1	D	338	LYS	2.1
1	H	315	TYR	2.1
1	L	44	THR	2.1
1	L	276	ILE	2.1
1	L	483	GLN	2.1
1	K	18	PHE	2.1
1	I	376	ASP	2.1
1	L	140	HIS	2.1
1	L	227	THR	2.1
1	F	465	PHE	2.1
1	I	248	GLU	2.1
1	J	34	ARG	2.1
1	J	424	THR	2.1
1	L	24	ILE	2.1
1	I	386	PHE	2.1
1	K	33	SER	2.1
1	K	483	GLN	2.1
1	A	359	THR	2.1
1	B	424	THR	2.1
1	L	51	VAL	2.1
1	L	247	THR	2.1
1	D	114	TYR	2.1
1	K	482	LEU	2.1
1	L	224	PHE	2.1
1	A	283	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	30	ASP	2.0
1	A	115	VAL	2.0
1	J	140	HIS	2.0
1	L	277	ILE	2.0
1	H	465	PHE	2.0
1	J	466	GLY	2.0
1	A	384	THR	2.0
1	G	248	GLU	2.0
1	A	311	GLN	2.0
1	D	467	GLY	2.0
1	L	199	LEU	2.0
1	L	298	GLN	2.0
1	K	37	PHE	2.0
1	K	480	TYR	2.0
1	D	248	GLU	2.0
1	L	334	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	J	610	1/1	0.56	0.12	75,75,75,75	0
2	NA	A	601	1/1	0.61	0.27	82,82,82,82	0
2	NA	C	603	1/1	0.67	0.23	54,54,54,54	0
2	NA	D	604	1/1	0.69	0.09	73,73,73,73	0
4	EDO	I	809	4/4	0.70	0.36	81,82,82,82	0
4	EDO	K	911	4/4	0.71	0.22	79,80,80,80	0
4	EDO	C	903	4/4	0.76	0.27	45,49,49,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	D	504[A]	27/27	0.76	0.29	79,81,86,86	27
3	ADP	D	504[B]	27/27	0.76	0.29	89,91,96,96	27
4	EDO	E	805	4/4	0.80	0.43	83,83,85,85	0
5	GAI	D	905	4/4	0.80	0.28	77,78,78,78	0
4	EDO	H	908	4/4	0.81	0.26	79,79,79,80	0
2	NA	I	609	1/1	0.81	0.13	54,54,54,54	0
2	NA	G	607	1/1	0.82	0.07	46,46,46,46	0
3	ADP	J	510	27/27	0.83	0.18	102,104,114,115	0
4	EDO	G	907	4/4	0.83	0.32	68,68,68,69	0
4	EDO	D	904	4/4	0.83	0.24	74,74,75,75	0
4	EDO	B	802	4/4	0.84	0.23	48,48,52,53	0
4	EDO	L	712	4/4	0.85	0.25	70,72,73,73	0
5	GAI	I	910	4/4	0.85	0.44	94,94,94,95	0
3	ADP	A	501[A]	27/27	0.86	0.20	78,80,81,81	27
4	EDO	F	706	4/4	0.86	0.38	74,76,79,80	0
3	ADP	A	501[B]	27/27	0.86	0.20	91,93,93,93	27
5	GAI	J	611	4/4	0.87	0.21	64,66,66,66	0
4	EDO	A	901	4/4	0.88	0.28	75,75,76,77	0
5	GAI	E	907	4/4	0.88	0.21	47,48,49,49	0
6	NAD	B	502	44/44	0.88	0.23	73,88,103,104	0
6	NAD	C	503	44/44	0.88	0.20	58,81,92,93	0
4	EDO	G	807	4/4	0.89	0.16	75,75,75,75	0
2	NA	L	612	1/1	0.89	0.17	80,80,80,80	0
2	NA	B	5003	1/1	0.89	0.17	55,55,55,55	0
6	NAD	H	508	44/44	0.89	0.16	49,81,89,90	0
5	GAI	H	909	4/4	0.90	0.32	95,95,95,95	0
3	ADP	L	512	27/27	0.90	0.21	89,97,112,113	0
4	EDO	H	808	4/4	0.90	0.21	63,64,64,65	0
4	EDO	F	707	4/4	0.90	0.29	59,59,61,61	0
5	GAI	E	906	4/4	0.90	0.31	51,54,55,55	0
6	NAD	G	507	44/44	0.90	0.19	61,77,91,92	0
3	ADP	K	511	27/27	0.90	0.18	94,99,105,106	0
4	EDO	E	705	4/4	0.91	0.34	77,80,80,80	0
3	ADP	I	509	27/27	0.91	0.16	79,81,94,95	0
2	NA	E	605	1/1	0.91	0.07	37,37,37,37	0
4	EDO	C	803	4/4	0.92	0.15	49,53,53,55	0
2	NA	H	608	1/1	0.92	0.10	46,46,46,46	0
6	NAD	F	506	44/44	0.92	0.17	38,68,81,84	0
3	ADP	E	505	27/27	0.92	0.15	43,52,79,80	0
4	EDO	I	909	4/4	0.92	0.15	62,62,63,64	0
2	NA	K	5012	1/1	0.93	0.16	60,60,60,60	0
2	NA	K	611	1/1	0.93	0.09	63,63,63,63	0

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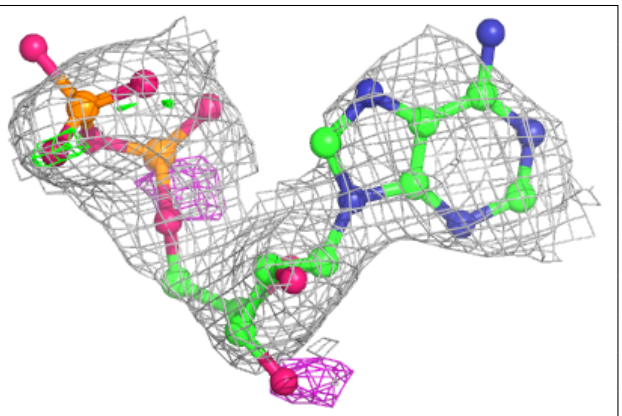
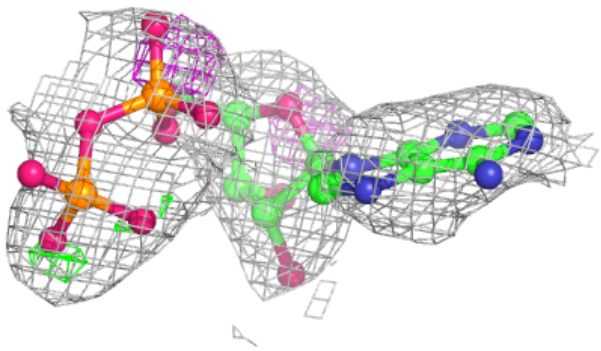
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	E	905	4/4	0.93	0.23	51,52,53,58	0
4	EDO	B	902	4/4	0.93	0.30	63,63,65,65	0
4	EDO	L	912	4/4	0.94	0.25	68,69,70,72	0
4	EDO	D	704	4/4	0.94	0.14	53,54,56,56	0
5	GAI	G	5009	4/4	0.94	0.25	76,76,76,76	0
5	GAI	G	5010	4/4	0.94	0.25	47,47,49,49	0
2	NA	F	606	1/1	0.95	0.08	32,32,32,32	0
2	NA	C	5004	1/1	0.95	0.44	51,51,51,51	0
5	GAI	A	902	4/4	0.95	0.18	63,64,64,65	0
2	NA	F	5007	1/1	0.95	0.20	54,54,54,54	0
4	EDO	B	701	4/4	0.96	0.19	67,67,67,68	0
4	EDO	F	906	4/4	0.96	0.18	63,63,65,65	0
4	EDO	H	708	4/4	0.96	0.19	47,49,51,53	0
2	NA	B	602	1/1	0.96	0.06	40,40,40,40	0
2	NA	G	5008	1/1	0.97	0.47	48,48,48,48	0
4	EDO	F	806	4/4	0.97	0.16	53,54,54,58	0

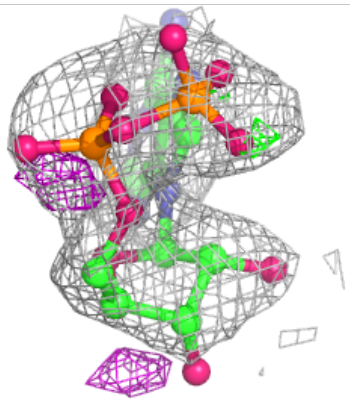
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 504 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

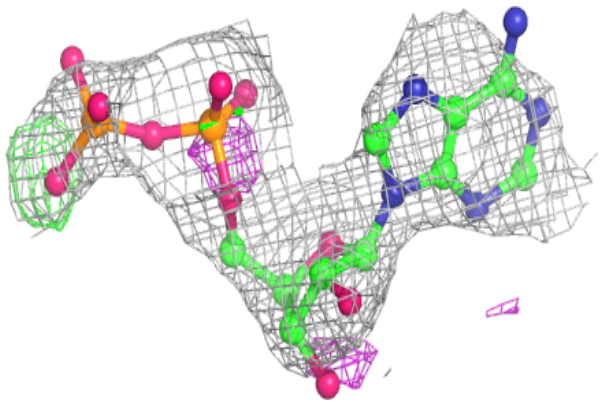


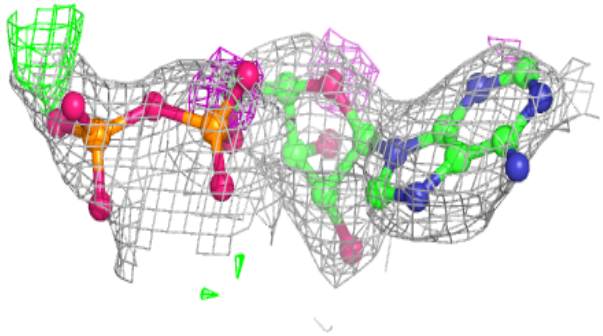


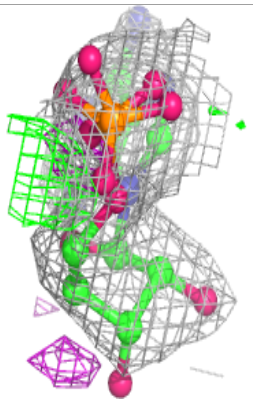


Electron density around ADP D 504 (B):

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

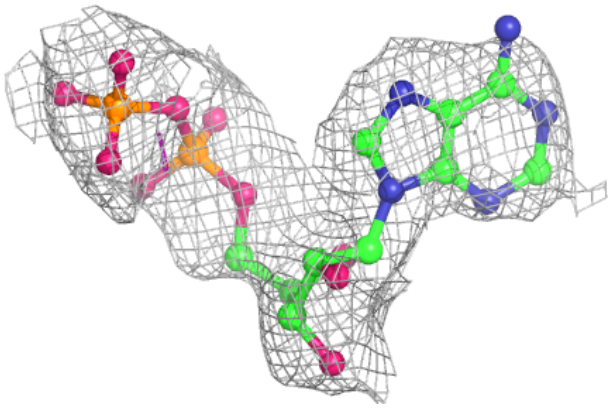


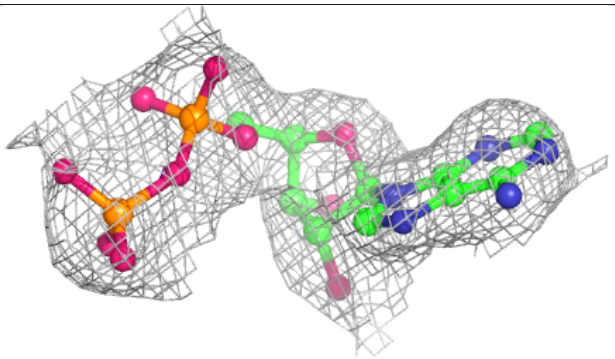


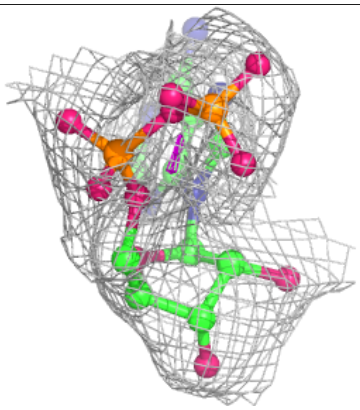


Electron density around ADP J 510:

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

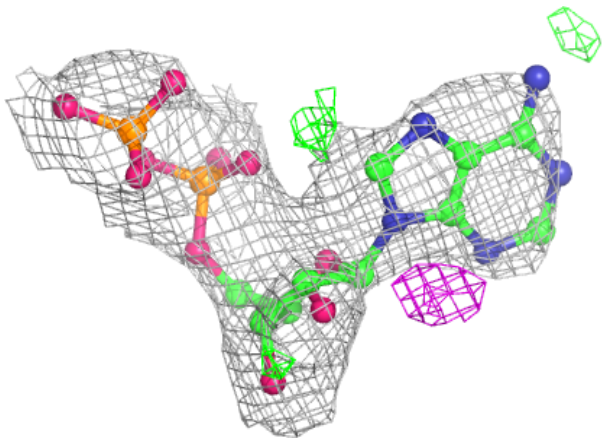


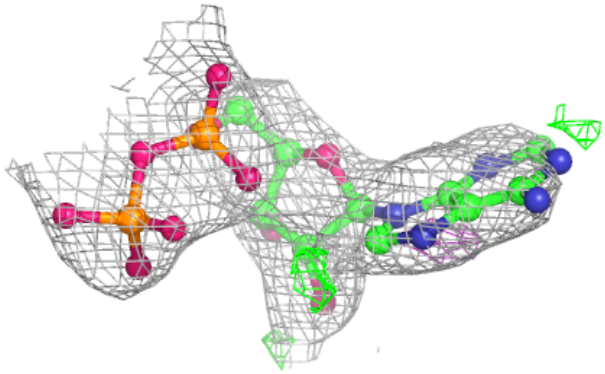


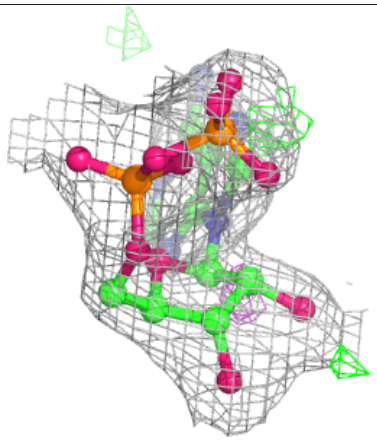


Electron density around ADP A 501 (A):

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

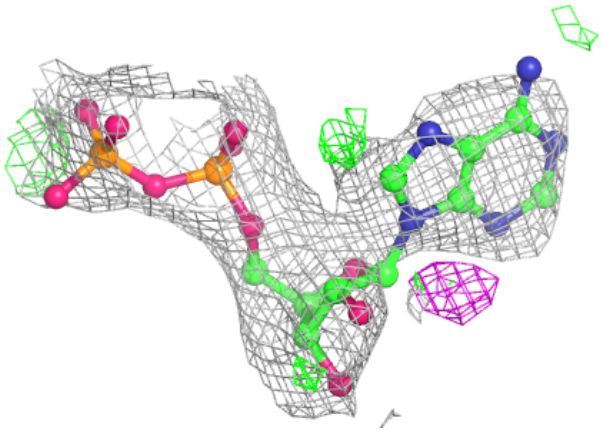


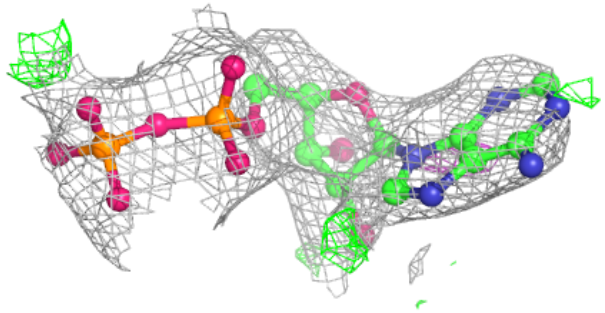


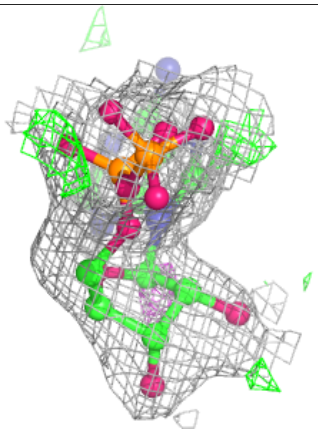


Electron density around ADP A 501 (B):

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

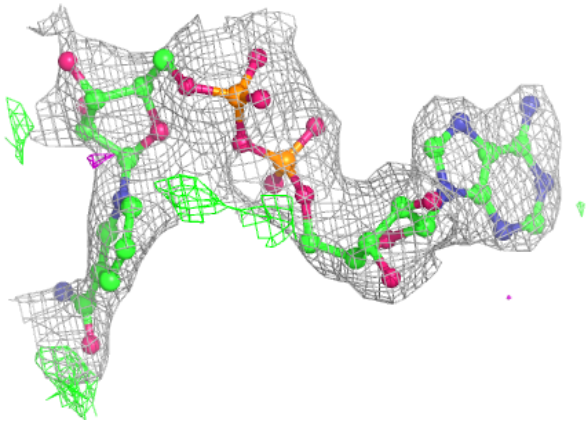


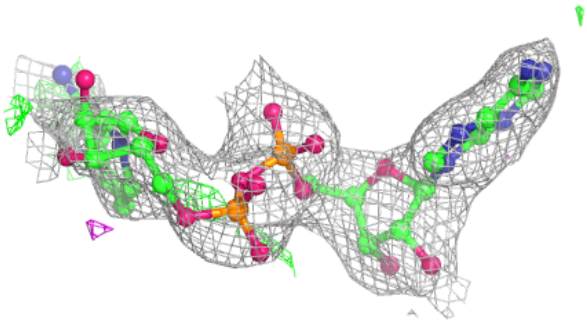


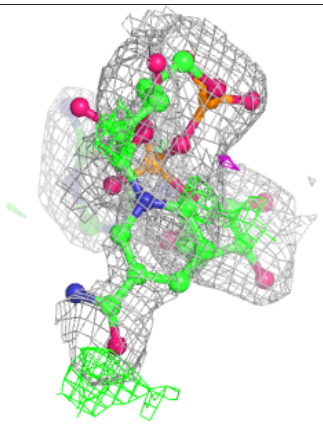


Electron density around NAD B 502:

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

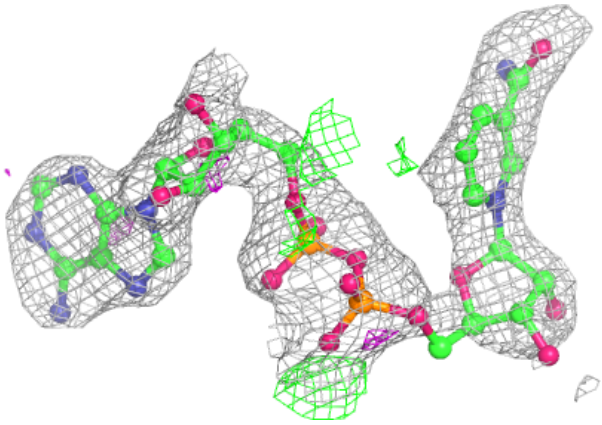


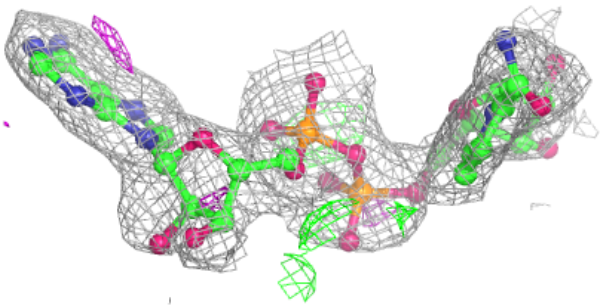


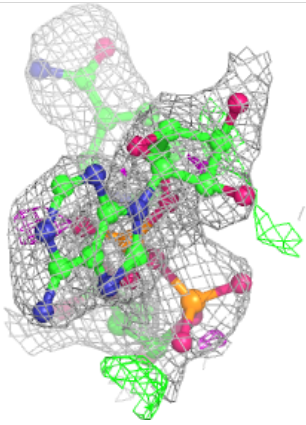


Electron density around NAD C 503:

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

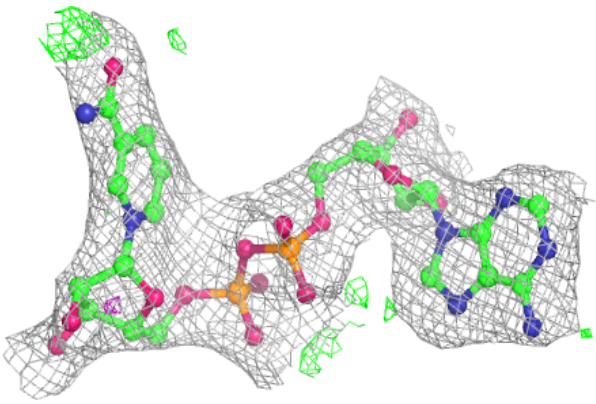


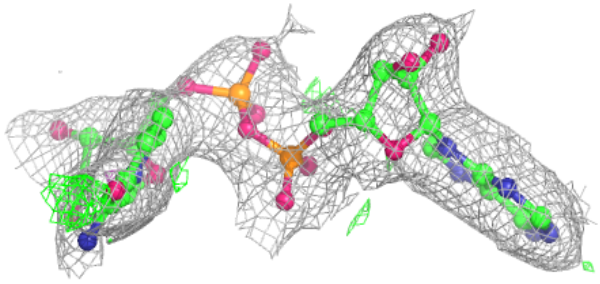


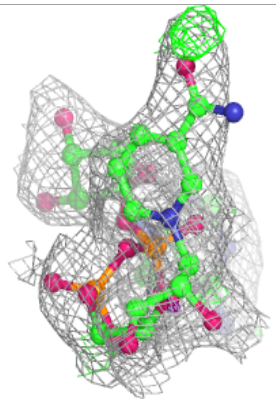


Electron density around NAD H 508:

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

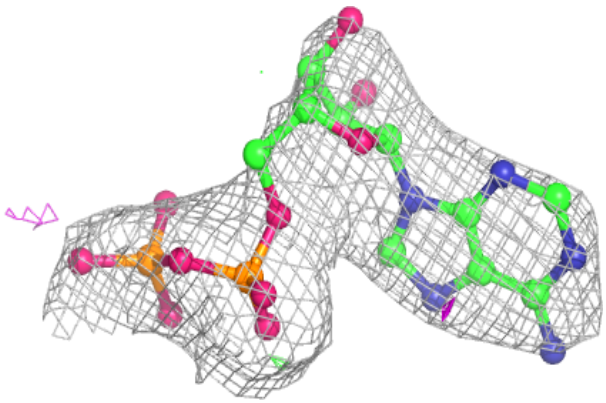


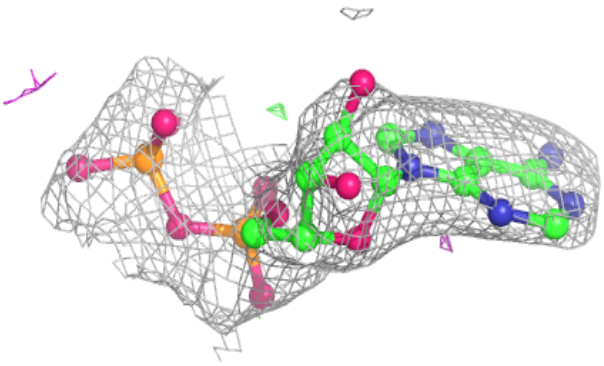


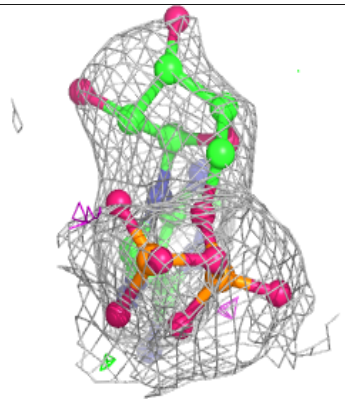


Electron density around ADP L 512:

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

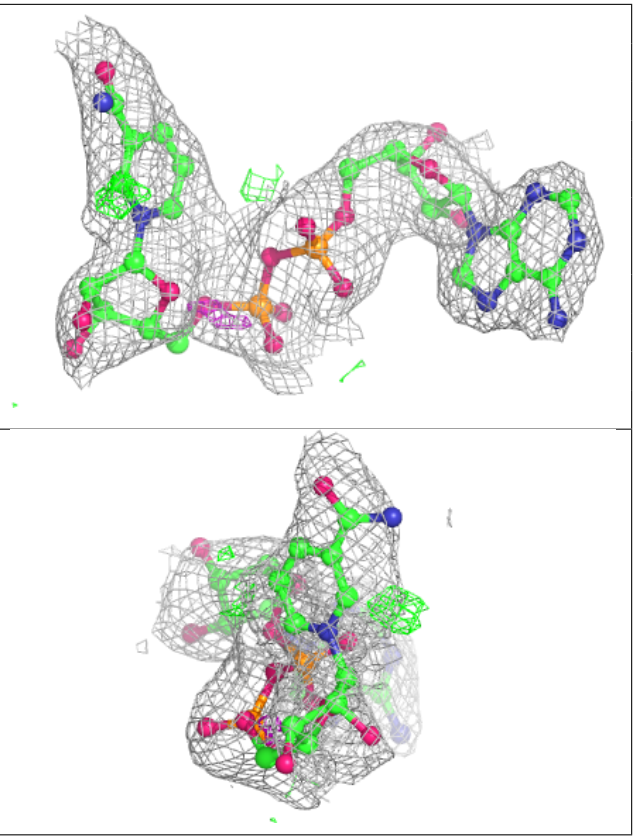






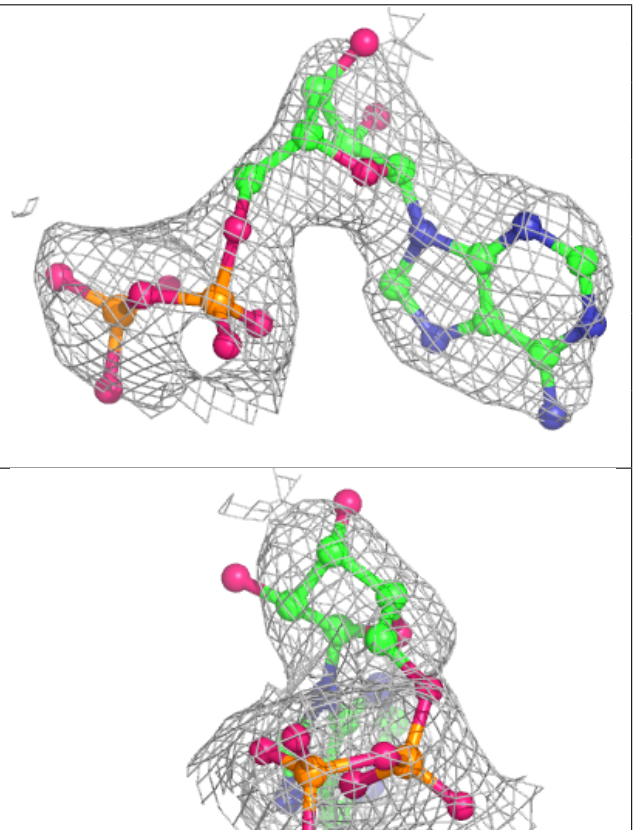
Electron density around NAD G 507:

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



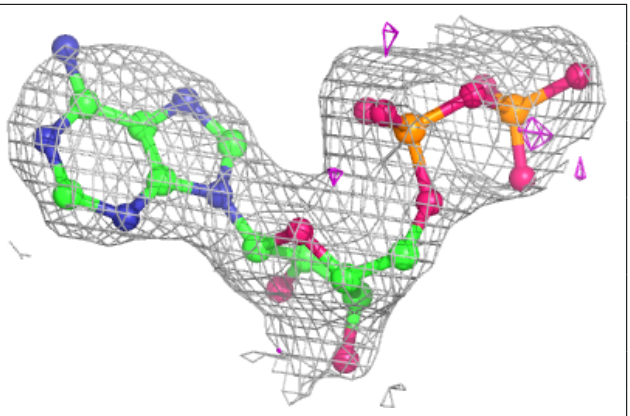
Electron density around ADP K 511:

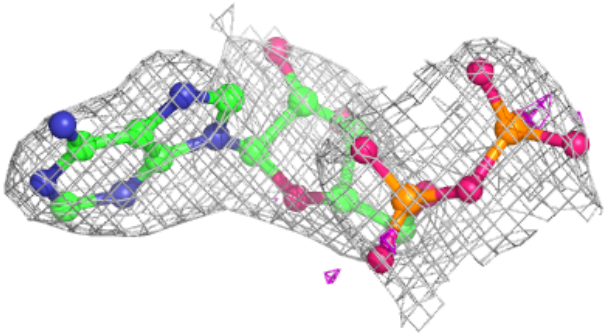
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

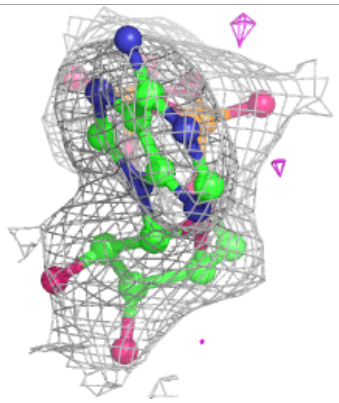


Electron density around ADP I 509:

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

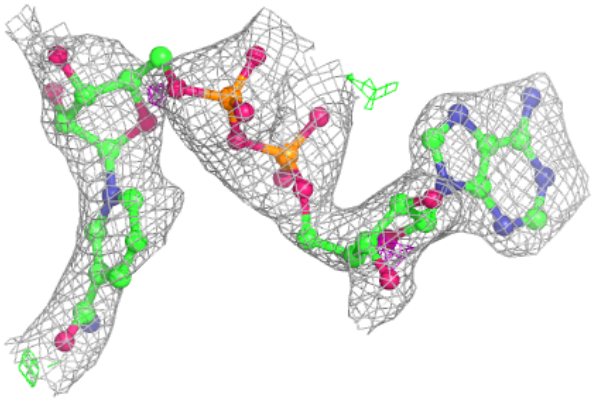


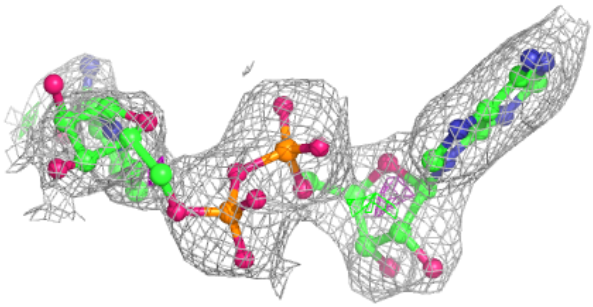


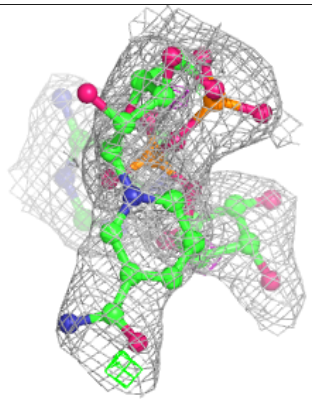


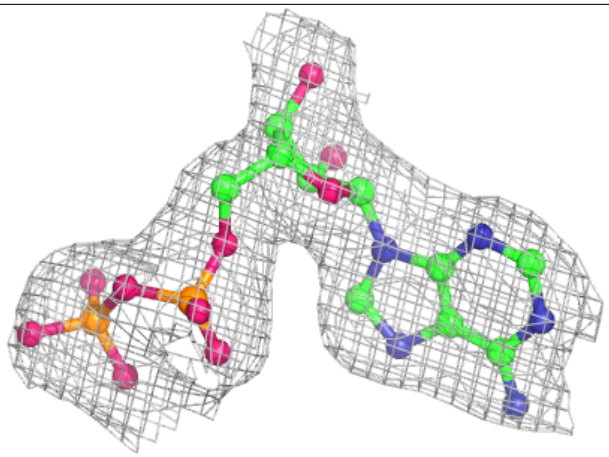
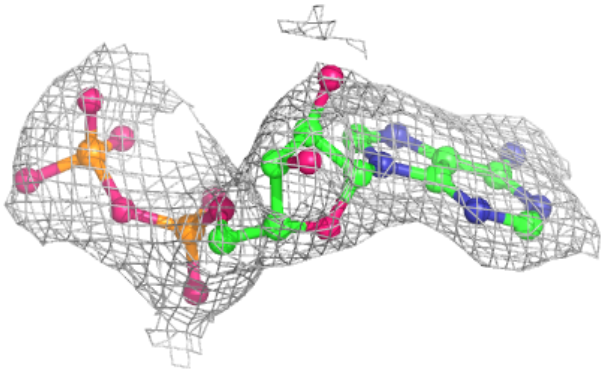
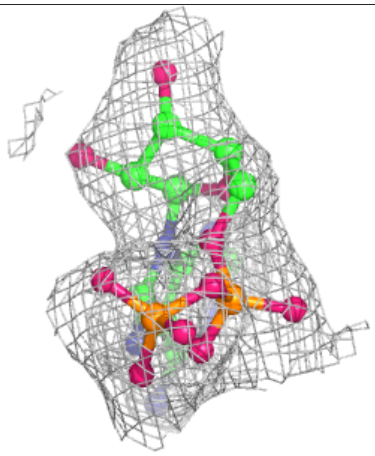
Electron density around NAD F 506:

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







Electron density around ADP E 505: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.