Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:35 pm BST

PDB ID	:	2IIR
Title	:	Acetate kinase from a hypothermophile Thermotoga maritima
Authors	:	Mukhopadhyay, S.; Hasson, M.S.; Sanders, D.A.
Deposited on	:	2006-09-28
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

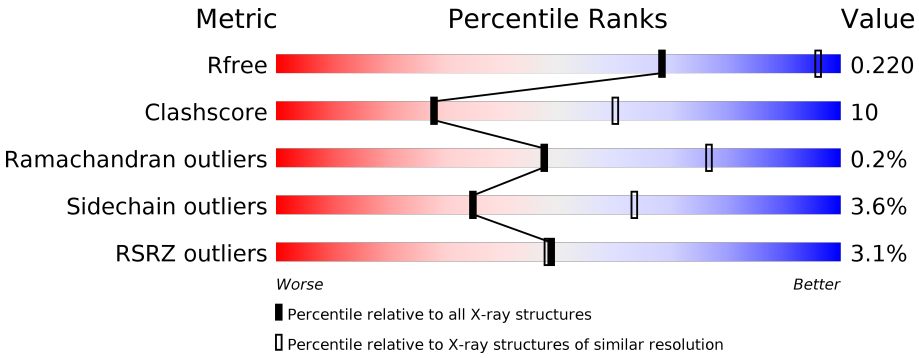
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	403	4% 79% 18%
1	B	403	6% 80% 17%
1	C	403	2% 81% 16%
1	D	403	81% 16%
1	E	403	2% 79% 19%
1	F	403	% 81% 16%

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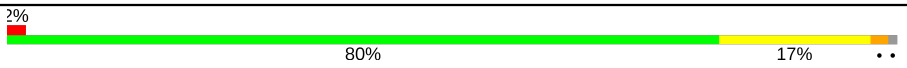
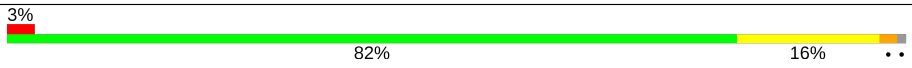
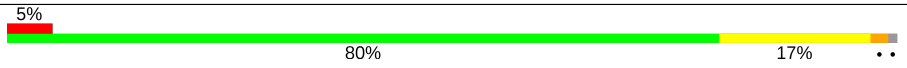
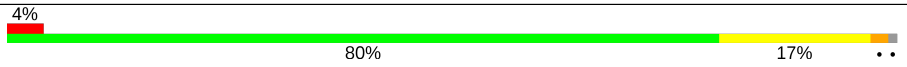
Mol	Chain	Length	Quality of chain
1	G	403	
1	H	403	
1	I	403	
1	J	403	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31280 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 Acetate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	B	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	C	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	D	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	E	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	F	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	G	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	H	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	I	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			
1	J	400	Total	C	N	O	S	0	0	0
			3123	1991	526	590	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	4	Total	O	0	0
			4	4		
2	C	7	Total	O	0	0
			7	7		
2	D	4	Total	O	0	0
			4	4		

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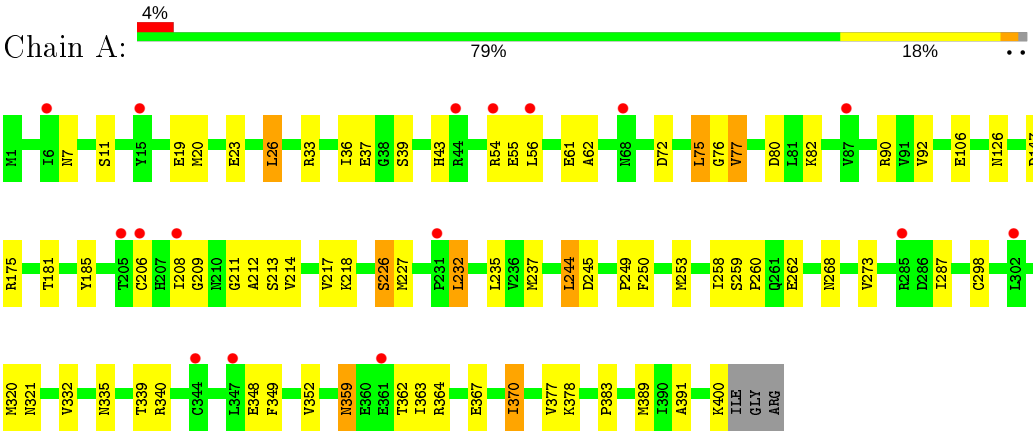
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	4	Total O 4 4	0	0
2	F	5	Total O 5 5	0	0
2	G	4	Total O 4 4	0	0
2	H	9	Total O 9 9	0	0
2	I	5	Total O 5 5	0	0
2	J	5	Total O 5 5	0	0

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.

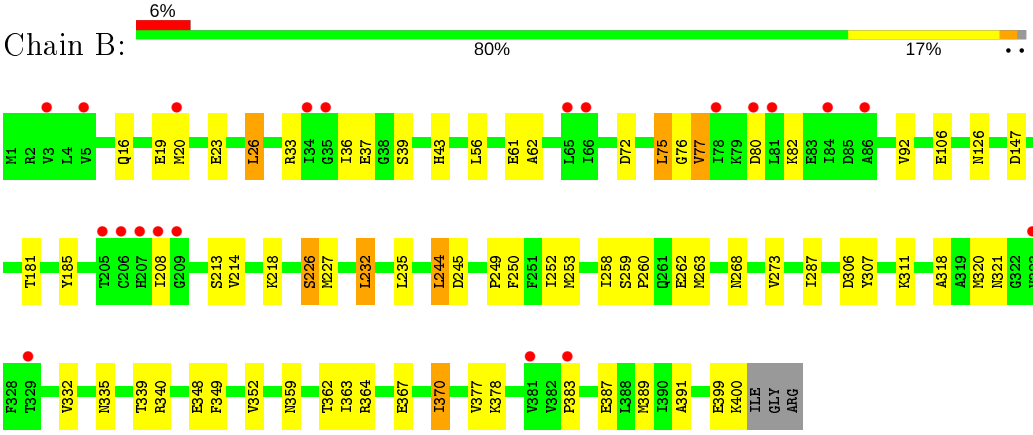
- Molecule 1: Acetate kinase

Chain A:



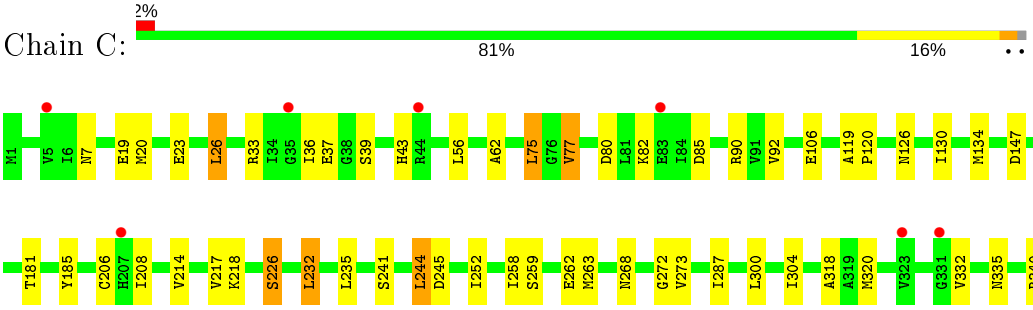
- Molecule 1: Acetate kinase

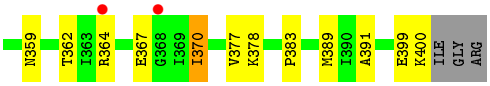
Chain B:



- Molecule 1: Acetate kinase

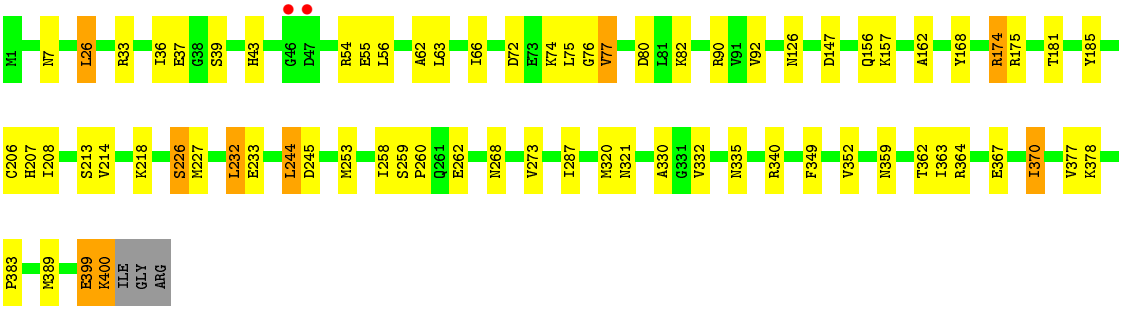
Chain C:





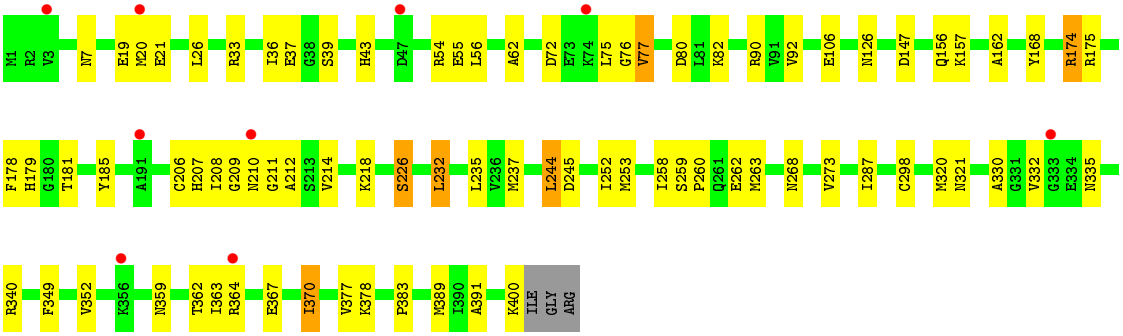
• Molecule 1: Acetate kinase

Chain D:



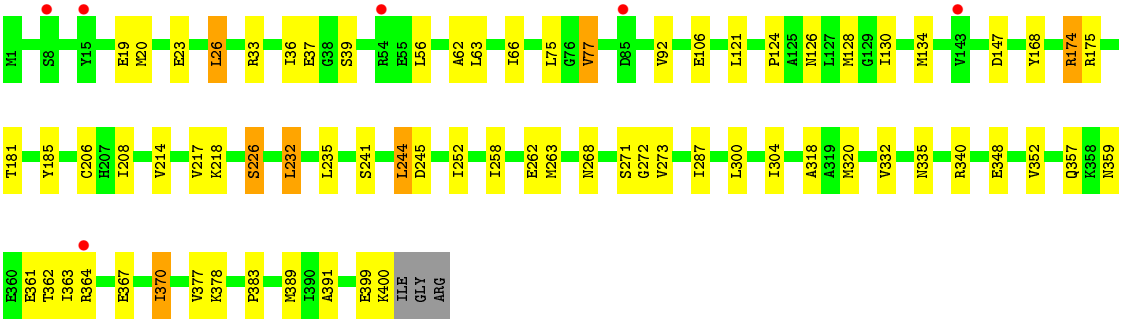
• Molecule 1: Acetate kinase

Chain E:



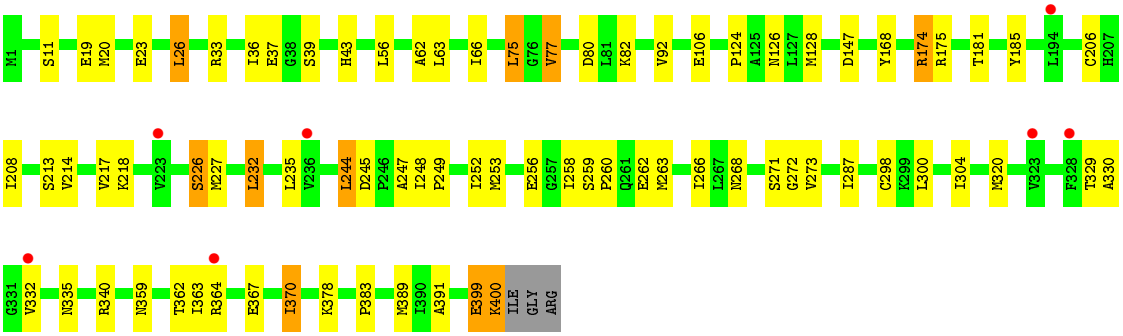
• Molecule 1: Acetate kinase

Chain F:



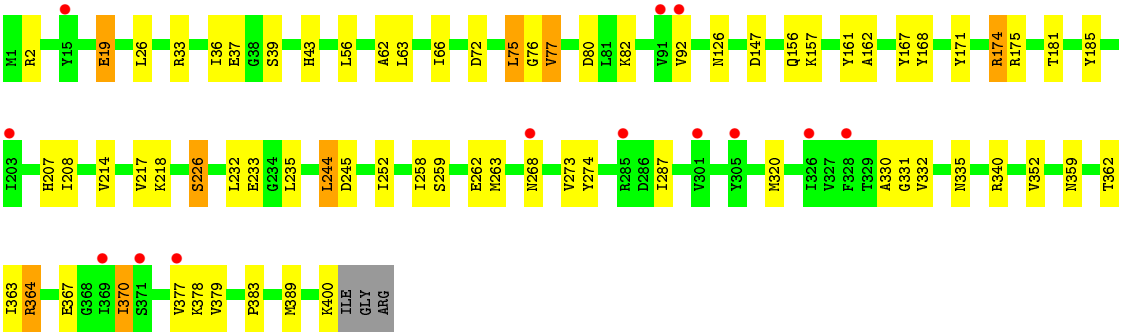
• Molecule 1: Acetate kinase

Chain G:



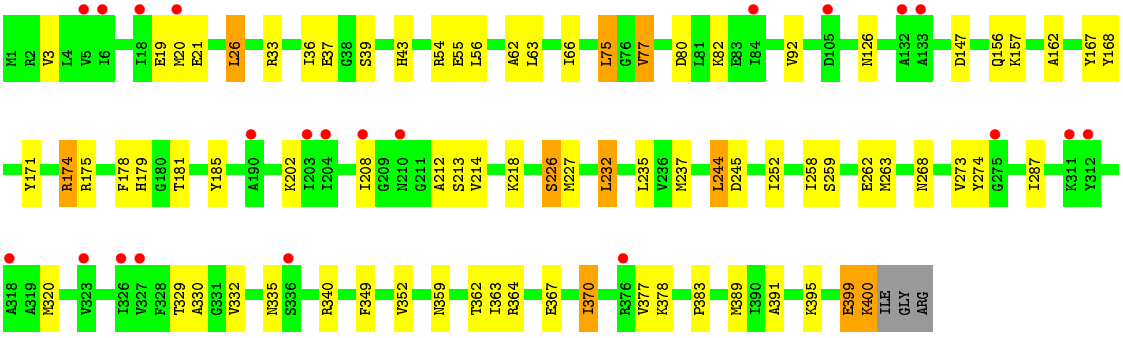
- Molecule 1: Acetate kinase

Chain H:



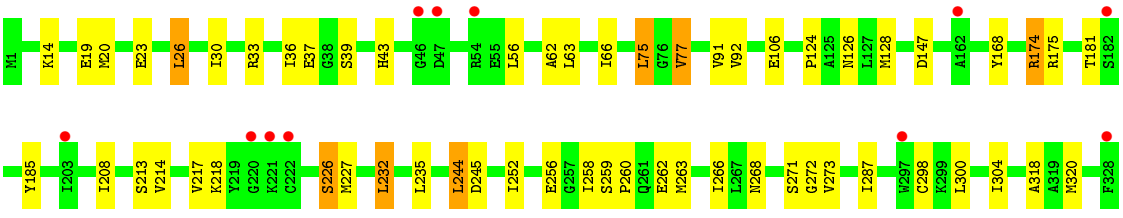
- Molecule 1: Acetate kinase

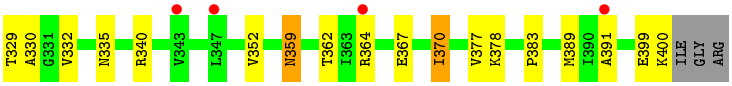
Chain I:



- Molecule 1: Acetate kinase

Chain J:




T329
A330
G331
V332
N335
R340
V343
L347
V352
N359
T362
I363
R364
E367
I370
V377
K378
P383
M389
I390
A391
E399
K400
ILE
GLY
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	105.43Å 300.33Å 334.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 95.36 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-3.30) 98.0 (95.36-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.94 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.253 0.221 , 0.220	Depositor DCC
R_{free} test set	3967 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 87.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31280	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1405e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	0/3176	0.62	0/4279
1	B	0.45	0/3176	0.61	0/4279
1	C	0.50	0/3176	0.62	0/4279
1	D	0.51	0/3176	0.62	0/4279
1	E	0.52	0/3176	0.64	0/4279
1	F	0.49	0/3176	0.62	0/4279
1	G	0.49	0/3176	0.63	0/4279
1	H	0.48	0/3176	0.62	0/4279
1	I	0.47	0/3176	0.63	0/4279
1	J	0.50	0/3176	0.62	0/4279
All	All	0.49	0/31760	0.62	0/42790

There are no bond length outliers.

There are no bond angle outliers.

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	3123	0	3194	70	0
1	B	3123	0	3194	75	0
1	C	3123	0	3194	63	0
1	D	3123	0	3194	68	1
1	E	3123	0	3194	69	1
1	F	3123	0	3194	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3123	0	3194	69	0
1	H	3123	0	3194	67	0
1	I	3123	0	3194	65	0
1	J	3123	0	3194	64	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	7	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	5	0	0	0	0
2	G	4	0	0	0	0
2	H	9	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
All	All	31280	0	31940	622	1

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 10.

All (622) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:MET:HE3	1:C:391:ALA:HB1	1.34	1.10
1:F:20:MET:HE3	1:F:391:ALA:HB1	1.38	1.04
1:D:74:LYS:NZ	1:D:75:LEU:HD21	1.72	1.03
1:D:74:LYS:HZ1	1:D:75:LEU:HD21	1.22	1.02
1:F:361:GLU:OE1	1:H:364:ARG:HD3	1.61	1.01
1:D:174:ARG:HG3	1:D:174:ARG:HH11	1.23	1.01
1:H:174:ARG:HH11	1:H:174:ARG:HG3	1.25	1.00
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.28	0.99
1:B:20:MET:HE3	1:B:391:ALA:HB1	1.42	0.98
1:E:174:ARG:HG3	1:E:174:ARG:HH11	1.24	0.98
1:C:174:ARG:HH11	1:C:174:ARG:HG3	1.27	0.98
1:H:2:ARG:HG3	1:H:19:GLU:OE2	1.65	0.97
1:A:174:ARG:HH11	1:A:174:ARG:HG3	1.27	0.97
1:B:16:GLN:HE21	1:B:387:GLU:HG2	1.30	0.97
1:G:174:ARG:HH11	1:G:174:ARG:HG3	1.29	0.96
1:A:20:MET:HE3	1:A:391:ALA:HB1	1.49	0.95
1:F:20:MET:CE	1:F:391:ALA:HB1	1.96	0.95
1:G:247:ALA:HB2	1:H:232:LEU:HD22	1.49	0.94
1:I:174:ARG:HG3	1:I:174:ARG:HH11	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:MET:CE	1:C:391:ALA:HB1	1.99	0.93
1:F:244:LEU:O	1:F:244:LEU:HD12	1.68	0.93
1:J:174:ARG:HH11	1:J:174:ARG:HG3	1.31	0.93
1:F:174:ARG:HH11	1:F:174:ARG:HG3	1.32	0.92
1:E:20:MET:HE3	1:E:391:ALA:HB1	1.52	0.92
1:I:20:MET:HA	1:I:20:MET:HE3	1.52	0.91
1:J:244:LEU:HD12	1:J:244:LEU:O	1.71	0.90
1:J:20:MET:CE	1:J:391:ALA:HB1	2.00	0.90
1:E:20:MET:CE	1:E:391:ALA:HB1	2.00	0.90
1:J:20:MET:HE3	1:J:391:ALA:HB1	1.50	0.90
1:I:19:GLU:OE1	1:I:21:GLU:HB2	1.72	0.89
1:G:244:LEU:HD12	1:G:244:LEU:O	1.73	0.89
1:B:244:LEU:HD12	1:B:244:LEU:O	1.74	0.88
1:G:20:MET:CE	1:G:391:ALA:HB1	2.03	0.88
1:B:16:GLN:NE2	1:B:387:GLU:HG2	1.87	0.88
1:F:361:GLU:OE1	1:H:364:ARG:CD	2.22	0.88
1:D:244:LEU:HD12	1:D:244:LEU:O	1.74	0.88
1:E:244:LEU:O	1:E:244:LEU:HD12	1.75	0.87
1:A:244:LEU:HD12	1:A:244:LEU:O	1.75	0.87
1:I:20:MET:HA	1:I:20:MET:CE	2.05	0.87
1:H:244:LEU:O	1:H:244:LEU:HD12	1.74	0.86
1:C:244:LEU:O	1:C:244:LEU:HD12	1.75	0.86
1:A:20:MET:CE	1:A:391:ALA:HB1	2.06	0.86
1:G:20:MET:HE3	1:G:391:ALA:HB1	1.55	0.85
1:B:20:MET:CE	1:B:391:ALA:HB1	2.06	0.84
1:F:357:GLN:NE2	1:H:364:ARG:NH2	2.24	0.84
1:I:244:LEU:O	1:I:244:LEU:HD12	1.77	0.83
1:F:174:ARG:NH1	1:F:175:ARG:O	2.11	0.83
1:D:174:ARG:HG3	1:D:174:ARG:NH1	1.94	0.81
1:A:174:ARG:NH1	1:A:175:ARG:O	2.15	0.80
1:E:174:ARG:NH1	1:E:175:ARG:O	2.15	0.79
1:B:16:GLN:NE2	1:B:387:GLU:CG	2.46	0.79
1:J:364:ARG:O	1:J:364:ARG:HG2	1.82	0.79
1:E:363:ILE:HG12	1:E:364:ARG:HG3	1.65	0.79
1:C:174:ARG:NH1	1:C:175:ARG:O	2.15	0.78
1:H:174:ARG:HG3	1:H:174:ARG:NH1	1.97	0.78
1:H:174:ARG:NH1	1:H:175:ARG:O	2.17	0.78
1:J:174:ARG:NH1	1:J:175:ARG:O	2.15	0.77
1:D:174:ARG:NH1	1:D:175:ARG:O	2.18	0.77
1:E:174:ARG:NH1	1:E:174:ARG:HG3	1.96	0.77
1:I:174:ARG:NH1	1:I:174:ARG:HG3	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:ARG:NH1	1:I:175:ARG:O	2.18	0.76
1:B:174:ARG:NH1	1:B:175:ARG:O	2.18	0.76
1:H:258:ILE:HG23	1:H:262:GLU:HB2	1.67	0.75
1:F:244:LEU:C	1:F:244:LEU:HD12	2.07	0.75
1:A:363:ILE:HG12	1:A:364:ARG:HG3	1.68	0.75
1:G:363:ILE:HG12	1:G:364:ARG:HG3	1.68	0.74
1:G:174:ARG:NH1	1:G:174:ARG:HG3	1.99	0.74
1:A:244:LEU:C	1:A:244:LEU:HD12	2.08	0.74
1:I:258:ILE:HG23	1:I:262:GLU:HB2	1.70	0.74
1:B:244:LEU:C	1:B:244:LEU:HD12	2.08	0.74
1:D:74:LYS:NZ	1:D:75:LEU:CD2	2.48	0.73
1:G:244:LEU:HD12	1:G:244:LEU:C	2.09	0.73
1:H:244:LEU:HD12	1:H:244:LEU:C	2.08	0.73
1:H:363:ILE:HG12	1:H:364:ARG:HG2	1.69	0.73
1:E:244:LEU:C	1:E:244:LEU:HD12	2.08	0.73
1:C:244:LEU:C	1:C:244:LEU:HD12	2.09	0.73
1:D:244:LEU:HD12	1:D:244:LEU:C	2.08	0.73
1:F:19:GLU:O	1:F:23:GLU:N	2.22	0.73
1:C:19:GLU:O	1:C:23:GLU:N	2.22	0.73
1:I:244:LEU:HD12	1:I:244:LEU:C	2.08	0.72
1:B:16:GLN:HE21	1:B:387:GLU:CG	2.01	0.72
1:B:174:ARG:HG3	1:B:174:ARG:NH1	2.02	0.72
1:F:258:ILE:HG23	1:F:262:GLU:HB2	1.72	0.72
1:G:19:GLU:O	1:G:23:GLU:N	2.22	0.72
1:J:258:ILE:HG23	1:J:262:GLU:HB2	1.72	0.72
1:A:321:ASN:HD21	1:B:348:GLU:HG2	1.54	0.72
1:B:19:GLU:O	1:B:23:GLU:N	2.23	0.71
1:F:357:GLN:NE2	1:H:364:ARG:HH22	1.85	0.71
1:H:2:ARG:CG	1:H:19:GLU:OE2	2.36	0.71
1:J:244:LEU:HD12	1:J:244:LEU:C	2.09	0.71
1:G:174:ARG:NH1	1:G:175:ARG:O	2.23	0.71
1:A:19:GLU:O	1:A:23:GLU:N	2.23	0.71
1:B:258:ILE:HG23	1:B:262:GLU:HB2	1.73	0.71
1:F:33:ARG:O	1:F:39:SER:HB3	1.91	0.70
1:A:174:ARG:HG3	1:A:174:ARG:NH1	2.00	0.70
1:C:258:ILE:HG23	1:C:262:GLU:HB2	1.73	0.70
1:G:258:ILE:HG23	1:G:262:GLU:HB2	1.72	0.70
1:A:258:ILE:HG23	1:A:262:GLU:HB2	1.72	0.70
1:E:367:GLU:HB2	1:E:383:PRO:HD2	1.73	0.69
1:I:33:ARG:O	1:I:39:SER:HB3	1.91	0.69
1:D:33:ARG:O	1:D:39:SER:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:GLU:HB2	1:G:383:PRO:HD2	1.74	0.69
1:H:33:ARG:O	1:H:39:SER:HB3	1.92	0.69
1:C:367:GLU:HB2	1:C:383:PRO:HD2	1.75	0.69
1:J:19:GLU:O	1:J:23:GLU:N	2.26	0.68
1:E:33:ARG:O	1:E:39:SER:HB3	1.93	0.68
1:G:340:ARG:HE	1:G:359:ASN:HD21	1.42	0.68
1:H:340:ARG:HE	1:H:359:ASN:HD21	1.41	0.68
1:C:33:ARG:O	1:C:39:SER:HB3	1.95	0.67
1:C:174:ARG:NH1	1:C:174:ARG:HG3	2.00	0.67
1:F:367:GLU:HB2	1:F:383:PRO:HD2	1.76	0.67
1:F:357:GLN:HE22	1:H:364:ARG:HH22	1.40	0.67
1:A:321:ASN:HD21	1:B:348:GLU:CG	2.08	0.66
1:F:174:ARG:NH1	1:F:174:ARG:HG3	2.05	0.66
1:A:348:GLU:HG2	1:B:321:ASN:HD21	1.60	0.66
1:D:258:ILE:HG23	1:D:262:GLU:HB2	1.77	0.66
1:B:33:ARG:O	1:B:39:SER:HB3	1.95	0.66
1:J:33:ARG:O	1:J:39:SER:HB3	1.96	0.66
1:D:340:ARG:HE	1:D:359:ASN:HD21	1.44	0.66
1:J:367:GLU:HB2	1:J:383:PRO:HD2	1.78	0.65
1:E:218:LYS:HB2	1:E:320:MET:HG2	1.78	0.65
1:G:218:LYS:HB2	1:G:320:MET:HG2	1.78	0.65
1:H:218:LYS:HB2	1:H:320:MET:HG2	1.79	0.65
1:H:367:GLU:HB2	1:H:383:PRO:HD2	1.79	0.65
1:I:162:ALA:HB1	1:J:272:GLY:HA2	1.79	0.65
1:D:174:ARG:CG	1:D:174:ARG:HH11	2.06	0.65
1:B:363:ILE:HG12	1:B:364:ARG:HG3	1.79	0.64
1:J:218:LYS:HB2	1:J:320:MET:HG2	1.79	0.64
1:A:33:ARG:O	1:A:39:SER:HB3	1.96	0.64
1:E:258:ILE:HG23	1:E:262:GLU:HB2	1.79	0.64
1:J:92:VAL:H	1:J:126:ASN:ND2	1.95	0.64
1:B:92:VAL:H	1:B:126:ASN:ND2	1.96	0.64
1:E:340:ARG:HE	1:E:359:ASN:HD21	1.46	0.64
1:A:218:LYS:HB2	1:A:320:MET:HG2	1.80	0.64
1:F:244:LEU:CD1	1:F:244:LEU:C	2.66	0.64
1:E:157:LYS:HA	1:F:304:ILE:HG13	1.78	0.63
1:B:218:LYS:HB2	1:B:320:MET:HG2	1.79	0.63
1:D:367:GLU:HB2	1:D:383:PRO:HD2	1.80	0.63
1:D:218:LYS:HB2	1:D:320:MET:HG2	1.78	0.63
1:D:74:LYS:HZ2	1:D:75:LEU:CD2	2.10	0.63
1:B:340:ARG:HE	1:B:359:ASN:HD21	1.47	0.63
1:D:92:VAL:H	1:D:126:ASN:ND2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:340:ARG:HE	1:I:359:ASN:HD21	1.45	0.63
1:I:367:GLU:HB2	1:I:383:PRO:HD2	1.81	0.62
1:C:340:ARG:HE	1:C:359:ASN:HD21	1.46	0.62
1:A:92:VAL:H	1:A:126:ASN:ND2	1.96	0.62
1:I:359:ASN:HA	1:I:370:ILE:HG21	1.81	0.62
1:J:174:ARG:NH1	1:J:174:ARG:HG3	2.02	0.62
1:I:157:LYS:HA	1:J:304:ILE:HG13	1.80	0.62
1:B:367:GLU:HB2	1:B:383:PRO:HD2	1.82	0.62
1:I:258:ILE:CG2	1:I:262:GLU:HB2	2.29	0.62
1:J:340:ARG:HE	1:J:359:ASN:HD21	1.46	0.62
1:I:157:LYS:HA	1:J:304:ILE:CG1	2.30	0.62
1:D:244:LEU:CD1	1:D:244:LEU:C	2.69	0.62
1:I:218:LYS:HB2	1:I:320:MET:HG2	1.81	0.61
1:C:244:LEU:C	1:C:244:LEU:CD1	2.69	0.61
1:G:244:LEU:CD1	1:G:244:LEU:C	2.69	0.61
1:J:244:LEU:C	1:J:244:LEU:CD1	2.69	0.61
1:B:244:LEU:C	1:B:244:LEU:CD1	2.69	0.61
1:C:218:LYS:HB2	1:C:320:MET:HG2	1.81	0.61
1:E:244:LEU:CD1	1:E:244:LEU:C	2.69	0.61
1:G:304:ILE:HG13	1:H:157:LYS:HA	1.82	0.61
1:A:340:ARG:HE	1:A:359:ASN:HD21	1.48	0.61
1:B:252:ILE:HG22	1:B:263:MET:HE1	1.82	0.61
1:H:244:LEU:C	1:H:244:LEU:CD1	2.69	0.61
1:I:244:LEU:CD1	1:I:244:LEU:C	2.69	0.61
1:J:258:ILE:CG2	1:J:262:GLU:HB2	2.31	0.61
1:J:92:VAL:H	1:J:126:ASN:HD21	1.49	0.61
1:C:185:TYR:HA	1:C:389:MET:CE	2.31	0.61
1:F:218:LYS:HB2	1:F:320:MET:HG2	1.83	0.61
1:A:244:LEU:C	1:A:244:LEU:CD1	2.69	0.60
1:E:92:VAL:H	1:E:126:ASN:ND2	1.99	0.60
1:F:340:ARG:HE	1:F:359:ASN:HD21	1.48	0.60
1:G:92:VAL:H	1:G:126:ASN:ND2	2.00	0.60
1:A:348:GLU:CG	1:B:321:ASN:HD21	2.14	0.60
1:G:359:ASN:HA	1:G:370:ILE:HG21	1.83	0.60
1:G:272:GLY:HA2	1:H:162:ALA:HB1	1.83	0.60
1:H:258:ILE:CG2	1:H:262:GLU:HB2	2.31	0.59
1:J:359:ASN:HA	1:J:370:ILE:HG21	1.84	0.59
1:F:36:ILE:HG22	1:F:37:GLU:N	2.17	0.59
1:G:174:ARG:HH11	1:G:174:ARG:CG	2.09	0.59
1:A:367:GLU:HB2	1:A:383:PRO:HD2	1.83	0.59
1:C:258:ILE:CG2	1:C:262:GLU:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:GLU:OE1	1:E:21:GLU:HB2	2.03	0.58
1:D:92:VAL:O	1:D:147:ASP:HB2	2.03	0.58
1:C:244:LEU:HD13	1:C:245:ASP:O	2.04	0.58
1:G:258:ILE:CG2	1:G:262:GLU:HB2	2.33	0.58
1:F:121:LEU:HD12	1:F:121:LEU:N	2.18	0.58
1:I:232:LEU:HD11	1:I:268:ASN:ND2	2.18	0.58
1:C:304:ILE:HG13	1:D:157:LYS:HA	1.86	0.58
1:F:92:VAL:O	1:F:147:ASP:HB2	2.04	0.58
1:C:92:VAL:O	1:C:147:ASP:HB2	2.03	0.58
1:G:304:ILE:CG1	1:H:157:LYS:HA	2.34	0.58
1:G:33:ARG:O	1:G:39:SER:HB3	2.04	0.58
1:H:359:ASN:HA	1:H:370:ILE:HG21	1.85	0.57
1:H:92:VAL:H	1:H:126:ASN:ND2	2.01	0.57
1:B:252:ILE:HB	1:B:263:MET:CE	2.34	0.57
1:E:214:VAL:H	1:E:226:SER:HB3	1.70	0.57
1:G:232:LEU:HD11	1:G:268:ASN:ND2	2.19	0.57
1:B:252:ILE:HB	1:B:263:MET:HE3	1.87	0.57
1:B:253:MET:HG3	1:B:263:MET:HE2	1.87	0.57
1:J:214:VAL:H	1:J:226:SER:HB3	1.69	0.57
1:D:214:VAL:H	1:D:226:SER:HB3	1.69	0.57
1:B:214:VAL:H	1:B:226:SER:HB3	1.70	0.57
1:F:36:ILE:HG22	1:F:37:GLU:H	1.69	0.57
1:I:92:VAL:H	1:I:126:ASN:ND2	2.03	0.57
1:C:36:ILE:HG22	1:C:37:GLU:N	2.20	0.56
1:G:36:ILE:HG22	1:G:37:GLU:N	2.20	0.56
1:J:92:VAL:O	1:J:147:ASP:HB2	2.05	0.56
1:A:92:VAL:O	1:A:147:ASP:HB2	2.05	0.56
1:A:359:ASN:HA	1:A:370:ILE:HG21	1.85	0.56
1:B:92:VAL:O	1:B:147:ASP:HB2	2.05	0.56
1:C:359:ASN:HA	1:C:370:ILE:HG21	1.87	0.56
1:A:258:ILE:CG2	1:A:262:GLU:HB2	2.36	0.56
1:G:92:VAL:O	1:G:147:ASP:HB2	2.04	0.56
1:G:214:VAL:H	1:G:226:SER:HB3	1.71	0.56
1:I:258:ILE:HG23	1:I:262:GLU:CB	2.35	0.56
1:E:321:ASN:HD21	1:F:348:GLU:HG2	1.71	0.56
1:D:258:ILE:CG2	1:D:262:GLU:HB2	2.36	0.56
1:A:349:PHE:HB3	1:B:321:ASN:O	2.06	0.56
1:C:367:GLU:CB	1:C:383:PRO:HD2	2.35	0.56
1:D:363:ILE:HG12	1:D:364:ARG:N	2.21	0.56
1:E:209:GLY:C	1:E:211:GLY:N	2.59	0.56
1:E:92:VAL:O	1:E:147:ASP:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:GLU:CB	1:F:383:PRO:HD2	2.37	0.55
1:I:214:VAL:H	1:I:226:SER:HB3	1.72	0.55
1:A:214:VAL:H	1:A:226:SER:HB3	1.71	0.55
1:B:359:ASN:HA	1:B:370:ILE:HG21	1.87	0.55
1:C:174:ARG:HH11	1:C:174:ARG:CG	2.11	0.55
1:C:214:VAL:H	1:C:226:SER:HB3	1.71	0.55
1:F:214:VAL:H	1:F:226:SER:HB3	1.70	0.55
1:D:185:TYR:HA	1:D:389:MET:CE	2.37	0.55
1:F:359:ASN:HA	1:F:370:ILE:HG21	1.88	0.55
1:G:256:GLU:HG2	1:H:171:TYR:OH	2.07	0.55
1:H:258:ILE:HG23	1:H:262:GLU:CB	2.36	0.55
1:B:258:ILE:CG2	1:B:262:GLU:HB2	2.37	0.55
1:E:335:ASN:OD1	1:E:364:ARG:HA	2.07	0.55
1:E:359:ASN:HA	1:E:370:ILE:HG21	1.88	0.55
1:E:174:ARG:CG	1:E:174:ARG:HH11	2.07	0.55
1:E:232:LEU:HD11	1:E:268:ASN:ND2	2.21	0.55
1:F:185:TYR:HA	1:F:389:MET:CE	2.36	0.55
1:D:359:ASN:HA	1:D:370:ILE:HG21	1.89	0.55
1:J:367:GLU:CB	1:J:383:PRO:HD2	2.37	0.55
1:B:253:MET:HG3	1:B:263:MET:CE	2.36	0.55
1:C:92:VAL:H	1:C:126:ASN:ND2	2.05	0.55
1:H:92:VAL:O	1:H:147:ASP:HB2	2.07	0.55
1:D:363:ILE:HG12	1:D:364:ARG:HG3	1.90	0.54
1:I:185:TYR:HA	1:I:389:MET:CE	2.37	0.54
1:G:92:VAL:H	1:G:126:ASN:HD21	1.55	0.54
1:I:359:ASN:HA	1:I:370:ILE:CG2	2.37	0.54
1:I:3:VAL:HG23	1:I:20:MET:HG2	1.89	0.54
1:A:321:ASN:O	1:B:349:PHE:HB3	2.07	0.54
1:E:185:TYR:HA	1:E:389:MET:CE	2.38	0.54
1:J:258:ILE:HG23	1:J:262:GLU:CB	2.38	0.54
1:A:92:VAL:H	1:A:126:ASN:HD21	1.55	0.54
1:B:232:LEU:HD11	1:B:268:ASN:ND2	2.22	0.54
1:D:335:ASN:OD1	1:D:364:ARG:HA	2.08	0.54
1:F:258:ILE:CG2	1:F:262:GLU:HB2	2.37	0.54
1:H:340:ARG:HE	1:H:359:ASN:ND2	2.06	0.54
1:J:232:LEU:HD11	1:J:268:ASN:ND2	2.23	0.53
1:D:359:ASN:HA	1:D:370:ILE:CG2	2.39	0.53
1:F:244:LEU:HD13	1:F:245:ASP:O	2.08	0.53
1:C:340:ARG:HE	1:C:359:ASN:ND2	2.06	0.53
1:G:252:ILE:CG2	1:G:263:MET:HE1	2.38	0.53
1:H:185:TYR:HA	1:H:389:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:ARG:CG	1:I:174:ARG:HH11	2.09	0.53
1:I:33:ARG:HB2	1:I:39:SER:HA	1.91	0.53
1:E:162:ALA:HB1	1:F:272:GLY:HA2	1.90	0.53
1:E:258:ILE:CG2	1:E:262:GLU:HB2	2.37	0.53
1:I:92:VAL:O	1:I:147:ASP:HB2	2.09	0.53
1:J:259:SER:HB2	1:J:260:PRO:HD2	1.91	0.53
1:B:92:VAL:H	1:B:126:ASN:HD21	1.55	0.52
1:D:92:VAL:H	1:D:126:ASN:HD21	1.55	0.52
1:F:20:MET:O	1:F:23:GLU:HG3	2.09	0.52
1:F:33:ARG:HB2	1:F:39:SER:HA	1.91	0.52
1:A:206:CYS:HB3	1:A:208:ILE:CD1	2.40	0.52
1:B:252:ILE:CG2	1:B:263:MET:HE1	2.39	0.52
1:F:363:ILE:HG12	1:F:364:ARG:HG3	1.91	0.52
1:J:36:ILE:HG22	1:J:37:GLU:N	2.23	0.52
1:J:33:ARG:HB2	1:J:39:SER:HA	1.92	0.52
1:E:359:ASN:HA	1:E:370:ILE:CG2	2.39	0.52
1:F:92:VAL:H	1:F:126:ASN:ND2	2.07	0.52
1:H:367:GLU:CB	1:H:383:PRO:HD2	2.39	0.52
1:J:340:ARG:HE	1:J:359:ASN:ND2	2.08	0.52
1:A:321:ASN:ND2	1:B:348:GLU:HG2	2.24	0.52
1:H:92:VAL:H	1:H:126:ASN:HD21	1.58	0.52
1:C:232:LEU:HD11	1:C:268:ASN:ND2	2.25	0.52
1:E:206:CYS:HB3	1:E:208:ILE:CD1	2.40	0.52
1:E:209:GLY:O	1:E:211:GLY:N	2.43	0.52
1:E:92:VAL:H	1:E:126:ASN:HD21	1.56	0.52
1:E:157:LYS:HA	1:F:304:ILE:CG1	2.38	0.52
1:I:20:MET:SD	1:I:391:ALA:HB1	2.50	0.52
1:F:340:ARG:HE	1:F:359:ASN:ND2	2.08	0.52
1:G:367:GLU:CB	1:G:383:PRO:HD2	2.39	0.52
1:H:363:ILE:HG12	1:H:364:ARG:CG	2.39	0.52
1:B:253:MET:CG	1:B:263:MET:HE2	2.39	0.51
1:G:359:ASN:HA	1:G:370:ILE:CG2	2.40	0.51
1:I:36:ILE:HG22	1:I:37:GLU:N	2.25	0.51
1:J:208:ILE:HG22	1:J:332:VAL:HB	1.91	0.51
1:C:36:ILE:HG22	1:C:37:GLU:H	1.74	0.51
1:I:208:ILE:HG22	1:I:332:VAL:HB	1.93	0.51
1:A:185:TYR:HA	1:A:389:MET:CE	2.41	0.51
1:C:258:ILE:HG23	1:C:262:GLU:CB	2.40	0.51
1:D:363:ILE:CG1	1:D:364:ARG:N	2.74	0.51
1:G:36:ILE:HG22	1:G:37:GLU:H	1.75	0.51
1:G:258:ILE:HG23	1:G:262:GLU:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:340:ARG:HE	1:I:359:ASN:ND2	2.09	0.51
1:A:232:LEU:HD11	1:A:268:ASN:ND2	2.26	0.51
1:G:20:MET:CE	1:G:391:ALA:CB	2.85	0.51
1:B:340:ARG:HE	1:B:359:ASN:ND2	2.08	0.51
1:B:185:TYR:HA	1:B:389:MET:CE	2.41	0.51
1:H:208:ILE:HG22	1:H:332:VAL:HB	1.93	0.51
1:H:359:ASN:HA	1:H:370:ILE:CG2	2.41	0.51
1:E:33:ARG:HB2	1:E:39:SER:HA	1.93	0.51
1:G:340:ARG:HE	1:G:359:ASN:ND2	2.07	0.51
1:H:33:ARG:HB2	1:H:39:SER:HA	1.93	0.51
1:H:80:ASP:HB3	1:H:82:LYS:H	1.76	0.51
1:A:273:VAL:HG13	1:A:287:ILE:CD1	2.42	0.50
1:B:36:ILE:HG22	1:B:37:GLU:N	2.26	0.50
1:A:33:ARG:HB2	1:A:39:SER:HA	1.94	0.50
1:G:244:LEU:HD13	1:G:245:ASP:O	2.11	0.50
1:B:367:GLU:CB	1:B:383:PRO:HD2	2.41	0.50
1:E:212:ALA:H	1:E:237:MET:HG2	1.76	0.50
1:A:212:ALA:H	1:A:237:MET:HG2	1.75	0.50
1:B:56:LEU:HD22	1:B:62:ALA:HA	1.93	0.50
1:B:258:ILE:HG23	1:B:262:GLU:CB	2.41	0.50
1:F:56:LEU:HD22	1:F:62:ALA:HA	1.93	0.50
1:G:259:SER:HB2	1:G:260:PRO:HD2	1.94	0.50
1:C:272:GLY:HA2	1:D:162:ALA:HB1	1.93	0.50
1:A:208:ILE:HG22	1:A:332:VAL:HB	1.94	0.50
1:H:244:LEU:HD13	1:H:245:ASP:O	2.11	0.50
1:H:259:SER:OG	1:H:262:GLU:HG3	2.11	0.50
1:J:185:TYR:HA	1:J:389:MET:CE	2.42	0.50
1:D:340:ARG:HE	1:D:359:ASN:ND2	2.08	0.49
1:I:367:GLU:CB	1:I:383:PRO:HD2	2.42	0.49
1:H:174:ARG:HH11	1:H:174:ARG:CG	2.07	0.49
1:H:214:VAL:H	1:H:226:SER:HB3	1.77	0.49
1:A:253:MET:HE1	1:A:260:PRO:HG3	1.94	0.49
1:C:56:LEU:HD22	1:C:62:ALA:HA	1.94	0.49
1:D:363:ILE:CG1	1:D:364:ARG:H	2.26	0.49
1:C:348:GLU:HG2	1:D:321:ASN:HD21	1.76	0.49
1:D:273:VAL:HG13	1:D:287:ILE:CD1	2.43	0.49
1:F:26:LEU:HB3	1:F:77:VAL:HG11	1.95	0.49
1:G:33:ARG:HB2	1:G:39:SER:HA	1.95	0.49
1:A:244:LEU:HD13	1:A:245:ASP:O	2.13	0.49
1:E:206:CYS:HB3	1:E:208:ILE:HD11	1.94	0.49
1:I:171:TYR:OH	1:J:256:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:SER:OG	1:D:262:GLU:HG3	2.13	0.49
1:G:208:ILE:HG22	1:G:332:VAL:HB	1.95	0.49
1:J:26:LEU:HB3	1:J:77:VAL:HG11	1.94	0.49
1:B:33:ARG:HB2	1:B:39:SER:HA	1.93	0.49
1:E:258:ILE:HG23	1:E:262:GLU:CB	2.43	0.49
1:E:259:SER:OG	1:E:262:GLU:HG3	2.13	0.49
1:H:56:LEU:HD22	1:H:62:ALA:HA	1.94	0.49
1:I:80:ASP:HB3	1:I:82:LYS:H	1.78	0.49
1:I:92:VAL:H	1:I:126:ASN:HD21	1.59	0.49
1:D:367:GLU:CB	1:D:383:PRO:HD2	2.43	0.49
1:J:244:LEU:HD13	1:J:245:ASP:O	2.13	0.49
1:A:259:SER:OG	1:A:262:GLU:HG3	2.13	0.48
1:D:56:LEU:HD22	1:D:62:ALA:HA	1.94	0.48
1:F:232:LEU:HD11	1:F:268:ASN:ND2	2.27	0.48
1:J:36:ILE:HG22	1:J:37:GLU:H	1.78	0.48
1:E:209:GLY:O	1:E:210:ASN:C	2.52	0.48
1:E:156:GLN:HB2	1:F:300:LEU:HD11	1.95	0.48
1:A:26:LEU:HB3	1:A:77:VAL:HG11	1.95	0.48
1:B:259:SER:OG	1:B:262:GLU:HG3	2.13	0.48
1:C:26:LEU:HB3	1:C:77:VAL:HG11	1.95	0.48
1:C:304:ILE:CG1	1:D:157:LYS:HA	2.43	0.48
1:I:273:VAL:HG13	1:I:287:ILE:CD1	2.43	0.48
1:A:168:TYR:HE1	1:A:174:ARG:HD2	1.78	0.48
1:A:36:ILE:HG22	1:A:37:GLU:N	2.28	0.48
1:A:349:PHE:CE2	1:B:318:ALA:HA	2.48	0.48
1:C:208:ILE:HG22	1:C:332:VAL:HB	1.95	0.48
1:D:74:LYS:HZ1	1:D:75:LEU:CD2	2.10	0.48
1:D:80:ASP:HB3	1:D:82:LYS:H	1.77	0.48
1:H:26:LEU:HB3	1:H:77:VAL:HG11	1.95	0.48
1:H:36:ILE:HG22	1:H:37:GLU:N	2.28	0.48
1:D:33:ARG:HB2	1:D:39:SER:HA	1.93	0.48
1:E:340:ARG:HE	1:E:359:ASN:ND2	2.09	0.48
1:E:54:ARG:HG2	1:E:55:GLU:N	2.29	0.48
1:F:208:ILE:HG22	1:F:332:VAL:HB	1.95	0.48
1:G:56:LEU:HD22	1:G:62:ALA:HA	1.95	0.48
1:H:352:VAL:HG22	1:H:377:VAL:HB	1.94	0.48
1:I:252:ILE:CG2	1:I:263:MET:HE1	2.44	0.48
1:G:185:TYR:HA	1:G:389:MET:CE	2.44	0.48
1:D:258:ILE:HG23	1:D:262:GLU:CB	2.42	0.48
1:D:363:ILE:HD13	1:D:364:ARG:NH1	2.28	0.48
1:E:208:ILE:HG22	1:E:332:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:GLU:CB	1:E:383:PRO:HD2	2.43	0.48
1:E:56:LEU:HD22	1:E:62:ALA:HA	1.96	0.48
1:J:335:ASN:OD1	1:J:364:ARG:HA	2.14	0.48
1:B:174:ARG:HH11	1:B:174:ARG:CG	2.11	0.48
1:B:214:VAL:HG23	1:B:235:LEU:HD11	1.96	0.48
1:F:168:TYR:HE1	1:F:174:ARG:HD2	1.78	0.48
1:B:335:ASN:OD1	1:B:364:ARG:HA	2.13	0.47
1:B:61:GLU:HG3	1:H:274:TYR:OH	2.14	0.47
1:A:367:GLU:CB	1:A:383:PRO:HD2	2.43	0.47
1:A:56:LEU:HD22	1:A:62:ALA:HA	1.95	0.47
1:E:352:VAL:HG22	1:E:377:VAL:HB	1.95	0.47
1:E:43:HIS:HE1	1:E:75:LEU:O	1.96	0.47
1:E:7:ASN:ND2	1:E:90:ARG:HD3	2.29	0.47
1:G:26:LEU:HB3	1:G:77:VAL:HG11	1.95	0.47
1:A:340:ARG:HE	1:A:359:ASN:ND2	2.10	0.47
1:C:168:TYR:HE1	1:C:174:ARG:HD2	1.80	0.47
1:C:33:ARG:HB2	1:C:39:SER:HA	1.96	0.47
1:J:124:PRO:O	1:J:128:MET:HG3	2.15	0.47
1:D:54:ARG:HG2	1:D:55:GLU:N	2.29	0.47
1:E:214:VAL:HG23	1:E:235:LEU:HD11	1.96	0.47
1:E:321:ASN:HD21	1:F:348:GLU:CG	2.27	0.47
1:G:259:SER:OG	1:G:262:GLU:HG3	2.15	0.47
1:I:178:PHE:O	1:I:179:HIS:HB2	2.15	0.47
1:I:352:VAL:HG22	1:I:377:VAL:HB	1.95	0.47
1:A:214:VAL:HG23	1:A:235:LEU:HD11	1.96	0.47
1:J:20:MET:CE	1:J:391:ALA:CB	2.85	0.47
1:A:206:CYS:HB3	1:A:208:ILE:HD11	1.96	0.47
1:H:273:VAL:HG13	1:H:287:ILE:CD1	2.45	0.47
1:I:244:LEU:HD13	1:I:245:ASP:O	2.14	0.47
1:B:306:ASP:OD1	1:B:339:THR:HG23	2.15	0.47
1:A:318:ALA:HA	1:B:349:PHE:CE2	2.50	0.47
1:B:16:GLN:NE2	1:B:387:GLU:CB	2.77	0.47
1:D:208:ILE:HG22	1:D:332:VAL:HB	1.97	0.47
1:D:232:LEU:HD11	1:D:268:ASN:ND2	2.30	0.47
1:B:26:LEU:HB3	1:B:77:VAL:HG11	1.96	0.47
1:B:168:TYR:HE1	1:B:174:ARG:HD2	1.80	0.47
1:I:363:ILE:HG12	1:I:364:ARG:HG2	1.97	0.47
1:I:162:ALA:O	1:J:271:SER:HB3	2.15	0.47
1:C:252:ILE:CG2	1:C:263:MET:HE1	2.44	0.47
1:J:168:TYR:HE1	1:J:174:ARG:HD2	1.80	0.47
1:A:258:ILE:HG23	1:A:262:GLU:CB	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG13	1:B:287:ILE:CD1	2.45	0.46
1:E:168:TYR:HE1	1:E:174:ARG:HD2	1.81	0.46
1:F:106:GLU:HA	1:F:106:GLU:OE2	2.16	0.46
1:F:258:ILE:HG23	1:F:262:GLU:CB	2.44	0.46
1:J:252:ILE:CG2	1:J:263:MET:HE1	2.44	0.46
1:A:335:ASN:OD1	1:A:364:ARG:HA	2.16	0.46
1:E:36:ILE:HG22	1:E:37:GLU:N	2.30	0.46
1:G:271:SER:HB3	1:H:162:ALA:O	2.16	0.46
1:A:61:GLU:HG3	1:I:274:TYR:OH	2.15	0.46
1:F:185:TYR:HA	1:F:389:MET:HE2	1.98	0.46
1:G:245:ASP:HB2	1:H:233:GLU:OE1	2.16	0.46
1:G:266:ILE:HD13	1:H:167:TYR:OH	2.15	0.46
1:H:335:ASN:OD1	1:H:364:ARG:HA	2.15	0.46
1:D:206:CYS:HB3	1:D:208:ILE:CD1	2.45	0.46
1:E:80:ASP:HB3	1:E:82:LYS:H	1.79	0.46
1:F:121:LEU:CD1	1:F:121:LEU:N	2.78	0.46
1:G:335:ASN:OD1	1:G:364:ARG:HA	2.15	0.46
1:F:217:VAL:C	1:F:320:MET:HE3	2.36	0.46
1:G:168:TYR:HE1	1:G:174:ARG:HD2	1.81	0.46
1:A:348:GLU:HG2	1:B:321:ASN:ND2	2.30	0.46
1:B:43:HIS:HE1	1:B:75:LEU:O	1.98	0.46
1:F:352:VAL:HG22	1:F:377:VAL:HB	1.97	0.46
1:F:252:ILE:CG2	1:F:263:MET:HE1	2.46	0.46
1:G:248:ILE:HD11	1:H:161:TYR:CE2	2.51	0.46
1:D:352:VAL:HG22	1:D:377:VAL:HB	1.98	0.45
1:C:214:VAL:HG23	1:C:235:LEU:HD11	1.97	0.45
1:C:335:ASN:OD1	1:C:364:ARG:HA	2.16	0.45
1:B:80:ASP:HB3	1:B:82:LYS:H	1.80	0.45
1:C:92:VAL:H	1:C:126:ASN:HD21	1.64	0.45
1:F:92:VAL:H	1:F:126:ASN:HD21	1.64	0.45
1:G:124:PRO:O	1:G:128:MET:HG3	2.16	0.45
1:A:352:VAL:HG22	1:A:377:VAL:HB	1.98	0.45
1:D:363:ILE:HG12	1:D:364:ARG:H	1.81	0.45
1:E:178:PHE:O	1:E:179:HIS:HB2	2.17	0.45
1:I:43:HIS:HE1	1:I:75:LEU:O	1.99	0.45
1:C:300:LEU:HD11	1:D:156:GLN:HB2	1.99	0.45
1:J:106:GLU:HA	1:J:106:GLU:OE2	2.17	0.45
1:J:174:ARG:HH11	1:J:174:ARG:CG	2.13	0.45
1:D:36:ILE:HG22	1:D:37:GLU:N	2.32	0.45
1:D:43:HIS:HE1	1:D:75:LEU:O	1.98	0.45
1:H:232:LEU:HD11	1:H:268:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:259:SER:OG	1:J:262:GLU:HG3	2.16	0.45
1:A:359:ASN:HA	1:A:370:ILE:CG2	2.47	0.45
1:B:249:PRO:O	1:B:263:MET:HE3	2.16	0.45
1:J:63:LEU:HA	1:J:66:ILE:HD12	1.99	0.45
1:C:217:VAL:C	1:C:320:MET:HE3	2.37	0.45
1:B:352:VAL:HG22	1:B:377:VAL:HB	1.99	0.45
1:C:106:GLU:OE2	1:C:106:GLU:HA	2.17	0.45
1:E:72:ASP:O	1:E:76:GLY:HA3	2.16	0.45
1:D:72:ASP:O	1:D:76:GLY:HA3	2.17	0.44
1:H:214:VAL:HG23	1:H:235:LEU:HD11	1.98	0.44
1:I:214:VAL:HG23	1:I:235:LEU:HD11	1.99	0.44
1:F:124:PRO:O	1:F:128:MET:HG3	2.18	0.44
1:B:253:MET:HE1	1:B:260:PRO:HG3	1.99	0.44
1:E:244:LEU:HD13	1:E:245:ASP:O	2.17	0.44
1:E:273:VAL:HG13	1:E:287:ILE:CD1	2.47	0.44
1:I:56:LEU:HD22	1:I:62:ALA:HA	2.00	0.44
1:J:56:LEU:HD22	1:J:62:ALA:HA	1.99	0.44
1:G:273:VAL:HG13	1:G:287:ILE:CD1	2.48	0.44
1:D:253:MET:HE1	1:D:260:PRO:HG3	2.00	0.44
1:G:206:CYS:HB3	1:G:208:ILE:HD11	1.99	0.44
1:G:206:CYS:HB3	1:G:208:ILE:CD1	2.48	0.44
1:I:36:ILE:HG22	1:I:37:GLU:H	1.82	0.44
1:A:249:PRO:HB3	1:B:250:PHE:HZ	1.83	0.44
1:F:273:VAL:HG13	1:F:287:ILE:CD1	2.48	0.44
1:A:306:ASP:OD1	1:A:339:THR:HG23	2.18	0.44
1:C:20:MET:CE	1:C:391:ALA:CB	2.85	0.44
1:C:359:ASN:HA	1:C:370:ILE:CG2	2.47	0.44
1:D:168:TYR:HE1	1:D:174:ARG:HD2	1.83	0.44
1:C:206:CYS:HB3	1:C:208:ILE:CD1	2.48	0.43
1:F:335:ASN:OD1	1:F:364:ARG:HA	2.18	0.43
1:B:359:ASN:HA	1:B:370:ILE:CG2	2.48	0.43
1:E:106:GLU:OE2	1:E:106:GLU:HA	2.18	0.43
1:C:85:ASP:HA	1:H:82:LYS:NZ	2.34	0.43
1:I:349:PHE:CE2	1:J:318:ALA:HA	2.53	0.43
1:C:43:HIS:HE1	1:C:75:LEU:O	2.01	0.43
1:I:335:ASN:OD1	1:I:364:ARG:HA	2.17	0.43
1:I:20:MET:HB3	1:I:395:LYS:HD2	2.00	0.43
1:C:130:ILE:O	1:C:134:MET:HG3	2.18	0.43
1:H:168:TYR:HE1	1:H:174:ARG:HD2	1.83	0.43
1:H:63:LEU:HA	1:H:66:ILE:HD12	1.99	0.43
1:J:273:VAL:HG13	1:J:287:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:HB3	1:A:82:LYS:H	1.83	0.43
1:I:167:TYR:OH	1:J:266:ILE:HD13	2.19	0.43
1:I:26:LEU:HB3	1:I:77:VAL:HG11	2.00	0.43
1:B:208:ILE:HG22	1:B:332:VAL:HB	2.01	0.43
1:C:259:SER:OG	1:C:262:GLU:HG3	2.19	0.43
1:D:206:CYS:HB3	1:D:208:ILE:HD11	1.99	0.43
1:E:36:ILE:HG22	1:E:37:GLU:H	1.83	0.43
1:E:162:ALA:O	1:F:271:SER:HB3	2.19	0.43
1:J:213:SER:HB3	1:J:227:MET:HG3	2.00	0.43
1:B:36:ILE:HG22	1:B:37:GLU:H	1.83	0.43
1:C:245:ASP:HB2	1:D:233:GLU:OE1	2.18	0.43
1:G:214:VAL:HG23	1:G:235:LEU:HD11	2.00	0.43
1:H:370:ILE:HD12	1:H:379:VAL:HG12	2.01	0.43
1:I:156:GLN:HB2	1:J:300:LEU:HD11	2.01	0.43
1:I:329:THR:O	1:I:330:ALA:HB3	2.19	0.43
1:J:359:ASN:HA	1:J:370:ILE:CG2	2.47	0.43
1:A:217:VAL:C	1:A:320:MET:HE3	2.39	0.42
1:C:185:TYR:HA	1:C:389:MET:HE2	2.00	0.42
1:D:207:HIS:CD2	1:D:330:ALA:HB2	2.54	0.42
1:E:207:HIS:CD2	1:E:330:ALA:HB2	2.54	0.42
1:F:174:ARG:HH11	1:F:174:ARG:CG	2.16	0.42
1:F:20:MET:HE1	1:F:391:ALA:HB1	1.94	0.42
1:G:106:GLU:HA	1:G:106:GLU:OE2	2.18	0.42
1:G:287:ILE:HG23	1:G:298:CYS:HB3	2.00	0.42
1:A:212:ALA:N	1:A:237:MET:HG2	2.34	0.42
1:J:287:ILE:HG23	1:J:298:CYS:HB3	2.01	0.42
1:A:43:HIS:HE1	1:A:75:LEU:O	2.02	0.42
1:B:106:GLU:OE2	1:B:106:GLU:HA	2.20	0.42
1:C:258:ILE:HD13	1:C:258:ILE:HG21	1.78	0.42
1:G:300:LEU:HD11	1:H:156:GLN:HB2	2.00	0.42
1:H:252:ILE:CG2	1:H:263:MET:HE1	2.49	0.42
1:I:168:TYR:HE1	1:I:174:ARG:HD2	1.84	0.42
1:I:259:SER:OG	1:I:262:GLU:HG3	2.19	0.42
1:A:209:GLY:C	1:A:211:GLY:N	2.72	0.42
1:A:250:PHE:HZ	1:B:249:PRO:HB3	1.85	0.42
1:E:253:MET:HE1	1:E:260:PRO:HG3	2.02	0.42
1:F:63:LEU:HA	1:F:66:ILE:HD12	2.02	0.42
1:C:7:ASN:ND2	1:C:90:ARG:HD3	2.34	0.42
1:E:209:GLY:C	1:E:211:GLY:H	2.22	0.42
1:G:20:MET:O	1:G:23:GLU:HG3	2.19	0.42
1:G:217:VAL:C	1:G:320:MET:HE3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:HIS:HE1	1:H:75:LEU:O	2.03	0.42
1:I:54:ARG:HG2	1:I:55:GLU:N	2.34	0.42
1:A:106:GLU:OE2	1:A:106:GLU:HA	2.20	0.42
1:B:72:ASP:O	1:B:76:GLY:N	2.53	0.42
1:I:63:LEU:HA	1:I:66:ILE:HD12	2.01	0.42
1:B:307:TYR:CZ	1:B:311:LYS:HD2	2.54	0.42
1:C:352:VAL:HG22	1:C:377:VAL:HB	2.01	0.42
1:D:26:LEU:HB3	1:D:77:VAL:HG11	2.02	0.42
1:F:359:ASN:HA	1:F:370:ILE:CG2	2.48	0.42
1:D:244:LEU:HD13	1:D:245:ASP:O	2.20	0.42
1:G:249:PRO:O	1:G:253:MET:HG3	2.19	0.42
1:I:399:GLU:O	1:I:400:LYS:HB2	2.19	0.42
1:A:54:ARG:HG2	1:A:55:GLU:N	2.35	0.42
1:A:72:ASP:O	1:A:76:GLY:N	2.53	0.42
1:C:273:VAL:HG13	1:C:287:ILE:CD1	2.50	0.42
1:E:252:ILE:CG2	1:E:263:MET:HE1	2.50	0.42
1:J:364:ARG:CG	1:J:364:ARG:O	2.53	0.42
1:F:20:MET:CE	1:F:391:ALA:CB	2.84	0.41
1:I:162:ALA:O	1:J:272:GLY:N	2.47	0.41
1:A:287:ILE:HG23	1:A:298:CYS:HB3	2.02	0.41
1:C:318:ALA:HA	1:D:349:PHE:CE2	2.55	0.41
1:I:212:ALA:H	1:I:237:MET:HG2	1.84	0.41
1:D:63:LEU:HA	1:D:66:ILE:HD12	2.02	0.41
1:F:214:VAL:HG23	1:F:235:LEU:HD11	2.02	0.41
1:A:72:ASP:O	1:A:76:GLY:HA3	2.20	0.41
1:C:119:ALA:N	1:C:120:PRO:HD3	2.35	0.41
1:C:80:ASP:HB3	1:C:82:LYS:H	1.86	0.41
1:C:241:SER:O	1:D:162:ALA:HB3	2.21	0.41
1:D:213:SER:HB3	1:D:227:MET:HG3	2.01	0.41
1:E:287:ILE:HG23	1:E:298:CYS:HB3	2.02	0.41
1:F:206:CYS:HB3	1:F:208:ILE:CD1	2.51	0.41
1:E:185:TYR:HA	1:E:389:MET:HE2	2.02	0.41
1:I:213:SER:HB3	1:I:227:MET:HG3	2.03	0.41
1:J:214:VAL:HG23	1:J:235:LEU:HD11	2.02	0.41
1:J:91:VAL:HA	1:J:126:ASN:ND2	2.36	0.41
1:B:213:SER:HB3	1:B:227:MET:HG3	2.03	0.41
1:G:213:SER:HB3	1:G:227:MET:HG3	2.02	0.41
1:H:207:HIS:CD2	1:H:330:ALA:HB2	2.55	0.41
1:D:258:ILE:HG21	1:D:258:ILE:HD13	1.75	0.41
1:E:349:PHE:CE2	1:F:318:ALA:HA	2.55	0.41
1:F:36:ILE:CG2	1:F:37:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:GLU:O	1:G:400:LYS:HB2	2.21	0.41
1:G:80:ASP:HB3	1:G:82:LYS:H	1.84	0.41
1:H:217:VAL:C	1:H:320:MET:HE3	2.41	0.41
1:J:329:THR:O	1:J:330:ALA:HB3	2.21	0.41
1:J:352:VAL:HG22	1:J:377:VAL:HB	2.03	0.41
1:J:43:HIS:HE1	1:J:75:LEU:O	2.02	0.41
1:E:26:LEU:HB3	1:E:77:VAL:HG11	2.03	0.41
1:F:130:ILE:O	1:F:134:MET:HG3	2.21	0.41
1:G:63:LEU:HA	1:G:66:ILE:HD12	2.03	0.41
1:H:36:ILE:HG22	1:H:37:GLU:H	1.84	0.41
1:C:206:CYS:HB3	1:C:208:ILE:HD11	2.03	0.41
1:E:162:ALA:HB3	1:F:241:SER:O	2.21	0.41
1:G:329:THR:O	1:G:330:ALA:HB3	2.21	0.41
1:G:20:MET:HE1	1:G:391:ALA:HB1	1.96	0.41
1:G:43:HIS:HE1	1:G:75:LEU:O	2.03	0.41
1:J:14:LYS:HE2	1:J:30:ILE:HD12	2.03	0.41
1:J:217:VAL:C	1:J:320:MET:HE3	2.40	0.41
1:B:244:LEU:HD13	1:B:245:ASP:O	2.21	0.40
1:D:185:TYR:HD1	1:D:389:MET:HE2	1.86	0.40
1:F:258:ILE:HD13	1:F:258:ILE:HG21	1.76	0.40
1:H:72:ASP:O	1:H:76:GLY:HA3	2.21	0.40
1:A:213:SER:HB3	1:A:227:MET:HG3	2.03	0.40
1:A:7:ASN:ND2	1:A:90:ARG:HD3	2.37	0.40
1:G:256:GLU:CG	1:H:171:TYR:OH	2.70	0.40
1:A:36:ILE:HG22	1:A:37:GLU:H	1.84	0.40
1:D:399:GLU:O	1:D:400:LYS:HB2	2.20	0.40
1:I:202:LYS:HB3	1:I:320:MET:HE1	2.04	0.40
1:C:185:TYR:HA	1:C:389:MET:HE3	2.01	0.40
1:D:7:ASN:ND2	1:D:90:ARG:HD3	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:GLY:O	1:E:364:ARG:NH2[7_655]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/403 (99%)	376 (94%)	22 (6%)	0	100	100
1	B	398/403 (99%)	373 (94%)	24 (6%)	1 (0%)	41	71
1	C	398/403 (99%)	374 (94%)	23 (6%)	1 (0%)	41	71
1	D	398/403 (99%)	377 (95%)	20 (5%)	1 (0%)	41	71
1	E	398/403 (99%)	376 (94%)	22 (6%)	0	100	100
1	F	398/403 (99%)	376 (94%)	21 (5%)	1 (0%)	41	71
1	G	398/403 (99%)	376 (94%)	21 (5%)	1 (0%)	41	71
1	H	398/403 (99%)	378 (95%)	19 (5%)	1 (0%)	41	71
1	I	398/403 (99%)	375 (94%)	22 (6%)	1 (0%)	41	71
1	J	398/403 (99%)	377 (95%)	20 (5%)	1 (0%)	41	71
All	All	3980/4030 (99%)	3758 (94%)	214 (5%)	8 (0%)	47	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	399	GLU
1	F	399	GLU
1	J	399	GLU
1	B	399	GLU
1	D	399	GLU
1	I	399	GLU
1	G	399	GLU
1	H	331	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/340 (99%)	324 (96%)	14 (4%)	30	61
1	B	338/340 (99%)	326 (96%)	12 (4%)	35	63
1	C	338/340 (99%)	326 (96%)	12 (4%)	35	63
1	D	338/340 (99%)	327 (97%)	11 (3%)	38	66
1	E	338/340 (99%)	328 (97%)	10 (3%)	41	68
1	F	338/340 (99%)	326 (96%)	12 (4%)	35	63
1	G	338/340 (99%)	325 (96%)	13 (4%)	33	62
1	H	338/340 (99%)	326 (96%)	12 (4%)	35	63
1	I	338/340 (99%)	326 (96%)	12 (4%)	35	63
1	J	338/340 (99%)	325 (96%)	13 (4%)	33	62
All	All	3380/3400 (99%)	3259 (96%)	121 (4%)	35	63

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	26	LEU
1	A	75	LEU
1	A	77	VAL
1	A	174	ARG
1	A	181	THR
1	A	226	SER
1	A	232	LEU
1	A	244	LEU
1	A	359	ASN
1	A	362	THR
1	A	370	ILE
1	A	378	LYS
1	A	400	LYS
1	B	26	LEU
1	B	75	LEU
1	B	77	VAL
1	B	174	ARG
1	B	181	THR
1	B	226	SER
1	B	232	LEU
1	B	244	LEU

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Mol	Chain	Res	Type
1	B	362	THR
1	B	370	ILE
1	B	378	LYS
1	B	400	LYS
1	C	26	LEU
1	C	75	LEU
1	C	77	VAL
1	C	174	ARG
1	C	181	THR
1	C	226	SER
1	C	232	LEU
1	C	244	LEU
1	C	362	THR
1	C	370	ILE
1	C	378	LYS
1	C	400	LYS
1	D	26	LEU
1	D	77	VAL
1	D	174	ARG
1	D	181	THR
1	D	226	SER
1	D	232	LEU
1	D	244	LEU
1	D	362	THR
1	D	370	ILE
1	D	378	LYS
1	D	400	LYS
1	E	77	VAL
1	E	174	ARG
1	E	181	THR
1	E	226	SER
1	E	232	LEU
1	E	244	LEU
1	E	362	THR
1	E	370	ILE
1	E	378	LYS
1	E	400	LYS
1	F	26	LEU
1	F	75	LEU
1	F	77	VAL
1	F	174	ARG
1	F	181	THR

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Mol	Chain	Res	Type
1	F	226	SER
1	F	232	LEU
1	F	244	LEU
1	F	362	THR
1	F	370	ILE
1	F	378	LYS
1	F	400	LYS
1	G	11	SER
1	G	26	LEU
1	G	75	LEU
1	G	77	VAL
1	G	174	ARG
1	G	181	THR
1	G	226	SER
1	G	232	LEU
1	G	244	LEU
1	G	362	THR
1	G	370	ILE
1	G	378	LYS
1	G	400	LYS
1	H	19	GLU
1	H	75	LEU
1	H	77	VAL
1	H	174	ARG
1	H	181	THR
1	H	226	SER
1	H	244	LEU
1	H	362	THR
1	H	364	ARG
1	H	370	ILE
1	H	378	LYS
1	H	400	LYS
1	I	26	LEU
1	I	75	LEU
1	I	77	VAL
1	I	174	ARG
1	I	181	THR
1	I	226	SER
1	I	232	LEU
1	I	244	LEU
1	I	362	THR
1	I	370	ILE

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Mol	Chain	Res	Type
1	I	378	LYS
1	I	400	LYS
1	J	26	LEU
1	J	75	LEU
1	J	77	VAL
1	J	174	ARG
1	J	181	THR
1	J	226	SER
1	J	232	LEU
1	J	244	LEU
1	J	359	ASN
1	J	362	THR
1	J	370	ILE
1	J	378	LYS
1	J	400	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	43	HIS
1	A	126	ASN
1	A	207	HIS
1	A	210	ASN
1	A	268	ASN
1	A	357	GLN
1	A	359	ASN
1	B	7	ASN
1	B	16	GLN
1	B	43	HIS
1	B	126	ASN
1	B	207	HIS
1	B	268	ASN
1	B	357	GLN
1	B	359	ASN
1	C	7	ASN
1	C	43	HIS
1	C	68	ASN
1	C	126	ASN
1	C	207	HIS
1	C	268	ASN
1	C	357	GLN

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Mol	Chain	Res	Type
1	C	359	ASN
1	D	7	ASN
1	D	43	HIS
1	D	126	ASN
1	D	207	HIS
1	D	268	ASN
1	D	357	GLN
1	D	359	ASN
1	E	7	ASN
1	E	43	HIS
1	E	126	ASN
1	E	207	HIS
1	E	210	ASN
1	E	268	ASN
1	E	357	GLN
1	E	359	ASN
1	F	7	ASN
1	F	43	HIS
1	F	126	ASN
1	F	207	HIS
1	F	268	ASN
1	F	357	GLN
1	F	359	ASN
1	G	7	ASN
1	G	43	HIS
1	G	126	ASN
1	G	207	HIS
1	G	268	ASN
1	G	357	GLN
1	G	359	ASN
1	H	7	ASN
1	H	43	HIS
1	H	126	ASN
1	H	207	HIS
1	H	268	ASN
1	H	357	GLN
1	H	359	ASN
1	I	7	ASN
1	I	43	HIS
1	I	126	ASN
1	I	207	HIS
1	I	268	ASN

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Mol	Chain	Res	Type
1	I	357	GLN
1	I	359	ASN
1	J	7	ASN
1	J	43	HIS
1	J	126	ASN
1	J	207	HIS
1	J	268	ASN
1	J	357	GLN
1	J	359	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	400/403 (99%)	0.53	16 (4%)	38	36	53, 71, 72, 73	0
1	B	400/403 (99%)	0.58	24 (6%)	21	21	53, 71, 72, 73	0
1	C	400/403 (99%)	0.44	9 (2%)	60	59	53, 71, 72, 73	0
1	D	400/403 (99%)	0.40	2 (0%)	91	91	53, 71, 72, 73	0
1	E	400/403 (99%)	0.41	9 (2%)	60	59	53, 71, 72, 73	0
1	F	400/403 (99%)	0.41	6 (1%)	73	72	53, 71, 72, 73	0
1	G	400/403 (99%)	0.49	7 (1%)	68	67	53, 71, 72, 73	0
1	H	400/403 (99%)	0.48	13 (3%)	46	44	53, 71, 72, 73	0
1	I	400/403 (99%)	0.60	22 (5%)	25	23	53, 71, 72, 73	0
1	J	400/403 (99%)	0.49	15 (3%)	40	37	53, 71, 72, 73	0
All	All	4000/4030 (99%)	0.48	123 (3%)	49	48	53, 71, 72, 73	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	THR	4.3
1	C	83	GLU	3.9
1	A	344	CYS	3.9
1	D	47	ASP	3.8
1	A	206	CYS	3.6
1	G	323	VAL	3.6
1	A	68	ASN	3.5
1	A	54	ARG	3.5
1	A	347	LEU	3.3
1	A	302	LEU	3.3
1	D	46	GLY	3.3
1	I	132	ALA	3.2
1	B	205	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	86	ALA	3.2
1	I	133	ALA	3.2
1	J	297	TRP	3.1
1	B	81	LEU	3.1
1	C	364	ARG	3.1
1	F	8	SER	3.0
1	B	84	ILE	3.0
1	H	15	TYR	3.0
1	G	364	ARG	2.9
1	J	46	GLY	2.9
1	C	5	VAL	2.9
1	F	85	ASP	2.9
1	G	332	VAL	2.9
1	E	20	MET	2.8
1	H	326	ILE	2.8
1	H	328	PHE	2.8
1	H	92	VAL	2.8
1	C	35	GLY	2.8
1	A	285	ARG	2.8
1	G	223	VAL	2.7
1	E	364	ARG	2.7
1	I	312	TYR	2.7
1	A	15	TYR	2.6
1	I	190	ALA	2.6
1	H	91	VAL	2.6
1	G	236	VAL	2.6
1	F	143	VAL	2.6
1	B	381	VAL	2.6
1	C	368	GLY	2.6
1	A	87	VAL	2.6
1	B	383	PRO	2.6
1	B	34	ILE	2.6
1	B	20	MET	2.5
1	J	221	LYS	2.5
1	I	376	ARG	2.5
1	I	5	VAL	2.5
1	B	206	CYS	2.5
1	B	326	ILE	2.5
1	J	364	ARG	2.5
1	B	35	GLY	2.4
1	J	328	PHE	2.4
1	B	66	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	2.4
1	I	326	ILE	2.4
1	I	84	ILE	2.4
1	I	336	SER	2.4
1	B	65	LEU	2.4
1	G	194	LEU	2.4
1	H	268	ASN	2.4
1	B	207	HIS	2.4
1	E	3	VAL	2.4
1	I	208	ILE	2.3
1	J	391	ALA	2.3
1	B	209	GLY	2.3
1	G	328	PHE	2.3
1	E	47	ASP	2.3
1	H	203	ILE	2.3
1	A	205	THR	2.3
1	A	56	LEU	2.3
1	A	231	PRO	2.3
1	E	333	GLY	2.3
1	J	54	ARG	2.3
1	B	5	VAL	2.3
1	H	301	VAL	2.3
1	C	331	GLY	2.3
1	H	377	VAL	2.3
1	I	18	ILE	2.3
1	H	305	TYR	2.3
1	B	323	VAL	2.2
1	E	74	LYS	2.2
1	B	3	VAL	2.2
1	I	327	VAL	2.2
1	B	327	VAL	2.2
1	J	343	VAL	2.2
1	A	361	GLU	2.2
1	A	6	ILE	2.2
1	I	323	VAL	2.2
1	J	182	SER	2.2
1	B	208	ILE	2.2
1	H	369	ILE	2.2
1	E	210	ASN	2.2
1	J	203	ILE	2.2
1	C	44	ARG	2.2
1	I	318	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	323	VAL	2.1
1	I	204	ILE	2.1
1	H	371	SER	2.1
1	I	203	ILE	2.1
1	I	105	ASP	2.1
1	J	47	ASP	2.1
1	B	325	ALA	2.1
1	I	6	ILE	2.1
1	I	275	GLY	2.1
1	A	208	ILE	2.1
1	B	78	ILE	2.1
1	I	20	MET	2.1
1	J	347	LEU	2.1
1	J	220	GLY	2.1
1	E	356	LYS	2.1
1	I	311	LYS	2.1
1	F	15	TYR	2.1
1	F	364	ARG	2.1
1	J	162	ALA	2.1
1	B	80	ASP	2.1
1	H	285	ARG	2.1
1	J	222	CYS	2.0
1	E	191	ALA	2.0
1	F	54	ARG	2.0
1	I	210	ASN	2.0
1	C	207	HIS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.