



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:14 am GMT

PDB ID : 1I10  
Title : HUMAN MUSCLE L-LACTATE DEHYDROGENASE M CHAIN,  
TERNARY COMPLEX WITH NADH AND OXAMATE  
Authors : Read, J.A.; Winter, V.J.; Eszes, C.M.; Sessions, R.B.; Brady, R.L.  
Deposited on : 2001-01-30  
Resolution : 2.30 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

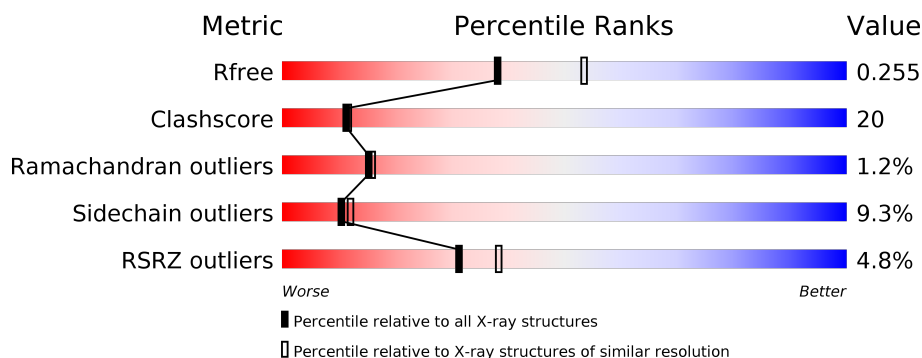
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	331	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>•</div> </div> </div>
1	B	331	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>•</div> </div> </div>
1	C	331	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>5%</div> <div>•</div> </div> </div>
1	D	331	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>5%</div> <div>•</div> </div> </div>
1	E	331	<div> <div>9%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>9%</div> <div>•</div> </div> </div>
1	F	331	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>6%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	331	
1	H	331	

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	ACT	A	803	-	-	X	X
2	ACT	B	806	-	-	X	X
2	ACT	C	809	-	-	X	X
2	ACT	D	812	-	-	X	X
2	ACT	E	815	-	-	-	X
2	ACT	F	818	-	-	X	X
2	ACT	G	821	-	-	-	X
2	ACT	H	824	-	-	-	X
4	OXM	D	811	-	-	X	X
4	OXM	E	814	-	-	X	-
4	OXM	G	820	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21581 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 L-LACTATE DEHYDROGENASE M CHAIN.

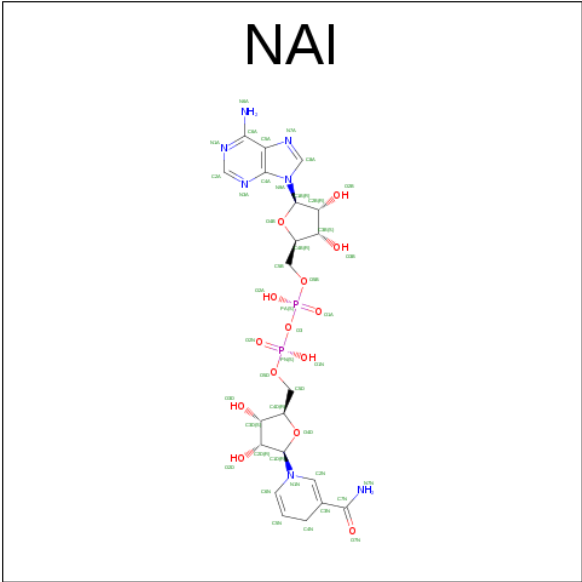
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	11	0	0
			2568	1639	439	477	13			
1	B	331	Total	C	N	O	S	21	0	0
			2568	1639	439	477	13			
1	C	331	Total	C	N	O	S	9	0	0
			2568	1639	439	477	13			
1	D	331	Total	C	N	O	S	60	0	0
			2568	1639	439	477	13			
1	E	331	Total	C	N	O	S	75	0	0
			2568	1639	439	477	13			
1	F	331	Total	C	N	O	S	36	0	0
			2568	1639	439	477	13			
1	G	325	Total	C	N	O	S	45	0	0
			2521	1612	430	466	13			
1	H	331	Total	C	N	O	S	36	0	0
			2568	1639	439	477	13			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



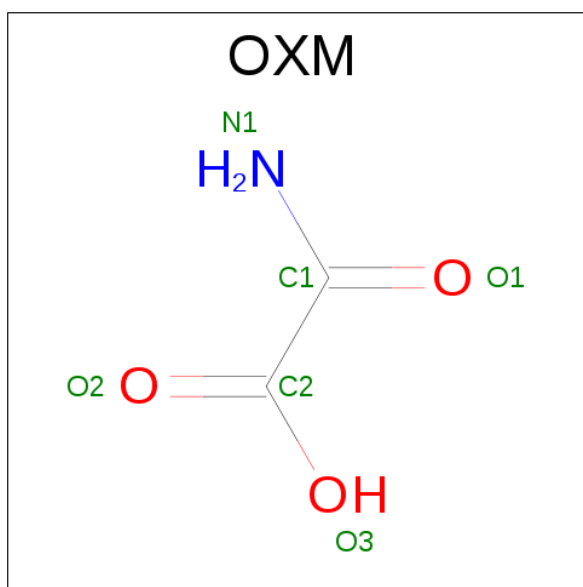
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 4 is OXAMIC ACID (three-letter code: OXM) (formula: C<sub>2</sub>H<sub>3</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	2	1	3		
4	B	1	Total	C	N	O	0	0
			6	2	1	3		
4	C	1	Total	C	N	O	0	0
			6	2	1	3		
4	D	1	Total	C	N	O	0	0
			6	2	1	3		
4	E	1	Total	C	N	O	0	0
			6	2	1	3		
4	F	1	Total	C	N	O	0	0
			6	2	1	3		
4	G	1	Total	C	N	O	0	0
			6	2	1	3		
4	H	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total	O	0	0
			135	135		
5	B	136	Total	O	0	0
			136	136		
5	C	78	Total	O	0	0
			78	78		
5	D	87	Total	O	0	0
			87	87		

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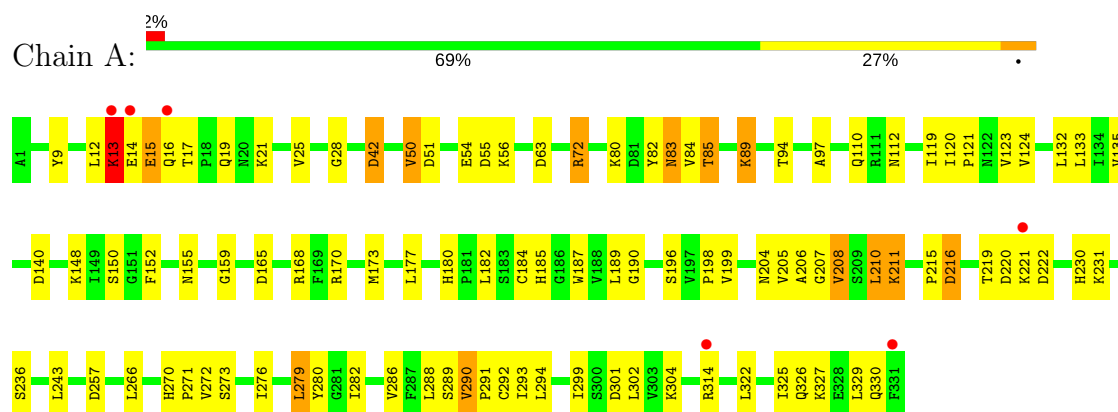
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	44	Total 44	O 44	0	0
5	F	51	Total 51	O 51	0	0
5	G	56	Total 56	O 56	0	0
5	H	65	Total 65	O 65	0	0



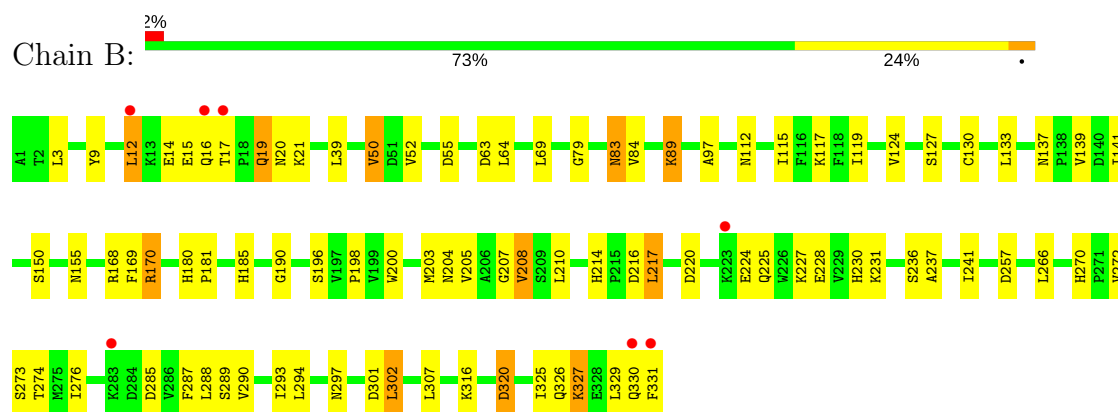
### 3 Residue-property plots

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.

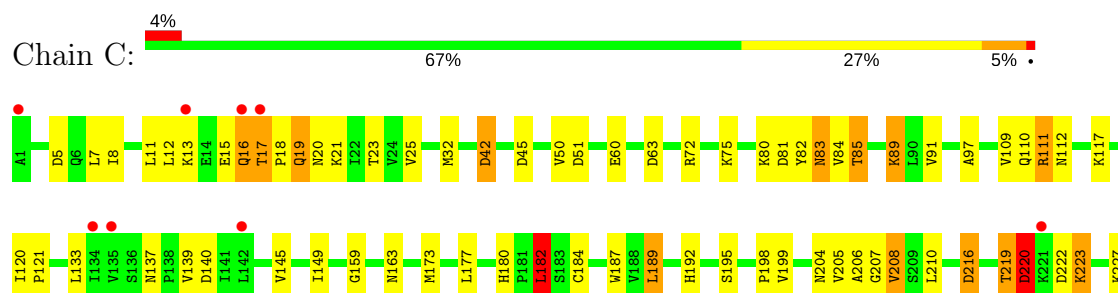
#### • Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

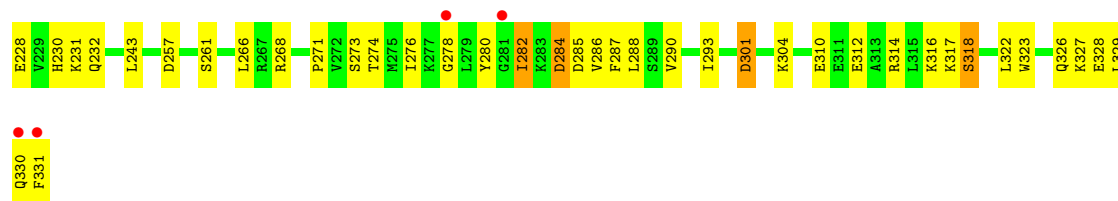


#### • Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

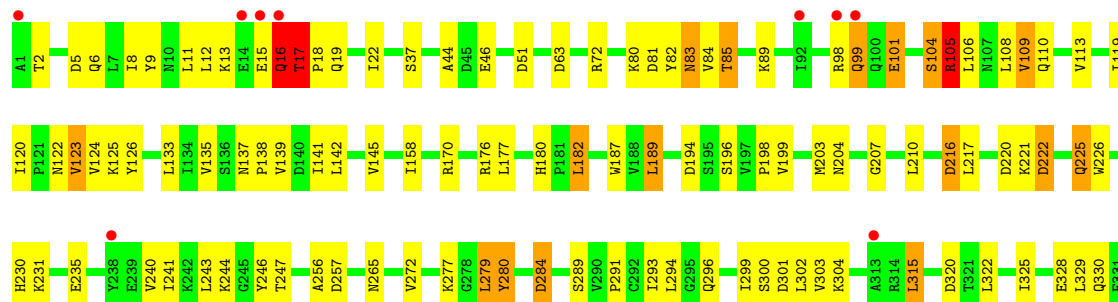


#### • Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

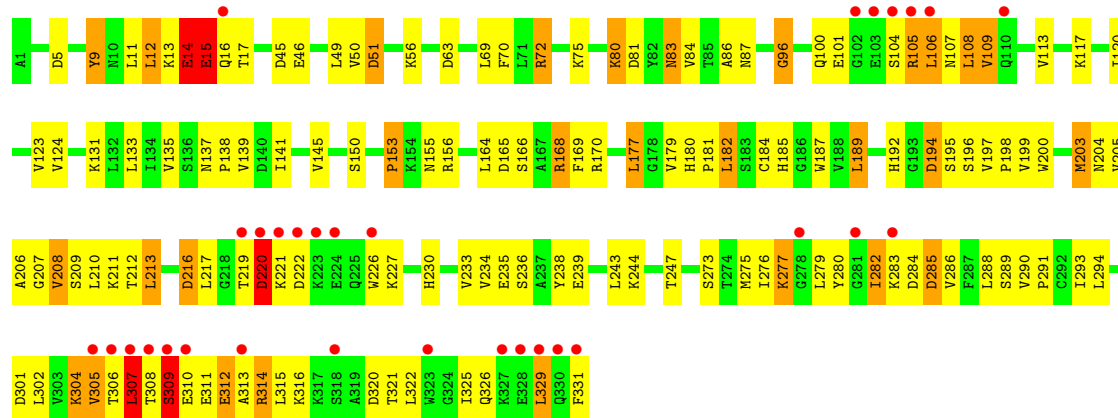




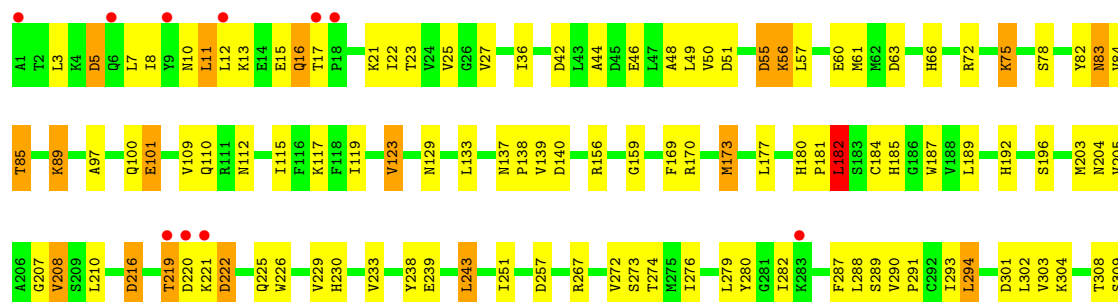
• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN



• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

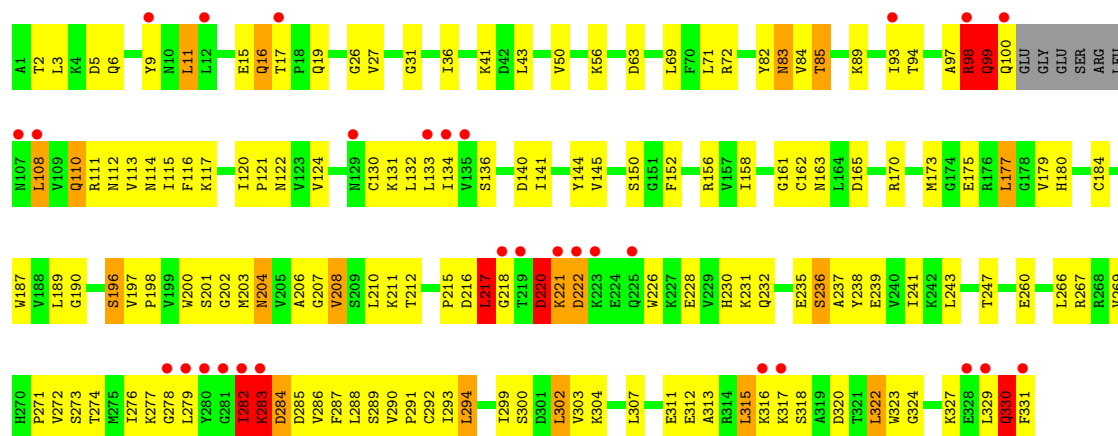


• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

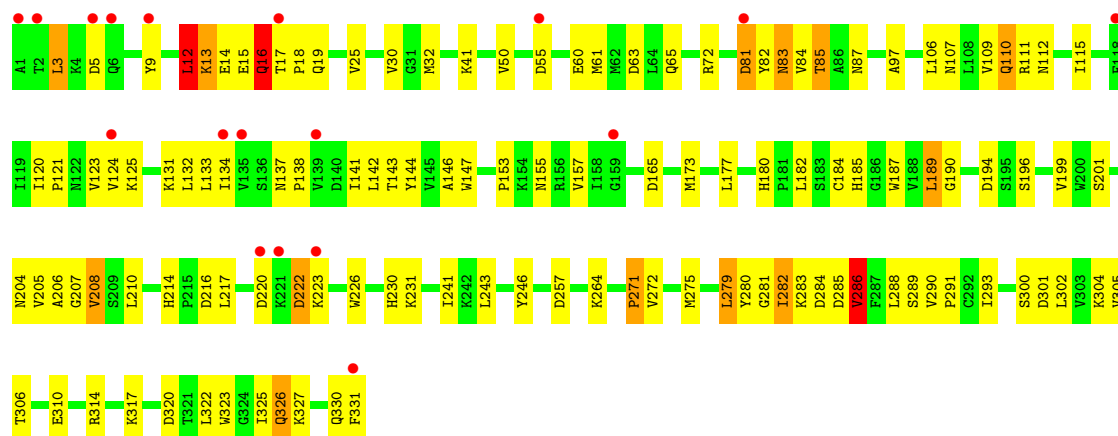




• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN



• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.94Å 158.54Å 266.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 29.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-2.30) 91.1 (29.94-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.98 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.197 , 0.257 0.197 , 0.255	Depositor DCC
$R_{free}$ test set	5588 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: OXM, NAI, ACT

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	0.89	1/2612 (0.0%)	1.02	10/3532 (0.3%)
1	B	0.85	0/2612	0.98	8/3532 (0.2%)
1	C	0.82	3/2612 (0.1%)	1.01	15/3532 (0.4%)
1	D	0.89	4/2612 (0.2%)	0.99	16/3532 (0.5%)
1	E	0.78	2/2612 (0.1%)	1.00	14/3532 (0.4%)
1	F	0.78	1/2612 (0.0%)	0.97	12/3532 (0.3%)
1	G	0.78	3/2564 (0.1%)	0.97	11/3467 (0.3%)
1	H	0.82	1/2612 (0.0%)	1.02	15/3532 (0.4%)
All	All	0.83	15/20848 (0.1%)	1.00	101/28191 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	E	0	1
1	F	0	1
1	H	0	3
All	All	0	7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	12	LEU	C-N	-18.70	0.91	1.34
1	D	231	LYS	C-O	-16.70	0.91	1.23
1	G	226	TRP	CB-CG	-14.33	1.24	1.50
1	A	13	LYS	CB-CG	-14.12	1.14	1.52
1	F	16	GLN	C-N	13.99	1.66	1.34
1	E	96	GLY	C-N	-11.45	1.07	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	104	SER	C-N	-11.34	1.07	1.34
1	G	226	TRP	NE1-CE2	9.23	1.49	1.37
1	D	99	GLN	C-N	-9.07	1.13	1.34
1	C	15	GLU	CB-CG	-8.41	1.36	1.52
1	G	217	LEU	CB-CG	7.76	1.75	1.52
1	D	231	LYS	CA-C	7.31	1.72	1.52
1	C	16	GLN	CG-CD	7.23	1.67	1.51
1	C	16	GLN	CB-CG	-6.14	1.35	1.52
1	E	14	GLU	CB-CG	5.12	1.61	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	217	LEU	CB-CG-CD1	14.68	135.96	111.00
1	H	16	GLN	O-C-N	-12.08	103.37	122.70
1	H	63	ASP	CB-CG-OD2	10.81	128.03	118.30
1	F	16	GLN	C-N-CA	-10.43	95.63	121.70
1	H	12	LEU	O-C-N	-10.34	106.16	122.70
1	E	96	GLY	O-C-N	-9.33	107.78	122.70
1	E	165	ASP	CB-CG-OD2	8.73	126.16	118.30
1	H	81	ASP	CB-CG-OD2	8.45	125.91	118.30
1	C	63	ASP	CB-CG-OD2	8.43	125.88	118.30
1	B	55	ASP	CB-CG-OD2	8.19	125.67	118.30
1	E	320	ASP	CB-CG-OD2	8.13	125.62	118.30
1	E	168	ARG	NE-CZ-NH1	-8.13	116.24	120.30
1	A	13	LYS	CA-CB-CG	8.03	131.07	113.40
1	F	16	GLN	O-C-N	7.82	135.22	122.70
1	F	63	ASP	CB-CG-OD2	7.80	125.32	118.30
1	D	320	ASP	CB-CG-OD2	7.73	125.26	118.30
1	B	170	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	D	231	LYS	O-C-N	-7.54	110.64	122.70
1	D	104	SER	O-C-N	-7.43	110.81	122.70
1	D	216	ASP	CB-CG-OD2	7.37	124.93	118.30
1	G	5	ASP	CB-CG-OD2	7.34	124.90	118.30
1	G	63	ASP	CB-CG-OD2	7.21	124.79	118.30
1	H	16	GLN	CA-C-N	7.17	132.98	117.20
1	F	257	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	257	ASP	CB-CG-OD2	7.01	124.61	118.30
1	E	285	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	285	ASP	CB-CG-OD2	6.92	124.53	118.30
1	C	285	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	42	ASP	CB-CG-OD2	6.76	124.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	5	ASP	CB-CG-OD2	6.72	124.35	118.30
1	H	165	ASP	CB-CG-OD2	6.67	124.30	118.30
1	G	220	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	170	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	A	140	ASP	CB-CG-OD2	6.58	124.22	118.30
1	F	16	GLN	CA-C-N	-6.47	102.96	117.20
1	D	194	ASP	CB-CG-OD2	6.45	124.11	118.30
1	C	284	ASP	CB-CG-OD2	6.39	124.05	118.30
1	D	284	ASP	CB-CG-OD2	6.37	124.04	118.30
1	C	216	ASP	CB-CG-OD2	6.34	124.00	118.30
1	C	182	LEU	CA-CB-CG	6.29	129.78	115.30
1	E	108	LEU	O-C-N	-6.29	112.63	122.70
1	A	51	ASP	CB-CG-OD2	6.28	123.95	118.30
1	H	222	ASP	CB-CG-OD2	6.26	123.93	118.30
1	C	257	ASP	CB-CG-OD2	6.10	123.79	118.30
1	H	271	PRO	N-CD-CG	-6.07	94.10	103.20
1	D	257	ASP	CB-CG-OD2	6.05	123.75	118.30
1	H	257	ASP	CB-CG-OD2	6.02	123.72	118.30
1	G	284	ASP	CB-CG-OD2	5.97	123.68	118.30
1	H	286	VAL	CB-CA-C	-5.97	100.05	111.40
1	G	217	LEU	CA-CB-CG	-5.94	101.65	115.30
1	H	16	GLN	C-N-CA	5.93	136.53	121.70
1	C	140	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	222	ASP	CB-CG-OD2	5.89	123.60	118.30
1	E	182	LEU	CA-CB-CG	5.79	128.62	115.30
1	D	220	ASP	CB-CG-OD2	5.79	123.51	118.30
1	F	5	ASP	CB-CG-OD2	5.76	123.49	118.30
1	C	111	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	F	55	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	42	ASP	CB-CG-OD2	5.73	123.45	118.30
1	D	105	ARG	CA-CB-CG	5.69	125.92	113.40
1	E	81	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	63	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	220	ASP	CB-CG-OD2	5.59	123.33	118.30
1	G	165	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	5	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	216	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	301	ASP	CB-CG-OD2	5.54	123.28	118.30
1	F	42	ASP	CB-CG-OD2	5.54	123.28	118.30
1	E	220	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	51	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	216	ASP	CB-CG-OD2	5.47	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	220	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	194	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	216	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	220	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	220	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	165	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	81	ASP	CB-CG-OD2	5.37	123.13	118.30
1	G	320	ASP	CB-CG-OD2	5.35	123.12	118.30
1	H	285	ASP	CB-CG-OD2	5.34	123.11	118.30
1	F	216	ASP	CB-CG-OD2	5.31	123.08	118.30
1	E	51	ASP	CB-CG-OD2	5.30	123.07	118.30
1	G	285	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	257	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	63	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	55	ASP	CB-CG-OD2	5.24	123.02	118.30
1	H	194	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	279	LEU	CA-CB-CG	5.22	127.31	115.30
1	F	222	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	63	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	5	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	51	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	231	LYS	CA-C-O	5.16	130.94	120.10
1	D	63	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	182	LEU	CA-CB-CG	5.14	127.12	115.30
1	E	156	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	G	98	ARG	CD-NE-CZ	-5.09	116.47	123.60
1	C	45	ASP	CB-CG-OD1	5.08	122.87	118.30
1	G	222	ASP	CB-CG-OD2	5.06	122.86	118.30
1	H	320	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	81	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	104	SER	Mainchain,Peptide
1	E	96	GLY	Mainchain
1	F	12	LEU	Peptide
1	H	12	LEU	Mainchain
1	H	16	GLN	Mainchain,Peptide



## 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	2568	0	2656	80	0
1	B	2568	0	2656	75	0
1	C	2568	0	2656	88	0
1	D	2568	0	2654	84	0
1	E	2568	0	2655	158	0
1	F	2568	0	2656	116	0
1	G	2521	0	2611	154	0
1	H	2568	0	2655	107	0
2	A	4	0	3	6	0
2	B	4	0	3	4	0
2	C	4	0	3	2	0
2	D	4	0	3	2	0
2	E	4	0	3	1	0
2	F	4	0	3	3	0
2	G	4	0	3	1	0
2	H	4	0	3	1	0
3	A	44	0	27	2	0
3	B	44	0	27	2	0
3	C	44	0	27	1	0
3	D	44	0	27	4	0
3	E	44	0	27	3	0
3	F	44	0	27	2	0
3	G	44	0	27	1	0
3	H	44	0	27	3	0
4	A	6	0	2	0	0
4	B	6	0	2	0	0
4	C	6	0	2	1	0
4	D	6	0	2	2	0
4	E	6	0	2	2	0
4	F	6	0	2	1	0
4	G	6	0	2	0	0
4	H	6	0	2	0	0
5	A	135	0	0	10	0
5	B	136	0	0	3	0
5	C	78	0	0	3	0
5	D	87	0	0	3	0
5	E	44	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	51	0	0	4	0
5	G	56	0	0	3	0
5	H	65	0	0	2	0
All	All	21581	0	21455	828	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 20.

All (828) 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:E:105:ARG:O	1:E:106:LEU:HG	1.20	1.29
1:D:279:LEU:HB3	1:D:280:TYR:CE1	1.74	1.22
1:E:308:THR:CA	1:E:309:SER:HB3	1.70	1.22
1:G:282:ILE:HG13	1:G:283:LYS:N	1.39	1.20
1:D:280:TYR:N	1:D:280:TYR:HD1	1.32	1.19
1:A:185:HIS:HD1	2:A:803:ACT:H2	1.01	1.14
1:G:282:ILE:CG1	1:G:283:LYS:H	1.62	1.12
1:A:21:LYS:H	1:A:89:LYS:HE3	1.01	1.11
1:D:280:TYR:N	1:D:280:TYR:CD1	2.08	1.10
1:E:276:ILE:HD13	1:E:288:LEU:HD11	1.32	1.09
1:E:105:ARG:O	1:E:106:LEU:CG	2.00	1.08
1:B:227:LYS:HE3	1:B:231:LYS:HE3	1.36	1.05
2:A:803:ACT:H1	5:A:898:HOH:O	1.58	1.03
1:G:110:GLN:OE1	1:G:330:GLN:NE2	1.91	1.03
1:E:308:THR:HA	1:E:309:SER:CB	1.82	1.02
1:A:21:LYS:N	1:A:89:LYS:HE3	1.75	1.00
1:F:276:ILE:HD12	1:F:282:ILE:HD12	1.43	1.00
1:B:270:HIS:HD2	1:B:294:LEU:HD13	1.25	0.99
1:G:283:LYS:HE3	1:G:283:LYS:HA	1.42	0.99
1:A:21:LYS:H	1:A:89:LYS:CE	1.77	0.97
1:E:310:GLU:HB3	1:E:313:ALA:H	1.29	0.97
1:E:308:THR:HA	1:E:309:SER:HB3	0.98	0.96
1:A:185:HIS:ND1	2:A:803:ACT:H2	1.80	0.96
1:C:97:ALA:H	1:C:112:ASN:HD21	1.02	0.95
1:E:104:SER:O	1:E:105:ARG:HG3	1.65	0.95
1:F:216:ASP:O	1:F:219:THR:HB	1.67	0.94
1:G:282:ILE:CG1	1:G:283:LYS:N	2.25	0.94
1:D:279:LEU:HB3	1:D:280:TYR:CD1	2.02	0.94
1:H:180:HIS:CE1	1:H:182:LEU:HD23	2.02	0.94
1:E:305:VAL:HG12	1:E:305:VAL:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:GLN:NE2	1:G:330:GLN:OE1	2.02	0.93
1:G:220:ASP:O	1:G:221:LYS:HB2	1.68	0.93
5:A:928:HOH:O	2:C:809:ACT:H3	1.68	0.93
1:E:198:PRO:HG3	1:E:230:HIS:CG	2.04	0.92
1:G:282:ILE:HG13	1:G:283:LYS:H	0.77	0.92
1:H:110:GLN:HA	1:H:110:GLN:HE21	1.34	0.92
1:B:270:HIS:CD2	1:B:294:LEU:HD13	2.06	0.91
1:H:187:TRP:CZ3	1:H:271:PRO:HG3	2.07	0.90
1:A:314:ARG:HG3	1:A:314:ARG:HH11	1.34	0.90
1:A:82:TYR:O	1:A:85:THR:HB	1.71	0.90
1:C:216:ASP:O	1:C:219:THR:HB	1.71	0.89
1:H:97:ALA:H	1:H:112:ASN:HD21	1.13	0.89
1:D:225:GLN:HA	1:D:225:GLN:OE1	1.73	0.89
1:E:192:HIS:O	1:E:192:HIS:CG	2.26	0.89
1:F:219:THR:HG22	1:F:221:LYS:H	1.36	0.88
1:G:330:GLN:H	1:G:330:GLN:HE21	0.92	0.88
1:D:280:TYR:H	1:D:280:TYR:HD1	1.18	0.88
1:E:117:LYS:HE2	1:E:331:PHE:CB	2.04	0.88
1:E:117:LYS:HE2	1:E:331:PHE:HB3	1.55	0.87
1:B:83:ASN:HD22	1:B:84:VAL:N	1.71	0.87
1:H:310:GLU:HG2	1:H:314:ARG:HH12	1.39	0.87
1:D:170:ARG:HH22	2:D:812:ACT:H1	1.37	0.87
1:A:85:THR:CG2	5:A:808:HOH:O	2.23	0.86
1:F:238:TYR:HD2	5:F:853:HOH:O	1.58	0.86
1:H:134:ILE:HD11	1:H:146:ALA:HB3	1.57	0.85
1:C:21:LYS:H	1:C:89:LYS:HE2	1.38	0.85
1:C:19:GLN:O	1:C:89:LYS:HE3	1.76	0.85
1:H:231:LYS:HE2	1:H:231:LYS:HA	1.56	0.85
1:H:310:GLU:HG2	1:H:314:ARG:NH1	1.90	0.85
1:B:203:MET:HG2	1:B:210:LEU:HD22	1.58	0.85
1:G:279:LEU:HD22	1:G:302:LEU:HD22	1.55	0.85
1:E:309:SER:HB2	1:E:312:GLU:HB2	1.59	0.84
1:A:302:LEU:HD13	1:D:11:LEU:HD11	1.57	0.84
1:C:97:ALA:N	1:C:112:ASN:HD21	1.74	0.83
1:B:227:LYS:CE	1:B:231:LYS:HE3	2.09	0.83
1:C:17:THR:HG22	1:C:18:PRO:HD2	1.61	0.82
1:D:99:GLN:HE22	1:D:108:LEU:HD22	1.44	0.82
1:E:306:THR:O	1:E:307:LEU:HB2	1.77	0.81
1:G:278:GLY:HA2	1:G:282:ILE:HG21	1.62	0.81
1:D:99:GLN:NE2	1:D:108:LEU:HD22	1.95	0.81
1:G:291:PRO:HB2	1:G:303:VAL:HB	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLY:HA3	5:C:881:HOH:O	1.80	0.80
1:F:117:LYS:HD3	1:F:331:PHE:HB2	1.62	0.80
1:F:61:MET:SD	1:F:78:SER:OG	2.38	0.80
1:D:279:LEU:C	1:D:280:TYR:CD1	2.54	0.80
1:D:279:LEU:CB	1:D:280:TYR:CE1	2.64	0.80
1:E:309:SER:CB	1:E:312:GLU:HB2	2.11	0.80
1:F:159:GLY:HA3	1:F:273:SER:HB2	1.64	0.80
1:E:304:LYS:HZ2	1:H:9:TYR:HB2	1.47	0.80
1:A:85:THR:HG23	5:A:808:HOH:O	1.80	0.79
1:E:106:LEU:HD22	1:E:325:ILE:HD13	1.65	0.79
1:F:97:ALA:H	1:F:112:ASN:HD21	1.28	0.79
1:C:21:LYS:H	1:C:89:LYS:CE	1.96	0.79
1:E:307:LEU:HD12	1:E:315:LEU:HD22	1.63	0.79
1:E:169:PHE:HD2	1:E:233:VAL:HG21	1.48	0.78
1:G:110:GLN:CD	1:G:330:GLN:HE22	1.85	0.78
1:F:185:HIS:ND1	2:F:818:ACT:H3	1.98	0.78
2:A:803:ACT:H3	5:A:900:HOH:O	1.84	0.77
1:H:110:GLN:HA	1:H:110:GLN:NE2	1.98	0.77
1:C:117:LYS:HD3	1:C:331:PHE:CB	2.15	0.77
1:E:276:ILE:CD1	1:E:288:LEU:HD11	2.11	0.77
1:G:97:ALA:H	1:G:112:ASN:HD21	1.32	0.77
1:D:2:THR:O	1:D:6:GLN:HG3	1.85	0.77
1:G:330:GLN:H	1:G:330:GLN:NE2	1.77	0.77
1:E:305:VAL:O	1:E:305:VAL:CG1	2.33	0.77
1:G:278:GLY:N	1:G:282:ILE:HB	2.00	0.76
1:B:155:ASN:ND2	1:C:12:LEU:HD11	2.00	0.76
1:D:110:GLN:HE22	1:D:330:GLN:H	1.34	0.76
1:E:180:HIS:CE1	1:E:182:LEU:HD23	2.20	0.76
1:B:17:THR:HG22	1:B:19:GLN:HE22	1.51	0.76
1:F:169:PHE:CE1	1:F:173:MET:CE	2.69	0.76
1:F:276:ILE:CD1	1:F:282:ILE:HD12	2.15	0.76
1:E:310:GLU:HB3	1:E:313:ALA:N	2.01	0.76
1:G:140:ASP:OD1	1:G:273:SER:OG	2.03	0.75
1:A:185:HIS:HD1	2:A:803:ACT:CH3	1.92	0.75
1:F:170:ARG:HD3	1:F:184:CYS:O	1.87	0.75
1:F:276:ILE:HD11	1:F:288:LEU:HD21	1.69	0.75
1:F:187:TRP:CZ2	1:H:206:ALA:HA	2.22	0.75
2:F:818:ACT:H2	5:F:838:HOH:O	1.86	0.75
1:C:182:LEU:HD21	5:D:877:HOH:O	1.87	0.74
1:G:121:PRO:HA	1:G:124:VAL:CG2	2.17	0.74
1:H:134:ILE:HD11	1:H:146:ALA:CB	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HD13	1:A:282:ILE:HD13	1.70	0.74
1:B:97:ALA:H	1:B:112:ASN:HD21	1.34	0.74
1:H:134:ILE:HD13	1:H:143:THR:HA	1.70	0.74
1:H:134:ILE:CD1	1:H:143:THR:HA	2.17	0.74
1:E:210:LEU:HD23	1:F:3:LEU:HD21	1.68	0.74
1:H:190:GLY:HA2	1:H:288:LEU:HD13	1.70	0.74
1:C:195:SER:HB2	1:C:317:LYS:HE3	1.70	0.73
1:F:21:LYS:H	1:F:89:LYS:CE	2.02	0.73
1:H:216:ASP:HB3	1:H:222:ASP:HB3	1.70	0.73
1:C:117:LYS:HD3	1:C:331:PHE:HB3	1.71	0.73
1:F:169:PHE:HE1	1:F:173:MET:CE	2.01	0.73
1:G:82:TYR:O	1:G:85:THR:HB	1.89	0.73
1:F:7:LEU:HG	1:F:8:ILE:HD12	1.70	0.73
1:H:180:HIS:HE1	1:H:182:LEU:HD23	1.54	0.73
1:F:169:PHE:CE1	1:F:173:MET:HE2	2.25	0.72
1:G:278:GLY:H	1:G:282:ILE:HB	1.55	0.72
1:B:196:SER:OG	1:B:230:HIS:HE1	1.72	0.72
1:E:212:THR:HG22	1:E:212:THR:O	1.88	0.72
1:F:82:TYR:O	1:F:85:THR:HB	1.89	0.72
1:H:115:ILE:HG23	3:H:822:NAI:N6A	2.04	0.72
1:G:330:GLN:N	1:G:330:GLN:HE21	1.78	0.71
1:H:138:PRO:HG2	1:H:141:ILE:HB	1.72	0.71
1:E:276:ILE:HD13	1:E:288:LEU:CD1	2.16	0.71
1:H:189:LEU:HD22	1:H:199:VAL:CG2	2.20	0.70
1:A:155:ASN:ND2	1:D:12:LEU:HD11	2.05	0.70
1:C:180:HIS:CE1	1:C:182:LEU:HD23	2.27	0.70
1:H:144:TYR:OH	1:H:330:GLN:HG2	1.91	0.70
1:G:278:GLY:HA2	1:G:282:ILE:CG2	2.22	0.70
1:A:314:ARG:HG3	1:A:314:ARG:NH1	2.06	0.70
1:G:216:ASP:HB3	1:G:222:ASP:HB3	1.73	0.70
1:B:9:TYR:HB2	1:C:304:LYS:HD2	1.72	0.69
1:B:227:LYS:HE3	1:B:231:LYS:CE	2.19	0.69
2:F:818:ACT:CH3	5:F:838:HOH:O	2.39	0.69
1:E:305:VAL:O	1:E:306:THR:OG1	2.10	0.69
1:H:134:ILE:CD1	1:H:146:ALA:HB3	2.22	0.69
1:H:97:ALA:N	1:H:112:ASN:HD21	1.88	0.69
1:E:308:THR:CB	1:E:309:SER:HB3	2.22	0.69
1:F:276:ILE:HD12	1:F:282:ILE:CD1	2.20	0.69
1:A:97:ALA:H	1:A:112:ASN:HD21	1.39	0.69
1:B:302:LEU:HD12	1:C:11:LEU:HD21	1.75	0.69
1:C:326:GLN:O	1:C:329:LEU:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:803:ACT:CH3	5:A:898:HOH:O	2.28	0.69
1:E:277:LYS:HA	1:E:282:ILE:CG2	2.23	0.69
1:G:220:ASP:O	1:G:221:LYS:CB	2.42	0.68
1:H:187:TRP:CE3	1:H:271:PRO:HG3	2.28	0.68
1:G:110:GLN:HA	1:G:110:GLN:NE2	2.07	0.68
1:E:109:VAL:O	1:E:113:VAL:HG23	1.93	0.68
1:F:22:ILE:HD12	1:F:44:ALA:HB2	1.76	0.68
1:E:198:PRO:HG3	1:E:230:HIS:ND1	2.08	0.68
1:E:105:ARG:O	1:E:106:LEU:CB	2.42	0.67
1:E:306:THR:O	1:E:307:LEU:CB	2.41	0.67
1:E:309:SER:HB2	1:E:312:GLU:CB	2.23	0.67
1:E:203:MET:SD	1:E:210:LEU:HD22	2.35	0.67
1:C:159:GLY:HA3	1:C:273:SER:OG	1.94	0.67
1:H:310:GLU:CG	1:H:314:ARG:NH1	2.58	0.67
1:G:173:MET:SD	1:G:184:CYS:HB3	2.34	0.67
1:A:173:MET:HE3	1:A:184:CYS:HB3	1.76	0.67
1:A:54:GLU:OE1	1:A:80:LYS:HE2	1.93	0.67
1:H:323:TRP:CE3	1:H:326:GLN:HB3	2.30	0.67
1:G:279:LEU:CD2	1:G:302:LEU:HD22	2.25	0.66
2:B:806:ACT:CH3	5:B:848:HOH:O	2.43	0.66
1:B:20:ASN:HA	1:B:89:LYS:HD2	1.76	0.66
1:C:25:VAL:HA	1:C:50:VAL:HG22	1.78	0.66
1:G:198:PRO:O	1:G:198:PRO:HG2	1.95	0.66
1:G:272:VAL:O	1:G:289:SER:HA	1.95	0.66
1:B:204:ASN:HA	1:B:210:LEU:HD13	1.78	0.66
1:E:192:HIS:O	1:E:192:HIS:CD2	2.49	0.66
1:G:203:MET:CE	1:G:210:LEU:HD22	2.26	0.66
1:H:310:GLU:CG	1:H:314:ARG:HH12	2.05	0.66
5:A:895:HOH:O	2:C:809:ACT:H1	1.96	0.66
1:F:276:ILE:CD1	1:F:282:ILE:CD1	2.74	0.66
1:D:216:ASP:HB3	1:D:222:ASP:HB2	1.78	0.66
1:B:169:PHE:HZ	1:B:203:MET:HE1	1.60	0.65
1:C:17:THR:HG22	1:C:18:PRO:CD	2.25	0.65
1:E:9:TYR:HB2	1:H:304:LYS:HE3	1.78	0.65
1:H:18:PRO:HG2	1:H:87:ASN:HB2	1.77	0.65
1:G:330:GLN:HG2	1:G:331:PHE:N	2.11	0.65
1:E:309:SER:HA	1:E:312:GLU:H	1.62	0.65
1:E:45:ASP:OD2	1:H:264:LYS:HA	1.96	0.65
1:G:121:PRO:HA	1:G:124:VAL:HG22	1.77	0.65
1:G:203:MET:HE2	1:G:210:LEU:HD22	1.79	0.65
1:H:106:LEU:O	1:H:109:VAL:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:HD22	1:A:84:VAL:N	1.95	0.65
1:H:41:LYS:NZ	5:H:829:HOH:O	2.23	0.65
1:A:170:ARG:HD3	1:A:184:CYS:O	1.96	0.65
1:G:196:SER:HB2	1:G:230:HIS:HE1	1.62	0.65
1:G:330:GLN:CG	1:G:331:PHE:N	2.59	0.65
1:H:216:ASP:HB3	1:H:222:ASP:CB	2.27	0.65
1:E:244:LYS:HB2	1:F:56:LYS:HE2	1.79	0.64
1:F:239:GLU:O	1:F:243:LEU:HD22	1.97	0.64
1:E:12:LEU:HD22	1:E:13:LYS:H	1.61	0.64
1:C:312:GLU:O	1:C:316:LYS:HG3	1.97	0.64
1:D:109:VAL:O	1:D:113:VAL:HG23	1.98	0.64
1:E:308:THR:CA	1:E:309:SER:CB	2.56	0.64
1:F:169:PHE:HE1	1:F:173:MET:HE1	1.62	0.64
1:F:204:ASN:HD22	1:F:207:GLY:H	1.44	0.64
1:G:114:ASN:HA	1:G:117:LYS:HE2	1.81	0.64
1:E:307:LEU:CD1	1:E:315:LEU:HD22	2.27	0.63
1:G:210:LEU:HG	1:H:3:LEU:HD11	1.80	0.63
1:H:282:ILE:HD11	1:H:286:VAL:HG23	1.81	0.63
1:F:229:VAL:O	1:F:233:VAL:HG23	1.98	0.63
1:H:107:ASN:O	1:H:111:ARG:NH2	2.29	0.63
1:G:323:TRP:CD1	1:G:327:LYS:HD2	2.34	0.63
1:H:25:VAL:HG13	1:H:50:VAL:HG22	1.80	0.63
1:E:212:THR:O	1:E:212:THR:CG2	2.46	0.63
1:G:98:ARG:O	1:G:111:ARG:NH2	2.31	0.63
1:F:117:LYS:HD3	1:F:331:PHE:O	1.98	0.63
1:G:282:ILE:O	1:G:283:LYS:HB3	1.99	0.63
1:B:83:ASN:HD22	1:B:84:VAL:H	1.44	0.63
1:B:200:TRP:CZ3	1:B:203:MET:HE1	2.34	0.62
1:G:56:LYS:NZ	5:G:855:HOH:O	2.31	0.62
1:A:276:ILE:HD11	1:A:286:VAL:HB	1.82	0.62
1:C:82:TYR:O	1:C:85:THR:HB	1.99	0.62
1:D:170:ARG:NH2	2:D:812:ACT:H1	2.12	0.62
1:G:93:ILE:HD12	1:G:134:ILE:CD1	2.30	0.62
3:D:810:NAI:H42N	4:D:811:OXM:C1	2.30	0.62
1:E:83:ASN:HD22	1:E:84:VAL:N	1.97	0.62
1:G:330:GLN:CG	1:G:331:PHE:H	2.12	0.62
1:C:19:GLN:C	1:C:89:LYS:HE3	2.21	0.62
1:G:204:ASN:HD22	1:G:207:GLY:H	1.48	0.62
1:D:203:MET:HG2	1:D:210:LEU:HD22	1.81	0.62
1:E:185:HIS:ND1	2:E:815:ACT:H3	2.15	0.61
1:E:305:VAL:HA	1:G:208:VAL:HG11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:LEU:HD21	1:E:302:LEU:HD21	1.81	0.61
1:A:327:LYS:HB3	1:A:327:LYS:NZ	2.14	0.61
1:D:180:HIS:CE1	1:D:182:LEU:HD23	2.35	0.61
3:D:810:NAI:H42N	4:D:811:OXM:C2	2.30	0.61
1:A:216:ASP:O	1:A:222:ASP:HB2	2.01	0.61
1:B:237:ALA:O	1:B:241:ILE:HG13	2.00	0.61
1:C:163:ASN:HA	1:C:271:PRO:HG2	1.81	0.61
1:G:279:LEU:HD22	1:G:302:LEU:CD2	2.28	0.61
1:H:173:MET:SD	1:H:184:CYS:HB3	2.41	0.61
1:H:82:TYR:O	1:H:85:THR:HB	1.99	0.61
1:B:205:VAL:O	1:B:208:VAL:CG1	2.49	0.61
1:G:170:ARG:HD3	1:G:184:CYS:O	2.00	0.60
1:E:194:ASP:OD1	1:E:238:TYR:OH	2.18	0.60
1:C:288:LEU:HD12	1:C:288:LEU:C	2.22	0.60
1:E:304:LYS:NZ	1:H:9:TYR:HB2	2.15	0.60
1:F:25:VAL:HG13	1:F:50:VAL:HG23	1.83	0.60
1:A:222:ASP:OD2	5:A:932:HOH:O	2.17	0.60
1:E:104:SER:O	1:E:105:ARG:CG	2.46	0.60
3:E:813:NAI:H42N	4:E:814:OXM:C1	2.31	0.60
1:F:159:GLY:CA	1:F:273:SER:HB2	2.31	0.60
1:F:204:ASN:HA	1:F:210:LEU:CD1	2.31	0.60
1:B:50:VAL:HB	1:B:79:GLY:O	2.01	0.60
1:F:317:LYS:HD3	1:F:318:SER:N	2.16	0.60
1:G:26:GLY:O	1:G:31:GLY:HA3	2.01	0.60
1:H:110:GLN:HE21	1:H:110:GLN:CA	2.09	0.60
1:H:32:MET:CE	1:H:60:GLU:HB3	2.31	0.60
1:E:168:ARG:NH1	1:F:66:HIS:ND1	2.50	0.60
1:E:211:LYS:C	1:E:213:LEU:H	2.04	0.60
1:E:235:GLU:O	1:E:239:GLU:HG2	2.01	0.60
1:A:54:GLU:CD	1:A:80:LYS:HE2	2.22	0.60
1:D:280:TYR:HD2	1:D:315:LEU:HD23	1.67	0.60
1:B:205:VAL:O	1:B:208:VAL:HG13	2.01	0.59
1:D:82:TYR:O	1:D:85:THR:HB	2.02	0.59
1:A:196:SER:OG	1:A:230:HIS:HE1	1.85	0.59
1:F:204:ASN:HA	1:F:210:LEU:HD13	1.84	0.59
1:F:21:LYS:H	1:F:89:LYS:HE3	1.65	0.59
1:A:120:ILE:HB	1:A:121:PRO:HD3	1.85	0.59
1:C:261:SER:OG	1:C:268:ARG:HD2	2.02	0.59
1:C:205:VAL:O	1:C:208:VAL:HG13	2.03	0.59
1:A:12:LEU:HD12	1:D:300:SER:HA	1.84	0.59
1:F:5:ASP:O	1:G:304:LYS:NZ	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:VAL:HG21	1:H:132:LEU:HD21	1.84	0.58
1:C:20:ASN:ND2	5:C:812:HOH:O	2.35	0.58
1:E:117:LYS:HE2	1:E:331:PHE:HB2	1.85	0.58
1:G:110:GLN:NE2	1:G:330:GLN:CD	2.56	0.58
1:H:310:GLU:CD	1:H:314:ARG:NH1	2.56	0.58
1:G:108:LEU:O	1:G:108:LEU:HD12	2.04	0.58
1:B:302:LEU:CD1	1:C:11:LEU:HD21	2.33	0.58
1:G:283:LYS:HA	1:G:283:LYS:CE	2.27	0.58
1:D:225:GLN:CA	1:D:225:GLN:OE1	2.50	0.58
1:D:106:LEU:HD13	1:D:328:GLU:OE1	2.03	0.58
1:F:180:HIS:CE1	1:F:182:LEU:HD22	2.39	0.58
1:G:120:ILE:O	1:G:124:VAL:HG22	2.03	0.58
1:H:272:VAL:O	1:H:289:SER:HA	2.03	0.58
1:C:17:THR:O	1:C:19:GLN:NE2	2.37	0.58
1:B:124:VAL:HG11	1:B:150:SER:HB2	1.85	0.57
1:E:208:VAL:HG21	1:F:7:LEU:HD13	1.86	0.57
1:E:310:GLU:HG3	1:E:312:GLU:HB3	1.85	0.57
1:E:329:LEU:HB3	1:E:331:PHE:CE1	2.39	0.57
1:C:23:THR:HB	1:C:91:VAL:HG22	1.87	0.57
1:E:313:ALA:O	1:E:315:LEU:N	2.37	0.57
1:G:179:VAL:CG1	1:G:180:HIS:N	2.67	0.57
1:A:159:GLY:HA3	1:A:273:SER:HB2	1.87	0.57
1:F:301:ASP:HA	1:G:11:LEU:HD23	1.87	0.57
1:G:239:GLU:O	1:G:243:LEU:CD2	2.52	0.57
1:B:168:ARG:HD3	1:B:236:SER:OG	2.04	0.57
1:B:297:ASN:ND2	1:C:16:GLN:OE1	2.37	0.57
1:G:97:ALA:N	1:G:112:ASN:HD21	2.01	0.57
1:G:284:ASP:HB3	1:G:323:TRP:CE3	2.39	0.57
1:E:105:ARG:C	1:E:106:LEU:CG	2.72	0.57
1:A:304:LYS:HD2	1:D:9:TYR:HB2	1.86	0.57
1:C:223:LYS:H	1:C:223:LYS:NZ	2.03	0.57
1:G:239:GLU:O	1:G:243:LEU:HD23	2.04	0.57
1:C:97:ALA:H	1:C:112:ASN:ND2	1.87	0.56
1:E:313:ALA:O	1:E:314:ARG:C	2.43	0.56
1:F:180:HIS:CG	1:F:181:PRO:HD2	2.40	0.56
1:B:20:ASN:HA	1:B:89:LYS:CD	2.35	0.56
1:D:279:LEU:C	1:D:280:TYR:HD1	1.97	0.56
1:A:89:LYS:N	1:A:89:LYS:HE2	2.20	0.56
1:F:204:ASN:ND2	1:F:207:GLY:H	2.03	0.56
1:F:293:ILE:HD12	1:F:301:ASP:HB2	1.86	0.56
1:G:11:LEU:HD22	1:G:11:LEU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:LYS:NZ	1:G:260:GLU:OE1	2.37	0.56
1:G:197:VAL:HG21	1:G:315:LEU:CD1	2.35	0.56
1:H:81:ASP:OD1	1:H:81:ASP:O	2.23	0.56
1:E:170:ARG:CD	1:E:184:CYS:O	2.54	0.56
1:E:199:VAL:HG12	1:E:199:VAL:O	2.04	0.56
1:H:147:TRP:HB2	1:H:157:VAL:HG11	1.88	0.56
1:A:42:ASP:OD2	1:A:72:ARG:HD3	2.06	0.56
1:B:12:LEU:N	1:B:12:LEU:HD12	2.20	0.56
1:D:272:VAL:O	1:D:289:SER:HA	2.06	0.56
1:E:236:SER:O	1:E:239:GLU:HB2	2.05	0.56
1:E:310:GLU:HB3	1:E:313:ALA:CB	2.36	0.56
3:F:816:NAI:H42N	4:F:817:OXM:C1	2.36	0.56
1:H:305:VAL:HG23	5:H:883:HOH:O	2.06	0.56
1:F:83:ASN:HD22	1:F:84:VAL:N	2.04	0.56
1:B:276:ILE:HD12	1:B:276:ILE:C	2.27	0.56
1:E:189:LEU:O	1:E:197:VAL:N	2.30	0.56
1:F:140:ASP:OD1	1:F:273:SER:OG	2.23	0.56
1:E:310:GLU:HA	1:E:312:GLU:N	2.20	0.56
1:C:117:LYS:HE2	1:C:330:GLN:O	2.06	0.55
1:E:135:VAL:O	3:E:813:NAI:H2N	2.06	0.55
1:F:89:LYS:HE2	1:F:89:LYS:H	1.71	0.55
1:A:292:CYS:HB3	1:A:299:ILE:HG23	1.88	0.55
1:C:204:ASN:HA	1:C:210:LEU:HD13	1.88	0.55
1:F:21:LYS:HG3	1:F:46:GLU:HB3	1.88	0.55
1:G:83:ASN:HD22	1:G:83:ASN:N	2.04	0.55
1:B:39:LEU:HD11	1:B:64:LEU:HD13	1.88	0.55
1:D:293:ILE:HD12	1:D:301:ASP:HB2	1.88	0.55
1:E:325:ILE:O	1:E:329:LEU:HD13	2.07	0.55
1:G:313:ALA:HA	1:G:316:LYS:HD3	1.88	0.55
1:F:173:MET:SD	1:F:203:MET:HE3	2.46	0.55
1:G:283:LYS:CA	1:G:283:LYS:HE3	2.26	0.55
1:H:187:TRP:HZ3	1:H:271:PRO:HG3	1.68	0.55
1:E:205:VAL:HB	1:F:7:LEU:HD21	1.87	0.55
1:H:282:ILE:CD1	1:H:286:VAL:HG23	2.37	0.55
1:H:325:ILE:N	1:H:325:ILE:HD12	2.21	0.55
1:G:202:GLY:HA3	5:G:866:HOH:O	2.06	0.55
1:D:277:LYS:HB2	1:D:284:ASP:O	2.07	0.55
1:E:277:LYS:HA	1:E:282:ILE:HG23	1.88	0.55
1:A:173:MET:CE	1:A:184:CYS:HB3	2.37	0.55
1:A:123:VAL:HG21	1:A:132:LEU:HD21	1.87	0.55
1:F:308:THR:HG23	1:F:311:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:TRP:CZ3	1:G:271:PRO:HD3	2.42	0.55
1:A:276:ILE:HD13	1:A:282:ILE:CD1	2.36	0.54
1:C:120:ILE:HB	1:C:121:PRO:HD3	1.89	0.54
1:F:314:ARG:O	1:F:317:LYS:HG3	2.06	0.54
1:G:278:GLY:CA	1:G:282:ILE:CG2	2.85	0.54
1:H:83:ASN:C	1:H:83:ASN:ND2	2.60	0.54
1:E:310:GLU:HA	1:E:311:GLU:HB2	1.88	0.54
1:E:329:LEU:HB3	1:E:331:PHE:CD1	2.42	0.54
1:G:277:LYS:HE2	1:G:282:ILE:HD12	1.88	0.54
1:H:327:LYS:O	1:H:330:GLN:HB2	2.07	0.54
1:H:282:ILE:HG13	1:H:282:ILE:O	2.06	0.54
1:C:223:LYS:H	1:C:223:LYS:CE	2.21	0.54
1:G:3:LEU:HD13	1:H:214:HIS:HB2	1.88	0.54
1:A:170:ARG:CD	1:A:184:CYS:O	2.56	0.54
1:F:276:ILE:HD13	1:F:288:LEU:HD11	1.88	0.54
1:A:279:LEU:HB3	1:A:280:TYR:CD1	2.43	0.54
1:B:137:ASN:HA	1:B:139:VAL:N	2.23	0.54
1:G:208:VAL:CG2	1:G:208:VAL:O	2.55	0.54
1:H:32:MET:HE1	1:H:60:GLU:HB3	1.90	0.54
1:H:81:ASP:OD1	1:H:84:VAL:HG13	2.07	0.54
1:A:198:PRO:HG2	1:A:198:PRO:O	2.08	0.54
1:E:280:TYR:HE2	1:E:306:THR:O	1.91	0.54
1:G:11:LEU:N	1:G:11:LEU:CD2	2.71	0.54
1:G:83:ASN:HD22	1:G:84:VAL:H	1.56	0.54
1:C:205:VAL:O	1:C:208:VAL:CG1	2.56	0.53
1:D:279:LEU:CG	1:D:280:TYR:HE1	2.21	0.53
1:E:280:TYR:CE2	1:E:307:LEU:HG	2.44	0.53
1:E:309:SER:HA	1:E:312:GLU:HB2	1.89	0.53
1:C:180:HIS:CE1	1:C:182:LEU:CD2	2.90	0.53
1:G:110:GLN:HE22	1:G:330:GLN:CD	2.10	0.53
1:C:83:ASN:HD22	1:C:84:VAL:N	2.06	0.53
1:D:198:PRO:HG3	1:D:230:HIS:CG	2.43	0.53
2:B:806:ACT:H3	5:B:848:HOH:O	2.08	0.53
1:A:124:VAL:HG12	1:A:152:PHE:CZ	2.43	0.53
1:C:312:GLU:O	1:C:316:LYS:CG	2.56	0.53
1:F:25:VAL:HG13	1:F:50:VAL:CG2	2.38	0.53
5:B:926:HOH:O	1:C:75:LYS:HB2	2.09	0.53
2:G:821:ACT:H1	5:G:822:HOH:O	2.09	0.53
1:E:164:LEU:O	1:E:164:LEU:HG	2.07	0.53
1:H:134:ILE:CD1	1:H:146:ALA:CB	2.85	0.53
1:A:124:VAL:HG11	1:A:150:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:HIS:CE1	1:D:182:LEU:CD2	2.92	0.53
1:H:282:ILE:HD12	1:H:284:ASP:H	1.72	0.53
1:H:223:LYS:NZ	1:H:223:LYS:HB2	2.24	0.53
1:C:317:LYS:HD3	1:C:318:SER:N	2.24	0.53
1:E:309:SER:N	1:E:311:GLU:HB2	2.24	0.52
1:G:163:ASN:HA	1:G:271:PRO:HG2	1.91	0.52
1:E:216:ASP:HB3	1:E:222:ASP:HB3	1.91	0.52
1:E:308:THR:HG1	1:E:309:SER:CB	2.22	0.52
1:F:219:THR:CG2	1:F:221:LYS:H	2.16	0.52
1:H:310:GLU:OE2	1:H:314:ARG:NH2	2.43	0.52
1:C:274:THR:O	1:C:287:PHE:HA	2.10	0.52
1:G:98:ARG:O	1:G:99:GLN:HB2	2.09	0.52
1:A:119:ILE:O	1:A:123:VAL:HG13	2.09	0.52
1:A:204:ASN:HD22	1:A:207:GLY:H	1.56	0.52
1:A:28:GLY:HA3	3:A:801:NAI:O5B	2.09	0.52
1:D:230:HIS:HD2	5:D:840:HOH:O	1.91	0.52
1:F:7:LEU:HG	1:F:8:ILE:CD1	2.37	0.52
1:G:212:THR:O	1:G:212:THR:HG22	2.09	0.52
1:G:110:GLN:CD	1:G:330:GLN:OE1	2.48	0.52
5:C:827:HOH:O	1:D:182:LEU:HD21	2.08	0.52
1:D:325:ILE:O	1:D:329:LEU:HD13	2.10	0.52
1:F:267:ARG:HA	1:F:294:LEU:O	2.10	0.52
1:G:121:PRO:CA	1:G:124:VAL:HG22	2.38	0.52
1:D:158:ILE:HG23	1:D:299:ILE:HD11	1.90	0.52
1:G:141:ILE:O	1:G:144:TYR:HB3	2.10	0.52
1:G:82:TYR:CG	1:G:122:ASN:HB3	2.44	0.52
1:H:180:HIS:ND1	1:H:182:LEU:HD23	2.25	0.52
1:H:204:ASN:HA	1:H:210:LEU:HD13	1.91	0.52
1:E:104:SER:C	1:E:105:ARG:HD2	2.30	0.52
1:E:70:PHE:O	1:E:72:ARG:NH2	2.43	0.52
1:F:115:ILE:HG22	1:F:119:ILE:HD12	1.91	0.52
1:H:189:LEU:HD22	1:H:199:VAL:HG21	1.90	0.52
1:H:97:ALA:H	1:H:112:ASN:ND2	1.95	0.52
1:B:200:TRP:CE3	1:B:203:MET:CE	2.93	0.52
1:D:99:GLN:NE2	1:D:108:LEU:HD13	2.24	0.52
1:E:9:TYR:C	1:E:9:TYR:CD2	2.82	0.52
1:F:85:THR:CG2	5:F:827:HOH:O	2.58	0.52
1:E:187:TRP:CZ2	1:G:206:ALA:HA	2.44	0.52
1:D:291:PRO:HB2	1:D:303:VAL:HB	1.91	0.51
1:G:276:ILE:HD12	1:G:276:ILE:O	2.10	0.51
1:B:17:THR:HG22	1:B:19:GLN:NE2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:MET:CG	1:B:210:LEU:HD22	2.35	0.51
1:C:145:VAL:HG12	1:C:149:ILE:HD12	1.92	0.51
1:D:265:ASN:CG	1:D:296:GLN:HG2	2.31	0.51
1:E:46:GLU:CD	1:E:75:LYS:HE3	2.29	0.51
1:F:8:ILE:HD12	1:F:8:ILE:N	2.26	0.51
1:B:204:ASN:HD22	1:B:207:GLY:H	1.56	0.51
1:E:106:LEU:HD13	1:E:325:ILE:HD11	1.91	0.51
1:E:120:ILE:O	1:E:123:VAL:HG22	2.10	0.51
1:G:110:GLN:NE2	1:G:110:GLN:CA	2.73	0.51
1:E:180:HIS:CE1	1:E:182:LEU:CD2	2.91	0.51
1:E:50:VAL:HG12	1:E:51:ASP:N	2.24	0.51
1:F:317:LYS:C	1:F:317:LYS:HD3	2.30	0.51
1:B:224:GLU:O	1:B:225:GLN:HB2	2.10	0.51
1:E:220:ASP:HA	1:E:227:LYS:HE3	1.91	0.51
1:F:97:ALA:N	1:F:112:ASN:HD21	2.05	0.51
1:G:110:GLN:CD	1:G:330:GLN:NE2	2.54	0.51
1:G:228:GLU:O	1:G:228:GLU:HG3	2.09	0.51
1:H:134:ILE:HD12	1:H:143:THR:HA	1.90	0.51
1:E:170:ARG:HD3	1:E:184:CYS:O	2.11	0.51
1:E:331:PHE:O	1:E:331:PHE:CG	2.63	0.51
1:E:293:ILE:HB	1:E:301:ASP:HB2	1.93	0.51
1:E:310:GLU:HG3	1:E:312:GLU:CB	2.40	0.51
1:E:106:LEU:CD2	1:E:325:ILE:HD13	2.37	0.51
1:F:129:ASN:HA	1:F:156:ARG:NH1	2.26	0.51
1:F:169:PHE:CE1	1:F:173:MET:HE1	2.41	0.50
1:A:189:LEU:HD22	1:A:199:VAL:HG21	1.93	0.50
1:D:204:ASN:HD22	1:D:207:GLY:H	1.58	0.50
1:E:208:VAL:CG2	1:F:7:LEU:HD13	2.41	0.50
1:E:5:ASP:O	1:H:304:LYS:NZ	2.44	0.50
1:A:293:ILE:HD12	1:A:301:ASP:HB2	1.94	0.50
1:H:115:ILE:HG23	3:H:822:NAI:H61A	1.71	0.50
1:C:210:LEU:N	1:C:210:LEU:CD1	2.74	0.50
1:E:196:SER:O	5:E:828:HOH:O	2.19	0.50
1:F:11:LEU:HB2	1:G:300:SER:O	2.11	0.50
1:F:49:LEU:O	1:F:78:SER:HA	2.12	0.50
1:F:180:HIS:ND1	1:F:181:PRO:HD2	2.27	0.50
1:D:135:VAL:O	3:D:810:NAI:H2N	2.12	0.50
1:E:170:ARG:HD2	1:E:184:CYS:O	2.11	0.50
1:E:219:THR:HG22	1:E:221:LYS:H	1.76	0.50
1:A:325:ILE:O	1:A:329:LEU:HD13	2.12	0.50
1:G:197:VAL:HG21	1:G:315:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:TYR:CG	1:H:326:GLN:HG2	2.47	0.50
1:C:322:LEU:O	1:C:326:GLN:HG3	2.12	0.50
1:H:120:ILE:HB	1:H:121:PRO:HD3	1.93	0.50
1:H:30:VAL:HG23	3:H:822:NAI:PN	2.51	0.50
1:E:14:GLU:O	1:E:15:GLU:HB2	2.12	0.50
1:A:210:LEU:HG	1:B:3:LEU:HD21	1.93	0.49
1:G:286:VAL:CG1	1:G:322:LEU:HD23	2.42	0.49
1:H:85:THR:CG2	1:H:85:THR:O	2.60	0.49
1:F:56:LYS:HD3	1:F:56:LYS:O	2.13	0.49
1:G:278:GLY:CA	1:G:282:ILE:HG21	2.39	0.49
1:G:324:GLY:HA2	1:G:327:LYS:HD3	1.94	0.49
1:G:330:GLN:O	1:G:331:PHE:O	2.30	0.49
1:B:115:ILE:CG2	1:B:119:ILE:HD12	2.42	0.49
1:C:228:GLU:O	1:C:232:GLN:HG3	2.12	0.49
1:E:310:GLU:CB	1:E:313:ALA:H	2.14	0.49
1:F:83:ASN:HD22	1:F:84:VAL:H	1.58	0.49
1:E:210:LEU:H	1:E:210:LEU:HD12	1.78	0.49
1:F:100:GLN:O	1:F:101:GLU:C	2.50	0.49
1:C:220:ASP:OD2	1:C:220:ASP:N	2.42	0.49
1:F:138:PRO:HG2	1:F:138:PRO:O	2.11	0.49
1:F:291:PRO:HB2	1:F:303:VAL:HB	1.93	0.49
1:F:46:GLU:HG3	1:F:75:LYS:HB3	1.93	0.49
1:G:196:SER:HB2	1:G:230:HIS:CE1	2.46	0.49
1:A:19:GLN:NE2	1:D:296:GLN:OE1	2.46	0.49
1:D:141:ILE:O	1:D:145:VAL:HG23	2.13	0.49
1:H:147:TRP:CZ2	1:H:275:MET:HE1	2.47	0.49
1:B:141:ILE:HD13	1:B:325:ILE:HG21	1.95	0.49
1:D:189:LEU:HD22	1:D:199:VAL:HG21	1.94	0.49
1:F:137:ASN:HA	1:F:139:VAL:N	2.27	0.49
1:H:241:ILE:HG12	1:H:246:TYR:HA	1.94	0.49
1:C:198:PRO:HD3	1:C:230:HIS:CE1	2.47	0.49
1:G:113:VAL:HG22	1:G:145:VAL:HG21	1.94	0.49
1:F:304:LYS:HD2	1:G:9:TYR:HB2	1.95	0.49
1:F:109:VAL:HG13	1:F:110:GLN:N	2.28	0.49
1:A:190:GLY:HA2	1:A:288:LEU:HD13	1.95	0.49
1:B:290:VAL:HG21	1:B:302:LEU:HD23	1.95	0.49
1:F:272:VAL:O	1:F:289:SER:HA	2.13	0.49
1:A:219:THR:HG23	1:A:221:LYS:H	1.78	0.48
1:E:304:LYS:NZ	1:H:9:TYR:N	2.61	0.48
1:B:119:ILE:HD11	3:B:804:NAI:N1A	2.28	0.48
1:G:235:GLU:HA	1:G:238:TYR:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:N	1:A:112:ASN:HD21	2.10	0.48
1:C:189:LEU:HD22	1:C:199:VAL:HG21	1.96	0.48
1:D:279:LEU:HB3	1:D:280:TYR:HE1	1.61	0.48
1:C:25:VAL:HA	1:C:50:VAL:CG2	2.42	0.48
1:D:230:HIS:CD2	5:D:840:HOH:O	2.65	0.48
1:E:331:PHE:CD2	1:E:331:PHE:O	2.66	0.48
1:E:309:SER:CA	1:E:312:GLU:HB2	2.43	0.48
1:F:27:VAL:HG22	1:F:51:ASP:OD2	2.14	0.48
1:F:302:LEU:HD13	1:G:11:LEU:HD21	1.95	0.48
1:B:200:TRP:CE3	1:B:203:MET:HE1	2.49	0.48
1:F:10:ASN:ND2	1:F:11:LEU:N	2.62	0.48
1:E:203:MET:HB3	1:E:210:LEU:HD13	1.94	0.48
1:E:209:SER:O	1:E:213:LEU:HB2	2.13	0.48
1:G:266:LEU:O	1:G:267:ARG:HB2	2.12	0.48
1:D:110:GLN:NE2	1:D:330:GLN:H	2.07	0.48
1:E:326:GLN:HA	1:E:329:LEU:HD22	1.95	0.48
5:E:834:HOH:O	1:F:182:LEU:HD21	2.14	0.48
1:D:125:LYS:HD3	1:D:126:TYR:CE1	2.49	0.48
1:G:215:PRO:C	1:G:217:LEU:H	2.17	0.48
1:B:83:ASN:HD22	1:B:83:ASN:C	2.15	0.47
1:G:110:GLN:NE2	1:G:330:GLN:NE2	2.62	0.47
1:D:120:ILE:O	1:D:124:VAL:HG13	2.14	0.47
1:G:162:CYS:N	1:G:289:SER:OG	2.46	0.47
1:A:19:GLN:O	1:A:89:LYS:HD2	2.14	0.47
1:C:276:ILE:HD12	1:C:276:ILE:C	2.35	0.47
1:C:187:TRP:N	1:C:187:TRP:CD1	2.82	0.47
1:E:69:LEU:HD12	1:F:182:LEU:HD13	1.96	0.47
1:F:173:MET:SD	1:F:184:CYS:HB3	2.54	0.47
1:G:179:VAL:HG12	1:G:180:HIS:N	2.28	0.47
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.95	0.47
1:F:57:LEU:HG	1:F:78:SER:HB2	1.96	0.47
1:G:232:GLN:O	1:G:236:SER:HB2	2.14	0.47
1:C:117:LYS:HD3	1:C:331:PHE:HB2	1.95	0.47
1:D:137:ASN:HA	1:D:139:VAL:N	2.30	0.47
1:E:206:ALA:HB3	1:G:303:VAL:HG11	1.95	0.47
1:E:9:TYR:CD2	1:E:11:LEU:HD22	2.50	0.47
1:E:179:VAL:HG22	1:G:293:ILE:CD1	2.45	0.47
1:H:331:PHE:CD2	1:H:331:PHE:O	2.68	0.47
1:E:138:PRO:HG2	1:E:141:ILE:HB	1.96	0.47
1:F:192:HIS:CG	1:F:192:HIS:O	2.63	0.47
1:H:137:ASN:O	1:H:142:LEU:CD1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:HIS:O	1:B:217:LEU:HB2	2.14	0.47
1:E:137:ASN:HA	1:E:139:VAL:N	2.29	0.47
1:E:284:ASP:O	1:E:286:VAL:N	2.47	0.47
1:G:69:LEU:HD12	1:H:182:LEU:HD22	1.97	0.47
1:H:204:ASN:HD22	1:H:207:GLY:H	1.62	0.47
1:E:198:PRO:HD3	1:E:230:HIS:CE1	2.50	0.47
1:E:211:LYS:C	1:E:213:LEU:N	2.67	0.47
1:G:282:ILE:O	1:G:283:LYS:CB	2.63	0.47
1:H:137:ASN:C	1:H:142:LEU:HD12	2.35	0.47
1:D:279:LEU:HG	1:D:280:TYR:HE1	1.80	0.47
1:E:310:GLU:HA	1:E:312:GLU:H	1.79	0.47
1:F:251:ILE:HD13	3:F:816:NAI:O7N	2.15	0.47
1:H:286:VAL:HA	1:H:326:GLN:OE1	2.15	0.47
1:B:266:LEU:O	1:D:180:HIS:HB2	2.14	0.46
1:C:195:SER:OG	1:C:318:SER:OG	2.32	0.46
1:C:223:LYS:H	1:C:223:LYS:HZ3	1.63	0.46
1:F:293:ILE:HD12	1:F:301:ASP:CB	2.45	0.46
1:G:201:SER:HA	1:G:211:LYS:HD3	1.97	0.46
1:C:173:MET:HB2	1:C:173:MET:HE2	1.56	0.46
1:F:276:ILE:HD11	1:F:288:LEU:CD2	2.44	0.46
1:A:180:HIS:HB2	1:C:266:LEU:O	2.16	0.46
1:A:25:VAL:HG13	1:A:50:VAL:HG22	1.97	0.46
1:B:204:ASN:ND2	1:B:207:GLY:H	2.14	0.46
1:E:177:LEU:O	1:E:179:VAL:HG23	2.15	0.46
1:F:279:LEU:HB3	1:F:280:TYR:CD1	2.50	0.46
1:G:198:PRO:HD3	1:G:230:HIS:CE1	2.50	0.46
1:A:42:ASP:OD2	1:A:72:ARG:CD	2.63	0.46
1:H:153:PRO:HB2	1:H:155:ASN:OD1	2.15	0.46
1:A:330:GLN:HA	1:A:330:GLN:OE1	2.15	0.46
1:B:272:VAL:O	1:B:289:SER:HA	2.16	0.46
1:E:180:HIS:CG	1:E:181:PRO:HD2	2.51	0.46
1:G:286:VAL:HG13	1:G:322:LEU:HD23	1.98	0.46
1:F:187:TRP:CD1	1:F:187:TRP:N	2.83	0.46
1:H:216:ASP:O	1:H:222:ASP:HB3	2.16	0.46
1:E:104:SER:C	1:E:105:ARG:CG	2.84	0.46
1:B:169:PHE:HZ	1:B:203:MET:CE	2.28	0.46
1:D:18:PRO:HG3	1:D:46:GLU:OE1	2.16	0.46
1:D:99:GLN:NE2	1:D:108:LEU:CD2	2.75	0.46
1:H:217:LEU:HD12	1:H:226:TRP:CB	2.45	0.46
1:A:206:ALA:HA	1:C:187:TRP:CZ2	2.51	0.46
1:A:270:HIS:CD2	1:A:294:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:SER:HB3	1:B:130:CYS:HB3	1.98	0.46
1:B:180:HIS:CG	1:B:181:PRO:HD2	2.51	0.46
1:D:119:ILE:O	1:D:123:VAL:HG22	2.16	0.46
1:H:204:ASN:ND2	1:H:207:GLY:H	2.14	0.46
1:B:180:HIS:ND1	1:B:181:PRO:HD2	2.31	0.45
1:C:280:TYR:C	1:C:282:ILE:H	2.20	0.45
1:C:42:ASP:CG	1:C:72:ARG:HE	2.19	0.45
1:F:82:TYR:CE2	1:F:123:VAL:HG12	2.50	0.45
1:G:16:GLN:HB3	1:G:17:THR:H	1.45	0.45
1:G:208:VAL:HG23	1:G:208:VAL:O	2.16	0.45
1:G:274:THR:HG21	1:G:302:LEU:HD11	1.97	0.45
1:G:83:ASN:HD22	1:G:84:VAL:N	2.14	0.45
1:H:124:VAL:O	1:H:125:LYS:C	2.53	0.45
1:D:119:ILE:HD11	3:D:810:NAI:C6A	2.46	0.45
1:F:170:ARG:CD	1:F:184:CYS:O	2.61	0.45
1:G:204:ASN:ND2	1:G:207:GLY:H	2.13	0.45
1:H:217:LEU:HD12	1:H:226:TRP:CG	2.51	0.45
1:B:21:LYS:H	1:B:89:LYS:CE	2.30	0.45
1:D:302:LEU:HD12	1:D:302:LEU:C	2.37	0.45
1:C:216:ASP:O	1:C:222:ASP:HB2	2.15	0.45
1:D:279:LEU:CB	1:D:280:TYR:CD1	2.89	0.45
1:G:200:TRP:CD1	1:G:218:GLY:HA3	2.51	0.45
1:E:179:VAL:HG22	1:G:293:ILE:HD11	1.98	0.45
1:B:274:THR:O	1:B:287:PHE:HA	2.16	0.45
1:D:120:ILE:O	1:D:123:VAL:HG23	2.17	0.45
1:D:240:VAL:CG1	1:D:247:THR:HG22	2.45	0.45
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.79	0.45
1:B:69:LEU:HD12	1:B:69:LEU:O	2.17	0.45
1:E:124:VAL:HG11	1:E:150:SER:HB2	1.99	0.45
1:E:321:THR:HA	5:E:849:HOH:O	2.16	0.45
1:E:9:TYR:HD2	1:E:9:TYR:C	2.19	0.45
1:C:117:LYS:CE	1:C:330:GLN:O	2.65	0.45
1:E:210:LEU:N	1:E:210:LEU:HD12	2.30	0.45
1:C:293:ILE:HB	1:C:301:ASP:HB2	1.99	0.45
1:E:313:ALA:O	1:E:316:LYS:N	2.50	0.45
1:F:109:VAL:HG13	1:F:110:GLN:H	1.82	0.45
1:E:164:LEU:O	1:E:168:ARG:HG3	2.17	0.44
1:F:23:THR:OG1	1:F:48:ALA:HB3	2.16	0.44
1:G:247:THR:OG1	3:G:819:NAI:H5N	2.17	0.44
1:G:85:THR:CG2	1:G:85:THR:O	2.64	0.44
1:H:280:TYR:H	1:H:282:ILE:HG23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:VAL:HG22	1:C:50:VAL:CG2	2.47	0.44
1:D:16:GLN:C	1:D:17:THR:OG1	2.54	0.44
1:E:9:TYR:HD2	1:E:11:LEU:HD22	1.82	0.44
1:E:305:VAL:HA	1:G:208:VAL:CG1	2.46	0.44
1:F:222:ASP:OD2	1:F:225:GLN:N	2.50	0.44
1:B:326:GLN:O	1:B:327:LYS:C	2.55	0.44
1:C:20:ASN:HA	1:C:89:LYS:HE3	2.00	0.44
1:C:32:MET:CE	1:C:60:GLU:HB3	2.48	0.44
1:F:85:THR:O	1:F:85:THR:HG23	2.16	0.44
1:G:93:ILE:HD12	1:G:134:ILE:HD13	1.98	0.44
1:B:198:PRO:HG3	1:B:230:HIS:CG	2.53	0.44
1:H:293:ILE:HD12	1:H:301:ASP:HB2	1.99	0.44
1:B:200:TRP:CE3	1:B:203:MET:HE3	2.53	0.44
1:B:89:LYS:HE3	1:B:89:LYS:N	2.33	0.44
1:A:266:LEU:O	1:C:180:HIS:HB2	2.18	0.44
1:D:196:SER:OG	1:D:230:HIS:HE1	2.00	0.44
1:G:116:PHE:O	1:G:120:ILE:HG12	2.18	0.44
1:E:309:SER:HA	1:E:310:GLU:HA	1.58	0.44
1:F:10:ASN:ND2	1:F:11:LEU:H	2.16	0.44
1:F:196:SER:OG	1:F:230:HIS:HE1	2.01	0.44
1:B:12:LEU:H	1:B:12:LEU:HD12	1.83	0.43
1:G:307:LEU:HD22	1:G:311:GLU:HB3	2.00	0.43
1:A:219:THR:CG2	1:A:221:LYS:HG2	2.48	0.43
1:E:312:GLU:O	1:E:312:GLU:OE1	2.37	0.43
1:G:200:TRP:C	1:G:202:GLY:H	2.20	0.43
1:G:204:ASN:HD22	1:G:207:GLY:N	2.16	0.43
1:G:276:ILE:CD1	1:G:276:ILE:O	2.66	0.43
1:H:290:VAL:HG13	1:H:291:PRO:HD2	2.00	0.43
1:C:109:VAL:HG13	1:C:110:GLN:N	2.33	0.43
1:E:277:LYS:HA	1:E:282:ILE:HG22	1.97	0.43
1:C:21:LYS:N	1:C:89:LYS:HE2	2.18	0.43
1:C:7:LEU:HD23	1:C:8:ILE:HG13	2.00	0.43
1:E:169:PHE:CD2	1:E:233:VAL:HG21	2.40	0.43
1:H:196:SER:OG	1:H:230:HIS:HE1	2.01	0.43
1:B:117:LYS:HD3	1:B:331:PHE:HB3	2.00	0.43
1:E:219:THR:O	1:E:220:ASP:C	2.57	0.43
1:E:217:LEU:HD12	1:E:226:TRP:CB	2.47	0.43
1:A:187:TRP:CZ2	1:C:206:ALA:HA	2.54	0.43
1:C:330:GLN:O	1:C:331:PHE:HB3	2.18	0.43
1:D:279:LEU:CG	1:D:280:TYR:CE1	3.00	0.43
1:E:315:LEU:HA	1:E:315:LEU:HD12	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ASP:OD2	1:G:220:ASP:N	2.52	0.43
1:H:137:ASN:HA	1:H:138:PRO:C	2.38	0.43
1:E:50:VAL:CG1	1:E:51:ASP:N	2.81	0.43
1:F:326:GLN:O	1:F:329:LEU:HB2	2.19	0.43
1:G:110:GLN:HE22	1:G:330:GLN:NE2	2.17	0.43
1:A:219:THR:HG23	1:A:221:LYS:N	2.34	0.43
1:B:290:VAL:HG21	1:B:302:LEU:CD2	2.49	0.43
1:D:80:LYS:O	1:D:80:LYS:HG2	2.18	0.43
1:E:308:THR:OG1	1:E:309:SER:CB	2.66	0.43
1:F:203:MET:HE2	1:F:226:TRP:CZ3	2.54	0.43
1:G:177:LEU:HD12	1:G:177:LEU:HA	1.75	0.43
1:H:205:VAL:O	1:H:208:VAL:HG13	2.18	0.43
1:H:279:LEU:HD22	1:H:302:LEU:HD23	1.99	0.43
1:H:185:HIS:CE1	2:H:824:ACT:H1	2.54	0.43
1:A:205:VAL:O	1:A:208:VAL:HG13	2.19	0.43
1:D:265:ASN:OD1	1:D:296:GLN:HG2	2.18	0.43
1:E:210:LEU:HD23	1:F:3:LEU:CD2	2.46	0.43
1:E:80:LYS:HG3	1:E:80:LYS:H	1.69	0.43
1:G:89:LYS:O	1:G:131:LYS:HE2	2.18	0.43
1:H:137:ASN:O	1:H:142:LEU:HD11	2.19	0.43
1:H:325:ILE:N	1:H:325:ILE:CD1	2.82	0.43
1:A:168:ARG:HD3	1:A:236:SER:OG	2.19	0.42
1:A:272:VAL:O	1:A:289:SER:HA	2.19	0.42
1:B:288:LEU:HD12	1:B:288:LEU:C	2.39	0.42
1:C:137:ASN:HA	1:C:139:VAL:N	2.34	0.42
1:D:244:LYS:HG3	1:D:246:TYR:O	2.19	0.42
3:E:813:NAI:H42N	4:E:814:OXM:C2	2.48	0.42
1:G:2:THR:O	1:G:6:GLN:HG3	2.19	0.42
1:H:83:ASN:C	1:H:83:ASN:HD22	2.21	0.42
1:B:316:LYS:O	1:B:320:ASP:OD2	2.38	0.42
1:C:280:TYR:O	1:C:316:LYS:HD3	2.19	0.42
1:C:286:VAL:CG2	1:C:323:TRP:HB2	2.49	0.42
3:C:807:NAI:H42N	4:C:808:OXM:C1	2.50	0.42
1:E:153:PRO:HB2	1:E:155:ASN:OD1	2.18	0.42
1:F:185:HIS:O	1:F:203:MET:HA	2.19	0.42
1:G:237:ALA:O	1:G:241:ILE:HG13	2.19	0.42
1:C:173:MET:SD	1:C:184:CYS:HB3	2.59	0.42
1:D:142:LEU:HD23	1:D:142:LEU:HA	1.71	0.42
1:G:150:SER:OG	1:G:152:PHE:HB2	2.19	0.42
1:E:291:PRO:HG2	1:E:305:VAL:HG21	2.02	0.42
1:G:112:ASN:HD22	1:G:115:ILE:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:CYS:O	1:G:156:ARG:HD2	2.19	0.42
1:C:192:HIS:O	1:C:192:HIS:CG	2.70	0.42
1:D:241:ILE:HG12	1:D:246:TYR:HA	2.01	0.42
1:F:173:MET:HE2	1:F:173:MET:HB2	1.83	0.42
1:G:278:GLY:HA2	1:G:282:ILE:CB	2.50	0.42
1:C:25:VAL:HG22	1:C:50:VAL:HG21	2.02	0.42
1:F:169:PHE:CD1	1:F:173:MET:CE	3.02	0.42
1:F:180:HIS:CE1	1:F:182:LEU:CD2	3.01	0.42
1:H:279:LEU:CD2	1:H:302:LEU:HD23	2.49	0.42
1:D:217:LEU:HD12	1:D:226:TRP:CG	2.55	0.42
1:E:166:SER:O	1:E:170:ARG:HG3	2.18	0.42
1:E:216:ASP:O	1:E:219:THR:HB	2.19	0.42
1:B:115:ILE:HG23	1:B:119:ILE:HD12	2.02	0.42
1:B:170:ARG:NH2	2:B:806:ACT:H1	2.34	0.42
1:B:228:GLU:O	1:B:228:GLU:HG3	2.20	0.42
1:H:124:VAL:CG2	1:H:125:LYS:N	2.82	0.42
1:A:211:LYS:HB3	5:A:931:HOH:O	2.18	0.42
1:C:327:LYS:HB3	1:C:327:LYS:HE2	1.84	0.42
1:D:137:ASN:HA	1:D:138:PRO:C	2.40	0.42
1:H:282:ILE:HD13	1:H:286:VAL:CG2	2.50	0.42
1:B:185:HIS:ND1	2:B:806:ACT:H2	2.35	0.42
1:C:310:GLU:O	1:C:314:ARG:HG3	2.20	0.42
1:E:308:THR:OG1	1:E:309:SER:HB3	2.18	0.42
1:F:85:THR:CG2	1:F:85:THR:O	2.66	0.42
1:G:294:LEU:HD12	1:G:294:LEU:HA	1.79	0.42
1:H:323:TRP:CZ3	1:H:326:GLN:HB3	2.54	0.42
1:A:326:GLN:HA	1:A:329:LEU:HD22	2.02	0.41
1:B:237:ALA:O	1:B:241:ILE:CG1	2.68	0.41
1:D:105:ARG:O	1:D:109:VAL:HG12	2.20	0.41
1:G:187:TRP:N	1:G:187:TRP:CD1	2.88	0.41
1:G:71:LEU:O	1:G:72:ARG:HG3	2.20	0.41
1:A:135:VAL:O	3:A:801:NAI:H2N	2.20	0.41
1:G:132:LEU:O	1:G:158:ILE:HD12	2.20	0.41
1:G:140:ASP:HB3	1:G:287:PHE:O	2.20	0.41
1:A:15:GLU:O	1:A:16:GLN:HG2	2.21	0.41
1:A:304:LYS:HE2	5:A:896:HOH:O	2.19	0.41
1:B:205:VAL:O	1:B:208:VAL:HG12	2.19	0.41
1:E:131:LYS:N	1:E:131:LYS:HD3	2.34	0.41
1:F:317:LYS:HB2	1:F:317:LYS:HE2	1.92	0.41
1:F:36:ILE:HA	1:F:36:ILE:HD12	1.93	0.41
1:G:317:LYS:HB3	1:G:317:LYS:HE2	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:HE3	1:A:173:MET:HB3	1.93	0.41
1:A:290:VAL:HG13	1:A:291:PRO:HD2	2.02	0.41
1:B:190:GLY:HA2	1:B:288:LEU:HD13	2.02	0.41
1:C:111:ARG:H	1:C:111:ARG:HG2	1.44	0.41
1:D:99:GLN:HE22	1:D:108:LEU:CD2	2.25	0.41
1:E:204:ASN:HD22	1:E:207:GLY:H	1.67	0.41
1:F:276:ILE:CD1	1:F:288:LEU:HD21	2.46	0.41
1:G:299:ILE:O	1:G:299:ILE:HG22	2.20	0.41
1:A:301:ASP:HA	1:D:11:LEU:HD13	2.03	0.41
1:A:9:TYR:HB2	1:D:304:LYS:HD2	2.01	0.41
1:E:106:LEU:CD1	1:E:325:ILE:HD11	2.50	0.41
1:E:86:ALA:O	1:E:87:ASN:HB2	2.20	0.41
1:B:307:LEU:HA	1:B:307:LEU:HD23	1.80	0.41
1:B:115:ILE:HG12	3:B:804:NAI:N6A	2.36	0.41
1:A:204:ASN:ND2	1:A:207:GLY:H	2.18	0.41
1:C:329:LEU:HA	1:C:329:LEU:HD12	1.81	0.41
1:D:187:TRP:N	1:D:187:TRP:CD1	2.89	0.41
1:H:300:SER:OG	1:H:301:ASP:OD1	2.31	0.41
1:A:301:ASP:HB3	1:D:8:ILE:CG2	2.51	0.41
1:D:22:ILE:HD12	1:D:44:ALA:HB2	2.02	0.41
1:E:294:LEU:HD12	1:E:294:LEU:HA	1.91	0.41
1:B:204:ASN:HD22	1:B:207:GLY:N	2.17	0.41
1:C:182:LEU:CD2	1:D:72:ARG:NH1	2.84	0.41
1:E:164:LEU:HD21	1:E:168:ARG:NH2	2.36	0.41
1:F:49:LEU:HB2	1:F:78:SER:HB3	2.03	0.41
1:G:237:ALA:O	1:G:238:TYR:C	2.59	0.41
1:H:189:LEU:CD2	1:H:199:VAL:HG21	2.51	0.41
1:C:204:ASN:HD22	1:C:207:GLY:H	1.69	0.41
1:F:129:ASN:HA	1:F:156:ARG:HH12	1.85	0.41
1:F:274:THR:O	1:F:287:PHE:HA	2.21	0.41
1:G:43:LEU:HD23	1:G:43:LEU:HA	1.70	0.41
1:C:20:ASN:CA	1:C:89:LYS:HE3	2.51	0.41
1:A:302:LEU:CD1	1:D:11:LEU:HD11	2.39	0.41
1:G:27:VAL:O	1:G:27:VAL:HG23	2.20	0.41
1:H:12:LEU:HA	1:H:12:LEU:HD23	1.94	0.41
1:E:9:TYR:CD2	1:E:11:LEU:CD2	3.05	0.40
1:G:217:LEU:HB3	1:G:218:GLY:H	1.75	0.40
1:D:37:SER:HB3	1:D:256:ALA:HB2	2.02	0.40
1:E:198:PRO:O	1:E:200:TRP:N	2.54	0.40
1:F:329:LEU:HD12	1:F:329:LEU:HA	1.86	0.40
1:G:190:GLY:O	1:G:289:SER:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:TYR:HA	1:G:287:PHE:CE2	2.55	0.40
1:G:269:VAL:HA	1:G:292:CYS:O	2.22	0.40
1:D:82:TYR:CG	1:D:122:ASN:HB3	2.56	0.40
1:D:83:ASN:HD22	1:D:84:VAL:N	2.18	0.40
1:E:141:ILE:O	1:E:145:VAL:HG23	2.21	0.40
1:F:221:LYS:HA	1:F:221:LYS:HD3	1.87	0.40
1:G:239:GLU:O	1:G:243:LEU:HD22	2.20	0.40
1:A:270:HIS:HB3	1:A:271:PRO:HD2	2.03	0.40
1:D:16:GLN:O	1:D:17:THR:CB	2.69	0.40
1:G:278:GLY:CA	1:G:282:ILE:HB	2.52	0.40
1:G:83:ASN:ND2	1:G:83:ASN:N	2.68	0.40
1:H:281:GLY:O	1:H:283:LYS:HG2	2.21	0.40
1:H:61:MET:O	1:H:65:GLN:HG3	2.22	0.40
1:A:210:LEU:HA	1:A:210:LEU:HD12	1.92	0.40
1:A:94:THR:HG22	1:A:135:VAL:HB	2.03	0.40
1:E:291:PRO:HG2	1:E:305:VAL:CG2	2.52	0.40
1:F:205:VAL:O	1:F:208:VAL:HG13	2.22	0.40
1:F:60:GLU:OE1	1:F:60:GLU:HA	2.22	0.40
1:G:113:VAL:HG21	1:G:329:LEU:HD21	2.04	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	329/331 (99%)	316 (96%)	11 (3%)	2 (1%)	28	34
1	B	329/331 (99%)	313 (95%)	12 (4%)	4 (1%)	15	16
1	C	329/331 (99%)	313 (95%)	15 (5%)	1 (0%)	44	55
1	D	329/331 (99%)	308 (94%)	16 (5%)	5 (2%)	12	11
1	E	329/331 (99%)	290 (88%)	30 (9%)	9 (3%)	6	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	329/331 (99%)	310 (94%)	17 (5%)	2 (1%)	28	34
1	G	321/331 (97%)	291 (91%)	23 (7%)	7 (2%)	8	6
1	H	329/331 (99%)	314 (95%)	13 (4%)	2 (1%)	28	34
All	All	2624/2648 (99%)	2455 (94%)	137 (5%)	32 (1%)	15	16

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	GLU
1	B	16	GLN
1	D	13	LYS
1	D	101	GLU
1	E	15	GLU
1	E	106	LEU
1	E	109	VAL
1	E	307	LEU
1	E	309	SER
1	G	99	GLN
1	G	217	LEU
1	G	221	LYS
1	G	282	ILE
1	G	283	LYS
1	G	330	GLN
1	H	13	LYS
1	H	16	GLN
1	A	13	LYS
1	C	282	ILE
1	D	16	GLN
1	D	105	ARG
1	E	314	ARG
1	F	329	LEU
1	E	101	GLU
1	E	285	ASP
1	E	305	VAL
1	A	215	PRO
1	B	14	GLU
1	B	327	LYS
1	F	101	GLU
1	D	17	THR
1	G	161	GLY

### 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	287/287 (100%)	264 (92%)	23 (8%)	14	17
1	B	287/287 (100%)	274 (96%)	13 (4%)	32	44
1	C	287/287 (100%)	265 (92%)	22 (8%)	15	18
1	D	287/287 (100%)	262 (91%)	25 (9%)	12	14
1	E	287/287 (100%)	247 (86%)	40 (14%)	4	4
1	F	287/287 (100%)	260 (91%)	27 (9%)	10	12
1	G	282/287 (98%)	245 (87%)	37 (13%)	5	5
1	H	287/287 (100%)	260 (91%)	27 (9%)	10	12
All	All	2291/2296 (100%)	2077 (91%)	214 (9%)	10	12

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	GLU
1	A	15	GLU
1	A	17	THR
1	A	50	VAL
1	A	56	LYS
1	A	72	ARG
1	A	83	ASN
1	A	85	THR
1	A	89	LYS
1	A	110	GLN
1	A	133	LEU
1	A	148	LYS
1	A	177	LEU
1	A	182	LEU
1	A	208	VAL
1	A	210	LEU
1	A	211	LYS
1	A	231	LYS

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	279	LEU
1	A	290	VAL
1	A	322	LEU
1	B	12	LEU
1	B	19	GLN
1	B	50	VAL
1	B	52	VAL
1	B	83	ASN
1	B	89	LYS
1	B	133	LEU
1	B	208	VAL
1	B	217	LEU
1	B	273	SER
1	B	302	LEU
1	B	320	ASP
1	B	330	GLN
1	C	13	LYS
1	C	17	THR
1	C	19	GLN
1	C	80	LYS
1	C	83	ASN
1	C	85	THR
1	C	89	LYS
1	C	133	LEU
1	C	177	LEU
1	C	182	LEU
1	C	189	LEU
1	C	208	VAL
1	C	219	THR
1	C	220	ASP
1	C	223	LYS
1	C	227	LYS
1	C	231	LYS
1	C	243	LEU
1	C	284	ASP
1	C	290	VAL
1	C	318	SER
1	C	328	GLU
1	D	15	GLU
1	D	16	GLN
1	D	17	THR

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Mol	Chain	Res	Type
1	D	19	GLN
1	D	83	ASN
1	D	85	THR
1	D	89	LYS
1	D	98	ARG
1	D	101	GLU
1	D	105	ARG
1	D	109	VAL
1	D	123	VAL
1	D	133	LEU
1	D	176	ARG
1	D	177	LEU
1	D	182	LEU
1	D	189	LEU
1	D	221	LYS
1	D	225	GLN
1	D	235	GLU
1	D	243	LEU
1	D	280	TYR
1	D	294	LEU
1	D	315	LEU
1	D	322	LEU
1	E	9	TYR
1	E	12	LEU
1	E	14	GLU
1	E	15	GLU
1	E	16	GLN
1	E	17	THR
1	E	49	LEU
1	E	56	LYS
1	E	72	ARG
1	E	80	LYS
1	E	83	ASN
1	E	100	GLN
1	E	105	ARG
1	E	107	ASN
1	E	108	LEU
1	E	133	LEU
1	E	153	PRO
1	E	177	LEU
1	E	189	LEU
1	E	195	SER

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Mol	Chain	Res	Type
1	E	203	MET
1	E	208	VAL
1	E	213	LEU
1	E	220	ASP
1	E	234	VAL
1	E	243	LEU
1	E	247	THR
1	E	273	SER
1	E	275	MET
1	E	277	LYS
1	E	282	ILE
1	E	283	LYS
1	E	289	SER
1	E	290	VAL
1	E	304	LYS
1	E	307	LEU
1	E	309	SER
1	E	312	GLU
1	E	322	LEU
1	E	329	LEU
1	F	11	LEU
1	F	13	LYS
1	F	15	GLU
1	F	16	GLN
1	F	17	THR
1	F	55	ASP
1	F	56	LYS
1	F	72	ARG
1	F	75	LYS
1	F	83	ASN
1	F	85	THR
1	F	89	LYS
1	F	123	VAL
1	F	133	LEU
1	F	173	MET
1	F	177	LEU
1	F	182	LEU
1	F	189	LEU
1	F	208	VAL
1	F	219	THR
1	F	243	LEU
1	F	290	VAL

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Mol	Chain	Res	Type
1	F	294	LEU
1	F	309	SER
1	F	317	LYS
1	F	329	LEU
1	F	331	PHE
1	G	11	LEU
1	G	15	GLU
1	G	16	GLN
1	G	19	GLN
1	G	36	ILE
1	G	50	VAL
1	G	83	ASN
1	G	85	THR
1	G	94	THR
1	G	98	ARG
1	G	99	GLN
1	G	100	GLN
1	G	108	LEU
1	G	110	GLN
1	G	133	LEU
1	G	136	SER
1	G	175	GLU
1	G	177	LEU
1	G	189	LEU
1	G	196	SER
1	G	204	ASN
1	G	208	VAL
1	G	217	LEU
1	G	220	ASP
1	G	231	LYS
1	G	236	SER
1	G	282	ILE
1	G	283	LYS
1	G	288	LEU
1	G	290	VAL
1	G	294	LEU
1	G	302	LEU
1	G	312	GLU
1	G	315	LEU
1	G	318	SER
1	G	322	LEU
1	G	330	GLN

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Mol	Chain	Res	Type
1	H	3	LEU
1	H	13	LYS
1	H	14	GLU
1	H	15	GLU
1	H	16	GLN
1	H	17	THR
1	H	19	GLN
1	H	55	ASP
1	H	72	ARG
1	H	83	ASN
1	H	85	THR
1	H	110	GLN
1	H	131	LYS
1	H	133	LEU
1	H	177	LEU
1	H	189	LEU
1	H	201	SER
1	H	208	VAL
1	H	220	ASP
1	H	243	LEU
1	H	279	LEU
1	H	282	ILE
1	H	286	VAL
1	H	306	THR
1	H	317	LYS
1	H	322	LEU
1	H	326	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	87	ASN
1	A	107	ASN
1	A	112	ASN
1	A	204	ASN
1	A	230	HIS
1	A	297	ASN
1	B	19	GLN
1	B	83	ASN
1	B	107	ASN
1	B	112	ASN

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Mol	Chain	Res	Type
1	B	122	ASN
1	B	204	ASN
1	B	230	HIS
1	B	297	ASN
1	C	6	GLN
1	C	16	GLN
1	C	83	ASN
1	C	112	ASN
1	C	122	ASN
1	C	204	ASN
1	C	230	HIS
1	C	297	ASN
1	C	326	GLN
1	D	83	ASN
1	D	99	GLN
1	D	110	GLN
1	D	122	ASN
1	D	204	ASN
1	D	230	HIS
1	D	330	GLN
1	E	20	ASN
1	E	83	ASN
1	E	110	GLN
1	E	112	ASN
1	E	129	ASN
1	E	326	GLN
1	F	6	GLN
1	F	10	ASN
1	F	20	ASN
1	F	83	ASN
1	F	112	ASN
1	F	129	ASN
1	F	204	ASN
1	F	230	HIS
1	G	20	ASN
1	G	83	ASN
1	G	107	ASN
1	G	110	GLN
1	G	112	ASN
1	G	122	ASN
1	G	204	ASN
1	G	230	HIS

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Mol	Chain	Res	Type
1	G	330	GLN
1	H	20	ASN
1	H	107	ASN
1	H	110	GLN
1	H	112	ASN
1	H	204	ASN
1	H	230	HIS

### 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 ⓘ

24 ligands are modelled in this entry.

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	NAI	A	801	-	40,48,48	1.58	5 (12%)	41,73,73	2.08	5 (12%)
4	OXM	A	802	-	2,5,5	0.77	0	2,6,6	0.81	0
2	ACT	A	803	-	1,3,3	1.05	0	0,3,3	0.00	-
3	NAI	B	804	-	40,48,48	1.73	5 (12%)	41,73,73	1.68	4 (9%)
4	OXM	B	805	-	2,5,5	1.26	0	2,6,6	1.31	0
2	ACT	B	806	-	1,3,3	0.67	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAI	C	807	-	40,48,48	1.85	8 (20%)	41,73,73	1.68	5 (12%)
4	OXM	C	808	-	2,5,5	0.69	0	2,6,6	2.03	1 (50%)
2	ACT	C	809	-	1,3,3	1.71	0	0,3,3	0.00	-
3	NAI	D	810	-	40,48,48	1.75	5 (12%)	41,73,73	1.87	6 (14%)
4	OXM	D	811	-	2,5,5	1.49	0	2,6,6	0.71	0
2	ACT	D	812	-	1,3,3	0.06	0	0,3,3	0.00	-
3	NAI	E	813	-	40,48,48	1.79	5 (12%)	41,73,73	1.73	5 (12%)
4	OXM	E	814	-	2,5,5	1.29	0	2,6,6	0.07	0
2	ACT	E	815	-	1,3,3	1.87	0	0,3,3	0.00	-
3	NAI	F	816	-	40,48,48	1.58	4 (10%)	41,73,73	2.23	4 (9%)
4	OXM	F	817	-	2,5,5	1.01	0	2,6,6	1.66	1 (50%)
2	ACT	F	818	-	1,3,3	0.49	0	0,3,3	0.00	-
3	NAI	G	819	-	40,48,48	1.70	5 (12%)	41,73,73	1.64	5 (12%)
4	OXM	G	820	-	2,5,5	0.27	0	2,6,6	1.99	1 (50%)
2	ACT	G	821	-	1,3,3	0.15	0	0,3,3	0.00	-
3	NAI	H	822	-	40,48,48	1.73	5 (12%)	41,73,73	1.96	7 (17%)
4	OXM	H	823	-	2,5,5	0.30	0	2,6,6	2.13	1 (50%)
2	ACT	H	824	-	1,3,3	0.98	0	0,3,3	0.00	-

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	NAI	A	801	-	-	0/25/72/72	0/5/5/5
4	OXM	A	802	-	-	0/0/4/4	0/0/0/0
2	ACT	A	803	-	-	0/0/0/0	0/0/0/0
3	NAI	B	804	-	-	0/25/72/72	0/5/5/5
4	OXM	B	805	-	-	0/0/4/4	0/0/0/0
2	ACT	B	806	-	-	0/0/0/0	0/0/0/0
3	NAI	C	807	-	-	0/25/72/72	0/5/5/5
4	OXM	C	808	-	-	0/0/4/4	0/0/0/0
2	ACT	C	809	-	-	0/0/0/0	0/0/0/0
3	NAI	D	810	-	-	0/25/72/72	0/5/5/5
4	OXM	D	811	-	-	0/0/4/4	0/0/0/0
2	ACT	D	812	-	-	0/0/0/0	0/0/0/0
3	NAI	E	813	-	-	0/25/72/72	0/5/5/5
4	OXM	E	814	-	-	0/0/4/4	0/0/0/0
2	ACT	E	815	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	F	816	-	-	0/25/72/72	0/5/5/5
4	OXM	F	817	-	-	0/0/4/4	0/0/0/0
2	ACT	F	818	-	-	0/0/0/0	0/0/0/0
3	NAI	G	819	-	-	0/25/72/72	0/5/5/5
4	OXM	G	820	-	-	0/0/4/4	0/0/0/0
2	ACT	G	821	-	-	0/0/0/0	0/0/0/0
3	NAI	H	822	-	-	0/25/72/72	0/5/5/5
4	OXM	H	823	-	-	0/0/4/4	0/0/0/0
2	ACT	H	824	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	822	NAI	C4N-C5N	-4.54	1.39	1.49
3	G	819	NAI	C4N-C5N	-4.53	1.39	1.49
3	D	810	NAI	C4N-C5N	-4.45	1.39	1.49
3	E	813	NAI	C4N-C5N	-4.39	1.39	1.49
3	F	816	NAI	C4N-C5N	-4.13	1.40	1.49
3	A	801	NAI	C4N-C5N	-3.59	1.41	1.49
3	C	807	NAI	C4N-C5N	-3.44	1.41	1.49
3	B	804	NAI	C4N-C5N	-3.38	1.41	1.49
3	C	807	NAI	C2B-C1B	-3.07	1.48	1.53
3	G	819	NAI	C2B-C1B	-2.23	1.50	1.53
3	C	807	NAI	O4B-C4B	-2.00	1.40	1.45
3	D	810	NAI	C2A-N1A	2.04	1.37	1.33
3	C	807	NAI	C2N-C3N	2.22	1.41	1.34
3	A	801	NAI	C2A-N1A	2.37	1.38	1.33
3	E	813	NAI	C2A-N1A	2.44	1.38	1.33
3	D	810	NAI	C2A-N3A	2.48	1.36	1.32
3	G	819	NAI	C2A-N3A	2.60	1.36	1.32
3	H	822	NAI	C2A-N1A	2.62	1.38	1.33
3	B	804	NAI	C2A-N1A	2.73	1.39	1.33
3	F	816	NAI	C2A-N3A	2.75	1.36	1.32
3	G	819	NAI	C6N-C5N	3.39	1.39	1.33
3	C	807	NAI	C2A-N1A	3.46	1.40	1.33
3	D	810	NAI	C6N-C5N	3.49	1.39	1.33
3	H	822	NAI	C2A-N3A	3.51	1.38	1.32
3	C	807	NAI	C2A-N3A	3.62	1.38	1.32
3	E	813	NAI	C6N-C5N	3.64	1.40	1.33
3	B	804	NAI	C2A-N3A	3.65	1.38	1.32
3	B	804	NAI	C6N-C5N	3.82	1.40	1.33
3	E	813	NAI	C2A-N3A	3.83	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	822	NAI	C6N-C5N	4.04	1.40	1.33
3	A	801	NAI	C6N-C5N	4.17	1.41	1.33
3	F	816	NAI	C6N-C5N	4.21	1.41	1.33
3	A	801	NAI	C2A-N3A	4.29	1.39	1.32
3	C	807	NAI	C6N-C5N	4.96	1.42	1.33
3	C	807	NAI	O7N-C7N	5.28	1.37	1.24
3	F	816	NAI	O7N-C7N	5.37	1.37	1.24
3	A	801	NAI	O7N-C7N	5.46	1.38	1.24
3	H	822	NAI	O7N-C7N	5.85	1.39	1.24
3	B	804	NAI	O7N-C7N	6.54	1.40	1.24
3	G	819	NAI	O7N-C7N	6.99	1.41	1.24
3	E	813	NAI	O7N-C7N	7.41	1.43	1.24
3	D	810	NAI	O7N-C7N	7.50	1.43	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	816	NAI	N3A-C2A-N1A	-12.01	118.40	128.86
3	A	801	NAI	N3A-C2A-N1A	-10.85	119.41	128.86
3	D	810	NAI	N3A-C2A-N1A	-9.38	120.69	128.86
3	H	822	NAI	N3A-C2A-N1A	-8.85	121.15	128.86
3	E	813	NAI	N3A-C2A-N1A	-8.79	121.20	128.86
3	B	804	NAI	N3A-C2A-N1A	-8.40	121.54	128.86
3	C	807	NAI	N3A-C2A-N1A	-7.51	122.32	128.86
3	G	819	NAI	N3A-C2A-N1A	-7.19	122.59	128.86
3	F	816	NAI	C1B-N9A-C4A	-3.68	120.27	126.64
3	H	822	NAI	C4A-C5A-N7A	-3.68	105.86	109.41
3	G	819	NAI	C1D-N1N-C2N	-3.24	115.60	121.09
3	H	822	NAI	O3D-C3D-C2D	-3.16	101.71	111.83
3	A	801	NAI	C1D-N1N-C2N	-3.13	115.77	121.09
3	C	807	NAI	O4D-C1D-C2D	-3.11	99.76	106.64
3	C	807	NAI	C4A-C5A-N7A	-2.94	106.57	109.41
3	E	813	NAI	C4B-O4B-C1B	-2.92	106.66	109.77
3	G	819	NAI	C1B-N9A-C4A	-2.85	121.71	126.64
3	D	810	NAI	O3D-C3D-C2D	-2.63	103.39	111.83
3	D	810	NAI	C4A-C5A-N7A	-2.63	106.87	109.41
3	A	801	NAI	O3D-C3D-C4D	-2.62	103.44	111.09
3	H	822	NAI	C4B-O4B-C1B	-2.61	106.99	109.77
3	C	807	NAI	C1D-N1N-C2N	-2.55	116.76	121.09
3	G	819	NAI	C4B-O4B-C1B	-2.44	107.17	109.77
3	H	822	NAI	C1D-N1N-C2N	-2.41	117.00	121.09
3	B	804	NAI	O4D-C1D-C2D	-2.41	101.31	106.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	807	NAI	C4B-O4B-C1B	-2.37	107.25	109.77
3	B	804	NAI	C1D-N1N-C2N	-2.36	117.09	121.09
3	D	810	NAI	C1B-N9A-C4A	-2.24	122.76	126.64
3	H	822	NAI	C3D-C2D-C1D	-2.23	97.14	101.43
3	F	816	NAI	O3D-C3D-C2D	-2.22	104.73	111.83
3	H	822	NAI	C3N-C2N-N1N	-2.19	119.91	123.08
3	B	804	NAI	C4A-C5A-N7A	-2.13	107.35	109.41
3	E	813	NAI	O3B-C3B-C4B	-2.09	104.99	111.09
3	A	801	NAI	C4A-C5A-N7A	-2.07	107.41	109.41
3	F	816	NAI	C4B-O4B-C1B	-2.05	107.58	109.77
3	E	813	NAI	C4A-C5A-N7A	-2.04	107.44	109.41
3	E	813	NAI	C1D-N1N-C2N	-2.04	117.64	121.09
3	D	810	NAI	C3N-C2N-N1N	-2.02	120.15	123.08
3	D	810	NAI	O2D-C2D-C1D	2.07	116.93	109.96
3	A	801	NAI	C1D-N1N-C6N	2.15	125.45	120.77
4	F	817	OXM	O1-C1-N1	2.32	125.88	122.58
4	G	820	OXM	C2-C1-N1	2.77	120.52	115.85
4	C	808	OXM	O1-C1-N1	2.86	126.64	122.58
4	H	823	OXM	C2-C1-N1	2.94	120.80	115.85
3	G	819	NAI	O4D-C1D-N1N	3.02	114.14	108.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	NAI	2	0
2	A	803	ACT	6	0
3	B	804	NAI	2	0
2	B	806	ACT	4	0
3	C	807	NAI	1	0
4	C	808	OXM	1	0
2	C	809	ACT	2	0
3	D	810	NAI	4	0
4	D	811	OXM	2	0
2	D	812	ACT	2	0
3	E	813	NAI	3	0
4	E	814	OXM	2	0
2	E	815	ACT	1	0
3	F	816	NAI	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	817	OXM	1	0
2	F	818	ACT	3	0
3	G	819	NAI	1	0
2	G	821	ACT	1	0
3	H	822	NAI	3	0
2	H	824	ACT	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	331/331 (100%)	-0.28	6 (1%) 69 74	5, 16, 37, 52	5 (1%)
1	B	330/331 (99%)	-0.26	7 (2%) 64 70	8, 16, 41, 66	5 (1%)
1	C	331/331 (100%)	-0.03	12 (3%) 43 50	11, 21, 49, 74	3 (0%)
1	D	326/331 (98%)	-0.08	9 (2%) 53 61	12, 22, 40, 56	6 (1%)
1	E	324/331 (97%)	0.30	31 (9%) 9 12	10, 29, 73, 150	4 (1%)
1	F	327/331 (98%)	0.02	14 (4%) 36 43	11, 24, 57, 79	0
1	G	325/331 (98%)	0.42	29 (8%) 10 14	12, 33, 67, 80	10 (3%)
1	H	327/331 (98%)	0.13	18 (5%) 26 32	11, 27, 52, 61	0
All	All	2621/2648 (98%)	0.02	126 (4%) 31 38	5, 23, 56, 150	33 (1%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	106	LEU	13.6
1	E	105	ARG	9.9
1	E	104	SER	6.5
1	D	14	GLU	6.1
1	H	331	PHE	6.0
1	E	222	ASP	5.3
1	G	331	PHE	5.3
1	A	16	GLN	5.0
1	B	330	GLN	5.0
1	G	222	ASP	5.0
1	G	279	LEU	4.9
1	C	331	PHE	4.9
1	G	100	GLN	4.9
1	H	1	ALA	4.8
1	F	331	PHE	4.8
1	D	15	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	16	GLN	4.4
1	E	313	ALA	4.3
1	C	330	GLN	4.2
1	E	307	LEU	4.2
1	F	329	LEU	4.0
1	C	1	ALA	4.0
1	G	280	TYR	3.9
1	C	13	LYS	3.9
1	A	14	GLU	3.8
1	H	2	THR	3.8
1	E	102	GLY	3.8
1	E	220	ASP	3.7
1	D	16	GLN	3.7
1	B	17	THR	3.6
1	F	330	GLN	3.6
1	E	224	GLU	3.6
1	C	17	THR	3.5
1	G	221	LYS	3.5
1	G	283	LYS	3.5
1	G	129	ASN	3.3
1	F	221	LYS	3.3
1	G	98	ARG	3.3
1	A	221	LYS	3.2
1	E	331	PHE	3.2
1	G	329	LEU	3.2
1	E	318	SER	3.2
1	H	9	TYR	3.1
1	E	310	GLU	3.1
1	G	219	THR	3.1
1	F	220	ASP	3.1
1	E	223	LYS	3.0
1	B	331	PHE	3.0
1	G	328	GLU	3.0
1	E	16	GLN	3.0
1	E	281	GLY	3.0
1	E	305	VAL	3.0
1	C	16	GLN	2.9
1	G	107	ASN	2.9
1	F	1	ALA	2.9
1	E	219	THR	2.9
1	G	134	ILE	2.9
1	F	17	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	330	GLN	2.9
1	G	93	ILE	2.8
1	H	135	VAL	2.8
1	H	134	ILE	2.8
1	B	223	LYS	2.8
1	D	238	TYR	2.8
1	F	18	PRO	2.7
1	E	323	TRP	2.7
1	F	6	GLN	2.7
1	H	220	ASP	2.7
1	A	331	PHE	2.7
1	C	221	LYS	2.6
1	G	282	ILE	2.6
1	E	329	LEU	2.6
1	H	221	LYS	2.6
1	D	98	ARG	2.6
1	F	12	LEU	2.6
1	H	5	ASP	2.6
1	C	281	GLY	2.6
1	E	110	GLN	2.6
1	E	103	GLU	2.6
1	E	278	GLY	2.5
1	G	9	TYR	2.5
1	B	283	LYS	2.5
1	E	226	TRP	2.5
1	C	278	GLY	2.5
1	G	17	THR	2.4
1	E	328	GLU	2.4
1	E	283	LYS	2.4
1	G	133	LEU	2.4
1	E	308	THR	2.4
1	G	135	VAL	2.4
1	H	118	PHE	2.4
1	F	219	THR	2.4
1	E	221	LYS	2.4
1	H	81	ASP	2.4
1	G	108	LEU	2.4
1	G	218	GLY	2.3
1	D	313	ALA	2.3
1	G	317	LYS	2.3
1	C	142	LEU	2.3
1	H	17	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	278	GLY	2.3
1	E	306	THR	2.3
1	G	225	GLN	2.3
1	G	223	LYS	2.3
1	G	316	LYS	2.2
1	H	124	VAL	2.2
1	H	159	GLY	2.2
1	D	92	ILE	2.2
1	H	55	ASP	2.2
1	F	283	LYS	2.1
1	F	323	TRP	2.1
1	H	139	VAL	2.1
1	D	99	GLN	2.1
1	C	134	ILE	2.1
1	H	223	LYS	2.1
1	H	6	GLN	2.1
1	C	135	VAL	2.1
1	E	309	SER	2.1
1	F	9	TYR	2.1
1	B	12	LEU	2.0
1	A	13	LYS	2.0
1	A	314	ARG	2.0
1	E	327	LYS	2.0
1	G	12	LEU	2.0
1	G	281	GLY	2.0
1	D	1	ALA	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	ACT	G	821	4/4	0.88	0.32	15.64	45,45,46,46	0
2	ACT	H	824	4/4	0.92	0.31	14.35	37,37,38,38	0
2	ACT	E	815	4/4	0.95	0.26	11.76	30,30,30,31	0
2	ACT	B	806	4/4	0.96	0.22	7.76	19,20,22,22	0
4	OXM	D	811	6/6	0.58	0.30	7.50	46,49,49,50	0
2	ACT	A	803	4/4	0.93	0.20	4.77	17,19,21,22	0
2	ACT	C	809	4/4	0.97	0.16	4.64	10,13,13,15	0
4	OXM	G	820	6/6	0.73	0.25	3.70	43,44,47,50	0
2	ACT	F	818	4/4	0.96	0.19	3.36	31,31,32,32	0
2	ACT	D	812	4/4	0.97	0.17	2.53	21,21,22,22	0
3	NAI	E	813	44/44	0.91	0.16	1.06	24,34,37,37	0
3	NAI	D	810	44/44	0.91	0.17	0.57	23,32,39,40	0
4	OXM	A	802	6/6	0.99	0.11	-0.02	5,9,11,12	0
4	OXM	E	814	6/6	0.89	0.16	-0.31	32,36,38,38	0
4	OXM	B	805	6/6	0.98	0.10	-0.31	7,12,13,15	0
3	NAI	A	801	44/44	0.97	0.10	-0.55	9,13,16,16	0
3	NAI	B	804	44/44	0.98	0.10	-0.63	8,13,21,21	0
3	NAI	G	819	44/44	0.94	0.11	-0.67	21,29,35,37	0
3	NAI	C	807	44/44	0.97	0.12	-0.69	15,18,21,22	0
3	NAI	F	816	44/44	0.96	0.09	-0.89	11,21,30,30	0
3	NAI	H	822	44/44	0.95	0.11	-0.91	16,21,32,34	0
4	OXM	F	817	6/6	0.98	0.08	-1.56	15,18,20,22	0
4	OXM	H	823	6/6	0.97	0.09	-2.24	15,17,17,18	0
4	OXM	C	808	6/6	0.98	0.07	-2.67	11,13,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.