



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:00 PM UTC

PDB ID : 2Z9S / pdb_00002z9s
Title : Crystal Structure Analysis of rat HBP23/Peroxiredoxin I, Cys52Ser mutant
Authors : Matsumura, T.; Okamoto, K.; Nishino, T.; Abe, Y.
Deposited on : 2007-09-25
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

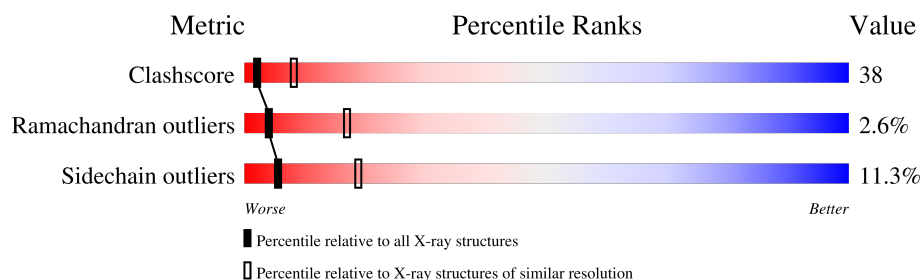
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	199	42% 45% 12% ..
1	B	199	46% 41% 12% ..
1	C	199	41% 47% 11% ..
1	D	199	48% 41% 10% ..
1	E	199	44% 42% 12% ..
1	F	199	44% 46% 9% .
1	G	199	39% 48% 12% .
1	H	199	44% 44% 10% ..

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Mol	Chain	Length	Quality of chain
1	I	199	44%44%10%..
1	J	199	45%42%13%. .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15460 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 Peroxiredoxin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	B	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	C	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	D	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	E	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	F	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	G	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	H	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	I	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			
1	J	197	Total	C	N	O	S	0	0	0
			1546	998	258	285	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	SER	CYS	engineered mutation	UNP Q63716
B	52	SER	CYS	engineered mutation	UNP Q63716
C	52	SER	CYS	engineered mutation	UNP Q63716
D	52	SER	CYS	engineered mutation	UNP Q63716
E	52	SER	CYS	engineered mutation	UNP Q63716
F	52	SER	CYS	engineered mutation	UNP Q63716
G	52	SER	CYS	engineered mutation	UNP Q63716
H	52	SER	CYS	engineered mutation	UNP Q63716
I	52	SER	CYS	engineered mutation	UNP Q63716

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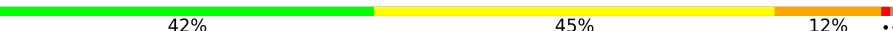
Chain	Residue	Modelled	Actual	Comment	Reference
J	52	SER	CYS	engineered mutation	UNP Q63716

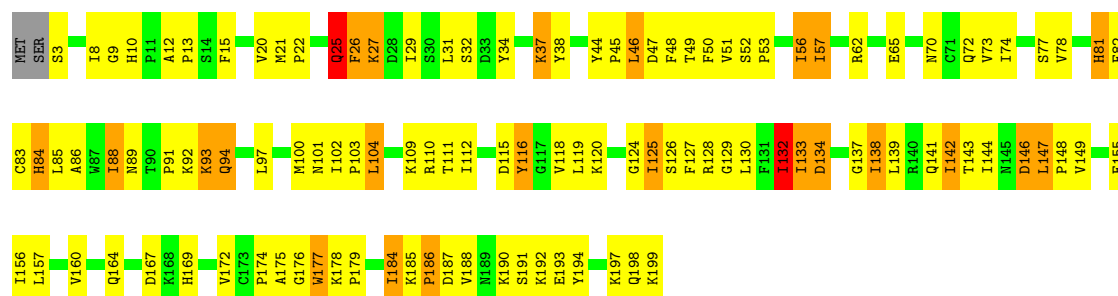
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

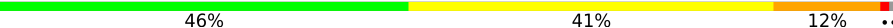
Note EDS was not executed.

• Molecule 1: Peroxiredoxin-1

Chain A: 



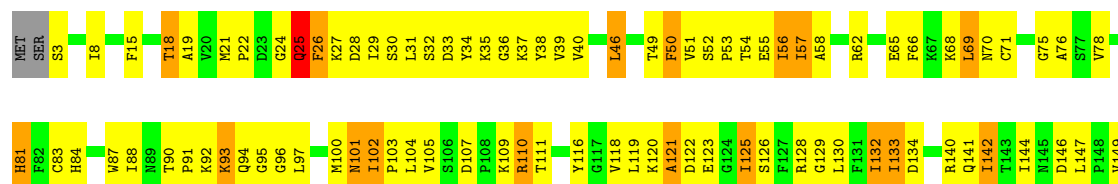
• Molecule 1: Peroxiredoxin-1

Chain B: 



• Molecule 1: Peroxiredoxin-1

Chain C: 





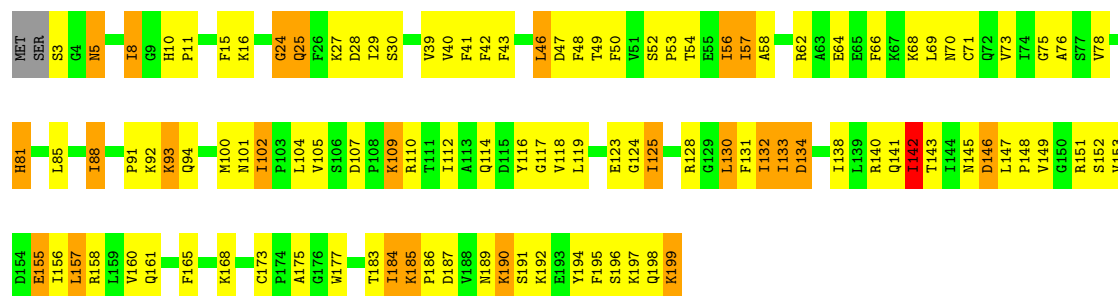
• Molecule 1: Peroxiredoxin-1

Chain D: 48% 41% 10% ..



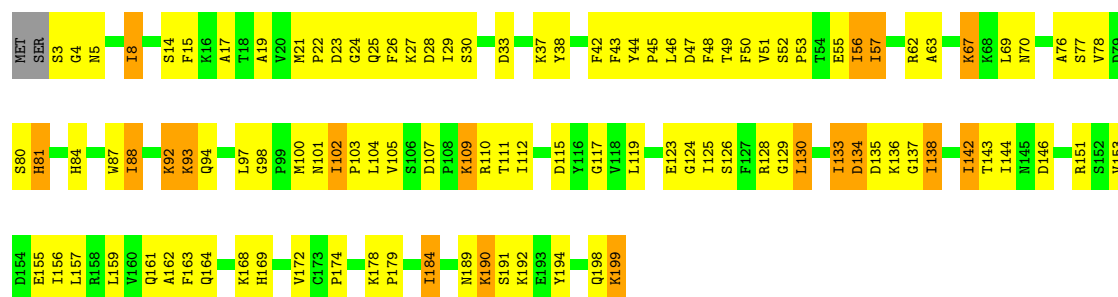
• Molecule 1: Peroxiredoxin-1

Chain E: 44% 42% 12% ..



• Molecule 1: Peroxiredoxin-1

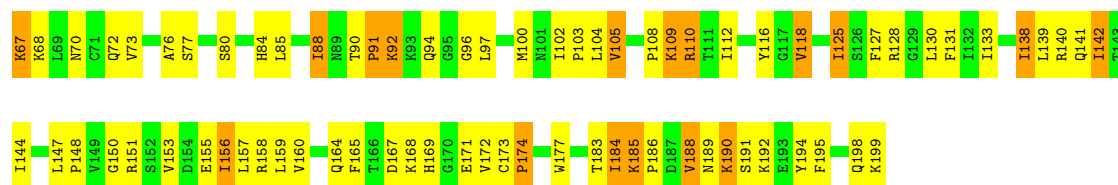
Chain F: 44% 46% 9% .



• Molecule 1: Peroxiredoxin-1

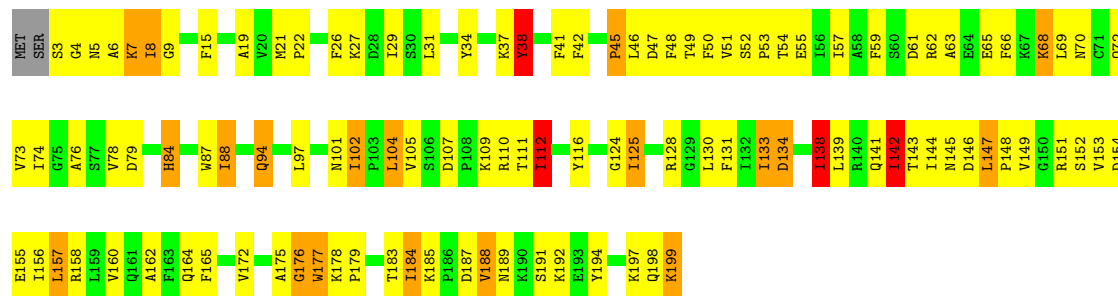
Chain G: 39% 48% 12% .





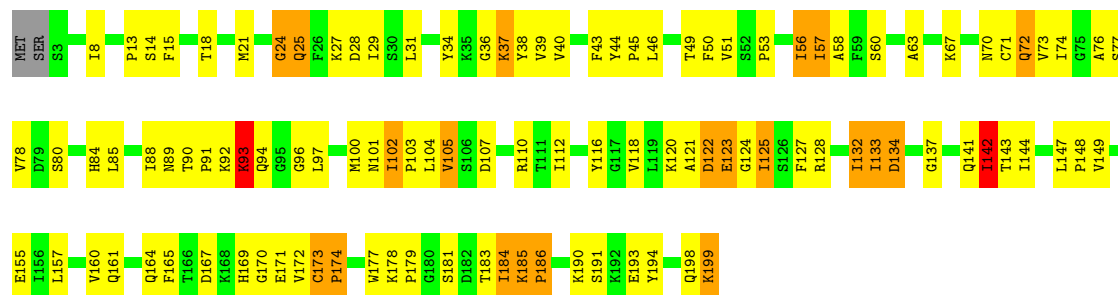
• Molecule 1: Peroxiredoxin-1

Chain H: 44% 44% 10% ..



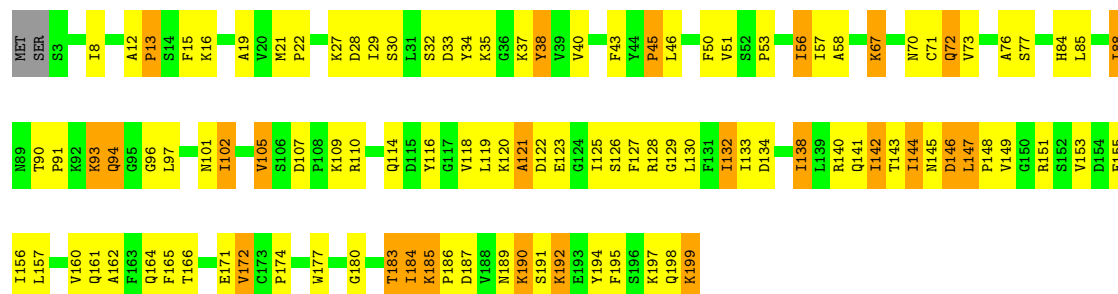
• Molecule 1: Peroxiredoxin-1

Chain I: 44% 44% 10% ..



• Molecule 1: Peroxiredoxin-1

Chain J: 45% 42% 13% .



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.31Å 111.64Å 120.74Å 90.00° 112.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15460	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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	0.55	1/1586 (0.1%)	1.07	11/2142 (0.5%)
1	B	0.56	1/1586 (0.1%)	1.04	7/2142 (0.3%)
1	C	0.52	0/1586	1.01	12/2142 (0.6%)
1	D	0.50	0/1586	1.04	8/2142 (0.4%)
1	E	0.53	1/1586 (0.1%)	1.01	14/2142 (0.7%)
1	F	0.49	0/1586	0.99	6/2142 (0.3%)
1	G	0.46	0/1586	0.99	2/2142 (0.1%)
1	H	0.50	1/1586 (0.1%)	1.06	12/2142 (0.6%)
1	I	0.55	1/1586 (0.1%)	1.08	9/2142 (0.4%)
1	J	0.54	0/1586	1.06	11/2142 (0.5%)
All	All	0.52	5/15860 (0.0%)	1.04	92/21420 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	142	ILE	CA-CB	6.16	1.62	1.54
1	H	112	ILE	CA-CB	5.64	1.61	1.54
1	A	132	ILE	CA-CB	5.20	1.60	1.54
1	E	142	ILE	CA-CB	5.19	1.60	1.54
1	B	132	ILE	CA-CB	5.16	1.61	1.54

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	VAL	N-CA-C	8.89	120.73	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	VAL	N-CA-C	8.02	119.43	107.80
1	I	134	ASP	N-CA-C	7.92	122.13	109.86
1	J	149	VAL	N-CA-C	7.60	117.64	106.85
1	H	134	ASP	N-CA-C	7.55	121.58	109.79
1	I	24	GLY	N-CA-C	-7.50	99.33	112.53
1	C	46	LEU	N-CA-C	7.33	120.50	108.99
1	D	147	LEU	N-CA-C	7.15	122.48	112.75
1	F	50	PHE	N-CA-C	6.93	121.55	111.02
1	J	180	GLY	N-CA-C	-6.91	106.19	113.58
1	A	146	ASP	N-CA-C	-6.87	101.97	110.41
1	H	149	VAL	N-CA-C	6.85	118.16	108.36
1	A	169	HIS	N-CA-C	6.83	121.78	113.38
1	B	147	LEU	N-CA-C	6.83	122.79	113.77
1	F	134	ASP	N-CA-C	6.82	119.77	110.35
1	E	146	ASP	N-CA-C	-6.71	101.49	110.55
1	F	109	LYS	N-CA-C	-6.58	105.07	113.23
1	C	149	VAL	N-CA-C	6.48	117.21	107.75
1	H	101	ASN	N-CA-C	-6.31	105.62	113.38
1	G	5	ASN	N-CA-C	-6.29	105.92	113.97
1	C	50	PHE	N-CA-C	6.22	120.46	112.12
1	C	83	CYS	N-CA-C	-6.16	104.48	111.07
1	A	81	HIS	N-CA-C	-6.15	104.12	111.69
1	A	147	LEU	N-CA-C	6.14	121.23	113.25
1	A	198	GLN	N-CA-C	6.14	118.53	109.69
1	D	44	TYR	CA-C-N	6.00	127.33	119.84
1	D	44	TYR	C-N-CA	6.00	127.33	119.84
1	J	172	VAL	N-CA-C	5.92	117.68	109.80
1	G	118	VAL	N-CA-C	-5.92	106.98	112.43
1	J	101	ASN	N-CA-C	-5.92	104.60	112.94
1	F	146	ASP	N-CA-C	-5.91	103.14	110.41
1	E	185	LYS	CA-C-N	5.86	127.16	119.84
1	E	185	LYS	C-N-CA	5.86	127.16	119.84
1	H	138	ILE	N-CA-C	5.86	116.37	108.17
1	I	147	LEU	N-CA-C	5.84	122.72	109.81
1	H	142	ILE	N-CA-C	5.84	116.53	108.12
1	A	147	LEU	CA-C-N	5.82	126.22	119.47
1	A	147	LEU	C-N-CA	5.82	126.22	119.47
1	D	134	ASP	N-CA-C	5.79	118.83	109.79
1	E	147	LEU	N-CA-C	5.78	121.48	113.45
1	D	146	ASP	N-CA-C	-5.72	103.37	110.41
1	H	198	GLN	CB-CA-C	-5.68	108.89	117.07
1	A	46	LEU	N-CA-C	5.67	117.80	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	101	ASN	N-CA-C	-5.65	105.73	113.30
1	I	36	GLY	N-CA-C	-5.63	107.60	114.92
1	B	177	TRP	N-CA-C	5.62	118.21	110.35
1	C	185	LYS	CA-C-N	5.59	126.83	119.84
1	C	185	LYS	C-N-CA	5.59	126.83	119.84
1	H	147	LEU	CA-C-N	5.57	125.03	119.24
1	H	147	LEU	C-N-CA	5.57	125.03	119.24
1	I	185	LYS	CA-C-N	5.55	126.77	119.84
1	I	185	LYS	C-N-CA	5.55	126.77	119.84
1	H	38	TYR	N-CA-C	-5.54	103.39	110.53
1	A	101	ASN	N-CA-C	-5.53	104.78	113.02
1	C	147	LEU	N-CA-C	5.51	121.99	109.81
1	H	111	THR	N-CA-C	5.49	117.07	111.14
1	C	69	LEU	N-CA-C	-5.49	105.21	112.94
1	E	46	LEU	N-CA-C	5.47	117.71	109.23
1	C	26	PHE	N-CA-C	5.42	122.33	110.80
1	F	26	PHE	N-CA-C	5.40	118.26	107.62
1	E	109	LYS	N-CA-C	-5.30	106.59	113.16
1	J	105	VAL	N-CA-C	5.26	116.16	108.53
1	J	185	LYS	CA-C-N	5.25	126.41	119.84
1	J	185	LYS	C-N-CA	5.25	126.41	119.84
1	D	148	PRO	N-CA-C	5.25	120.92	114.35
1	E	134	ASP	N-CA-C	5.25	118.19	110.59
1	B	184	ILE	N-CA-C	5.24	117.40	108.86
1	J	107	ASP	CA-C-N	5.23	124.55	118.85
1	J	107	ASP	C-N-CA	5.23	124.55	118.85
1	J	35	LYS	N-CA-C	-5.23	102.65	110.23
1	C	146	ASP	N-CA-C	-5.21	103.16	110.50
1	I	149	VAL	N-CA-C	5.20	115.98	107.24
1	I	148	PRO	N-CA-C	5.20	120.69	113.98
1	J	146	ASP	N-CA-C	-5.18	104.04	110.41
1	D	56	ILE	N-CA-C	5.17	115.94	110.72
1	B	191	SER	N-CA-C	-5.16	105.73	111.36
1	H	198	GLN	CA-C-O	5.15	120.93	117.94
1	B	146	ASP	N-CA-C	-5.15	103.69	110.43
1	A	134	ASP	N-CA-C	5.13	117.14	110.53
1	D	184	ILE	N-CA-C	5.11	116.07	108.46
1	C	173	CYS	N-CA-C	5.10	117.87	108.69
1	E	107	ASP	CA-C-N	5.10	124.71	119.56
1	E	107	ASP	C-N-CA	5.10	124.71	119.56
1	E	173	CYS	N-CA-C	5.08	116.76	109.04
1	B	90	THR	CA-C-N	5.07	125.35	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	THR	C-N-CA	5.07	125.35	119.93
1	C	101	ASN	N-CA-C	-5.06	105.81	112.94
1	H	148	PRO	N-CA-C	5.04	121.95	113.78
1	E	24	GLY	N-CA-C	-5.04	103.00	112.22
1	E	148	PRO	N-CA-C	5.03	120.44	113.65
1	I	173	CYS	N-CA-C	5.02	117.46	108.47
1	F	57	ILE	N-CA-C	-5.01	105.96	110.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1546	0	1540	134	0
1	B	1546	0	1541	116	0
1	C	1546	0	1540	129	0
1	D	1546	0	1541	123	0
1	E	1546	0	1541	120	0
1	F	1546	0	1541	140	0
1	G	1546	0	1541	139	0
1	H	1546	0	1541	115	0
1	I	1546	0	1541	131	0
1	J	1546	0	1541	114	0
All	All	15460	0	15408	1159	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 38.

All (1159) 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:91:PRO:HG2	1:A:94:GLN:HG3	1.29	1.11
1:H:8:ILE:HD13	1:H:8:ILE:H	1.21	1.06
1:A:97:LEU:HB3	1:A:100:MET:HE3	1.41	1.02
1:H:73:VAL:HB	1:H:102:ILE:HD11	1.44	1.00
1:E:91:PRO:HG2	1:E:94:GLN:HG3	1.44	0.99
1:E:93:LYS:H	1:E:93:LYS:HD3	1.27	0.98
1:I:132:ILE:HG23	1:I:141:GLN:HB3	1.47	0.96
1:J:94:GLN:HA	1:J:94:GLN:HE21	1.31	0.96
1:A:133:ILE:HD12	1:A:134:ASP:N	1.81	0.95
1:I:184:ILE:HD13	1:I:185:LYS:N	1.82	0.94
1:A:3:SER:HB3	1:B:3:SER:HB2	1.50	0.94
1:A:56:ILE:HD11	1:A:100:MET:SD	2.08	0.93
1:E:155:GLU:HG3	1:F:155:GLU:HG2	1.50	0.93
1:G:110:ARG:NH1	1:G:110:ARG:HB3	1.84	0.92
1:J:93:LYS:HZ1	1:J:93:LYS:H	1.09	0.92
1:E:78:VAL:HB	1:E:110:ARG:NH1	1.84	0.91
1:G:46:LEU:HD21	1:G:125:ILE:HD11	1.53	0.91
1:I:8:ILE:HD11	1:J:127:PHE:CD1	2.06	0.90
1:G:92:LYS:H	1:G:92:LYS:HD3	1.33	0.90
1:I:46:LEU:HD21	1:I:125:ILE:HD11	1.50	0.90
1:G:184:ILE:HD11	1:G:191:SER:HB2	1.54	0.89
1:C:46:LEU:HD21	1:C:125:ILE:HD11	1.55	0.89
1:B:78:VAL:HB	1:B:110:ARG:HH12	1.38	0.89
1:F:93:LYS:HE3	1:F:93:LYS:H	1.38	0.88
1:A:93:LYS:H	1:A:93:LYS:HZ2	1.21	0.88
1:A:46:LEU:HD21	1:A:125:ILE:HD11	1.54	0.87
1:A:184:ILE:HD11	1:A:191:SER:HB2	1.56	0.86
1:I:57:ILE:HD13	1:I:58:ALA:H	1.40	0.85
1:A:15:PHE:CE2	1:A:31:LEU:HB2	2.12	0.85
1:J:90:THR:O	1:J:96:GLY:HA3	1.77	0.85
1:B:56:ILE:HD11	1:B:100:MET:SD	2.17	0.84
1:F:110:ARG:HG2	1:F:110:ARG:HH11	1.41	0.84
1:C:92:LYS:HE3	1:D:199:LYS:HE2	1.57	0.84
1:F:42:PHE:HB3	1:F:130:LEU:HD12	1.60	0.83
1:J:93:LYS:H	1:J:93:LYS:NZ	1.75	0.83
1:C:53:PRO:O	1:C:57:ILE:HG22	1.77	0.83
1:H:131:PHE:HD1	1:H:142:ILE:HG22	1.43	0.83
1:J:38:TYR:HD2	1:J:132:ILE:HD11	1.44	0.82
1:D:56:ILE:HD11	1:D:100:MET:SD	2.20	0.82
1:E:130:LEU:HD13	1:E:131:PHE:N	1.94	0.82
1:G:65:GLU:HA	1:G:68:LYS:HE2	1.61	0.82
1:I:133:ILE:HD12	1:I:134:ASP:N	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:8:ILE:HD11	1:J:142:ILE:HG22	1.60	0.81
1:F:56:ILE:HD12	1:F:97:LEU:HD22	1.62	0.81
1:A:20:VAL:HG22	1:A:81:HIS:CE1	2.16	0.81
1:J:132:ILE:HG23	1:J:141:GLN:HB3	1.63	0.81
1:F:37:LYS:HG2	1:F:70:ASN:HD21	1.44	0.80
1:G:85:LEU:HA	1:G:88:ILE:HD11	1.63	0.80
1:H:5:ASN:O	1:H:7:LYS:HE2	1.80	0.80
1:J:53:PRO:O	1:J:57:ILE:HG23	1.80	0.80
1:C:93:LYS:H	1:C:93:LYS:HD2	1.46	0.80
1:A:53:PRO:O	1:A:57:ILE:HG22	1.82	0.80
1:H:131:PHE:CD1	1:H:142:ILE:HG22	2.16	0.80
1:D:184:ILE:HD11	1:D:191:SER:HA	1.62	0.80
1:A:91:PRO:HG2	1:A:94:GLN:CG	2.11	0.79
1:A:138:ILE:HD12	1:A:139:LEU:N	1.97	0.79
1:B:53:PRO:HA	1:B:56:ILE:HG23	1.64	0.79
1:F:52:SER:O	1:F:56:ILE:HG22	1.83	0.79
1:J:38:TYR:CD2	1:J:132:ILE:HD11	2.17	0.79
1:B:132:ILE:HG23	1:B:141:GLN:HB3	1.63	0.79
1:G:53:PRO:HA	1:G:56:ILE:HG23	1.65	0.79
1:G:52:SER:O	1:G:56:ILE:HG22	1.83	0.79
1:I:37:LYS:HD2	1:I:70:ASN:ND2	1.99	0.78
1:B:78:VAL:HB	1:B:110:ARG:NH1	1.97	0.78
1:C:29:ILE:HD11	1:C:105:VAL:HG12	1.66	0.78
1:C:187:ASP:HB3	1:C:190:LYS:HB2	1.66	0.78
1:C:125:ILE:HG23	1:C:126:SER:N	1.97	0.77
1:D:24:GLY:O	1:D:25:GLN:HG2	1.84	0.77
1:G:160:VAL:O	1:G:164:GLN:HG3	1.82	0.77
1:J:76:ALA:HB2	1:J:105:VAL:HB	1.66	0.77
1:H:145:ASN:HD22	1:H:151:ARG:HG3	1.49	0.77
1:C:15:PHE:CE2	1:C:31:LEU:HB2	2.20	0.77
1:D:125:ILE:HG22	1:D:126:SER:N	1.97	0.77
1:G:171:GLU:HG2	1:G:185:LYS:HG3	1.65	0.76
1:I:37:LYS:HD2	1:I:70:ASN:HD21	1.50	0.76
1:I:92:LYS:HE2	1:J:199:LYS:HD2	1.68	0.76
1:J:56:ILE:HD11	1:J:97:LEU:HD13	1.68	0.76
1:I:93:LYS:H	1:I:93:LYS:HD2	1.51	0.76
1:B:132:ILE:HD13	1:B:132:ILE:O	1.86	0.76
1:G:53:PRO:HA	1:G:56:ILE:CG2	2.16	0.75
1:B:165:PHE:CE2	1:B:183:THR:HG21	2.21	0.75
1:I:93:LYS:H	1:I:93:LYS:CD	1.99	0.75
1:I:78:VAL:HB	1:I:110:ARG:NH1	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:MET:HG2	1:I:104:LEU:HD21	1.67	0.75
1:C:132:ILE:C	1:C:132:ILE:HD13	2.11	0.75
1:E:42:PHE:HB3	1:E:130:LEU:HD22	1.69	0.75
1:E:132:ILE:HD12	1:E:160:VAL:HG22	1.69	0.75
1:I:50:PHE:HB3	1:J:184:ILE:HD12	1.68	0.75
1:D:56:ILE:HD12	1:D:97:LEU:HD22	1.67	0.75
1:E:142:ILE:HD12	1:F:144:ILE:HD12	1.69	0.74
1:F:56:ILE:C	1:F:56:ILE:HD13	2.12	0.74
1:C:29:ILE:HD11	1:C:105:VAL:CG1	2.18	0.74
1:G:85:LEU:HD12	1:G:88:ILE:HD11	1.68	0.74
1:H:130:LEU:HB3	1:H:143:THR:HB	1.70	0.74
1:J:88:ILE:HA	1:J:97:LEU:HB2	1.69	0.74
1:G:57:ILE:HG21	1:H:199:LYS:HE2	1.69	0.73
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.53	0.73
1:A:110:ARG:HD2	1:C:110:ARG:HD2	1.70	0.73
1:J:132:ILE:CG2	1:J:141:GLN:HB3	2.19	0.73
1:F:97:LEU:HB3	1:F:100:MET:HE3	1.69	0.73
1:D:194:TYR:HA	1:D:197:LYS:HE2	1.71	0.73
1:A:9:GLY:C	1:A:138:ILE:HD13	2.13	0.72
1:J:184:ILE:C	1:J:184:ILE:HD13	2.14	0.72
1:E:142:ILE:HD11	1:F:142:ILE:HD11	1.71	0.72
1:C:91:PRO:HG2	1:C:94:GLN:HG2	1.71	0.72
1:G:19:ALA:HB2	1:G:105:VAL:HG12	1.72	0.72
1:D:184:ILE:HD12	1:D:185:LYS:H	1.55	0.71
1:G:90:THR:O	1:G:96:GLY:HA3	1.89	0.71
1:H:42:PHE:HB3	1:H:130:LEU:CD2	2.20	0.71
1:B:194:TYR:O	1:B:198:GLN:HB2	1.90	0.71
1:J:199:LYS:HE2	1:J:199:LYS:H	1.53	0.71
1:E:50:PHE:HB3	1:F:184:ILE:HD12	1.70	0.71
1:G:76:ALA:HB2	1:G:105:VAL:HG22	1.72	0.71
1:E:116:TYR:O	1:E:118:VAL:HG13	1.91	0.71
1:B:142:ILE:HD13	1:B:142:ILE:C	2.16	0.70
1:E:93:LYS:HD3	1:E:93:LYS:N	2.02	0.70
1:J:73:VAL:HB	1:J:102:ILE:HD11	1.72	0.70
1:D:125:ILE:CG2	1:D:126:SER:N	2.54	0.70
1:G:27:LYS:HG3	1:G:28:ASP:H	1.56	0.70
1:I:93:LYS:HD2	1:I:93:LYS:N	2.06	0.70
1:C:184:ILE:HG12	1:D:50:PHE:HB3	1.74	0.70
1:A:26:PHE:HD1	1:A:26:PHE:H	1.39	0.70
1:E:78:VAL:HB	1:E:110:ARG:HH12	1.53	0.70
1:F:42:PHE:CB	1:F:130:LEU:HD12	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:PRO:HA	1:G:138:ILE:HA	1.72	0.70
1:D:140:ARG:HH11	1:D:140:ARG:HB3	1.56	0.69
1:C:62:ARG:HB3	1:C:65:GLU:HG3	1.73	0.69
1:G:27:LYS:HG3	1:G:28:ASP:N	2.07	0.69
1:C:196:SER:O	1:D:93:LYS:HE2	1.92	0.69
1:B:46:LEU:HD22	1:F:80:SER:HB3	1.72	0.69
1:H:53:PRO:HB3	1:H:87:TRP:CZ2	2.27	0.69
1:D:125:ILE:CG2	1:D:126:SER:H	2.06	0.69
1:E:57:ILE:C	1:E:57:ILE:HD13	2.18	0.69
1:B:138:ILE:HD12	1:B:139:LEU:N	2.09	0.68
1:B:187:ASP:O	1:B:191:SER:HB3	1.92	0.68
1:H:8:ILE:H	1:H:8:ILE:CD1	1.98	0.68
1:B:62:ARG:HD2	1:B:65:GLU:OE1	1.94	0.68
1:C:91:PRO:HG2	1:C:94:GLN:CG	2.24	0.68
1:D:97:LEU:HB3	1:D:100:MET:HE3	1.76	0.68
1:E:53:PRO:O	1:E:57:ILE:HG22	1.93	0.68
1:A:132:ILE:HG23	1:A:141:GLN:HB3	1.75	0.68
1:C:46:LEU:CD2	1:C:125:ILE:HD11	2.22	0.68
1:G:9:GLY:C	1:G:138:ILE:HD13	2.19	0.68
1:B:57:ILE:HD13	1:B:58:ALA:N	2.09	0.68
1:G:155:GLU:HG2	1:H:155:GLU:HG2	1.75	0.68
1:C:132:ILE:HD13	1:C:132:ILE:O	1.93	0.68
1:I:155:GLU:HG2	1:J:155:GLU:HG2	1.75	0.68
1:I:73:VAL:O	1:I:102:ILE:HG13	1.93	0.68
1:B:24:GLY:O	1:B:25:GLN:HB3	1.92	0.68
1:C:56:ILE:HD11	1:C:100:MET:SD	2.33	0.68
1:D:164:GLN:O	1:D:168:LYS:HD3	1.94	0.68
1:E:78:VAL:HB	1:E:110:ARG:CZ	2.24	0.68
1:C:3:SER:HA	1:D:3:SER:N	2.09	0.67
1:C:184:ILE:HD13	1:C:191:SER:CB	2.24	0.67
1:B:8:ILE:C	1:B:8:ILE:HD12	2.19	0.67
1:E:184:ILE:HD11	1:E:191:SER:HB2	1.76	0.67
1:F:110:ARG:HG2	1:F:110:ARG:NH1	2.07	0.67
1:D:53:PRO:O	1:D:57:ILE:HG23	1.95	0.67
1:J:165:PHE:CE2	1:J:183:THR:HG21	2.28	0.67
1:E:81:HIS:H	1:E:81:HIS:CD2	2.12	0.67
1:C:88:ILE:HD13	1:C:97:LEU:HD12	1.77	0.67
1:G:55:GLU:OE2	1:G:150:GLY:HA2	1.95	0.67
1:E:132:ILE:HG23	1:E:141:GLN:HB3	1.75	0.67
1:B:142:ILE:HD11	1:B:144:ILE:HG13	1.75	0.67
1:A:8:ILE:HD12	1:B:146:ASP:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HD11	1:B:127:PHE:CD1	2.30	0.66
1:E:184:ILE:HD12	1:E:185:LYS:N	2.10	0.66
1:F:81:HIS:CD2	1:F:81:HIS:H	2.12	0.66
1:I:85:LEU:O	1:I:88:ILE:HG13	1.96	0.66
1:D:128:ARG:HH11	1:D:128:ARG:HG2	1.58	0.66
1:A:8:ILE:HD11	1:B:127:PHE:CG	2.31	0.66
1:E:199:LYS:O	1:F:93:LYS:HE2	1.96	0.66
1:I:184:ILE:HD13	1:I:185:LYS:H	1.59	0.66
1:F:93:LYS:HE3	1:F:93:LYS:N	2.11	0.66
1:H:189:ASN:O	1:H:192:LYS:HG2	1.96	0.66
1:J:91:PRO:HG2	1:J:94:GLN:HB2	1.77	0.66
1:E:91:PRO:HG2	1:E:94:GLN:CG	2.25	0.66
1:F:8:ILE:C	1:F:8:ILE:HD13	2.21	0.65
1:G:51:VAL:HB	1:G:128:ARG:NH2	2.11	0.65
1:H:59:PHE:CE1	1:H:153:VAL:HG22	2.32	0.65
1:B:9:GLY:C	1:B:138:ILE:HD13	2.22	0.65
1:C:56:ILE:HD12	1:C:97:LEU:HD22	1.76	0.65
1:I:76:ALA:HB2	1:I:105:VAL:HG13	1.77	0.65
1:A:91:PRO:CG	1:A:94:GLN:HG3	2.18	0.65
1:B:53:PRO:O	1:B:57:ILE:HG23	1.97	0.65
1:C:133:ILE:HD13	1:C:133:ILE:O	1.96	0.65
1:F:133:ILE:CD1	1:F:137:GLY:HA2	2.26	0.65
1:J:189:ASN:C	1:J:191:SER:H	2.04	0.65
1:G:37:LYS:HZ2	1:G:70:ASN:ND2	1.95	0.65
1:A:138:ILE:HD12	1:A:138:ILE:C	2.22	0.65
1:G:67:LYS:HE3	1:G:67:LYS:HA	1.79	0.65
1:I:90:THR:O	1:I:96:GLY:HA3	1.97	0.65
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.62	0.65
1:J:142:ILE:HD11	1:J:144:ILE:HD11	1.77	0.65
1:G:184:ILE:HD13	1:G:185:LYS:N	2.11	0.65
1:D:123:GLU:HG2	1:D:125:ILE:HD13	1.80	0.64
1:G:110:ARG:HB3	1:G:110:ARG:HH11	1.61	0.64
1:I:88:ILE:HA	1:I:97:LEU:HB2	1.78	0.64
1:D:66:PHE:CZ	1:D:157:LEU:HD13	2.33	0.64
1:E:124:GLY:O	1:E:125:ILE:HD12	1.97	0.64
1:J:94:GLN:HA	1:J:94:GLN:NE2	2.10	0.64
1:I:133:ILE:HD11	1:I:137:GLY:HA2	1.80	0.64
1:J:184:ILE:HD13	1:J:185:LYS:N	2.13	0.64
1:A:57:ILE:O	1:A:57:ILE:HD13	1.98	0.64
1:A:185:LYS:HD3	1:A:190:LYS:HE2	1.79	0.64
1:H:199:LYS:HZ2	1:H:199:LYS:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ILE:HD13	1:E:57:ILE:O	1.98	0.64
1:H:124:GLY:O	1:H:125:ILE:HD12	1.98	0.64
1:D:53:PRO:HA	1:D:56:ILE:HG23	1.79	0.64
1:D:187:ASP:O	1:D:191:SER:HB3	1.98	0.64
1:H:160:VAL:O	1:H:164:GLN:HG3	1.98	0.64
1:E:132:ILE:CG2	1:E:141:GLN:HB3	2.28	0.64
1:B:57:ILE:HD13	1:B:58:ALA:H	1.63	0.64
1:C:132:ILE:HG23	1:C:141:GLN:HB3	1.80	0.64
1:C:196:SER:HA	1:D:93:LYS:HG2	1.80	0.63
1:E:152:SER:O	1:E:156:ILE:HG12	1.97	0.63
1:I:102:ILE:HG13	1:I:103:PRO:HD2	1.79	0.63
1:E:93:LYS:H	1:E:93:LYS:CD	1.99	0.63
1:F:43:PHE:HZ	1:F:112:ILE:HG22	1.62	0.63
1:E:46:LEU:HD21	1:E:125:ILE:HD11	1.80	0.63
1:I:8:ILE:HD11	1:J:127:PHE:CG	2.32	0.63
1:F:62:ARG:HD3	1:F:153:VAL:HG11	1.79	0.63
1:H:72:GLN:HE21	1:H:73:VAL:H	1.45	0.63
1:A:132:ILE:CG2	1:A:141:GLN:HB3	2.29	0.63
1:B:27:LYS:HB3	1:B:29:ILE:CD1	2.28	0.63
1:B:131:PHE:HB3	1:B:139:LEU:HD11	1.81	0.63
1:G:32:SER:C	1:G:34:TYR:H	2.06	0.63
1:J:199:LYS:HE2	1:J:199:LYS:N	2.14	0.63
1:A:10:HIS:N	1:A:138:ILE:HD13	2.14	0.63
1:A:142:ILE:HD11	1:A:144:ILE:HG13	1.81	0.63
1:C:184:ILE:HD12	1:C:185:LYS:N	2.13	0.63
1:E:42:PHE:HB3	1:E:130:LEU:CD2	2.28	0.63
1:G:158:ARG:HD2	1:G:177:TRP:O	1.99	0.63
1:H:9:GLY:C	1:H:138:ILE:HD13	2.24	0.63
1:F:134:ASP:OD2	1:F:138:ILE:HG13	1.99	0.63
1:I:56:ILE:HD12	1:I:104:LEU:HD11	1.81	0.62
1:A:38:TYR:OH	1:A:167:ASP:OD2	2.15	0.62
1:A:133:ILE:HD11	1:A:137:GLY:CA	2.29	0.62
1:B:110:ARG:NE	1:F:110:ARG:HE	1.97	0.62
1:J:73:VAL:O	1:J:102:ILE:HG13	1.98	0.62
1:C:84:HIS:CD2	1:C:104:LEU:HB3	2.34	0.62
1:C:125:ILE:CG2	1:C:126:SER:N	2.62	0.62
1:D:199:LYS:H	1:D:199:LYS:HD3	1.64	0.62
1:J:93:LYS:HZ1	1:J:93:LYS:N	1.89	0.62
1:A:85:LEU:HA	1:A:88:ILE:HG23	1.81	0.62
1:B:84:HIS:O	1:B:88:ILE:HG23	2.00	0.62
1:D:195:PHE:O	1:D:198:GLN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ILE:HD12	1:E:88:ILE:C	2.25	0.62
1:E:175:ALA:HB2	1:F:55:GLU:HB3	1.81	0.62
1:H:184:ILE:C	1:H:184:ILE:HD13	2.24	0.62
1:B:50:PHE:O	1:B:53:PRO:HD2	1.99	0.62
1:B:132:ILE:CG2	1:B:141:GLN:HB3	2.29	0.62
1:D:184:ILE:HD11	1:D:191:SER:CA	2.30	0.62
1:F:46:LEU:HD21	1:F:125:ILE:HD12	1.82	0.62
1:I:132:ILE:CG2	1:I:141:GLN:HB3	2.27	0.62
1:J:165:PHE:HE2	1:J:183:THR:HG21	1.65	0.61
1:C:3:SER:N	1:D:3:SER:N	2.48	0.61
1:D:64:GLU:O	1:D:68:LYS:HG3	2.00	0.61
1:G:109:LYS:HZ3	1:G:109:LYS:HB3	1.65	0.61
1:A:133:ILE:HD12	1:A:133:ILE:C	2.25	0.61
1:D:138:ILE:HG13	1:D:140:ARG:HD3	1.81	0.61
1:B:94:GLN:HA	1:B:94:GLN:HE21	1.64	0.61
1:D:56:ILE:C	1:D:56:ILE:HD13	2.25	0.61
1:F:184:ILE:HD11	1:F:191:SER:HB2	1.81	0.61
1:G:37:LYS:NZ	1:G:70:ASN:ND2	2.49	0.61
1:G:85:LEU:HA	1:G:88:ILE:CD1	2.31	0.61
1:G:184:ILE:HD13	1:G:184:ILE:C	2.25	0.61
1:H:84:HIS:CD2	1:H:104:LEU:HB3	2.36	0.61
1:C:125:ILE:HG23	1:C:126:SER:H	1.63	0.61
1:I:56:ILE:HG12	1:I:97:LEU:HD22	1.82	0.61
1:A:15:PHE:CZ	1:A:31:LEU:HB2	2.34	0.61
1:A:142:ILE:CD1	1:A:144:ILE:HG13	2.30	0.61
1:D:132:ILE:HG12	1:D:141:GLN:HB3	1.82	0.61
1:F:157:LEU:C	1:F:161:GLN:HE21	2.09	0.61
1:G:73:VAL:HB	1:G:102:ILE:HD12	1.81	0.61
1:H:68:LYS:HB2	1:H:68:LYS:NZ	2.14	0.61
1:A:25:GLN:O	1:A:25:GLN:HG2	1.99	0.61
1:F:24:GLY:O	1:F:25:GLN:HB2	2.01	0.61
1:F:189:ASN:O	1:F:192:LYS:HG3	2.00	0.61
1:B:138:ILE:HD12	1:B:138:ILE:C	2.26	0.61
1:G:109:LYS:C	1:G:110:ARG:HD2	2.26	0.60
1:J:146:ASP:OD1	1:J:147:LEU:N	2.33	0.60
1:F:67:LYS:HB2	1:F:67:LYS:NZ	2.16	0.60
1:B:120:LYS:HE2	1:B:123:GLU:OE2	2.02	0.60
1:D:51:VAL:HB	1:D:128:ARG:NH2	2.17	0.60
1:G:37:LYS:HZ2	1:G:70:ASN:HD21	1.47	0.60
1:H:78:VAL:HB	1:H:110:ARG:CZ	2.31	0.60
1:H:145:ASN:ND2	1:H:151:ARG:HG3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HB3	1:A:179:PRO:HD2	1.84	0.60
1:E:165:PHE:CE2	1:E:183:THR:HG21	2.36	0.60
1:F:133:ILE:HD11	1:F:137:GLY:HA2	1.83	0.60
1:G:142:ILE:HG23	1:H:144:ILE:HB	1.82	0.60
1:B:114:GLN:HG3	1:B:119:LEU:HD12	1.83	0.60
1:D:142:ILE:HD13	1:D:142:ILE:C	2.26	0.60
1:E:91:PRO:HB2	1:E:93:LYS:HE2	1.83	0.60
1:D:142:ILE:HD13	1:D:142:ILE:O	2.02	0.60
1:D:184:ILE:HD12	1:D:185:LYS:N	2.17	0.60
1:E:155:GLU:HG3	1:F:155:GLU:CG	2.27	0.60
1:A:21:MET:HB3	1:A:22:PRO:HD2	1.83	0.59
1:D:125:ILE:HG22	1:D:126:SER:H	1.65	0.59
1:D:128:ARG:HG2	1:D:128:ARG:NH1	2.17	0.59
1:G:97:LEU:HB3	1:G:100:MET:HE3	1.84	0.59
1:G:156:ILE:HG12	1:G:156:ILE:O	2.01	0.59
1:A:133:ILE:CD1	1:A:137:GLY:C	2.75	0.59
1:A:184:ILE:CD1	1:A:191:SER:HB2	2.29	0.59
1:A:3:SER:HB3	1:B:3:SER:CB	2.30	0.59
1:A:124:GLY:O	1:A:125:ILE:HD12	2.02	0.59
1:B:114:GLN:HG3	1:B:119:LEU:CD1	2.32	0.59
1:H:152:SER:O	1:H:156:ILE:HD13	2.02	0.59
1:J:130:LEU:HD11	1:J:156:ILE:HG13	1.84	0.59
1:H:78:VAL:HB	1:H:110:ARG:NH1	2.17	0.59
1:A:132:ILE:HD13	1:A:132:ILE:O	2.02	0.59
1:B:8:ILE:HD12	1:B:9:GLY:N	2.18	0.59
1:I:63:ALA:O	1:I:67:LYS:HG2	2.02	0.59
1:I:73:VAL:HB	1:I:102:ILE:HD11	1.85	0.59
1:I:184:ILE:HD11	1:I:191:SER:HB2	1.85	0.59
1:J:197:LYS:O	1:J:197:LYS:HG2	2.03	0.59
1:D:52:SER:O	1:D:56:ILE:HG22	2.03	0.59
1:D:84:HIS:O	1:D:88:ILE:HG23	2.02	0.59
1:F:78:VAL:CB	1:F:110:ARG:HH12	2.15	0.59
1:E:140:ARG:HG3	1:E:140:ARG:HH11	1.68	0.59
1:C:3:SER:HB3	1:D:3:SER:OG	2.03	0.59
1:C:8:ILE:HD11	1:C:142:ILE:HG22	1.85	0.58
1:G:8:ILE:HD12	1:G:139:LEU:O	2.03	0.58
1:G:110:ARG:HB3	1:G:110:ARG:CZ	2.32	0.58
1:B:119:LEU:HD23	1:B:120:LYS:N	2.18	0.58
1:I:120:LYS:HD2	1:I:127:PHE:CE1	2.39	0.58
1:B:46:LEU:HD22	1:F:80:SER:CB	2.33	0.58
1:C:75:GLY:O	1:C:105:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:LEU:HD11	1:E:161:GLN:HE21	1.68	0.58
1:G:3:SER:HB3	1:H:3:SER:HB2	1.86	0.58
1:I:57:ILE:HD13	1:I:58:ALA:N	2.14	0.58
1:D:56:ILE:HD13	1:D:57:ILE:N	2.18	0.58
1:G:195:PHE:O	1:G:198:GLN:HG2	2.03	0.58
1:E:187:ASP:O	1:E:191:SER:HB3	2.03	0.58
1:F:88:ILE:HD12	1:F:88:ILE:O	2.04	0.58
1:I:186:PRO:HA	1:J:50:PHE:CD2	2.39	0.58
1:G:128:ARG:C	1:G:151:ARG:NH1	2.62	0.58
1:J:132:ILE:HD12	1:J:133:ILE:N	2.19	0.58
1:A:78:VAL:HB	1:A:110:ARG:NH1	2.19	0.58
1:D:172:VAL:HG22	1:D:184:ILE:HG23	1.86	0.58
1:G:31:LEU:HD11	1:G:133:ILE:HD11	1.85	0.58
1:B:51:VAL:HB	1:B:128:ARG:NH2	2.19	0.58
1:C:93:LYS:H	1:C:93:LYS:CD	2.11	0.58
1:D:118:VAL:HG12	1:D:144:ILE:HD12	1.86	0.58
1:G:16:LYS:HE3	1:G:28:ASP:HB3	1.84	0.58
1:H:72:GLN:NE2	1:H:73:VAL:H	2.02	0.58
1:E:184:ILE:HD11	1:E:191:SER:CB	2.34	0.57
1:F:46:LEU:HD21	1:F:125:ILE:CD1	2.34	0.57
1:J:189:ASN:O	1:J:191:SER:N	2.37	0.57
1:C:87:TRP:CE3	1:C:97:LEU:HD11	2.38	0.57
1:C:132:ILE:CG2	1:C:141:GLN:HB3	2.34	0.57
1:B:90:THR:O	1:B:96:GLY:HA3	2.03	0.57
1:E:75:GLY:O	1:E:105:VAL:HG22	2.04	0.57
1:E:142:ILE:HD13	1:E:142:ILE:O	2.04	0.57
1:H:107:ASP:CG	1:H:112:ILE:HG23	2.29	0.57
1:C:34:TYR:O	1:C:36:GLY:N	2.37	0.57
1:D:184:ILE:CD1	1:D:191:SER:HA	2.31	0.57
1:F:27:LYS:HG2	1:F:28:ASP:N	2.18	0.57
1:C:110:ARG:HG2	1:C:110:ARG:NH1	2.16	0.57
1:D:46:LEU:HG	1:D:125:ILE:HG13	1.86	0.57
1:D:157:LEU:O	1:D:161:GLN:HG3	2.03	0.57
1:A:133:ILE:HD13	1:A:137:GLY:C	2.30	0.57
1:F:78:VAL:HG11	1:F:110:ARG:HH12	1.70	0.57
1:H:158:ARG:HD2	1:H:177:TRP:O	2.05	0.57
1:C:81:HIS:H	1:C:81:HIS:CD2	2.20	0.57
1:D:7:LYS:HD3	1:D:10:HIS:ND1	2.20	0.57
1:B:81:HIS:CD2	1:B:81:HIS:H	2.22	0.57
1:C:87:TRP:CH2	1:C:97:LEU:HD21	2.39	0.57
1:E:185:LYS:HD3	1:E:190:LYS:HZ3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:GLY:O	1:G:25:GLN:O	2.23	0.57
1:G:110:ARG:HH11	1:G:110:ARG:CB	2.17	0.57
1:I:142:ILE:CD1	1:I:144:ILE:HG13	2.35	0.57
1:C:3:SER:CA	1:D:3:SER:N	2.68	0.57
1:C:87:TRP:CZ2	1:C:97:LEU:HD21	2.40	0.57
1:D:27:LYS:HE2	1:D:29:ILE:HD11	1.87	0.57
1:D:133:ILE:HD13	1:D:137:GLY:C	2.30	0.57
1:J:84:HIS:O	1:J:88:ILE:HG23	2.05	0.57
1:J:142:ILE:HD13	1:J:142:ILE:C	2.29	0.57
1:I:132:ILE:HG13	1:I:132:ILE:O	2.04	0.56
1:A:133:ILE:HD12	1:A:134:ASP:H	1.67	0.56
1:C:84:HIS:O	1:C:88:ILE:HG12	2.05	0.56
1:C:133:ILE:HD13	1:C:133:ILE:C	2.29	0.56
1:H:47:ASP:O	1:H:48:PHE:HB2	2.05	0.56
1:H:138:ILE:HD12	1:H:138:ILE:C	2.30	0.56
1:A:9:GLY:H	1:A:138:ILE:HD11	1.70	0.56
1:A:160:VAL:HG12	1:A:164:GLN:NE2	2.21	0.56
1:B:94:GLN:HE21	1:B:94:GLN:CA	2.16	0.56
1:D:57:ILE:HD13	1:D:58:ALA:N	2.21	0.56
1:F:199:LYS:HB2	1:F:199:LYS:HZ3	1.71	0.56
1:I:97:LEU:HB3	1:I:100:MET:CE	2.35	0.56
1:C:32:SER:C	1:C:34:TYR:H	2.14	0.56
1:C:130:LEU:HD23	1:C:130:LEU:C	2.31	0.56
1:E:199:LYS:HD3	1:F:92:LYS:HB3	1.87	0.56
1:G:109:LYS:HB3	1:G:109:LYS:NZ	2.21	0.56
1:I:97:LEU:HB3	1:I:100:MET:HE1	1.87	0.56
1:F:51:VAL:HB	1:F:128:ARG:NH2	2.20	0.56
1:F:134:ASP:CG	1:F:138:ILE:HG13	2.31	0.56
1:I:50:PHE:O	1:I:53:PRO:HD2	2.06	0.56
1:E:156:ILE:O	1:E:160:VAL:HG23	2.05	0.56
1:I:93:LYS:H	1:I:93:LYS:CE	2.18	0.56
1:A:118:VAL:HG23	1:A:126:SER:HB2	1.86	0.55
1:E:24:GLY:O	1:E:25:GLN:HB3	2.04	0.55
1:E:47:ASP:O	1:E:48:PHE:HB2	2.06	0.55
1:F:190:LYS:HB2	1:F:190:LYS:NZ	2.21	0.55
1:I:120:LYS:HE3	1:I:123:GLU:OE2	2.06	0.55
1:I:132:ILE:HD13	1:I:160:VAL:HG22	1.88	0.55
1:D:53:PRO:O	1:D:57:ILE:HD12	2.06	0.55
1:F:78:VAL:HG11	1:F:110:ARG:NH1	2.20	0.55
1:G:44:TYR:HB2	1:G:52:SER:OG	2.06	0.55
1:G:172:VAL:O	1:G:174:PRO:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:GLU:HA	1:H:175:ALA:HB2	1.88	0.55
1:A:127:PHE:CE1	1:B:8:ILE:HD11	2.41	0.55
1:E:158:ARG:HD2	1:E:177:TRP:O	2.06	0.55
1:I:185:LYS:HG3	1:I:190:LYS:HB3	1.87	0.55
1:J:13:PRO:HB2	1:J:116:TYR:CE1	2.42	0.55
1:J:199:LYS:O	1:J:199:LYS:HG2	2.07	0.55
1:B:27:LYS:HB3	1:B:29:ILE:HD11	1.87	0.55
1:E:130:LEU:HD13	1:E:131:PHE:H	1.70	0.55
1:F:76:ALA:HB2	1:F:105:VAL:HB	1.89	0.55
1:G:46:LEU:HB2	1:G:49:THR:HG21	1.89	0.55
1:J:172:VAL:CG2	1:J:184:ILE:HG23	2.36	0.55
1:E:100:MET:HE2	1:E:100:MET:HA	1.89	0.55
1:F:46:LEU:HB2	1:F:49:THR:HG21	1.89	0.55
1:H:42:PHE:HB3	1:H:130:LEU:HD23	1.87	0.55
1:H:138:ILE:HD12	1:H:139:LEU:O	2.06	0.55
1:J:46:LEU:HD21	1:J:125:ILE:CD1	2.36	0.55
1:E:114:GLN:OE1	1:E:119:LEU:HD23	2.07	0.55
1:A:56:ILE:HD12	1:A:56:ILE:O	2.06	0.55
1:E:3:SER:HA	1:F:3:SER:N	2.22	0.55
1:H:184:ILE:HD13	1:H:185:LYS:N	2.22	0.55
1:G:62:ARG:HD3	1:G:153:VAL:HG11	1.89	0.54
1:H:165:PHE:CE2	1:H:183:THR:HG21	2.42	0.54
1:B:131:PHE:HB3	1:B:139:LEU:CD1	2.38	0.54
1:B:196:SER:O	1:B:198:GLN:N	2.40	0.54
1:E:28:ASP:C	1:E:29:ILE:HD12	2.32	0.54
1:G:13:PRO:HG2	1:G:116:TYR:CZ	2.43	0.54
1:F:194:TYR:O	1:F:198:GLN:HG2	2.08	0.54
1:G:91:PRO:HB2	1:G:94:GLN:HB2	1.90	0.54
1:G:173:CYS:HB3	1:G:177:TRP:CG	2.41	0.54
1:G:192:LYS:C	1:G:194:TYR:H	2.15	0.54
1:D:140:ARG:HB3	1:D:140:ARG:NH1	2.20	0.54
1:E:52:SER:O	1:E:56:ILE:HG22	2.07	0.54
1:F:119:LEU:HD12	1:F:125:ILE:O	2.07	0.54
1:I:53:PRO:O	1:I:57:ILE:HG23	2.08	0.54
1:I:72:GLN:HE21	1:I:73:VAL:N	2.05	0.54
1:I:161:GLN:OE1	1:I:179:PRO:HG2	2.08	0.54
1:I:21:MET:HE2	1:I:21:MET:HA	1.89	0.54
1:I:73:VAL:HB	1:I:102:ILE:CD1	2.38	0.54
1:C:109:LYS:HB3	1:C:111:THR:HG23	1.90	0.54
1:E:8:ILE:HD12	1:E:8:ILE:C	2.33	0.54
1:I:8:ILE:O	1:I:8:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:PHE:HB2	1:B:112:ILE:HD13	1.90	0.54
1:F:37:LYS:HG2	1:F:70:ASN:ND2	2.16	0.54
1:G:10:HIS:HB3	1:G:11:PRO:HD2	1.90	0.54
1:H:116:TYR:HB3	1:H:131:PHE:CZ	2.43	0.54
1:C:119:LEU:HD12	1:C:125:ILE:O	2.08	0.54
1:F:172:VAL:CG2	1:F:184:ILE:HG23	2.38	0.54
1:G:43:PHE:CD2	1:G:118:VAL:HG21	2.43	0.54
1:G:88:ILE:HA	1:G:97:LEU:HB2	1.90	0.54
1:I:40:VAL:HB	1:I:73:VAL:HG22	1.90	0.54
1:I:88:ILE:C	1:I:88:ILE:HD12	2.33	0.54
1:J:72:GLN:HE21	1:J:73:VAL:N	2.05	0.54
1:A:172:VAL:CG2	1:A:184:ILE:HG23	2.38	0.53
1:E:130:LEU:HB3	1:E:143:THR:HB	1.90	0.53
1:G:189:ASN:C	1:G:191:SER:H	2.16	0.53
1:J:189:ASN:C	1:J:191:SER:N	2.67	0.53
1:C:21:MET:HB3	1:C:22:PRO:HD2	1.90	0.53
1:H:61:ASP:C	1:H:63:ALA:H	2.15	0.53
1:I:185:LYS:HE2	1:I:190:LYS:HD3	1.90	0.53
1:G:32:SER:C	1:G:34:TYR:N	2.66	0.53
1:G:60:SER:HA	1:G:102:ILE:HG12	1.90	0.53
1:H:109:LYS:HD2	1:I:124:GLY:N	2.22	0.53
1:J:88:ILE:HG22	1:J:97:LEU:HD12	1.89	0.53
1:B:110:ARG:CZ	1:F:110:ARG:HH21	2.21	0.53
1:E:54:THR:HG21	1:F:174:PRO:HB3	1.91	0.53
1:I:199:LYS:OXT	1:J:93:LYS:HE3	2.08	0.53
1:A:78:VAL:HB	1:A:110:ARG:HH12	1.73	0.53
1:I:51:VAL:HB	1:I:128:ARG:NH2	2.23	0.53
1:C:55:GLU:O	1:C:58:ALA:HB3	2.09	0.53
1:C:184:ILE:HD12	1:C:185:LYS:C	2.34	0.53
1:E:43:PHE:HZ	1:E:112:ILE:HG22	1.72	0.53
1:G:140:ARG:HG3	1:G:140:ARG:HH11	1.73	0.53
1:A:62:ARG:HB3	1:A:65:GLU:OE2	2.08	0.53
1:C:184:ILE:HD13	1:C:191:SER:HB2	1.91	0.53
1:C:184:ILE:HD12	1:C:184:ILE:C	2.33	0.53
1:E:92:LYS:HE2	1:F:199:LYS:HD2	1.90	0.53
1:C:66:PHE:CE2	1:C:157:LEU:HD13	2.44	0.53
1:D:133:ILE:CD1	1:D:137:GLY:HA2	2.39	0.53
1:E:185:LYS:HD3	1:E:190:LYS:NZ	2.24	0.53
1:F:142:ILE:HD11	1:F:144:ILE:HG13	1.91	0.53
1:G:142:ILE:HD13	1:G:142:ILE:C	2.33	0.53
1:I:133:ILE:CD1	1:I:137:GLY:C	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD13	1:A:57:ILE:C	2.34	0.53
1:C:81:HIS:CD2	1:C:81:HIS:N	2.77	0.53
1:G:110:ARG:NH1	1:G:110:ARG:CB	2.65	0.53
1:I:133:ILE:HD13	1:I:137:GLY:C	2.33	0.53
1:J:51:VAL:HB	1:J:128:ARG:NH2	2.24	0.53
1:A:34:TYR:CE1	1:A:72:GLN:HG2	2.44	0.52
1:A:175:ALA:O	1:A:177:TRP:N	2.42	0.52
1:C:37:LYS:HG2	1:C:70:ASN:HD21	1.74	0.52
1:C:55:GLU:OE1	1:C:128:ARG:HD3	2.09	0.52
1:D:34:TYR:CD1	1:D:72:GLN:HG3	2.44	0.52
1:E:58:ALA:O	1:E:62:ARG:HG2	2.09	0.52
1:F:142:ILE:HD12	1:F:143:THR:N	2.24	0.52
1:I:133:ILE:HD11	1:I:137:GLY:CA	2.39	0.52
1:A:26:PHE:CD1	1:A:26:PHE:N	2.77	0.52
1:C:18:THR:HB	1:C:28:ASP:OD1	2.10	0.52
1:G:31:LEU:HD11	1:G:133:ILE:CD1	2.40	0.52
1:C:174:PRO:HD2	1:C:183:THR:HG22	1.91	0.52
1:G:24:GLY:O	1:G:25:GLN:HG2	2.09	0.52
1:I:93:LYS:HA	1:J:195:PHE:O	2.08	0.52
1:A:81:HIS:O	1:A:84:HIS:HB2	2.09	0.52
1:B:109:LYS:HB3	1:B:111:THR:HG23	1.90	0.52
1:B:190:LYS:CD	1:B:190:LYS:H	2.23	0.52
1:F:44:TYR:CZ	1:F:77:SER:HB3	2.44	0.52
1:F:112:ILE:HD12	1:F:112:ILE:N	2.24	0.52
1:D:53:PRO:HB3	1:D:87:TRP:CZ2	2.45	0.52
1:H:55:GLU:OE1	1:H:128:ARG:NH1	2.42	0.52
1:I:44:TYR:CZ	1:I:77:SER:HB3	2.45	0.52
1:B:46:LEU:HD21	1:B:125:ILE:HD11	1.92	0.52
1:C:84:HIS:HD2	1:C:104:LEU:HB3	1.72	0.52
1:C:116:TYR:O	1:C:118:VAL:HG13	2.09	0.52
1:E:192:LYS:O	1:E:196:SER:HB2	2.09	0.52
1:I:184:ILE:HD11	1:I:191:SER:CB	2.39	0.52
1:J:189:ASN:O	1:J:192:LYS:HG2	2.10	0.52
1:A:93:LYS:HB2	1:A:93:LYS:NZ	2.24	0.52
1:D:99:PRO:O	1:D:100:MET:HE2	2.10	0.52
1:A:9:GLY:C	1:A:138:ILE:CD1	2.83	0.52
1:A:197:LYS:CB	1:A:197:LYS:NZ	2.73	0.52
1:F:17:ALA:HB3	1:F:105:VAL:HG13	1.92	0.52
1:F:159:LEU:O	1:F:162:ALA:HB3	2.09	0.52
1:G:3:SER:HA	1:H:3:SER:N	2.25	0.52
1:G:172:VAL:HG21	1:H:51:VAL:HG23	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:LEU:N	1:I:104:LEU:HD22	2.25	0.52
1:E:50:PHE:O	1:E:53:PRO:HG2	2.09	0.51
1:A:92:LYS:HD3	1:B:199:LYS:HD2	1.92	0.51
1:E:43:PHE:CZ	1:E:112:ILE:HG22	2.46	0.51
1:G:27:LYS:CG	1:G:28:ASP:N	2.72	0.51
1:H:62:ARG:NE	1:H:65:GLU:OE2	2.40	0.51
1:E:184:ILE:HD12	1:E:184:ILE:C	2.36	0.51
1:F:48:PHE:CE1	1:F:87:TRP:CD1	2.98	0.51
1:F:125:ILE:HG22	1:F:126:SER:N	2.25	0.51
1:B:178:LYS:HB3	1:B:179:PRO:HD2	1.93	0.51
1:C:199:LYS:HB2	1:C:199:LYS:NZ	2.25	0.51
1:C:199:LYS:NZ	1:D:92:LYS:NZ	2.58	0.51
1:D:88:ILE:HA	1:D:97:LEU:HB2	1.92	0.51
1:E:128:ARG:HG2	1:E:151:ARG:CZ	2.40	0.51
1:F:184:ILE:C	1:F:184:ILE:HD13	2.36	0.51
1:A:134:ASP:OD1	1:A:138:ILE:HG23	2.10	0.51
1:C:39:VAL:HB	1:C:133:ILE:HD12	1.93	0.51
1:D:90:THR:O	1:D:96:GLY:HA3	2.11	0.51
1:G:39:VAL:HB	1:G:133:ILE:CG1	2.40	0.51
1:A:88:ILE:HD12	1:A:88:ILE:O	2.11	0.51
1:A:110:ARG:HG3	1:A:110:ARG:NH1	2.23	0.51
1:E:41:PHE:HE1	1:E:76:ALA:HB2	1.76	0.51
1:E:165:PHE:CZ	1:E:183:THR:HG21	2.46	0.51
1:F:78:VAL:HB	1:F:110:ARG:NH1	2.25	0.51
1:I:24:GLY:O	1:I:25:GLN:HB2	2.11	0.51
1:A:12:ALA:O	1:A:13:PRO:C	2.54	0.51
1:A:184:ILE:HD13	1:B:50:PHE:HB3	1.93	0.51
1:B:93:LYS:HB2	1:B:93:LYS:NZ	2.25	0.51
1:C:8:ILE:HD11	1:C:142:ILE:CG2	2.41	0.51
1:F:21:MET:SD	1:F:29:ILE:HD11	2.51	0.51
1:F:56:ILE:CD1	1:F:97:LEU:HD13	2.40	0.51
1:H:145:ASN:ND2	1:H:151:ARG:CG	2.74	0.51
1:J:32:SER:C	1:J:34:TYR:H	2.18	0.51
1:A:3:SER:HA	1:B:3:SER:N	2.26	0.51
1:G:109:LYS:O	1:G:110:ARG:HG2	2.11	0.51
1:H:88:ILE:HA	1:H:97:LEU:HB2	1.93	0.51
1:I:56:ILE:HD11	1:I:97:LEU:HD13	1.93	0.51
1:A:92:LYS:HB3	1:B:199:LYS:HG3	1.92	0.51
1:A:109:LYS:HB3	1:A:111:THR:HG23	1.91	0.51
1:C:142:ILE:HG12	1:C:142:ILE:O	2.11	0.51
1:G:30:SER:N	1:G:33:ASP:OD2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:VAL:HB	1:I:110:ARG:HH12	1.76	0.51
1:C:128:ARG:HG2	1:C:151:ARG:CZ	2.40	0.51
1:D:88:ILE:HG13	1:D:89:ASN:N	2.26	0.51
1:C:30:SER:O	1:C:31:LEU:C	2.54	0.50
1:F:112:ILE:HD12	1:F:112:ILE:H	1.75	0.50
1:G:21:MET:HE2	1:G:21:MET:HA	1.93	0.50
1:I:133:ILE:HD12	1:I:134:ASP:H	1.75	0.50
1:J:12:ALA:O	1:J:13:PRO:C	2.53	0.50
1:J:67:LYS:HB2	1:J:67:LYS:NZ	2.26	0.50
1:E:40:VAL:HG23	1:E:71:CYS:SG	2.51	0.50
1:A:133:ILE:HD11	1:A:137:GLY:C	2.37	0.50
1:H:46:LEU:HB2	1:H:49:THR:CG2	2.41	0.50
1:I:44:TYR:OH	1:I:84:HIS:CE1	2.63	0.50
1:E:123:GLU:O	1:E:125:ILE:HD13	2.11	0.50
1:F:199:LYS:HB2	1:F:199:LYS:NZ	2.25	0.50
1:H:88:ILE:HD12	1:H:88:ILE:C	2.36	0.50
1:I:93:LYS:HE3	1:J:199:LYS:HE3	1.94	0.50
1:C:66:PHE:HB3	1:C:71:CYS:HB3	1.94	0.50
1:G:21:MET:HE1	1:G:103:PRO:HB3	1.93	0.50
1:G:32:SER:O	1:G:34:TYR:N	2.45	0.50
1:G:50:PHE:O	1:G:53:PRO:HD2	2.11	0.50
1:I:194:TYR:C	1:I:194:TYR:CD1	2.89	0.50
1:J:94:GLN:HE21	1:J:94:GLN:CA	2.07	0.50
1:A:50:PHE:C	1:A:53:PRO:HD2	2.36	0.50
1:A:132:ILE:HD13	1:A:132:ILE:C	2.36	0.50
1:A:146:ASP:OD1	1:A:147:LEU:N	2.43	0.50
1:B:35:LYS:HD2	1:B:35:LYS:C	2.37	0.50
1:B:93:LYS:HB2	1:B:93:LYS:HZ3	1.76	0.50
1:G:184:ILE:HD11	1:G:191:SER:CB	2.34	0.50
1:J:187:ASP:O	1:J:191:SER:HB3	2.12	0.50
1:E:69:LEU:CD1	1:E:157:LEU:HD12	2.42	0.50
1:F:133:ILE:HD12	1:F:133:ILE:C	2.36	0.50
1:G:92:LYS:HD3	1:G:92:LYS:N	2.15	0.50
1:G:92:LYS:HG2	1:H:199:LYS:NZ	2.27	0.50
1:I:50:PHE:CD2	1:J:186:PRO:HA	2.46	0.50
1:B:27:LYS:O	1:B:29:ILE:HD13	2.10	0.50
1:B:34:TYR:CE1	1:B:72:GLN:HG2	2.47	0.50
1:F:172:VAL:O	1:F:174:PRO:HD3	2.12	0.50
1:H:187:ASP:O	1:H:188:VAL:C	2.55	0.50
1:B:15:PHE:CE2	1:B:31:LEU:HB2	2.47	0.50
1:C:66:PHE:CZ	1:C:157:LEU:HD13	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:PHE:CZ	1:G:157:LEU:HG	2.47	0.50
1:H:184:ILE:HD11	1:H:191:SER:CB	2.42	0.50
1:J:46:LEU:HD21	1:J:125:ILE:HD11	1.94	0.50
1:C:19:ALA:HB3	1:C:21:MET:CE	2.41	0.49
1:F:56:ILE:HD11	1:F:97:LEU:HD13	1.94	0.49
1:G:72:GLN:HE21	1:G:72:GLN:HA	1.76	0.49
1:H:50:PHE:O	1:H:53:PRO:HG2	2.12	0.49
1:B:120:LYS:HG3	1:B:127:PHE:CZ	2.47	0.49
1:H:37:LYS:HG2	1:H:70:ASN:HD21	1.77	0.49
1:A:119:LEU:HD12	1:A:120:LYS:N	2.27	0.49
1:G:72:GLN:HA	1:G:72:GLN:NE2	2.26	0.49
1:I:15:PHE:CD1	1:I:15:PHE:C	2.90	0.49
1:A:49:THR:OG1	1:A:52:SER:HB2	2.12	0.49
1:C:24:GLY:O	1:C:25:GLN:HG3	2.12	0.49
1:C:76:ALA:HB2	1:C:105:VAL:CG2	2.43	0.49
1:D:184:ILE:HD13	1:D:194:TYR:HB3	1.94	0.49
1:F:21:MET:N	1:F:21:MET:HE2	2.27	0.49
1:G:173:CYS:HB3	1:G:177:TRP:CB	2.41	0.49
1:H:69:LEU:O	1:H:70:ASN:C	2.54	0.49
1:F:78:VAL:CG1	1:F:110:ARG:HH12	2.24	0.49
1:G:186:PRO:HA	1:H:50:PHE:CD2	2.48	0.49
1:H:19:ALA:HB3	1:H:21:MET:CE	2.43	0.49
1:I:199:LYS:HA	1:I:199:LYS:NZ	2.27	0.49
1:A:112:ILE:O	1:A:116:TYR:HD1	1.96	0.49
1:A:172:VAL:HG23	1:A:184:ILE:HG23	1.93	0.49
1:B:107:ASP:CG	1:B:112:ILE:HG13	2.37	0.49
1:F:119:LEU:HG	1:F:119:LEU:O	2.13	0.49
1:D:184:ILE:HD11	1:D:191:SER:CB	2.42	0.49
1:G:66:PHE:CZ	1:G:156:ILE:HD11	2.47	0.49
1:G:140:ARG:HG3	1:G:140:ARG:NH1	2.27	0.49
1:H:15:PHE:CE2	1:H:31:LEU:HB2	2.47	0.49
1:A:175:ALA:C	1:A:177:TRP:H	2.20	0.49
1:D:50:PHE:O	1:D:53:PRO:HD2	2.11	0.49
1:F:142:ILE:CD1	1:F:144:ILE:HG13	2.43	0.49
1:E:52:SER:N	1:E:53:PRO:HD2	2.27	0.49
1:G:165:PHE:CE2	1:G:183:THR:HG21	2.48	0.49
1:C:101:ASN:O	1:C:102:ILE:HD12	2.13	0.49
1:D:125:ILE:N	1:D:125:ILE:HD12	2.28	0.49
1:H:110:ARG:NH1	1:I:110:ARG:NH2	2.60	0.49
1:J:192:LYS:C	1:J:194:TYR:H	2.21	0.49
1:F:29:ILE:N	1:F:29:ILE:CD1	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:ILE:C	1:G:138:ILE:HD12	2.37	0.48
1:G:141:GLN:HG2	1:H:145:ASN:OD1	2.13	0.48
1:J:40:VAL:HG23	1:J:71:CYS:SG	2.53	0.48
1:J:125:ILE:HG22	1:J:126:SER:N	2.28	0.48
1:I:13:PRO:HB2	1:I:116:TYR:CE1	2.48	0.48
1:I:184:ILE:HD12	1:J:50:PHE:HB3	1.95	0.48
1:A:147:LEU:HB2	1:A:148:PRO:HD3	1.96	0.48
1:E:73:VAL:O	1:E:102:ILE:HG13	2.13	0.48
1:G:109:LYS:NZ	1:G:109:LYS:CB	2.77	0.48
1:H:61:ASP:C	1:H:63:ALA:N	2.70	0.48
1:J:8:ILE:CD1	1:J:142:ILE:HG22	2.39	0.48
1:D:172:VAL:CG2	1:D:184:ILE:HG23	2.43	0.48
1:E:199:LYS:HE3	1:E:199:LYS:HA	1.95	0.48
1:I:15:PHE:CE2	1:I:31:LEU:HB2	2.48	0.48
1:I:133:ILE:HD12	1:I:133:ILE:C	2.38	0.48
1:J:147:LEU:N	1:J:148:PRO:HD2	2.27	0.48
1:E:46:LEU:HD21	1:E:125:ILE:CG1	2.43	0.48
1:F:15:PHE:CD1	1:F:15:PHE:C	2.92	0.48
1:F:107:ASP:OD1	1:F:112:ILE:HD13	2.13	0.48
1:G:110:ARG:HH11	1:G:110:ARG:N	2.11	0.48
1:I:43:PHE:CD2	1:I:118:VAL:HG21	2.49	0.48
1:A:32:SER:C	1:A:34:TYR:H	2.21	0.48
1:A:92:LYS:HB3	1:B:199:LYS:CG	2.44	0.48
1:A:197:LYS:NZ	1:A:197:LYS:HB3	2.28	0.48
1:A:197:LYS:HZ3	1:A:197:LYS:HB3	1.78	0.48
1:F:178:LYS:O	1:F:179:PRO:C	2.57	0.48
1:G:15:PHE:CD1	1:G:15:PHE:C	2.91	0.48
1:I:164:GLN:HA	1:I:167:ASP:OD2	2.13	0.48
1:E:128:ARG:HB3	1:E:145:ASN:HB2	1.95	0.48
1:F:109:LYS:HB3	1:F:111:THR:HG23	1.95	0.48
1:H:131:PHE:HD1	1:H:142:ILE:CG2	2.19	0.48
1:F:84:HIS:O	1:F:88:ILE:HG22	2.14	0.48
1:B:116:TYR:HB3	1:B:131:PHE:CZ	2.49	0.47
1:G:56:ILE:HD11	1:G:104:LEU:HD11	1.95	0.47
1:G:188:VAL:HG11	1:I:85:LEU:HD23	1.95	0.47
1:H:38:TYR:CZ	1:H:134:ASP:HB3	2.49	0.47
1:I:178:LYS:O	1:I:181:SER:OG	2.29	0.47
1:B:122:ASP:HA	1:F:109:LYS:HZ1	1.79	0.47
1:C:103:PRO:O	1:C:104:LEU:HD12	2.14	0.47
1:I:21:MET:HE2	1:I:21:MET:CA	2.43	0.47
1:I:199:LYS:HA	1:I:199:LYS:HZ3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:43:PHE:CD2	1:J:118:VAL:HG21	2.49	0.47
1:B:99:PRO:O	1:B:100:MET:HE2	2.13	0.47
1:D:53:PRO:HA	1:D:56:ILE:CG2	2.44	0.47
1:E:146:ASP:HB3	1:F:163:PHE:HE1	1.79	0.47
1:F:78:VAL:CG1	1:F:110:ARG:NH1	2.77	0.47
1:F:94:GLN:HA	1:F:94:GLN:NE2	2.30	0.47
1:G:128:ARG:C	1:G:151:ARG:HH12	2.22	0.47
1:I:142:ILE:HG13	1:J:144:ILE:HG12	1.96	0.47
1:F:81:HIS:H	1:F:81:HIS:HD2	1.62	0.47
1:E:93:LYS:HD2	1:F:199:LYS:OXT	2.14	0.47
1:E:189:ASN:C	1:E:191:SER:H	2.23	0.47
1:I:165:PHE:CE2	1:I:183:THR:HG21	2.50	0.47
1:A:56:ILE:HD12	1:A:56:ILE:C	2.39	0.47
1:B:157:LEU:O	1:B:161:GLN:HG3	2.15	0.47
1:D:199:LYS:H	1:D:199:LYS:CD	2.26	0.47
1:E:128:ARG:HG2	1:E:151:ARG:NE	2.30	0.47
1:F:133:ILE:HD12	1:F:134:ASP:N	2.30	0.47
1:F:133:ILE:HD13	1:F:137:GLY:C	2.40	0.47
1:F:135:ASP:OD1	1:F:136:LYS:HG3	2.14	0.47
1:G:27:LYS:HG2	1:G:29:ILE:HD13	1.95	0.47
1:G:37:LYS:NZ	1:G:70:ASN:HD21	2.11	0.47
1:G:43:PHE:HZ	1:G:112:ILE:HG22	1.79	0.47
1:G:192:LYS:C	1:G:194:TYR:N	2.72	0.47
1:H:133:ILE:HD13	1:H:133:ILE:O	2.14	0.47
1:I:38:TYR:CD2	1:I:132:ILE:HD11	2.50	0.47
1:I:40:VAL:HG23	1:I:71:CYS:SG	2.55	0.47
1:I:165:PHE:CZ	1:I:183:THR:HG21	2.50	0.47
1:A:51:VAL:HB	1:A:128:ARG:NH2	2.29	0.47
1:C:46:LEU:CG	1:C:125:ILE:HD11	2.45	0.47
1:C:90:THR:HG22	1:C:96:GLY:HA3	1.96	0.47
1:C:199:LYS:HG3	1:C:199:LYS:O	2.14	0.47
1:G:144:ILE:O	1:H:141:GLN:HG2	2.15	0.47
1:G:189:ASN:O	1:G:191:SER:N	2.48	0.47
1:H:15:PHE:CD1	1:H:15:PHE:C	2.92	0.47
1:J:28:ASP:C	1:J:29:ILE:HD12	2.40	0.47
1:H:42:PHE:HB3	1:H:130:LEU:HD22	1.95	0.47
1:H:184:ILE:HD13	1:H:185:LYS:C	2.39	0.47
1:I:107:ASP:OD1	1:I:112:ILE:HG13	2.14	0.47
1:B:91:PRO:HB2	1:B:94:GLN:HB2	1.97	0.47
1:F:84:HIS:O	1:F:88:ILE:CG2	2.63	0.47
1:F:103:PRO:O	1:F:104:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ALA:O	1:C:165:PHE:HB3	2.16	0.46
1:E:187:ASP:HB3	1:E:190:LYS:HB2	1.96	0.46
1:H:19:ALA:HB3	1:H:21:MET:HE1	1.97	0.46
1:H:146:ASP:OD1	1:H:147:LEU:N	2.46	0.46
1:J:192:LYS:C	1:J:194:TYR:N	2.72	0.46
1:B:23:ASP:C	1:B:24:GLY:O	2.56	0.46
1:E:184:ILE:CD1	1:E:191:SER:HB2	2.44	0.46
1:I:21:MET:HE2	1:I:21:MET:N	2.30	0.46
1:I:34:TYR:CD1	1:I:72:GLN:HG3	2.51	0.46
1:I:60:SER:HG	1:I:101:ASN:H	1.59	0.46
1:B:76:ALA:CB	1:B:105:VAL:HG22	2.45	0.46
1:C:66:PHE:HA	1:C:69:LEU:HD12	1.97	0.46
1:H:188:VAL:O	1:H:192:LYS:HE2	2.16	0.46
1:J:198:GLN:HB2	1:J:199:LYS:NZ	2.30	0.46
1:B:94:GLN:HA	1:B:94:GLN:NE2	2.28	0.46
1:E:140:ARG:HG3	1:E:140:ARG:NH1	2.29	0.46
1:F:190:LYS:HB2	1:F:190:LYS:HZ3	1.80	0.46
1:H:46:LEU:HD22	1:I:80:SER:CB	2.46	0.46
1:J:162:ALA:O	1:J:166:THR:HG23	2.15	0.46
1:A:85:LEU:O	1:A:86:ALA:C	2.58	0.46
1:I:73:VAL:CG1	1:I:102:ILE:HG12	2.46	0.46
1:A:120:LYS:HG3	1:A:127:PHE:CZ	2.51	0.46
1:B:46:LEU:CD2	1:F:80:SER:HB3	2.41	0.46
1:D:196:SER:C	1:D:198:GLN:H	2.24	0.46
1:G:184:ILE:HD13	1:G:185:LYS:C	2.40	0.46
1:H:6:ALA:HB1	1:H:139:LEU:HD22	1.97	0.46
1:A:82:PHE:O	1:A:83:CYS:C	2.57	0.46
1:C:24:GLY:C	1:C:25:GLN:HG3	2.40	0.46
1:F:29:ILE:N	1:F:29:ILE:HD12	2.29	0.46
1:F:43:PHE:CZ	1:F:112:ILE:HG22	2.48	0.46
1:I:8:ILE:HD12	1:J:146:ASP:HA	1.96	0.46
1:I:57:ILE:CD1	1:I:58:ALA:H	2.21	0.46
1:J:194:TYR:CD1	1:J:194:TYR:C	2.93	0.46
1:A:47:ASP:O	1:A:48:PHE:HB2	2.16	0.46
1:A:194:TYR:CD1	1:A:194:TYR:C	2.93	0.46
1:B:56:ILE:HD12	1:B:56:ILE:O	2.15	0.46
1:E:15:PHE:CD1	1:E:15:PHE:C	2.94	0.46
1:E:46:LEU:HB2	1:E:49:THR:CG2	2.46	0.46
1:E:141:GLN:HG2	1:F:144:ILE:O	2.16	0.46
1:F:17:ALA:HB3	1:F:105:VAL:CG1	2.46	0.46
1:F:38:TYR:CE1	1:F:134:ASP:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:GLY:O	1:F:125:ILE:HD13	2.15	0.46
1:I:142:ILE:HD12	1:I:143:THR:N	2.31	0.46
1:J:16:LYS:HG3	1:J:30:SER:OG	2.16	0.46
1:C:109:LYS:C	1:C:110:ARG:HG3	2.41	0.46
1:G:92:LYS:HG2	1:H:199:LYS:HZ1	1.81	0.46
1:G:147:LEU:N	1:G:148:PRO:HD2	2.31	0.46
1:H:46:LEU:HD22	1:I:80:SER:HB3	1.98	0.46
1:A:46:LEU:HB2	1:A:49:THR:HG21	1.98	0.46
1:B:44:TYR:CZ	1:B:77:SER:HB3	2.51	0.46
1:E:53:PRO:HA	1:E:56:ILE:CG2	2.46	0.46
1:E:110:ARG:CZ	1:J:110:ARG:NH1	2.79	0.46
1:E:116:TYR:O	1:E:117:GLY:C	2.59	0.46
1:F:123:GLU:HB3	1:F:125:ILE:HG12	1.98	0.46
1:F:133:ILE:CD1	1:F:137:GLY:CA	2.94	0.46
1:G:46:LEU:HB2	1:G:49:THR:CG2	2.46	0.46
1:I:169:HIS:O	1:I:170:GLY:C	2.56	0.46
1:J:21:MET:HE2	1:J:21:MET:N	2.31	0.46
1:C:164:GLN:O	1:C:168:LYS:HB2	2.16	0.45
1:F:21:MET:C	1:F:23:ASP:H	2.24	0.45
1:F:55:GLU:OE1	1:F:128:ARG:NH1	2.49	0.45
1:H:5:ASN:O	1:H:7:LYS:CE	2.60	0.45
1:H:172:VAL:CG2	1:H:184:ILE:HG23	2.46	0.45
1:I:73:VAL:HG12	1:I:102:ILE:HG12	1.98	0.45
1:J:19:ALA:HB3	1:J:21:MET:CE	2.46	0.45
1:B:97:LEU:HB3	1:B:100:MET:HE3	1.97	0.45
1:C:30:SER:C	1:C:32:SER:N	2.72	0.45
1:E:146:ASP:OD1	1:F:8:ILE:HD11	2.16	0.45
1:J:72:GLN:NE2	1:J:73:VAL:N	2.64	0.45
1:A:26:PHE:O	1:A:27:LYS:HB2	2.16	0.45
1:D:133:ILE:HD12	1:D:134:ASP:O	2.17	0.45
1:D:157:LEU:HD12	1:D:157:LEU:HA	1.83	0.45
1:A:110:ARG:CZ	1:C:110:ARG:NH1	2.79	0.45
1:B:132:ILE:HD13	1:B:132:ILE:C	2.41	0.45
1:F:46:LEU:CD2	1:F:125:ILE:HD12	2.44	0.45
1:I:34:TYR:HD1	1:I:72:GLN:HG3	1.81	0.45
1:J:184:ILE:C	1:J:184:ILE:CD1	2.86	0.45
1:A:20:VAL:HG22	1:A:81:HIS:NE2	2.32	0.45
1:A:184:ILE:HG13	1:A:185:LYS:N	2.31	0.45
1:B:37:LYS:HE2	1:B:37:LYS:HB3	1.84	0.45
1:C:173:CYS:HA	1:C:174:PRO:HD2	1.87	0.45
1:G:15:PHE:O	1:G:30:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:ALA:O	1:H:26:PHE:HA	2.16	0.45
1:B:19:ALA:HB3	1:B:21:MET:CE	2.46	0.45
1:E:175:ALA:HB2	1:F:55:GLU:HA	1.98	0.45
1:G:66:PHE:HZ	1:G:156:ILE:CD1	2.30	0.45
1:H:66:PHE:CE2	1:H:157:LEU:HD13	2.51	0.45
1:A:44:TYR:CZ	1:A:77:SER:HB3	2.51	0.45
1:D:43:PHE:HZ	1:D:112:ILE:HG22	1.82	0.45
1:D:46:LEU:HD22	1:G:80:SER:HB3	1.97	0.45
1:F:168:LYS:O	1:F:169:HIS:CD2	2.69	0.45
1:G:147:LEU:N	1:G:148:PRO:CD	2.79	0.45
1:I:88:ILE:HD12	1:I:89:ASN:N	2.32	0.45
1:A:104:LEU:HD12	1:A:104:LEU:HA	1.73	0.45
1:B:187:ASP:HB3	1:B:190:LYS:HD3	1.99	0.45
1:D:62:ARG:NH2	1:D:157:LEU:HD23	2.32	0.45
1:H:107:ASP:OD1	1:H:112:ILE:HG23	2.17	0.45
1:B:177:TRP:CE3	1:B:177:TRP:C	2.95	0.45
1:D:47:ASP:OD2	1:D:84:HIS:ND1	2.49	0.45
1:E:27:LYS:HD3	1:E:29:ILE:HD11	1.99	0.45
1:F:57:ILE:HD13	1:F:92:LYS:HD2	1.99	0.45
1:H:53:PRO:O	1:H:57:ILE:HG13	2.17	0.45
1:A:73:VAL:HB	1:A:102:ILE:HD12	1.99	0.45
1:C:76:ALA:HB2	1:C:105:VAL:HG22	1.99	0.45
1:D:19:ALA:HB3	1:D:21:MET:CE	2.47	0.45
1:D:84:HIS:CD2	1:D:104:LEU:HB3	2.51	0.45
1:G:5:ASN:O	1:G:7:LYS:HG3	2.16	0.45
1:I:73:VAL:O	1:I:74:ILE:HD13	2.16	0.45
1:J:118:VAL:O	1:J:126:SER:HA	2.16	0.45
1:B:66:PHE:CZ	1:B:157:LEU:HD22	2.51	0.44
1:C:46:LEU:HB2	1:C:49:THR:HG21	1.99	0.44
1:D:80:SER:HB3	1:G:46:LEU:HD22	1.98	0.44
1:J:19:ALA:HB2	1:J:105:VAL:HG22	1.99	0.44
1:C:68:LYS:CB	1:C:68:LYS:NZ	2.80	0.44
1:D:34:TYR:O	1:D:37:LYS:HG2	2.17	0.44
1:D:66:PHE:CE2	1:D:157:LEU:HD13	2.52	0.44
1:D:72:GLN:NE2	1:D:73:VAL:O	2.50	0.44
1:D:194:TYR:HA	1:D:197:LYS:CE	2.45	0.44
1:E:81:HIS:H	1:E:81:HIS:HD2	1.61	0.44
1:E:195:PHE:O	1:E:199:LYS:HB2	2.17	0.44
1:J:129:GLY:HA2	1:J:143:THR:O	2.17	0.44
1:A:109:LYS:HB3	1:A:109:LYS:HE3	1.81	0.44
1:B:37:LYS:HE2	1:B:70:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:PRO:O	1:B:94:GLN:N	2.50	0.44
1:B:98:GLY:O	1:B:99:PRO:C	2.61	0.44
1:E:184:ILE:HB	1:E:194:TYR:CG	2.53	0.44
1:G:13:PRO:HG2	1:G:116:TYR:CE1	2.53	0.44
1:G:62:ARG:O	1:G:63:ALA:C	2.61	0.44
1:J:46:LEU:HD21	1:J:125:ILE:HD12	2.00	0.44
1:J:172:VAL:HG23	1:J:184:ILE:HG23	1.99	0.44
1:J:174:PRO:O	1:J:177:TRP:HB2	2.17	0.44
1:A:199:LYS:HD3	1:B:92:LYS:NZ	2.33	0.44
1:D:116:TYR:O	1:D:118:VAL:HG13	2.17	0.44
1:D:133:ILE:HD13	1:D:137:GLY:HA2	1.98	0.44
1:F:63:ALA:HB2	1:F:102:ILE:HD13	1.99	0.44
1:F:81:HIS:CD2	1:F:81:HIS:N	2.85	0.44
1:G:77:SER:OG	1:G:84:HIS:HE1	2.01	0.44
1:H:31:LEU:HD12	1:H:31:LEU:O	2.17	0.44
1:J:123:GLU:O	1:J:125:ILE:HG12	2.17	0.44
1:C:121:ALA:O	1:C:123:GLU:N	2.50	0.44
1:E:185:LYS:CD	1:E:190:LYS:HZ3	2.28	0.44
1:F:129:GLY:HA2	1:F:143:THR:O	2.17	0.44
1:B:52:SER:O	1:B:56:ILE:HG22	2.18	0.44
1:D:119:LEU:HD12	1:D:125:ILE:O	2.18	0.44
1:D:194:TYR:C	1:D:194:TYR:CD1	2.95	0.44
1:I:57:ILE:CD1	1:I:58:ALA:N	2.79	0.44
1:J:85:LEU:HD23	1:J:85:LEU:O	2.18	0.44
1:E:41:PHE:CE1	1:E:76:ALA:HB2	2.53	0.44
1:F:93:LYS:N	1:F:93:LYS:CE	2.80	0.44
1:F:156:ILE:HD12	1:F:156:ILE:N	2.32	0.44
1:H:52:SER:HB2	1:H:53:PRO:CD	2.48	0.44
1:D:47:ASP:N	1:D:79:ASP:OD2	2.51	0.44
1:F:56:ILE:HD12	1:F:97:LEU:CD2	2.39	0.44
1:F:133:ILE:HD13	1:F:137:GLY:HA2	2.00	0.44
1:H:47:ASP:HB2	1:H:79:ASP:CG	2.43	0.44
1:J:57:ILE:HG13	1:J:58:ALA:N	2.33	0.44
1:J:77:SER:OG	1:J:84:HIS:HE1	2.01	0.44
1:A:129:GLY:HA2	1:A:143:THR:O	2.17	0.44
1:B:50:PHE:O	1:B:51:VAL:C	2.61	0.44
1:B:122:ASP:HA	1:F:109:LYS:NZ	2.33	0.44
1:B:135:ASP:OD1	1:B:136:LYS:HD2	2.18	0.44
1:C:19:ALA:HB3	1:C:21:MET:HE1	1.99	0.44
1:C:55:GLU:HA	1:D:175:ALA:HB2	1.99	0.44
1:C:140:ARG:HG3	1:C:140:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLY:C	1:D:25:GLN:HG2	2.43	0.44
1:D:27:LYS:HE2	1:D:29:ILE:CD1	2.48	0.44
1:D:116:TYR:HB3	1:D:131:PHE:CZ	2.53	0.44
1:D:194:TYR:O	1:D:198:GLN:HG2	2.18	0.44
1:F:56:ILE:HD11	1:F:100:MET:SD	2.57	0.44
1:G:64:GLU:HA	1:G:64:GLU:OE1	2.17	0.44
1:H:178:LYS:O	1:H:179:PRO:C	2.60	0.44
1:I:57:ILE:CG1	1:I:58:ALA:N	2.81	0.43
1:I:173:CYS:HB3	1:I:177:TRP:CG	2.53	0.43
1:C:128:ARG:HG2	1:C:151:ARG:NH2	2.34	0.43
1:G:156:ILE:HA	1:G:159:LEU:HD12	2.00	0.43
1:H:34:TYR:CD1	1:H:72:GLN:HG2	2.53	0.43
1:H:112:ILE:HD12	1:H:112:ILE:O	2.19	0.43
1:H:177:TRP:O	1:H:177:TRP:HE3	2.01	0.43
1:J:34:TYR:CE1	1:J:72:GLN:HG3	2.53	0.43
1:B:146:ASP:OD1	1:B:147:LEU:N	2.51	0.43
1:C:81:HIS:O	1:C:84:HIS:HB2	2.18	0.43
1:C:92:LYS:HA	1:C:96:GLY:O	2.17	0.43
1:C:175:ALA:HB2	1:D:55:GLU:HA	2.00	0.43
1:D:44:TYR:CZ	1:D:77:SER:HB2	2.52	0.43
1:D:199:LYS:HD3	1:D:199:LYS:N	2.32	0.43
1:A:52:SER:O	1:A:53:PRO:C	2.62	0.43
1:A:84:HIS:CD2	1:A:104:LEU:HB3	2.53	0.43
1:A:119:LEU:HD12	1:A:120:LYS:H	1.82	0.43
1:D:187:ASP:OD1	1:D:189:ASN:N	2.50	0.43
1:I:46:LEU:HB2	1:I:49:THR:HG21	2.00	0.43
1:I:178:LYS:O	1:I:179:PRO:C	2.61	0.43
1:J:172:VAL:HG22	1:J:184:ILE:O	2.18	0.43
1:A:46:LEU:HB2	1:A:49:THR:CG2	2.48	0.43
1:C:78:VAL:HA	1:C:107:ASP:O	2.18	0.43
1:C:177:TRP:CD1	1:C:181:SER:HB2	2.54	0.43
1:E:46:LEU:HD21	1:E:125:ILE:CD1	2.45	0.43
1:H:68:LYS:HB2	1:H:68:LYS:HZ2	1.81	0.43
1:H:109:LYS:NZ	1:I:121:ALA:O	2.44	0.43
1:J:15:PHE:CD1	1:J:15:PHE:C	2.96	0.43
1:A:9:GLY:N	1:A:138:ILE:HD11	2.33	0.43
1:C:38:TYR:OH	1:C:167:ASP:OD2	2.37	0.43
1:D:193:GLU:O	1:D:197:LYS:HG2	2.19	0.43
1:F:19:ALA:HB3	1:F:21:MET:HE1	2.00	0.43
1:J:85:LEU:HD23	1:J:85:LEU:C	2.43	0.43
1:A:155:GLU:O	1:A:156:ILE:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ALA:HB2	1:B:105:VAL:HG22	2.01	0.43
1:D:5:ASN:N	1:D:5:ASN:HD22	2.15	0.43
1:D:134:ASP:OD1	1:D:138:ILE:HG12	2.17	0.43
1:G:39:VAL:HB	1:G:133:ILE:HD11	2.00	0.43
1:H:76:ALA:HB2	1:H:105:VAL:HB	2.01	0.43
1:A:32:SER:C	1:A:34:TYR:N	2.76	0.43
1:C:19:ALA:HB2	1:C:105:VAL:HG12	2.00	0.43
1:C:62:ARG:HB3	1:C:65:GLU:CG	2.45	0.43
1:E:57:ILE:C	1:E:57:ILE:CD1	2.88	0.43
1:E:175:ALA:HB2	1:F:55:GLU:CB	2.49	0.43
1:F:67:LYS:C	1:F:69:LEU:H	2.26	0.43
1:F:133:ILE:O	1:F:133:ILE:HG13	2.18	0.43
1:I:185:LYS:HG3	1:I:190:LYS:CB	2.48	0.43
1:A:142:ILE:HD11	1:A:144:ILE:CG1	2.48	0.43
1:B:29:ILE:CD1	1:B:29:ILE:N	2.82	0.43
1:C:120:LYS:O	1:C:121:ALA:C	2.62	0.43
1:F:30:SER:HB2	1:F:33:ASP:OD1	2.18	0.43
1:G:7:LYS:C	1:G:139:LEU:HD23	2.44	0.43
1:H:175:ALA:O	1:H:176:GLY:C	2.62	0.43
1:I:169:HIS:C	1:I:171:GLU:N	2.76	0.43
1:I:184:ILE:HG12	1:I:194:TYR:HB3	2.00	0.43
1:A:88:ILE:HG13	1:A:89:ASN:N	2.32	0.43
1:B:15:PHE:C	1:B:15:PHE:CD1	2.96	0.43
1:F:55:GLU:CD	1:F:151:ARG:HH21	2.26	0.43
1:F:110:ARG:NH1	1:F:110:ARG:CG	2.74	0.43
1:H:131:PHE:CD1	1:H:142:ILE:CG2	2.95	0.43
1:H:139:LEU:HD11	1:H:142:ILE:HG23	2.00	0.43
1:B:53:PRO:O	1:B:57:ILE:HD12	2.18	0.42
1:C:109:LYS:C	1:C:111:THR:N	2.77	0.42
1:C:157:LEU:O	1:C:161:GLN:HG3	2.19	0.42
1:D:124:GLY:HA3	1:G:108:PRO:O	2.19	0.42
1:E:197:LYS:HG2	1:E:198:GLN:H	1.84	0.42
1:H:94:GLN:HE21	1:H:94:GLN:HB3	1.57	0.42
1:I:27:LYS:O	1:I:29:ILE:HG23	2.19	0.42
1:A:91:PRO:HB2	1:A:93:LYS:NZ	2.33	0.42
1:A:144:ILE:HB	1:B:142:ILE:HG23	2.01	0.42
1:B:157:LEU:HD13	1:B:157:LEU:HA	1.88	0.42
1:C:189:ASN:O	1:C:192:LYS:HB2	2.18	0.42
1:D:133:ILE:HD13	1:D:137:GLY:CA	2.49	0.42
1:G:188:VAL:HG11	1:I:85:LEU:CD2	2.50	0.42
1:I:161:GLN:OE1	1:I:179:PRO:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PHE:CD1	1:D:149:VAL:HG21	2.55	0.42
1:F:22:PRO:HB3	1:F:101:ASN:HA	2.01	0.42
1:A:85:LEU:CA	1:A:88:ILE:HG23	2.49	0.42
1:E:184:ILE:CD1	1:E:191:SER:HA	2.49	0.42
1:F:53:PRO:O	1:F:57:ILE:HG13	2.19	0.42
1:G:43:PHE:O	1:G:151:ARG:NH2	2.41	0.42
1:I:125:ILE:HD12	1:I:125:ILE:HA	1.69	0.42
1:J:120:LYS:HE3	1:J:147:LEU:HD11	2.00	0.42
1:J:134:ASP:OD2	1:J:140:ARG:HD3	2.19	0.42
1:C:52:SER:O	1:C:56:ILE:HG22	2.20	0.42
1:E:16:LYS:HD3	1:E:30:SER:OG	2.19	0.42
1:G:168:LYS:O	1:G:169:HIS:HD2	2.02	0.42
1:H:199:LYS:HB2	1:H:199:LYS:NZ	2.32	0.42
1:I:172:VAL:O	1:I:174:PRO:HD3	2.19	0.42
1:A:46:LEU:HD21	1:A:125:ILE:CD1	2.37	0.42
1:B:142:ILE:HD11	1:B:144:ILE:CG1	2.45	0.42
1:E:68:LYS:C	1:E:70:ASN:H	2.27	0.42
1:E:153:VAL:HG12	1:E:157:LEU:CD2	2.50	0.42
1:F:155:GLU:O	1:F:159:LEU:HG	2.19	0.42
1:H:145:ASN:HD22	1:H:151:ARG:CG	2.25	0.42
1:I:91:PRO:HB2	1:I:93:LYS:CD	2.50	0.42
1:I:141:GLN:HG2	1:J:145:ASN:OD1	2.20	0.42
1:I:172:VAL:HG23	1:I:184:ILE:CG2	2.50	0.42
1:B:198:GLN:OE1	1:B:199:LYS:HD3	2.20	0.42
1:C:37:LYS:HE3	1:C:70:ASN:ND2	2.35	0.42
1:G:67:LYS:HE2	1:G:72:GLN:NE2	2.33	0.42
1:H:87:TRP:CE3	1:H:97:LEU:HD11	2.55	0.42
1:H:194:TYR:CD1	1:H:194:TYR:C	2.97	0.42
1:I:157:LEU:HG	1:I:161:GLN:HE21	1.84	0.42
1:J:37:LYS:HG2	1:J:70:ASN:ND2	2.34	0.42
1:A:56:ILE:HG13	1:A:97:LEU:HD22	2.02	0.42
1:B:124:GLY:O	1:B:125:ILE:HD12	2.19	0.42
1:C:50:PHE:C	1:C:53:PRO:HD2	2.44	0.42
1:D:24:GLY:O	1:D:25:GLN:CG	2.61	0.42
1:E:66:PHE:CE2	1:E:157:LEU:HD13	2.55	0.42
1:F:4:GLY:CA	1:F:117:GLY:HA3	2.50	0.42
1:F:107:ASP:OD2	1:F:110:ARG:HA	2.20	0.42
1:I:190:LYS:O	1:I:193:GLU:HB2	2.19	0.42
1:J:160:VAL:O	1:J:164:GLN:HG3	2.19	0.42
1:D:158:ARG:HD2	1:D:177:TRP:O	2.19	0.42
1:D:189:ASN:C	1:D:191:SER:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:VAL:CB	1:F:110:ARG:NH1	2.79	0.42
1:G:151:ARG:H	1:G:151:ARG:HG2	1.75	0.42
1:H:46:LEU:HB2	1:H:49:THR:HG23	2.01	0.42
1:H:172:VAL:HG23	1:H:184:ILE:CG2	2.50	0.42
1:J:29:ILE:HD12	1:J:29:ILE:N	2.35	0.42
1:J:120:LYS:O	1:J:121:ALA:C	2.63	0.42
1:A:26:PHE:HA	1:A:81:HIS:NE2	2.35	0.42
1:C:129:GLY:HA2	1:C:144:ILE:HA	2.01	0.42
1:G:127:PHE:CZ	1:H:8:ILE:HG12	2.54	0.42
1:G:141:GLN:CG	1:H:145:ASN:OD1	2.68	0.42
1:J:138:ILE:O	1:J:138:ILE:HG13	2.16	0.42
1:A:133:ILE:HD11	1:A:137:GLY:HA2	2.00	0.41
1:C:51:VAL:HG23	1:D:172:VAL:HG21	2.01	0.41
1:D:130:LEU:C	1:D:130:LEU:HD23	2.45	0.41
1:F:47:ASP:O	1:F:48:PHE:HB2	2.20	0.41
1:H:21:MET:HB3	1:H:22:PRO:HD2	2.02	0.41
1:A:102:ILE:HG23	1:A:103:PRO:HD2	2.03	0.41
1:B:110:ARG:HB3	1:B:119:LEU:HD11	2.02	0.41
1:C:199:LYS:HZ3	1:D:92:LYS:NZ	2.18	0.41
1:E:8:ILE:O	1:E:8:ILE:HG13	2.20	0.41
1:E:73:VAL:HB	1:E:102:ILE:HD11	2.02	0.41
1:I:18:THR:HA	1:I:28:ASP:HA	2.02	0.41
1:J:128:ARG:HB3	1:J:151:ARG:CZ	2.49	0.41
1:B:114:GLN:HG3	1:B:119:LEU:HD13	2.03	0.41
1:C:163:PHE:O	1:C:164:GLN:C	2.62	0.41
1:D:107:ASP:OD2	1:D:112:ILE:HB	2.21	0.41
1:D:199:LYS:O	1:D:199:LYS:HG2	2.19	0.41
1:H:38:TYR:CE1	1:H:134:ASP:HB2	2.55	0.41
1:H:162:ALA:O	1:H:165:PHE:HB3	2.19	0.41
1:H:177:TRP:C	1:H:177:TRP:CE3	2.98	0.41
1:A:37:LYS:NZ	1:A:70:ASN:ND2	2.69	0.41
1:A:142:ILE:HD11	1:A:144:ILE:CD1	2.50	0.41
1:B:189:ASN:C	1:B:191:SER:H	2.28	0.41
1:C:54:THR:O	1:C:58:ALA:HB2	2.20	0.41
1:E:39:VAL:HB	1:E:133:ILE:CD1	2.50	0.41
1:E:69:LEU:HD12	1:E:157:LEU:HD12	2.02	0.41
1:G:76:ALA:CB	1:G:105:VAL:HG22	2.47	0.41
1:H:41:PHE:HE2	1:H:112:ILE:HD11	1.85	0.41
1:I:184:ILE:HD13	1:I:184:ILE:C	2.40	0.41
1:J:153:VAL:O	1:J:153:VAL:HG12	2.19	0.41
1:J:157:LEU:O	1:J:161:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PHE:O	1:A:53:PRO:HG2	2.20	0.41
1:A:130:LEU:CD2	1:A:156:ILE:HD12	2.50	0.41
1:D:13:PRO:HD2	1:D:116:TYR:CZ	2.55	0.41
1:F:88:ILE:HD12	1:F:98:GLY:C	2.45	0.41
1:G:50:PHE:O	1:G:54:THR:HG23	2.20	0.41
1:J:29:ILE:CG2	1:J:30:SER:N	2.83	0.41
1:J:114:GLN:CG	1:J:119:LEU:HD22	2.50	0.41
1:J:194:TYR:O	1:J:198:GLN:HG2	2.20	0.41
1:A:172:VAL:O	1:A:174:PRO:HD3	2.21	0.41
1:A:177:TRP:CE3	1:A:177:TRP:C	2.98	0.41
1:D:108:PRO:O	1:G:110:ARG:NH2	2.50	0.41
1:J:134:ASP:OD1	1:J:134:ASP:C	2.64	0.41
1:A:70:ASN:OD1	1:A:70:ASN:O	2.38	0.41
1:E:85:LEU:O	1:E:88:ILE:HG13	2.20	0.41
1:F:57:ILE:HD13	1:F:92:LYS:CD	2.51	0.41
1:H:72:GLN:HE21	1:H:73:VAL:N	2.14	0.41
1:B:64:GLU:O	1:B:68:LYS:HG3	2.20	0.41
1:B:77:SER:OG	1:B:84:HIS:HE1	2.04	0.41
1:C:32:SER:C	1:C:34:TYR:N	2.76	0.41
1:C:130:LEU:HD22	1:C:156:ILE:HD12	2.01	0.41
1:D:54:THR:HA	1:D:57:ILE:HD12	2.03	0.41
1:G:29:ILE:HD13	1:G:29:ILE:N	2.36	0.41
1:H:45:PRO:HG2	1:H:147:LEU:HD13	2.03	0.41
1:H:138:ILE:O	1:H:138:ILE:HG13	2.21	0.41
1:I:92:LYS:C	1:I:94:GLN:H	2.29	0.41
1:I:93:LYS:H	1:I:93:LYS:HE3	1.85	0.41
1:A:110:ARG:NH1	1:A:110:ARG:CG	2.82	0.41
1:B:8:ILE:C	1:B:8:ILE:CD1	2.85	0.41
1:B:73:VAL:C	1:B:74:ILE:HG13	2.46	0.41
1:B:132:ILE:HD13	1:B:140:ARG:HB2	2.03	0.41
1:B:189:ASN:C	1:B:191:SER:N	2.77	0.41
1:C:95:GLY:HA2	1:D:195:PHE:CG	2.56	0.41
1:C:133:ILE:HG12	1:C:134:ASP:N	2.36	0.41
1:D:45:PRO:HD2	1:D:128:ARG:NH1	2.36	0.41
1:D:102:ILE:HA	1:D:103:PRO:HD3	1.94	0.41
1:E:10:HIS:HB3	1:E:11:PRO:CD	2.51	0.41
1:E:46:LEU:HB2	1:E:49:THR:HG21	2.02	0.41
1:E:133:ILE:O	1:E:133:ILE:HD13	2.20	0.41
1:G:64:GLU:C	1:G:66:PHE:N	2.77	0.41
1:G:130:LEU:HD23	1:G:131:PHE:N	2.36	0.41
1:J:185:LYS:HB2	1:J:190:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HB	1:A:102:ILE:CD1	2.51	0.41
1:C:185:LYS:O	1:C:187:ASP:N	2.45	0.41
1:D:133:ILE:HD12	1:D:134:ASP:N	2.36	0.41
1:D:134:ASP:OD2	1:D:138:ILE:CG1	2.69	0.41
1:D:184:ILE:HD11	1:D:191:SER:HB2	2.02	0.41
1:E:124:GLY:C	1:E:125:ILE:HD12	2.45	0.41
1:E:134:ASP:CG	1:E:138:ILE:HG13	2.46	0.41
1:A:192:LYS:C	1:A:194:TYR:H	2.28	0.40
1:B:130:LEU:C	1:B:130:LEU:HD23	2.46	0.40
1:C:24:GLY:O	1:C:25:GLN:O	2.38	0.40
1:F:8:ILE:C	1:F:8:ILE:CD1	2.90	0.40
1:G:138:ILE:O	1:G:138:ILE:HG13	2.21	0.40
1:G:172:VAL:CG2	1:H:51:VAL:HG23	2.52	0.40
1:I:50:PHE:HB3	1:J:184:ILE:CD1	2.46	0.40
1:I:121:ALA:C	1:I:123:GLU:H	2.29	0.40
1:I:184:ILE:HG12	1:I:194:TYR:CB	2.50	0.40
1:C:78:VAL:HB	1:C:110:ARG:NH2	2.36	0.40
1:G:34:TYR:O	1:G:35:LYS:C	2.64	0.40
1:H:27:LYS:HD3	1:H:29:ILE:HD11	2.04	0.40
1:H:138:ILE:HD12	1:H:139:LEU:N	2.36	0.40
1:J:67:LYS:HB2	1:J:67:LYS:HZ2	1.85	0.40
1:A:187:ASP:O	1:A:188:VAL:C	2.64	0.40
1:A:190:LYS:O	1:A:193:GLU:HG2	2.21	0.40
1:B:146:ASP:C	1:B:148:PRO:HD2	2.46	0.40
1:C:8:ILE:HG21	1:D:146:ASP:HA	2.02	0.40
1:E:46:LEU:O	1:E:49:THR:HG23	2.21	0.40
1:E:66:PHE:CZ	1:E:157:LEU:HD22	2.56	0.40
1:E:175:ALA:HB2	1:F:55:GLU:CA	2.51	0.40
1:J:38:TYR:CE2	1:J:132:ILE:HD11	2.56	0.40
1:J:72:GLN:HE21	1:J:72:GLN:C	2.28	0.40
1:A:50:PHE:HB3	1:B:184:ILE:HD13	2.03	0.40
1:B:190:LYS:H	1:B:190:LYS:HD2	1.85	0.40
1:C:37:LYS:HG2	1:C:70:ASN:ND2	2.35	0.40
1:C:40:VAL:HG23	1:C:71:CYS:SG	2.61	0.40
1:D:110:ARG:N	1:D:110:ARG:HD2	2.36	0.40
1:G:172:VAL:HG22	1:G:184:ILE:HG23	2.03	0.40
1:H:112:ILE:HD12	1:H:116:TYR:CD1	2.56	0.40
1:I:39:VAL:HA	1:I:72:GLN:O	2.22	0.40
1:I:121:ALA:O	1:I:123:GLU:N	2.54	0.40
1:J:27:LYS:O	1:J:29:ILE:HD13	2.22	0.40
1:A:74:ILE:HG23	1:A:103:PRO:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HA	1:A:186:PRO:HD2	1.91	0.40
1:B:155:GLU:OE1	1:B:158:ARG:NH2	2.55	0.40
1:C:93:LYS:HE3	1:D:199:LYS:OXT	2.21	0.40
1:C:140:ARG:HG3	1:C:140:ARG:NH1	2.36	0.40
1:D:133:ILE:HD12	1:D:133:ILE:C	2.46	0.40
1:E:3:SER:CA	1:F:3:SER:N	2.84	0.40
1:E:78:VAL:HB	1:E:110:ARG:NH2	2.36	0.40
1:E:110:ARG:NH2	1:J:110:ARG:HH12	2.19	0.40
1:F:14:SER:O	1:F:15:PHE:HB3	2.20	0.40
1:F:52:SER:O	1:F:53:PRO:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/199 (98%)	168 (86%)	21 (11%)	6 (3%)	3	14
1	B	195/199 (98%)	176 (90%)	15 (8%)	4 (2%)	5	21
1	C	195/199 (98%)	167 (86%)	20 (10%)	8 (4%)	2	9
1	D	195/199 (98%)	171 (88%)	19 (10%)	5 (3%)	4	17
1	E	195/199 (98%)	171 (88%)	20 (10%)	4 (2%)	5	21
1	F	195/199 (98%)	172 (88%)	22 (11%)	1 (0%)	24	54
1	G	195/199 (98%)	167 (86%)	23 (12%)	5 (3%)	4	17
1	H	195/199 (98%)	168 (86%)	23 (12%)	4 (2%)	5	21
1	I	195/199 (98%)	167 (86%)	20 (10%)	8 (4%)	2	9
1	J	195/199 (98%)	168 (86%)	22 (11%)	5 (3%)	4	17
All	All	1950/1990 (98%)	1695 (87%)	205 (10%)	50 (3%)	4	17

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	PRO
1	B	196	SER
1	B	198	GLN
1	C	25	GLN
1	C	26	PHE
1	C	35	LYS
1	F	45	PRO
1	G	25	GLN
1	G	190	LYS
1	J	190	LYS
1	A	176	GLY
1	C	121	ALA
1	C	122	ASP
1	C	186	PRO
1	D	121	ALA
1	G	45	PRO
1	I	198	GLN
1	J	121	ALA
1	J	122	ASP
1	A	177	TRP
1	B	197	LYS
1	C	27	LYS
1	C	33	ASP
1	D	24	GLY
1	D	25	GLN
1	D	45	PRO
1	E	5	ASN
1	G	33	ASP
1	H	4	GLY
1	I	25	GLN
1	I	122	ASP
1	J	33	ASP
1	J	45	PRO
1	A	27	LYS
1	A	45	PRO
1	E	25	GLN
1	E	190	LYS
1	I	93	LYS
1	A	25	GLN
1	H	45	PRO
1	I	45	PRO
1	I	174	PRO

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Mol	Chain	Res	Type
1	I	123	GLU
1	I	186	PRO
1	D	186	PRO
1	H	176	GLY
1	A	186	PRO
1	E	186	PRO
1	H	188	VAL
1	G	174	PRO

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	169/171 (99%)	150 (89%)	19 (11%)	6	19
1	B	169/171 (99%)	147 (87%)	22 (13%)	4	13
1	C	169/171 (99%)	154 (91%)	15 (9%)	9	28
1	D	169/171 (99%)	154 (91%)	15 (9%)	9	28
1	E	169/171 (99%)	148 (88%)	21 (12%)	4	15
1	F	169/171 (99%)	151 (89%)	18 (11%)	6	22
1	G	169/171 (99%)	147 (87%)	22 (13%)	4	13
1	H	169/171 (99%)	147 (87%)	22 (13%)	4	13
1	I	169/171 (99%)	154 (91%)	15 (9%)	9	28
1	J	169/171 (99%)	147 (87%)	22 (13%)	4	13
All	All	1690/1710 (99%)	1499 (89%)	191 (11%)	5	19

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	PHE
1	A	29	ILE
1	A	37	LYS
1	A	56	ILE

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Mol	Chain	Res	Type
1	A	57	ILE
1	A	84	HIS
1	A	88	ILE
1	A	93	LYS
1	A	94	GLN
1	A	104	LEU
1	A	115	ASP
1	A	125	ILE
1	A	132	ILE
1	A	133	ILE
1	A	138	ILE
1	A	142	ILE
1	A	157	LEU
1	A	184	ILE
1	B	8	ILE
1	B	45	PRO
1	B	49	THR
1	B	56	ILE
1	B	57	ILE
1	B	62	ARG
1	B	77	SER
1	B	81	HIS
1	B	88	ILE
1	B	94	GLN
1	B	104	LEU
1	B	105	VAL
1	B	112	ILE
1	B	125	ILE
1	B	132	ILE
1	B	133	ILE
1	B	138	ILE
1	B	142	ILE
1	B	157	LEU
1	B	168	LYS
1	B	185	LYS
1	B	188	VAL
1	C	18	THR
1	C	25	GLN
1	C	56	ILE
1	C	57	ILE
1	C	81	HIS
1	C	93	LYS

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Mol	Chain	Res	Type
1	C	102	ILE
1	C	110	ARG
1	C	125	ILE
1	C	132	ILE
1	C	133	ILE
1	C	142	ILE
1	C	164	GLN
1	C	184	ILE
1	C	199	LYS
1	D	8	ILE
1	D	37	LYS
1	D	56	ILE
1	D	57	ILE
1	D	72	GLN
1	D	88	ILE
1	D	104	LEU
1	D	105	VAL
1	D	130	LEU
1	D	133	ILE
1	D	140	ARG
1	D	142	ILE
1	D	144	ILE
1	D	157	LEU
1	D	172	VAL
1	E	5	ASN
1	E	8	ILE
1	E	56	ILE
1	E	57	ILE
1	E	64	GLU
1	E	81	HIS
1	E	88	ILE
1	E	93	LYS
1	E	102	ILE
1	E	104	LEU
1	E	109	LYS
1	E	125	ILE
1	E	130	LEU
1	E	132	ILE
1	E	133	ILE
1	E	142	ILE
1	E	155	GLU
1	E	157	LEU

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Mol	Chain	Res	Type
1	E	168	LYS
1	E	184	ILE
1	E	199	LYS
1	F	5	ASN
1	F	8	ILE
1	F	56	ILE
1	F	67	LYS
1	F	81	HIS
1	F	88	ILE
1	F	92	LYS
1	F	93	LYS
1	F	102	ILE
1	F	115	ASP
1	F	130	LEU
1	F	133	ILE
1	F	138	ILE
1	F	142	ILE
1	F	164	GLN
1	F	184	ILE
1	F	190	LYS
1	F	199	LYS
1	G	8	ILE
1	G	26	PHE
1	G	29	ILE
1	G	52	SER
1	G	56	ILE
1	G	67	LYS
1	G	88	ILE
1	G	91	PRO
1	G	92	LYS
1	G	105	VAL
1	G	109	LYS
1	G	110	ARG
1	G	125	ILE
1	G	138	ILE
1	G	142	ILE
1	G	156	ILE
1	G	167	ASP
1	G	184	ILE
1	G	185	LYS
1	G	188	VAL
1	G	190	LYS

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Mol	Chain	Res	Type
1	G	199	LYS
1	H	7	LYS
1	H	8	ILE
1	H	38	TYR
1	H	54	THR
1	H	68	LYS
1	H	74	ILE
1	H	84	HIS
1	H	88	ILE
1	H	94	GLN
1	H	102	ILE
1	H	104	LEU
1	H	112	ILE
1	H	125	ILE
1	H	133	ILE
1	H	138	ILE
1	H	142	ILE
1	H	154	ASP
1	H	157	LEU
1	H	177	TRP
1	H	184	ILE
1	H	197	LYS
1	H	199	LYS
1	I	14	SER
1	I	37	LYS
1	I	56	ILE
1	I	57	ILE
1	I	72	GLN
1	I	93	LYS
1	I	102	ILE
1	I	105	VAL
1	I	122	ASP
1	I	125	ILE
1	I	132	ILE
1	I	133	ILE
1	I	142	ILE
1	I	184	ILE
1	I	199	LYS
1	J	13	PRO
1	J	22	PRO
1	J	38	TYR
1	J	45	PRO

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Mol	Chain	Res	Type
1	J	56	ILE
1	J	67	LYS
1	J	72	GLN
1	J	88	ILE
1	J	93	LYS
1	J	94	GLN
1	J	102	ILE
1	J	109	LYS
1	J	132	ILE
1	J	138	ILE
1	J	142	ILE
1	J	144	ILE
1	J	147	LEU
1	J	171	GLU
1	J	183	THR
1	J	184	ILE
1	J	192	LYS
1	J	199	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	70	ASN
1	A	164	GLN
1	B	70	ASN
1	B	72	GLN
1	B	81	HIS
1	B	94	GLN
1	B	114	GLN
1	B	164	GLN
1	C	25	GLN
1	C	70	ASN
1	C	72	GLN
1	C	81	HIS
1	C	141	GLN
1	C	198	GLN
1	D	5	ASN
1	D	70	ASN
1	D	72	GLN
1	D	101	ASN
1	D	164	GLN

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Mol	Chain	Res	Type
1	E	5	ASN
1	E	70	ASN
1	E	81	HIS
1	E	141	GLN
1	E	145	ASN
1	E	161	GLN
1	F	70	ASN
1	F	81	HIS
1	F	94	GLN
1	F	114	GLN
1	F	161	GLN
1	G	10	HIS
1	G	70	ASN
1	G	72	GLN
1	G	84	HIS
1	G	164	GLN
1	H	70	ASN
1	H	72	GLN
1	I	10	HIS
1	I	70	ASN
1	I	72	GLN
1	I	84	HIS
1	I	114	GLN
1	J	70	ASN
1	J	72	GLN
1	J	94	GLN
1	J	114	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.