



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:22 am GMT

PDB ID : 3FA4  
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](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  
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

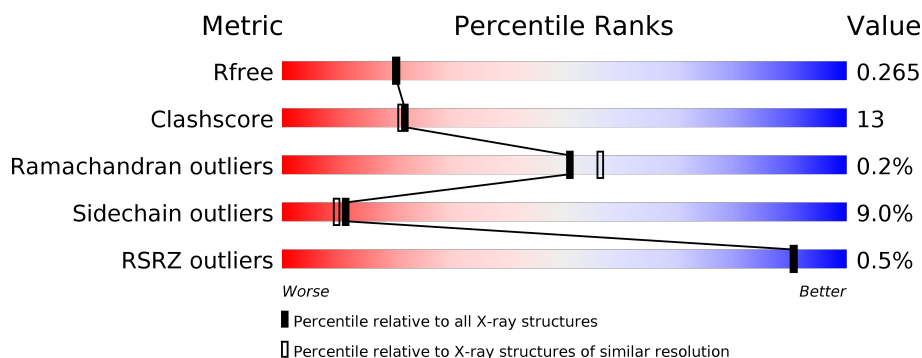
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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))
$R_{free}$	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (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 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	302	<div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div>
1	B	302	<div> <div>%</div> <div>73%</div> <div>21%</div> <div>• 5%</div> </div>
1	C	302	<div> <div>%</div> <div>69%</div> <div>22%</div> <div>• 6%</div> </div>
1	D	302	<div> <div>%</div> <div>72%</div> <div>19%</div> <div>• 6%</div> </div>
1	E	302	<div> <div>70%</div> <div>21%</div> <div>• • 5%</div> </div>
1	F	302	<div> <div>73%</div> <div>18%</div> <div>• • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	302	<div><div></div><div>69%22%6%</div></div>
1	H	302	<div><div></div><div>65%26%7%</div></div>
1	I	302	<div><div></div><div>67%21%6%7%</div></div>
1	J	302	<div><div></div><div>62%26%5%7%</div></div>
1	K	302	<div><div></div><div>72%16%7%</div></div>
1	L	302	<div><div></div><div>69%23%5%</div></div>

## 2 Entry composition

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Mg 1	0	0
2	K	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0
2	F	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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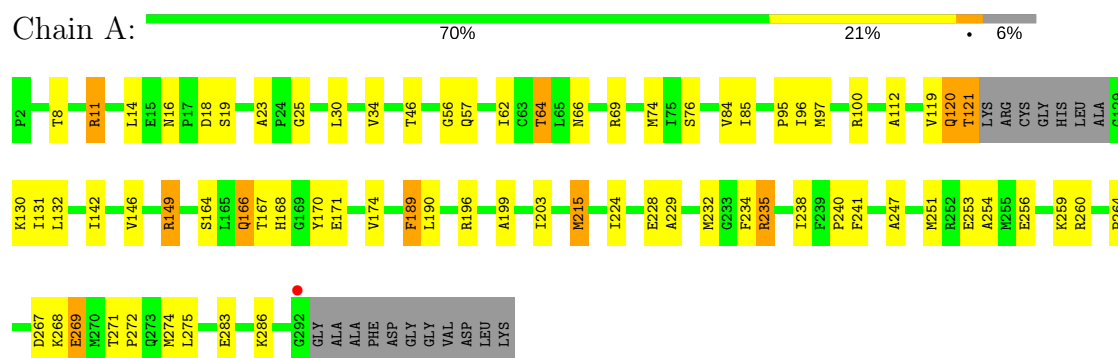
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	83	Total 83	O 83	0	0
3	K	61	Total 61	O 61	0	0
3	L	64	Total 64	O 64	0	0

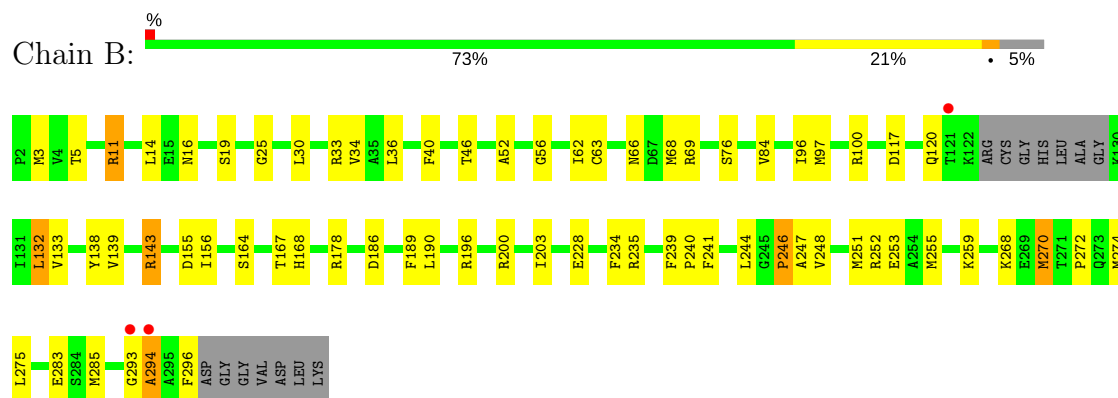
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

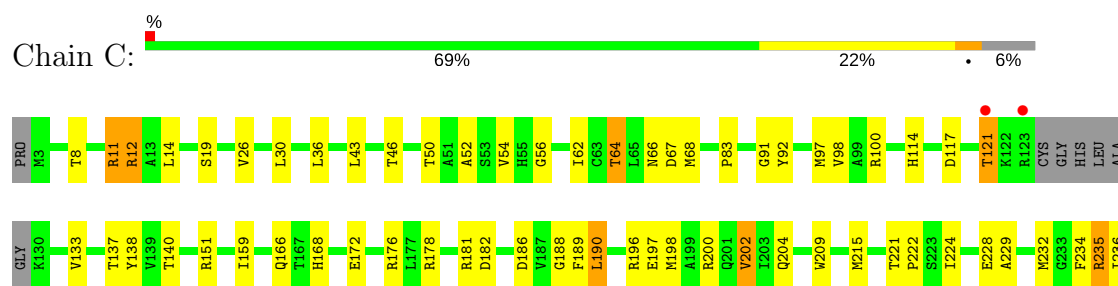
#### • Molecule 1: 2,3-dimethylmalate lyase

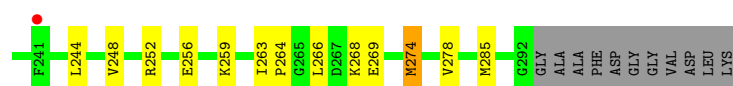


#### • Molecule 1: 2,3-dimethylmalate lyase

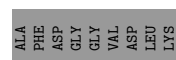
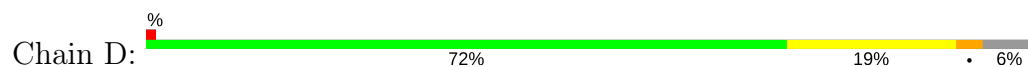


#### • Molecule 1: 2,3-dimethylmalate lyase

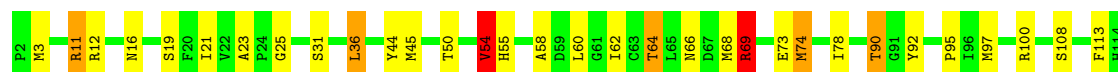




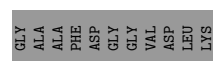
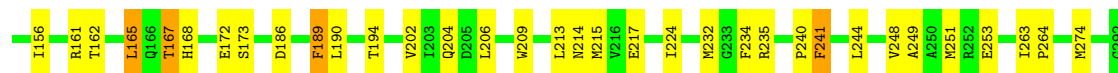
- Molecule 1: 2,3-dimethylmalate lyase



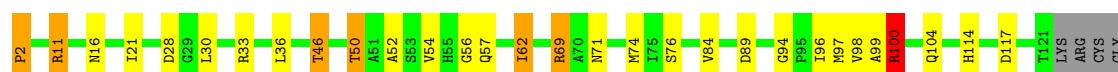
- Molecule 1: 2,3-dimethylmalate lyase



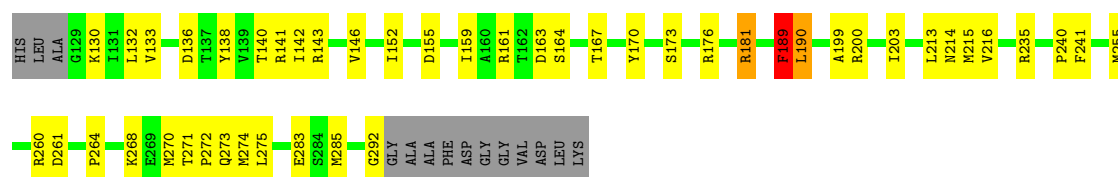
- Molecule 1: 2,3-dimethylmalate lyase



- Molecule 1: 2,3-dimethylmalate lyase

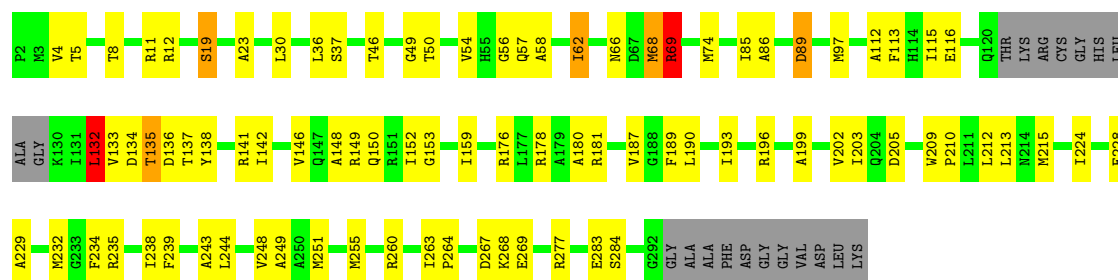






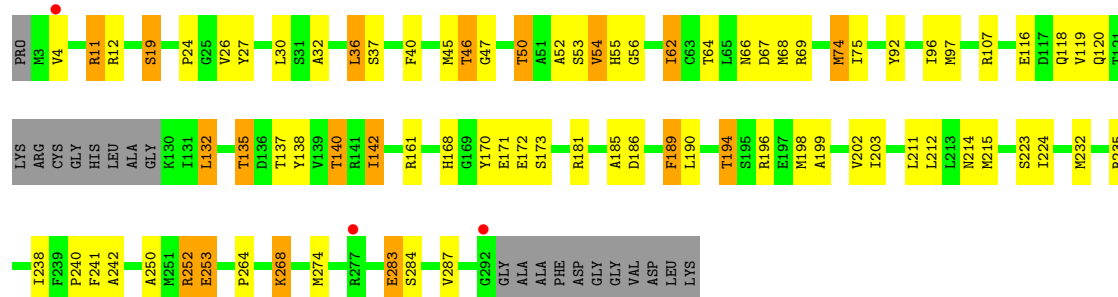
• Molecule 1: 2,3-dimethylmalate lyase

Chain H: 65% 26% 7%



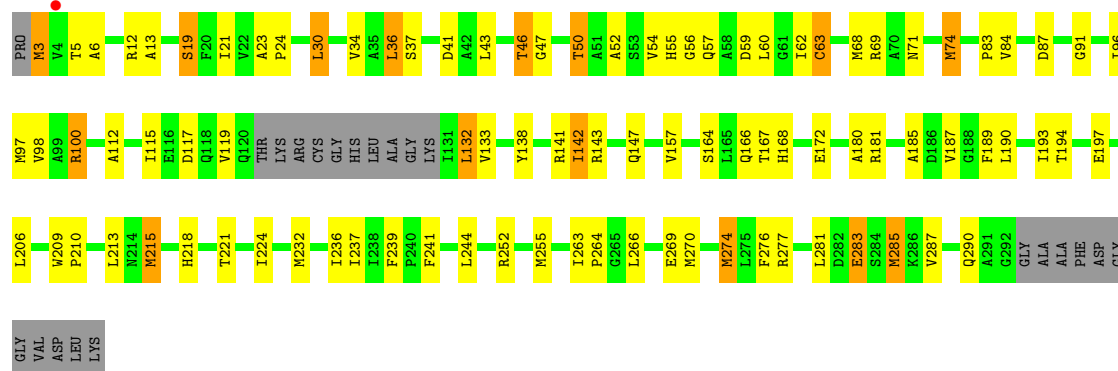
• Molecule 1: 2,3-dimethylmalate lyase

Chain I: 67% 21% 6% 7%



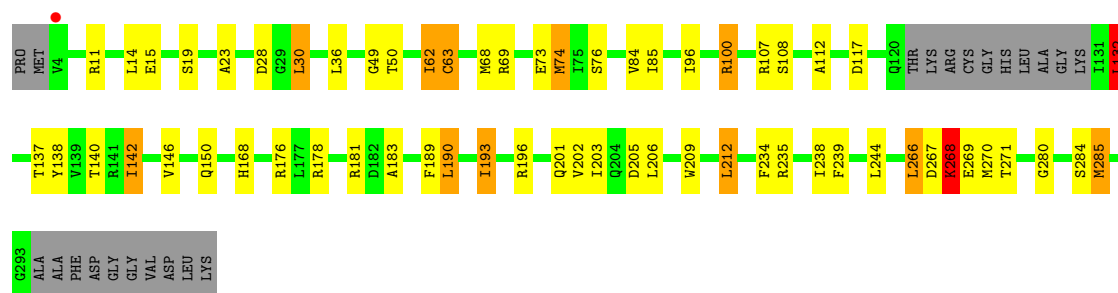
• Molecule 1: 2,3-dimethylmalate lyase

Chain J: 62% 26% 5% 7%



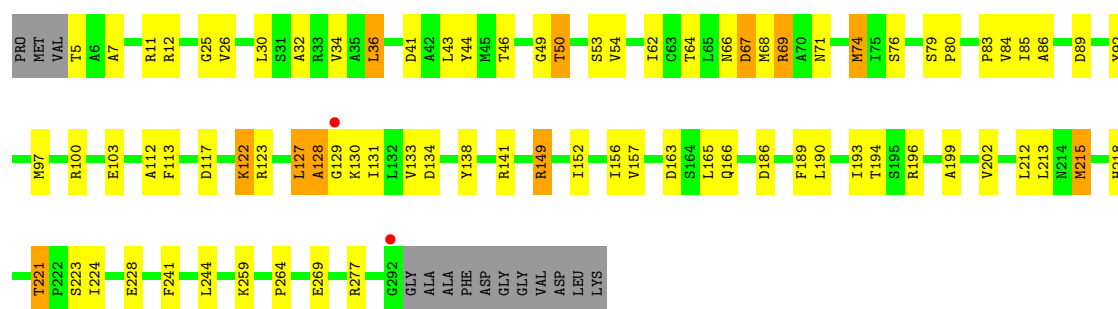
• Molecule 1: 2,3-dimethylmalate lyase

Chain K:  72% 16% 7%



• Molecule 1: 2,3-dimethylmalate lyase

Chain L:  69% 23% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.09Å 115.47Å 115.75Å 119.66° 90.71° 96.28°	Depositor
Resolution (Å)	46.83 – 2.18 46.81 – 2.18	Depositor EDS
% Data completeness (in resolution range)	93.2 (46.83-2.18) 75.4 (46.81-2.18)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.18Å)	Xtriage
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 (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.159 for -h,-k-l,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage'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.*

<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: 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	1.09	1/2141 (0.0%)	1.04	5/2898 (0.2%)
1	B	1.11	1/2168 (0.0%)	1.03	2/2935 (0.1%)
1	C	1.08	2/2141 (0.1%)	1.08	8/2898 (0.3%)
1	D	1.12	2/2141 (0.1%)	1.06	5/2898 (0.2%)
1	E	1.07	4/2148 (0.2%)	1.08	8/2907 (0.3%)
1	F	1.02	0/2146	1.03	4/2905 (0.1%)
1	G	1.16	4/2137 (0.2%)	1.08	8/2893 (0.3%)
1	H	1.09	2/2110 (0.1%)	1.06	4/2861 (0.1%)
1	I	0.93	1/2129 (0.0%)	0.96	1/2882 (0.0%)
1	J	0.97	1/2097 (0.0%)	0.95	3/2841 (0.1%)
1	K	0.96	1/2101 (0.0%)	0.94	3/2846 (0.1%)
1	L	0.92	1/2157 (0.0%)	0.96	4/2922 (0.1%)
All	All	1.05	20/25616 (0.1%)	1.02	55/34686 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	15	GLU	CG-CD	5.95	1.60	1.51
1	J	63	CYS	CB-SG	-5.88	1.72	1.81
1	G	283	GLU	CG-CD	5.88	1.60	1.51
1	E	54	VAL	CB-CG2	-5.87	1.40	1.52
1	B	283	GLU	CG-CD	5.77	1.60	1.51
1	E	253	GLU	CG-CD	5.64	1.60	1.51
1	H	4	VAL	CA-CB	5.51	1.66	1.54
1	I	253	GLU	CG-CD	5.46	1.60	1.51
1	C	269	GLU	CD-OE2	5.39	1.31	1.25
1	E	253	GLU	CD-OE2	5.34	1.31	1.25
1	H	283	GLU	CG-CD	5.30	1.59	1.51
1	K	63	CYS	CB-SG	-5.26	1.73	1.81
1	D	254	ALA	CA-CB	-5.22	1.41	1.52
1	G	189	PHE	CE2-CZ	-5.19	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	128	ALA	CA-CB	5.16	1.63	1.52
1	G	99	ALA	CA-CB	-5.15	1.41	1.52
1	E	253	GLU	CB-CG	5.11	1.61	1.52
1	A	189	PHE	CB-CG	5.09	1.60	1.51
1	G	100	ARG	CG-CD	5.02	1.64	1.51
1	C	256	GLU	CG-CD	5.01	1.59	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	C	235	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	C	235	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	E	235	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	L	149	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	E	235	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	L	149	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	H	132	LEU	CB-CG-CD2	-5.83	101.09	111.00
1	E	45	MET	CG-SD-CE	5.79	109.46	100.20
1	G	176	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	149	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	L	212	LEU	CA-CB-CG	5.62	128.22	115.30
1	C	178	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	L	67	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	H	69	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	G	176	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	H	68	MET	CG-SD-CE	-5.49	91.42	100.20
1	G	190	LEU	CA-CB-CG	5.41	127.75	115.30
1	J	59	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	41	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	J	132	LEU	CA-CB-CG	5.35	127.61	115.30
1	D	252	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	E	69	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	235	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	132	LEU	CA-CB-CG	5.29	127.48	115.30
1	K	132	LEU	CA-CB-CG	5.29	127.48	115.30
1	B	178	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	132	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	G	261	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	292	GLY	N-CA-C	5.24	126.19	113.10
1	A	215	MET	CG-SD-CE	-5.23	91.83	100.20
1	I	74	MET	CG-SD-CE	-5.22	91.84	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	176	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	K	28	ASP	CB-CG-OD1	5.20	122.98	118.30
1	F	74	MET	CG-SD-CE	-5.20	91.88	100.20
1	E	143	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	E	36	LEU	CA-CB-CG	5.17	127.20	115.30
1	F	121	THR	N-CA-C	5.16	124.93	111.00
1	C	151	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	190	LEU	CB-CG-CD2	5.15	119.75	111.00
1	D	213	LEU	CA-CB-CG	5.11	127.05	115.30
1	G	28	ASP	CB-CG-OD1	5.09	122.89	118.30
1	H	176	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	K	212	LEU	CA-CB-CG	5.09	127.00	115.30
1	E	149	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	235	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	120	GLN	C-N-CA	5.04	134.30	121.70
1	F	12	ARG	CG-CD-NE	5.03	122.37	111.80
1	D	235	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	G	181	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	182	ASP	CB-CG-OD1	5.02	122.82	118.30
1	J	36	LEU	CA-CB-CG	5.01	126.83	115.30
1	G	141	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	G	89	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2111	0	2110	71	0
1	B	2137	0	2131	79	0
1	C	2112	0	2107	61	0
1	D	2111	0	2110	53	0
1	E	2118	0	2113	68	0
1	F	2116	0	2112	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2107	0	2106	53	0
1	H	2080	0	2057	72	0
1	I	2100	0	2099	72	0
1	J	2068	0	2046	85	0
1	K	2072	0	2053	48	0
1	L	2126	0	2119	74	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	7	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	678	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 13.

All (678) 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
1:A:97:MET:HE2	1:A:100:ARG:HD3	1.19	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG22	1:D:97:MET:HE3	1.30	1.12
1:B:97:MET:HE1	1:B:100:ARG:HD3	1.34	1.09
1:H:260:ARG:HB3	3:H:1097:HOH:O	1.49	1.08
1:B:293:GLY:HA3	1:B:294:ALA:HB2	1.25	1.08
1:B:62:ILE:HG22	1:C:97:MET:HE3	1.36	1.08
1:I:62:ILE:HD12	1:L:97:MET:HE1	1.33	1.06
1:I:46:THR:O	1:I:50:THR:HG22	1.57	1.04
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:74:MET:HE2	1:E:78:ILE:HD11	1.41	0.99
1:A:120:GLN:HB3	1:A:121:THR:HB	1.45	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: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: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:F:224:ILE:HG21	1:F:232:MET:HE2	1.56	0.88
1:I:66:ASN:OD1	1:L:64:THR:HG21	1.73	0.87
1:A:97:MET:HE1	1:A:100:ARG:HD3	1.53	0.87
1:F:190:LEU:HG	3:F:1093:HOH:O	1.74	0.85
1:F:62:ILE:HG23	1:G:97:MET:HE1	1.55	0.85
1:J:142:ILE:HD13	1:J:185:ALA:HB2	1.57	0.85
1:J:60:LEU:HB2	1:J:62:ILE:HD12	1.57	0.84
1:C:229:ALA:HA	1:C:232:MET:HE2	1.60	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:E:62:ILE:HA	1:H:97:MET:HE3	1.60	0.83
1:I:212:LEU:HD21	1:I:238:ILE:HG12	1.62	0.82
1:B:274:MET:HE2	1:B:275:LEU:HG	1.60	0.82
1:I:64:THR:HG21	1:L:66:ASN:OD1	1.81	0.81
1:J:224:ILE:HG21	1:J:232:MET:HE3	1.63	0.81
1:E:97:MET:HE2	1:H:62:ILE:HG22	1.61	0.81
1:F:62:ILE:HD12	1:G:97:MET:CE	2.11	0.80
1:H:132:LEU:HD12	1:H:132:LEU:C	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:ARG:HD3	3:H:419:HOH:O	1.80	0.80
1:J:97:MET:CE	1:K:62:ILE:HG12	2.12	0.80
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:E:62:ILE:HA	1:H:97:MET:HE1	1.65	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:J:215:MET:HE3	1:J:215:MET:HA	1.64	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: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:C:274:MET:HE3	1:D:248:VAL:HG11	1.67	0.77
1:J:97:MET:HE1	1:K:62:ILE:HG12	1.66	0.76
1:I:242:ALA:HB1	1:J:255:MET:HE1	1.68	0.76
1:B:293:GLY:CA	1:B:294:ALA:HB2	2.13	0.76
1:B:120:GLN:OE1	1:C:121:THR:HG21	1.86	0.76
1:G:97:MET:HE2	1:G:100:ARG:HD2	1.68	0.76
1:E:74:MET:HE2	1:E:78:ILE:CD1	2.15	0.75
1:E:74:MET:HE3	1:E:78:ILE:HD11	1.69	0.75
1:L:97:MET:HE2	1:L:100:ARG:HD3	1.68	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:F:74:MET:HE2	1:F:78:ILE:HD11	1.68	0.73
1:B:19:SER:O	1:B:235:ARG:NH1	2.22	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: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: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:A:97:MET:HE1	1:D:62:ILE:HD12	1.73	0.70
1:A:97:MET:CE	1:A:100:ARG:CD	2.58	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:MET:HE2	1:C:100:ARG:HG3	1.74	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: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:C:97:MET:HE2	1:C:97:MET:HA	1.74	0.69
1:E:74:MET:CE	1:E:78:ILE:CD1	2.63	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:F:62:ILE:CD1	1:G:97:MET:HE3	2.24	0.68
1:B:16:ASN:OD1	1:B:16:ASN:C	2.32	0.68
1:B:68:MET:HE3	3:B:896:HOH:O	1.93	0.68
1:H:142:ILE:HD13	1:H:180:ALA:HB1	1.76	0.68
1:E:62:ILE:HD13	1:H:97:MET:HE2	1.76	0.68
1:A:97:MET:CE	1:D:62:ILE:HD12	2.24	0.67
1:A:97:MET:HE2	1:A:100:ARG:CD	2.13	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:H:199:ALA:O	1:H:203:ILE:HD12	1.95	0.67
1:F:167:THR:CG2	1:F:168:HIS:ND1	2.57	0.67
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:A:62:ILE:CG2	1:D:97:MET:HE3	2.17	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:B:63:CYS:SG	1:B:68:MET:CE	2.84	0.66
1:K:63:CYS:CB	1:K:68:MET:HE3	2.25	0.66
1:A:120:GLN:CB	1:A:121:THR:HB	2.23	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:F:19:SER:O	1:F:235:ARG:NH1	2.28	0.65
1:A:97:MET:HE1	1:A:100:ARG:CD	2.23	0.65
1:I:171:GLU:OE1	1:I:171:GLU:HA	1.97	0.65
1:B:270:MET:HE2	1:B:275:LEU:HD11	1.79	0.65
1:H:58:ALA:O	1:H:62:ILE:HD11	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:SER:O	1:G:96:ILE:HD11	1.96	0.64
1:E:277:ARG:HG3	1:E:277:ARG:HH11	1.63	0.64
1:F:173:SER:HB3	3:F:1093:HOH:O	1.97	0.64
1:B:97:MET:HE3	1:C:62:ILE:HG23	1.80	0.64
1:E:196:ARG:O	1:E:200:ARG:HG3	1.98	0.64
1:H:263:ILE:HD12	1:H:264:PRO:CD	2.28	0.63
1:H:50:THR:HB	1:H:68:MET:HE1	1.80	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:F:12:ARG:HH11	1:F:12:ARG:CG	2.10	0.63
1:K:142:ILE:HD11	1:K:183:ALA:HB3	1.79	0.63
1:L:127:LEU:O	1:L:127:LEU:HD12	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
1:A:196:ARG:HD3	1:A:228:GLU:OE1	1.99	0.63
1:F:62:ILE:HD12	1:G:97:MET:HE3	1.79	0.63
1:K:63:CYS:SG	1:K:68:MET:HE3	2.38	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:H:267:ASP:C	1:H:269:GLU:H	2.02	0.62
1:F:74:MET:HE2	1:F:78:ILE:CD1	2.29	0.62
1:I:170:TYR:O	1:I:173:SER:HB2	1.99	0.62
1:L:122:LYS:HE2	1:L:129:GLY:O	2.00	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:B:120:GLN:OE1	1:C:121:THR:CG2	2.48	0.61
1:H:203:ILE:HD11	1:H:234:PHE:CE1	2.36	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: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: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:L:196:ARG:NH1	1:L:228:GLU:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:MET:HE1	1:H:224:ILE:HB	1.82	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: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
1:E:97:MET:CE	1:H:62:ILE:HG22	2.31	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:J:274:MET:HE2	3:J:396:HOH:O	2.01	0.59
1:B:63:CYS:SG	1:B:68:MET:HE3	2.43	0.59
1:D:247:ALA:O	1:D:251:MET:HG3	2.02	0.59
1:J:215:MET:CA	1:J:215:MET:CE	2.80	0.59
1:F:74:MET:HE1	1:F:78:ILE:HD11	1.83	0.59
1:F:96:ILE:HD11	1:H:284:SER:O	2.03	0.59
1:D:132:LEU:HD11	1:D:164:SER:HA	1.84	0.59
1:C:248:VAL:HG11	1:D:274:MET:HE3	1.85	0.59
1:A:215:MET:CE	1:A:224:ILE:HB	2.33	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: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:B:97:MET:HE3	1:C:62:ILE:CD1	2.34	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:HH11	1:E:200:ARG:HG2	1.67	0.57
1:I:27:TYR:HD2	1:I:53:SER:HG	1.52	0.57
1:J:215:MET:HA	1:J:215:MET:CE	2.31	0.57
1:J:97:MET:HE3	1:K:62:ILE:HG12	1.85	0.57
1:L:166:GLN:HB2	3:L:968:HOH:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG3	1:F:12:ARG:HH11	1.69	0.56
1:J:266:LEU:HG	1:J:270:MET:HE3	1.83	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:E:55:HIS:C	1:F:74:MET:HE3	2.26	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:G:170:TYR:O	1:G:173:SER:HB2	2.05	0.56
1:E:62:ILE:HD13	1:H:97:MET:CE	2.36	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:H:132:LEU:CD1	1:H:132:LEU:C	2.72	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:B:293:GLY:CA	1:B:294:ALA:CB	2.80	0.55
1:F:96:ILE:HG12	3:F:416:HOH:O	2.06	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:A:171:GLU:CD	1:A:171:GLU:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:210:PRO:HB3	1:H:235:ARG:HG3	1.88	0.55
1:K:146:VAL:O	1:K:150:GLN:HG3	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: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:L:97:MET:CE	1:L:100:ARG:HD3	2.37	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:J:266:LEU:CG	1:J:270:MET:CE	2.81	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:I:27:TYR:CD2	1:I:53:SER:OG	2.61	0.54
1:B:97:MET:HE3	1:C:62:ILE:HD12	1.90	0.54
1:E:11:ARG:HB2	1:E:11:ARG:HH11	1.73	0.54
1:I:268:LYS:HA	1:J:218:HIS:CE1	2.43	0.54
1:L:269:GLU:HG2	1:L:269:GLU:O	2.08	0.54
1:A:62:ILE:HG22	1:D:97:MET:CE	2.20	0.54
1:E:50:THR:O	1:E:54:VAL:HG13	2.08	0.54
1:C:274:MET:CE	1:D:248:VAL:HG11	2.36	0.53
1:G:52:ALA:O	1:G:56:GLY:HA2	2.09	0.53
1:F:62:ILE:HD11	1:G:96:ILE:HG21	1.91	0.53
1:G:285:MET:HE3	3:G:927:HOH:O	2.07	0.53
1:B:255:MET:CE	1:B:255:MET:HA	2.38	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
1:D:168:HIS:CB	1:D:172:GLU:HG2	2.39	0.53
1:D:11:ARG:NH2	1:D:186:ASP:OD1	2.42	0.53
3:C:495:HOH:O	1:D:57:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:224:ILE:CG2	1:J:232:MET:CE	2.86	0.53
1:C:200:ARG:O	1:C:204:GLN:NE2	2.41	0.53
1:I:215:MET:HE2	1:J:263:ILE:HD11	1.91	0.52
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:F:232:MET:CE	1:F:234:PHE:HE1	2.23	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:H:229:ALA:HA	1:H:232:MET:HE2	1.92	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:C:232:MET:HE3	1:C:234:PHE:CE1	2.44	0.52
1:J:266:LEU:HG	1:J:270:MET:HE1	1.89	0.52
1:H:50:THR:CB	1:H:68:MET:HE1	2.40	0.52
1:D:264:PRO:HB2	1:D:266:LEU:HG	1.91	0.52
1:E:264:PRO:HB2	1:E:266:LEU:HD13	1.92	0.52
1:E:97:MET:CE	1:E:100:ARG:HD3	2.40	0.52
1:H:50:THR:CG2	1:H:68:MET:HE1	2.40	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:H:224:ILE:HG21	1:H:232:MET:HE1	1.92	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: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:B:285:MET:CE	1:B:296:PHE:HB3	2.39	0.51
1:B:97:MET:CE	1:C:62:ILE:CD1	2.89	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:294:ALA:HB3	3:B:1230:HOH:O	2.09	0.51
1:H:115:ILE:HD11	1:H:142:ILE:CG1	2.39	0.51
1:A:97:MET:HE2	1:A:97:MET:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:GLU:CB	1:I:161:ARG:HG2	2.41	0.51
1:I:96:ILE:HD11	1:K:284:SER:O	2.11	0.51
1:L:97:MET:HE2	1:L:97:MET:HA	1.92	0.51
1:J:276:PHE:O	1:J:281:LEU:HB2	2.11	0.51
1:B:96:ILE:CG2	1:C:62:ILE:HD11	2.40	0.51
1:E:55:HIS:O	1:F:74:MET:HE3	2.11	0.51
1:H:267:ASP:O	1:H:269:GLU:N	2.43	0.51
1:J:3:MET:HE3	1:L:152:ILE:HD12	1.93	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:G:270:MET:CE	1:H:249:ALA:HB2	2.41	0.50
1:A:132:LEU:HD12	1:A:168:HIS:CE1	2.46	0.50
1:B:63:CYS:CB	1:B:68:MET:HE3	2.41	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:B:62:ILE:HG22	1:C:97:MET:HE1	1.89	0.50
1:E:294:ALA:HB2	3:E:447:HOH:O	2.10	0.50
1:F:224:ILE:HG21	1:F:232:MET:CE	2.35	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:224:ILE:HG21	1:A:232:MET:CE	2.41	0.50
1:A:275:LEU:HG	1:A:275:LEU:O	2.10	0.50
1:F:224:ILE:CG2	1:F:232:MET:HE2	2.36	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:B:270:MET:CE	1:B:275:LEU:HD21	2.41	0.50
1:K:19:SER:O	1:K:235:ARG:NH1	2.45	0.50
1:E:267:ASP:HB3	3:E:879:HOH:O	2.12	0.50
1:J:62:ILE:HD11	1:K:96:ILE:HG21	1.93	0.50
1:F:62:ILE:HD13	1:G:97:MET:HE3	1.92	0.50
1:A:224:ILE:HG21	1:A:232:MET:HE1	1.94	0.49
1:B:62:ILE:CG2	1:C:97:MET:CE	2.82	0.49
1:G:46:THR:O	1:G:50:THR:CG2	2.60	0.49
1:A:97:MET:HE1	1:D:62:ILE:HG23	1.94	0.49
1:D:168:HIS:HB3	1:D:172:GLU:HG2	1.92	0.49
1:D:64:THR:CG2	1:D:66:ASN:H	2.23	0.49
1:A:215:MET:HE3	1:A:224:ILE:HB	1.93	0.49
1:E:16:ASN:C	1:E:16:ASN:OD1	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:O	1:A:121:THR:CG2	2.60	0.49
1:B:97:MET:CE	1:C:62:ILE:HD12	2.43	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:J:142:ILE:HD11	1:J:180:ALA:O	2.13	0.49
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:B:270:MET:HE2	1:B:275:LEU:HD21	1.94	0.49
1:B:63:CYS:SG	1:B:68:MET:HE2	2.52	0.49
1:E:291:ALA:O	1:G:143:ARG:HD2	2.13	0.49
1:I:62:ILE:HD12	1:L:97:MET:HE3	1.87	0.49
1:J:55:HIS:O	1:J:57:GLN:HG2	2.12	0.49
1:C:196:ARG:HD3	1:C:228:GLU:OE2	2.13	0.49
1:F:32:ALA:O	1:F:36:LEU:HD22	2.13	0.49
1:L:49:GLY:CA	1:L:244:LEU:HD11	2.43	0.49
1:B:97:MET:HE1	1:B:100:ARG:CD	2.24	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:F:62:ILE:CD1	1:G:97:MET:CE	2.83	0.48
1:H:267:ASP:C	1:H:269:GLU:N	2.66	0.48
1:I:97:MET:CE	1:L:62:ILE:HA	2.44	0.48
1:I:97:MET:HE1	1:L:62:ILE:HD12	1.93	0.48
1:J:215:MET:HE2	1:J:215:MET:C	2.33	0.48
1:E:54:VAL:CG2	1:E:55:HIS:CD2	2.96	0.48
1:F:232:MET:HE3	1:F:234:PHE:CE1	2.49	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:E:69:ARG:C	1:E:69:ARG:HD3	2.34	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: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:275:LEU:CB	1:F:241:PHE:HZ	2.26	0.48
1:E:68:MET:HG3	1:E:92:TYR:OH	2.14	0.48
1:L:97:MET:CE	1:L:97:MET:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:MET:O	1:B:274:MET:HE3	2.14	0.48
1:C:168:HIS:HB3	1:C:172:GLU:HG2	1.95	0.48
1:H:212:LEU:HD23	1:H:212:LEU:C	2.34	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:B:3:MET:CE	1:D:152:ILE:HD12	2.44	0.47
1:F:214:ASN:OD1	1:F:240:PRO:HG2	2.14	0.47
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:189:PHE:HD2	1:I:189:PHE:C	2.17	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:J:142:ILE:CD1	1:J:185:ALA:HB2	2.38	0.47
1:K:267:ASP:C	1:K:269:GLU:H	2.18	0.47
1:D:43:LEU:HB2	1:D:84:VAL:HG22	1.97	0.47
1:E:216:VAL:HG22	1:E:240:PRO:HD2	1.97	0.47
1:A:85:ILE:HG12	1:A:112:ALA:HB3	1.97	0.47
1:D:63:CYS:HB3	1:D:68:MET:HG2	1.97	0.47
1:H:133:VAL:HG22	1:H:134:ASP:H	1.79	0.47
1:C:263:ILE:HD11	1:D:223:SER:HB3	1.97	0.47
1:I:189:PHE:C	1:I:189:PHE:CD2	2.88	0.47
1:I:50:THR:O	1:I:54:VAL:HG13	2.14	0.47
1:D:121:THR:O	1:D:121:THR:HG23	2.15	0.47
1:G:76:SER:HA	1:G:84:VAL:HG21	1.96	0.47
1:J:12:ARG:HG3	3:J:1257:HOH:O	2.15	0.47
1:J:47:GLY:HA3	1:J:87:ASP:OD2	2.15	0.47
1:J:41:ASP:O	1:J:83:PRO:HD2	2.14	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:D:130:LYS:C	1:D:131:ILE:HD12	2.35	0.46
1:J:266:LEU:HG	1:J:270:MET:HE2	1.93	0.46
1:A:97:MET:CE	1:A:97:MET:HA	2.46	0.46
1:B:96:ILE:HD11	1:D:284:SER:O	2.15	0.46
1:I:215:MET:HE2	1:I:223:SER:HA	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ILE:CG1	1:E:264:PRO:HD2	2.43	0.46
1:F:62:ILE:CG2	1:F:62:ILE:O	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:I:64:THR:HG22	1:I:67:ASP:CG	2.36	0.46
1:J:52:ALA:O	1:J:56:GLY:HA2	2.14	0.46
1:B:196:ARG:NH1	1:B:228:GLU:OE2	2.43	0.46
1:B:285:MET:HE3	1:B:296:PHE:HB3	1.98	0.46
1:D:19:SER:O	1:D:235:ARG:NH1	2.48	0.46
1:B:244:LEU:O	1:B:248:VAL:HG23	2.15	0.46
1:A:241:PHE:CE1	1:B:272:PRO:HA	2.50	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:264:PRO:HB2	1:C:266:LEU:HG	1.98	0.46
1:C:26:VAL:HG21	1:C:43:LEU:HD22	1.97	0.46
1:G:216:VAL:HG22	1:G:240:PRO:HD2	1.98	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:J:23:ALA:HA	1:J:24:PRO:HD2	1.87	0.45
1:L:215:MET:HE3	1:L:224:ILE:HB	1.98	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:F:213:LEU:HD21	1:F:215:MET:HE2	1.97	0.45
1:I:30:LEU:HD11	1:J:244:LEU:HD23	1.99	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:I:97:MET:HE3	1:L:62:ILE:HA	1.97	0.45
1:E:277:ARG:CG	1:E:277:ARG:HH11	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:A:247:ALA:O	1:A:251:MET:HG3	2.17	0.45
1:C:114:HIS:HB3	1:C:159:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:MET:HA	1:C:97:MET:CE	2.45	0.45
1:I:92:TYR:O	1:I:97:MET:HG3	2.17	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:J:74:MET:C	1:J:74:MET:HE2	2.37	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: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:47:GLY:HA2	1:I:50:THR:CG2	2.47	0.45
1:A:215:MET:HE1	1:A:224:ILE:HB	1.99	0.44
1:I:224:ILE:HG21	1:I:232:MET:HE2	1.99	0.44
1:D:96:ILE:O	1:D:100:ARG:HG3	2.17	0.44
1:J:63:CYS:CB	1:J:68:MET:HE3	2.48	0.44
1:L:7:ALA:HB1	1:L:156:ILE:HA	1.99	0.44
1:B:63:CYS:HB2	1:B:68:MET:HE3	1.98	0.44
1:I:62:ILE:CD1	1:L:97:MET:CE	2.82	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:HH11	1:I:12:ARG:HG3	1.83	0.44
1:K:117:ASP:HB3	1:K:138:TYR:CE1	2.52	0.44
1:K:30:LEU:HD23	1:K:30:LEU:HA	1.71	0.44
1:K:63:CYS:HB3	1:K:68:MET:HE3	1.99	0.44
1:E:142:ILE:O	1:E:146:VAL:HG23	2.18	0.44
1:E:23:ALA:HB3	1:E:238:ILE:HG22	2.00	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:K:181:ARG:NH1	1:K:209:TRP:HB2	2.33	0.44
1:L:69:ARG:HD3	1:L:69:ARG:C	2.38	0.44
1:C:198:MET:O	1:C:202:VAL:HG23	2.18	0.43
1:C:97:MET:HA	1:C:100:ARG:HG3	2.00	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
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:103:GLU:HG2	1:L:152:ILE:HD13	2.00	0.43
1:L:11:ARG:NH2	1:L:149:ARG:CZ	2.81	0.43
1:D:36:LEU:HD13	1:D:43:LEU:HD11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:L:194:THR:O	2.18	0.43
1:L:196:ARG:NH2	1:L:223:SER:O	2.45	0.43
1:G:117:ASP:HB3	1:G:138:TYR:CG	2.53	0.43
1:G:16:ASN:O	1:G:235:ARG:NH1	2.51	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:J:215:MET:HG3	1:J:237:ILE:HD11	2.00	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:11:ARG:HH22	1:I:186:ASP:CG	2.20	0.43
1:J:266:LEU:CB	1:J:270:MET:HE2	2.48	0.43
1:J:285:MET:HG2	1:J:285:MET:H	1.73	0.43
1:C:215:MET:CE	1:C:224:ILE:HB	2.48	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:D:170:TYR:HE1	1:D:202:VAL:HG22	1.84	0.43
1:F:161:ARG:HA	1:F:189:PHE:HB3	2.01	0.43
1:A:271:THR:HB	1:A:272:PRO:CD	2.49	0.42
1:F:232:MET:CE	1:F:234:PHE:CE1	3.02	0.42
1:F:57:GLN:HG2	1:F:62:ILE:HG13	2.01	0.42
1:B:274:MET:HE2	1:B:275:LEU:CG	2.40	0.42
1:B:97:MET:CE	1:C:62:ILE:HD13	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PRO:HG2	3:C:635:HOH:O	2.18	0.42
1:G:214:ASN:OD1	1:G:240:PRO:HG2	2.20	0.42
1:L:30:LEU:O	1:L:34:VAL:HG23	2.19	0.42
1:I:32:ALA:O	1:I:36:LEU:HB2	2.19	0.42
1:K:96:ILE:O	1:K:100:ARG:HG3	2.19	0.42
1:K:23:ALA:HB3	1:K:238:ILE:HG22	2.01	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:C:232:MET:HE3	1:C:234:PHE:CD1	2.55	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:I:264:PRO:HD3	1:J:239:PHE:CD2	2.54	0.42
1:I:107:ARG:O	1:K:107:ARG:HB3	2.20	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:E:275:LEU:HB2	1:F:241:PHE:HZ	1.85	0.42
1:E:31:SER:HB3	1:F:251:MET:SD	2.60	0.42
1:E:3:MET:CE	1:G:152:ILE:HD12	2.50	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: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:G:161:ARG:HA	1:G:189:PHE:HB3	2.01	0.41
1:G:57:GLN:HB3	1:G:62:ILE:HD11	2.02	0.41
1:G:117:ASP:HB3	1:G:138:TYR:CD1	2.56	0.41
1:G:270:MET:HE3	1:H:249:ALA:HB2	2.01	0.41
1:G:30:LEU:HD22	1:H:248:VAL:CG2	2.50	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:D:196:ARG:HD3	1:D:228:GLU:OE2	2.20	0.41
1:D:196:ARG:HH11	1:D:228:GLU:CD	2.24	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:H:69:ARG:C	1:H:69:ARG:HD3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:LEU:HD12	1:K:202:VAL:HG21	2.02	0.41
1:K:76:SER:HA	1:K:84: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:B:285:MET:HE2	1:B:296:PHE:HB3	2.02	0.41
1:K:137:THR:O	1:K:140:THR:HB	2.20	0.41
1:K:285:MET:CG	1:L:127:LEU:HD11	2.48	0.41
1:A:229:ALA:HA	1:A:232:MET:CE	2.51	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:149:ARG:NH1	3:H:385:HOH:O	2.52	0.41
1:H:148:ALA:O	1:H:152:ILE:HG12	2.20	0.41
1:H:181:ARG:CZ	1:H:209:TRP:HB2	2.51	0.41
1:C:274:MET:HE3	1:C:278:VAL:HG21	2.02	0.41
1:F:244:LEU:O	1:F:248:VAL:HG23	2.21	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:I:55:HIS:O	1:J:74:MET:CE	2.69	0.41
1:K:74:MET:HE1	1:L:53:SER:O	2.20	0.41
1:L:127:LEU:O	1:L:128:ALA:CB	2.69	0.41
1:E:200:ARG:CG	1:E:200:ARG:HH11	2.28	0.41
1:F:115:ILE:HG21	1:F:115:ILE:HD13	1.78	0.41
1:H:178:ARG:NH2	1:H:205:ASP:O	2.53	0.41
1:G:33:ARG:NE	1:H:56:GLY:O	2.42	0.41
1:L:193:ILE:O	1:L:221:THR:CB	2.51	0.41
1:C:232:MET:CE	1:C:234:PHE:CE1	3.04	0.41
1:E:113:PHE:HE1	1:E:115:ILE:HD11	1.86	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:97:MET:HE2	1:E:100:ARG:HD3	2.03	0.41
1:G:292:GLY:CA	3:G:543:HOH:O	2.69	0.41
1:J:193:ILE:O	1:J:221:THR:HA	2.21	0.41
1:J:187:VAL:HG22	1:J:210:PRO:HB2	2.02	0.41
1:A:64:THR:HG22	1:A:66:ASN:N	2.36	0.41
1:C:117:ASP:HB3	1:C:138:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:97:MET:HE3	1:D:62:ILE:CD1	2.51	0.40
1:B:155:ASP:O	1:B:156:ILE:C	2.58	0.40
1:B:62:ILE:CG2	1:C:97:MET:HE1	2.49	0.40
1:D:272:PRO:O	1:D:273:GLN:C	2.60	0.40
1:E:58:ALA:HB3	1:E:60:LEU:HG	2.04	0.40
1:H:50:THR:HG21	1:H:68:MET:HE1	2.02	0.40
1:J:143:ARG:O	1:J:147:GLN:HG3	2.22	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:H:229:ALA:HA	1:H:232:MET:CE	2.52	0.40
1:J:218:HIS:N	1:J:218:HIS:ND1	2.70	0.40
1:J:283:GLU:O	1:J:287:VAL:HG23	2.21	0.40
1:J:30:LEU:HA	1:J:30:LEU:HD23	1.85	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%)	38	39
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	25	22
1	I	278/302 (92%)	268 (96%)	10 (4%)	0	100	100
1	J	276/302 (91%)	263 (95%)	12 (4%)	1 (0%)	38	39
1	K	276/302 (91%)	268 (97%)	6 (2%)	2 (1%)	25	22
1	L	286/302 (95%)	276 (96%)	10 (4%)	0	100	100
All	All	3361/3624 (93%)	3246 (97%)	109 (3%)	6 (0%)	51	56

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 ⓘ

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%)	201 (93%)	16 (7%)	16	15
1	B	218/228 (96%)	203 (93%)	15 (7%)	18	17
1	C	216/228 (95%)	198 (92%)	18 (8%)	13	11
1	D	217/228 (95%)	202 (93%)	15 (7%)	18	17
1	E	216/228 (95%)	196 (91%)	20 (9%)	10	9
1	F	217/228 (95%)	200 (92%)	17 (8%)	15	13
1	G	216/228 (95%)	196 (91%)	20 (9%)	10	9
1	H	211/228 (92%)	193 (92%)	18 (8%)	12	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	216/228 (95%)	189 (88%)	27 (12%)	5	4
1	J	209/228 (92%)	181 (87%)	28 (13%)	4	3
1	K	210/228 (92%)	193 (92%)	17 (8%)	14	12
1	L	215/228 (94%)	193 (90%)	22 (10%)	8	7
All	All	2578/2736 (94%)	2345 (91%)	233 (9%)	11	10

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	46	THR
1	A	64	THR
1	A	69	ARG
1	A	74	MET
1	A	95	PRO
1	A	121	THR
1	A	166	GLN
1	A	167	THR
1	A	189	PHE
1	A	190	LEU
1	A	253	GLU
1	A	269	GLU
1	A	274	MET
1	A	283	GLU
1	A	286	LYS
1	B	5	THR
1	B	11	ARG
1	B	36	LEU
1	B	46	THR
1	B	69	ARG
1	B	133	VAL
1	B	143	ARG
1	B	167	THR
1	B	189	PHE
1	B	190	LEU
1	B	246	PRO
1	B	253	GLU
1	B	259	LYS
1	B	268	LYS
1	B	270	MET
1	C	11	ARG

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Mol	Chain	Res	Type
1	C	12	ARG
1	C	30	LEU
1	C	36	LEU
1	C	46	THR
1	C	64	THR
1	C	121	THR
1	C	140	THR
1	C	166	GLN
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	2	PRO
1	D	11	ARG
1	D	36	LEU
1	D	46	THR
1	D	64	THR
1	D	69	ARG
1	D	100	ARG
1	D	115	ILE
1	D	189	PHE
1	D	190	LEU
1	D	202	VAL
1	D	213	LEU
1	D	241	PHE
1	D	268	LYS
1	D	274	MET
1	E	11	ARG
1	E	36	LEU
1	E	54	VAL
1	E	64	THR
1	E	69	ARG
1	E	74	MET
1	E	90	THR
1	E	130	LYS
1	E	132	LEU
1	E	133	VAL

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Mol	Chain	Res	Type
1	E	167	THR
1	E	189	PHE
1	E	190	LEU
1	E	194	THR
1	E	195	SER
1	E	202	VAL
1	E	215	MET
1	E	241	PHE
1	E	267	ASP
1	E	268	LYS
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	69	ARG
1	F	74	MET
1	F	121	THR
1	F	133	VAL
1	F	165	LEU
1	F	167	THR
1	F	189	PHE
1	F	194	THR
1	F	204	GLN
1	F	241	PHE
1	F	274	MET
1	G	2	PRO
1	G	11	ARG
1	G	36	LEU
1	G	46	THR
1	G	50	THR
1	G	54	VAL
1	G	62	ILE
1	G	69	ARG
1	G	74	MET
1	G	100	ARG
1	G	133	VAL
1	G	136	ASP
1	G	140	THR
1	G	167	THR
1	G	189	PHE

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Mol	Chain	Res	Type
1	G	190	LEU
1	G	241	PHE
1	G	260	ARG
1	G	273	GLN
1	G	275	LEU
1	H	5	THR
1	H	11	ARG
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	69	ARG
1	H	74	MET
1	H	132	LEU
1	H	135	THR
1	H	136	ASP
1	H	189	PHE
1	H	190	LEU
1	H	202	VAL
1	H	213	LEU
1	I	4	VAL
1	I	11	ARG
1	I	19	SER
1	I	26	VAL
1	I	36	LEU
1	I	37	SER
1	I	46	THR
1	I	50	THR
1	I	54	VAL
1	I	62	ILE
1	I	69	ARG
1	I	74	MET
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

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Mol	Chain	Res	Type
1	I	190	LEU
1	I	194	THR
1	I	196	ARG
1	I	241	PHE
1	I	252	ARG
1	I	268	LYS
1	I	274	MET
1	I	283	GLU
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	69	ARG
1	J	74	MET
1	J	96	ILE
1	J	100	ARG
1	J	133	VAL
1	J	142	ILE
1	J	167	THR
1	J	168	HIS
1	J	189	PHE
1	J	190	LEU
1	J	194	THR
1	J	206	LEU
1	J	215	MET
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	74	MET

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Mol	Chain	Res	Type
1	K	100	ARG
1	K	132	LEU
1	K	142	ILE
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	285	MET
1	L	26	VAL
1	L	36	LEU
1	L	50	THR
1	L	54	VAL
1	L	69	ARG
1	L	71	ASN
1	L	74	MET
1	L	122	LYS
1	L	123	ARG
1	L	127	LEU
1	L	133	VAL
1	L	134	ASP
1	L	165	LEU
1	L	189	PHE
1	L	190	LEU
1	L	202	VAL
1	L	213	LEU
1	L	215	MET
1	L	221	THR
1	L	241	PHE
1	L	259	LYS
1	L	277	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	G	273	GLN
1	H	118	GLN
1	L	71	ASN

### 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 carbohydrates 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 ⓘ

### 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	284/302 (94%)	-0.32	1 (0%) 92 92	30, 36, 43, 54	0
1	B	288/302 (95%)	-0.29	3 (1%) 82 82	29, 36, 44, 53	0
1	C	284/302 (94%)	-0.29	3 (1%) 80 81	30, 36, 43, 50	0
1	D	284/302 (94%)	-0.32	2 (0%) 87 87	31, 36, 43, 50	0
1	E	286/302 (94%)	-0.26	1 (0%) 93 93	31, 36, 43, 52	0
1	F	285/302 (94%)	-0.30	1 (0%) 92 92	28, 36, 44, 52	0
1	G	284/302 (94%)	-0.34	0 100 100	27, 36, 43, 49	0
1	H	282/302 (93%)	-0.32	0 100 100	29, 36, 43, 48	0
1	I	282/302 (93%)	-0.15	3 (1%) 80 81	30, 37, 43, 49	0
1	J	280/302 (92%)	-0.21	1 (0%) 92 92	29, 36, 42, 49	0
1	K	280/302 (92%)	-0.24	1 (0%) 92 92	31, 36, 42, 46	0
1	L	288/302 (95%)	-0.19	2 (0%) 87 87	30, 36, 43, 52	0
All	All	3407/3624 (94%)	-0.27	18 (0%) 90 90	27, 36, 43, 54	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	4	VAL	5.3
1	L	129	GLY	4.9
1	E	129	GLY	4.6
1	C	123	ARG	3.3
1	I	4	VAL	3.2
1	I	292	GLY	2.7
1	D	273	GLN	2.6
1	B	293	GLY	2.5
1	C	121	THR	2.4
1	F	2	PRO	2.4
1	B	121	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	121	THR	2.3
1	L	292	GLY	2.2
1	B	294	ALA	2.2
1	J	4	VAL	2.2
1	A	292	GLY	2.1
1	C	241	PHE	2.1
1	I	277	ARG	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	MG	K	401	1/1	0.97	0.10	0.98	46,46,46,46	0
2	MG	H	401	1/1	0.98	0.10	-0.17	43,43,43,43	0
2	MG	E	401	1/1	0.96	0.07	-0.92	40,40,40,40	0
2	MG	C	401	1/1	0.97	0.06	-2.32	46,46,46,46	0
2	MG	G	401	1/1	0.99	0.05	-2.82	37,37,37,37	0
2	MG	F	401	1/1	0.91	0.07	-3.99	44,44,44,44	0
2	MG	L	401	1/1	0.86	0.08	-	48,48,48,48	0
2	MG	I	401	1/1	0.96	0.07	-	42,42,42,42	0
2	MG	B	401	1/1	0.93	0.06	-	35,35,35,35	0
2	MG	D	401	1/1	0.88	0.07	-	40,40,40,40	0
2	MG	A	401	1/1	0.91	0.07	-	51,51,51,51	0
2	MG	J	401	1/1	0.87	0.07	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.