



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2014 – 03:30 AM EST

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

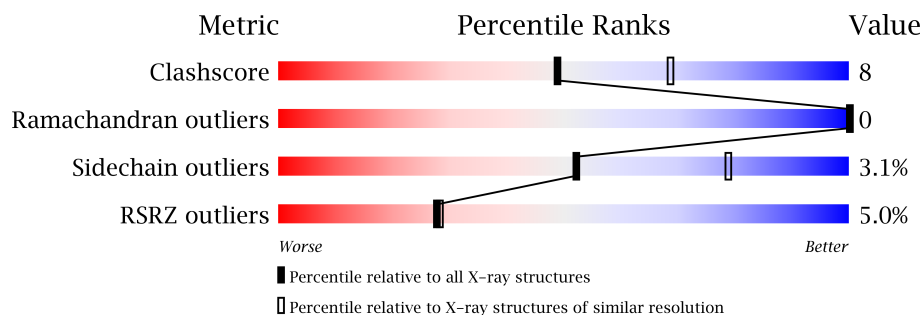
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	
1	C	500	
1	D	500	
1	E	500	
1	F	500	
1	G	500	
1	H	500	
1	I	500	
1	J	500	
1	K	500	
1	L	500	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NA	A	601	-	X
2	NA	B	5003	-	X
2	NA	C	5004	-	X
2	NA	C	603	-	X
2	NA	F	5007	-	X
2	NA	G	5008	-	X
3	ADP	D	504[A]	-	X
3	ADP	D	504[B]	-	X
5	EDO	A	901	-	X
5	EDO	B	701	-	X
5	EDO	B	802	-	X
5	EDO	B	902	-	X
5	EDO	C	903	-	X
5	EDO	E	705	-	X
5	EDO	E	805	-	X
5	EDO	E	905	-	X
5	EDO	F	706	-	X
5	EDO	F	707	-	X
5	EDO	G	907	-	X
5	EDO	I	809	-	X
5	EDO	L	712	-	X
5	EDO	L	912	-	X
6	GAI	D	905	-	X
6	GAI	E	906	-	X
6	GAI	E	907	-	X
6	GAI	G	5009	-	X
6	GAI	G	5010	-	X
6	GAI	H	909	-	X
6	GAI	I	910	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 48124 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Aldehyde dehydrogenase, mitochondrial precursor.

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

There are 12 discrepancies between the modelled and reference sequences:

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

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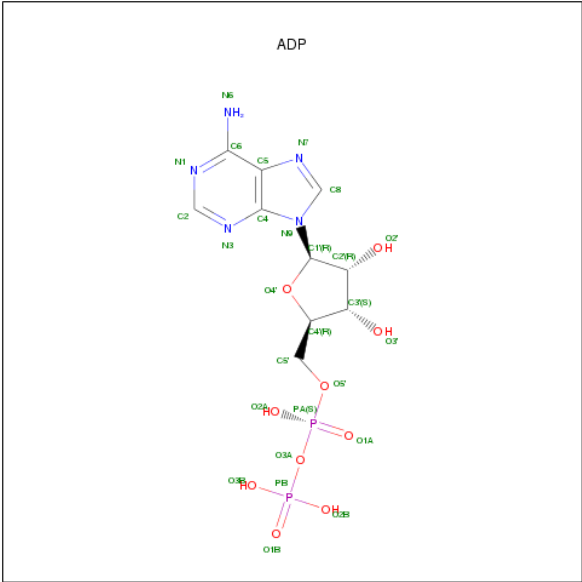
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Chain	Residue	Modelled	Actual	Comment	Reference
F	487	LYS	GLU	ENGINEERED	UNP P05091
G	487	LYS	GLU	ENGINEERED	UNP P05091
H	487	LYS	GLU	ENGINEERED	UNP P05091
I	487	LYS	GLU	ENGINEERED	UNP P05091
J	487	LYS	GLU	ENGINEERED	UNP P05091
K	487	LYS	GLU	ENGINEERED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

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

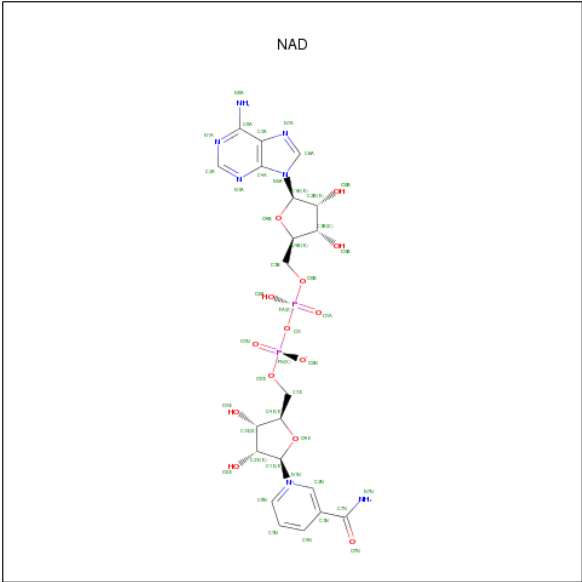
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Na 2 2	0	0
2	J	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	K	2	Total Na 2 2	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	2	Total Na 2 2	0	0
2	I	1	Total Na 1 1	0	0
2	C	2	Total Na 2 2	0	0
2	A	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0
2	F	2	Total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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



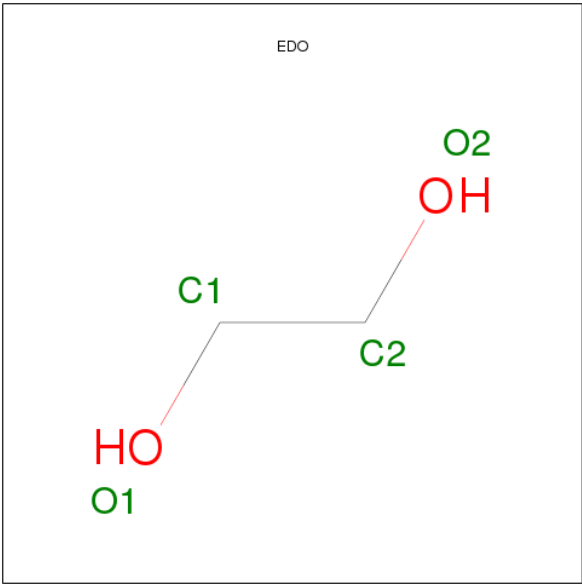
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	D	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



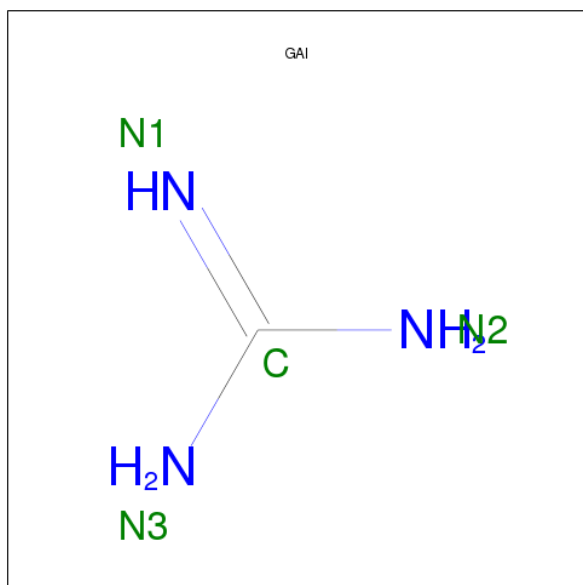
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	N	0	0
			4	1	3		

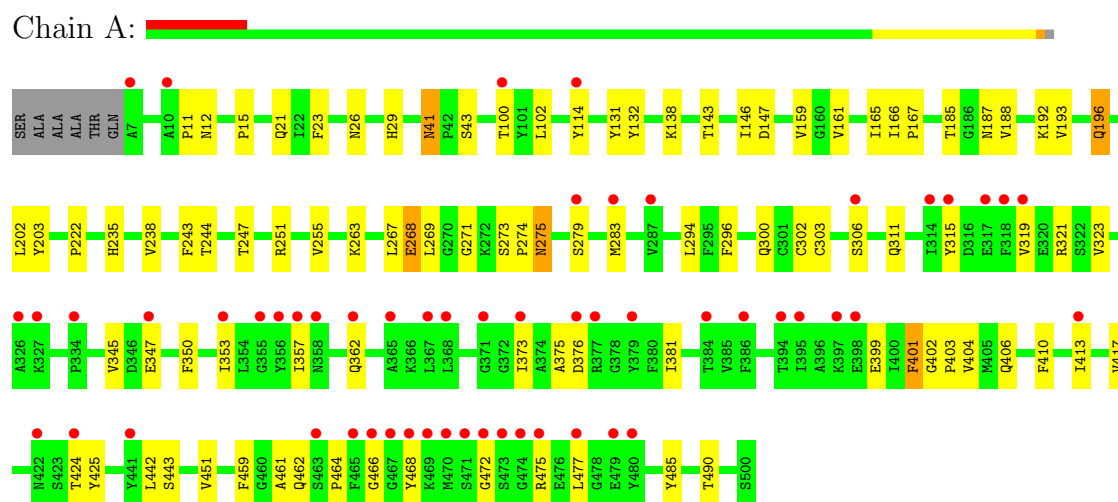
- Molecule 7 is water.

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

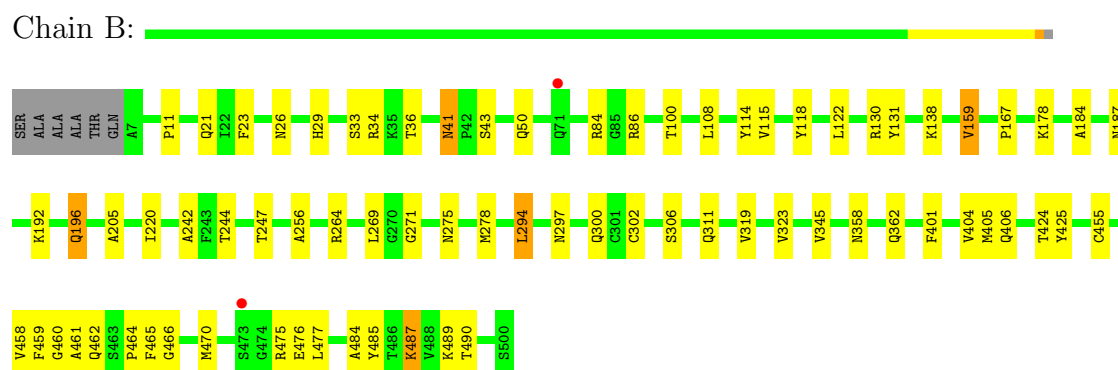
3 Residue-property plots

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

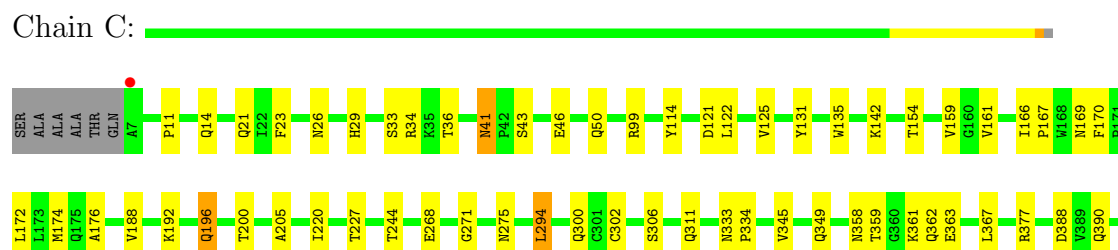
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



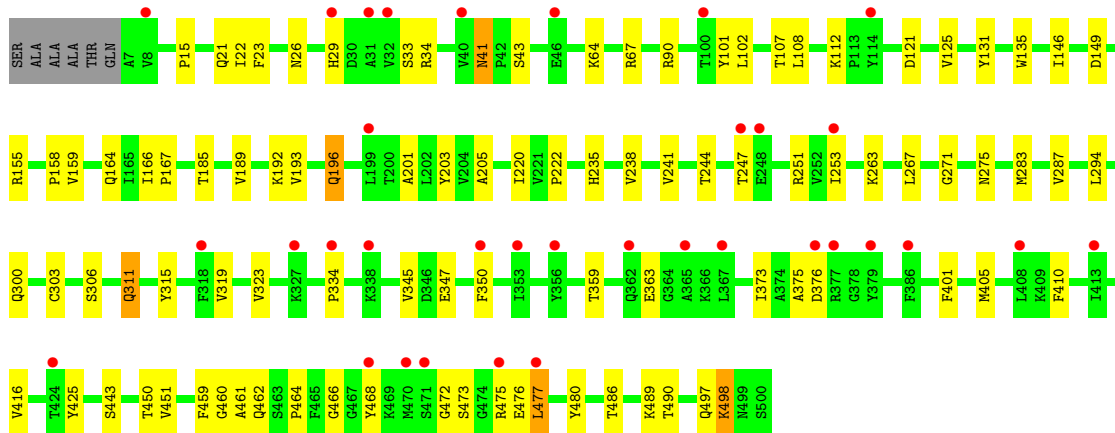
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor





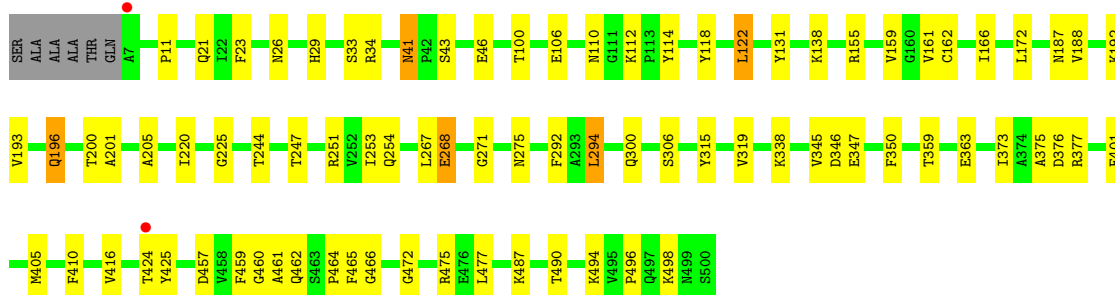
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain D:



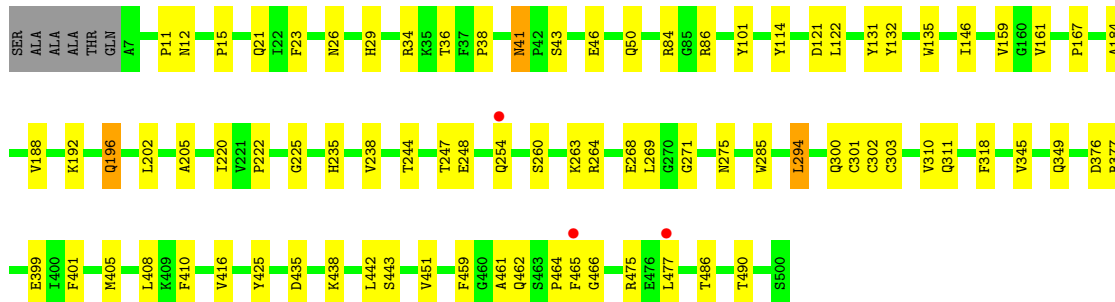
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain E:



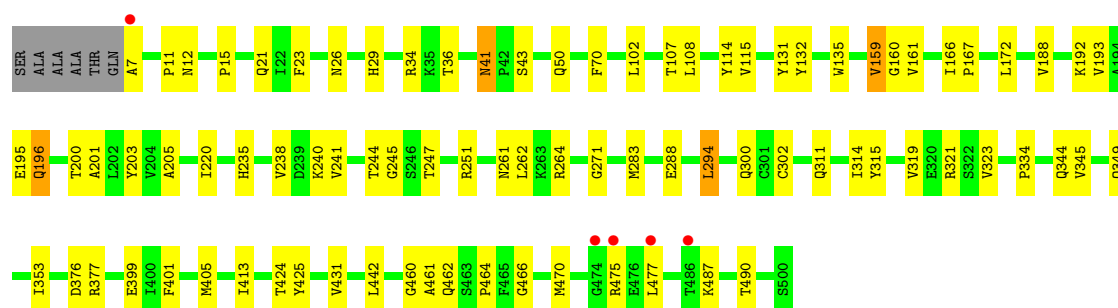
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain F:



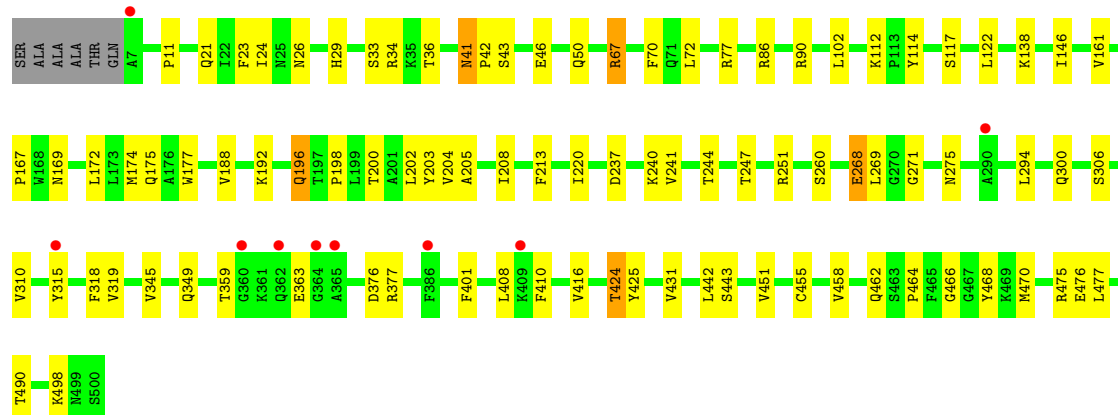
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain G:



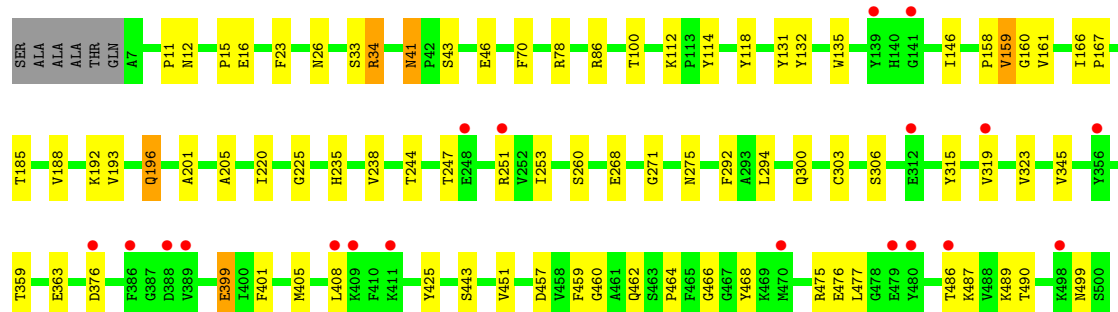
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain H:



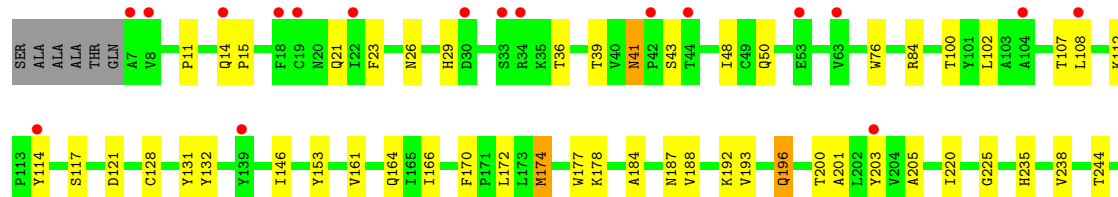
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

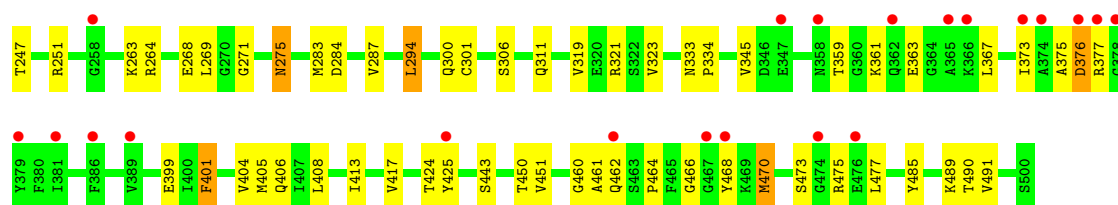
Chain I:



- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

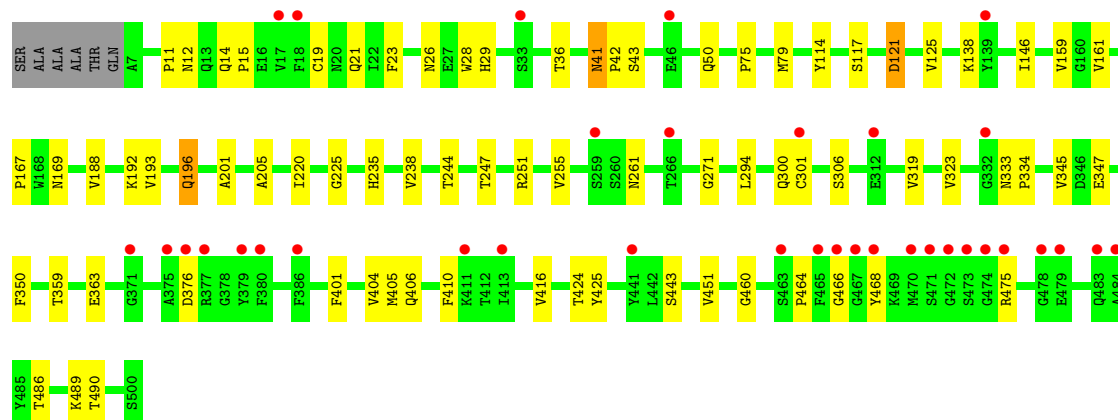
Chain J:





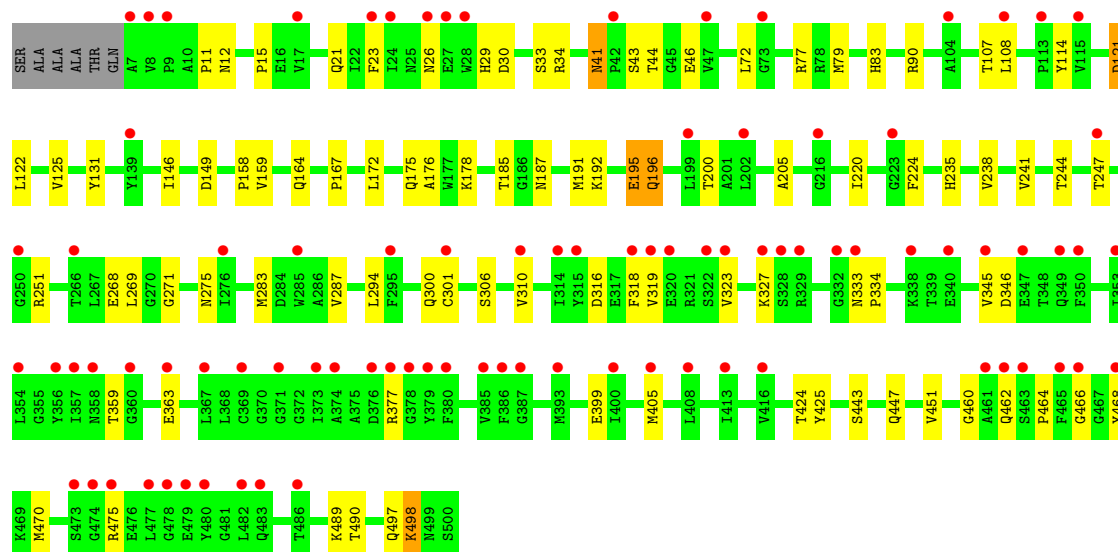
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain K:



- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.20Å 104.85Å 162.36Å 78.99° 82.14° 88.55°	Depositor
Resolution (Å)	44.01 – 2.50 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
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.271 0.250 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 207756 reflections	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 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GAI, ADP, NAD, 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(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	B	44	0	26	5	0
4	C	44	0	26	1	0
4	F	44	0	26	2	0
4	G	44	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	44	0	26	2	0
5	A	4	0	6	0	0
5	B	12	0	18	2	0
5	C	8	0	12	1	0
5	D	8	0	12	2	0
5	E	12	0	18	1	0
5	F	16	0	24	2	0
5	G	8	0	12	1	0
5	H	12	0	18	1	0
5	I	8	0	12	2	0
5	K	4	0	6	0	0
5	L	8	0	12	0	0
6	A	4	0	4	0	0
6	D	4	0	5	0	0
6	E	8	0	10	0	0
6	G	8	0	10	0	0
6	H	4	0	5	0	0
6	I	4	0	5	0	0
6	J	4	0	5	0	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (702) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	5: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	Distance(Å)	Clash(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:HE21	1:A:196:GLN:H	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:HE21	1:I:196:GLN:H	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:HD22	1:B:41:ASN:C	1.87	0.76
1:J:196:GLN:H	1:J:196:GLN:NE2	1.83	0.76
1:C:196:GLN:NE2	1:C:196:GLN:H	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	5: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	5:I:809:EDO:H11	1.71	0.72
1:J:196:GLN:N	1:J:196:GLN:HE21	1.87	0.71
1:L:196:GLN:H	1:L:196:GLN:HE21	1.38	0.71
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.72	0.71
1:C:205:ALA:HB2	1:C:220:ILE:HD12	1.72	0.71
1:H:41:ASN:C	1:H:41:ASN:HD22	1.94	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:NE2	1:A:196:GLN:H	1.82	0.69
1:G:196:GLN:H	1:G:196:GLN:HE21	1.40	0.69
1:E:100:THR:HG21	1:I:16:GLU:OE1	1.91	0.69
1:C:41:ASN:ND2	1:C:43:SER:H	1.90	0.69
1:G:349:GLN:NE2	4: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:NE2	1:L:196:GLN:H	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	5:D:704:EDO:O2	1.95	0.65
1:I:489:LYS:HB2	1:J:468:TYR:OH	1.96	0.65
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.79	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	4: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	4: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:HD22	1:K:41:ASN:C	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:NE2	1:I:196:GLN:H	1.95	0.57
1:L:247:THR:O	1:L:251:ARG:HG3	2.05	0.57
1:L:443:SER:HA	1:L:451:VAL:HG11	1.86	0.57
1:C:172:LEU:HD21	1:C:200:THR:HB	1.86	0.57
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.87	0.57
1: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:196:GLN:HE21	1:I:196:GLN:N	1.95	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:46:GLU:HB2	5:I:809:EDO:C1	2.35	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:NH1	1:L:34:ARG:HG3	2.20	0.56
4:H:508:NAD:H6N	4:H:508:NAD:O5D	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	5: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:349:GLN:HG3	7:F:1196:HOH:O	2.06	0.55
1:F:38:PRO:HD3	1:F:50:GLN:HE22	1.70	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	5:B:802:EDO:H12	1.90	0.54
1:F:443:SER:HA	1:F:451:VAL:HG11	1.90	0.54
1:F:41:ASN:ND2	1:F:43:SER:H	2.05	0.54
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.43	0.54
1:L:41:ASN:ND2	1:L:43:SER:H	2.05	0.54
1:D:319:VAL:O	1:D:323:VAL:HG23	2.07	0.54
1:F:46:GLU:HB2	5: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	4: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:N	1:D:196:GLN:HE21	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:H:21:GLN:HB3	1:H:29:HIS:O	2.09	0.53
1:G:251:ARG:NH1	1:H:260:SER:O	2.41	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:121:ASP:O	1:L:125:VAL:HG23	2.10	0.52
1:L:41:ASN:HD22	1:L:41:ASN:C	2.13	0.52
1:C:489:LYS:HB2	1:D:468:TYR:OH	2.09	0.52
1:E:196:GLN:HE21	1:E:196:GLN:N	1.94	0.52
1:H:67:ARG:HD2	1:H:237:ASP:OD2	2.10	0.52
1:I:70:PHE:CZ	1:I:160:GLY:HA2	2.44	0.52
1:C:302:CYS:SG	7:C:2137:HOH:O	2.59	0.52
1:H:41:ASN:HD21	1:H:43:SER:HB2	1.75	0.52
1:I:159:VAL:HA	1:I:487:LYS:HG3	1.90	0.52
1:A:12:ASN:O	1:A:15:PRO:HD3	2.10	0.52
1:A:146:ILE:HG13	1:B:460:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:K:23:PHE:CZ	1:K:26:ASN:HA	2.45	0.51
1:L:399:GLU:OE1	1:L:399:GLU:HA	2.10	0.51
1:I:499:ASN:HA	1:L:77:ARG:O	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:N	1:B:196:GLN:HE21	1.97	0.51
1:B:278:MET:HE3	7:B:1529:HOH:O	2.11	0.51
1:E:193:VAL:HG11	1:E:201:ALA:CB	2.41	0.51
1:E:41:ASN:C	1:E:41:ASN:ND2	2.61	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:HH11	1:I:34:ARG:HG3	1.75	0.51
1:J:41:ASN:ND2	1:J:43:SER:H	2.08	0.51
1:F:247:THR:HA	1:F:269:LEU:HD22	1.94	0.51
1:G:424:THR:HG22	1:G:470:MET:HB2	1.93	0.51
1:H:310:VAL:HG21	1:H:318:PHE:CD2	2.46	0.51
1:A: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:254:GLN:HE21	1:F:254:GLN:HE21	1.58	0.50
1:F:302:CYS:HB3	4:F:506:NAD:O7N	2.11	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:K:146:ILE:HG13	1:L:460:GLY:HA3	1.94	0.50
1:F:196:GLN:N	1:F:196:GLN:HE21	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:115:VAL:HG23	7:B:1146:HOH:O	2.12	0.50
1:B:100:THR:HG22	1:B:118:TYR:HE1	1.77	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:267:LEU:O	1:A:472:GLY:HA3	2.13	0.49
1:A:187:ASN:HD21	1:A:485:TYR:HB3	1.76	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
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:H	1:G:195:GLU:CD	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:294:LEU:HD12	1:E:306:SER:HA	1.94	0.48
1:F:377:ARG:HB2	7:F:2647:HOH:O	2.14	0.48
1:I:294:LEU:HD13	1:I:405:MET:HA	1.94	0.48
1:K:11:PRO:HB3	1:K:114:TYR:CZ	2.47	0.48
1:F:459:PHE:HE2	1:F:465:PHE:CE1	2.32	0.48
1:I:468:TYR:OH	1:J:489:LYS:HB2	2.12	0.48
1:J:41:ASN:HD22	1:J:41:ASN:C	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:121:ASP:O	1:C:125:VAL:HG23	2.14	0.48
1:C:36:THR:CB	1:C:50:GLN:HG3	2.43	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:ND2	1:G:41:ASN:C	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:L:149:ASP:HA	1:L:498:LYS:HB2	1.97	0.47
1:K:489:LYS:HB2	1:L:468:TYR:OH	2.13	0.47
1:B:300:GLN:HE22	1:B:345:VAL:N	1.96	0.47
1:C:131:TYR:CE1	1:C:462:GLN:HB3	2.49	0.47
1:G:464:PRO:HG2	1:H:490:THR:OG1	2.15	0.47
1:I:193:VAL:HG11	1:I:201:ALA:CB	2.45	0.47
1:D:238:VAL:O	1:D:263:LYS:HE3	2.13	0.47
1:F:301:CYS:HB2	7:F:2754:HOH:O	2.14	0.47
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.95	0.47
1:J:461:ALA:HA	1:J:477:LEU:HD22	1.96	0.47
1:A:247:THR:HG23	1:A:269:LEU:HD13	1.97	0.47
1:A:283:MET:CG	1:A:321:ARG:NH1	2.78	0.47
1:G:41:ASN:HD21	1:G:43:SER:HB2	1.78	0.47
1:B:297:ASN:HA	7:B:1057:HOH:O	2.14	0.47
1:C:159:VAL:HA	1:C:487:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:302:CYS:HB3	4:C:503:NAD:O7N	2.13	0.47
1:F:435:ASP:HB3	1:F:438:LYS:HD2	1.97	0.47
1:G:349:GLN:O	1:G:353:ILE:HG13	2.14	0.47
1:J:164:GLN:CD	1:J:178:LYS:HB3	2.35	0.47
1:J:132:TYR:OH	1:J:477:LEU:HA	2.14	0.47
1:G:302:CYS:HB3	4: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: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:I:33:SER:O	1:I:34:ARG:HB2	2.15	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	4: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:N	1:H:408:LEU:HD12	2.30	0.46
1:E:292:PHE:HE1	1:E:457:ASP:HB2	1.79	0.46
1:E:253:ILE:HD11	3:E:505:ADP:C2	2.50	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:319:VAL:O	1:G:323:VAL:HG23	2.15	0.46
1:G:271:GLY:HA2	1:G:425:TYR:CD2	2.50	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
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:107:THR:HG23	1:G:334:PRO:HB2	1.98	0.45
1:G:36:THR:CB	1:G:50:GLN:HG3	2.45	0.45
1:I:292:PHE:HE1	1:I:457:ASP:HB2	1.81	0.45
1:J:301:CYS:C	1:J:401:PHE:HE1	2.20	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:84:ARG:NH1	1:J:184:ALA:O	2.50	0.45
1:L:15:PRO:HG2	1:L:108:LEU:HD22	1.99	0.45
1:L:316:ASP:N	7:L:2214:HOH:O	2.49	0.45
1:B:178:LYS:HE3	1:B:242:ALA:HB1	1.97	0.45
1:L:247:THR:HA	1:L:269:LEU:HD13	1.98	0.45
1:B:264:ARG:NH1	1:B:484:ALA:O	2.50	0.45
1:E:338:LYS:HD2	1:I:34:ARG:NH2	2.21	0.45
1:K:12:ASN:O	1:K:15:PRO:HD3	2.17	0.45
1:A:353:ILE:O	1:A:357:ILE:HG13	2.16	0.45
1: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	4: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	4:B:502:NAD:H5N	1.99	0.44
1:D:102:LEU:HD21	1:D:203:TYR:HD2	1.81	0.44
1:D:22:ILE:HG12	1:D:222:PRO:HD2	1.99	0.44
1:E:498:LYS:HE2	1:E:498:LYS:HB3	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:46:GLU:HG3	7:C:2480:HOH:O	2.17	0.44
1:G:159:VAL:CG2	1:G:264:ARG:HH11	2.31	0.44
1:G:167:PRO:HD3	1:G:244:THR:HB	1.99	0.44
1:I:100:THR:HG22	1:I:118:TYR:HE1	1.83	0.44
1:J:102:LEU:HD21	1:J:203:TYR:CD2	2.51	0.44
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.53	0.43
1:C:170:PHE:O	1:C:174:MET:HG2	2.17	0.43
1:C:41:ASN:C	1:C:41:ASN:ND2	2.66	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	5: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:N	1:H:169:ASN:OD1	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:167:PRO:HD3	1:L:244:THR:HB	2.00	0.43
1:I:78:ARG:NH1	1:L:497:GLN:NE2	2.62	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	5: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
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:ND2	1:H:41:ASN:C	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:377:ARG:NH1	7:E:1554:HOH:O	2.51	0.42
1:E:254:GLN:HE21	1:F:254:GLN:NE2	2.17	0.42
1:A:167:PRO:HD3	1:A:244:THR:HB	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:443:SER:HA	1:H:451:VAL:HG11	2.01	0.42
1:H:70:PHE:CD1	1:H:77:ARG:HD3	2.55	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:F:101:TYR:CG	5:F:906:EDO:H11	2.54	0.42
1:E:138:LYS:HE3	1:G:135:TRP:CD1	2.55	0.42
1:B:108:LEU:HD11	5: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:347:GLU:O	1:K:350:PHE:HB3	2.19	0.41
1:K:75:PRO:O	1:K:79:MET:HB2	2.20	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
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:N	1:I:462:GLN:OE1	2.50	0.41
1:K:193:VAL:HG11	1:K:201:ALA:CB	2.50	0.41
1:K:167:PRO:HD3	1:K:244:THR:HB	2.01	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:167:PRO:HD3	1:C:244:THR:HB	2.02	0.41
1:C:154:THR:HA	1:C:489:LYS:O	2.20	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:359:THR:O	1:J:363:GLU:HG3	2.20	0.41
1:J:39:THR:HG23	1:J:48:ILE:HB	2.01	0.41
1:K:19:CYS:HB3	1:K:28:TRP:CH2	2.56	0.41
1:B:187:ASN:HD21	1:B:485:TYR:HB3	1.86	0.41
1:B:33:SER:O	1:B:34:ARG:HB2	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:C:358:ASN:O	1:C:362:GLN:HG2	2.21	0.41
1:H:42:PRO:HB3	1:H:345:VAL:O	2.21	0.41
1:I:294:LEU:HD22	1:I:405:MET:HB2	2.02	0.41
1:L:333:ASN:HA	1:L:334:PRO:HD2	1.91	0.41
1:A: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:HE2	1:H:112:LYS:HB3	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:HE2	1:L:498:LYS:HB3	1.87	0.40
1:E:100:THR:HG23	7:E:1808:HOH:O	2.21	0.40
1:F:442:LEU:HA	1:F:442:LEU:HD23	1.96	0.40
1:G:245:GLY:HA2	4:G:507:NAD:C4N	2.51	0.40
1:I:196:GLN:NE2	1:I:196:GLN:N	2.63	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:303:CYS:SG	1:I:459:PHE:HZ	2.43	0.40
1:J:166:ILE:HD11	1:J:193:VAL:HG12	2.04	0.40
1:J:128:CYS:SG	1:J:177:TRP:HD1	2.44	0.40
1:L:164:GLN:OE1	1:L:178:LYS:HB3	2.21	0.40
1:L:79:MET:SD	1:L:83:HIS:HD2	2.44	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	4: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
1:J:376:ASP:N	1:J:376:ASP:OD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	56	82
1	B	399/402 (99%)	389 (98%)	10 (2%)	60	85
1	C	399/402 (99%)	391 (98%)	8 (2%)	68	89
1	D	399/402 (99%)	384 (96%)	15 (4%)	44	71
1	E	399/402 (99%)	388 (97%)	11 (3%)	56	82
1	F	399/402 (99%)	384 (96%)	15 (4%)	44	71
1	G	399/402 (99%)	390 (98%)	9 (2%)	63	87
1	H	399/402 (99%)	383 (96%)	16 (4%)	42	68
1	I	399/402 (99%)	389 (98%)	10 (2%)	60	85
1	J	399/402 (99%)	384 (96%)	15 (4%)	44	71
1	K	399/402 (99%)	388 (97%)	11 (3%)	56	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	399/402 (99%)	383 (96%)	16 (4%)	42 68
All	All	4788/4824 (99%)	4641 (97%)	147 (3%)	52 79

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

Some 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	501[A]	-	29,29,29	1.87	7 (24%)	45,45,45	2.18	10 (22%)
3	ADP	A	501[B]	-	29,29,29	1.62	8 (27%)	45,45,45	1.94	7 (15%)
5	EDO	A	901	-	3,3,3	0.58	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAI	A	902	-	3,3,3	1.50	1 (33%)	3,3,3	1.46	1 (33%)
4	NAD	B	502	-	48,48,48	2.05	11 (22%)	73,73,73	2.00	17 (23%)
5	EDO	B	701	-	3,3,3	0.48	0	2,2,2	0.44	0
5	EDO	B	802	-	3,3,3	0.45	0	2,2,2	0.54	0
5	EDO	B	902	-	3,3,3	0.34	0	2,2,2	0.51	0
4	NAD	C	503	-	48,48,48	2.00	9 (18%)	73,73,73	2.11	21 (28%)
5	EDO	C	803	-	3,3,3	0.50	0	2,2,2	0.38	0
5	EDO	C	903	-	3,3,3	0.68	0	2,2,2	0.39	0
3	ADP	D	504[A]	-	29,29,29	1.83	7 (24%)	45,45,45	1.99	10 (22%)
3	ADP	D	504[B]	-	29,29,29	1.53	5 (17%)	45,45,45	1.67	7 (15%)
5	EDO	D	704	-	3,3,3	0.64	0	2,2,2	0.34	0
5	EDO	D	904	-	3,3,3	0.46	0	2,2,2	0.43	0
6	GAI	D	905	-	3,3,3	1.60	1 (33%)	3,3,3	1.50	1 (33%)
3	ADP	E	505	-	29,29,29	1.68	7 (24%)	45,45,45	2.12	9 (20%)
5	EDO	E	705	-	3,3,3	0.61	0	2,2,2	0.32	0
5	EDO	E	805	-	3,3,3	0.69	0	2,2,2	0.25	0
5	EDO	E	905	-	3,3,3	0.17	0	2,2,2	0.63	0
6	GAI	E	906	-	3,3,3	1.42	1 (33%)	3,3,3	1.55	1 (33%)
6	GAI	E	907	-	3,3,3	1.60	1 (33%)	3,3,3	1.63	1 (33%)
4	NAD	F	506	-	48,48,48	2.17	11 (22%)	73,73,73	1.90	14 (19%)
5	EDO	F	706	-	3,3,3	0.47	0	2,2,2	0.45	0
5	EDO	F	707	-	3,3,3	0.80	0	2,2,2	0.19	0
5	EDO	F	806	-	3,3,3	0.49	0	2,2,2	0.39	0
5	EDO	F	906	-	3,3,3	0.45	0	2,2,2	0.44	0
6	GAI	G	5009	-	3,3,3	1.44	1 (33%)	3,3,3	1.38	1 (33%)
6	GAI	G	5010	-	3,3,3	1.59	1 (33%)	3,3,3	1.43	1 (33%)
4	NAD	G	507	-	48,48,48	2.25	13 (27%)	73,73,73	1.66	15 (20%)
5	EDO	G	807	-	3,3,3	0.64	0	2,2,2	0.27	0
5	EDO	G	907	-	3,3,3	0.41	0	2,2,2	0.50	0
4	NAD	H	508	-	48,48,48	2.19	14 (29%)	73,73,73	1.93	16 (21%)
5	EDO	H	708	-	3,3,3	0.51	0	2,2,2	0.36	0
5	EDO	H	808	-	3,3,3	0.72	0	2,2,2	0.27	0
5	EDO	H	908	-	3,3,3	0.47	0	2,2,2	0.43	0
6	GAI	H	909	-	3,3,3	1.45	1 (33%)	3,3,3	1.40	1 (33%)
3	ADP	I	509	-	29,29,29	1.67	7 (24%)	45,45,45	2.25	10 (22%)
5	EDO	I	809	-	3,3,3	0.71	0	2,2,2	0.21	0
5	EDO	I	909	-	3,3,3	0.44	0	2,2,2	0.43	0
6	GAI	I	910	-	3,3,3	1.58	1 (33%)	3,3,3	1.25	0
3	ADP	J	510	-	29,29,29	1.85	7 (24%)	45,45,45	1.78	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAI	J	611	-	3,3,3	1.41	1 (33%)	3,3,3	1.46	1 (33%)
3	ADP	K	511	-	29,29,29	1.62	6 (20%)	45,45,45	1.81	9 (20%)
5	EDO	K	911	-	3,3,3	0.66	0	2,2,2	0.32	0
3	ADP	L	512	-	29,29,29	1.59	5 (17%)	45,45,45	1.86	8 (17%)
5	EDO	L	712	-	3,3,3	0.60	0	2,2,2	0.33	0
5	EDO	L	912	-	3,3,3	0.48	0	2,2,2	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	501[A]	-	-	0/16/32/32	0/3/3/3
3	ADP	A	501[B]	-	-	0/16/32/32	0/3/3/3
5	EDO	A	901	-	-	0/1/1/1	0/0/0/0
6	GAI	A	902	-	-	0/0/0/0	0/0/0/0
4	NAD	B	502	-	-	0/30/62/62	0/5/5/5
5	EDO	B	701	-	-	0/1/1/1	0/0/0/0
5	EDO	B	802	-	-	0/1/1/1	0/0/0/0
5	EDO	B	902	-	-	0/1/1/1	0/0/0/0
4	NAD	C	503	-	-	0/30/62/62	0/5/5/5
5	EDO	C	803	-	-	0/1/1/1	0/0/0/0
5	EDO	C	903	-	-	0/1/1/1	0/0/0/0
3	ADP	D	504[A]	-	-	0/16/32/32	0/3/3/3
3	ADP	D	504[B]	-	-	0/16/32/32	0/3/3/3
5	EDO	D	704	-	-	0/1/1/1	0/0/0/0
5	EDO	D	904	-	-	0/1/1/1	0/0/0/0
6	GAI	D	905	-	-	0/0/0/0	0/0/0/0
3	ADP	E	505	-	-	0/16/32/32	0/3/3/3
5	EDO	E	705	-	-	0/1/1/1	0/0/0/0
5	EDO	E	805	-	-	0/1/1/1	0/0/0/0
5	EDO	E	905	-	-	0/1/1/1	0/0/0/0
6	GAI	E	906	-	-	0/0/0/0	0/0/0/0
6	GAI	E	907	-	-	0/0/0/0	0/0/0/0
4	NAD	F	506	-	-	0/30/62/62	0/5/5/5
5	EDO	F	706	-	-	0/1/1/1	0/0/0/0
5	EDO	F	707	-	-	0/1/1/1	0/0/0/0
5	EDO	F	806	-	-	0/1/1/1	0/0/0/0
5	EDO	F	906	-	-	0/1/1/1	0/0/0/0
6	GAI	G	5009	-	-	0/0/0/0	0/0/0/0
6	GAI	G	5010	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	G	507	-	-	0/30/62/62	0/5/5/5
5	EDO	G	807	-	-	0/1/1/1	0/0/0/0
5	EDO	G	907	-	-	0/1/1/1	0/0/0/0
4	NAD	H	508	-	-	0/30/62/62	0/5/5/5
5	EDO	H	708	-	-	0/1/1/1	0/0/0/0
5	EDO	H	808	-	-	0/1/1/1	0/0/0/0
5	EDO	H	908	-	-	0/1/1/1	0/0/0/0
6	GAI	H	909	-	-	0/0/0/0	0/0/0/0
3	ADP	I	509	-	-	0/16/32/32	0/3/3/3
5	EDO	I	809	-	-	0/1/1/1	0/0/0/0
5	EDO	I	909	-	-	0/1/1/1	0/0/0/0
6	GAI	I	910	-	-	0/0/0/0	0/0/0/0
3	ADP	J	510	-	-	0/16/32/32	0/3/3/3
6	GAI	J	611	-	-	0/0/0/0	0/0/0/0
3	ADP	K	511	-	-	0/16/32/32	0/3/3/3
5	EDO	K	911	-	-	0/1/1/1	0/0/0/0
3	ADP	L	512	-	-	0/16/32/32	0/3/3/3
5	EDO	L	712	-	-	0/1/1/1	0/0/0/0
5	EDO	L	912	-	-	0/1/1/1	0/0/0/0

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	507	NAD	C3N-C7N	-10.94	1.32	1.50
4	H	508	NAD	C3N-C7N	-9.58	1.34	1.50
4	B	502	NAD	C3N-C7N	-9.25	1.35	1.50
4	F	506	NAD	C3N-C7N	-8.87	1.36	1.50
4	C	503	NAD	C3N-C7N	-8.63	1.36	1.50
4	C	503	NAD	C2A-N3A	5.04	1.41	1.32
4	F	506	NAD	PN-O3	4.74	1.70	1.60
4	F	506	NAD	C2A-N3A	4.64	1.40	1.32
3	A	501[A]	ADP	C2-N3	4.61	1.40	1.32
4	B	502	NAD	C2A-N3A	4.47	1.40	1.32
3	D	504[A]	ADP	C2-N3	4.46	1.40	1.32
3	L	512	ADP	C2-N3	4.39	1.39	1.32
3	D	504[A]	ADP	PB-O3B	4.35	1.70	1.54
3	I	509	ADP	C2-N3	4.35	1.39	1.32
3	A	501[B]	ADP	C2-N3	4.29	1.39	1.32
3	J	510	ADP	C2-N3	4.26	1.39	1.32
3	K	511	ADP	C2-N3	4.17	1.39	1.32
3	D	504[B]	ADP	C2-N3	4.16	1.39	1.32
4	H	508	NAD	O4D-C1D	4.14	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	510	ADP	PA-O3A	4.09	1.67	1.59
4	G	507	NAD	C2A-N3A	3.98	1.39	1.32
4	F	506	NAD	PA-O3	3.97	1.66	1.59
4	B	502	NAD	PN-O3	3.92	1.68	1.60
3	J	510	ADP	PB-O3A	3.81	1.66	1.60
3	A	501[A]	ADP	PB-O3A	3.71	1.66	1.60
3	D	504[A]	ADP	PB-O3A	3.61	1.66	1.60
3	A	501[A]	ADP	C2-N1	3.56	1.40	1.33
4	C	503	NAD	O4D-C1D	3.50	1.45	1.41
3	E	505	ADP	PB-O3A	3.37	1.65	1.60
4	G	507	NAD	C5N-C4N	-3.37	1.32	1.38
4	C	503	NAD	C2A-N1A	3.37	1.40	1.33
4	C	503	NAD	C4A-N3A	3.37	1.40	1.35
4	F	506	NAD	O4D-C1D	3.36	1.45	1.41
4	G	507	NAD	O4D-C1D	3.35	1.45	1.41
4	H	508	NAD	C4N-C3N	-3.34	1.33	1.39
3	D	504[A]	ADP	C2-N1	3.32	1.40	1.33
3	E	505	ADP	C2-N3	3.31	1.38	1.32
3	A	501[B]	ADP	C2-N1	3.29	1.40	1.33
4	H	508	NAD	C5N-C4N	-3.28	1.32	1.38
4	B	502	NAD	PA-O3	3.28	1.65	1.59
3	E	505	ADP	C8-N9	3.27	1.41	1.36
3	A	501[A]	ADP	C4-N3	3.24	1.40	1.35
4	H	508	NAD	C2A-N3A	3.22	1.37	1.32
3	I	509	ADP	PB-O3B	3.21	1.66	1.54
3	I	509	ADP	C2-N1	3.19	1.40	1.33
4	G	507	NAD	C2A-N1A	3.18	1.40	1.33
3	E	505	ADP	C8-N7	3.16	1.40	1.34
3	J	510	ADP	C2-N1	3.14	1.40	1.33
3	K	511	ADP	C8-N7	3.12	1.40	1.34
4	H	508	NAD	C2N-C3N	-3.10	1.34	1.39
3	L	512	ADP	C2-N1	3.10	1.40	1.33
3	L	512	ADP	C8-N7	3.09	1.40	1.34
4	H	508	NAD	C2N-N1N	-3.05	1.31	1.35
4	G	507	NAD	C4N-C3N	-3.05	1.34	1.39
3	A	501[A]	ADP	C8-N7	3.04	1.40	1.34
3	K	511	ADP	C2-N1	3.02	1.39	1.33
4	F	506	NAD	C8A-N7A	3.01	1.40	1.34
3	I	509	ADP	C8-N7	2.99	1.40	1.34
4	H	508	NAD	O4B-C1B	2.99	1.45	1.41
3	E	505	ADP	PB-O3B	2.97	1.65	1.54
3	D	504[B]	ADP	C2-N1	2.95	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	506	NAD	O4B-C1B	2.91	1.44	1.41
4	H	508	NAD	C8A-N7A	2.89	1.40	1.34
4	B	502	NAD	C2A-N1A	2.86	1.39	1.33
4	B	502	NAD	O4D-C1D	2.85	1.44	1.41
4	B	502	NAD	C4N-C3N	-2.84	1.34	1.39
3	J	510	ADP	C8-N7	2.84	1.40	1.34
3	K	511	ADP	PB-O3B	2.83	1.65	1.54
3	E	505	ADP	C2-N1	2.83	1.39	1.33
4	F	506	NAD	C5N-C4N	-2.82	1.33	1.38
3	L	512	ADP	PB-O3B	2.80	1.64	1.54
3	D	504[A]	ADP	C8-N7	2.78	1.39	1.34
4	G	507	NAD	PN-O3	2.74	1.66	1.60
4	F	506	NAD	C4N-C3N	-2.74	1.34	1.39
4	C	503	NAD	C8A-N7A	2.71	1.39	1.34
3	A	501[B]	ADP	C8-N7	2.69	1.39	1.34
3	A	501[A]	ADP	PB-O3B	2.69	1.64	1.54
6	I	910	GAI	C-N1	2.65	1.36	1.30
3	D	504[B]	ADP	C8-N7	2.64	1.39	1.34
4	G	507	NAD	C8A-N7A	2.63	1.39	1.34
3	A	501[A]	ADP	C8-N9	2.62	1.40	1.36
3	A	501[B]	ADP	PB-O3A	-2.61	1.55	1.60
3	I	509	ADP	PB-O3A	2.61	1.64	1.60
4	C	503	NAD	C5N-C4N	-2.61	1.33	1.38
6	D	905	GAI	C-N1	2.59	1.36	1.30
3	J	510	ADP	C4-N3	2.59	1.39	1.35
4	H	508	NAD	C2A-N1A	2.58	1.39	1.33
3	K	511	ADP	C8-N9	2.57	1.40	1.36
3	E	505	ADP	PA-O3A	2.57	1.64	1.59
3	D	504[B]	ADP	PB-O2B	-2.56	1.45	1.54
4	B	502	NAD	C2N-C3N	-2.55	1.35	1.39
4	H	508	NAD	PN-O3	2.54	1.65	1.60
4	F	506	NAD	C4A-N3A	2.51	1.39	1.35
4	F	506	NAD	C2A-N1A	2.48	1.38	1.33
4	B	502	NAD	C8A-N7A	2.47	1.39	1.34
3	J	510	ADP	C8-N9	2.47	1.40	1.36
6	G	5010	GAI	C-N1	2.46	1.35	1.30
3	I	509	ADP	C8-N9	2.44	1.40	1.36
4	B	502	NAD	C2N-N1N	-2.43	1.32	1.35
6	E	907	GAI	C-N1	2.42	1.35	1.30
3	D	504[A]	ADP	C8-N9	2.42	1.40	1.36
3	D	504[A]	ADP	C4-N3	2.39	1.39	1.35
6	J	611	GAI	C-N1	2.38	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	507	NAD	C2N-C3N	-2.37	1.35	1.39
4	G	507	NAD	PA-O3	2.37	1.64	1.59
6	H	909	GAI	C-N1	2.35	1.35	1.30
6	G	5009	GAI	C-N1	2.34	1.35	1.30
6	E	906	GAI	C-N1	2.33	1.35	1.30
3	A	501[B]	ADP	C4-N3	2.32	1.39	1.35
4	C	503	NAD	C4N-C3N	-2.31	1.35	1.39
4	H	508	NAD	C8A-N9A	2.30	1.40	1.36
3	A	501[B]	ADP	PB-O2B	-2.27	1.46	1.54
4	B	502	NAD	C8A-N9A	2.26	1.40	1.36
4	H	508	NAD	PN-O5D	2.20	1.66	1.59
6	A	902	GAI	C-N1	2.18	1.35	1.30
4	G	507	NAD	C8A-N9A	2.16	1.40	1.36
3	L	512	ADP	PB-O3A	2.16	1.63	1.60
3	D	504[B]	ADP	PA-O2A	-2.16	1.45	1.55
4	G	507	NAD	C2N-N1N	-2.11	1.32	1.35
3	I	509	ADP	C4-N3	2.10	1.38	1.35
3	K	511	ADP	PB-O3A	2.09	1.63	1.60
4	C	503	NAD	C8A-N9A	2.07	1.39	1.36
3	A	501[B]	ADP	PA-O2A	-2.06	1.46	1.55
4	G	507	NAD	C4A-N3A	2.05	1.38	1.35
4	H	508	NAD	C2D-C1D	2.02	1.56	1.53
3	A	501[B]	ADP	C8-N9	2.01	1.39	1.36

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	505	ADP	N3-C2-N1	-9.51	120.52	128.89
3	A	501[B]	ADP	N3-C2-N1	-8.22	121.66	128.89
4	H	508	NAD	N3A-C2A-N1A	-8.22	121.66	128.89
3	I	509	ADP	O4'-C1'-C2'	-8.19	94.77	106.69
4	B	502	NAD	O4B-C1B-C2B	-8.19	94.77	106.69
3	D	504[A]	ADP	N3-C2-N1	-7.91	121.93	128.89
3	J	510	ADP	N3-C2-N1	-7.17	122.59	128.89
3	A	501[A]	ADP	O4'-C1'-C2'	-7.00	96.51	106.69
4	C	503	NAD	N3A-C2A-N1A	-6.78	122.92	128.89
3	A	501[A]	ADP	N3-C2-N1	-6.66	123.03	128.89
4	G	507	NAD	N3A-C2A-N1A	-6.57	123.11	128.89
4	F	506	NAD	N3A-C2A-N1A	-6.54	123.14	128.89
3	L	512	ADP	N3-C2-N1	-6.26	123.38	128.89
3	K	511	ADP	N3-C2-N1	-6.22	123.42	128.89
4	B	502	NAD	N3A-C2A-N1A	-5.94	123.66	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	NAD	C8A-N9A-C4A	-5.86	102.19	106.96
3	I	509	ADP	N3-C2-N1	-5.65	123.92	128.89
3	A	501[A]	ADP	C4'-O4'-C1'	-5.55	103.62	109.72
3	D	504[B]	ADP	N3-C2-N1	-5.54	124.02	128.89
3	I	509	ADP	C8-N9-C4	-5.50	102.49	106.96
4	B	502	NAD	C8A-N9A-C4A	-5.47	102.51	106.96
3	A	501[B]	ADP	C8-N9-C4	-5.42	102.55	106.96
4	H	508	NAD	C8A-N9A-C4A	-5.34	102.62	106.96
3	J	510	ADP	C8-N9-C4	-4.94	102.94	106.96
4	C	503	NAD	O4B-C1B-C2B	-4.89	99.57	106.69
4	F	506	NAD	C8A-N9A-C4A	-4.85	103.01	106.96
4	C	503	NAD	O7N-C7N-N7N	-4.69	115.89	122.59
3	K	511	ADP	C2'-C3'-C4'	-4.69	93.28	102.64
3	D	504[B]	ADP	O4'-C1'-C2'	-4.63	99.95	106.69
3	L	512	ADP	C8-N9-C1'	4.56	134.74	126.15
3	L	512	ADP	C8-N9-C4	-4.54	103.26	106.96
3	E	505	ADP	C8-N9-C4	-4.51	103.29	106.96
3	I	509	ADP	PA-O3A-PB	-4.49	119.50	131.93
4	G	507	NAD	C8A-N9A-C4A	-4.47	103.32	106.96
3	K	511	ADP	C8-N9-C4	-4.45	103.34	106.96
3	I	509	ADP	C3'-C2'-C1'	4.42	107.86	100.92
3	D	504[A]	ADP	PA-O3A-PB	-4.39	119.76	131.93
3	A	501[A]	ADP	PA-O3A-PB	-4.34	119.91	131.93
3	E	505	ADP	O4'-C1'-C2'	-4.33	100.39	106.69
4	F	506	NAD	O4B-C1B-C2B	-4.27	100.47	106.69
3	L	512	ADP	PA-O3A-PB	-4.25	120.16	131.93
3	D	504[B]	ADP	C8-N9-C4	-4.22	103.53	106.96
4	G	507	NAD	C2N-C3N-C4N	4.10	122.91	118.31
4	H	508	NAD	C5A-C4A-N3A	-4.06	122.03	125.98
4	C	503	NAD	O4D-C4D-C3D	-3.95	97.12	105.16
4	F	506	NAD	C3B-C2B-C1B	3.95	107.11	100.92
4	H	508	NAD	O4B-C1B-C2B	-3.94	100.95	106.69
3	D	504[A]	ADP	C8-N9-C4	-3.94	103.76	106.96
4	F	506	NAD	C2B-C3B-C4B	-3.84	94.97	102.64
3	D	504[A]	ADP	O4'-C1'-C2'	-3.83	101.12	106.69
4	C	503	NAD	C2D-C1D-N1N	3.81	121.11	113.48
4	C	503	NAD	C2B-C3B-C4B	-3.81	95.04	102.64
4	H	508	NAD	PN-O3-PA	-3.76	118.04	133.17
4	F	506	NAD	O4B-C4B-C3B	3.74	112.77	105.16
4	H	508	NAD	O7N-C7N-N7N	-3.69	117.32	122.59
4	B	502	NAD	O4D-C4D-C3D	-3.69	97.67	105.16
4	B	502	NAD	O7N-C7N-C3N	3.65	123.67	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	NAD	O2N-PN-O1N	-3.64	107.83	118.70
3	A	501[B]	ADP	O4'-C1'-C2'	-3.58	101.48	106.69
3	L	512	ADP	C5-C4-N9	3.57	112.04	107.09
4	C	503	NAD	C3N-C7N-N7N	3.57	121.76	117.78
3	E	505	ADP	PA-O3A-PB	-3.56	122.08	131.93
4	F	506	NAD	C3N-C7N-N7N	3.56	121.74	117.78
3	A	501[A]	ADP	C8-N9-C4	-3.51	104.10	106.96
4	F	506	NAD	C5A-C4A-N3A	-3.50	122.57	125.98
4	C	503	NAD	C5A-C4A-N3A	-3.43	122.64	125.98
4	F	506	NAD	O2N-PN-O1N	-3.39	108.58	118.70
3	K	511	ADP	PA-O3A-PB	-3.39	122.56	131.93
4	C	503	NAD	O2N-PN-O1N	-3.33	108.77	118.70
4	G	507	NAD	C2D-C1D-N1N	3.30	120.09	113.48
3	A	501[B]	ADP	C2'-C3'-C4'	-3.30	96.04	102.64
4	B	502	NAD	C6A-C5A-C4A	3.31	121.26	117.55
4	C	503	NAD	C6A-C5A-C4A	3.24	121.18	117.55
4	H	508	NAD	O2N-PN-O1N	-3.23	109.05	118.70
3	K	511	ADP	O4'-C1'-C2'	-3.23	101.99	106.69
3	A	501[B]	ADP	C5-C4-N3	-3.17	122.89	125.98
4	H	508	NAD	O7N-C7N-C3N	3.08	123.04	119.59
4	B	502	NAD	C1B-N9A-C4A	3.07	131.95	126.64
3	A	501[A]	ADP	C3'-C2'-C1'	3.06	105.72	100.92
4	B	502	NAD	C5A-C4A-N3A	-3.04	123.01	125.98
4	G	507	NAD	O2N-PN-O1N	-3.02	109.68	118.70
3	D	504[A]	ADP	O3A-PA-O5'	-3.00	94.97	102.91
3	E	505	ADP	C5-C4-N3	-3.00	123.06	125.98
4	F	506	NAD	O7N-C7N-N7N	-2.99	118.31	122.59
3	J	510	ADP	C5-C4-N3	-2.99	123.06	125.98
3	I	509	ADP	C6-C5-C4	2.93	120.84	117.55
4	H	508	NAD	C5A-C4A-N9A	2.93	111.15	107.09
3	I	509	ADP	C5-C4-N3	-2.91	123.14	125.98
4	F	506	NAD	C6A-C5A-C4A	2.90	120.81	117.55
4	G	507	NAD	C6A-C5A-C4A	2.85	120.75	117.55
3	D	504[A]	ADP	C6-C5-C4	2.83	120.73	117.55
3	J	510	ADP	C2'-C3'-C4'	-2.82	97.02	102.64
3	I	509	ADP	C4'-O4'-C1'	-2.81	106.63	109.72
3	D	504[B]	ADP	C6-C5-C4	2.80	120.69	117.55
4	G	507	NAD	C6N-C5N-C4N	-2.80	115.11	119.44
3	A	501[B]	ADP	C6-C5-C4	2.77	120.66	117.55
3	J	510	ADP	C6-C5-C4	2.75	120.63	117.55
3	J	510	ADP	O4'-C1'-C2'	-2.72	102.73	106.69
3	L	512	ADP	C1'-N9-C4	-2.71	121.95	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[A]	ADP	C6-C5-C4	2.71	120.59	117.55
3	K	511	ADP	C8-N9-C1'	2.69	131.22	126.15
3	E	505	ADP	C5-C4-N9	2.69	110.81	107.09
3	L	512	ADP	C2'-C3'-C4'	-2.68	97.30	102.64
4	C	503	NAD	O5B-C5B-C4B	2.67	118.79	108.96
4	F	506	NAD	C5A-C4A-N9A	2.67	110.78	107.09
4	G	507	NAD	C2D-C3D-C4D	-2.65	97.34	102.64
3	A	501[A]	ADP	C2'-C3'-C4'	-2.65	97.34	102.64
3	I	509	ADP	C2'-C3'-C4'	-2.61	97.42	102.64
3	E	505	ADP	C2'-C3'-C4'	-2.61	97.43	102.64
4	B	502	NAD	O7N-C7N-N7N	-2.61	118.86	122.59
3	D	504[B]	ADP	C2'-C3'-C4'	-2.60	97.45	102.64
3	K	511	ADP	C6-C5-C4	2.60	120.47	117.55
4	H	508	NAD	C6N-N1N-C2N	-2.58	118.41	121.79
4	B	502	NAD	C3B-C2B-C1B	2.58	104.97	100.92
3	L	512	ADP	C6-C5-C4	2.57	120.43	117.55
3	J	510	ADP	O3A-PA-O5'	2.55	109.68	102.91
3	D	504[A]	ADP	C5-C4-N3	-2.55	123.50	125.98
6	E	907	GAI	N3-C-N2	2.53	120.82	115.83
4	H	508	NAD	C6A-C5A-C4A	2.52	120.38	117.55
4	B	502	NAD	C6N-N1N-C1D	2.51	125.56	119.33
3	A	501[A]	ADP	C5-C4-N3	-2.51	123.54	125.98
4	B	502	NAD	C2D-C3D-C4D	-2.49	97.66	102.64
4	H	508	NAD	C6N-C5N-C4N	-2.49	115.59	119.44
3	D	504[B]	ADP	C5-C4-N3	-2.47	123.58	125.98
4	C	503	NAD	O7N-C7N-C3N	2.45	122.33	119.59
4	G	507	NAD	C4N-C3N-C7N	-2.45	114.62	121.11
4	H	508	NAD	C2B-C3B-C4B	-2.45	97.75	102.64
4	G	507	NAD	PN-O3-PA	-2.44	123.34	133.17
4	H	508	NAD	C8A-N9A-C1B	2.44	130.75	126.15
3	A	501[B]	ADP	C5-C4-N9	2.43	110.45	107.09
4	H	508	NAD	C2D-C1D-N1N	2.40	118.28	113.48
6	E	906	GAI	N3-C-N2	2.39	120.56	115.83
4	F	506	NAD	C4B-O4B-C1B	-2.38	107.10	109.72
3	K	511	ADP	C5-C4-N9	2.37	110.38	107.09
4	G	507	NAD	O4B-C1B-C2B	-2.36	103.25	106.69
3	A	501[A]	ADP	O4'-C1'-N9	-2.35	102.97	108.10
3	I	509	ADP	C5-C4-N9	2.35	110.35	107.09
3	E	505	ADP	C8-N9-C1'	2.35	130.57	126.15
3	K	511	ADP	O5'-C5'-C4'	2.34	117.58	108.96
4	C	503	NAD	C6N-C5N-C4N	-2.33	115.83	119.44
3	D	504[A]	ADP	C2'-C3'-C4'	-2.31	98.02	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	505	ADP	C6-C5-C4	2.31	120.14	117.55
6	D	905	GAI	N3-C-N2	2.30	120.38	115.83
4	G	507	NAD	C5A-C4A-N9A	2.29	110.26	107.09
3	D	504[B]	ADP	PA-O3A-PB	2.27	138.22	131.93
4	C	503	NAD	C5N-C4N-C3N	2.27	123.18	120.34
6	J	611	GAI	N3-C-N2	2.27	120.31	115.83
4	C	503	NAD	O5D-C5D-C4D	2.27	117.30	108.96
6	A	902	GAI	N3-C-N2	2.27	120.31	115.83
4	B	502	NAD	C2B-C3B-C4B	-2.26	98.12	102.64
4	G	507	NAD	C3N-C2N-N1N	-2.23	117.39	120.36
4	B	502	NAD	C4B-O4B-C1B	2.22	112.16	109.72
4	G	507	NAD	C5A-C4A-N3A	-2.20	123.84	125.98
4	C	503	NAD	C5A-C4A-N9A	2.19	110.12	107.09
4	C	503	NAD	PN-O3-PA	-2.17	124.43	133.17
6	H	909	GAI	N3-C-N2	2.17	120.12	115.83
4	B	502	NAD	C5A-C4A-N9A	2.17	110.10	107.09
6	G	5010	GAI	N3-C-N2	2.17	120.11	115.83
4	B	502	NAD	O4D-C1D-N1N	2.16	110.51	108.13
4	F	506	NAD	PN-O3-PA	-2.16	124.49	133.17
6	G	5009	GAI	N3-C-N2	2.14	120.06	115.83
3	D	504[A]	ADP	C4-C5-N7	2.12	111.45	109.41
4	C	503	NAD	C3B-C2B-C1B	2.12	104.24	100.92
3	D	504[A]	ADP	O2A-PA-O3A	2.08	115.02	105.14
4	C	503	NAD	C8A-N9A-C1B	2.07	130.05	126.15
4	H	508	NAD	C2N-C3N-C4N	2.07	120.63	118.31
4	G	507	NAD	C5N-C6N-N1N	2.02	123.89	120.49
4	C	503	NAD	O3-PA-O5B	-2.02	97.55	102.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/500 (98%)	0.70	56 (11%) 6 5	21, 67, 104, 123	0
1	B	494/500 (98%)	-0.14	2 (0%) 90 92	24, 40, 78, 98	0
1	C	494/500 (98%)	-0.10	2 (0%) 90 92	23, 40, 72, 88	0
1	D	494/500 (98%)	0.63	34 (6%) 17 16	25, 68, 97, 118	0
1	E	494/500 (98%)	-0.16	2 (0%) 90 92	23, 41, 68, 96	0
1	F	494/500 (98%)	-0.08	3 (0%) 86 88	21, 37, 66, 94	0
1	G	494/500 (98%)	0.09	5 (1%) 79 81	26, 46, 68, 98	0
1	H	494/500 (98%)	0.09	9 (1%) 65 68	24, 46, 77, 91	0
1	I	494/500 (98%)	0.37	19 (3%) 38 40	36, 58, 82, 105	0
1	J	494/500 (98%)	0.74	39 (7%) 13 12	44, 77, 104, 114	0
1	K	494/500 (98%)	0.60	35 (7%) 16 15	44, 71, 96, 115	0
1	L	494/500 (98%)	1.12	89 (18%) 2 2	47, 89, 115, 127	0
All	All	5928/6000 (98%)	0.32	295 (4%) 28 28	21, 55, 99, 127	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	378	GLY	6.6
1	L	369	CYS	6.1
1	A	371	GLY	5.6
1	G	474	GLY	5.3
1	L	373	ILE	5.0
1	L	223	GLY	4.7
1	D	356	TYR	4.7
1	K	376	ASP	4.7
1	L	386	PHE	4.6
1	K	377	ARG	4.5
1	A	362	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	424	THR	4.5
1	K	474	GLY	4.4
1	K	371	GLY	4.4
1	A	470	MET	4.3
1	L	295	PHE	4.3
1	A	473	SER	4.2
1	D	470	MET	4.1
1	K	475	ARG	4.0
1	K	470	MET	4.0
1	J	7	ALA	4.0
1	A	468	TYR	3.9
1	G	7	ALA	3.9
1	J	365	ALA	3.9
1	E	7	ALA	3.9
1	A	424	THR	3.9
1	A	353	ILE	3.9
1	L	285	TRP	3.9
1	L	356	TYR	3.8
1	A	477	LEU	3.8
1	L	350	PHE	3.8
1	L	327	LYS	3.7
1	I	408	LEU	3.7
1	L	478	GLY	3.7
1	D	376	ASP	3.7
1	A	315	TYR	3.6
1	J	108	LEU	3.6
1	L	380	PHE	3.6
1	A	469	LYS	3.6
1	D	327	LYS	3.6
1	L	377	ARG	3.6
1	K	473	SER	3.6
1	A	474	GLY	3.6
1	L	332	GLY	3.5
1	A	367	LEU	3.5
1	L	376	ASP	3.5
1	L	357	ILE	3.5
1	J	362	GLN	3.5
1	L	349	GLN	3.5
1	L	108	LEU	3.5
1	L	333	ASN	3.4
1	L	354	LEU	3.4
1	A	376	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	394	THR	3.4
1	L	322	SER	3.4
1	A	334	PRO	3.3
1	L	482	LEU	3.3
1	K	379	TYR	3.3
1	L	468	TYR	3.3
1	L	310	VAL	3.2
1	I	389	VAL	3.2
1	L	413	ILE	3.2
1	A	7	ALA	3.2
1	H	386	PHE	3.2
1	A	475	ARG	3.2
1	A	356	TYR	3.2
1	H	365	ALA	3.1
1	L	340	GLU	3.1
1	J	476	GLU	3.0
1	I	470	MET	3.0
1	D	379	TYR	3.0
1	J	425	TYR	3.0
1	K	468	TYR	3.0
1	D	199	LEU	3.0
1	L	360	GLY	3.0
1	K	471	SER	3.0
1	L	408	LEU	3.0
1	L	329	ARG	2.9
1	K	380	PHE	2.9
1	L	367	LEU	2.9
1	A	377	ARG	2.9
1	A	373	ILE	2.9
1	K	139	TYR	2.9
1	H	362	GLN	2.9
1	K	472	GLY	2.9
1	L	328	SER	2.9
1	L	480	TYR	2.9
1	A	386	PHE	2.8
1	L	462	GLN	2.8
1	L	479	GLU	2.8
1	A	395	ILE	2.8
1	A	10	ALA	2.8
1	H	7	ALA	2.8
1	A	358	ASN	2.8
1	I	480	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	463	SER	2.8
1	D	29	HIS	2.8
1	L	115	VAL	2.8
1	K	386	PHE	2.8
1	J	139	TYR	2.8
1	K	46	GLU	2.7
1	J	468	TYR	2.7
1	J	22	ILE	2.7
1	L	301	CYS	2.7
1	L	475	ARG	2.7
1	D	350	PHE	2.7
1	L	318	PHE	2.7
1	D	32	VAL	2.7
1	J	203	TYR	2.7
1	I	139	TYR	2.7
1	D	471	SER	2.7
1	J	347	GLU	2.6
1	D	468	TYR	2.6
1	L	9	PRO	2.6
1	L	73	GLY	2.6
1	J	44	THR	2.6
1	A	326	ALA	2.6
1	L	28	TRP	2.6
1	K	463	SER	2.6
1	L	199	LEU	2.6
1	L	216	GLY	2.6
1	L	353	ILE	2.6
1	L	385	VAL	2.6
1	G	475	ARG	2.6
1	A	472	GLY	2.6
1	L	387	GLY	2.6
1	L	315	TYR	2.6
1	K	413	ILE	2.6
1	H	290	ALA	2.6
1	D	40	VAL	2.6
1	K	465	PHE	2.6
1	A	365	ALA	2.6
1	D	365	ALA	2.6
1	F	477	LEU	2.6
1	G	477	LEU	2.6
1	L	113	PRO	2.6
1	J	386	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	279	SER	2.6
1	L	477	LEU	2.5
1	D	353	ILE	2.5
1	H	364	GLY	2.5
1	K	478	GLY	2.5
1	A	379	TYR	2.5
1	L	379	TYR	2.5
1	J	376	ASP	2.5
1	K	17	VAL	2.5
1	K	18	PHE	2.5
1	I	248	GLU	2.5
1	D	31	ALA	2.5
1	L	314	ILE	2.5
1	L	139	TYR	2.5
1	J	378	GLY	2.5
1	J	42	PRO	2.5
1	L	466	GLY	2.5
1	L	473	SER	2.5
1	L	347	GLU	2.5
1	D	475	ARG	2.4
1	I	411	LYS	2.4
1	L	7	ALA	2.4
1	L	345	VAL	2.4
1	D	247	THR	2.4
1	A	465	PHE	2.4
1	L	358	ASN	2.4
1	I	386	PHE	2.4
1	D	413	ILE	2.4
1	A	471	SER	2.4
1	A	287	VAL	2.4
1	L	47	VAL	2.4
1	L	323	VAL	2.4
1	J	30	ASP	2.4
1	K	259	SER	2.4
1	A	317	GLU	2.4
1	E	424	THR	2.4
1	J	358	ASN	2.4
1	L	266	THR	2.4
1	L	486	THR	2.4
1	I	319	VAL	2.4
1	L	416	VAL	2.4
1	D	248	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	253	ILE	2.4
1	K	467	GLY	2.4
1	I	486	THR	2.3
1	J	366	LYS	2.3
1	L	338	LYS	2.3
1	B	473	SER	2.3
1	A	466	GLY	2.3
1	L	26	ASN	2.3
1	A	327	LYS	2.3
1	D	334	PRO	2.3
1	L	319	VAL	2.3
1	D	114	TYR	2.3
1	J	258	GLY	2.3
1	L	465	PHE	2.3
1	D	8	VAL	2.3
1	L	363	GLU	2.3
1	L	400	ILE	2.3
1	I	251	ARG	2.3
1	D	408	LEU	2.3
1	J	18	PHE	2.3
1	J	373	ILE	2.3
1	L	320	GLU	2.3
1	D	362	GLN	2.3
1	H	315	TYR	2.3
1	A	314	ILE	2.3
1	L	8	VAL	2.3
1	D	377	ARG	2.2
1	L	42	PRO	2.2
1	L	371	GLY	2.2
1	L	247	THR	2.2
1	C	477	LEU	2.2
1	K	484	ALA	2.2
1	L	27	GLU	2.2
1	A	357	ILE	2.2
1	A	368	LEU	2.2
1	J	467	GLY	2.2
1	I	409	LYS	2.2
1	K	375	ALA	2.2
1	A	318	PHE	2.2
1	A	319	VAL	2.2
1	K	266	THR	2.2
1	J	374	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	283	MET	2.2
1	J	53	GLU	2.2
1	K	479	GLU	2.2
1	J	33	SER	2.2
1	D	46	GLU	2.2
1	L	104	ALA	2.2
1	A	306	SER	2.2
1	A	467	GLY	2.2
1	A	398	GLU	2.2
1	A	114	TYR	2.2
1	K	441	TYR	2.2
1	L	461	ALA	2.2
1	K	332	GLY	2.1
1	A	100	THR	2.1
1	I	479	GLU	2.1
1	L	24	ILE	2.1
1	L	202	LEU	2.1
1	A	422	ASN	2.1
1	A	384	THR	2.1
1	F	254	GLN	2.1
1	G	486	THR	2.1
1	A	413	ILE	2.1
1	J	381	ILE	2.1
1	D	477	LEU	2.1
1	A	441	TYR	2.1
1	I	141	GLY	2.1
1	I	498	LYS	2.1
1	J	462	GLN	2.1
1	K	483	GLN	2.1
1	L	374	ALA	2.1
1	A	397	LYS	2.1
1	J	474	GLY	2.1
1	L	474	GLY	2.1
1	L	405	MET	2.1
1	J	63	VAL	2.1
1	H	409	LYS	2.1
1	I	388	ASP	2.1
1	K	411	LYS	2.1
1	J	104	ALA	2.1
1	J	379	TYR	2.1
1	J	389	VAL	2.1
1	B	71	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	463	SER	2.1
1	D	367	LEU	2.1
1	L	393	MET	2.1
1	A	355	GLY	2.1
1	D	386	PHE	2.1
1	F	465	PHE	2.1
1	K	466	GLY	2.1
1	I	312	GLU	2.1
1	K	312	GLU	2.1
1	D	338	LYS	2.1
1	D	100	THR	2.0
1	L	17	VAL	2.0
1	I	356	TYR	2.0
1	C	7	ALA	2.0
1	K	301	CYS	2.0
1	L	23	PHE	2.0
1	L	276	ILE	2.0
1	J	377	ARG	2.0
1	A	479	GLU	2.0
1	H	360	GLY	2.0
1	J	14	GLN	2.0
1	L	250	GLY	2.0
1	J	8	VAL	2.0
1	A	480	TYR	2.0
1	I	376	ASP	2.0
1	A	347	GLU	2.0
1	D	318	PHE	2.0
1	J	34	ARG	2.0
1	J	114	TYR	2.0
1	K	33	SER	2.0
1	L	483	GLN	2.0
1	J	19	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NA	G	5008	1/1	0.53	24.21	48,48,48,48	0
2	NA	C	5004	1/1	0.44	19.46	51,51,51,51	0
2	NA	F	5007	1/1	0.40	17.26	54,54,54,54	0
6	GAI	I	910	4/4	0.40	9.03	94,94,94,95	0
2	NA	C	603	1/1	0.21	8.37	54,54,54,54	0
5	EDO	E	905	4/4	0.20	7.66	51,52,53,58	0
5	EDO	F	706	4/4	0.35	7.57	74,76,79,80	0
5	EDO	E	805	4/4	0.47	6.88	83,83,85,85	0
5	EDO	B	902	4/4	0.29	6.26	63,63,65,65	0
5	EDO	E	705	4/4	0.31	6.22	77,80,80,80	0
6	GAI	E	906	4/4	0.29	6.15	51,54,55,55	0
5	EDO	G	907	4/4	0.37	5.62	68,68,68,69	0
6	GAI	H	909	4/4	0.30	4.89	95,95,95,95	0
5	EDO	A	901	4/4	0.33	4.56	75,75,76,77	0
5	EDO	I	809	4/4	0.35	4.55	81,82,82,82	0
6	GAI	G	5010	4/4	0.23	3.93	47,47,49,49	0
6	GAI	G	5009	4/4	0.28	3.60	76,76,76,76	0
2	NA	A	601	1/1	0.26	3.51	82,82,82,82	0
5	EDO	B	802	4/4	0.22	3.04	48,48,52,53	0
5	EDO	F	707	4/4	0.24	2.94	59,59,61,61	0
6	GAI	E	907	4/4	0.20	2.86	47,48,49,49	0
2	NA	B	5003	1/1	0.14	2.68	55,55,55,55	0
5	EDO	L	712	4/4	0.26	2.63	70,72,73,73	0
5	EDO	B	701	4/4	0.21	2.51	67,67,67,68	0
3	ADP	D	504[A]	27/27	0.28	2.29	79,81,86,86	27
6	GAI	D	905	4/4	0.26	2.26	77,78,78,78	0
3	ADP	D	504[B]	27/27	0.28	2.19	89,91,96,96	27
5	EDO	C	903	4/4	0.22	2.18	45,49,49,52	0
5	EDO	L	912	4/4	0.26	2.02	68,69,70,72	0
4	NAD	B	502	44/44	0.23	1.96	73,88,103,104	0
5	EDO	F	906	4/4	0.17	1.83	63,63,65,65	0
5	EDO	D	904	4/4	0.24	1.72	74,74,75,75	0
6	GAI	A	902	4/4	0.15	1.20	63,64,64,65	0
6	GAI	J	611	4/4	0.21	1.13	64,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	I	909	4/4	0.15	0.94	62,62,63,64	0
5	EDO	H	908	4/4	0.23	0.91	79,79,79,80	0
4	NAD	C	503	44/44	0.20	0.80	58,81,92,93	0
3	ADP	A	501[A]	27/27	0.21	0.80	78,80,81,81	27
3	ADP	A	501[B]	27/27	0.21	0.80	91,93,93,93	27
5	EDO	K	911	4/4	0.26	0.75	79,80,80,80	0
4	NAD	G	507	44/44	0.18	0.73	61,77,91,92	0
5	EDO	C	803	4/4	0.16	0.70	49,53,53,55	0
5	EDO	H	708	4/4	0.17	0.55	47,49,51,53	0
2	NA	K	5012	1/1	0.16	0.42	60,60,60,60	0
3	ADP	K	511	27/27	0.18	0.41	94,99,105,106	0
4	NAD	F	506	44/44	0.17	0.38	38,68,81,84	0
3	ADP	E	505	27/27	0.14	0.11	43,52,79,80	0
4	NAD	H	508	44/44	0.15	0.06	49,81,89,90	0
5	EDO	H	808	4/4	0.19	0.01	63,64,64,65	0
3	ADP	I	509	27/27	0.17	0.00	79,81,94,95	0
3	ADP	L	512	27/27	0.21	-0.15	89,97,112,113	0
5	EDO	F	806	4/4	0.13	-0.62	53,54,54,58	0
2	NA	I	609	1/1	0.11	-0.76	54,54,54,54	0
3	ADP	J	510	27/27	0.17	-0.80	102,104,114,115	0
5	EDO	D	704	4/4	0.13	-0.83	53,54,56,56	0
5	EDO	G	807	4/4	0.17	-1.03	75,75,75,75	0
2	NA	L	612	1/1	0.15	-1.35	80,80,80,80	0
2	NA	J	610	1/1	0.13	-1.73	75,75,75,75	0
2	NA	D	604	1/1	0.10	-1.89	73,73,73,73	0
2	NA	H	608	1/1	0.09	-2.23	46,46,46,46	0
2	NA	K	611	1/1	0.09	-2.49	63,63,63,63	0
2	NA	F	606	1/1	0.08	-2.51	32,32,32,32	0
2	NA	B	602	1/1	0.06	-2.66	40,40,40,40	0
2	NA	E	605	1/1	0.07	-2.75	37,37,37,37	0
2	NA	G	607	1/1	0.08	-2.98	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.