Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:56 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

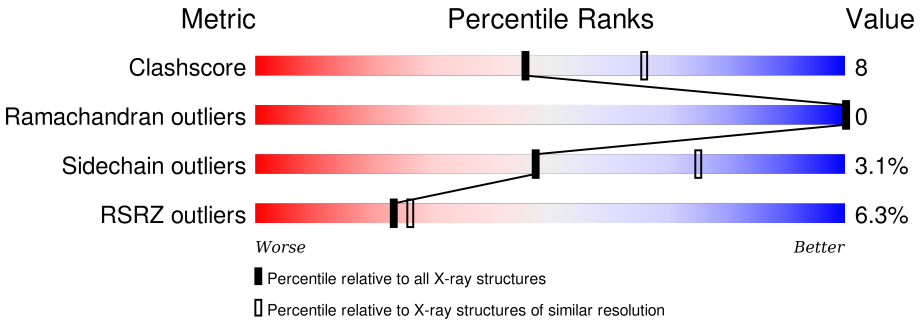
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	13% 80% 18%
1	B	500	% 84% 14%
1	C	500	% 82% 16%
1	D	500	9% 80% 18%
1	E	500	% 82% 16%
1	F	500	% 82% 16%
1	G	500	2% 82% 16%

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Mol	Chain	Length	Quality of chain
1	H	500	3% 80% 17%
1	I	500	5% 83% 15%
1	J	500	9% 77% 20%
1	K	500	9% 84% 14%
1	L	500	22% 80% 18%

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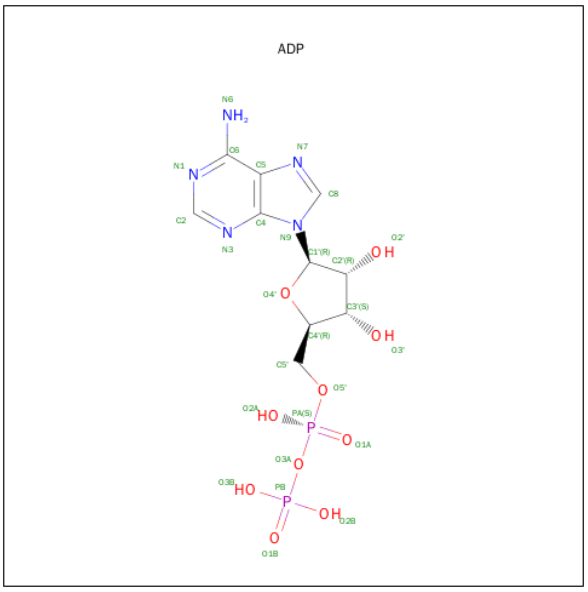
Chain	Residue	Modelled	Actual	Comment	Reference
F	487	LYS	GLU	ENGINEERED	UNP P05091
G	487	LYS	GLU	ENGINEERED	UNP P05091
H	487	LYS	GLU	ENGINEERED	UNP P05091
I	487	LYS	GLU	ENGINEERED	UNP P05091
J	487	LYS	GLU	ENGINEERED	UNP P05091
K	487	LYS	GLU	ENGINEERED	UNP P05091
L	487	LYS	GLU	ENGINEERED	UNP P05091

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

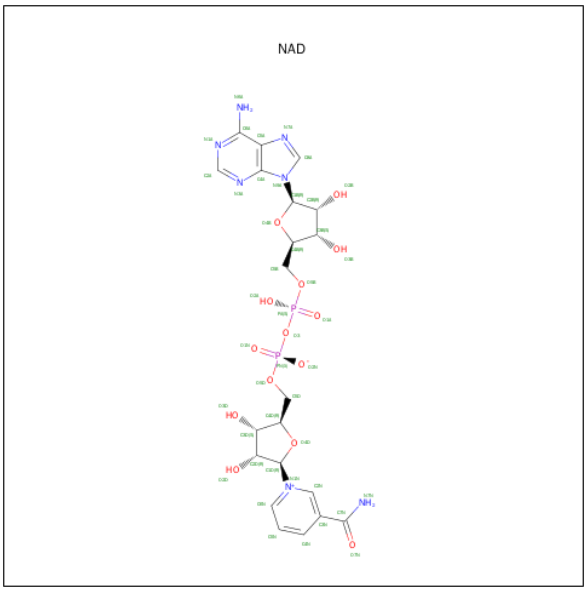
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Na 2 2	0	0
2	J	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	K	2	Total Na 2 2	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	2	Total Na 2 2	0	0
2	I	1	Total Na 1 1	0	0
2	C	2	Total Na 2 2	0	0
2	A	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0
2	F	2	Total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

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



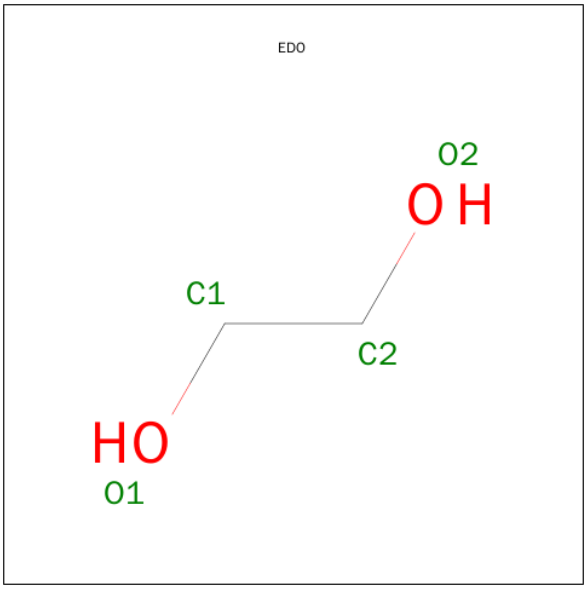
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	D	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	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: $C_{21}H_{27}N_7O_{14}P_2$).



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: $C_2H_6O_2$).



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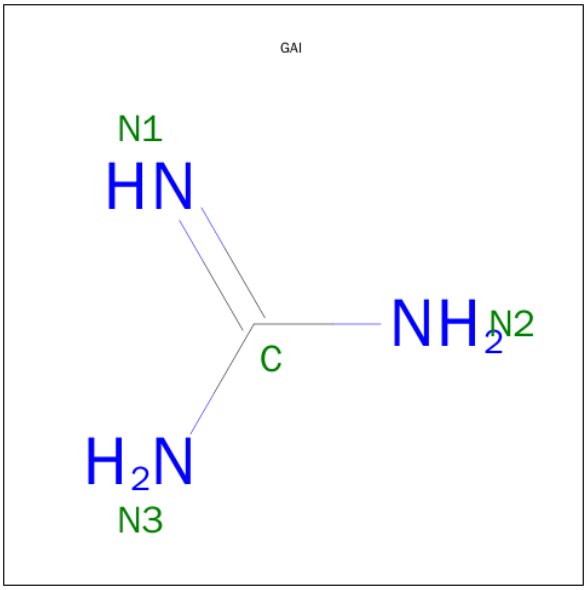
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0

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



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

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

- Molecule 7 is water.

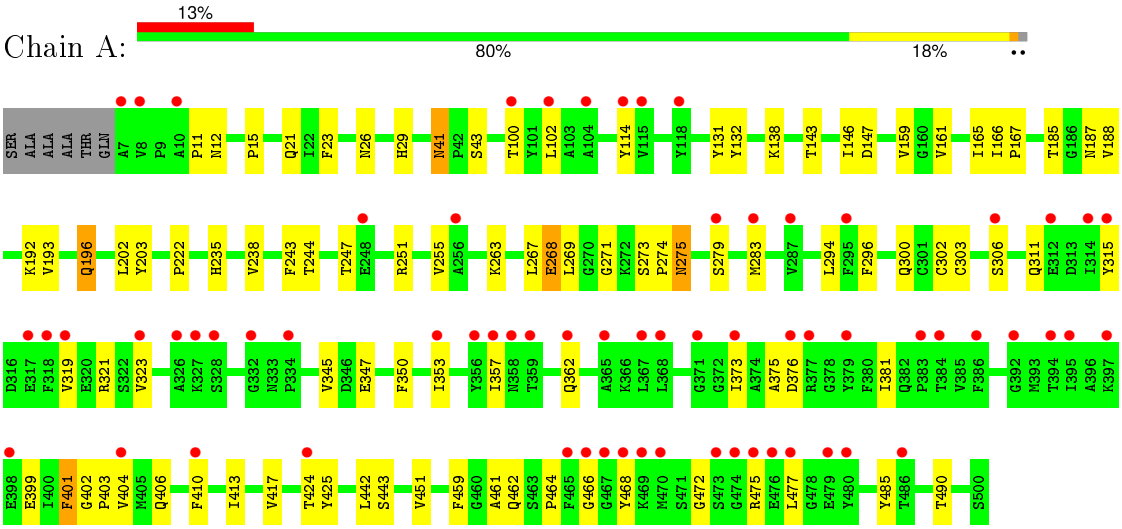
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	121	Total O 121 121	0	0
7	B	223	Total O 223 223	0	0
7	C	232	Total O 232 232	0	0
7	D	133	Total O 133 133	0	0
7	E	264	Total O 264 264	0	0
7	F	251	Total O 251 251	0	0
7	G	186	Total O 186 186	0	0
7	H	185	Total O 185 185	0	0
7	I	131	Total O 131 131	0	0
7	J	63	Total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

3 Residue-property plots (i)

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.

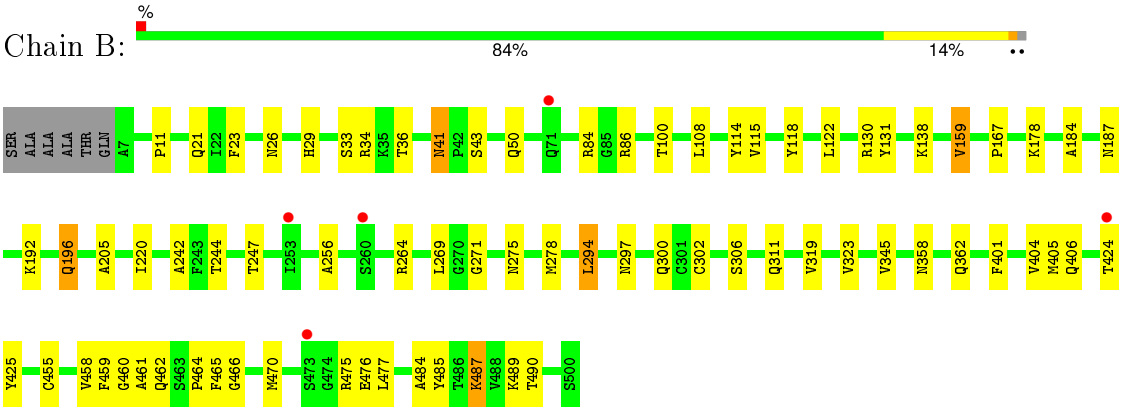
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain A:



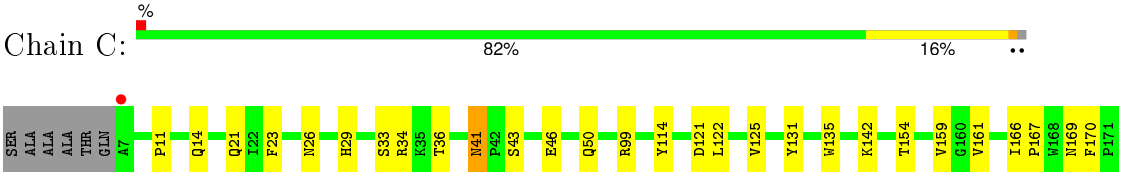
- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

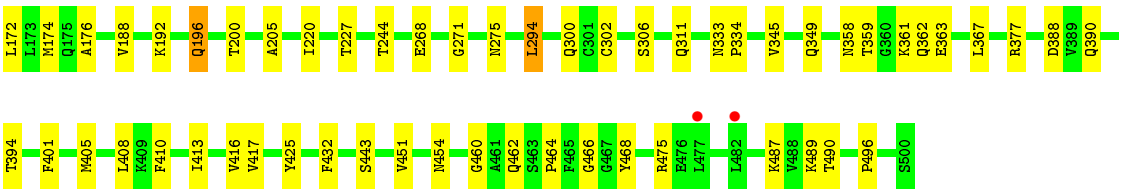
Chain B:



- Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

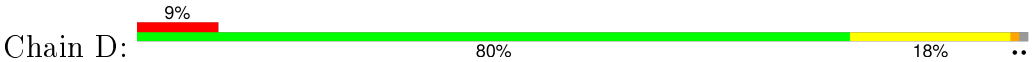
Chain C:

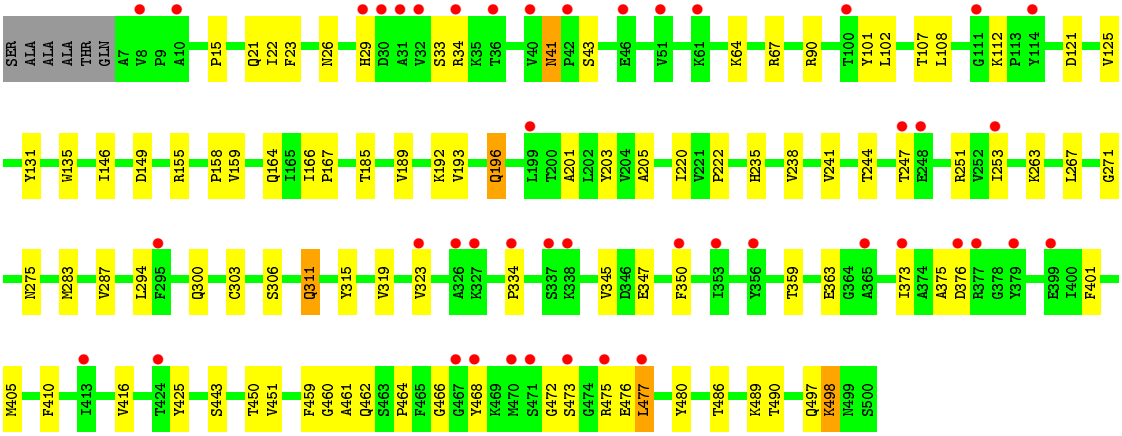




• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

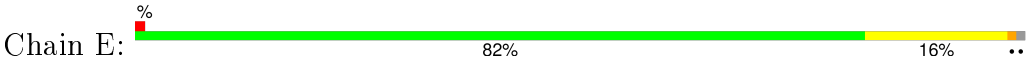
Chain D:

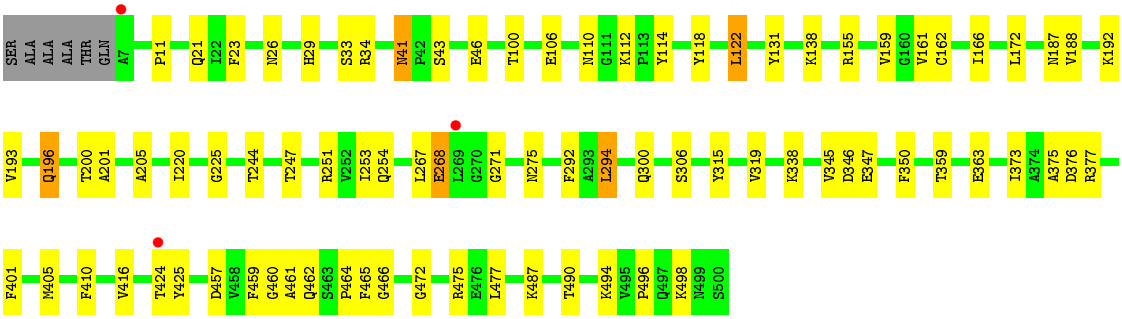




• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

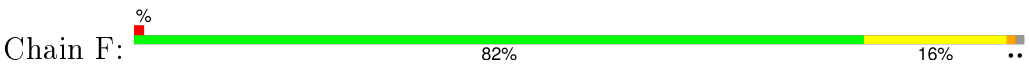
Chain E:

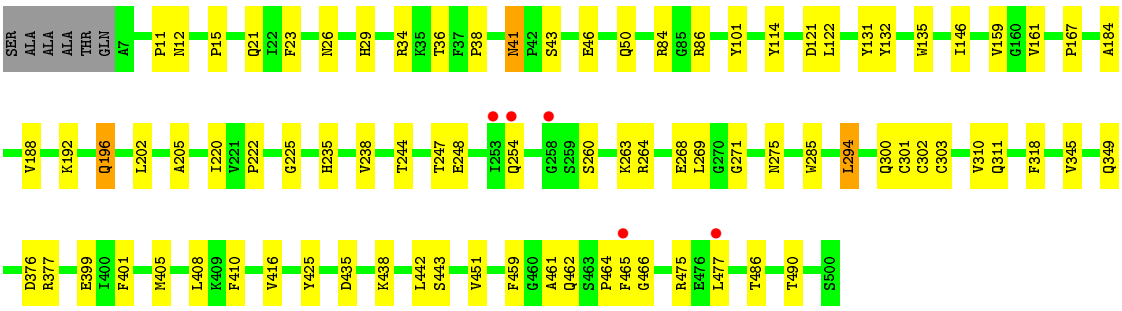




• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

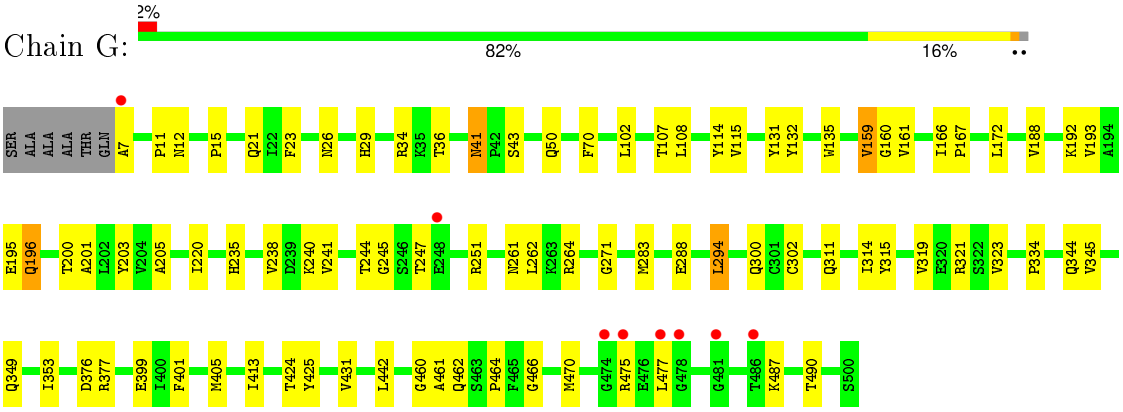
Chain F:





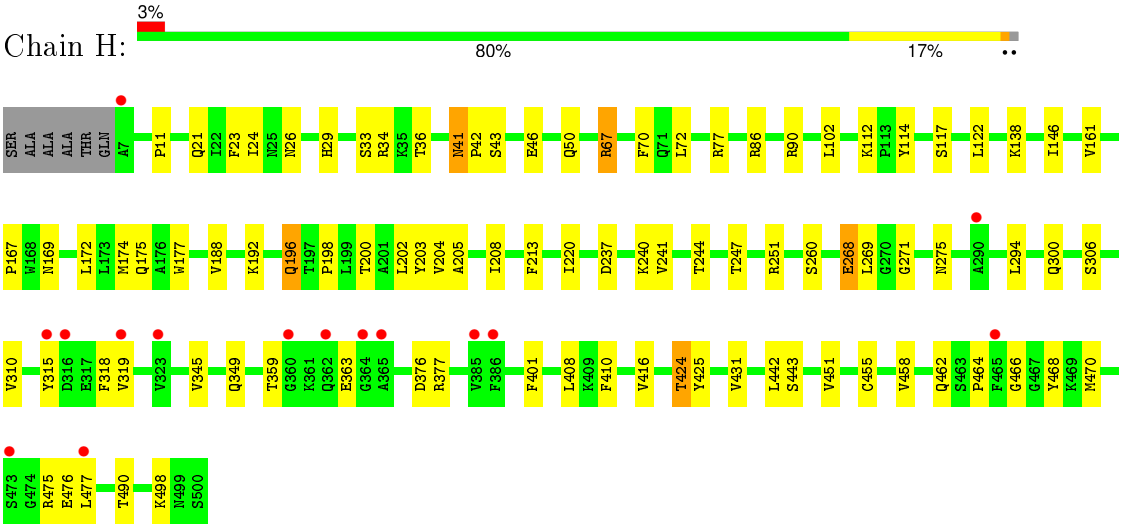
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain G:



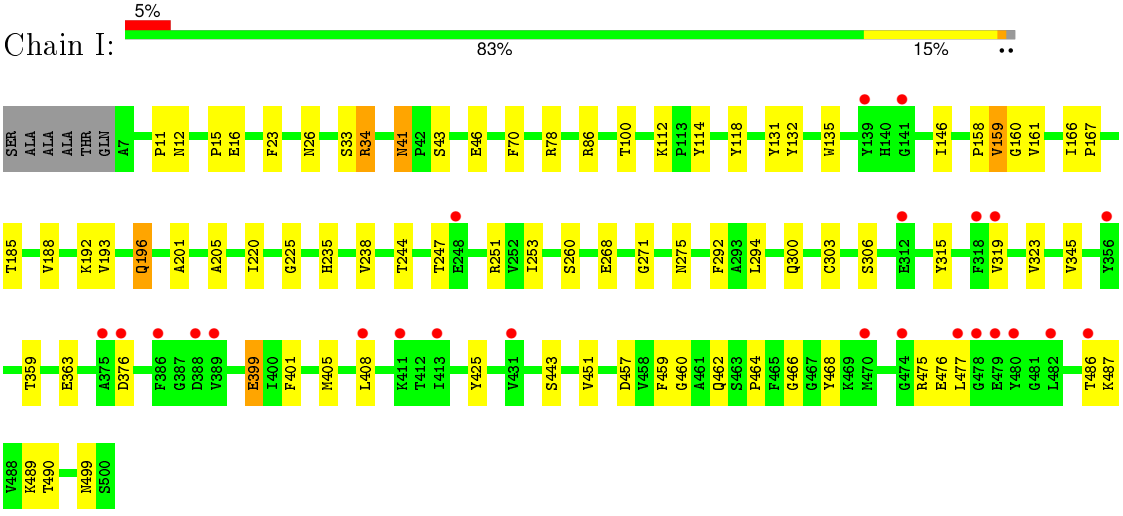
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

Chain H:

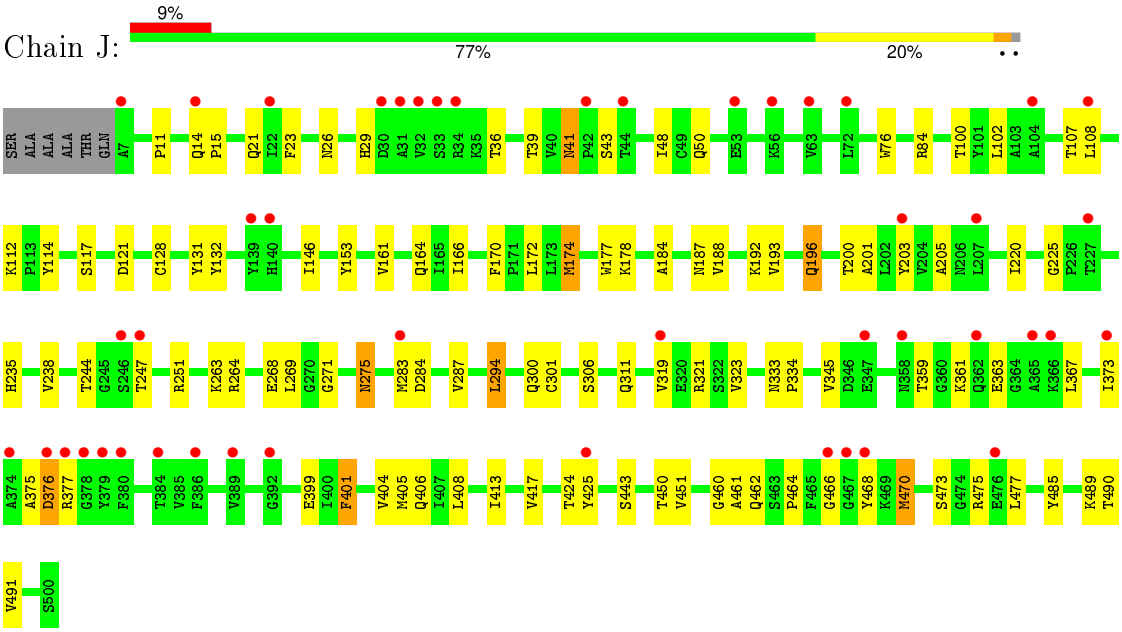


• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

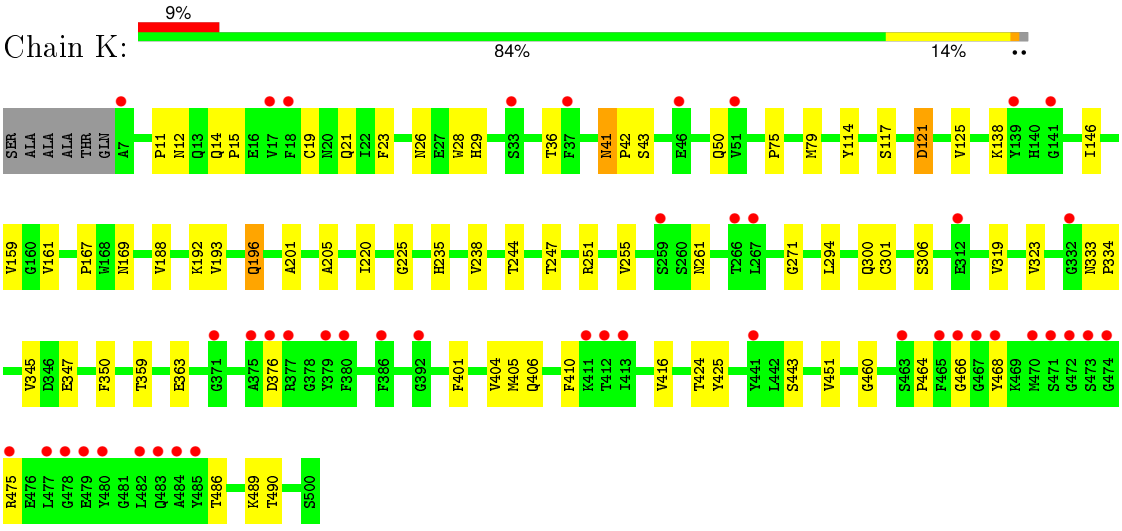
Chain I:



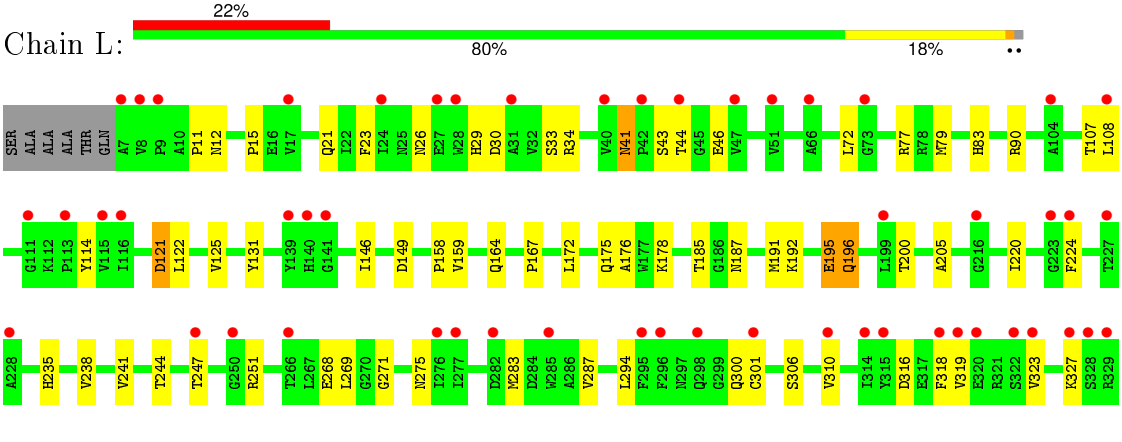
• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor

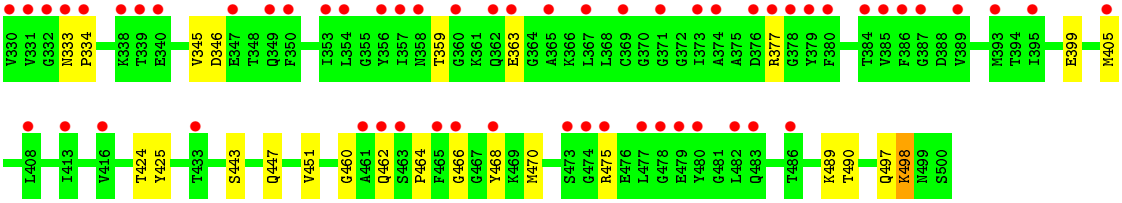


• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor



• Molecule 1: Aldehyde dehydrogenase, mitochondrial precursor




V330
V331
G332
N333
P334
K338
T339
E340
V345
D346
E347
T348
Q349
F350
I353
L354
G355
Y356
I357
N358
T359
G360
K361
Q362
E363
G364
A365
K366
L367
L368
C369
G370
G371
G372
I373
A374
A375
D376
R377
G378
Y379
F380
T384
V385
F386
G387
D388
V389
N393
T394
I395
E399
M405
L408
I413
V416
T424
Y425
T433
S443
Q447
V451
G460
A461
Q462
S463
P464
F465
G466
G467
Y468
K469
M470
S473
G474
R475
E476
L477
G478
E479
Y480
G481
L482
Q483
T486
K489
T490
Q497
K498
N499
S500

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	96.20Å 104.85Å 162.36Å 78.99° 82.14° 88.55°	Depositor
Resolution (Å)	44.01 – 2.50 48.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.01-2.50) 88.2 (48.95-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
1	J	264	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	E	122	LEU	CA-CB-CG	-5.51	102.63	115.30
1	A	143	THR	N-CA-C	-5.17	97.04	111.00
1	B	130	ARG	NE-CZ-NH1	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3752	78	0
1	B	3798	0	3752	57	0
1	C	3798	0	3752	63	0
1	D	3798	0	3752	63	0
1	E	3798	0	3752	67	0
1	F	3798	0	3752	55	0
1	G	3798	0	3752	64	0
1	H	3798	0	3752	56	0
1	I	3798	0	3752	74	0
1	J	3798	0	3752	75	0
1	K	3798	0	3752	46	0
1	L	3798	0	3752	62	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
3	A	54	0	24	3	0
3	D	54	0	24	1	0
3	E	27	0	12	2	0
3	I	27	0	12	2	0
3	J	27	0	12	1	0
3	K	27	0	12	1	0
3	L	27	0	12	0	0
4	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:HD22	1:E:41:ASN:C	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: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	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.72	0.71
1:C:41:ASN:HD22	1:C:43:SER:H	1.39	0.71
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.73	0.71
1:G:41:ASN:C	1:G:41:ASN:HD22	1.94	0.71
1:D:41:ASN:HD22	1:D:43:SER:H	1.39	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:466:GLY:HA3	1:F:475:ARG:HD3	1.76	0.67
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.75	0.67
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.30	0.67
1:L:196:GLN:NE2	1:L:196:GLN:H	1.92	0.67
1:A:41:ASN:HD22	1:A:43:SER:H	1.43	0.67
1:C:14:GLN:HG2	7:C:2212:HOH:O	1.95	0.67
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:A:131:TYR:CE1	1:A:462:GLN:HG3	2.30	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:NE2	1:B:196:GLN:H	1.91	0.66
1:J:36:THR:HB	1:J:50:GLN:HG3	1.77	0.66
1:D:166:ILE:HD11	1:D:193:VAL:HG12	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:K:196:GLN:HE21	1:K:196:GLN:N	1.91	0.65
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.79	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:K:36:THR:HB	1:K:50:GLN:HG3	1.78	0.64
1:D:443:SER:HA	1:D:451:VAL:HG11	1.80	0.64
1:I:41:ASN:C	1:I:41:ASN:HD22	2.01	0.64
1:B:461:ALA:HA	1:B:477:LEU:HD22	1.79	0.64
1:I:464:PRO:HG2	1:J:490:THR:OG1	1.97	0.64
1:A:350:PHE:O	1:A:353:ILE:HG22	1.96	0.64
1:K:294:LEU:HD12	1:K:306:SER:HA	1.79	0.64
1:A:41:ASN:ND2	1:A:43:SER:H	1.96	0.63
1:L:271:GLY:HA2	1:L:425:TYR:CG	2.32	0.63
1:G:271:GLY:HA2	1:G:425:TYR:CG	2.33	0.63
1:A:102:LEU:HD21	1:A:203:TYR:HD2	1.62	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: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:A:353:ILE:HD11	1:A:403:PRO:HD2	1.82	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:L:23:PHE:CZ	1:L:26:ASN:HA	2.35	0.61
1:I:23:PHE:CZ	1:I: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:D:23:PHE:CZ	1:D:26:ASN:HA	2.36	0.61
1:K:121:ASP:O	1:K:125:VAL:HG23	2.01	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:B:34:ARG:HG2	1:B:34:ARG:HH11	1.64	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:I:78:ARG:HH11	1:L:497:GLN:NE2	1.98	0.60
1:B:36:THR:OG1	1:B:50:GLN:HG3	2.01	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:E:159:VAL:HG12	1:E:187:ASN:OD1	2.02	0.60
1:C:125:VAL:HG13	1:C:176:ALA:HB2	1.83	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: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:D:271:GLY:HA2	1:D:425:TYR:CG	2.37	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:J:102:LEU:HD21	1:J:203:TYR:HD2	1.68	0.58
1:G:166:ILE:HD11	1:G:193:VAL:HG12	1.85	0.58
1:K:247:THR:O	1:K:251:ARG:HG3	2.03	0.58
1:K:41:ASN:HD22	1:K:41:ASN:C	2.06	0.58
1:G:36:THR:HB	1:G:50:GLN:HG3	1.86	0.58
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.39	0.58
1:L:466:GLY:HA3	1:L:475:ARG:HD3	1.86	0.58
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.39	0.57
1: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:H:208:ILE:HG23	1:H:213:PHE:CD1	2.39	0.57
1:K:41:ASN:ND2	1:K:43:SER:H	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:36:THR:HB	1:C:50:GLN:HG3	1.87	0.56
1:A:279:SER:HB3	1:A:311:GLN:HG2	1.88	0.56
1:L:34:ARG:NH1	1:L:34:ARG:HG3	2.20	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
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:D:311:GLN:HG2	1:D:410:PHE:CZ	2.41	0.55
1:J:244:THR:HG23	1:J:268:GLU:HB2	1.88	0.55
1:C:443:SER:HA	1:C:451:VAL:HG11	1.87	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:I:460:GLY:HA3	1:J:146:ILE:HG13	1.87	0.55
1:F:38:PRO:HD3	1:F:50:GLN:HE22	1.70	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:K:490:THR:OG1	1:L:464:PRO:HG2	2.07	0.55
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.42	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:F:443:SER:HA	1:F:451:VAL:HG11	1.90	0.54
1:B:108:LEU:HD11	5:B:802:EDO:H12	1.90	0.54
1:F:41:ASN:ND2	1:F:43:SER:H	2.05	0.54
1:L:41:ASN:ND2	1:L:43:SER:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.43	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:D:319:VAL:O	1:D:323:VAL:HG23	2.07	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:L:319:VAL:O	1:L:323:VAL:HG23	2.08	0.54
1:I:399:GLU:OE1	1:I:399:GLU:HA	2.06	0.54
1:I:12:ASN:O	1:I:15:PRO:HD3	2.08	0.53
1:E:21:GLN:HB3	1:E:29:HIS:O	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:K:443:SER:HA	1:K:451:VAL:HG11	1.91	0.53
1:F:264:ARG:NH2	7:F:2163:HOH:O	2.40	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:G:251:ARG:NH1	1:H:260:SER:O	2.41	0.53
1:F:12:ASN:O	1:F:15:PRO:HD3	2.09	0.53
1:I:294:LEU:HD12	1:I:306:SER:HA	1.91	0.53
1:H:21:GLN:HB3	1:H:29:HIS:O	2.09	0.53
1:J:187:ASN:ND2	1:J:485:TYR:HB3	2.23	0.53
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:490:THR:OG1	1:D:464:PRO:HG2	2.09	0.52
1:J:76:TRP:CH2	1:J:84:ARG:HG2	2.44	0.52
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.44	0.52
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.73	0.52
1:L:235:HIS:HB3	1:L:238:VAL:HG23	1.91	0.52
1:D:167:PRO:HD3	1:D:244:THR:HB	1.90	0.52
1:I:41:ASN:HD22	1:I:43:SER:H	1.57	0.52
1:L:41:ASN:HD22	1:L:41:ASN:C	2.13	0.52
1:L:121:ASP:O	1:L:125:VAL:HG23	2.10	0.52
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.45	0.52
1:E:196:GLN:HE21	1:E:196:GLN:N	1.94	0.52
1:C:489:LYS:HB2	1:D:468:TYR:OH	2.09	0.52
1:I:70:PHE:CZ	1:I:160:GLY:HA2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:ARG:HD2	1:H:237:ASP:OD2	2.10	0.52
1:H:41:ASN:HD21	1:H:43:SER:HB2	1.75	0.52
1:C:302:CYS:SG	7:C:2137:HOH:O	2.59	0.52
1:I:159:VAL:HA	1:I:487:LYS:HG3	1.90	0.52
1:A:146:ILE:HG13	1:B:460:GLY:HA3	1.91	0.52
1:A:12:ASN:O	1:A:15:PRO:HD3	2.10	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:G:21:GLN:HB3	1:G:29:HIS:O	2.09	0.52
1:E:464:PRO:HG2	1:F:490:THR:OG1	2.09	0.52
1:J:247:THR:O	1:J:251:ARG:HG3	2.09	0.52
1:D:33:SER:O	1:D:34:ARG:HB2	2.10	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:L:399:GLU:OE1	1:L:399:GLU:HA	2.10	0.51
1:K:23:PHE:CZ	1:K:26:ASN:HA	2.45	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:E:41:ASN:ND2	1:E:41:ASN:C	2.61	0.51
1:I:167:PRO:HD3	1:I:244:THR:HB	1.93	0.51
1:E:193:VAL:HG11	1:E:201:ALA:CB	2.41	0.51
1:B:278:MET:HE3	7:B:1529:HOH:O	2.11	0.51
1:K:41:ASN:HD22	1:K:43:SER:H	1.57	0.51
1:H:175:GLN:HE22	1:H:204:VAL:HB	1.76	0.51
1:D:41:ASN:HD21	1:D:43:SER:HB2	1.76	0.51
1:A:353:ILE:HD12	1:A:402:GLY:HA3	1.91	0.51
1:G:399:GLU:HG3	7:G:1106:HOH:O	2.10	0.51
1:C:460:GLY:HA3	1:D:146:ILE:HG13	1.92	0.51
1:B:159:VAL:HA	1:B:487:LYS:HD3	1.93	0.51
1:A:21:GLN:HB3	1:A:29:HIS:O	2.11	0.51
1:C:349:GLN:HB3	7:C:1069:HOH:O	2.11	0.51
1:F:86:ARG:HD2	7:F:2867:HOH:O	2.10	0.51
1:C:408:LEU:HD12	1:C:408:LEU:N	2.25	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:H:310:VAL:HG21	1:H:318:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:283:MET:HG3	1:A:321:ARG:HH11	1.76	0.50
1:A:187:ASN:ND2	1:A:485:TYR:HB3	2.26	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:K:300:GLN:NE2	1:K:345:VAL:H	2.01	0.50
1:E:254:GLN:HE21	1:F:254:GLN:HE21	1.58	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:302:CYS:HB3	4:F:506:NAD:O7N	2.11	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: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:B:84:ARG:NH1	1:B:184:ALA:O	2.44	0.49
1:I:268:GLU:OE2	1:I:476:GLU:HG3	2.12	0.49
1:L:271:GLY:HA2	1:L:425:TYR:CD2	2.48	0.49
1:B:424:THR:HG22	1:B:470:MET:HB2	1.93	0.49
1:I:33:SER:O	1:I:34:ARG:CB	2.60	0.49
1:D:294:LEU:CD1	1:D:306:SER:HA	2.41	0.49
1:A:296:PHE:HA	7:A:2378:HOH:O	2.12	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:I:78:ARG:NH1	1:L:497:GLN:HE21	2.09	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: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:L:294:LEU:CD1	1:L:306:SER:HA	2.39	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:D:149:ASP:HA	1:D:498:LYS:HB2	1.95	0.48
1:I:132:TYR:OH	1:I:477:LEU:HA	2.12	0.48
1:E:494:LYS:HE3	1:F:285:TRP:CZ2	2.48	0.48
1:K:235:HIS:HB3	1:K:238:VAL:HG23	1.95	0.48
1:G:195:GLU:H	1:G:195:GLU:CD	2.16	0.48
1:I:294:LEU:HD13	1:I:405:MET:HA	1.94	0.48
1:E:294:LEU:HD12	1:E:306:SER:HA	1.94	0.48
1:C:468:TYR:OH	1:D:489:LYS:HB2	2.13	0.48
1:F:377:ARG:HB2	7:F:2647:HOH:O	2.14	0.48
1:K:11:PRO:HB3	1:K:114:TYR:CZ	2.47	0.48
1:J:41:ASN:HD22	1:J:41:ASN:C	2.16	0.48
1:F:459:PHE:HE2	1:F:465:PHE:CE1	2.32	0.48
1:K:261:ASN:HA	1:L:470:MET:CE	2.44	0.48
1:I:468:TYR:OH	1:J:489:LYS:HB2	2.12	0.48
1:E:338:LYS:CD	1:I:34:ARG:NH2	2.75	0.48
1:E:172:LEU:HD21	1:E:200:THR:HB	1.94	0.48
1:D:247:THR:O	1:D:251:ARG:HG3	2.13	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:I:253:ILE:HD11	3:I:509:ADP:C2	2.49	0.48
1:L:125:VAL:HG13	1:L:176:ALA:HB2	1.96	0.48
1:G:159:VAL:HG23	1:G:264:ARG:NH1	2.28	0.48
1:J:193:VAL:HG11	1:J:201:ALA:CB	2.43	0.48
1:B:41:ASN:HD21	1:B:43:SER:HB2	1.78	0.48
1:G:41:ASN:ND2	1:G:41:ASN:C	2.64	0.47
1:A:319:VAL:O	1:A:323:VAL:HG23	2.14	0.47
1:J:319:VAL:O	1:J:323:VAL:HG23	2.14	0.47
1:J:408:LEU:N	1:J:408:LEU:HD12	2.28	0.47
1:B:294:LEU:HD12	1:B:306:SER:HA	1.96	0.47
1: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:I:193:VAL:HG11	1:I:201:ALA:CB	2.45	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

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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:J:461:ALA:HA	1:J:477:LEU:HD22	1.96	0.47
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.95	0.47
1:G:41:ASN:HD21	1:G:43:SER:HB2	1.78	0.47
1:G:349:GLN:O	1:G:353:ILE:HG13	2.14	0.47
1:C:302:CYS:HB3	4:C:503:NAD:O7N	2.13	0.47
1:A:283:MET:CG	1:A:321:ARG:NH1	2.78	0.47
1:J:132:TYR:OH	1:J:477:LEU:HA	2.14	0.47
1:A:247:THR:HG23	1:A:269:LEU:HD13	1.97	0.47
1:F:435:ASP:HB3	1:F:438:LYS:HD2	1.97	0.47
1:C:159:VAL:HA	1:C:487:LYS:HD2	1.97	0.47
1:B:297:ASN:HA	7:B:1057:HOH:O	2.14	0.47
1:J:164:GLN:CD	1:J:178:LYS:HB3	2.35	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:G:302:CYS:HB3	4:G:507:NAD:O7N	2.14	0.47
1:J:247:THR:HG23	1:J:269:LEU:HD13	1.96	0.47
1:G:413:ILE:HD11	1:G:442:LEU:HG	1.97	0.47
1:I:158:PRO:HG3	1:I:185:THR:O	2.15	0.47
1:G:460:GLY:HA3	1:H:146:ILE:HG13	1.97	0.47
1:J:161:VAL:HA	1:J:188:VAL:HG23	1.97	0.47
1:I:100:THR:HG22	1:I:118:TYR:CE1	2.50	0.47
1:L:11:PRO:HB3	1:L:114:TYR:CZ	2.50	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: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:L:21:GLN:HB3	1:L:29:HIS:O	2.15	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: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:A:302:CYS:HA	1:A:401:PHE:CZ	2.50	0.46
1:H:408:LEU:N	1:H:408:LEU:HD12	2.30	0.46
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.97	0.46
1:J:36:THR:CB	1:J:50:GLN:HG3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:SER:O	1:J:251:ARG:NH1	2.48	0.46
1:G:431:VAL:HG21	1:G:442:LEU:HB3	1.97	0.46
1:G:235:HIS:HB3	1:G:238:VAL:HG23	1.97	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:C:413:ILE:O	1:C:417:VAL:HG23	2.16	0.46
1:B:247:THR:HA	1:B:269:LEU:HD13	1.98	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:J:187:ASN:HD21	1:J:485:TYR:HB3	1.80	0.46
1:D:461:ALA:HA	1:D:477:LEU:CD1	2.46	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: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:B:459:PHE:HE2	1:B:465:PHE:CE1	2.34	0.46
1:A:294:LEU:CD1	1:A:306:SER:HA	2.44	0.46
1:G:271:GLY:HA2	1:G:425:TYR:CD2	2.50	0.46
1:G:319:VAL:O	1:G:323:VAL:HG23	2.15	0.46
1:C:294:LEU:HD12	1:C:306:SER:HA	1.98	0.46
1:A:161:VAL:HA	1:A:188:VAL:HG23	1.98	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: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:F:235:HIS:HB3	1:F:238:VAL:HG23	1.98	0.45
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.16	0.45
1:J:235:HIS:HB3	1:J:238:VAL:HG23	1.98	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:A:283:MET:HG3	1:A:321:ARG:NH1	2.31	0.45
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.16	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: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:L:310:VAL:HG21	1:L:318:PHE:CD2	2.51	0.45
1:K:359:THR:O	1:K:363:GLU:HG3	2.16	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:L:172:LEU:HD21	1:L:200:THR:HB	1.97	0.45
1:G:172:LEU:HD21	1:G:200:THR:HB	1.98	0.45
1:K:225:GLY:HA3	3:K:511:ADP:C8	2.51	0.45
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.17	0.45
1:L:15:PRO:HG2	1:L:108:LEU:HD22	1.99	0.45
1:G:36:THR:CB	1:G:50:GLN:HG3	2.45	0.45
1:A:413:ILE:HD11	1:A:442:LEU:HG	1.99	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: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:L:316:ASP:N	7:L:2214:HOH:O	2.49	0.45
1:I:292:PHE:HE1	1:I:457:ASP:HB2	1.81	0.45
1:A:202:LEU:HD21	1:A:222:PRO:HG3	1.99	0.45
1:L:247:THR:HA	1:L:269:LEU:HD13	1.98	0.45
1:B:178:LYS:HE3	1:B:242:ALA:HB1	1.97	0.45
1:E:338:LYS:HD2	1:I:34:ARG:NH2	2.21	0.45
1:B:264:ARG:NH1	1:B:484:ALA:O	2.50	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: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:C:358:ASN:ND2	7:C:2390:HOH:O	2.48	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:E:315:TYR:O	1:E:319:VAL:HG23	2.17	0.44
1:D:359:THR:O	1:D:363:GLU:HG3	2.17	0.44
1:D:347:GLU:O	1:D:350:PHE:HB3	2.17	0.44
1:J:131:TYR:CZ	1:J:462:GLN:HA	2.52	0.44
1:D:460:GLY:O	1:D:477:LEU:HD12	2.17	0.44
1:C:294:LEU:HD22	1:C:405:MET:HB2	2.00	0.44
1:H:86:ARG:HG3	7:H:1869:HOH:O	2.18	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:D:107:THR:HG23	1:D:112:LYS:O	2.17	0.44
1:C:166:ILE:HD11	7:C:1483:HOH:O	2.17	0.44
1:K:294:LEU:HD22	1:K:405:MET:HB2	1.99	0.44
1:B:167:PRO:HB2	4:B:502:NAD:H5N	1.99	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:D:102:LEU:HD21	1:D:203:TYR:HD2	1.81	0.44
1:H:247:THR:O	1:H:251:ARG:HG3	2.17	0.44
1:E:498:LYS:HE2	1:E:498:LYS:HB3	1.75	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:J:15:PRO:HD2	1:J:108:LEU:HD22	2.00	0.44
1:D:373:ILE:HG22	1:D:375:ALA:H	1.82	0.44
1:A:315:TYR:O	1:A:319:VAL:HG23	2.17	0.44
1:A:165:ILE:HG22	3:A:501[B]:ADP:H4'	2.00	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:J:102:LEU:HD21	1:J:203:TYR:CD2	2.51	0.44
1:I:100:THR:HG22	1:I:118:TYR:HE1	1.83	0.44
1:G:167:PRO:HD3	1:G:244:THR:HB	1.99	0.44
1:C:41:ASN:C	1:C:41:ASN:ND2	2.66	0.43
1:D:235:HIS:HB3	1:D:238:VAL:HG23	2.00	0.43
1:C:170:PHE:O	1:C:174:MET:HG2	2.17	0.43
1:F:131:TYR:CE1	1:F:462:GLN:HG3	2.53	0.43
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.53	0.43
1:D:158:PRO:HG3	1:D:185:THR:O	2.17	0.43
1:A:347:GLU:O	1:A:350:PHE:HB3	2.17	0.43
1:E:338:LYS:NZ	1:I:34:ARG:NE	2.66	0.43
1:A:353:ILE:CG2	1:A:381:ILE:CD1	2.95	0.43
1:I:490:THR:HG1	1:J:464:PRO:HG2	1.81	0.43
1:A:238:VAL:O	1:A:263:LYS:HE3	2.18	0.43
1:L:283:MET:O	1:L:287:VAL:HG23	2.19	0.43
1:D:294:LEU:HD13	1:D:405:MET:HA	2.00	0.43
1:A:353:ILE:CG2	1:A:381:ILE:HD13	2.49	0.43
1:F:36:THR:HB	1:F:50:GLN:HG3	2.00	0.43
1:B:86:ARG:HD3	7:B:2785:HOH:O	2.19	0.43
1:D:267:LEU:O	1:D:472:GLY:HA3	2.18	0.43
1:D:101:TYR:CG	5:D:904:EDO:H11	2.54	0.43
1:C:361:LYS:HE2	1:C:367:LEU:HD22	2.01	0.43
1:H:169:ASN:OD1	1:H:169:ASN:N	2.49	0.43
1:L:345:VAL:HG13	1:L:346:ASP:N	2.34	0.43
1:K:251:ARG:O	1:K:255:VAL:HG23	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:159:VAL:HG12	1:L:187:ASN:OD1	2.19	0.43
1:K:404:VAL:HG12	1:K:406:GLN:OE1	2.18	0.43
1:E:244:THR:HG23	1:E:268:GLU:HB3	2.01	0.43
1:J:238:VAL:O	1:J:263:LYS:HE3	2.18	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:D:311:GLN:HG2	1:D:410:PHE:CE1	2.53	0.43
1:A:302:CYS:HA	1:A:401:PHE:HZ	1.84	0.43
1:K:161:VAL:HA	1:K:188:VAL:HG23	2.00	0.43
1:H:315:TYR:CE1	1:H:319:VAL:HG21	2.54	0.43
1:I:78:ARG:NH1	1:L:497:GLN:NE2	2.62	0.43
1:H:244:THR:HG23	1:H:268:GLU:HB3	2.01	0.43
1:E:461:ALA:HA	1:E:477:LEU:HD22	2.01	0.43
1:A:273:SER:HA	1:A:274:PRO:HD2	1.95	0.43
1:L:167:PRO:HD3	1:L:244:THR:HB	2.00	0.43
1:A:185:THR:OG1	1:A:187:ASN:ND2	2.52	0.42
1: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:H:455:CYS:SG	1:H:458:VAL:HG21	2.59	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:D:461:ALA:HA	1:D:477:LEU:HD13	2.01	0.42
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.19	0.42
1:E:106:GLU:O	1:E:110:ASN:HB3	2.19	0.42
1:G:108:LEU:HD11	5:G:807:EDO:O1	2.19	0.42
1:K:36:THR:CB	1:K:50:GLN:HG3	2.47	0.42
1:F:36:THR:CB	1:F:50:GLN:HG3	2.49	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:G:261:ASN:HA	1:H:470:MET:HE2	2.01	0.42
1:L:195:GLU:HG2	1:L:224:PHE:HA	2.01	0.42
1:I:408:LEU:N	1:I:408:LEU:HD12	2.33	0.42
1:E:345:VAL:HG13	1:E:346:ASP:N	2.33	0.42
1:C:41:ASN:HD21	1:C:43:SER:HB2	1.84	0.42
1:L:41:ASN:HD22	1:L:43:SER:H	1.68	0.42
1:L:11:PRO:HB3	1:L:114:TYR:CE1	2.54	0.42
1:A:167:PRO:HD3	1:A:244:THR:O	2.20	0.42
1:E:315:TYR:CE1	1:E:319:VAL:HG21	2.54	0.42
1:G:240:LYS:HG2	1:G:241:VAL:N	2.34	0.42
1:E:131:TYR:CE1	1:E:462:GLN:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:373:ILE:HG22	1:J:375:ALA:H	1.85	0.42
1:D:476:GLU:O	1:D:477:LEU:HB2	2.19	0.42
1:C:142:LYS:HE2	1:D:480:TYR:CZ	2.55	0.42
1:K:410:PHE:CD1	1:K:416:VAL:HB	2.55	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:L:158:PRO:HG3	1:L:185:THR:O	2.19	0.42
1:K:42:PRO:HB3	1:K:345:VAL:O	2.19	0.42
1:H:41:ASN:ND2	1:H:41:ASN:C	2.66	0.42
1:C:271:GLY:HA2	1:C:425:TYR:CD2	2.54	0.42
1:E:254:GLN:HE21	1:F:254:GLN:NE2	2.17	0.42
1:E:377:ARG:NH1	7:E:1554:HOH:O	2.51	0.42
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.55	0.42
1:B:476:GLU:O	1:B:477:LEU:HB2	2.20	0.42
1:J:41:ASN:HD22	1:J:43:SER:H	1.68	0.42
1:A:167:PRO:HD3	1:A:244:THR:HB	2.00	0.42
1:C:99:ARG:HG3	1:C:122:LEU:HD22	2.01	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:H:443:SER:HA	1:H:451:VAL:HG11	2.01	0.42
1:B:455:CYS:SG	1:B:458:VAL:HG21	2.59	0.42
1:A:404:VAL:HG12	1:A:406:GLN:OE1	2.20	0.42
1:H:70:PHE:CD1	1:H:77:ARG:HD3	2.55	0.42
1:D:283:MET:O	1:D:287:VAL:HG23	2.19	0.42
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.55	0.42
1:A:235:HIS:HB3	1:A:238:VAL:HG23	2.01	0.42
1:F:101:TYR:CG	5:F:906:EDO:H11	2.54	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:138:LYS:HE3	1:G:135:TRP:CD1	2.55	0.42
1:I:490:THR:O	1:J:450:THR:HA	2.20	0.41
1:D:410:PHE:CD1	1:D:416:VAL:HB	2.55	0.41
1:B:108:LEU:HD11	5:B:802:EDO:C1	2.50	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:D:164:GLN:OE1	1:D:189:VAL:HG11	2.20	0.41
1:L:294:LEU:HD13	1:L:405:MET:HA	2.02	0.41
1:I:319:VAL:O	1:I:323:VAL:HG23	2.20	0.41
1:C:410:PHE:CD1	1:C:416:VAL:HB	2.55	0.41
1:I:462:GLN:OE1	1:I:462:GLN:N	2.50	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:A:247:THR:HA	1:A:269:LEU:HD22	2.01	0.41
1:E:225:GLY:HA3	3:E:505:ADP:C8	2.56	0.41
1:I:315:TYR:O	1:I:319:VAL:HG23	2.20	0.41
1:K:193:VAL:HG11	1:K:201:ALA:CB	2.50	0.41
1:D:64:LYS:HA	7:D:1478:HOH:O	2.21	0.41
1:H:431:VAL:HG21	1:H:442:LEU:HB3	2.01	0.41
1:K:167:PRO:HD3	1:K:244:THR:HB	2.01	0.41
1:C:169:ASN:OD1	1:C:169:ASN:N	2.52	0.41
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.79	0.41
1:C:154:THR:HA	1:C:489:LYS:O	2.20	0.41
1:J:301:CYS:O	1:J:401:PHE:HE1	2.03	0.41
1:L:175:GLN:HG3	1:L:191:MET:SD	2.60	0.41
1: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:J:153:TYR:CZ	1:J:491:VAL:HB	2.56	0.41
1:G:201:ALA:HB2	7:G:1228:HOH:O	2.21	0.41
1:J:11:PRO:HB3	1:J:114:TYR:CZ	2.56	0.41
1:G:262:LEU:HD13	1:H:269:LEU:HD11	2.01	0.41
1:E:347:GLU:O	1:E:350:PHE:HB3	2.20	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:L:323:VAL:O	1:L:327:LYS:HG3	2.21	0.41
1:H:161:VAL:HA	1:H:188:VAL:HG23	2.02	0.41
1:I:205:ALA:HB2	1:I:220:ILE:HD12	2.02	0.41
1:C:333:ASN:HA	1:C:334:PRO:HD2	1.92	0.41
1:K:333:ASN:HA	1:K:334:PRO:HD2	1.93	0.41
1:J:23:PHE:CE1	1:J:26:ASN:HA	2.55	0.41
1:C:363:GLU:CD	1:C:394:THR:H	2.23	0.41
1:J:359:THR:O	1:J:363:GLU:HG3	2.20	0.41
1:K:19:CYS:HB3	1:K:28:TRP:CH2	2.56	0.41
1:I:112:LYS:HB3	1:I:112:LYS:HE2	1.91	0.41
1:J:39:THR:HG23	1:J:48:ILE:HB	2.01	0.41
1:H:42:PRO:HB3	1:H:345:VAL:O	2.21	0.41
1:B:33:SER:O	1:B:34:ARG:HB2	2.21	0.41
1:I:294:LEU:HD22	1:I:405:MET:HB2	2.02	0.41
1:C:358:ASN:O	1:C:362:GLN:HG2	2.21	0.41
1:D:107:THR:HG23	1:D:334:PRO:HB2	2.02	0.41
1:L:333:ASN:HA	1:L:334:PRO:HD2	1.91	0.41
1:B:187:ASN:HD21	1:B:485:TYR:HB3	1.86	0.41
1:G:115:VAL:HG23	7:G:1190:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:ARG:NH1	7:G:1164:HOH:O	2.54	0.41
1:J:164:GLN:NE2	1:J:178:LYS:HB3	2.36	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:A:311:GLN:OE1	1:A:410:PHE:CE1	2.75	0.40
1:E:373:ILE:HG22	1:E:375:ALA:H	1.86	0.40
1:C:227:THR:HG21	7:C:1394:HOH:O	2.21	0.40
1:J:413:ILE:O	1:J:417:VAL:HG23	2.21	0.40
1:H:112:LYS:HE2	1:H:112:LYS:HB3	1.86	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:F:238:VAL:O	1:F:263:LYS:HE3	2.21	0.40
1:I:196:GLN:NE2	1:I:196:GLN:N	2.63	0.40
1:E:100:THR:HG23	7:E:1808:HOH:O	2.21	0.40
1:G:245:GLY:HA2	4:G:507:NAD:C4N	2.51	0.40
1:J:166:ILE:HD11	1:J:193:VAL:HG12	2.04	0.40
1:L:164:GLN:OE1	1:L:178:LYS:HB3	2.21	0.40
1:I:303:CYS:SG	1:I:459:PHE:HZ	2.43	0.40
1:J:128:CYS:SG	1:J:177:TRP:HD1	2.44	0.40
1:L:79:MET:SD	1:L:83:HIS:HD2	2.44	0.40
1:F:442:LEU:HA	1:F:442:LEU:HD23	1.96	0.40
1:E:159:VAL:CG1	1:E:162:CYS:SG	3.10	0.40
1:F:225:GLY:HA3	4:F:506:NAD:C8A	2.51	0.40
1:J:333:ASN:HA	1:J:334:PRO:HD2	1.96	0.40
1:F:303:CYS:SG	1:F:459:PHE:HZ	2.44	0.40
1:A:399:GLU:CD	1:A:401:PHE:CE1	2.95	0.40
1:H:424:THR:CG2	1:H:470:MET:SD	3.10	0.40
1:K:466:GLY:HA3	1:K:475:ARG:HD3	2.03	0.40
1:D:497:GLN:HB3	7:D:2272:HOH:O	2.21	0.40
1:K:169:ASN:ND2	7:K:2893:HOH:O	2.54	0.40
1:I:161:VAL:HA	1:I:188:VAL:HG23	2.03	0.40
1:E:112:LYS:HB3	1:E:112:LYS:HE2	1.77	0.40
1:E:267:LEU:O	1:E:472:GLY:HA3	2.21	0.40
1:A:146:ILE:HG12	1:A:147:ASP:N	2.37	0.40
1:D:112:LYS:HB3	1:D:112:LYS:HE2	1.92	0.40
1:H:410:PHE:CD1	1:H:416:VAL:HB	2.57	0.40
1:A:251:ARG:O	1:A:255:VAL:HG23	2.20	0.40
1:H:174:MET:HE2	1:H:177:TRP:CE3	2.56	0.40
1:F:310:VAL:HG21	1:F:318:PHE:CD2	2.57	0.40
1:G:70:PHE:CZ	1:G:160:GLY:HA2	2.56	0.40
1:J:376:ASP:N	1:J:376:ASP:OD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:LEU:HD12	1:F:408:LEU:N	2.36	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
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%)	51	78
1	B	399/402 (99%)	389 (98%)	10 (2%)	55	82
1	C	399/402 (99%)	391 (98%)	8 (2%)	63	86
1	D	399/402 (99%)	384 (96%)	15 (4%)	40	67
1	E	399/402 (99%)	388 (97%)	11 (3%)	51	78
1	F	399/402 (99%)	384 (96%)	15 (4%)	40	67
1	G	399/402 (99%)	390 (98%)	9 (2%)	58	83
1	H	399/402 (99%)	383 (96%)	16 (4%)	38	64
1	I	399/402 (99%)	389 (98%)	10 (2%)	55	82
1	J	399/402 (99%)	384 (96%)	15 (4%)	40	67
1	K	399/402 (99%)	388 (97%)	11 (3%)	51	78
1	L	399/402 (99%)	383 (96%)	16 (4%)	38	64
All	All	4788/4824 (99%)	4641 (97%)	147 (3%)	47	75

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 (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	501[A]	-	22,29,29	1.88	5 (22%)	27,45,45	2.25	6 (22%)
3	ADP	A	501[B]	-	22,29,29	1.69	6 (27%)	27,45,45	2.11	2 (7%)
5	EDO	A	901	-	3,3,3	0.54	0	2,2,2	0.43	0
6	GAI	A	902	-	0,3,3	0.00	-	0,3,3	0.00	-
4	NAD	B	502	-	38,48,48	2.13	7 (18%)	47,73,73	1.76	9 (19%)
5	EDO	B	701	-	3,3,3	0.45	0	2,2,2	0.46	0
5	EDO	B	802	-	3,3,3	0.42	0	2,2,2	0.56	0
5	EDO	B	902	-	3,3,3	0.31	0	2,2,2	0.53	0
4	NAD	C	503	-	38,48,48	2.20	8 (21%)	47,73,73	2.16	13 (27%)
5	EDO	C	803	-	3,3,3	0.46	0	2,2,2	0.40	0
5	EDO	C	903	-	3,3,3	0.64	0	2,2,2	0.41	0
3	ADP	D	504[A]	-	22,29,29	1.86	5 (22%)	27,45,45	2.29	6 (22%)
3	ADP	D	504[B]	-	22,29,29	1.65	5 (22%)	27,45,45	1.63	3 (11%)
5	EDO	D	704	-	3,3,3	0.60	0	2,2,2	0.37	0
5	EDO	D	904	-	3,3,3	0.43	0	2,2,2	0.45	0
6	GAI	D	905	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	E	505	-	22,29,29	1.53	4 (18%)	27,45,45	2.41	3 (11%)
5	EDO	E	705	-	3,3,3	0.57	0	2,2,2	0.34	0
5	EDO	E	805	-	3,3,3	0.65	0	2,2,2	0.27	0
5	EDO	E	905	-	3,3,3	0.14	0	2,2,2	0.65	0
6	GAI	E	906	-	0,3,3	0.00	-	0,3,3	0.00	-
6	GAI	E	907	-	0,3,3	0.00	-	0,3,3	0.00	-
4	NAD	F	506	-	38,48,48	2.20	9 (23%)	47,73,73	1.93	7 (14%)
5	EDO	F	706	-	3,3,3	0.43	0	2,2,2	0.47	0
5	EDO	F	707	-	3,3,3	0.76	0	2,2,2	0.21	0
5	EDO	F	806	-	3,3,3	0.45	0	2,2,2	0.41	0
5	EDO	F	906	-	3,3,3	0.41	0	2,2,2	0.46	0
6	GAI	G	5009	-	0,3,3	0.00	-	0,3,3	0.00	-
6	GAI	G	5010	-	0,3,3	0.00	-	0,3,3	0.00	-
4	NAD	G	507	-	38,48,48	2.43	9 (23%)	47,73,73	1.76	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	G	807	-	3,3,3	0.60	0	2,2,2	0.29	0
5	EDO	G	907	-	3,3,3	0.38	0	2,2,2	0.53	0
4	NAD	H	508	-	38,48,48	2.33	9 (23%)	47,73,73	2.01	7 (14%)
5	EDO	H	708	-	3,3,3	0.48	0	2,2,2	0.38	0
5	EDO	H	808	-	3,3,3	0.68	0	2,2,2	0.30	0
5	EDO	H	908	-	3,3,3	0.43	0	2,2,2	0.46	0
6	GAI	H	909	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	I	509	-	22,29,29	1.76	5 (22%)	27,45,45	1.84	5 (18%)
5	EDO	I	809	-	3,3,3	0.67	0	2,2,2	0.24	0
5	EDO	I	909	-	3,3,3	0.40	0	2,2,2	0.46	0
6	GAI	I	910	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	J	510	-	22,29,29	1.67	4 (18%)	27,45,45	1.93	3 (11%)
6	GAI	J	611	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	K	511	-	22,29,29	1.66	4 (18%)	27,45,45	1.94	4 (14%)
5	EDO	K	911	-	3,3,3	0.62	0	2,2,2	0.34	0
3	ADP	L	512	-	22,29,29	1.67	4 (18%)	27,45,45	1.88	4 (14%)
5	EDO	L	712	-	3,3,3	0.56	0	2,2,2	0.35	0
5	EDO	L	912	-	3,3,3	0.44	0	2,2,2	0.45	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
6	GAI	D	905	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	507	NAD	C3N-C7N	-11.37	1.32	1.50
4	H	508	NAD	C3N-C7N	-9.96	1.34	1.50
4	B	502	NAD	C3N-C7N	-9.62	1.35	1.50
4	F	506	NAD	C3N-C7N	-9.22	1.36	1.50
4	C	503	NAD	C3N-C7N	-8.97	1.36	1.50
4	H	508	NAD	C4N-C3N	-3.37	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	507	NAD	C5N-C4N	-3.34	1.32	1.38
4	H	508	NAD	C5N-C4N	-3.25	1.32	1.38
4	H	508	NAD	C2N-C3N	-3.08	1.34	1.39
4	G	507	NAD	C4N-C3N	-3.08	1.34	1.39
4	B	502	NAD	C4N-C3N	-2.86	1.34	1.39
4	F	506	NAD	C5N-C4N	-2.79	1.33	1.38
4	F	506	NAD	C4N-C3N	-2.76	1.34	1.39
4	C	503	NAD	C5N-C4N	-2.58	1.33	1.38
3	D	504[B]	ADP	PB-O2B	-2.57	1.45	1.54
4	B	502	NAD	C2N-C3N	-2.54	1.35	1.39
4	G	507	NAD	C2N-C3N	-2.35	1.35	1.39
4	C	503	NAD	C4N-C3N	-2.32	1.35	1.39
3	A	501[B]	ADP	PB-O2B	-2.27	1.46	1.54
3	D	504[B]	ADP	PA-O2A	-2.21	1.45	1.54
3	A	501[B]	ADP	PA-O2A	-2.10	1.46	1.54
4	G	507	NAD	C4A-N3A	2.11	1.38	1.35
3	I	509	ADP	C4-N3	2.17	1.38	1.35
3	A	501[B]	ADP	C4-N3	2.39	1.39	1.35
3	D	504[A]	ADP	C4-N3	2.46	1.39	1.35
4	B	502	NAD	C8A-N7A	2.47	1.39	1.34
4	F	506	NAD	C2A-N1A	2.56	1.38	1.33
4	F	506	NAD	C4A-N3A	2.59	1.39	1.35
4	G	507	NAD	C8A-N7A	2.63	1.39	1.34
3	D	504[B]	ADP	C8-N7	2.64	1.39	1.34
3	J	510	ADP	C4-N3	2.66	1.39	1.35
4	H	508	NAD	C2A-N1A	2.67	1.39	1.33
3	A	501[B]	ADP	C8-N7	2.69	1.39	1.34
3	A	501[A]	ADP	PB-O3B	2.71	1.64	1.54
4	C	503	NAD	C8A-N7A	2.71	1.39	1.34
3	D	504[A]	ADP	C8-N7	2.78	1.39	1.34
3	L	512	ADP	PB-O3B	2.83	1.64	1.54
3	J	510	ADP	C8-N7	2.84	1.40	1.34
4	B	502	NAD	O4D-C1D	2.85	1.44	1.41
3	K	511	ADP	PB-O3B	2.85	1.65	1.54
4	H	508	NAD	C8A-N7A	2.89	1.40	1.34
4	F	506	NAD	O4B-C1B	2.91	1.44	1.41
3	E	505	ADP	C2-N1	2.92	1.39	1.33
4	B	502	NAD	C2A-N1A	2.96	1.39	1.33
4	H	508	NAD	O4B-C1B	2.99	1.45	1.41
3	I	509	ADP	C8-N7	2.99	1.40	1.34
3	E	505	ADP	PB-O3B	3.00	1.65	1.54
4	F	506	NAD	C8A-N7A	3.01	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501[A]	ADP	C8-N7	3.04	1.40	1.34
3	D	504[B]	ADP	C2-N1	3.05	1.39	1.33
3	L	512	ADP	C8-N7	3.10	1.40	1.34
3	K	511	ADP	C2-N1	3.12	1.39	1.33
3	K	511	ADP	C8-N7	3.12	1.40	1.34
3	E	505	ADP	C8-N7	3.17	1.40	1.34
4	H	508	NAD	C2A-N3A	3.18	1.37	1.32
3	L	512	ADP	C2-N1	3.20	1.40	1.33
3	I	509	ADP	PB-O3B	3.23	1.66	1.54
3	J	510	ADP	C2-N1	3.24	1.40	1.33
3	E	505	ADP	C2-N3	3.26	1.38	1.32
4	G	507	NAD	C2A-N1A	3.28	1.40	1.33
3	I	509	ADP	C2-N1	3.29	1.40	1.33
3	A	501[A]	ADP	C4-N3	3.34	1.40	1.35
4	G	507	NAD	O4D-C1D	3.35	1.45	1.41
4	F	506	NAD	O4D-C1D	3.36	1.45	1.41
3	A	501[B]	ADP	C2-N1	3.40	1.40	1.33
3	D	504[A]	ADP	C2-N1	3.43	1.40	1.33
4	C	503	NAD	C4A-N3A	3.47	1.40	1.35
4	C	503	NAD	C2A-N1A	3.48	1.40	1.33
4	C	503	NAD	O4D-C1D	3.50	1.45	1.41
3	A	501[A]	ADP	C2-N1	3.68	1.40	1.33
4	G	507	NAD	C2A-N3A	3.95	1.39	1.32
4	H	508	NAD	O4D-C1D	4.14	1.46	1.41
3	D	504[B]	ADP	C2-N3	4.14	1.39	1.32
3	K	511	ADP	C2-N3	4.15	1.39	1.32
3	J	510	ADP	C2-N3	4.23	1.39	1.32
3	A	501[B]	ADP	C2-N3	4.26	1.39	1.32
3	I	509	ADP	C2-N3	4.33	1.39	1.32
3	L	512	ADP	C2-N3	4.37	1.39	1.32
3	D	504[A]	ADP	PB-O3B	4.39	1.70	1.54
3	D	504[A]	ADP	C2-N3	4.44	1.40	1.32
4	B	502	NAD	C2A-N3A	4.45	1.40	1.32
3	A	501[A]	ADP	C2-N3	4.60	1.40	1.32
4	F	506	NAD	C2A-N3A	4.63	1.40	1.32
4	C	503	NAD	C2A-N3A	5.04	1.41	1.32

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	505	ADP	N3-C2-N1	-10.93	120.52	128.89
3	A	501[B]	ADP	N3-C2-N1	-9.45	121.66	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	508	NAD	N3A-C2A-N1A	-9.45	121.66	128.89
3	D	504[A]	ADP	N3-C2-N1	-9.09	121.93	128.89
3	J	510	ADP	N3-C2-N1	-8.24	122.59	128.89
4	C	503	NAD	N3A-C2A-N1A	-7.80	122.92	128.89
3	A	501[A]	ADP	N3-C2-N1	-7.66	123.03	128.89
4	G	507	NAD	N3A-C2A-N1A	-7.55	123.11	128.89
4	F	506	NAD	N3A-C2A-N1A	-7.52	123.14	128.89
3	L	512	ADP	N3-C2-N1	-7.20	123.38	128.89
3	K	511	ADP	N3-C2-N1	-7.15	123.42	128.89
4	B	502	NAD	N3A-C2A-N1A	-6.83	123.66	128.89
3	I	509	ADP	N3-C2-N1	-6.50	123.92	128.89
3	D	504[B]	ADP	N3-C2-N1	-6.37	124.02	128.89
3	A	501[A]	ADP	C4'-O4'-C1'	-5.55	103.62	109.72
4	H	508	NAD	PN-O3-PA	-5.23	118.04	132.73
4	C	503	NAD	O7N-C7N-N7N	-4.76	115.89	122.59
3	K	511	ADP	C2'-C3'-C4'	-4.54	93.28	102.61
4	C	503	NAD	O4D-C4D-C3D	-3.98	97.12	105.15
3	I	509	ADP	PA-O3A-PB	-3.93	119.50	132.67
3	D	504[A]	ADP	PA-O3A-PB	-3.85	119.76	132.67
3	A	501[A]	ADP	PA-O3A-PB	-3.81	119.91	132.67
4	H	508	NAD	O7N-C7N-N7N	-3.75	117.32	122.59
3	L	512	ADP	PA-O3A-PB	-3.73	120.16	132.67
4	F	506	NAD	C2B-C3B-C4B	-3.72	94.97	102.61
4	B	502	NAD	O4D-C4D-C3D	-3.71	97.67	105.15
4	C	503	NAD	C2B-C3B-C4B	-3.69	95.04	102.61
4	C	503	NAD	C2B-C1B-N9A	-3.36	109.16	114.29
4	G	507	NAD	PN-O3-PA	-3.34	123.34	132.73
3	L	512	ADP	C1'-N9-C4	-3.31	121.95	126.94
3	A	501[B]	ADP	C2'-C3'-C4'	-3.20	96.04	102.61
3	E	505	ADP	PA-O3A-PB	-3.16	122.08	132.67
4	F	506	NAD	O7N-C7N-N7N	-3.04	118.31	122.59
3	K	511	ADP	PA-O3A-PB	-3.02	122.56	132.67
3	D	504[A]	ADP	O3A-PA-O5'	-3.00	94.97	102.94
4	C	503	NAD	PN-O3-PA	-2.96	124.43	132.73
4	F	506	NAD	PN-O3-PA	-2.93	124.49	132.73
4	G	507	NAD	C6N-C5N-C4N	-2.87	115.11	119.44
3	I	509	ADP	C4'-O4'-C1'	-2.81	106.63	109.72
3	J	510	ADP	C2'-C3'-C4'	-2.72	97.02	102.61
4	B	502	NAD	O7N-C7N-N7N	-2.65	118.86	122.59
3	L	512	ADP	C2'-C3'-C4'	-2.59	97.30	102.61
4	G	507	NAD	C3N-C2N-N1N	-2.58	117.39	120.36
4	G	507	NAD	C2D-C3D-C4D	-2.56	97.34	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501[A]	ADP	C2'-C3'-C4'	-2.56	97.34	102.61
4	H	508	NAD	C6N-C5N-C4N	-2.55	115.59	119.44
3	I	509	ADP	C2'-C3'-C4'	-2.52	97.42	102.61
3	E	505	ADP	C2'-C3'-C4'	-2.52	97.43	102.61
3	D	504[B]	ADP	C2'-C3'-C4'	-2.51	97.45	102.61
4	G	507	NAD	C4N-C3N-C7N	-2.45	114.62	121.09
3	A	501[A]	ADP	O4'-C1'-N9	-2.45	102.97	108.10
4	B	502	NAD	C2D-C3D-C4D	-2.41	97.66	102.61
4	C	503	NAD	C6N-C5N-C4N	-2.39	115.83	119.44
4	F	506	NAD	C4B-O4B-C1B	-2.38	107.10	109.72
4	H	508	NAD	C2B-C3B-C4B	-2.36	97.75	102.61
3	D	504[A]	ADP	C2'-C3'-C4'	-2.23	98.02	102.61
4	B	502	NAD	C2B-C3B-C4B	-2.19	98.12	102.61
3	I	509	ADP	C2'-C1'-N9	-2.13	111.04	114.29
4	C	503	NAD	O3-PA-O5B	-2.03	97.55	102.94
3	D	504[B]	ADP	O2A-PA-O3A	2.03	114.28	105.09
4	H	508	NAD	C2N-C3N-C4N	2.10	120.63	118.29
3	D	504[A]	ADP	C4-C5-N7	2.15	111.45	109.48
4	B	502	NAD	O4D-C1D-N1N	2.16	110.51	108.13
3	D	504[A]	ADP	O2A-PA-O3A	2.19	115.02	105.09
4	B	502	NAD	C4B-O4B-C1B	2.22	112.16	109.72
4	C	503	NAD	O5D-C5D-C4D	2.22	117.30	109.12
4	C	503	NAD	C5N-C4N-C3N	2.26	123.18	120.33
3	K	511	ADP	O5'-C5'-C4'	2.29	117.58	109.12
3	A	501[A]	ADP	C2'-C1'-N9	2.48	118.08	114.29
4	C	503	NAD	O7N-C7N-C3N	2.52	122.33	119.59
3	J	510	ADP	O3A-PA-O5'	2.54	109.68	102.94
4	C	503	NAD	O5B-C5B-C4B	2.62	118.79	109.12
4	H	508	NAD	O7N-C7N-C3N	3.16	123.04	119.59
4	B	502	NAD	C1B-N9A-C4A	3.32	131.95	126.94
4	F	506	NAD	C3N-C7N-N7N	3.59	121.74	117.82
4	C	503	NAD	C3N-C7N-N7N	3.60	121.76	117.82
4	B	502	NAD	O7N-C7N-C3N	3.74	123.67	119.59
4	F	506	NAD	O4B-C4B-C3B	3.78	112.77	105.15
4	G	507	NAD	C2N-C3N-C4N	4.15	122.91	118.29

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^{th} 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%)	0.77	67 (13%) 4 4	21, 67, 104, 123	0
1	B	494/500 (98%)	-0.11	5 (1%) 84 86	24, 40, 78, 98	0
1	C	494/500 (98%)	-0.08	3 (0%) 90 91	23, 40, 72, 88	0
1	D	494/500 (98%)	0.67	45 (9%) 11 12	25, 68, 97, 118	0
1	E	494/500 (98%)	-0.13	3 (0%) 90 91	23, 41, 68, 96	0
1	F	494/500 (98%)	-0.05	5 (1%) 84 86	21, 37, 66, 94	0
1	G	494/500 (98%)	0.12	8 (1%) 74 78	26, 46, 68, 98	0
1	H	494/500 (98%)	0.15	15 (3%) 54 59	24, 46, 77, 91	0
1	I	494/500 (98%)	0.43	24 (4%) 33 38	36, 58, 82, 105	0
1	J	494/500 (98%)	0.83	46 (9%) 11 11	44, 77, 104, 114	0
1	K	494/500 (98%)	0.62	45 (9%) 11 12	44, 71, 96, 115	0
1	L	494/500 (98%)	1.22	110 (22%) 1 1	47, 89, 115, 127	0
All	All	5928/6000 (98%)	0.37	376 (6%) 23 26	21, 55, 99, 127	0

All (376) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	378	GLY	7.7
1	L	369	CYS	6.2
1	L	223	GLY	5.4
1	G	474	GLY	5.2
1	L	386	PHE	5.2
1	L	373	ILE	5.1
1	A	371	GLY	5.1
1	D	424	THR	5.0
1	A	362	GLN	4.9
1	L	295	PHE	4.9
1	K	377	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	K	475	ARG	4.8
1	A	477	LEU	4.7
1	A	470	MET	4.7
1	J	365	ALA	4.7
1	L	333	ASN	4.6
1	D	327	LYS	4.5
1	A	353	ILE	4.5
1	L	332	GLY	4.4
1	L	360	GLY	4.4
1	A	473	SER	4.4
1	D	356	TYR	4.4
1	K	376	ASP	4.4
1	J	108	LEU	4.3
1	E	7	ALA	4.3
1	A	315	TYR	4.2
1	K	371	GLY	4.2
1	D	470	MET	4.2
1	L	285	TRP	4.1
1	K	474	GLY	4.1
1	A	468	TYR	4.1
1	L	356	TYR	4.1
1	L	482	LEU	4.1
1	D	376	ASP	4.1
1	L	350	PHE	4.1
1	J	7	ALA	4.1
1	L	478	GLY	4.0
1	L	318	PHE	4.0
1	L	387	GLY	4.0
1	L	327	LYS	4.0
1	L	354	LEU	4.0
1	L	357	ILE	4.0
1	L	380	PHE	4.0
1	K	470	MET	3.9
1	K	473	SER	3.9
1	G	7	ALA	3.9
1	J	362	GLN	3.9
1	L	310	VAL	3.9
1	A	424	THR	3.8
1	L	377	ARG	3.8
1	A	394	THR	3.8
1	L	322	SER	3.8
1	A	474	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	475	ARG	3.7
1	I	319	VAL	3.7
1	L	358	ASN	3.6
1	I	408	LEU	3.6
1	A	334	PRO	3.6
1	A	7	ALA	3.6
1	K	413	ILE	3.6
1	A	358	ASN	3.6
1	L	108	LEU	3.5
1	A	367	LEU	3.5
1	K	463	SER	3.5
1	A	377	ARG	3.4
1	L	468	TYR	3.4
1	L	480	TYR	3.4
1	J	425	TYR	3.4
1	D	32	VAL	3.4
1	A	404	VAL	3.3
1	K	471	SER	3.3
1	A	356	TYR	3.3
1	L	479	GLU	3.3
1	J	139	TYR	3.3
1	J	42	PRO	3.3
1	L	340	GLU	3.3
1	A	376	ASP	3.3
1	H	364	GLY	3.3
1	A	365	ALA	3.3
1	I	389	VAL	3.2
1	I	480	TYR	3.2
1	J	378	GLY	3.2
1	A	319	VAL	3.2
1	K	379	TYR	3.2
1	K	380	PHE	3.2
1	D	29	HIS	3.2
1	L	349	GLN	3.2
1	A	10	ALA	3.2
1	L	314	ILE	3.2
1	J	468	TYR	3.2
1	H	362	GLN	3.2
1	L	9	PRO	3.2
1	L	353	ILE	3.2
1	H	386	PHE	3.2
1	D	247	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	365	ALA	3.1
1	L	408	LEU	3.1
1	A	395	ILE	3.1
1	J	104	ALA	3.1
1	D	350	PHE	3.1
1	L	367	LEU	3.1
1	A	373	ILE	3.1
1	K	468	TYR	3.1
1	A	386	PHE	3.1
1	K	466	GLY	3.1
1	L	475	ARG	3.1
1	A	469	LYS	3.1
1	K	472	GLY	3.1
1	J	373	ILE	3.1
1	L	347	GLU	3.1
1	D	31	ALA	3.0
1	H	7	ALA	3.0
1	J	22	ILE	3.0
1	A	279	SER	3.0
1	D	365	ALA	3.0
1	K	375	ALA	3.0
1	D	353	ILE	3.0
1	H	290	ALA	3.0
1	K	484	ALA	3.0
1	J	476	GLU	3.0
1	F	477	LEU	3.0
1	I	139	TYR	3.0
1	L	216	GLY	3.0
1	J	30	ASP	3.0
1	J	247	THR	2.9
1	K	139	TYR	2.9
1	L	28	TRP	2.9
1	L	8	VAL	2.9
1	L	376	ASP	2.9
1	G	477	LEU	2.9
1	K	17	VAL	2.9
1	A	326	ALA	2.9
1	L	115	VAL	2.9
1	L	329	ARG	2.8
1	I	470	MET	2.8
1	J	32	VAL	2.8
1	L	113	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	253	ILE	2.8
1	D	471	SER	2.8
1	L	139	TYR	2.8
1	A	287	VAL	2.8
1	K	46	GLU	2.8
1	L	465	PHE	2.8
1	K	467	GLY	2.8
1	L	463	SER	2.8
1	L	385	VAL	2.8
1	J	31	ALA	2.8
1	J	44	THR	2.8
1	L	319	VAL	2.8
1	K	465	PHE	2.8
1	D	475	ARG	2.8
1	K	7	ALA	2.8
1	L	413	ILE	2.7
1	L	466	GLY	2.7
1	A	295	PHE	2.7
1	J	33	SER	2.7
1	J	376	ASP	2.7
1	J	392	GLY	2.7
1	J	374	ALA	2.7
1	A	398	GLU	2.7
1	I	486	THR	2.7
1	L	27	GLU	2.7
1	A	100	THR	2.7
1	G	486	THR	2.7
1	L	461	ALA	2.7
1	A	256	ALA	2.7
1	A	379	TYR	2.7
1	L	365	ALA	2.7
1	L	363	GLU	2.7
1	D	468	TYR	2.7
1	L	462	GLN	2.6
1	L	301	CYS	2.6
1	J	347	GLU	2.6
1	D	334	PRO	2.6
1	L	47	VAL	2.6
1	D	379	TYR	2.6
1	A	327	LYS	2.6
1	B	253	ILE	2.6
1	D	199	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	8	VAL	2.6
1	L	40	VAL	2.6
1	L	66	ALA	2.6
1	A	397	LYS	2.6
1	I	141	GLY	2.6
1	D	100	THR	2.6
1	J	203	TYR	2.6
1	H	360	GLY	2.6
1	K	332	GLY	2.6
1	E	424	THR	2.6
1	J	386	PHE	2.6
1	K	478	GLY	2.6
1	A	357	ILE	2.6
1	L	339	THR	2.6
1	D	399	GLU	2.6
1	J	53	GLU	2.6
1	A	323	VAL	2.5
1	L	266	THR	2.5
1	L	486	THR	2.5
1	L	393	MET	2.5
1	L	7	ALA	2.5
1	D	51	VAL	2.5
1	L	323	VAL	2.5
1	L	42	PRO	2.5
1	K	479	GLU	2.5
1	J	63	VAL	2.5
1	A	332	GLY	2.5
1	I	318	PHE	2.5
1	A	480	TYR	2.5
1	J	283	MET	2.5
1	I	411	LYS	2.5
1	L	338	LYS	2.5
1	L	473	SER	2.5
1	A	114	TYR	2.5
1	I	474	GLY	2.5
1	L	141	GLY	2.5
1	I	479	GLU	2.5
1	J	56	LYS	2.5
1	F	254	GLN	2.4
1	L	405	MET	2.4
1	B	473	SER	2.4
1	D	337	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	259	SER	2.4
1	I	388	ASP	2.4
1	A	317	GLU	2.4
1	L	320	GLU	2.4
1	D	40	VAL	2.4
1	J	389	VAL	2.4
1	C	477	LEU	2.4
1	L	328	SER	2.4
1	G	475	ARG	2.4
1	J	377	ARG	2.4
1	L	296	PHE	2.4
1	J	467	GLY	2.4
1	I	482	LEU	2.4
1	D	413	ILE	2.4
1	A	465	PHE	2.4
1	K	386	PHE	2.4
1	D	477	LEU	2.4
1	J	72	LEU	2.4
1	L	384	THR	2.4
1	K	392	GLY	2.3
1	L	315	TYR	2.3
1	H	316	ASP	2.3
1	A	314	ILE	2.3
1	J	358	ASN	2.3
1	L	104	ALA	2.3
1	L	73	GLY	2.3
1	J	319	VAL	2.3
1	D	46	GLU	2.3
1	B	260	SER	2.3
1	D	111	GLY	2.3
1	I	248	GLU	2.3
1	L	228	ALA	2.3
1	L	395	ILE	2.3
1	A	328	SER	2.3
1	K	477	LEU	2.3
1	D	36	THR	2.3
1	H	323	VAL	2.3
1	A	476	GLU	2.3
1	K	312	GLU	2.3
1	L	250	GLY	2.3
1	L	433	THR	2.3
1	A	466	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	371	GLY	2.3
1	L	276	ILE	2.3
1	J	379	TYR	2.3
1	D	473	SER	2.2
1	I	477	LEU	2.2
1	K	482	LEU	2.2
1	L	44	THR	2.2
1	D	377	ARG	2.2
1	I	312	GLU	2.2
1	H	473	SER	2.2
1	D	30	ASP	2.2
1	A	102	LEU	2.2
1	D	42	PRO	2.2
1	L	51	VAL	2.2
1	I	478	GLY	2.2
1	J	34	ARG	2.2
1	D	338	LYS	2.2
1	L	227	THR	2.2
1	B	71	GLN	2.2
1	H	315	TYR	2.2
1	L	379	TYR	2.2
1	A	283	MET	2.2
1	L	24	ILE	2.2
1	L	199	LEU	2.2
1	A	384	THR	2.2
1	C	7	ALA	2.2
1	J	246	SER	2.2
1	L	140	HIS	2.2
1	D	467	GLY	2.2
1	J	466	GLY	2.2
1	F	465	PHE	2.2
1	A	359	THR	2.2
1	A	306	SER	2.2
1	A	392	GLY	2.2
1	K	483	GLN	2.2
1	A	479	GLU	2.2
1	D	295	PHE	2.2
1	K	18	PHE	2.2
1	D	323	VAL	2.1
1	I	375	ALA	2.1
1	K	412	THR	2.1
1	L	247	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	334	PRO	2.1
1	J	140	HIS	2.1
1	A	115	VAL	2.1
1	K	33	SER	2.1
1	A	118	TYR	2.1
1	I	356	TYR	2.1
1	L	277	ILE	2.1
1	I	376	ASP	2.1
1	I	386	PHE	2.1
1	L	224	PHE	2.1
1	D	248	GLU	2.1
1	L	111	GLY	2.1
1	L	374	ALA	2.1
1	K	441	TYR	2.1
1	A	312	GLU	2.1
1	J	207	LEU	2.1
1	B	424	THR	2.1
1	K	266	THR	2.1
1	F	258	GLY	2.1
1	L	474	GLY	2.1
1	H	385	VAL	2.1
1	L	389	VAL	2.1
1	G	248	GLU	2.1
1	H	477	LEU	2.1
1	K	37	PHE	2.1
1	K	267	LEU	2.1
1	A	383	PRO	2.1
1	A	248	GLU	2.1
1	K	411	LYS	2.1
1	L	17	VAL	2.1
1	L	330	VAL	2.1
1	L	331	VAL	2.1
1	D	114	TYR	2.1
1	A	318	PHE	2.1
1	C	482	LEU	2.1
1	E	269	LEU	2.1
1	K	51	VAL	2.1
1	L	298	GLN	2.1
1	L	362	GLN	2.1
1	D	373	ILE	2.1
1	L	477	LEU	2.1
1	A	486	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	384	THR	2.1
1	D	61	LYS	2.0
1	F	253	ILE	2.0
1	G	478	GLY	2.0
1	G	481	GLY	2.0
1	K	485	TYR	2.0
1	A	410	PHE	2.0
1	L	282	ASP	2.0
1	J	14	GLN	2.0
1	D	34	ARG	2.0
1	A	104	ALA	2.0
1	L	31	ALA	2.0
1	J	366	LYS	2.0
1	H	319	VAL	2.0
1	I	431	VAL	2.0
1	I	413	ILE	2.0
1	K	480	TYR	2.0
1	H	465	PHE	2.0
1	J	227	THR	2.0
1	L	483	GLN	2.0
1	D	10	ALA	2.0
1	D	326	ALA	2.0
1	A	8	VAL	2.0
1	A	467	GLY	2.0
1	K	141	GLY	2.0
1	L	416	VAL	2.0
1	L	116	ILE	2.0
1	A	368	LEU	2.0
1	J	380	PHE	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^{th} 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^2)	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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	-0.21	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
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.