



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:03 PM UTC

PDB ID : 3FA4 / pdb_00003fa4
Title : Crystal structure of 2,3-dimethylmalate lyase, a PEP mutase/isocitrate lyase superfamily member, triclinic crystal form
Authors : Narayanan, B.C.; Herzberg, O.
Deposited on : 2008-11-14
Resolution : 2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

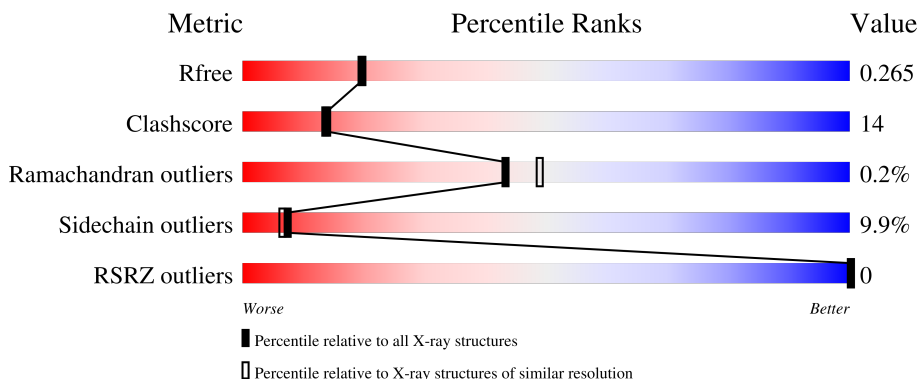
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	302	 66% 24% 6%
1	B	302	 67% 25% 5%
1	C	302	 66% 24% 6%
1	D	302	 69% 20% 5% 6%
1	E	302	 64% 25% 5% 6%

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Mol	Chain	Length	Quality of chain
1	F	302	 71% 20% • • 6%
1	G	302	 63% 27% • 6%
1	H	302	 60% 29% • • 7%
1	I	302	 63% 23% 6% • 7%
1	J	302	 59% 28% 6% 7%
1	K	302	 70% 18% 5% 7%
1	L	302	 65% 25% 5% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26432 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 2,3-dimethylmalate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2111	1312	375	409	15	0	0	0
1	B	288	2137	1330	379	413	15	0	0	0
1	C	284	2112	1313	375	409	15	0	0	0
1	D	284	2111	1312	375	409	15	0	0	0
1	E	286	2118	1316	377	410	15	0	0	0
1	F	285	2116	1315	376	410	15	0	0	0
1	G	284	2107	1310	375	407	15	0	0	0
1	H	282	2080	1293	369	403	15	0	0	0
1	I	282	2100	1305	373	407	15	0	0	0
1	J	280	2068	1284	369	400	15	0	0	0
1	K	280	2072	1287	368	403	14	0	0	0
1	L	288	2126	1320	384	407	15	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0
3	B	115	Total 115	O 115	0	0
3	C	109	Total 109	O 109	0	0
3	D	135	Total 135	O 135	0	0
3	E	104	Total 104	O 104	0	0
3	F	109	Total 109	O 109	0	0
3	G	124	Total 124	O 124	0	0
3	H	104	Total 104	O 104	0	0
3	I	38	Total 38	O 38	0	0

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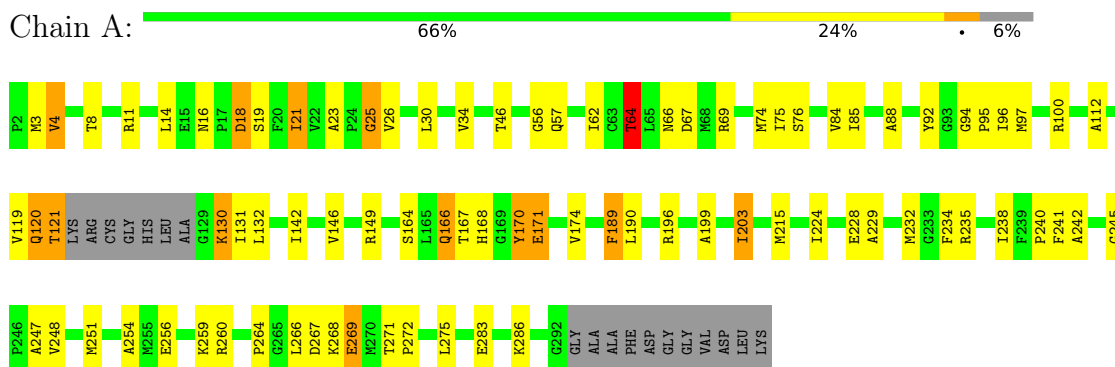
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	83	Total 83	O 83	0	0
3	K	61	Total 61	O 61	0	0
3	L	64	Total 64	O 64	0	0

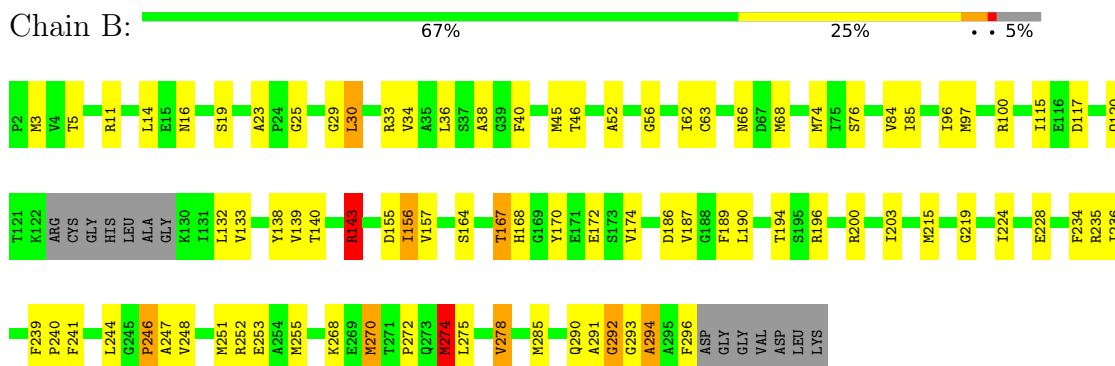
3 Residue-property plots i

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

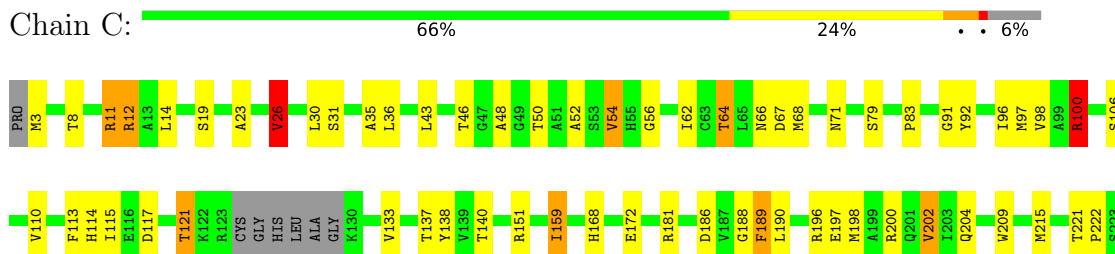
- Molecule 1: 2,3-dimethylmalate lyase



- Molecule 1: 2,3-dimethylmalate lyase



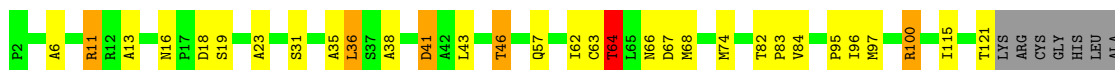
- Molecule 1: 2,3-dimethylmalate lyase





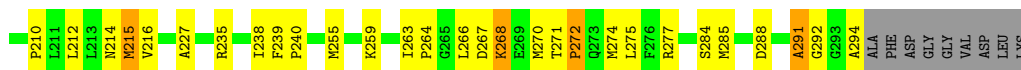
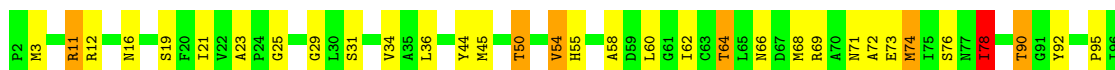
- Molecule 1: 2,3-dimethylmalate lyase

Chain D: 69% 20% 5% 6%



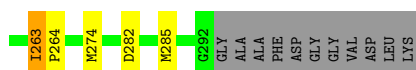
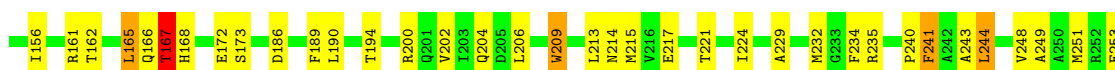
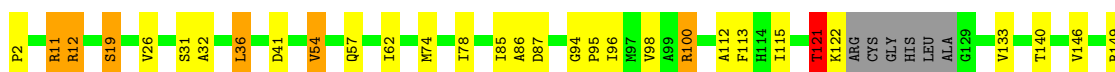
- Molecule 1: 2,3-dimethylmalate lyase

Chain E: 64% 25% 5% 6%



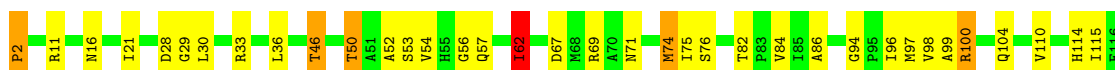
- Molecule 1: 2,3-dimethylmalate lyase

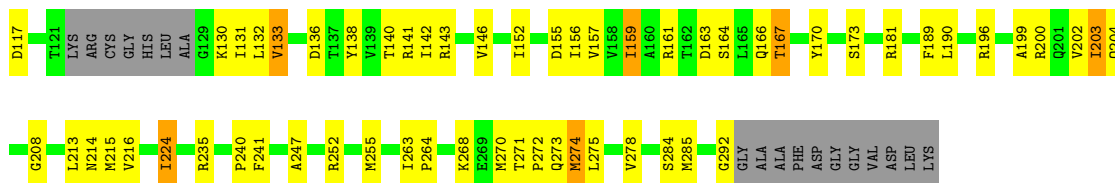
Chain F: 71% 20% 5% 6%



- Molecule 1: 2,3-dimethylmalate lyase

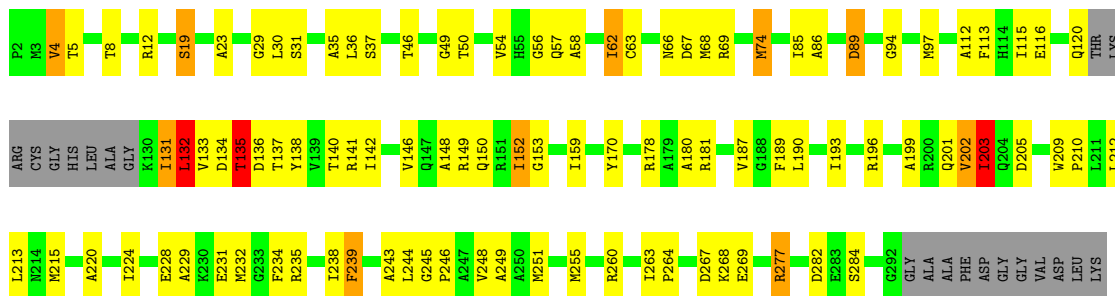
Chain G: 63% 27% 6% 4%





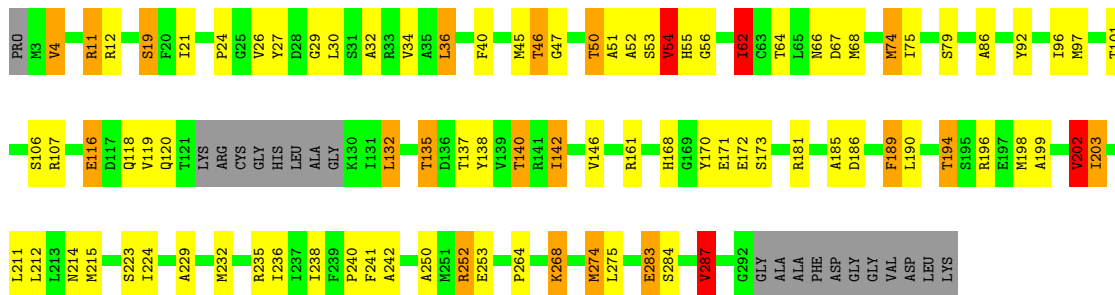
- Molecule 1: 2,3-dimethylmalate lyase

Chain H: 60% 29% 7%



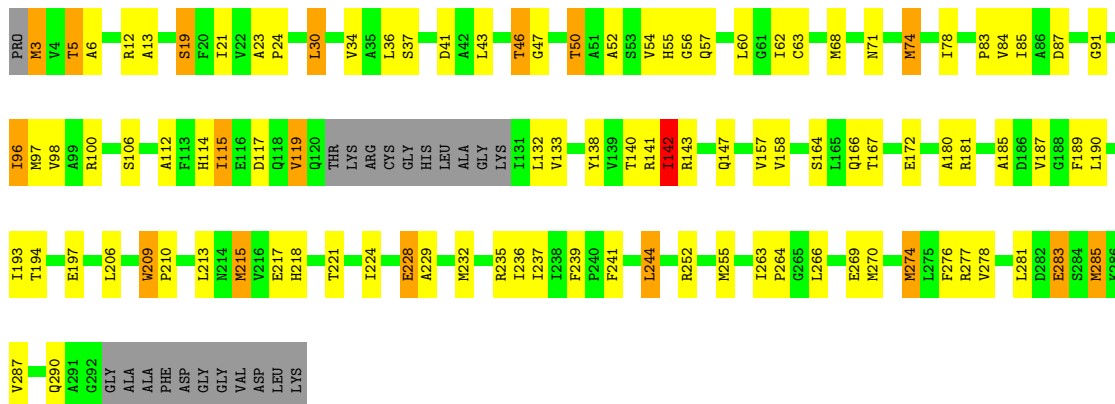
- Molecule 1: 2,3-dimethylmalate lyase

Chain I: 63% 23% 6% 7%



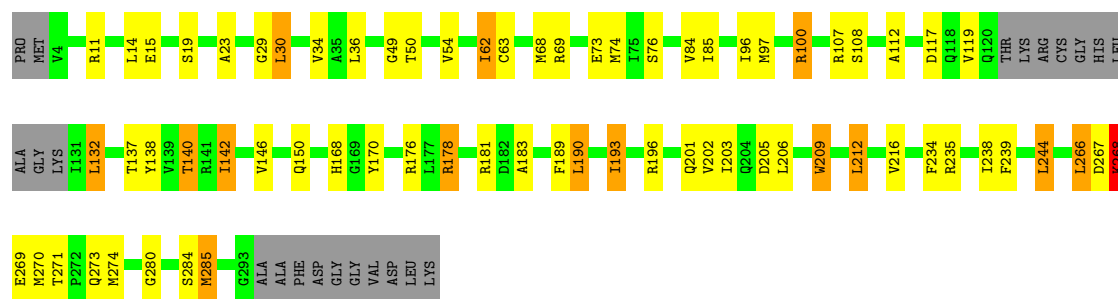
- Molecule 1: 2,3-dimethylmalate lyase

Chain J: 59% 28% 6% 7%



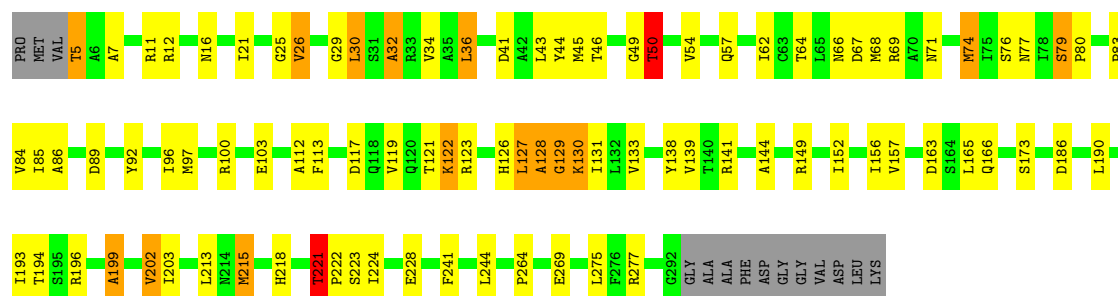
- Molecule 1: 2,3-dimethylmalate lyase

Chain K:  70% 18% 5% 7%



● Molecule 1: 2,3-dimethylmalate lyase

Chain L:  65% 25% 5% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.09Å 115.47Å 115.75Å 119.66° 90.71° 96.28°	Depositor
Resolution (Å)	46.83 – 2.18 46.83 – 2.18	Depositor EDS
% Data completeness (in resolution range)	93.2 (46.83-2.18) 91.8 (46.83-2.18)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.265 0.202 , 0.265	Depositor DCC
R_{free} test set	8603 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.159 for -h,-k-l,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26432	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.43	5/2141 (0.2%)	1.41	17/2898 (0.6%)
1	B	1.44	11/2168 (0.5%)	1.38	10/2935 (0.3%)
1	C	1.40	9/2141 (0.4%)	1.37	13/2898 (0.4%)
1	D	1.45	16/2141 (0.7%)	1.43	10/2898 (0.3%)
1	E	1.42	12/2148 (0.6%)	1.43	12/2907 (0.4%)
1	F	1.33	3/2146 (0.1%)	1.37	13/2905 (0.4%)
1	G	1.52	15/2137 (0.7%)	1.42	13/2893 (0.4%)
1	H	1.41	7/2110 (0.3%)	1.40	14/2861 (0.5%)
1	I	1.21	7/2129 (0.3%)	1.32	7/2882 (0.2%)
1	J	1.27	6/2097 (0.3%)	1.34	11/2841 (0.4%)
1	K	1.25	2/2101 (0.1%)	1.27	5/2846 (0.2%)
1	L	1.24	6/2157 (0.3%)	1.35	20/2922 (0.7%)
All	All	1.37	99/25616 (0.4%)	1.38	145/34686 (0.4%)

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	142	ILE	CA-CB	7.63	1.64	1.54
1	D	254	ALA	CA-CB	-7.41	1.41	1.53
1	G	99	ALA	CA-CB	-7.41	1.41	1.53
1	A	21	ILE	CA-CB	7.34	1.62	1.54
1	A	189	PHE	CA-C	7.19	1.60	1.53
1	L	119	VAL	CA-CB	7.01	1.61	1.54
1	J	85	ILE	CA-CB	6.99	1.62	1.54
1	E	34	VAL	CA-CB	6.94	1.62	1.54
1	G	86	ALA	C-O	-6.92	1.15	1.24
1	E	148	ALA	CA-CB	-6.82	1.42	1.53
1	H	4	VAL	CA-CB	6.72	1.66	1.54
1	H	231	GLU	C-O	-6.71	1.16	1.24
1	E	71	ASN	C-O	-6.65	1.16	1.24
1	G	131	ILE	C-O	-6.58	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	224	ILE	CA-CB	6.49	1.62	1.54
1	B	143	ARG	C-O	-6.45	1.16	1.24
1	D	23	ALA	C-O	-6.43	1.19	1.25
1	H	67	ASP	N-CA	6.40	1.53	1.46
1	G	202	VAL	CA-CB	6.34	1.62	1.54
1	K	54	VAL	CA-CB	6.33	1.63	1.54
1	L	129	GLY	N-CA	6.32	1.50	1.45
1	B	23	ALA	N-CA	-6.27	1.40	1.46
1	F	54	VAL	CA-CB	6.25	1.62	1.54
1	I	4	VAL	CA-CB	6.25	1.61	1.54
1	D	23	ALA	CA-CB	6.25	1.60	1.53
1	J	158	VAL	CA-CB	6.24	1.60	1.53
1	H	152	ILE	CA-CB	6.22	1.62	1.54
1	I	287	VAL	CA-CB	6.17	1.62	1.54
1	H	239	PHE	CA-C	6.12	1.59	1.52
1	C	113	PHE	CA-C	-6.04	1.45	1.52
1	J	158	VAL	CA-C	6.03	1.59	1.53
1	B	156	ILE	CA-CB	6.02	1.60	1.54
1	G	157	VAL	CA-CB	5.98	1.61	1.54
1	D	289	ALA	C-O	-5.90	1.17	1.24
1	H	31	SER	N-CA	5.88	1.53	1.46
1	B	167	THR	CA-CB	5.87	1.62	1.53
1	D	6	ALA	CA-CB	-5.86	1.42	1.53
1	B	157	VAL	CA-CB	5.86	1.60	1.54
1	C	11	ARG	C-O	-5.85	1.17	1.24
1	C	100	ARG	C-O	-5.84	1.17	1.24
1	L	121	THR	CA-CB	5.83	1.62	1.53
1	A	69	ARG	C-O	-5.81	1.17	1.24
1	L	128	ALA	CA-CB	5.81	1.63	1.53
1	G	156	ILE	CA-CB	5.80	1.61	1.54
1	G	67	ASP	C-O	-5.79	1.17	1.24
1	G	196	ARG	C-O	-5.78	1.17	1.24
1	E	102	THR	CA-CB	5.74	1.62	1.53
1	C	159	ILE	CA-CB	5.67	1.60	1.53
1	C	71	ASN	N-CA	5.66	1.53	1.46
1	F	167	THR	CA-C	5.62	1.59	1.52
1	L	221	THR	CA-CB	5.61	1.62	1.52
1	D	35	ALA	C-O	-5.57	1.17	1.24
1	C	35	ALA	N-CA	5.57	1.53	1.46
1	D	224	ILE	C-O	-5.54	1.18	1.24
1	L	96	ILE	CA-CB	5.54	1.61	1.54
1	E	255	MET	CA-C	5.53	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	SER	C-O	5.50	1.30	1.24
1	B	85	ILE	C-O	-5.49	1.18	1.24
1	C	247	ALA	C-O	-5.47	1.17	1.24
1	D	143	ARG	C-O	-5.44	1.17	1.24
1	H	131	ILE	CA-CB	5.43	1.60	1.54
1	I	54	VAL	CA-CB	5.42	1.61	1.54
1	I	101	THR	CA-CB	5.41	1.61	1.53
1	J	278	VAL	CA-CB	5.37	1.61	1.54
1	E	200	ARG	C-O	-5.36	1.17	1.24
1	G	252	ARG	N-CA	5.32	1.52	1.46
1	I	51	ALA	CA-CB	5.29	1.61	1.53
1	D	46	THR	CA-CB	5.28	1.61	1.53
1	B	219	GLY	N-CA	5.27	1.50	1.45
1	A	88	ALA	CA-CB	-5.27	1.46	1.53
1	G	263	ILE	CA-CB	5.27	1.60	1.54
1	D	224	ILE	CA-CB	5.25	1.60	1.54
1	I	21	ILE	CA-CB	5.25	1.60	1.54
1	B	224	ILE	CA-CB	5.24	1.60	1.54
1	D	152	ILE	CA-CB	5.22	1.61	1.54
1	D	236	ILE	CA-CB	5.22	1.61	1.54
1	G	247	ALA	CA-CB	-5.22	1.45	1.53
1	D	16	ASN	C-O	-5.21	1.18	1.24
1	E	142	ILE	CA-CB	5.18	1.59	1.54
1	B	187	VAL	C-O	5.17	1.29	1.24
1	G	110	VAL	CA-CB	5.16	1.60	1.54
1	E	71	ASN	N-CA	5.16	1.52	1.46
1	K	34	VAL	CA-CB	5.16	1.60	1.54
1	J	96	ILE	CA-CB	5.15	1.60	1.54
1	C	23	ALA	CA-C	5.15	1.59	1.52
1	G	133	VAL	CA-CB	5.13	1.62	1.54
1	E	50	THR	CA-C	5.09	1.59	1.52
1	E	149	ARG	C-O	-5.08	1.18	1.24
1	B	45	MET	CA-C	-5.06	1.46	1.52
1	I	236	ILE	CA-CB	5.06	1.62	1.54
1	E	76	SER	N-CA	5.05	1.52	1.46
1	G	159	ILE	CA-CB	5.05	1.60	1.54
1	D	171	GLU	CA-C	5.04	1.59	1.52
1	D	140	THR	CA-C	5.03	1.59	1.52
1	C	3	MET	N-CA	5.02	1.55	1.46
1	A	26	VAL	CA-C	5.01	1.59	1.52
1	B	274	MET	C-O	-5.01	1.18	1.24
1	E	239	PHE	N-CA	5.01	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	ASP	CA-C	5.00	1.59	1.52

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	79	SER	CA-C-N	10.09	129.75	119.56
1	L	79	SER	C-N-CA	10.09	129.75	119.56
1	F	121	THR	N-CA-C	9.15	124.93	111.02
1	H	170	TYR	N-CA-C	8.11	119.75	111.07
1	A	170	TYR	N-CA-C	7.84	119.51	110.97
1	E	202	VAL	CB-CA-C	-7.82	101.96	111.97
1	A	120	GLN	N-CA-C	7.29	123.33	111.37
1	A	245	GLY	CA-C-N	7.22	126.75	119.24
1	A	245	GLY	C-N-CA	7.22	126.75	119.24
1	H	132	LEU	N-CA-C	7.19	119.10	108.60
1	H	203	ILE	N-CA-C	-7.16	103.48	110.72
1	G	141	ARG	N-CA-C	7.13	118.70	111.07
1	E	291	ALA	N-CA-C	7.13	120.09	111.82
1	D	202	VAL	CB-CA-C	-7.10	102.88	111.97
1	C	100	ARG	N-CA-C	7.00	119.51	111.11
1	A	120	GLN	CA-C-N	7.00	134.30	121.70
1	A	120	GLN	C-N-CA	7.00	134.30	121.70
1	E	149	ARG	N-CA-C	6.76	118.30	111.07
1	G	166	GLN	N-CA-C	6.75	118.30	111.07
1	E	45	MET	N-CA-C	6.73	119.11	108.67
1	F	221	THR	CA-C-N	6.68	128.19	119.84
1	F	221	THR	C-N-CA	6.68	128.19	119.84
1	D	38	ALA	N-CA-C	-6.61	105.25	113.38
1	F	263	ILE	CA-C-N	-6.60	111.66	118.85
1	F	263	ILE	C-N-CA	-6.60	111.66	118.85
1	J	5	THR	N-CA-C	6.39	119.13	109.41
1	L	202	VAL	CB-CA-C	-6.39	103.52	112.14
1	H	94	GLY	CA-C-N	6.39	127.83	119.84
1	H	94	GLY	C-N-CA	6.39	127.83	119.84
1	G	274	MET	N-CA-C	6.36	119.20	111.82
1	E	78	ILE	N-CA-CB	6.35	117.28	110.62
1	B	38	ALA	N-CA-C	-6.29	105.61	113.28
1	J	244	LEU	N-CA-C	6.29	117.80	111.07
1	A	67	ASP	N-CA-C	6.27	118.64	111.11
1	L	77	ASN	N-CA-C	6.27	121.09	113.38
1	H	201	GLN	N-CA-C	6.24	118.16	111.36
1	E	72	ALA	N-CA-C	6.23	118.07	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	135	THR	N-CA-C	6.21	119.33	111.69
1	D	202	VAL	N-CA-CB	6.17	117.77	110.55
1	J	115	ILE	CB-CA-C	-6.17	102.28	110.98
1	D	31	SER	N-CA-C	-6.14	105.27	112.89
1	G	82	THR	CA-C-N	6.11	127.47	119.84
1	G	82	THR	C-N-CA	6.11	127.47	119.84
1	B	194	THR	N-CA-C	6.09	120.71	113.28
1	B	292	GLY	N-CA-C	-6.06	103.84	112.81
1	G	133	VAL	CB-CA-C	6.04	119.83	111.19
1	I	86	ALA	N-CA-C	5.99	119.17	109.40
1	L	32	ALA	CA-C-N	5.96	128.27	120.28
1	L	32	ALA	C-N-CA	5.96	128.27	120.28
1	J	114	HIS	N-CA-C	5.96	118.12	108.41
1	H	245	GLY	CA-C-N	5.95	126.10	119.32
1	H	245	GLY	C-N-CA	5.95	126.10	119.32
1	H	220	ALA	N-CA-C	5.95	118.55	111.71
1	E	202	VAL	N-CA-CB	5.94	117.50	110.55
1	K	209	TRP	CA-C-N	5.91	126.22	119.83
1	K	209	TRP	C-N-CA	5.91	126.22	119.83
1	G	204	GLN	N-CA-C	5.91	117.39	111.07
1	H	74	MET	N-CA-CB	5.89	118.89	110.16
1	L	221	THR	N-CA-C	5.86	117.05	109.72
1	E	175	ALA	CA-C-N	5.82	128.40	120.54
1	E	175	ALA	C-N-CA	5.82	128.40	120.54
1	G	53	SER	N-CA-C	5.82	118.50	111.40
1	A	4	VAL	N-CA-C	5.81	116.85	108.48
1	K	170	TYR	N-CA-C	5.80	117.69	111.36
1	A	75	ILE	N-CA-C	-5.78	104.89	110.72
1	B	172	GLU	N-CA-C	-5.74	105.11	111.36
1	B	291	ALA	N-CA-C	-5.73	106.33	113.15
1	F	54	VAL	N-CA-C	5.71	116.49	110.72
1	E	227	ALA	N-CA-C	5.70	117.49	111.28
1	J	228	GLU	N-CA-C	5.69	117.16	111.07
1	H	202	VAL	CB-CA-C	-5.67	103.36	112.16
1	F	243	ALA	CA-C-N	5.67	128.20	120.54
1	F	243	ALA	C-N-CA	5.67	128.20	120.54
1	F	146	VAL	N-CA-C	-5.66	105.01	110.72
1	A	94	GLY	CA-C-N	5.65	126.90	119.84
1	A	94	GLY	C-N-CA	5.65	126.90	119.84
1	A	64	THR	N-CA-C	-5.59	102.19	110.46
1	L	199	ALA	N-CA-C	5.58	117.81	111.11
1	H	282	ASP	N-CA-C	5.58	117.36	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	35	ALA	N-CA-C	5.54	117.00	111.07
1	B	170	TYR	N-CA-C	5.54	117.76	111.11
1	C	79	SER	CA-C-N	5.54	125.38	119.28
1	C	79	SER	C-N-CA	5.54	125.38	119.28
1	B	29	GLY	CA-C-N	5.53	127.63	120.44
1	B	29	GLY	C-N-CA	5.53	127.63	120.44
1	C	31	SER	CA-C-N	5.52	127.61	120.44
1	C	31	SER	C-N-CA	5.52	127.61	120.44
1	D	82	THR	N-CA-C	5.50	117.56	109.42
1	D	292	GLY	N-CA-C	5.49	126.19	113.18
1	L	30	LEU	N-CA-C	5.49	116.94	111.07
1	J	217	GLU	CA-C-N	5.45	131.50	121.70
1	J	217	GLU	C-N-CA	5.45	131.50	121.70
1	A	248	VAL	N-CA-C	5.44	115.64	110.42
1	G	133	VAL	N-CA-C	-5.43	100.79	109.20
1	F	209	TRP	N-CA-C	-5.42	100.73	109.40
1	L	26	VAL	N-CA-CB	-5.42	102.56	111.45
1	A	25	GLY	N-CA-C	5.39	119.37	110.97
1	G	167	THR	CB-CA-C	-5.36	102.43	110.90
1	I	79	SER	CA-C-N	5.36	125.03	119.56
1	I	79	SER	C-N-CA	5.36	125.03	119.56
1	I	146	VAL	N-CA-C	5.36	116.08	110.62
1	C	253	GLU	N-CA-C	5.34	117.10	111.28
1	D	64	THR	N-CA-CB	-5.33	102.64	110.85
1	C	48	ALA	CA-C-N	5.30	125.87	119.98
1	C	48	ALA	C-N-CA	5.30	125.87	119.98
1	L	16	ASN	CA-C-N	5.30	126.46	119.84
1	L	16	ASN	C-N-CA	5.30	126.46	119.84
1	E	215	MET	N-CA-C	5.27	118.06	107.41
1	A	92	TYR	N-CA-C	5.27	119.28	112.86
1	C	110	VAL	N-CA-C	-5.26	101.94	108.89
1	C	268	LYS	CA-C-N	-5.22	113.58	122.56
1	C	268	LYS	C-N-CA	-5.22	113.58	122.56
1	F	31	SER	CA-C-N	5.22	127.54	120.65
1	F	31	SER	C-N-CA	5.22	127.54	120.65
1	L	79	SER	O-C-N	5.22	124.40	121.27
1	G	62	ILE	N-CA-C	5.21	117.98	112.83
1	D	248	VAL	N-CA-C	5.20	115.41	110.42
1	J	209	TRP	CA-C-N	5.18	126.31	119.84
1	J	209	TRP	C-N-CA	5.18	126.31	119.84
1	I	106	SER	N-CA-C	5.17	116.61	110.97
1	C	241	PHE	N-CA-C	5.17	118.62	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	21	ILE	CB-CA-C	5.17	118.53	110.83
1	G	208	GLY	N-CA-C	5.16	121.92	115.21
1	K	216	VAL	N-CA-C	-5.15	100.33	107.80
1	C	26	VAL	N-CA-CB	-5.15	103.00	111.44
1	G	284	SER	N-CA-C	5.15	117.79	111.82
1	F	244	LEU	CB-CA-C	-5.14	102.59	110.81
1	A	18	ASP	N-CA-C	5.13	119.59	113.23
1	L	50	THR	CB-CA-C	5.12	119.30	110.79
1	D	284	SER	N-CA-C	5.11	117.51	111.33
1	L	126	HIS	N-CA-C	5.11	119.05	112.41
1	L	144	ALA	CA-C-N	5.11	127.58	120.63
1	L	144	ALA	C-N-CA	5.11	127.58	120.63
1	L	275	LEU	CA-C-N	5.11	127.08	120.44
1	L	275	LEU	C-N-CA	5.11	127.08	120.44
1	B	30	LEU	N-CA-C	5.09	116.52	111.07
1	I	62	ILE	N-CA-C	-5.08	106.19	111.58
1	A	242	ALA	N-CA-C	5.08	116.82	111.28
1	D	41	ASP	CB-CA-C	-5.08	102.14	110.72
1	B	174	VAL	CB-CA-C	5.07	118.99	112.14
1	E	214	ASN	N-CA-C	5.07	116.57	108.41
1	I	202	VAL	CB-CA-C	-5.06	102.13	111.79
1	K	244	LEU	N-CA-C	5.04	116.46	111.07
1	J	106	SER	CA-C-N	5.03	127.02	120.28
1	J	106	SER	C-N-CA	5.03	127.02	120.28

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	2111	0	2110	73	0
1	B	2137	0	2131	79	0
1	C	2112	0	2107	66	0
1	D	2111	0	2110	61	0
1	E	2118	0	2113	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2116	0	2112	67	0
1	G	2107	0	2106	61	0
1	H	2080	0	2057	76	0
1	I	2100	0	2099	76	0
1	J	2068	0	2046	93	0
1	K	2072	0	2053	52	0
1	L	2126	0	2119	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	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	1	0	0	0	0
2	L	1	0	0	0	0
3	A	116	0	0	3	0
3	B	115	0	0	4	0
3	C	109	0	0	3	0
3	D	135	0	0	2	0
3	E	104	0	0	3	0
3	F	109	0	0	6	0
3	G	124	0	0	6	0
3	H	104	0	0	8	0
3	I	38	0	0	6	0
3	J	83	0	0	10	0
3	K	61	0	0	2	0
3	L	64	0	0	4	0
All	All	26432	0	25163	727	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 14.

All (727) 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:A:97:MET:CE	1:A:100:ARG:HD3	1.65	1.25
1:E:74:MET:CE	1:E:78:ILE:HD11	1.72	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:ILE:HD12	1:L:97:MET:HE3	1.33	1.11
1:A:97:MET:HE1	1:A:100:ARG:HD3	1.15	1.09
1:B:293:GLY:HA3	1:B:294:ALA:HB2	1.25	1.08
1:H:260:ARG:HB3	3:H:1097:HOH:O	1.49	1.08
1:A:62:ILE:HG22	1:D:97:MET:HE3	1.30	1.08
1:B:62:ILE:HG22	1:C:97:MET:HE3	1.12	1.05
1:I:46:THR:O	1:I:50:THR:HG22	1.57	1.04
1:A:97:MET:HE1	1:A:100:ARG:CD	1.88	1.02
1:B:143:ARG:HH11	1:D:293:GLY:HA3	1.21	1.02
1:L:193:ILE:O	1:L:221:THR:HB	1.62	1.00
1:E:97:MET:HE3	1:H:62:ILE:HG22	1.44	0.98
1:A:120:GLN:HB3	1:A:121:THR:HB	1.45	0.97
1:F:74:MET:HE1	1:F:78:ILE:HD11	1.46	0.97
1:I:137:THR:O	1:I:140:THR:HG22	1.65	0.96
1:I:199:ALA:O	1:I:203:ILE:HD12	1.65	0.96
1:B:143:ARG:NH1	1:D:293:GLY:HA3	1.79	0.96
1:B:62:ILE:HG22	1:C:97:MET:CE	1.96	0.95
1:I:62:ILE:HD12	1:L:97:MET:CE	1.94	0.95
1:E:74:MET:HE3	1:E:78:ILE:HD11	1.45	0.95
1:L:122:LYS:HE3	1:L:131:ILE:H	1.32	0.94
1:J:266:LEU:HG	1:J:270:MET:CE	1.97	0.93
1:E:62:ILE:HA	1:H:97:MET:CE	1.98	0.93
1:J:97:MET:HE3	1:K:62:ILE:HG12	1.49	0.93
1:B:97:MET:HE3	1:C:62:ILE:CD1	1.99	0.93
1:E:12:ARG:HG3	3:E:889:HOH:O	1.67	0.93
1:L:12:ARG:HG2	3:L:975:HOH:O	1.69	0.92
1:B:97:MET:CE	1:B:100:ARG:HD3	2.02	0.89
1:B:97:MET:HE3	1:C:62:ILE:HD13	1.52	0.89
1:I:62:ILE:CD1	1:L:97:MET:HE3	2.02	0.87
1:I:66:ASN:OD1	1:L:64:THR:HG21	1.73	0.87
1:I:242:ALA:HB1	1:J:255:MET:HE1	1.57	0.87
1:A:97:MET:HE3	1:D:62:ILE:HD12	1.56	0.86
1:B:255:MET:HA	1:B:255:MET:HE2	1.55	0.86
1:E:62:ILE:HA	1:H:97:MET:HE3	1.57	0.86
1:B:97:MET:HE1	1:B:100:ARG:HD3	1.56	0.86
1:F:190:LEU:HG	3:F:1093:HOH:O	1.74	0.85
1:J:142:ILE:HD13	1:J:185:ALA:HB2	1.57	0.85
1:H:132:LEU:C	1:H:132:LEU:HD12	2.01	0.85
1:F:62:ILE:HG23	1:G:97:MET:HE1	1.59	0.85
1:A:229:ALA:HA	1:A:232:MET:HE3	1.59	0.84
1:C:229:ALA:HA	1:C:232:MET:HE2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:LEU:HB2	1:J:62:ILE:HD12	1.57	0.84
1:B:293:GLY:HA3	1:B:294:ALA:CB	2.06	0.84
1:I:194:THR:CG2	3:I:586:HOH:O	2.24	0.84
1:I:142:ILE:HD13	1:I:185:ALA:HB2	1.58	0.83
1:B:3:MET:HE3	1:D:152:ILE:HD12	1.59	0.83
1:E:55:HIS:C	1:F:74:MET:HE3	2.04	0.83
1:A:97:MET:HE2	1:A:100:ARG:HD3	1.58	0.82
1:I:212:LEU:HD21	1:I:238:ILE:HG12	1.62	0.82
1:A:97:MET:HE3	1:D:62:ILE:CD1	2.09	0.82
1:I:64:THR:HG21	1:L:66:ASN:OD1	1.81	0.81
1:A:97:MET:HE2	1:A:97:MET:HA	1.62	0.81
1:F:62:ILE:HD12	1:G:97:MET:CE	2.11	0.80
1:A:62:ILE:CG2	1:D:97:MET:HE3	2.10	0.80
1:H:181:ARG:HD3	3:H:419:HOH:O	1.80	0.80
1:E:74:MET:HE2	1:E:78:ILE:HD11	1.64	0.80
1:J:97:MET:CE	1:K:62:ILE:HG12	2.12	0.80
1:L:97:MET:HE2	1:L:97:MET:HA	1.63	0.79
1:F:74:MET:CE	1:F:78:ILE:HD11	2.13	0.79
1:J:46:THR:O	1:J:50:THR:CG2	2.30	0.79
1:C:8:THR:O	1:C:12:ARG:HD3	1.82	0.78
1:C:97:MET:HA	1:C:97:MET:HE2	1.64	0.78
1:A:241:PHE:CD1	1:B:275:LEU:HD13	2.19	0.78
1:A:199:ALA:O	1:A:203:ILE:HD12	1.83	0.78
1:F:12:ARG:HD3	3:F:1062:HOH:O	1.84	0.78
1:F:165:LEU:HD22	1:F:190:LEU:HD21	1.66	0.78
1:H:215:MET:HE3	1:H:224:ILE:HB	1.66	0.77
1:I:29:GLY:N	1:I:74:MET:HE1	1.99	0.77
1:J:264:PRO:HB2	1:J:266:LEU:HD13	1.65	0.77
1:J:100:ARG:CZ	1:K:62:ILE:HD11	2.15	0.77
1:B:120:GLN:OE1	1:C:121:THR:HG21	1.86	0.76
1:B:293:GLY:CA	1:B:294:ALA:HB2	2.13	0.76
1:H:229:ALA:HA	1:H:232:MET:HE3	1.67	0.76
1:E:62:ILE:HA	1:H:97:MET:HE1	1.68	0.75
1:A:224:ILE:HG21	1:A:232:MET:HE1	1.67	0.75
1:F:249:ALA:O	1:F:253:GLU:HG3	1.87	0.74
1:J:264:PRO:HB2	1:J:266:LEU:CD1	2.17	0.74
1:C:19:SER:O	1:C:235:ARG:NH1	2.21	0.73
1:E:263:ILE:HG13	1:E:264:PRO:HD2	1.69	0.73
1:K:29:GLY:N	1:K:74:MET:HE1	2.03	0.73
1:F:232:MET:HE3	1:F:234:PHE:CE1	2.23	0.73
1:B:19:SER:O	1:B:235:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASN:C	1:B:16:ASN:OD1	2.32	0.73
1:B:285:MET:HE3	1:B:296:PHE:HB3	1.70	0.73
1:F:167:THR:HG23	1:F:168:HIS:ND1	2.03	0.72
1:E:19:SER:O	1:E:235:ARG:NH1	2.22	0.72
1:J:46:THR:O	1:J:50:THR:HG22	1.89	0.72
1:F:11:ARG:NH2	1:F:186:ASP:OD1	2.22	0.72
1:L:5:THR:HG21	3:L:553:HOH:O	1.88	0.72
1:C:64:THR:HG23	1:C:66:ASN:H	1.54	0.72
1:G:97:MET:CE	1:G:100:ARG:HD2	2.20	0.72
1:B:68:MET:HE3	3:B:896:HOH:O	1.89	0.72
1:D:100:ARG:HD2	3:D:313:HOH:O	1.90	0.71
1:J:224:ILE:HG21	1:J:232:MET:CE	2.20	0.71
1:L:215:MET:HE1	1:L:222:PRO:O	1.91	0.71
1:H:196:ARG:HD3	1:H:228:GLU:OE1	1.89	0.71
1:J:115:ILE:HG12	3:J:877:HOH:O	1.91	0.71
1:F:62:ILE:CD1	1:G:97:MET:HE3	2.22	0.70
1:B:96:ILE:HG21	1:C:62:ILE:HD11	1.72	0.69
1:I:181:ARG:HD3	3:I:988:HOH:O	1.91	0.69
1:D:64:THR:HG23	1:D:66:ASN:H	1.57	0.69
1:J:50:THR:HB	1:J:71:ASN:ND2	2.07	0.69
1:B:62:ILE:CG2	1:C:97:MET:HE3	2.07	0.69
1:H:57:GLN:NE2	3:H:369:HOH:O	2.24	0.69
1:J:100:ARG:NH1	1:K:62:ILE:HD11	2.07	0.69
1:B:139:VAL:HG12	1:B:143:ARG:HH21	1.56	0.69
1:E:74:MET:CE	1:E:78:ILE:CD1	2.63	0.69
1:B:274:MET:HE2	1:B:275:LEU:HG	1.75	0.69
1:H:159:ILE:HG12	1:H:187:VAL:HB	1.74	0.69
1:L:11:ARG:NH2	1:L:149:ARG:NH2	2.40	0.68
1:H:142:ILE:HD13	1:H:180:ALA:HB1	1.76	0.68
1:A:97:MET:CE	1:D:62:ILE:HD12	2.24	0.67
1:G:29:GLY:N	1:G:74:MET:HE1	2.09	0.67
1:J:224:ILE:HG21	1:J:232:MET:HE1	1.76	0.67
1:F:232:MET:HE3	1:F:234:PHE:HE1	1.57	0.67
1:E:62:ILE:HD13	1:H:97:MET:HE2	1.77	0.67
1:I:242:ALA:HB1	1:J:255:MET:CE	2.24	0.67
1:J:50:THR:HB	1:J:71:ASN:HD22	1.59	0.67
1:A:14:LEU:O	1:A:235:ARG:NH2	2.27	0.67
1:B:97:MET:HE3	1:C:62:ILE:HD12	1.75	0.67
1:H:199:ALA:O	1:H:203:ILE:HD12	1.95	0.67
1:H:267:ASP:C	1:H:269:GLU:H	2.02	0.67
1:F:167:THR:CG2	1:F:168:HIS:ND1	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG13	1:B:252:ARG:HG2	1.77	0.67
1:D:64:THR:HG22	1:D:67:ASP:H	1.59	0.67
1:G:270:MET:HE2	1:H:249:ALA:HB2	1.77	0.67
1:L:5:THR:HG22	1:L:7:ALA:H	1.58	0.66
1:K:280:GLY:HA2	3:K:623:HOH:O	1.95	0.66
1:L:193:ILE:HG21	1:L:199:ALA:HB2	1.78	0.66
1:J:274:MET:HE2	3:J:396:HOH:O	1.96	0.66
1:B:63:CYS:SG	1:B:68:MET:CE	2.84	0.66
1:A:120:GLN:CB	1:A:121:THR:HB	2.23	0.66
1:E:97:MET:HE2	1:E:100:ARG:HD3	1.78	0.66
1:L:215:MET:HE3	1:L:224:ILE:HB	1.77	0.66
1:B:270:MET:HE1	1:B:275:LEU:HD21	1.77	0.66
1:I:283:GLU:O	1:I:287:VAL:HG13	1.95	0.66
1:E:11:ARG:NH1	1:E:155:ASP:O	2.30	0.65
1:I:252:ARG:NH1	1:J:34:VAL:O	2.29	0.65
1:A:228:GLU:HG2	1:A:232:MET:HE2	1.77	0.65
1:F:19:SER:O	1:F:235:ARG:NH1	2.28	0.65
1:C:274:MET:HE3	1:C:278:VAL:HG21	1.77	0.65
1:I:171:GLU:HA	1:I:171:GLU:OE1	1.97	0.65
1:H:58:ALA:O	1:H:62:ILE:HD11	1.97	0.65
1:J:215:MET:C	1:J:215:MET:HE2	2.22	0.65
1:J:215:MET:HE3	1:J:215:MET:HA	1.77	0.65
1:E:284:SER:O	1:G:96:ILE:HD11	1.96	0.64
1:L:29:GLY:N	1:L:74:MET:HE1	2.11	0.64
1:E:277:ARG:HG3	1:E:277:ARG:HH11	1.63	0.64
1:F:62:ILE:HD12	1:G:97:MET:HE3	1.79	0.64
1:F:224:ILE:HG21	1:F:232:MET:HE2	1.79	0.64
1:F:173:SER:HB3	3:F:1093:HOH:O	1.97	0.64
1:E:196:ARG:O	1:E:200:ARG:HG3	1.98	0.64
1:K:63:CYS:SG	1:K:68:MET:HE3	2.37	0.64
1:D:274:MET:HE3	1:D:278:VAL:HG21	1.81	0.63
1:H:263:ILE:HD12	1:H:264:PRO:CD	2.28	0.63
1:G:11:ARG:NH1	1:G:155:ASP:O	2.30	0.63
1:H:251:MET:O	1:H:255:MET:HG2	1.98	0.63
1:I:250:ALA:HA	1:I:253:GLU:HG2	1.79	0.63
1:E:3:MET:HE3	1:G:152:ILE:HD12	1.80	0.63
1:F:12:ARG:CG	1:F:12:ARG:HH11	2.10	0.63
1:K:142:ILE:HD11	1:K:183:ALA:HB3	1.79	0.63
1:L:127:LEU:HD12	1:L:127:LEU:O	1.99	0.63
1:J:181:ARG:CZ	1:J:209:TRP:HB2	2.28	0.63
1:J:269:GLU:O	1:J:274:MET:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HD3	1:A:228:GLU:OE1	1.99	0.63
1:I:242:ALA:CB	1:J:255:MET:HE1	2.26	0.63
1:E:288:ASP:O	1:E:292:GLY:HA2	1.99	0.62
1:F:62:ILE:O	1:F:62:ILE:HG22	1.98	0.62
1:J:132:LEU:HD21	1:J:164:SER:HA	1.82	0.62
1:I:170:TYR:O	1:I:173:SER:HB2	1.99	0.62
1:K:97:MET:HE2	1:K:97:MET:HA	1.82	0.62
1:L:122:LYS:HE2	1:L:129:GLY:O	2.00	0.62
1:C:215:MET:HE3	1:C:224:ILE:HB	1.81	0.62
1:A:149:ARG:NH1	3:A:349:HOH:O	2.32	0.61
1:E:210:PRO:HB3	1:E:235:ARG:HG3	1.82	0.61
1:A:121:THR:HG23	1:A:121:THR:O	1.99	0.61
1:H:224:ILE:HG21	1:H:232:MET:HE1	1.82	0.61
1:B:120:GLN:OE1	1:C:121:THR:CG2	2.48	0.61
1:L:45:MET:HE3	1:L:50:THR:HG21	1.82	0.61
1:H:203:ILE:HD11	1:H:234:PHE:CE1	2.36	0.61
1:B:97:MET:HE2	1:B:100:ARG:HD3	1.83	0.61
1:J:228:GLU:HG2	1:J:232:MET:HE2	1.81	0.61
1:H:115:ILE:HD11	1:H:142:ILE:HG13	1.83	0.61
1:H:215:MET:CE	1:H:224:ILE:HB	2.31	0.61
1:J:215:MET:HA	1:J:215:MET:CE	2.31	0.61
1:J:285:MET:HB2	3:J:501:HOH:O	2.00	0.61
1:B:247:ALA:O	1:B:251:MET:HG3	1.99	0.61
1:D:18:ASP:HB3	3:D:626:HOH:O	2.00	0.61
1:E:97:MET:HE3	1:H:62:ILE:CG2	2.26	0.61
1:G:200:ARG:NH1	3:G:930:HOH:O	2.32	0.61
1:F:41:ASP:HB2	3:F:812:HOH:O	2.00	0.61
1:A:16:ASN:OD1	1:A:18:ASP:HB2	2.01	0.60
1:C:62:ILE:HG22	1:C:62:ILE:O	1.99	0.60
1:A:8:THR:O	1:A:11:ARG:HB3	2.01	0.60
1:E:74:MET:HE2	1:E:78:ILE:CD1	2.29	0.60
1:L:196:ARG:NH1	1:L:228:GLU:OE1	2.34	0.60
1:K:63:CYS:CB	1:K:68:MET:HE3	2.30	0.60
1:H:132:LEU:C	1:H:132:LEU:CD1	2.72	0.60
1:K:196:ARG:HD2	3:K:996:HOH:O	2.01	0.60
1:F:165:LEU:HD22	1:F:190:LEU:CD2	2.31	0.60
1:G:2:PRO:HB2	3:G:886:HOH:O	2.02	0.60
1:I:198:MET:O	1:I:202:VAL:HG23	2.02	0.60
1:I:215:MET:HE2	1:J:263:ILE:HD11	1.83	0.60
1:A:19:SER:O	1:A:235:ARG:NH1	2.33	0.60
1:D:283:GLU:OE2	1:D:286:LYS:NZ	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLU:CD	1:A:171:GLU:H	2.10	0.60
1:L:46:THR:O	1:L:50:THR:CG2	2.49	0.60
1:H:19:SER:O	1:H:235:ARG:NH1	2.35	0.59
1:L:46:THR:O	1:L:50:THR:HG23	2.02	0.59
1:G:142:ILE:O	1:G:146:VAL:HG23	2.02	0.59
1:D:247:ALA:O	1:D:251:MET:HG3	2.02	0.59
1:J:215:MET:CE	1:J:215:MET:CA	2.80	0.59
1:J:3:MET:HE3	1:L:152:ILE:HD12	1.84	0.59
1:F:96:ILE:HD11	1:H:284:SER:O	2.03	0.59
1:J:266:LEU:HG	1:J:270:MET:HE3	1.82	0.59
1:D:132:LEU:HD11	1:D:164:SER:HA	1.84	0.59
1:A:215:MET:CE	1:A:224:ILE:HB	2.33	0.59
1:F:213:LEU:HD21	1:F:215:MET:HE2	1.85	0.59
1:J:91:GLY:HA3	1:J:98:VAL:HG22	1.85	0.59
1:L:68:MET:HG3	1:L:92:TYR:OH	2.02	0.59
1:A:267:ASP:HB3	1:A:269:GLU:OE1	2.03	0.58
1:F:213:LEU:HD21	1:F:215:MET:CE	2.34	0.58
1:B:97:MET:HE2	1:B:97:MET:HA	1.86	0.58
1:H:263:ILE:HD12	1:H:264:PRO:HD2	1.85	0.58
1:B:139:VAL:CG1	1:B:143:ARG:HH21	2.16	0.58
1:A:23:ALA:HB3	1:A:238:ILE:HG22	1.86	0.58
1:C:133:VAL:HG21	1:C:137:THR:HG21	1.84	0.58
1:D:170:TYR:O	1:D:173:SER:HB2	2.04	0.57
1:E:200:ARG:HG2	1:E:200:ARG:HH11	1.67	0.57
1:I:27:TYR:HD2	1:I:53:SER:HG	1.52	0.57
1:L:166:GLN:HB2	3:L:968:HOH:O	2.04	0.57
1:A:215:MET:HE3	1:A:224:ILE:HB	1.84	0.57
1:J:3:MET:CE	1:L:152:ILE:HD12	2.35	0.57
1:A:256:GLU:O	1:A:260:ARG:HG3	2.04	0.57
1:E:263:ILE:HG13	1:E:264:PRO:CD	2.33	0.57
1:L:85:ILE:HG12	1:L:112:ALA:HB3	1.86	0.57
1:A:241:PHE:CD1	1:B:275:LEU:CD1	2.87	0.57
1:B:66:ASN:OD1	1:C:64:THR:HG21	2.05	0.57
1:G:181:ARG:HD3	3:G:874:HOH:O	2.03	0.57
1:K:11:ARG:O	1:K:15:GLU:HG3	2.04	0.57
1:E:90:THR:HG21	1:E:120:GLN:HG2	1.86	0.56
1:F:224:ILE:HG21	1:F:232:MET:CE	2.35	0.56
1:L:11:ARG:NH2	1:L:149:ARG:HH22	2.02	0.56
1:D:131:ILE:HD12	1:D:131:ILE:N	2.20	0.56
1:E:54:VAL:HG22	1:E:55:HIS:CD2	2.40	0.56
1:F:12:ARG:HH11	1:F:12:ARG:HG3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:MET:HE3	1:F:224:ILE:HB	1.86	0.56
1:H:63:CYS:SG	1:H:68:MET:HE3	2.45	0.56
1:I:135:THR:HG22	3:I:428:HOH:O	2.04	0.56
1:A:259:LYS:HG2	1:B:40:PHE:CZ	2.40	0.56
1:B:63:CYS:SG	1:B:68:MET:HE3	2.46	0.56
1:H:49:GLY:HA2	1:H:244:LEU:HD11	1.87	0.56
1:I:97:MET:CE	1:L:62:ILE:HD12	2.35	0.56
1:C:64:THR:HG23	1:C:66:ASN:N	2.21	0.56
1:D:198:MET:O	1:D:202:VAL:HG23	2.06	0.56
1:E:266:LEU:HG	1:E:270:MET:SD	2.45	0.56
1:H:277:ARG:HG3	3:H:944:HOH:O	2.04	0.56
1:E:62:ILE:HD13	1:H:97:MET:CE	2.36	0.56
1:G:170:TYR:O	1:G:173:SER:HB2	2.05	0.56
1:K:178:ARG:HG2	1:K:206:LEU:HD21	1.87	0.56
1:A:272:PRO:HA	1:B:241:PHE:CZ	2.41	0.56
1:C:232:MET:HE3	1:C:234:PHE:CE1	2.40	0.56
1:C:274:MET:CE	1:D:248:VAL:HG11	2.36	0.56
1:I:62:ILE:HD12	1:L:97:MET:HE1	1.86	0.56
1:J:263:ILE:CG1	1:J:264:PRO:HD2	2.36	0.56
1:C:11:ARG:NH2	1:C:186:ASP:OD1	2.39	0.55
1:G:274:MET:O	1:G:274:MET:HG2	2.05	0.55
1:H:133:VAL:HG21	1:H:137:THR:HG21	1.88	0.55
1:H:146:VAL:O	1:H:150:GLN:HG3	2.06	0.55
1:K:285:MET:HG3	1:L:127:LEU:HD11	1.86	0.55
1:F:96:ILE:HG12	3:F:416:HOH:O	2.06	0.55
1:H:50:THR:HG21	1:H:68:MET:HE2	1.87	0.55
1:K:117:ASP:HB3	1:K:138:TYR:CD1	2.41	0.55
1:G:94:GLY:O	1:G:98:VAL:HG23	2.05	0.55
1:I:116:GLU:HB2	1:I:161:ARG:HG2	1.89	0.55
1:J:197:GLU:HB2	3:J:316:HOH:O	2.04	0.55
1:C:14:LEU:O	1:C:235:ARG:NH2	2.40	0.55
1:A:119:VAL:HB	1:A:121:THR:HG22	1.89	0.55
1:I:170:TYR:HE1	1:I:202:VAL:HG22	1.71	0.55
1:J:197:GLU:CB	3:J:316:HOH:O	2.54	0.55
1:E:25:GLY:HA2	1:E:44:TYR:O	2.05	0.55
1:F:62:ILE:HA	1:G:97:MET:HE3	1.89	0.55
1:G:271:THR:HB	1:G:272:PRO:HD2	1.89	0.55
1:A:166:GLN:HG3	3:A:926:HOH:O	2.06	0.55
1:E:159:ILE:HG12	1:E:187:VAL:HB	1.87	0.55
1:H:142:ILE:HD13	1:H:180:ALA:CB	2.36	0.55
1:L:97:MET:HE2	1:L:97:MET:CA	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:PRO:HB3	1:H:235:ARG:HG3	1.88	0.55
1:H:228:GLU:HG2	1:H:232:MET:HE2	1.88	0.55
1:K:146:VAL:O	1:K:150:GLN:HG3	2.07	0.55
1:A:97:MET:HE1	1:A:100:ARG:NE	2.22	0.55
1:G:285:MET:HE3	3:G:927:HOH:O	2.07	0.55
1:G:132:LEU:HD11	1:G:164:SER:HA	1.89	0.54
1:I:27:TYR:HD2	1:I:53:SER:OG	1.90	0.54
1:L:97:MET:CE	1:L:100:ARG:HD3	2.37	0.54
1:A:241:PHE:CE1	1:B:275:LEU:HD13	2.43	0.54
1:B:11:ARG:NH2	1:B:186:ASP:OD1	2.40	0.54
1:C:181:ARG:HD3	3:C:937:HOH:O	2.08	0.54
1:I:68:MET:HG3	1:I:92:TYR:OH	2.08	0.54
1:D:149:ARG:HB2	1:D:154:SER:HB3	1.89	0.54
1:J:12:ARG:HD3	3:J:959:HOH:O	2.06	0.54
1:K:203:ILE:HD11	1:K:234:PHE:CE1	2.42	0.54
1:L:64:THR:HG22	1:L:67:ASP:OD2	2.07	0.54
1:E:16:ASN:C	1:E:16:ASN:OD1	2.50	0.54
1:J:266:LEU:CG	1:J:270:MET:CE	2.81	0.54
1:K:97:MET:HE1	1:K:100:ARG:HE	1.73	0.54
1:F:96:ILE:O	1:F:100:ARG:HG3	2.08	0.54
1:E:73:GLU:HB2	1:E:108:SER:HB3	1.88	0.54
1:J:46:THR:O	1:J:50:THR:HG23	2.05	0.54
1:J:63:CYS:SG	1:J:68:MET:HE2	2.48	0.54
1:H:50:THR:HB	1:H:68:MET:HE1	1.90	0.54
1:I:27:TYR:CD2	1:I:53:SER:OG	2.61	0.54
1:E:11:ARG:HH11	1:E:11:ARG:HB2	1.73	0.54
1:I:268:LYS:HA	1:J:218:HIS:CE1	2.43	0.54
1:L:269:GLU:O	1:L:269:GLU:HG2	2.08	0.54
1:E:50:THR:O	1:E:54:VAL:HG13	2.08	0.54
1:H:267:ASP:C	1:H:269:GLU:N	2.66	0.54
1:F:62:ILE:HD13	1:G:97:MET:HE3	1.89	0.53
1:F:62:ILE:HD11	1:G:96:ILE:HG21	1.91	0.53
1:G:52:ALA:O	1:G:56:GLY:HA2	2.09	0.53
1:I:274:MET:HE3	1:I:275:LEU:N	2.24	0.53
1:J:74:MET:C	1:J:74:MET:HE2	2.34	0.53
1:A:62:ILE:HG22	1:D:97:MET:CE	2.20	0.53
1:G:199:ALA:O	1:G:203:ILE:HD12	2.08	0.53
1:J:98:VAL:HG11	1:J:141:ARG:O	2.09	0.53
1:L:127:LEU:O	1:L:128:ALA:HB3	2.09	0.53
1:A:130:LYS:O	1:A:131:ILE:HD13	2.08	0.53
1:G:268:LYS:HG3	3:G:950:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:HIS:CB	1:D:172:GLU:HG2	2.39	0.53
3:C:495:HOH:O	1:D:57:GLN:HG3	2.08	0.53
1:D:11:ARG:NH2	1:D:186:ASP:OD1	2.42	0.53
1:J:224:ILE:CG2	1:J:232:MET:CE	2.86	0.53
1:B:63:CYS:SG	1:B:68:MET:HE2	2.48	0.53
1:C:200:ARG:O	1:C:204:GLN:NE2	2.41	0.53
1:E:69:ARG:HD3	1:E:69:ARG:C	2.34	0.53
1:A:132:LEU:HD11	1:A:164:SER:HA	1.91	0.52
1:I:194:THR:HG22	3:I:586:HOH:O	2.01	0.52
1:L:74:MET:HB3	3:L:1030:HOH:O	2.07	0.52
1:B:14:LEU:O	1:B:235:ARG:NH2	2.42	0.52
1:D:196:ARG:NH1	1:D:228:GLU:OE1	2.42	0.52
1:E:95:PRO:HG3	1:E:140:THR:HG22	1.91	0.52
1:H:212:LEU:C	1:H:212:LEU:HD23	2.34	0.52
1:J:263:ILE:HG13	1:J:264:PRO:CD	2.40	0.52
1:B:248:VAL:O	1:B:252:ARG:HG3	2.09	0.52
1:E:64:THR:HG21	1:H:66:ASN:OD1	2.08	0.52
1:F:94:GLY:O	1:F:98:VAL:HG23	2.09	0.52
1:J:263:ILE:HG12	1:J:264:PRO:HD2	1.91	0.52
1:L:11:ARG:HH22	1:L:149:ARG:NH1	2.06	0.52
1:B:274:MET:HE3	1:B:278:VAL:HG23	1.91	0.52
1:I:189:PHE:HD2	1:I:189:PHE:C	2.17	0.52
1:K:267:ASP:C	1:K:269:GLU:H	2.18	0.52
1:D:130:LYS:C	1:D:131:ILE:HD12	2.35	0.52
1:D:264:PRO:HB2	1:D:266:LEU:HG	1.91	0.52
1:E:97:MET:CE	1:E:100:ARG:HD3	2.40	0.52
1:E:264:PRO:HB2	1:E:266:LEU:HD13	1.92	0.52
1:I:52:ALA:O	1:I:56:GLY:HA2	2.09	0.52
1:J:172:GLU:HB2	3:J:742:HOH:O	2.10	0.52
1:K:142:ILE:HD11	1:K:183:ALA:CB	2.40	0.52
1:G:30:LEU:HD11	1:H:244:LEU:CD2	2.40	0.52
1:G:97:MET:HE2	1:G:100:ARG:HD2	1.91	0.52
1:B:76:SER:HA	1:B:84:VAL:HG21	1.92	0.51
1:G:264:PRO:HD3	1:H:239:PHE:CD2	2.45	0.51
1:I:189:PHE:C	1:I:189:PHE:CD2	2.88	0.51
1:I:194:THR:HG23	3:I:586:HOH:O	1.96	0.51
1:I:214:ASN:OD1	1:I:240:PRO:HG2	2.10	0.51
1:K:239:PHE:CD2	1:L:264:PRO:HD3	2.45	0.51
1:C:62:ILE:O	1:C:62:ILE:CG2	2.59	0.51
1:F:162:THR:HG23	3:F:1093:HOH:O	2.09	0.51
1:B:270:MET:HE2	1:B:275:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:MET:CE	1:B:296:PHE:HB3	2.39	0.51
1:B:294:ALA:HB3	3:B:1230:HOH:O	2.09	0.51
1:F:232:MET:CE	1:F:234:PHE:HE1	2.23	0.51
1:H:115:ILE:HD11	1:H:142:ILE:CG1	2.39	0.51
1:I:96:ILE:HD11	1:K:284:SER:O	2.11	0.51
1:I:116:GLU:CB	1:I:161:ARG:HG2	2.41	0.51
1:B:274:MET:HE3	1:B:278:VAL:CG2	2.41	0.51
1:J:276:PHE:O	1:J:281:LEU:HB2	2.11	0.51
1:E:55:HIS:O	1:F:74:MET:HE3	2.10	0.51
1:I:64:THR:HG22	1:I:67:ASP:CG	2.36	0.51
1:B:96:ILE:CG2	1:C:62:ILE:HD11	2.40	0.51
1:H:267:ASP:O	1:H:269:GLU:N	2.43	0.51
1:I:97:MET:CE	1:L:62:ILE:CD1	2.88	0.51
1:F:121:THR:O	1:F:122:LYS:CB	2.57	0.51
1:F:168:HIS:HB3	1:F:172:GLU:HG2	1.93	0.51
1:G:57:GLN:HG2	1:G:62:ILE:HD12	1.93	0.50
1:H:29:GLY:N	1:H:74:MET:HE1	2.26	0.50
1:A:132:LEU:HD12	1:A:168:HIS:CE1	2.46	0.50
1:B:132:LEU:HD12	1:B:168:HIS:NE2	2.25	0.50
1:C:64:THR:HG22	1:C:67:ASP:H	1.75	0.50
1:H:89:ASP:O	1:H:116:GLU:HG2	2.12	0.50
1:E:294:ALA:HB2	3:E:447:HOH:O	2.10	0.50
1:C:68:MET:HG3	1:C:92:TYR:OH	2.11	0.50
1:D:244:LEU:O	1:D:248:VAL:HG23	2.12	0.50
1:A:275:LEU:O	1:A:275:LEU:HG	2.10	0.50
1:I:203:ILE:HG13	1:I:211:LEU:HD12	1.93	0.50
1:L:76:SER:HA	1:L:84:VAL:HG21	1.94	0.50
1:K:19:SER:O	1:K:235:ARG:NH1	2.45	0.50
1:B:270:MET:CE	1:B:275:LEU:HD21	2.41	0.50
1:E:267:ASP:HB3	3:E:879:HOH:O	2.12	0.50
1:G:215:MET:HE3	1:G:224:ILE:HB	1.94	0.50
1:G:270:MET:CE	1:H:249:ALA:HB2	2.41	0.50
1:J:62:ILE:HD11	1:K:96:ILE:HG21	1.93	0.50
1:G:46:THR:O	1:G:50:THR:CG2	2.60	0.49
1:D:64:THR:CG2	1:D:66:ASN:H	2.23	0.49
1:D:168:HIS:HB3	1:D:172:GLU:HG2	1.92	0.49
1:A:121:THR:O	1:A:121:THR:CG2	2.60	0.49
1:E:266:LEU:HD23	1:E:270:MET:HB3	1.95	0.49
1:H:224:ILE:HG21	1:H:232:MET:CE	2.42	0.49
1:F:224:ILE:HD13	1:F:232:MET:HE1	1.95	0.49
1:J:142:ILE:HD11	1:J:180:ALA:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:ARG:NH1	1:K:205:ASP:O	2.46	0.49
1:A:241:PHE:HD1	1:B:275:LEU:HD13	1.73	0.49
1:E:291:ALA:O	1:G:143:ARG:HD2	2.13	0.49
1:J:55:HIS:O	1:J:57:GLN:HG2	2.12	0.49
1:J:215:MET:HE2	1:J:215:MET:CA	2.40	0.49
1:L:97:MET:HE1	1:L:100:ARG:HD3	1.94	0.49
1:C:196:ARG:HD3	1:C:228:GLU:OE2	2.13	0.49
1:D:274:MET:C	1:D:274:MET:HE2	2.38	0.49
1:F:32:ALA:O	1:F:36:LEU:HD22	2.13	0.49
1:I:97:MET:HE1	1:L:62:ILE:HD12	1.93	0.49
1:L:49:GLY:CA	1:L:244:LEU:HD11	2.43	0.49
1:I:118:GLN:HA	1:I:132:LEU:HB3	1.95	0.49
1:F:95:PRO:HG3	1:F:140:THR:HG22	1.94	0.49
1:J:13:ALA:HB1	1:J:19:SER:OG	2.12	0.49
1:G:30:LEU:HD22	1:H:248:VAL:HG22	1.94	0.48
1:I:212:LEU:HD21	1:I:238:ILE:CG1	2.41	0.48
1:E:132:LEU:HD21	1:E:164:SER:HA	1.94	0.48
1:E:190:LEU:HD12	1:E:202:VAL:CG1	2.43	0.48
1:E:190:LEU:HD12	1:E:202:VAL:HG11	1.95	0.48
1:I:97:MET:CE	1:L:62:ILE:HA	2.44	0.48
1:J:224:ILE:CG2	1:J:232:MET:HE1	2.43	0.48
1:L:69:ARG:HD3	1:L:69:ARG:C	2.38	0.48
1:E:54:VAL:CG2	1:E:55:HIS:CD2	2.96	0.48
1:G:130:LYS:HD3	1:G:163:ASP:HB3	1.93	0.48
1:A:96:ILE:CG2	1:D:62:ILE:HD11	2.42	0.48
1:B:30:LEU:O	1:B:34:VAL:HG23	2.13	0.48
1:G:213:LEU:HD21	1:G:215:MET:CE	2.43	0.48
1:J:74:MET:HE1	1:J:78:ILE:HD11	1.96	0.48
1:J:263:ILE:CG1	1:J:264:PRO:CD	2.92	0.48
1:L:41:ASP:O	1:L:83:PRO:HD2	2.14	0.48
1:E:68:MET:HG3	1:E:92:TYR:OH	2.14	0.48
1:E:275:LEU:CB	1:F:241:PHE:HZ	2.26	0.48
1:C:168:HIS:HB3	1:C:172:GLU:HG2	1.95	0.48
1:I:11:ARG:HH22	1:I:186:ASP:CG	2.20	0.48
1:J:21:ILE:HB	1:J:236:ILE:HG12	1.96	0.48
1:K:73:GLU:HG3	1:K:108:SER:HB3	1.96	0.48
1:A:241:PHE:HD1	1:B:275:LEU:CD1	2.26	0.47
1:C:97:MET:HE2	1:C:100:ARG:HG3	1.96	0.47
1:F:214:ASN:OD1	1:F:240:PRO:HG2	2.14	0.47
1:C:97:MET:HE2	1:C:97:MET:CA	2.39	0.47
1:A:3:MET:HE1	1:C:106:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:ILE:HD11	1:K:234:PHE:CD1	2.49	0.47
1:C:52:ALA:O	1:C:56:GLY:HA2	2.15	0.47
1:D:64:THR:CG2	1:D:66:ASN:HB2	2.44	0.47
1:F:149:ARG:HD2	1:F:156:ILE:O	2.15	0.47
1:A:76:SER:HA	1:A:84:VAL:HG21	1.95	0.47
1:I:54:VAL:HG22	1:I:55:HIS:CD2	2.49	0.47
1:L:127:LEU:O	1:L:127:LEU:CD1	2.63	0.47
1:D:74:MET:HE3	1:D:74:MET:HB3	1.86	0.47
1:J:142:ILE:CD1	1:J:185:ALA:HB2	2.38	0.47
1:A:85:ILE:HG12	1:A:112:ALA:HB3	1.97	0.47
1:D:43:LEU:HB2	1:D:84:VAL:HG22	1.97	0.47
1:D:63:CYS:HB3	1:D:68:MET:HG2	1.97	0.47
1:E:216:VAL:HG22	1:E:240:PRO:HD2	1.97	0.47
1:G:97:MET:HE1	1:G:100:ARG:HD2	1.95	0.47
1:H:133:VAL:HG22	1:H:134:ASP:H	1.79	0.47
1:K:270:MET:HA	1:K:274:MET:HE3	1.97	0.47
1:A:3:MET:HE1	1:C:106:SER:CB	2.45	0.47
1:C:263:ILE:HD11	1:D:223:SER:HB3	1.97	0.47
1:I:50:THR:O	1:I:54:VAL:HG13	2.14	0.47
1:D:121:THR:HG23	1:D:121:THR:O	2.15	0.47
1:G:76:SER:HA	1:G:84:VAL:HG21	1.96	0.47
1:I:97:MET:HE3	1:L:62:ILE:HA	1.95	0.47
1:J:12:ARG:HG3	3:J:1257:HOH:O	2.15	0.47
1:J:41:ASP:O	1:J:83:PRO:HD2	2.14	0.47
1:J:47:GLY:HA3	1:J:87:ASP:OD2	2.15	0.47
1:A:268:LYS:HB2	3:A:1035:HOH:O	2.14	0.47
1:B:117:ASP:HB3	1:B:138:TYR:CD1	2.50	0.47
1:K:49:GLY:HA2	1:K:244:LEU:HD21	1.96	0.47
1:I:64:THR:OG1	1:L:64:THR:OG1	2.26	0.46
1:J:266:LEU:HG	1:J:270:MET:HE2	1.92	0.46
1:B:96:ILE:HD11	1:D:284:SER:O	2.15	0.46
1:K:14:LEU:O	1:K:235:ARG:NH2	2.48	0.46
1:C:14:LEU:HD21	1:C:236:ILE:HD11	1.98	0.46
1:E:263:ILE:CG1	1:E:264:PRO:HD2	2.43	0.46
1:F:62:ILE:O	1:F:62:ILE:CG2	2.63	0.46
1:G:50:THR:HB	1:G:71:ASN:ND2	2.31	0.46
1:J:112:ALA:HB2	1:J:157:VAL:HB	1.97	0.46
1:J:117:ASP:HB3	1:J:138:TYR:CD1	2.50	0.46
1:A:96:ILE:HG21	1:D:62:ILE:HD11	1.96	0.46
1:C:274:MET:HE3	1:D:248:VAL:HG11	1.96	0.46
1:J:52:ALA:O	1:J:56:GLY:HA2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:NH1	1:B:228:GLU:OE2	2.43	0.46
1:D:19:SER:O	1:D:235:ARG:NH1	2.48	0.46
1:D:196:ARG:HH11	1:D:228:GLU:CD	2.24	0.46
1:D:274:MET:HE3	1:D:278:VAL:CG2	2.45	0.46
1:B:244:LEU:O	1:B:248:VAL:HG23	2.15	0.46
1:C:274:MET:HE2	1:C:275:LEU:HA	1.97	0.46
1:A:241:PHE:CE1	1:B:272:PRO:HA	2.50	0.46
1:B:97:MET:CE	1:C:62:ILE:HD12	2.43	0.46
1:E:270:MET:HA	1:E:274:MET:HE2	1.97	0.46
1:H:138:TYR:O	1:H:141:ARG:HB2	2.16	0.46
1:B:11:ARG:NH1	1:B:155:ASP:O	2.48	0.46
1:G:69:ARG:HG3	1:G:104:GLN:HB3	1.97	0.46
1:A:241:PHE:CE1	1:B:275:LEU:CD1	2.99	0.46
1:C:26:VAL:HG21	1:C:43:LEU:HD22	1.97	0.46
1:C:264:PRO:HB2	1:C:266:LEU:HG	1.98	0.46
1:G:216:VAL:HG22	1:G:240:PRO:HD2	1.98	0.46
1:H:69:ARG:HD3	1:H:69:ARG:C	2.41	0.46
1:J:43:LEU:HB2	1:J:84:VAL:HG22	1.97	0.46
1:A:57:GLN:HB2	1:A:62:ILE:HD11	1.98	0.45
1:C:274:MET:HE1	1:D:248:VAL:HG11	1.97	0.45
1:F:229:ALA:HA	1:F:232:MET:HE2	1.98	0.45
1:J:23:ALA:HA	1:J:24:PRO:HD2	1.87	0.45
1:A:30:LEU:HD21	1:A:275:LEU:HD11	1.99	0.45
1:F:168:HIS:CB	1:F:172:GLU:HG2	2.46	0.45
1:F:263:ILE:HG12	1:F:264:PRO:CD	2.45	0.45
1:J:6:ALA:HB1	1:J:83:PRO:HA	1.97	0.45
1:K:85:ILE:HG12	1:K:112:ALA:HB3	1.99	0.45
1:F:86:ALA:O	1:F:113:PHE:HA	2.16	0.45
1:I:30:LEU:HD11	1:J:244:LEU:HD23	1.99	0.45
1:J:266:LEU:HG	1:J:270:MET:HE1	1.91	0.45
1:L:25:GLY:HA2	1:L:44:TYR:O	2.16	0.45
1:E:212:LEU:HD21	1:E:238:ILE:HG12	1.98	0.45
1:A:224:ILE:HG21	1:A:232:MET:CE	2.41	0.45
1:E:277:ARG:HH11	1:E:277:ARG:CG	2.28	0.45
1:I:135:THR:CG2	3:I:428:HOH:O	2.64	0.45
1:L:11:ARG:HH22	1:L:149:ARG:CZ	2.29	0.45
1:B:132:LEU:HD11	1:B:164:SER:HA	1.97	0.45
1:C:248:VAL:HG11	1:D:274:MET:HE1	1.99	0.45
1:D:272:PRO:O	1:D:273:GLN:C	2.60	0.45
1:A:247:ALA:O	1:A:251:MET:HG3	2.17	0.45
1:B:63:CYS:CB	1:B:68:MET:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:HIS:HB3	1:C:159:ILE:HB	1.98	0.45
1:I:92:TYR:O	1:I:97:MET:HG3	2.17	0.45
1:J:266:LEU:CB	1:J:270:MET:HE2	2.46	0.45
1:B:155:ASP:O	1:B:156:ILE:C	2.58	0.45
1:E:29:GLY:HA2	1:E:74:MET:HE1	1.97	0.45
1:F:232:MET:HE3	1:F:234:PHE:CD1	2.51	0.45
1:I:97:MET:HE1	1:L:62:ILE:HG23	1.99	0.45
1:L:46:THR:O	1:L:50:THR:HG22	2.16	0.45
1:A:142:ILE:O	1:A:146:VAL:HG23	2.17	0.45
1:B:97:MET:HE1	1:C:62:ILE:HG23	1.98	0.45
1:B:215:MET:HE3	1:B:215:MET:HA	1.98	0.45
1:L:138:TYR:O	1:L:141:ARG:HB2	2.17	0.45
1:L:194:THR:O	1:L:194:THR:CG2	2.65	0.45
1:I:47:GLY:HA2	1:I:50:THR:CG2	2.47	0.45
1:I:138:TYR:O	1:I:142:ILE:HG23	2.17	0.45
1:I:224:ILE:HG21	1:I:232:MET:CE	2.47	0.45
1:I:55:HIS:O	1:J:74:MET:HE3	2.17	0.44
1:D:96:ILE:O	1:D:100:ARG:HG3	2.17	0.44
1:G:28:ASP:C	1:G:74:MET:HE1	2.42	0.44
1:L:7:ALA:HB1	1:L:156:ILE:HA	1.99	0.44
1:F:282:ASP:HA	1:F:285:MET:HE2	2.00	0.44
1:I:284:SER:O	1:K:96:ILE:HD11	2.18	0.44
1:K:268:LYS:HA	1:L:218:HIS:CE1	2.53	0.44
1:L:89:ASP:OD2	1:L:92:TYR:OH	2.25	0.44
1:F:206:LEU:HD22	1:F:209:TRP:CE3	2.52	0.44
1:I:12:ARG:HG3	1:I:12:ARG:HH11	1.83	0.44
1:K:117:ASP:HB3	1:K:138:TYR:CE1	2.52	0.44
1:K:30:LEU:HA	1:K:30:LEU:HD23	1.71	0.44
1:E:23:ALA:HB3	1:E:238:ILE:HG22	2.00	0.44
1:E:142:ILE:O	1:E:146:VAL:HG23	2.18	0.44
1:H:193:ILE:HG21	1:H:199:ALA:HB2	2.00	0.44
1:I:168:HIS:HB2	1:I:172:GLU:HG2	2.00	0.44
1:G:74:MET:HE3	1:G:75:ILE:HG13	1.99	0.44
1:J:97:MET:HE2	1:J:97:MET:HA	2.00	0.44
1:K:181:ARG:NH1	1:K:209:TRP:HB2	2.33	0.44
1:A:97:MET:CE	1:A:100:ARG:CD	2.58	0.43
1:B:235:ARG:C	1:B:236:ILE:HG13	2.43	0.43
1:C:97:MET:HA	1:C:100:ARG:HG3	2.00	0.43
1:C:198:MET:O	1:C:202:VAL:HG23	2.18	0.43
1:C:263:ILE:CD1	1:D:223:SER:HB3	2.48	0.43
1:E:275:LEU:HB2	1:F:241:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:ILE:HG12	1:H:112:ALA:HB3	2.00	0.43
1:J:263:ILE:HG13	1:J:264:PRO:HD2	2.00	0.43
1:L:11:ARG:NH2	1:L:149:ARG:CZ	2.81	0.43
1:L:103:GLU:HG2	1:L:152:ILE:HD13	2.00	0.43
1:D:36:LEU:HD13	1:D:43:LEU:HD11	1.98	0.43
1:G:97:MET:HE1	1:G:100:ARG:CD	2.48	0.43
1:H:8:THR:O	1:H:12:ARG:HG3	2.18	0.43
1:I:168:HIS:CB	1:I:172:GLU:HG2	2.49	0.43
1:J:30:LEU:O	1:J:34:VAL:HG23	2.18	0.43
3:B:542:HOH:O	1:D:96:ILE:HG12	2.18	0.43
1:J:181:ARG:HD3	3:J:713:HOH:O	2.17	0.43
1:L:157:VAL:HG13	1:L:186:ASP:HB2	2.00	0.43
1:L:194:THR:O	1:L:194:THR:HG22	2.18	0.43
1:L:196:ARG:NH2	1:L:223:SER:O	2.45	0.43
1:G:16:ASN:O	1:G:235:ARG:NH1	2.51	0.43
1:G:117:ASP:HB3	1:G:138:TYR:CG	2.53	0.43
1:I:19:SER:O	1:I:235:ARG:NH1	2.51	0.43
1:J:213:LEU:HD11	1:J:221:THR:HG21	2.00	0.43
1:K:285:MET:SD	1:L:127:LEU:HD11	2.59	0.43
1:D:13:ALA:O	1:D:19:SER:HB2	2.19	0.43
1:D:274:MET:HE2	1:D:275:LEU:HA	1.99	0.43
1:J:215:MET:HG3	1:J:237:ILE:HD11	2.00	0.43
1:A:97:MET:HE3	1:D:62:ILE:HD13	1.95	0.43
1:C:232:MET:HE3	1:C:234:PHE:HE1	1.82	0.43
1:E:263:ILE:HG12	1:F:217:GLU:OE2	2.19	0.43
1:G:114:HIS:HB3	1:G:159:ILE:HB	2.00	0.43
1:H:235:ARG:NH1	3:H:780:HOH:O	2.35	0.43
1:K:117:ASP:OD2	1:K:176:ARG:NH1	2.50	0.43
1:L:64:THR:HG23	1:L:67:ASP:H	1.83	0.43
1:A:120:GLN:CA	1:A:121:THR:HB	2.49	0.43
1:A:170:TYR:O	1:A:174:VAL:HG23	2.18	0.43
1:C:50:THR:O	1:C:54:VAL:HG13	2.19	0.43
1:F:85:ILE:HG12	1:F:112:ALA:HB3	2.00	0.43
1:I:229:ALA:HA	1:I:232:MET:HE2	2.00	0.43
1:J:285:MET:H	1:J:285:MET:HG2	1.73	0.43
1:J:166:GLN:HB3	3:J:798:HOH:O	2.18	0.43
1:H:23:ALA:HB3	1:H:238:ILE:HG22	2.01	0.43
1:J:229:ALA:HA	1:J:232:MET:HE3	2.01	0.43
1:D:170:TYR:HE1	1:D:202:VAL:HG22	1.84	0.43
1:D:274:MET:HE2	1:D:275:LEU:N	2.33	0.43
1:F:161:ARG:HA	1:F:189:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:HB	1:A:272:PRO:CD	2.49	0.42
1:F:57:GLN:HG2	1:F:62:ILE:HG13	2.01	0.42
1:K:212:LEU:HD13	1:K:212:LEU:C	2.43	0.42
1:A:56:GLY:O	1:B:33:ARG:NH2	2.52	0.42
1:I:24:PRO:HG3	1:I:40:PHE:CD1	2.55	0.42
1:I:252:ARG:NH1	1:J:37:SER:OG	2.53	0.42
1:L:117:ASP:HB3	1:L:138:TYR:CD1	2.54	0.42
1:C:83:PRO:HG2	3:C:635:HOH:O	2.18	0.42
1:C:232:MET:HE3	1:C:234:PHE:CD1	2.55	0.42
1:G:214:ASN:OD1	1:G:240:PRO:HG2	2.20	0.42
1:H:50:THR:CG2	1:H:68:MET:HE2	2.49	0.42
1:L:30:LEU:O	1:L:34:VAL:HG23	2.19	0.42
1:C:189:PHE:C	1:C:189:PHE:CD2	2.97	0.42
1:C:282:ASP:HA	1:C:285:MET:HE2	2.01	0.42
1:I:32:ALA:O	1:I:36:LEU:HB2	2.19	0.42
1:K:23:ALA:HB3	1:K:238:ILE:HG22	2.01	0.42
1:K:96:ILE:O	1:K:100:ARG:HG3	2.19	0.42
1:K:266:LEU:HG	1:K:270:MET:SD	2.59	0.42
1:L:130:LYS:HD3	1:L:163:ASP:HB3	2.01	0.42
1:G:21:ILE:HD12	1:G:21:ILE:N	2.34	0.42
1:A:203:ILE:HD11	1:A:234:PHE:CD1	2.55	0.42
1:C:215:MET:CE	1:C:224:ILE:HB	2.48	0.42
1:I:107:ARG:O	1:K:107:ARG:HB3	2.20	0.42
1:I:264:PRO:HD3	1:J:239:PHE:CD2	2.54	0.42
1:L:79:SER:HA	1:L:80:PRO:HD3	1.61	0.42
1:E:268:LYS:H	1:E:268:LYS:HG3	1.36	0.42
1:F:190:LEU:HD12	1:F:202:VAL:HG21	2.01	0.42
1:B:97:MET:HE1	1:B:100:ARG:CD	2.40	0.42
1:E:31:SER:HB3	1:F:251:MET:SD	2.60	0.42
1:E:275:LEU:HB2	1:F:241:PHE:HZ	1.85	0.42
1:H:135:THR:O	1:H:138:TYR:HB3	2.20	0.42
1:H:263:ILE:HD12	1:H:264:PRO:HD3	1.98	0.42
1:K:190:LEU:HD13	1:K:193:ILE:HG12	2.02	0.42
1:L:86:ALA:O	1:L:113:PHE:HA	2.20	0.42
1:C:64:THR:CG2	1:C:66:ASN:HB2	2.50	0.42
1:E:97:MET:CE	1:H:62:ILE:HG22	2.31	0.42
1:I:45:MET:HG3	1:I:75:ILE:HD12	2.02	0.42
1:K:132:LEU:HD22	1:K:168:HIS:CE1	2.55	0.42
1:A:254:ALA:CB	1:B:246:PRO:HG2	2.50	0.41
1:C:221:THR:HA	1:C:222:PRO:HD2	1.87	0.41
1:F:11:ARG:HH22	1:F:186:ASP:CG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:GLN:HB3	1:G:62:ILE:HD11	2.02	0.41
1:G:161:ARG:HA	1:G:189:PHE:HB3	2.01	0.41
1:G:30:LEU:HD22	1:H:248:VAL:CG2	2.50	0.41
1:G:117:ASP:HB3	1:G:138:TYR:CD1	2.56	0.41
1:I:215:MET:CE	1:I:223:SER:HA	2.50	0.41
1:B:200:ARG:HD2	3:B:789:HOH:O	2.19	0.41
1:B:203:ILE:HD11	1:B:234:PHE:CE1	2.55	0.41
1:B:290:GLN:C	1:B:292:GLY:H	2.27	0.41
1:D:196:ARG:HD3	1:D:228:GLU:OE2	2.20	0.41
1:F:2:PRO:HB3	1:H:153:GLY:O	2.19	0.41
1:G:46:THR:O	1:G:50:THR:HG22	2.20	0.41
1:K:76:SER:HA	1:K:84:VAL:HG21	2.02	0.41
1:K:190:LEU:HD12	1:K:202:VAL:HG21	2.02	0.41
1:L:36:LEU:HD13	1:L:43:LEU:HD21	2.02	0.41
1:A:25:GLY:HA3	1:A:240:PRO:HA	2.01	0.41
1:A:264:PRO:HD3	1:B:239:PHE:CD2	2.55	0.41
1:K:137:THR:O	1:K:140:THR:HB	2.20	0.41
1:K:212:LEU:C	1:K:212:LEU:CD1	2.93	0.41
1:K:285:MET:CG	1:L:127:LEU:HD11	2.48	0.41
1:B:52:ALA:O	1:B:56:GLY:HA2	2.20	0.41
1:C:244:LEU:O	1:C:248:VAL:HG23	2.20	0.41
1:H:148:ALA:O	1:H:152:ILE:HG12	2.20	0.41
1:H:149:ARG:NH1	3:H:385:HOH:O	2.52	0.41
1:H:181:ARG:CZ	1:H:209:TRP:HB2	2.51	0.41
1:F:244:LEU:O	1:F:248:VAL:HG23	2.21	0.41
1:H:120:GLN:C	3:H:830:HOH:O	2.63	0.41
1:L:32:ALA:O	1:L:36:LEU:HD22	2.20	0.41
1:C:274:MET:O	1:C:278:VAL:HG23	2.21	0.41
1:D:41:ASP:O	1:D:83:PRO:HD2	2.20	0.41
1:H:260:ARG:NH2	3:H:1026:HOH:O	2.53	0.41
1:K:239:PHE:CE2	1:L:264:PRO:HD3	2.55	0.41
1:A:196:ARG:NH1	1:A:228:GLU:OE2	2.53	0.41
1:G:255:MET:CE	1:H:243:ALA:HB2	2.51	0.41
1:G:270:MET:HE2	1:H:249:ALA:CB	2.48	0.41
1:I:55:HIS:O	1:J:74:MET:CE	2.69	0.41
1:L:127:LEU:O	1:L:128:ALA:CB	2.69	0.41
1:C:232:MET:CE	1:C:234:PHE:CE1	3.04	0.41
1:E:21:ILE:N	1:E:21:ILE:HD12	2.36	0.41
1:E:64:THR:HG22	1:E:66:ASN:HB2	2.03	0.41
1:E:113:PHE:HE1	1:E:115:ILE:HD11	1.86	0.41
1:E:200:ARG:HH11	1:E:200:ARG:CG	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:THR:O	1:E:272:PRO:C	2.63	0.41
1:F:115:ILE:HG21	1:F:115:ILE:HD13	1.78	0.41
1:G:33:ARG:NE	1:H:56:GLY:O	2.42	0.41
1:G:292:GLY:CA	3:G:543:HOH:O	2.69	0.41
1:H:178:ARG:NH2	1:H:205:ASP:O	2.53	0.41
1:J:187:VAL:HG22	1:J:210:PRO:HB2	2.02	0.41
1:J:193:ILE:O	1:J:221:THR:HA	2.21	0.41
1:K:97:MET:HE1	1:K:100:ARG:NE	2.34	0.41
1:L:193:ILE:O	1:L:221:THR:CB	2.51	0.41
1:A:64:THR:HG22	1:A:66:ASN:N	2.36	0.41
1:B:74:MET:HE3	1:B:74:MET:HB3	1.94	0.41
1:C:117:ASP:HB3	1:C:138:TYR:CD1	2.56	0.41
1:B:25:GLY:HA3	1:B:240:PRO:HA	2.03	0.40
1:C:188:GLY:HA3	1:C:209:TRP:CZ3	2.56	0.40
1:E:11:ARG:NH1	1:E:11:ARG:HB2	2.36	0.40
1:G:274:MET:HE3	1:G:278:VAL:CG2	2.51	0.40
1:E:58:ALA:HB3	1:E:60:LEU:HG	2.04	0.40
1:J:143:ARG:O	1:J:147:GLN:HG3	2.22	0.40
1:A:62:ILE:CB	1:D:97:MET:HE3	2.51	0.40
1:C:91:GLY:HA3	1:C:98:VAL:HG22	2.02	0.40
1:F:62:ILE:HA	1:G:97:MET:CE	2.52	0.40
1:J:30:LEU:HA	1:J:30:LEU:HD23	1.85	0.40
1:J:218:HIS:ND1	1:J:218:HIS:N	2.70	0.40
1:J:266:LEU:CG	1:J:270:MET:HE2	2.51	0.40
1:J:283:GLU:O	1:J:287:VAL:HG23	2.21	0.40
1:B:139:VAL:HG12	1:B:143:ARG:NH2	2.30	0.40
1:D:95:PRO:HG3	1:D:140:THR:CG2	2.51	0.40
1:H:86:ALA:O	1:H:113:PHE:HA	2.22	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	280/302 (93%)	273 (98%)	7 (2%)	0	100	100
1	B	284/302 (94%)	270 (95%)	13 (5%)	1 (0%)	30	31
1	C	280/302 (93%)	273 (98%)	7 (2%)	0	100	100
1	D	280/302 (93%)	267 (95%)	13 (5%)	0	100	100
1	E	282/302 (93%)	276 (98%)	6 (2%)	0	100	100
1	F	281/302 (93%)	273 (97%)	8 (3%)	0	100	100
1	G	280/302 (93%)	274 (98%)	6 (2%)	0	100	100
1	H	278/302 (92%)	265 (95%)	11 (4%)	2 (1%)	18	17
1	I	278/302 (92%)	268 (96%)	10 (4%)	0	100	100
1	J	276/302 (91%)	263 (95%)	12 (4%)	1 (0%)	30	31
1	K	276/302 (91%)	268 (97%)	6 (2%)	2 (1%)	18	17
1	L	286/302 (95%)	276 (96%)	10 (4%)	0	100	100
All	All	3361/3624 (93%)	3246 (97%)	109 (3%)	6 (0%)	43	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	ALA
1	H	268	LYS
1	J	119	VAL
1	K	268	LYS
1	H	89	ASP
1	K	193	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/228 (95%)	199 (92%)	18 (8%)	10	10
1	B	218/228 (96%)	202 (93%)	16 (7%)	13	13
1	C	216/228 (95%)	194 (90%)	22 (10%)	7	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	217/228 (95%)	202 (93%)	15 (7%)	14	14
1	E	216/228 (95%)	191 (88%)	25 (12%)	5	4
1	F	217/228 (95%)	200 (92%)	17 (8%)	11	11
1	G	216/228 (95%)	198 (92%)	18 (8%)	10	10
1	H	211/228 (92%)	190 (90%)	21 (10%)	7	6
1	I	216/228 (95%)	186 (86%)	30 (14%)	3	2
1	J	209/228 (92%)	181 (87%)	28 (13%)	4	3
1	K	210/228 (92%)	190 (90%)	20 (10%)	8	7
1	L	215/228 (94%)	191 (89%)	24 (11%)	6	4
All	All	2578/2736 (94%)	2324 (90%)	254 (10%)	7	6

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	21	ILE
1	A	46	THR
1	A	64	THR
1	A	74	MET
1	A	95	PRO
1	A	121	THR
1	A	130	LYS
1	A	166	GLN
1	A	167	THR
1	A	171	GLU
1	A	189	PHE
1	A	190	LEU
1	A	203	ILE
1	A	266	LEU
1	A	269	GLU
1	A	283	GLU
1	A	286	LYS
1	B	5	THR
1	B	36	LEU
1	B	46	THR
1	B	115	ILE
1	B	133	VAL
1	B	140	THR
1	B	143	ARG

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Mol	Chain	Res	Type
1	B	167	THR
1	B	189	PHE
1	B	190	LEU
1	B	246	PRO
1	B	253	GLU
1	B	268	LYS
1	B	270	MET
1	B	274	MET
1	B	278	VAL
1	C	12	ARG
1	C	26	VAL
1	C	30	LEU
1	C	36	LEU
1	C	46	THR
1	C	54	VAL
1	C	64	THR
1	C	96	ILE
1	C	100	ARG
1	C	115	ILE
1	C	121	THR
1	C	140	THR
1	C	151	ARG
1	C	189	PHE
1	C	190	LEU
1	C	197	GLU
1	C	202	VAL
1	C	252	ARG
1	C	259	LYS
1	C	268	LYS
1	C	274	MET
1	C	285	MET
1	D	11	ARG
1	D	36	LEU
1	D	46	THR
1	D	64	THR
1	D	100	ARG
1	D	115	ILE
1	D	131	ILE
1	D	189	PHE
1	D	190	LEU
1	D	202	VAL
1	D	213	LEU

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Mol	Chain	Res	Type
1	D	235	ARG
1	D	268	LYS
1	D	274	MET
1	D	286	LYS
1	E	11	ARG
1	E	36	LEU
1	E	54	VAL
1	E	64	THR
1	E	74	MET
1	E	78	ILE
1	E	90	THR
1	E	130	LYS
1	E	131	ILE
1	E	132	LEU
1	E	133	VAL
1	E	139	VAL
1	E	167	THR
1	E	174	VAL
1	E	189	PHE
1	E	190	LEU
1	E	194	THR
1	E	195	SER
1	E	200	ARG
1	E	202	VAL
1	E	215	MET
1	E	259	LYS
1	E	268	LYS
1	E	272	PRO
1	E	285	MET
1	F	11	ARG
1	F	12	ARG
1	F	19	SER
1	F	26	VAL
1	F	36	LEU
1	F	54	VAL
1	F	100	ARG
1	F	121	THR
1	F	133	VAL
1	F	165	LEU
1	F	166	GLN
1	F	167	THR
1	F	194	THR

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Mol	Chain	Res	Type
1	F	200	ARG
1	F	204	GLN
1	F	241	PHE
1	F	274	MET
1	G	2	PRO
1	G	36	LEU
1	G	46	THR
1	G	50	THR
1	G	54	VAL
1	G	62	ILE
1	G	74	MET
1	G	100	ARG
1	G	115	ILE
1	G	133	VAL
1	G	136	ASP
1	G	140	THR
1	G	167	THR
1	G	190	LEU
1	G	203	ILE
1	G	241	PHE
1	G	273	GLN
1	G	275	LEU
1	H	4	VAL
1	H	5	THR
1	H	19	SER
1	H	30	LEU
1	H	36	LEU
1	H	37	SER
1	H	46	THR
1	H	54	VAL
1	H	62	ILE
1	H	131	ILE
1	H	132	LEU
1	H	135	THR
1	H	136	ASP
1	H	140	THR
1	H	189	PHE
1	H	190	LEU
1	H	202	VAL
1	H	203	ILE
1	H	213	LEU
1	H	246	PRO

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Mol	Chain	Res	Type
1	H	277	ARG
1	I	4	VAL
1	I	11	ARG
1	I	19	SER
1	I	26	VAL
1	I	34	VAL
1	I	36	LEU
1	I	46	THR
1	I	50	THR
1	I	54	VAL
1	I	62	ILE
1	I	74	MET
1	I	116	GLU
1	I	119	VAL
1	I	120	GLN
1	I	132	LEU
1	I	135	THR
1	I	140	THR
1	I	142	ILE
1	I	189	PHE
1	I	190	LEU
1	I	194	THR
1	I	196	ARG
1	I	202	VAL
1	I	203	ILE
1	I	241	PHE
1	I	252	ARG
1	I	268	LYS
1	I	274	MET
1	I	283	GLU
1	I	287	VAL
1	J	3	MET
1	J	5	THR
1	J	19	SER
1	J	30	LEU
1	J	36	LEU
1	J	46	THR
1	J	50	THR
1	J	54	VAL
1	J	74	MET
1	J	96	ILE
1	J	119	VAL

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Mol	Chain	Res	Type
1	J	133	VAL
1	J	140	THR
1	J	142	ILE
1	J	167	THR
1	J	189	PHE
1	J	190	LEU
1	J	194	THR
1	J	206	LEU
1	J	215	MET
1	J	235	ARG
1	J	241	PHE
1	J	252	ARG
1	J	274	MET
1	J	277	ARG
1	J	283	GLU
1	J	285	MET
1	J	290	GLN
1	K	30	LEU
1	K	36	LEU
1	K	50	THR
1	K	62	ILE
1	K	69	ARG
1	K	100	ARG
1	K	119	VAL
1	K	132	LEU
1	K	140	THR
1	K	142	ILE
1	K	178	ARG
1	K	189	PHE
1	K	190	LEU
1	K	201	GLN
1	K	212	LEU
1	K	266	LEU
1	K	268	LYS
1	K	271	THR
1	K	273	GLN
1	K	285	MET
1	L	5	THR
1	L	26	VAL
1	L	36	LEU
1	L	50	THR
1	L	54	VAL

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Mol	Chain	Res	Type
1	L	57	GLN
1	L	71	ASN
1	L	74	MET
1	L	122	LYS
1	L	123	ARG
1	L	127	LEU
1	L	130	LYS
1	L	133	VAL
1	L	139	VAL
1	L	165	LEU
1	L	173	SER
1	L	190	LEU
1	L	202	VAL
1	L	203	ILE
1	L	213	LEU
1	L	215	MET
1	L	221	THR
1	L	241	PHE
1	L	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	B	118	GLN
1	B	150	GLN
1	B	201	GLN
1	B	204	GLN
1	D	273	GLN
1	G	71	ASN
1	G	273	GLN
1	H	204	GLN
1	J	57	GLN
1	J	71	ASN
1	J	118	GLN
1	K	290	GLN
1	L	71	ASN
1	L	290	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/302 (94%)	-1.38	0 100 100	30, 36, 43, 54	0
1	B	288/302 (95%)	-1.38	0 100 100	29, 36, 44, 53	0
1	C	284/302 (94%)	-1.39	0 100 100	29, 36, 43, 50	0
1	D	284/302 (94%)	-1.40	0 100 100	31, 36, 43, 50	0
1	E	286/302 (94%)	-1.36	0 100 100	31, 36, 43, 52	0
1	F	285/302 (94%)	-1.35	0 100 100	28, 36, 44, 52	0
1	G	284/302 (94%)	-1.42	0 100 100	27, 36, 43, 49	0
1	H	282/302 (93%)	-1.37	0 100 100	29, 36, 43, 48	0
1	I	282/302 (93%)	-1.40	0 100 100	30, 37, 43, 49	0
1	J	280/302 (92%)	-1.40	0 100 100	29, 36, 42, 49	0
1	K	280/302 (92%)	-1.39	0 100 100	31, 36, 42, 46	0
1	L	288/302 (95%)	-1.37	0 100 100	30, 36, 43, 52	0
All	All	3407/3624 (94%)	-1.38	0 100 100	27, 36, 43, 54	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	401	1/1	0.97	0.04	51,51,51,51	0
2	MG	F	401	1/1	0.97	0.05	44,44,44,44	0
2	MG	H	401	1/1	0.97	0.04	43,43,43,43	0
2	MG	I	401	1/1	0.97	0.04	42,42,42,42	0
2	MG	J	401	1/1	0.97	0.05	47,47,47,47	0
2	MG	E	401	1/1	0.98	0.04	40,40,40,40	0
2	MG	K	401	1/1	0.98	0.05	46,46,46,46	0
2	MG	L	401	1/1	0.98	0.05	48,48,48,48	0
2	MG	C	401	1/1	0.99	0.06	46,46,46,46	0
2	MG	D	401	1/1	0.99	0.02	40,40,40,40	0
2	MG	B	401	1/1	0.99	0.05	35,35,35,35	0
2	MG	G	401	1/1	1.00	0.03	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.