



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:12 am GMT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

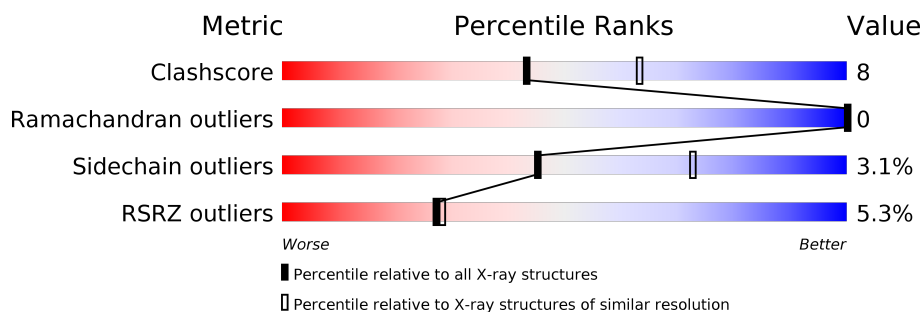
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	<div> <div>11%</div> <div>80%18%..</div> </div>
1	B	500	<div> <div>%</div> <div>84%14%..</div> </div>
1	C	500	<div> <div>82%16%..</div> </div>
1	D	500	<div> <div>8%80%18%..</div> </div>
1	E	500	<div> <div>82%16%..</div> </div>
1	F	500	<div> <div>%82%16%..</div> </div>
1	G	500	<div> <div>%82%16%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	500	
1	I	500	
1	J	500	
1	K	500	
1	L	500	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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	B	802	-	-	-	X
5	EDO	B	902	-	-	-	X
5	EDO	E	705	-	-	-	X
5	EDO	E	805	-	-	-	X
5	EDO	F	706	-	-	-	X
5	EDO	F	707	-	-	-	X
5	EDO	I	809	-	-	-	X
6	GAI	A	902	-	-	-	X
6	GAI	D	905	-	-	-	X
6	GAI	E	906	-	-	-	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 hydrogens and 0 are deuteriums.

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

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

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

There are 12 discrepancies between the modelled and reference sequences:

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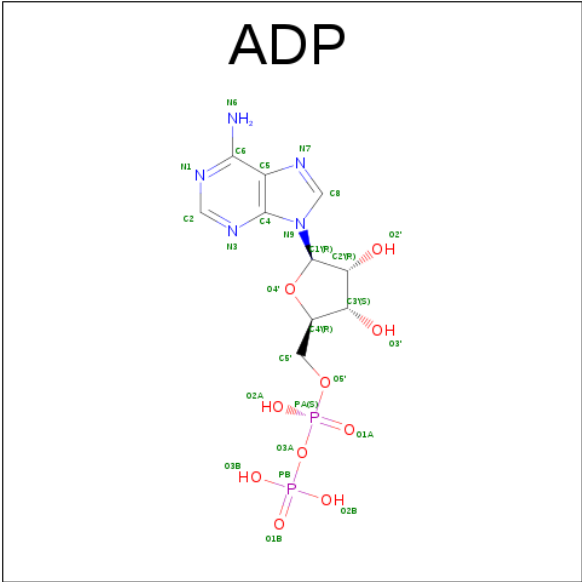
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Chain	Residue	Modelled	Actual	Comment	Reference
F	487	LYS	GLU	ENGINEERED	UNP P05091
G	487	LYS	GLU	ENGINEERED	UNP P05091
H	487	LYS	GLU	ENGINEERED	UNP P05091
I	487	LYS	GLU	ENGINEERED	UNP P05091
J	487	LYS	GLU	ENGINEERED	UNP P05091
K	487	LYS	GLU	ENGINEERED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

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

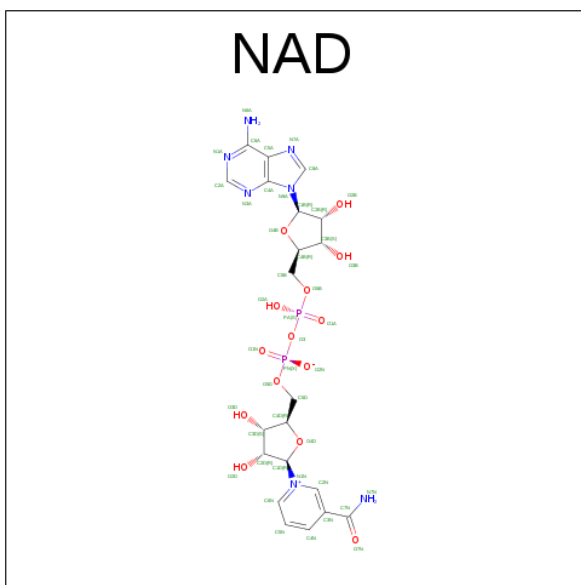
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Na 2 2	0	0
2	J	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	K	2	Total Na 2 2	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	2	Total Na 2 2	0	0
2	I	1	Total Na 1 1	0	0
2	C	2	Total Na 2 2	0	0
2	A	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0
2	F	2	Total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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



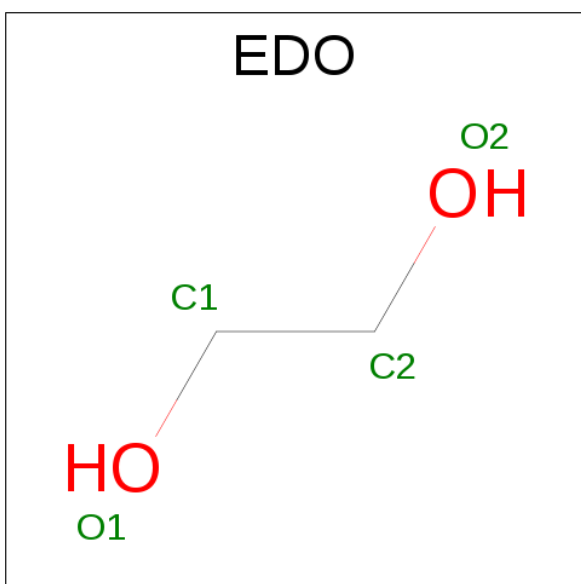
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	D	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	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: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



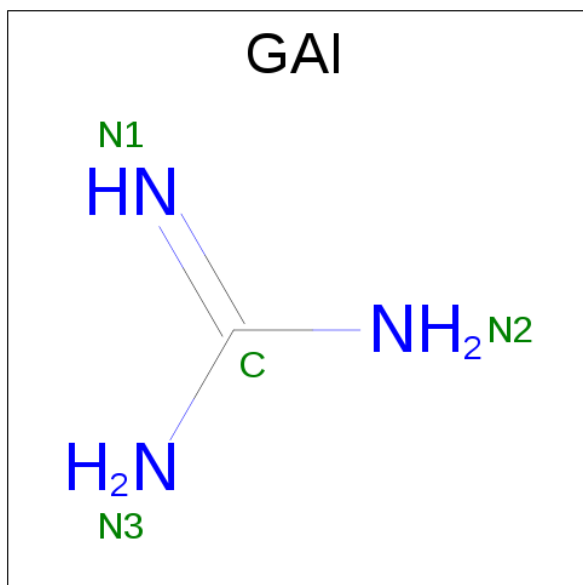
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
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:  $\text{CH}_5\text{N}_3$ ).



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		

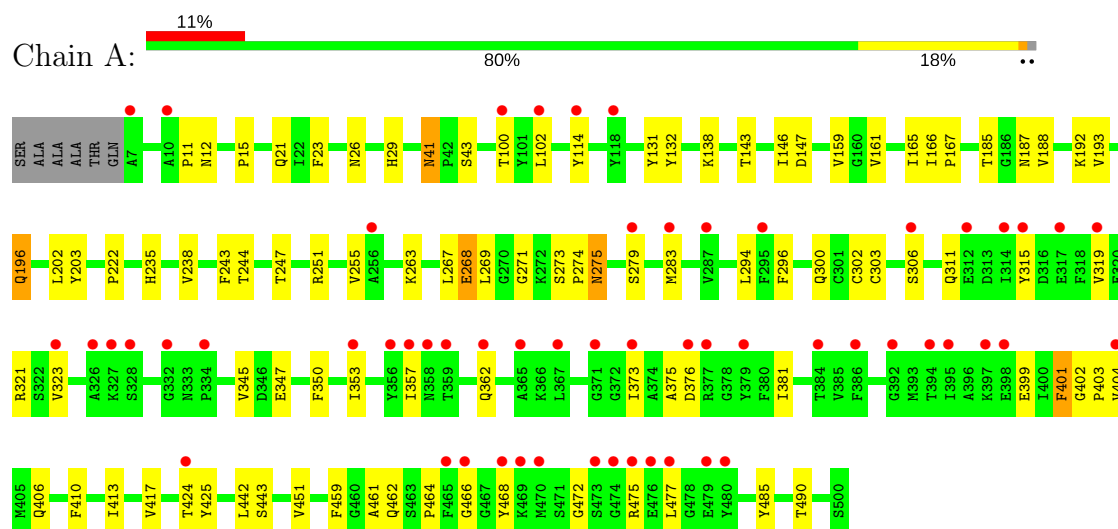
- Molecule 7 is water.

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		

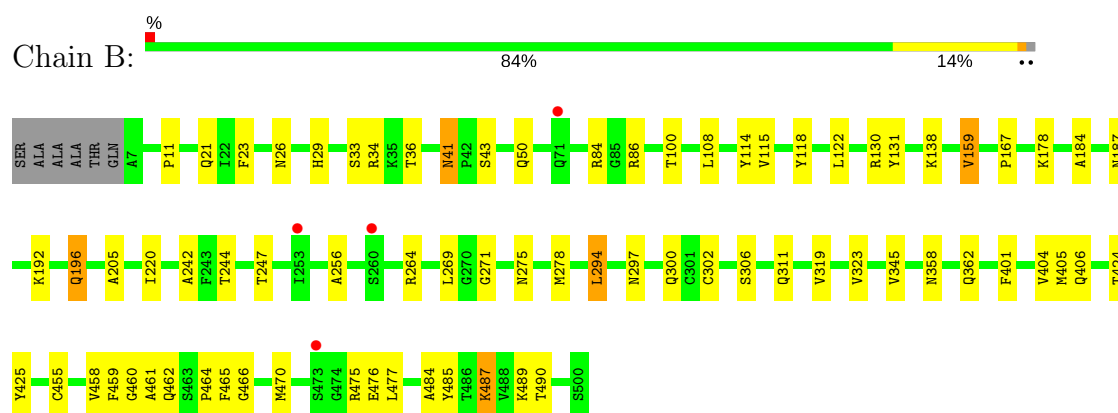
### 3 Residue-property plots

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

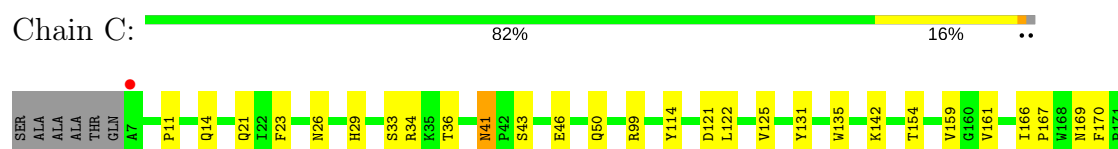
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

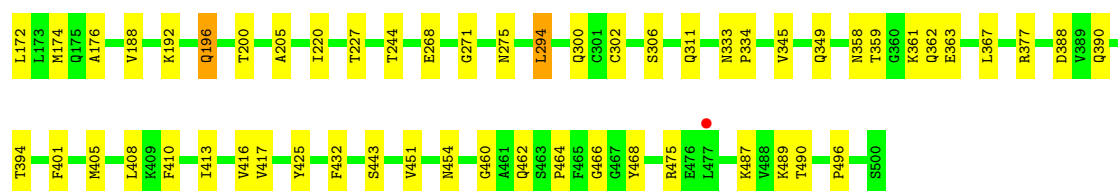


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

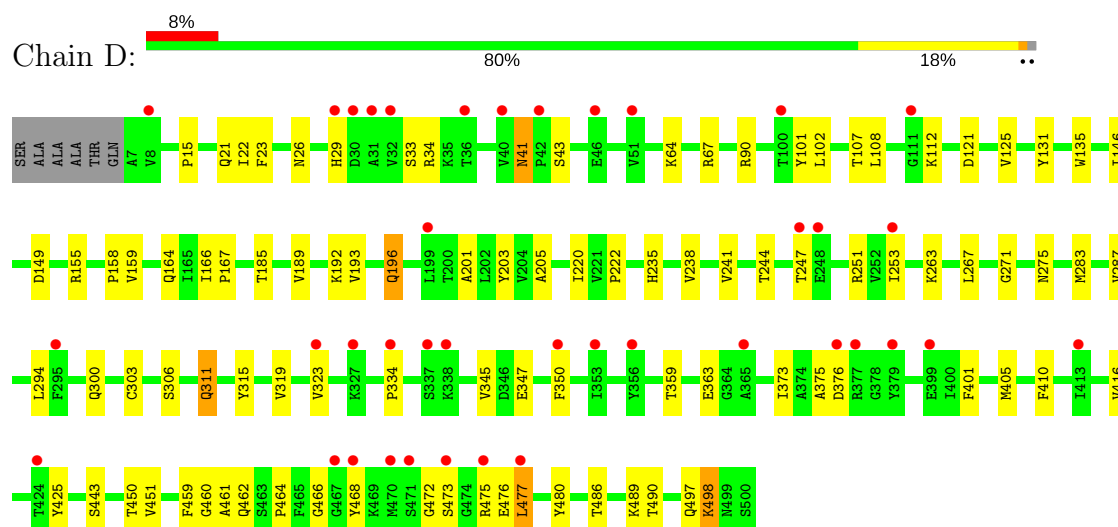


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

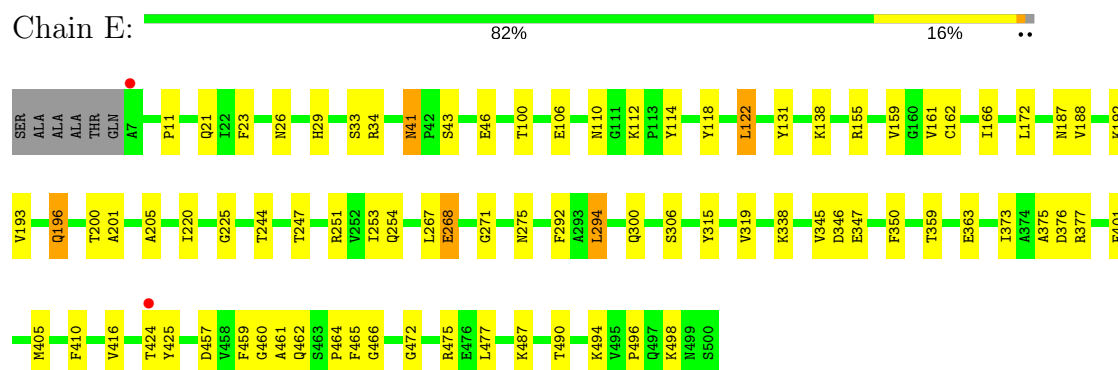




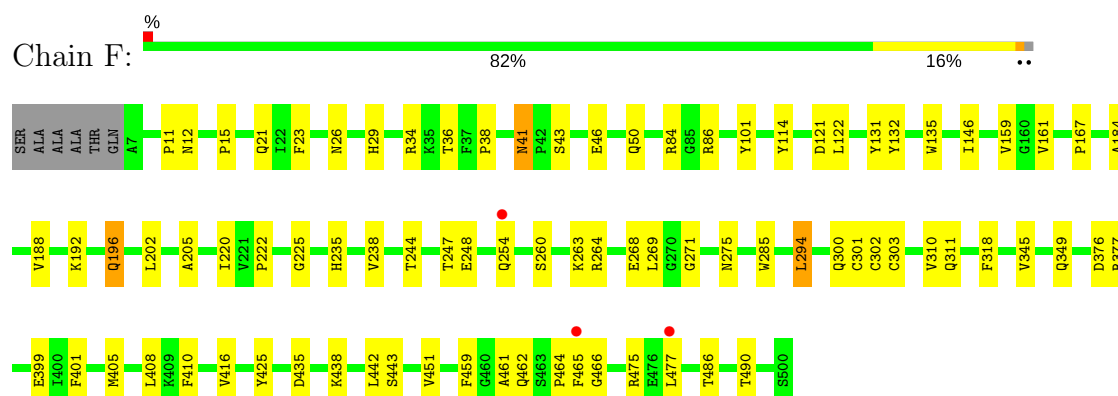
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



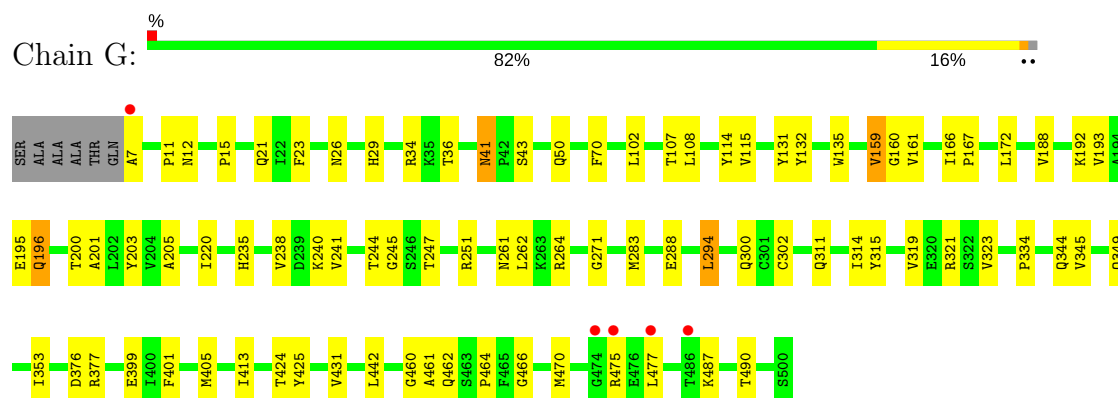
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



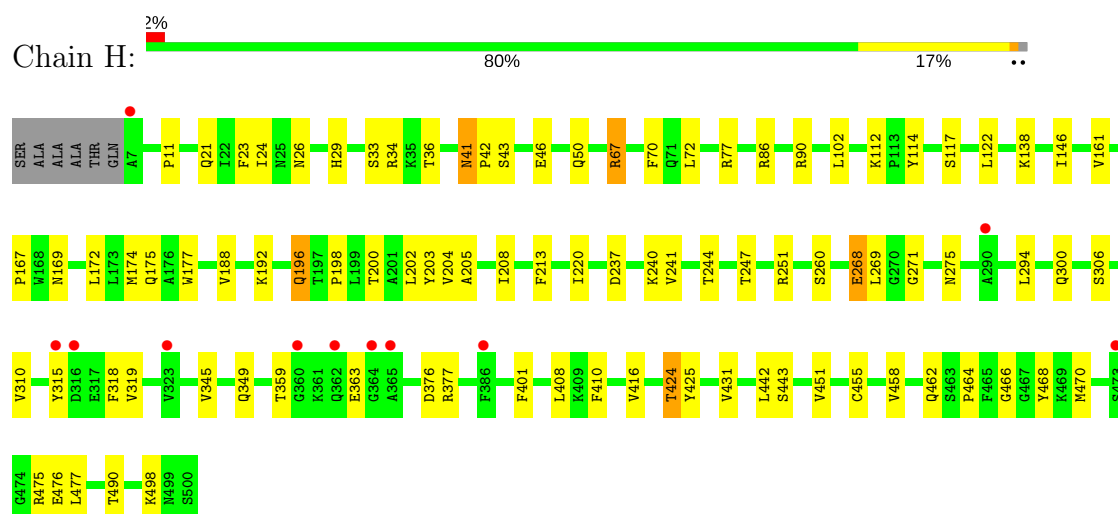
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



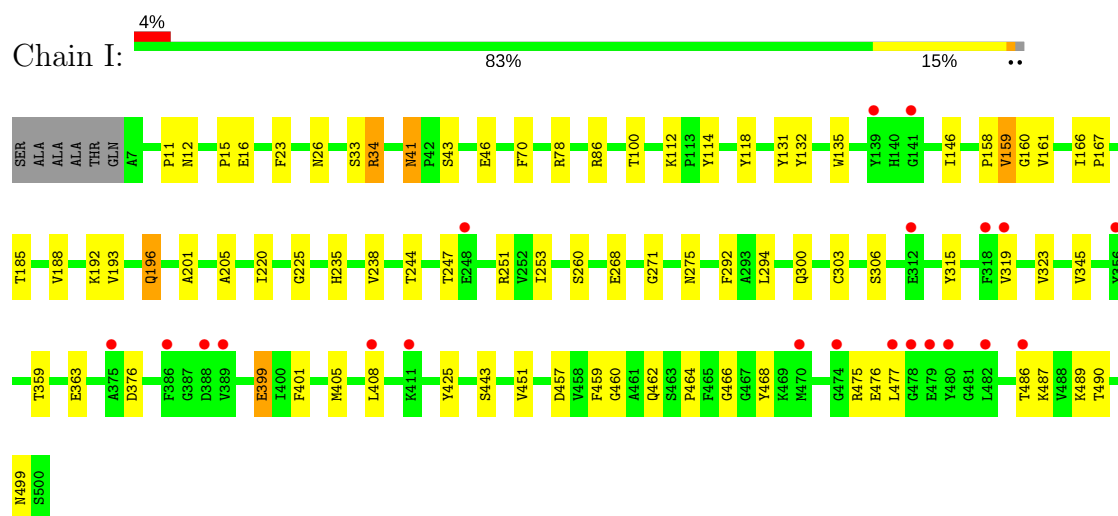
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

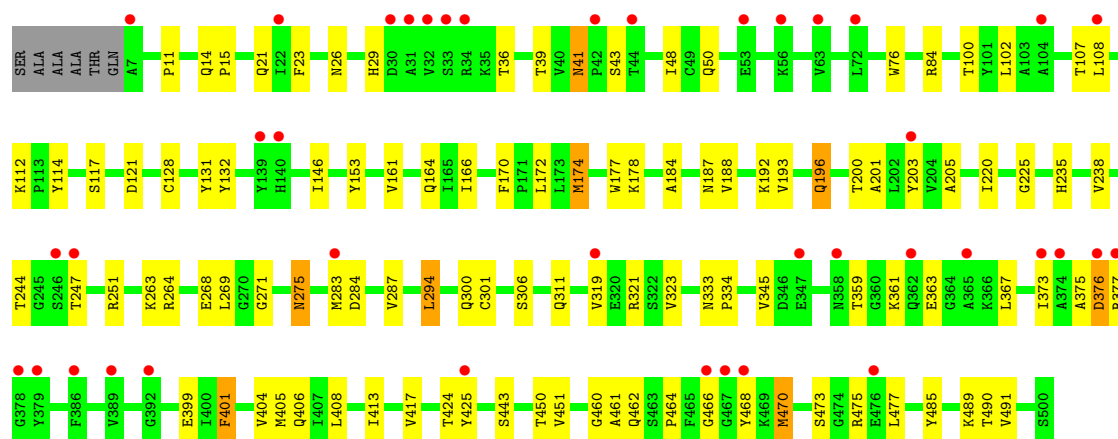


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

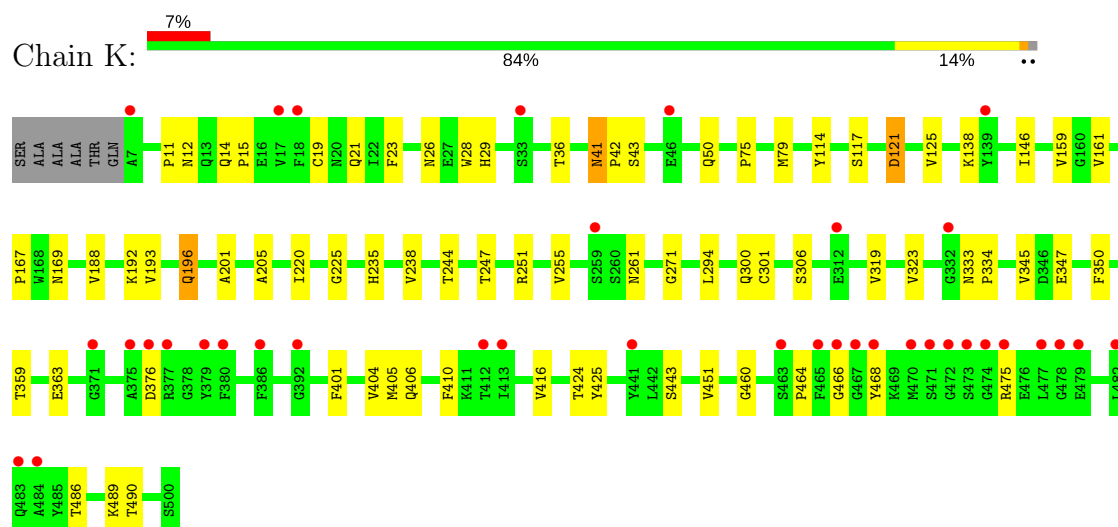


- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

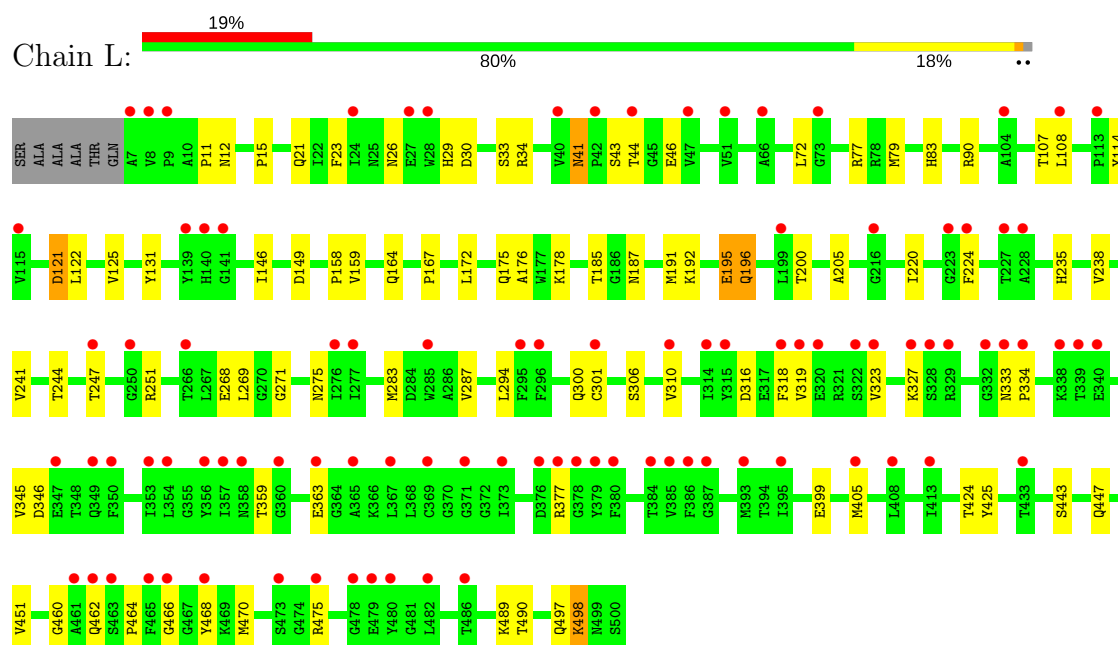




- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 88.2 (48.95-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3752	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
4	H	44	0	26	2	0
5	A	4	0	6	0	0

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

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	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	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: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

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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:NE2	1:A:196:GLN:H	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	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

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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	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

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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:196:GLN:HE21	1:I:196:GLN:N	1.95	0.57
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

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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	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
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: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: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

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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:OE1	1:L:399:GLU:HA	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

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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	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: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:353:ILE:CD1	1:A:403:PRO:HD2	2.41	0.49
1:A:132:TYR:OH	1:A:477:LEU:HA	2.13	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: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
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:J:41:ASN:HD22	1:J:41:ASN:C	2.16	0.48
1:I:468:TYR:OH	1:J:489:LYS:HB2	2.12	0.48
1:K:261:ASN:HA	1:L:470:MET:CE	2.44	0.48
1:D:247:THR:O	1:D:251:ARG:HG3	2.13	0.48
1:E:172:LEU:HD21	1:E:200:THR:HB	1.94	0.48
1:E:338:LYS:CD	1:I:34:ARG:NH2	2.75	0.48
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.49	0.48
1:G:12:ASN:O	1:G:15:PRO:HD3	2.14	0.48
1:A:271:GLY:HA2	1:A:425:TYR:CD2	2.49	0.48
1:C: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: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: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
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:413:ILE:HD11	1:G:442:LEU:HG	1.97	0.47
1:G:302:CYS:HB3	4:G:507:NAD:O7N	2.14	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: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:G:159:VAL:HG23	1:G:264:ARG:HH11	1.80	0.46
1:E:338:LYS:NZ	1:I:34:ARG:HE	2.13	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:235:HIS:HB3	1:F:238:VAL:HG23	1.98	0.45
1:F:21:GLN:HB3	1:F:29:HIS:O	2.16	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: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: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	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:319:VAL:O	1:B:323:VAL:HG23	2.17	0.44
1:A:468:TYR:OH	1:B:489:LYS:HB2	2.17	0.44
1:D:373:ILE:HG22	1:D:375:ALA:H	1.82	0.44
1:J:15:PRO:HD2	1:J:108:LEU:HD22	2.00	0.44
1:A:165:ILE:HG22	3:A:501[B]:ADP:H4'	2.00	0.44
1:A:315:TYR:O	1:A:319:VAL:HG23	2.17	0.44
1:F:167:PRO:HD3	1:F:244:THR:HB	2.00	0.44
1:H:359:THR:O	1:H:363:GLU:HG3	2.18	0.44
1:C:46:GLU:HG3	7:C:2480:HOH:O	2.17	0.44
1:G:159:VAL:CG2	1:G:264:ARG:HH11	2.31	0.44
1:G:167:PRO:HD3	1:G:244:THR:HB	1.99	0.44
1:I:100:THR:HG22	1:I:118:TYR:HE1	1.83	0.44
1:J:102:LEU:HD21	1:J:203:TYR:CD2	2.51	0.44
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.53	0.43
1:C:170:PHE:O	1:C:174:MET:HG2	2.17	0.43
1: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

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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: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:135:TRP:CE2	1:H:138:LYS:HD3	2.54	0.42
1:F:36:THR:CB	1:F:50:GLN:HG3	2.49	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: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:E:131:TYR:CE1	1:E:462:GLN:HG3	2.54	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: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
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

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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: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: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:301:CYS:O	1:J:401:PHE:HE1	2.03	0.41
1:J:153:TYR:CZ	1:J:491:VAL:HB	2.56	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: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

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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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:376:ASP:N	1:J:376:ASP:OD1	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%)	49	76
1	B	399/402 (99%)	389 (98%)	10 (2%)	53	79
1	C	399/402 (99%)	391 (98%)	8 (2%)	60	84
1	D	399/402 (99%)	384 (96%)	15 (4%)	38	64
1	E	399/402 (99%)	388 (97%)	11 (3%)	49	76
1	F	399/402 (99%)	384 (96%)	15 (4%)	38	64
1	G	399/402 (99%)	390 (98%)	9 (2%)	56	81
1	H	399/402 (99%)	383 (96%)	16 (4%)	36	62
1	I	399/402 (99%)	389 (98%)	10 (2%)	53	79
1	J	399/402 (99%)	384 (96%)	15 (4%)	38	64
1	K	399/402 (99%)	388 (97%)	11 (3%)	49	76
1	L	399/402 (99%)	383 (96%)	16 (4%)	36	62
All	All	4788/4824 (99%)	4641 (97%)	147 (3%)	45	73

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

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
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 ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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]	-	25,29,29	1.96	6 (24%)	24,45,45	2.01	3 (12%)
3	ADP	A	501[B]	-	25,29,29	1.69	6 (24%)	24,45,45	2.00	2 (8%)
5	EDO	A	901	-	3,3,3	0.53	0	2,2,2	0.36	0
6	GAI	A	902	-	3,3,3	1.36	1 (33%)	3,3,3	1.18	0
4	NAD	B	502	-	41,48,48	2.09	8 (19%)	43,73,73	1.67	8 (18%)
5	EDO	B	701	-	3,3,3	0.43	0	2,2,2	0.40	0
5	EDO	B	802	-	3,3,3	0.40	0	2,2,2	0.49	0
5	EDO	B	902	-	3,3,3	0.30	0	2,2,2	0.47	0
4	NAD	C	503	-	41,48,48	2.17	8 (19%)	43,73,73	2.02	10 (23%)
5	EDO	C	803	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	C	903	-	3,3,3	0.62	0	2,2,2	0.35	0
3	ADP	D	504[A]	-	25,29,29	1.90	6 (24%)	24,45,45	1.91	3 (12%)
3	ADP	D	504[B]	-	25,29,29	1.59	4 (16%)	24,45,45	1.49	2 (8%)
5	EDO	D	704	-	3,3,3	0.59	0	2,2,2	0.30	0
5	EDO	D	904	-	3,3,3	0.41	0	2,2,2	0.38	0
6	GAI	D	905	-	3,3,3	1.56	1 (33%)	3,3,3	1.22	0
3	ADP	E	505	-	25,29,29	1.60	5 (20%)	24,45,45	2.19	2 (8%)
5	EDO	E	705	-	3,3,3	0.55	0	2,2,2	0.28	0
5	EDO	E	805	-	3,3,3	0.63	0	2,2,2	0.21	0
5	EDO	E	905	-	3,3,3	0.13	0	2,2,2	0.59	0
6	GAI	E	906	-	3,3,3	1.39	1 (33%)	3,3,3	1.26	0
6	GAI	E	907	-	3,3,3	1.55	1 (33%)	3,3,3	1.32	0
4	NAD	F	506	-	41,48,48	2.16	9 (21%)	43,73,73	1.85	7 (16%)
5	EDO	F	706	-	3,3,3	0.41	0	2,2,2	0.41	0
5	EDO	F	707	-	3,3,3	0.75	0	2,2,2	0.15	0
5	EDO	F	806	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	F	906	-	3,3,3	0.40	0	2,2,2	0.40	0
6	GAI	G	5009	-	3,3,3	1.37	1 (33%)	3,3,3	1.11	0
6	GAI	G	5010	-	3,3,3	1.52	1 (33%)	3,3,3	1.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAD	G	507	-	41,48,48	2.39	9 (21%)	43,73,73	1.69	7 (16%)
5	EDO	G	807	-	3,3,3	0.59	0	2,2,2	0.23	0
5	EDO	G	907	-	3,3,3	0.36	0	2,2,2	0.46	0
4	NAD	H	508	-	41,48,48	2.28	9 (21%)	43,73,73	1.77	7 (16%)
5	EDO	H	708	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	H	808	-	3,3,3	0.66	0	2,2,2	0.23	0
5	EDO	H	908	-	3,3,3	0.42	0	2,2,2	0.39	0
6	GAI	H	909	-	3,3,3	1.38	1 (33%)	3,3,3	1.13	0
3	ADP	I	509	-	25,29,29	1.75	6 (24%)	24,45,45	1.60	3 (12%)
5	EDO	I	809	-	3,3,3	0.66	0	2,2,2	0.18	0
5	EDO	I	909	-	3,3,3	0.38	0	2,2,2	0.39	0
6	GAI	I	910	-	3,3,3	1.53	1 (33%)	3,3,3	0.99	0
3	ADP	J	510	-	25,29,29	1.78	5 (20%)	24,45,45	1.76	2 (8%)
6	GAI	J	611	-	3,3,3	1.39	1 (33%)	3,3,3	1.18	0
3	ADP	K	511	-	25,29,29	1.63	5 (20%)	24,45,45	1.82	3 (12%)
5	EDO	K	911	-	3,3,3	0.60	0	2,2,2	0.28	0
3	ADP	L	512	-	25,29,29	1.64	5 (20%)	24,45,45	1.64	3 (12%)
5	EDO	L	712	-	3,3,3	0.55	0	2,2,2	0.29	0
5	EDO	L	912	-	3,3,3	0.43	0	2,2,2	0.39	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]	-	-	0/12/32/32	0/3/3/3
3	ADP	A	501[B]	-	-	0/12/32/32	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	-	-	0/22/62/62	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	-	-	0/22/62/62	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]	-	-	0/12/32/32	0/3/3/3
3	ADP	D	504[B]	-	-	0/12/32/32	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GAI	D	905	-	-	0/0/0/0	0/0/0/0
3	ADP	E	505	-	-	0/12/32/32	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	-	-	0/22/62/62	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
4	NAD	G	507	-	-	0/22/62/62	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	-	-	0/22/62/62	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	-	-	0/12/32/32	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	-	-	0/12/32/32	0/3/3/3
6	GAI	J	611	-	-	0/0/0/0	0/0/0/0
3	ADP	K	511	-	-	0/12/32/32	0/3/3/3
5	EDO	K	911	-	-	0/1/1/1	0/0/0/0
3	ADP	L	512	-	-	0/12/32/32	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 (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	507	NAD	C3N-C7N	-11.54	1.32	1.50
4	H	508	NAD	C3N-C7N	-10.11	1.34	1.50
4	B	502	NAD	C3N-C7N	-9.76	1.35	1.50
4	F	506	NAD	C3N-C7N	-9.35	1.36	1.50
4	C	503	NAD	C3N-C7N	-9.10	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	507	NAD	C5N-C4N	-3.58	1.32	1.38
4	H	508	NAD	C4N-C3N	-3.53	1.33	1.39
4	H	508	NAD	C5N-C4N	-3.49	1.32	1.38
4	G	507	NAD	C4N-C3N	-3.22	1.34	1.39
4	H	508	NAD	C2N-C3N	-3.09	1.34	1.39
4	B	502	NAD	C4N-C3N	-3.00	1.34	1.39
4	F	506	NAD	C5N-C4N	-3.00	1.33	1.38
4	F	506	NAD	C4N-C3N	-2.89	1.34	1.39
4	C	503	NAD	C5N-C4N	-2.77	1.33	1.38
3	A	501[B]	ADP	PB-O3A	-2.63	1.55	1.60
4	B	502	NAD	C2N-C3N	-2.55	1.35	1.39
4	C	503	NAD	C4N-C3N	-2.44	1.35	1.39
4	G	507	NAD	C2N-C3N	-2.37	1.35	1.39
3	D	504[B]	ADP	PB-O2B	-2.27	1.45	1.54
4	B	502	NAD	C5N-C4N	-2.10	1.34	1.38
3	A	501[B]	ADP	PB-O2B	-2.01	1.46	1.54
4	G	507	NAD	C4A-N3A	2.15	1.38	1.35
6	A	902	GAI	C-N1	2.15	1.35	1.30
3	I	509	ADP	C4-N3	2.20	1.38	1.35
3	K	511	ADP	PB-O3A	2.27	1.63	1.60
6	E	906	GAI	C-N1	2.31	1.35	1.30
6	G	5009	GAI	C-N1	2.31	1.35	1.30
6	H	909	GAI	C-N1	2.33	1.35	1.30
3	L	512	ADP	PB-O3A	2.34	1.63	1.60
3	A	501[A]	ADP	PB-O3B	2.34	1.64	1.54
6	J	611	GAI	C-N1	2.35	1.35	1.30
6	E	907	GAI	C-N1	2.40	1.35	1.30
3	A	501[B]	ADP	C4-N3	2.42	1.39	1.35
6	G	5010	GAI	C-N1	2.43	1.35	1.30
3	L	512	ADP	PB-O3B	2.45	1.64	1.54
3	K	511	ADP	PB-O3B	2.47	1.65	1.54
4	B	502	NAD	C8A-N7A	2.49	1.39	1.34
3	D	504[A]	ADP	C4-N3	2.50	1.39	1.35
4	B	502	NAD	O4D-C1D	2.56	1.44	1.41
6	D	905	GAI	C-N1	2.57	1.36	1.30
4	F	506	NAD	C2A-N1A	2.59	1.38	1.33
3	E	505	ADP	PB-O3B	2.60	1.65	1.54
4	F	506	NAD	C4A-N3A	2.62	1.39	1.35
4	F	506	NAD	O4B-C1B	2.62	1.44	1.41
6	I	910	GAI	C-N1	2.62	1.36	1.30
4	G	507	NAD	C8A-N7A	2.66	1.39	1.34
3	D	504[B]	ADP	C8-N7	2.67	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	508	NAD	O4B-C1B	2.69	1.45	1.41
3	J	510	ADP	C4-N3	2.70	1.39	1.35
4	H	508	NAD	C2A-N1A	2.70	1.39	1.33
3	A	501[B]	ADP	C8-N7	2.72	1.39	1.34
4	C	503	NAD	C8A-N7A	2.74	1.39	1.34
3	I	509	ADP	PB-O3B	2.80	1.66	1.54
3	I	509	ADP	PB-O3A	2.80	1.64	1.60
3	D	504[A]	ADP	C8-N7	2.81	1.39	1.34
3	J	510	ADP	C8-N7	2.87	1.40	1.34
4	H	508	NAD	C8A-N7A	2.92	1.40	1.34
3	E	505	ADP	C2-N1	2.96	1.39	1.33
4	B	502	NAD	C2A-N1A	2.99	1.39	1.33
4	G	507	NAD	O4D-C1D	3.02	1.45	1.41
4	F	506	NAD	O4D-C1D	3.03	1.45	1.41
3	I	509	ADP	C8-N7	3.03	1.40	1.34
4	F	506	NAD	C8A-N7A	3.05	1.40	1.34
3	A	501[A]	ADP	C8-N7	3.08	1.40	1.34
3	D	504[B]	ADP	C2-N1	3.08	1.39	1.33
3	L	512	ADP	C8-N7	3.14	1.40	1.34
3	K	511	ADP	C2-N1	3.15	1.39	1.33
4	C	503	NAD	O4D-C1D	3.16	1.45	1.41
3	K	511	ADP	C8-N7	3.16	1.40	1.34
3	E	505	ADP	C8-N7	3.21	1.40	1.34
3	L	512	ADP	C2-N1	3.24	1.40	1.33
3	J	510	ADP	C2-N1	3.28	1.40	1.33
4	G	507	NAD	C2A-N1A	3.32	1.40	1.33
3	I	509	ADP	C2-N1	3.33	1.40	1.33
4	H	508	NAD	C2A-N3A	3.38	1.37	1.32
3	A	501[A]	ADP	C4-N3	3.39	1.40	1.35
3	A	501[B]	ADP	C2-N1	3.44	1.40	1.33
3	D	504[A]	ADP	C2-N1	3.47	1.40	1.33
3	E	505	ADP	C2-N3	3.47	1.38	1.32
4	C	503	NAD	C4A-N3A	3.51	1.40	1.35
4	C	503	NAD	C2A-N1A	3.52	1.40	1.33
3	E	505	ADP	PB-O3A	3.60	1.65	1.60
3	A	501[A]	ADP	C2-N1	3.72	1.40	1.33
4	H	508	NAD	O4D-C1D	3.74	1.46	1.41
3	D	504[A]	ADP	PB-O3B	3.81	1.70	1.54
3	D	504[A]	ADP	PB-O3A	3.84	1.66	1.60
3	A	501[A]	ADP	PB-O3A	3.95	1.66	1.60
3	J	510	ADP	PB-O3A	4.06	1.66	1.60
4	G	507	NAD	C2A-N3A	4.21	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504[B]	ADP	C2-N3	4.41	1.39	1.32
3	K	511	ADP	C2-N3	4.42	1.39	1.32
3	J	510	ADP	C2-N3	4.51	1.39	1.32
3	A	501[B]	ADP	C2-N3	4.54	1.39	1.32
3	I	509	ADP	C2-N3	4.61	1.39	1.32
3	L	512	ADP	C2-N3	4.65	1.39	1.32
3	D	504[A]	ADP	C2-N3	4.73	1.40	1.32
4	B	502	NAD	C2A-N3A	4.74	1.40	1.32
3	A	501[A]	ADP	C2-N3	4.90	1.40	1.32
4	F	506	NAD	C2A-N3A	4.93	1.40	1.32
4	C	503	NAD	C2A-N3A	5.37	1.41	1.32

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	505	ADP	N3-C2-N1	-9.57	120.52	128.86
3	A	501[B]	ADP	N3-C2-N1	-8.27	121.66	128.86
4	H	508	NAD	N3A-C2A-N1A	-8.27	121.66	128.86
3	D	504[A]	ADP	N3-C2-N1	-7.95	121.93	128.86
3	J	510	ADP	N3-C2-N1	-7.20	122.59	128.86
4	C	503	NAD	N3A-C2A-N1A	-6.81	122.92	128.86
3	A	501[A]	ADP	N3-C2-N1	-6.69	123.03	128.86
4	G	507	NAD	N3A-C2A-N1A	-6.60	123.11	128.86
4	F	506	NAD	N3A-C2A-N1A	-6.57	123.14	128.86
3	L	512	ADP	N3-C2-N1	-6.29	123.38	128.86
3	K	511	ADP	N3-C2-N1	-6.24	123.42	128.86
4	B	502	NAD	N3A-C2A-N1A	-5.97	123.66	128.86
3	A	501[A]	ADP	C4'-O4'-C1'	-5.77	103.62	109.77
3	I	509	ADP	N3-C2-N1	-5.67	123.92	128.86
3	D	504[B]	ADP	N3-C2-N1	-5.56	124.02	128.86
3	K	511	ADP	C2'-C3'-C4'	-4.79	93.28	102.62
4	C	503	NAD	O7N-C7N-N7N	-4.70	115.89	122.58
4	C	503	NAD	O4D-C4D-C3D	-4.05	97.12	105.17
4	F	506	NAD	C2B-C3B-C4B	-3.93	94.97	102.62
4	C	503	NAD	C2B-C3B-C4B	-3.89	95.04	102.62
4	B	502	NAD	O4D-C4D-C3D	-3.77	97.67	105.17
4	H	508	NAD	O7N-C7N-N7N	-3.70	117.32	122.58
3	A	501[B]	ADP	C2'-C3'-C4'	-3.38	96.04	102.62
4	G	507	NAD	C3N-C2N-N1N	-3.02	117.39	120.43
4	F	506	NAD	O7N-C7N-N7N	-3.00	118.31	122.58
3	I	509	ADP	C4'-O4'-C1'	-2.95	106.63	109.77
3	J	510	ADP	C2'-C3'-C4'	-2.88	97.02	102.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	507	NAD	C6N-C5N-C4N	-2.87	115.11	119.44
3	L	512	ADP	C2'-C3'-C4'	-2.73	97.30	102.62
3	L	512	ADP	C1'-N9-C4	-2.71	121.95	126.64
4	G	507	NAD	C2D-C3D-C4D	-2.71	97.34	102.62
3	A	501[A]	ADP	C2'-C3'-C4'	-2.71	97.34	102.62
3	I	509	ADP	C2'-C3'-C4'	-2.67	97.42	102.62
3	E	505	ADP	C2'-C3'-C4'	-2.66	97.43	102.62
3	D	504[B]	ADP	C2'-C3'-C4'	-2.66	97.45	102.62
4	B	502	NAD	O7N-C7N-N7N	-2.61	118.86	122.58
4	H	508	NAD	C6N-C5N-C4N	-2.55	115.59	119.44
4	B	502	NAD	C2D-C3D-C4D	-2.55	97.66	102.62
4	F	506	NAD	C4B-O4B-C1B	-2.50	107.10	109.77
4	H	508	NAD	C2B-C3B-C4B	-2.50	97.75	102.62
4	G	507	NAD	C4N-C3N-C7N	-2.43	114.62	121.07
4	C	503	NAD	C6N-C5N-C4N	-2.39	115.83	119.44
3	D	504[A]	ADP	C2'-C3'-C4'	-2.36	98.02	102.62
4	B	502	NAD	C2B-C3B-C4B	-2.31	98.12	102.62
4	F	506	NAD	C5N-C4N-C3N	2.03	122.74	120.35
4	H	508	NAD	O5D-C5D-C4D	2.04	116.24	109.00
4	H	508	NAD	C2N-C3N-C4N	2.08	120.63	118.26
3	D	504[A]	ADP	C4-C5-N7	2.12	111.45	109.41
4	B	502	NAD	C4B-O4B-C1B	2.24	112.16	109.77
4	G	507	NAD	C5N-C6N-N1N	2.27	123.89	120.40
4	C	503	NAD	O7N-C7N-C3N	2.32	122.33	119.62
4	C	503	NAD	O5D-C5D-C4D	2.34	117.30	109.00
4	C	503	NAD	C5N-C4N-C3N	2.40	123.18	120.35
3	K	511	ADP	O5'-C5'-C4'	2.42	117.58	109.00
4	C	503	NAD	O5B-C5B-C4B	2.76	118.79	109.00
4	H	508	NAD	O7N-C7N-C3N	2.92	123.04	119.62
4	B	502	NAD	C1B-N9A-C4A	3.07	131.95	126.64
4	B	502	NAD	O7N-C7N-C3N	3.46	123.67	119.62
4	F	506	NAD	C3N-C7N-N7N	3.48	121.74	117.77
4	C	503	NAD	C3N-C7N-N7N	3.49	121.76	117.77
4	F	506	NAD	O4B-C4B-C3B	3.83	112.77	105.17
4	G	507	NAD	C2N-C3N-C4N	4.07	122.91	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 35 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	494/500 (98%)	0.69	57 (11%) 5 5	21, 67, 104, 123	0
1	B	494/500 (98%)	-0.16	4 (0%) 86 86	24, 40, 78, 98	0
1	C	494/500 (98%)	-0.13	2 (0%) 92 92	23, 40, 72, 88	0
1	D	494/500 (98%)	0.59	39 (7%) 13 13	25, 68, 97, 118	0
1	E	494/500 (98%)	-0.18	2 (0%) 92 92	23, 41, 68, 96	0
1	F	494/500 (98%)	-0.10	3 (0%) 89 89	21, 37, 66, 94	0
1	G	494/500 (98%)	0.06	5 (1%) 82 83	26, 46, 68, 98	0
1	H	494/500 (98%)	0.09	11 (2%) 62 64	24, 46, 77, 91	0
1	I	494/500 (98%)	0.36	21 (4%) 36 38	36, 58, 82, 105	0
1	J	494/500 (98%)	0.75	40 (8%) 13 12	44, 77, 104, 114	0
1	K	494/500 (98%)	0.55	37 (7%) 15 15	44, 71, 96, 115	0
1	L	494/500 (98%)	1.13	95 (19%) 1 1	47, 89, 115, 127	0
All	All	5928/6000 (98%)	0.31	316 (5%) 27 28	21, 55, 99, 127	0

All (316) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	378	GLY	7.3
1	L	369	CYS	6.0
1	L	223	GLY	5.2
1	L	386	PHE	5.0
1	G	474	GLY	5.0
1	L	373	ILE	4.9
1	A	371	GLY	4.8
1	D	424	THR	4.8
1	A	362	GLN	4.8
1	L	295	PHE	4.7
1	K	377	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	K	475	ARG	4.6
1	A	477	LEU	4.5
1	A	470	MET	4.4
1	L	333	ASN	4.4
1	J	365	ALA	4.4
1	D	327	LYS	4.3
1	A	353	ILE	4.3
1	A	473	SER	4.3
1	D	356	TYR	4.3
1	L	332	GLY	4.2
1	L	360	GLY	4.2
1	K	376	ASP	4.2
1	J	108	LEU	4.1
1	E	7	ALA	4.1
1	A	315	TYR	4.1
1	L	285	TRP	4.0
1	K	371	GLY	4.0
1	A	468	TYR	3.9
1	L	356	TYR	3.9
1	D	470	MET	3.9
1	L	350	PHE	3.9
1	L	482	LEU	3.9
1	K	474	GLY	3.9
1	D	376	ASP	3.9
1	L	318	PHE	3.9
1	J	7	ALA	3.8
1	L	327	LYS	3.8
1	L	380	PHE	3.8
1	L	478	GLY	3.8
1	L	387	GLY	3.8
1	L	354	LEU	3.8
1	L	357	ILE	3.8
1	K	473	SER	3.8
1	J	362	GLN	3.7
1	G	7	ALA	3.7
1	K	470	MET	3.7
1	L	310	VAL	3.7
1	L	377	ARG	3.7
1	A	424	THR	3.7
1	L	322	SER	3.6
1	A	394	THR	3.6
1	A	475	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	474	GLY	3.5
1	L	358	ASN	3.5
1	I	408	LEU	3.5
1	I	319	VAL	3.5
1	K	413	ILE	3.4
1	A	7	ALA	3.4
1	A	334	PRO	3.4
1	A	358	ASN	3.4
1	L	108	LEU	3.3
1	K	463	SER	3.3
1	A	367	LEU	3.3
1	L	468	TYR	3.3
1	L	480	TYR	3.3
1	A	377	ARG	3.3
1	J	425	TYR	3.2
1	K	471	SER	3.2
1	A	356	TYR	3.2
1	L	479	GLU	3.2
1	D	32	VAL	3.2
1	J	139	TYR	3.2
1	L	340	GLU	3.2
1	A	404	VAL	3.2
1	J	42	PRO	3.1
1	A	376	ASP	3.1
1	I	480	TYR	3.1
1	K	380	PHE	3.1
1	K	379	TYR	3.1
1	A	365	ALA	3.1
1	H	364	GLY	3.1
1	D	29	HIS	3.1
1	L	349	GLN	3.1
1	I	389	VAL	3.1
1	J	378	GLY	3.1
1	A	319	VAL	3.1
1	L	314	ILE	3.0
1	J	468	TYR	3.0
1	A	10	ALA	3.0
1	H	362	GLN	3.0
1	H	386	PHE	3.0
1	L	353	ILE	3.0
1	D	350	PHE	3.0
1	D	247	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	408	LEU	3.0
1	L	9	PRO	3.0
1	A	386	PHE	3.0
1	A	395	ILE	3.0
1	K	468	TYR	3.0
1	H	365	ALA	3.0
1	L	367	LEU	3.0
1	A	469	LYS	3.0
1	L	475	ARG	3.0
1	A	373	ILE	3.0
1	J	104	ALA	3.0
1	J	373	ILE	2.9
1	K	466	GLY	2.9
1	L	347	GLU	2.9
1	K	472	GLY	2.9
1	A	279	SER	2.9
1	J	22	ILE	2.9
1	D	31	ALA	2.9
1	H	7	ALA	2.9
1	J	476	GLU	2.9
1	D	353	ILE	2.9
1	D	365	ALA	2.9
1	F	477	LEU	2.9
1	K	375	ALA	2.9
1	I	139	TYR	2.9
1	H	290	ALA	2.8
1	K	484	ALA	2.8
1	J	30	ASP	2.8
1	J	247	THR	2.8
1	L	216	GLY	2.8
1	L	28	TRP	2.8
1	K	139	TYR	2.8
1	G	477	LEU	2.8
1	L	376	ASP	2.7
1	L	8	VAL	2.7
1	L	329	ARG	2.7
1	K	17	VAL	2.7
1	A	326	ALA	2.7
1	L	115	VAL	2.7
1	D	471	SER	2.7
1	L	465	PHE	2.7
1	L	139	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	46	GLU	2.7
1	D	253	ILE	2.7
1	J	32	VAL	2.7
1	L	463	SER	2.7
1	L	113	PRO	2.7
1	I	470	MET	2.7
1	A	287	VAL	2.6
1	K	465	PHE	2.6
1	D	475	ARG	2.6
1	K	467	GLY	2.6
1	A	295	PHE	2.6
1	J	33	SER	2.6
1	J	31	ALA	2.6
1	L	385	VAL	2.6
1	J	44	THR	2.6
1	L	413	ILE	2.6
1	K	7	ALA	2.6
1	L	319	VAL	2.6
1	A	398	GLU	2.6
1	L	466	GLY	2.6
1	J	376	ASP	2.6
1	L	27	GLU	2.6
1	J	392	GLY	2.6
1	I	486	THR	2.6
1	J	374	ALA	2.6
1	A	379	TYR	2.6
1	A	100	THR	2.5
1	G	486	THR	2.5
1	L	363	GLU	2.5
1	D	468	TYR	2.5
1	L	461	ALA	2.5
1	A	256	ALA	2.5
1	L	365	ALA	2.5
1	L	462	GLN	2.5
1	J	347	GLU	2.5
1	A	327	LYS	2.5
1	D	379	TYR	2.5
1	A	397	LYS	2.5
1	D	199	LEU	2.5
1	B	253	ILE	2.5
1	D	334	PRO	2.5
1	L	301	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	203	TYR	2.5
1	L	47	VAL	2.5
1	J	386	PHE	2.5
1	D	100	THR	2.5
1	L	66	ALA	2.5
1	D	8	VAL	2.4
1	L	40	VAL	2.4
1	D	399	GLU	2.4
1	J	53	GLU	2.4
1	I	141	GLY	2.4
1	E	424	THR	2.4
1	A	357	ILE	2.4
1	H	360	GLY	2.4
1	K	332	GLY	2.4
1	L	339	THR	2.4
1	K	478	GLY	2.4
1	L	266	THR	2.4
1	L	486	THR	2.4
1	K	479	GLU	2.4
1	A	323	VAL	2.4
1	I	318	PHE	2.4
1	L	7	ALA	2.4
1	I	411	LYS	2.4
1	L	338	LYS	2.4
1	D	51	VAL	2.4
1	L	323	VAL	2.4
1	A	480	TYR	2.4
1	L	42	PRO	2.4
1	L	393	MET	2.4
1	L	473	SER	2.4
1	J	63	VAL	2.4
1	J	56	LYS	2.4
1	A	114	TYR	2.4
1	I	479	GLU	2.4
1	A	332	GLY	2.3
1	F	254	GLN	2.3
1	J	283	MET	2.3
1	B	473	SER	2.3
1	D	337	SER	2.3
1	K	259	SER	2.3
1	I	474	GLY	2.3
1	L	141	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	317	GLU	2.3
1	L	320	GLU	2.3
1	L	296	PHE	2.3
1	L	328	SER	2.3
1	G	475	ARG	2.3
1	J	377	ARG	2.3
1	C	477	LEU	2.3
1	I	388	ASP	2.3
1	L	405	MET	2.3
1	A	465	PHE	2.3
1	K	386	PHE	2.3
1	I	482	LEU	2.3
1	D	40	VAL	2.3
1	J	389	VAL	2.3
1	D	413	ILE	2.3
1	D	477	LEU	2.3
1	J	467	GLY	2.2
1	J	72	LEU	2.2
1	L	315	TYR	2.2
1	L	384	THR	2.2
1	J	358	ASN	2.2
1	A	314	ILE	2.2
1	D	46	GLU	2.2
1	H	316	ASP	2.2
1	K	392	GLY	2.2
1	B	260	SER	2.2
1	L	104	ALA	2.2
1	I	248	GLU	2.2
1	L	73	GLY	2.2
1	A	328	SER	2.2
1	J	319	VAL	2.2
1	A	476	GLU	2.2
1	K	312	GLU	2.2
1	L	395	ILE	2.2
1	K	477	LEU	2.2
1	L	228	ALA	2.2
1	D	36	THR	2.2
1	D	111	GLY	2.2
1	J	379	TYR	2.1
1	H	323	VAL	2.1
1	L	250	GLY	2.1
1	L	276	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	433	THR	2.1
1	D	473	SER	2.1
1	D	377	ARG	2.1
1	A	466	GLY	2.1
1	L	371	GLY	2.1
1	I	477	LEU	2.1
1	K	482	LEU	2.1
1	H	473	SER	2.1
1	I	312	GLU	2.1
1	D	338	LYS	2.1
1	L	44	THR	2.1
1	A	102	LEU	2.1
1	J	34	ARG	2.1
1	B	71	GLN	2.1
1	H	315	TYR	2.1
1	L	379	TYR	2.1
1	D	30	ASP	2.1
1	D	42	PRO	2.1
1	L	51	VAL	2.1
1	L	227	THR	2.1
1	L	24	ILE	2.1
1	F	465	PHE	2.1
1	J	246	SER	2.1
1	L	140	HIS	2.1
1	L	199	LEU	2.1
1	I	478	GLY	2.1
1	A	384	THR	2.1
1	A	306	SER	2.1
1	D	295	PHE	2.1
1	K	18	PHE	2.1
1	K	483	GLN	2.1
1	A	479	GLU	2.1
1	A	283	MET	2.0
1	C	7	ALA	2.0
1	A	359	THR	2.0
1	D	467	GLY	2.0
1	J	466	GLY	2.0
1	J	140	HIS	2.0
1	K	33	SER	2.0
1	A	118	TYR	2.0
1	A	392	GLY	2.0
1	I	356	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	386	PHE	2.0
1	L	224	PHE	2.0
1	D	248	GLU	2.0
1	L	334	PRO	2.0
1	I	375	ALA	2.0
1	K	412	THR	2.0
1	L	247	THR	2.0
1	D	323	VAL	2.0
1	L	277	ILE	2.0
1	K	441	TYR	2.0
1	A	312	GLU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	G	5008	1/1	0.97	0.48	20.55	48,48,48,48	0
2	NA	C	5004	1/1	0.94	0.47	19.94	51,51,51,51	0
2	NA	C	603	1/1	0.69	0.23	10.47	54,54,54,54	0
5	EDO	F	706	4/4	0.87	0.37	8.94	74,76,79,80	0
5	EDO	E	705	4/4	0.91	0.34	8.59	77,80,80,80	0
6	GAI	I	910	4/4	0.87	0.43	7.36	94,94,94,95	0
5	EDO	E	805	4/4	0.81	0.44	7.33	83,83,85,85	0
5	EDO	B	902	4/4	0.94	0.30	6.93	63,63,65,65	0
6	GAI	E	906	4/4	0.90	0.32	6.79	51,54,55,55	0
2	NA	B	5003	1/1	0.88	0.18	6.64	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GAI	H	909	4/4	0.89	0.31	5.44	95,95,95,95	0
5	EDO	I	809	4/4	0.69	0.35	5.05	81,82,82,82	0
2	NA	F	5007	1/1	0.92	0.22	5.05	54,54,54,54	0
6	GAI	G	5010	4/4	0.94	0.24	4.28	47,47,49,49	0
2	NA	A	601	1/1	0.62	0.27	3.89	82,82,82,82	0
5	EDO	F	707	4/4	0.90	0.29	3.65	59,59,61,61	0
6	GAI	D	905	4/4	0.80	0.28	3.03	77,78,78,78	0
5	EDO	B	802	4/4	0.83	0.23	2.79	48,48,52,53	0
6	GAI	G	5009	4/4	0.93	0.24	2.55	76,76,76,76	0
3	ADP	D	504[A]	27/27	0.76	0.29	2.45	79,81,86,86	27
3	ADP	D	504[B]	27/27	0.76	0.29	2.28	89,91,96,96	27
6	GAI	A	902	4/4	0.95	0.18	2.21	63,64,64,65	0
5	EDO	L	712	4/4	0.84	0.25	1.88	70,72,73,73	0
5	EDO	B	701	4/4	0.95	0.20	1.69	67,67,67,68	0
4	NAD	B	502	44/44	0.88	0.23	1.56	73,88,103,104	0
5	EDO	H	908	4/4	0.83	0.26	1.53	79,79,79,80	0
6	GAI	E	907	4/4	0.89	0.20	1.52	47,48,49,49	0
6	GAI	J	611	4/4	0.87	0.22	1.23	64,66,66,66	0
2	NA	K	5012	1/1	0.92	0.18	1.20	60,60,60,60	0
5	EDO	H	708	4/4	0.96	0.19	1.08	47,49,51,53	0
3	ADP	A	501[A]	27/27	0.87	0.20	0.88	78,80,81,81	27
3	ADP	A	501[B]	27/27	0.87	0.20	0.88	91,93,93,93	27
4	NAD	G	507	44/44	0.90	0.19	0.80	61,77,91,92	0
5	EDO	H	808	4/4	0.92	0.20	0.75	63,64,64,65	0
4	NAD	C	503	44/44	0.88	0.20	0.63	58,81,92,93	0
4	NAD	F	506	44/44	0.92	0.17	0.39	38,68,81,84	0
2	NA	I	609	1/1	0.82	0.15	0.31	54,54,54,54	0
5	EDO	F	806	4/4	0.97	0.16	0.31	53,54,54,58	0
3	ADP	E	505	27/27	0.92	0.15	0.25	43,52,79,80	0
4	NAD	H	508	44/44	0.90	0.16	0.24	49,81,89,90	0
5	EDO	C	803	4/4	0.93	0.14	0.14	49,53,53,55	0
3	ADP	K	511	27/27	0.91	0.17	0.05	94,99,105,106	0
3	ADP	L	512	27/27	0.91	0.21	-0.22	89,97,112,113	0
3	ADP	I	509	27/27	0.92	0.16	-0.39	79,81,94,95	0
2	NA	L	612	1/1	0.88	0.18	-0.57	80,80,80,80	0
3	ADP	J	510	27/27	0.84	0.18	-0.71	102,104,114,115	0
5	EDO	D	704	4/4	0.95	0.13	-1.07	53,54,56,56	0
5	EDO	G	807	4/4	0.89	0.16	-1.35	75,75,75,75	0
2	NA	D	604	1/1	0.70	0.10	-1.94	73,73,73,73	0
2	NA	H	608	1/1	0.93	0.10	-2.00	46,46,46,46	0
2	NA	J	610	1/1	0.57	0.12	-2.17	75,75,75,75	0
2	NA	E	605	1/1	0.91	0.07	-2.61	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	K	611	1/1	0.92	0.09	-2.78	63,63,63,63	0
2	NA	F	606	1/1	0.95	0.07	-2.97	32,32,32,32	0
2	NA	G	607	1/1	0.84	0.07	-3.07	46,46,46,46	0
2	NA	B	602	1/1	0.97	0.05	-3.62	40,40,40,40	0
5	EDO	I	909	4/4	0.93	0.14	-	62,62,63,64	0
5	EDO	F	906	4/4	0.96	0.18	-	63,63,65,65	0
5	EDO	E	905	4/4	0.93	0.23	-	51,52,53,58	0
5	EDO	K	911	4/4	0.69	0.23	-	79,80,80,80	0
5	EDO	G	907	4/4	0.85	0.33	-	68,68,68,69	0
5	EDO	A	901	4/4	0.89	0.29	-	75,75,76,77	0
5	EDO	C	903	4/4	0.76	0.27	-	45,49,49,52	0
5	EDO	D	904	4/4	0.82	0.24	-	74,74,75,75	0
5	EDO	L	912	4/4	0.95	0.26	-	68,69,70,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.