Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 12:25 AM EDT

PDB ID	:	3KCV
Title	:	Structure of formate channel
Authors	:	Wang, Y.; Huang, Y.; Wang, J.; Yan, N.; Shi, Y.
Deposited on	:	2009-10-22
Resolution	:	3.20 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:

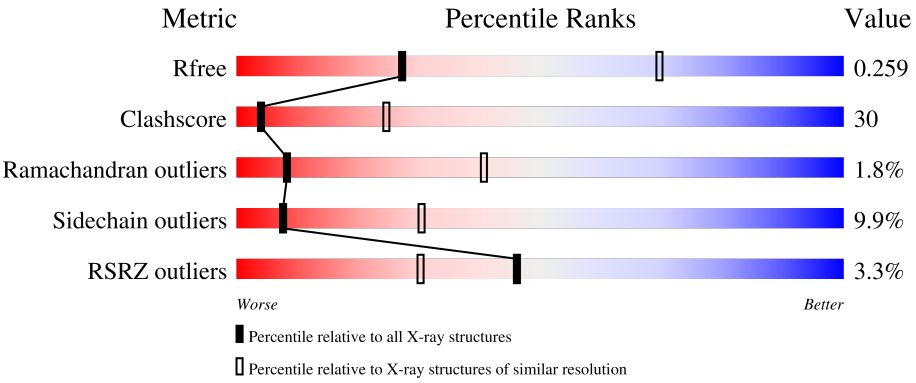
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	285	% 41% 42% • 12%
1	B	285	3% 47% 34% 6% 12%
1	C	285	6% 47% 34% 6% • 12%
1	D	285	4% 41% 42% 5% 12%
1	E	285	4% 41% 41% 6% 12%

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Mol	Chain	Length	Quality of chain
1	F	285	2% 47% 35% 5% 12%
1	G	285	4% 46% 38% 5% 12%
1	H	285	3% 42% 39% 7% 12%
1	I	285	% 43% 39% 6% 12%
1	J	285	% 46% 36% 5% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19120 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 Probable formate transporter 1.

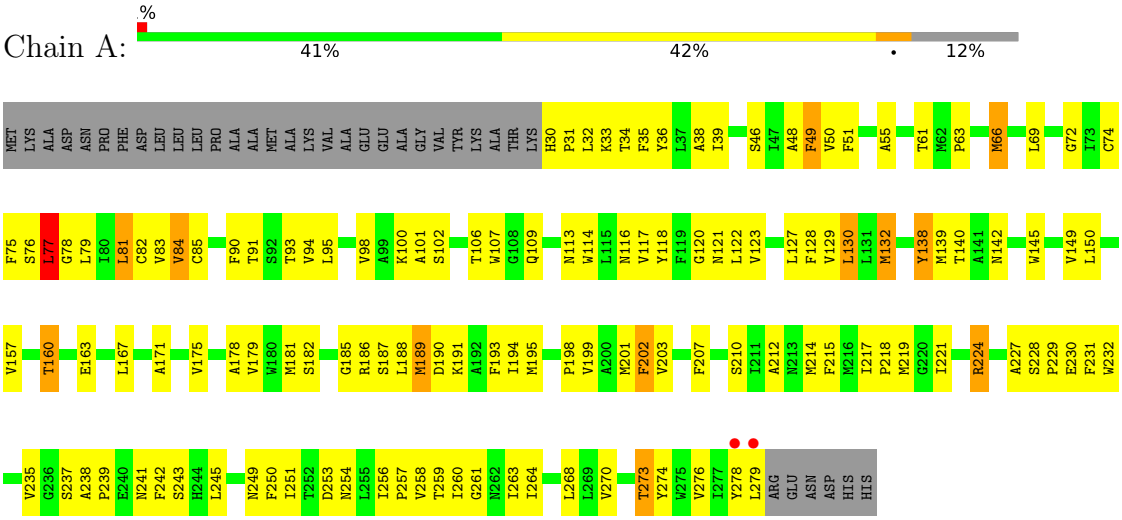
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1907	1269	298	322	18			
1	B	250	Total	C	N	O	S	0	0	0
			1907	1269	298	322	18			
1	C	250	Total	C	N	O	S	0	0	0
			1907	1269	298	322	18			
1	D	251	Total	C	N	O	S	0	0	0
			1912	1272	299	323	18			
1	E	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	F	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	G	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	H	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	I	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	J	249	Total	C	N	O	S	0	0	0
			1902	1267	297	320	18			

3 Residue-property plots (i)

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

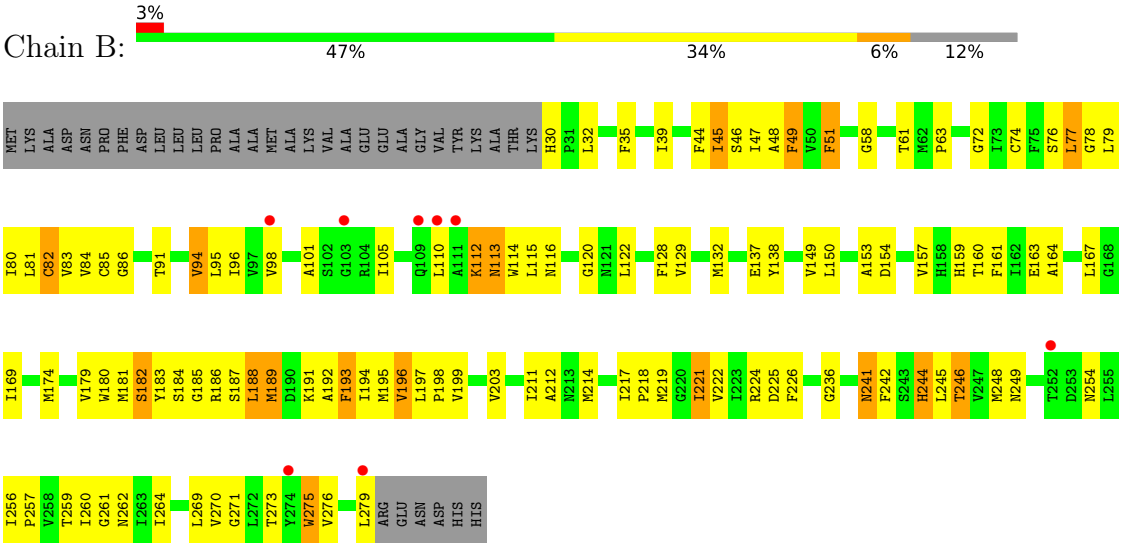
• Molecule 1: Probable formate transporter 1

Chain A:



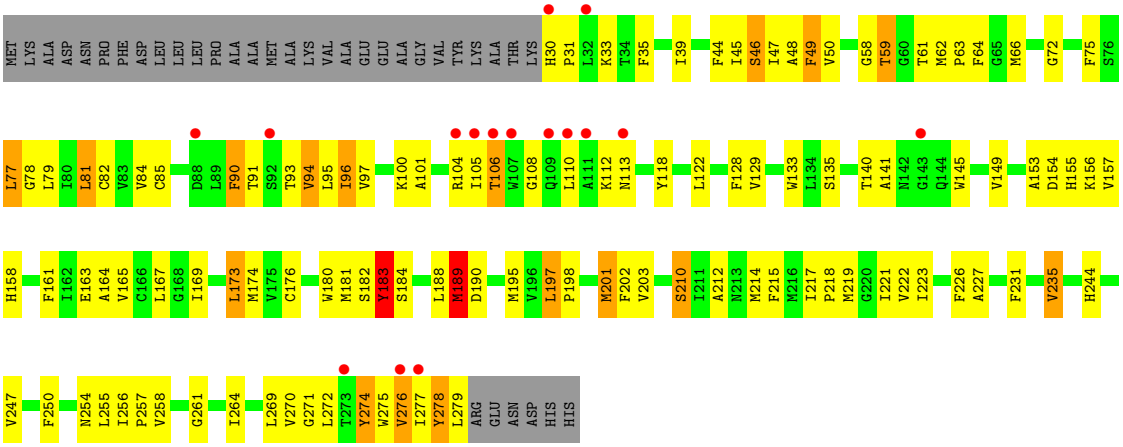
• Molecule 1: Probable formate transporter 1

Chain B:



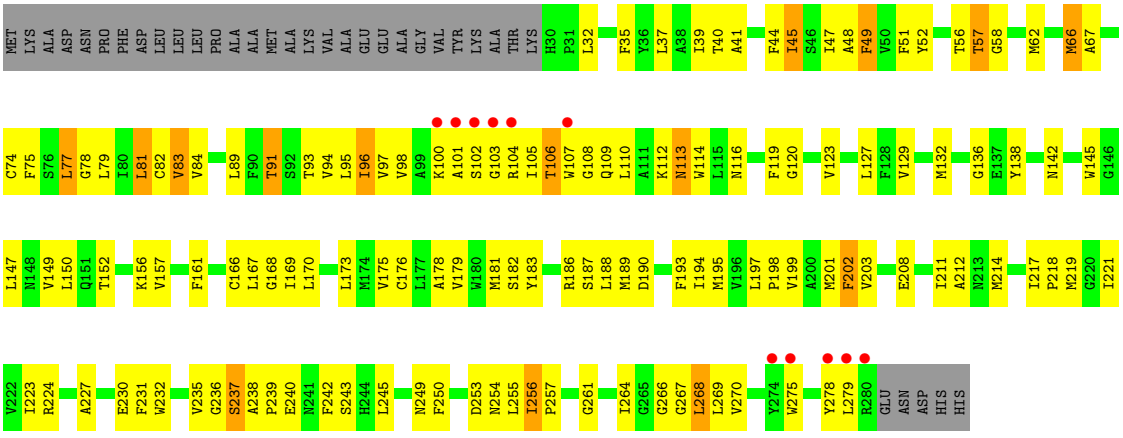
• Molecule 1: Probable formate transporter 1

Chain C:



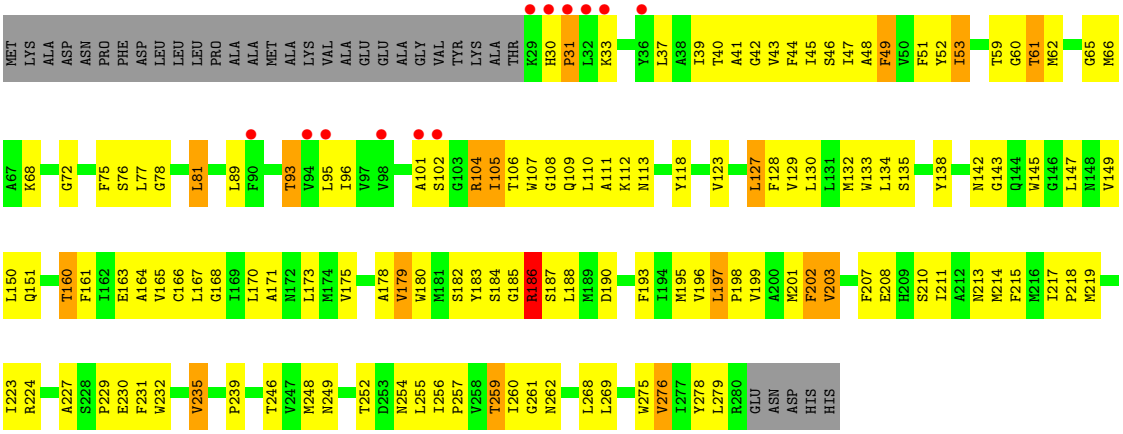
• Molecule 1: Probable formate transporter 1

Chain D:



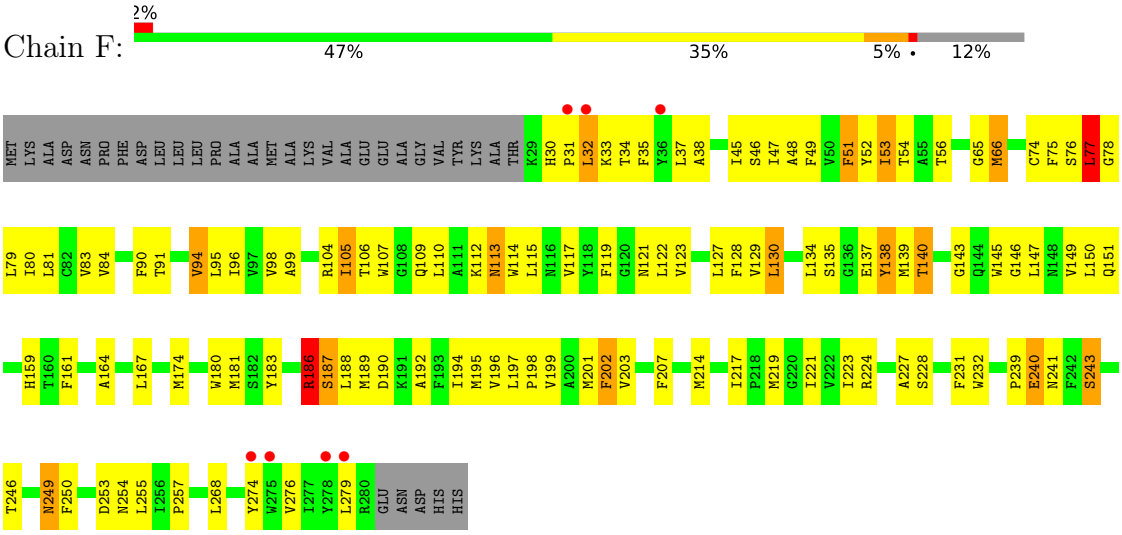
• Molecule 1: Probable formate transporter 1

Chain E:



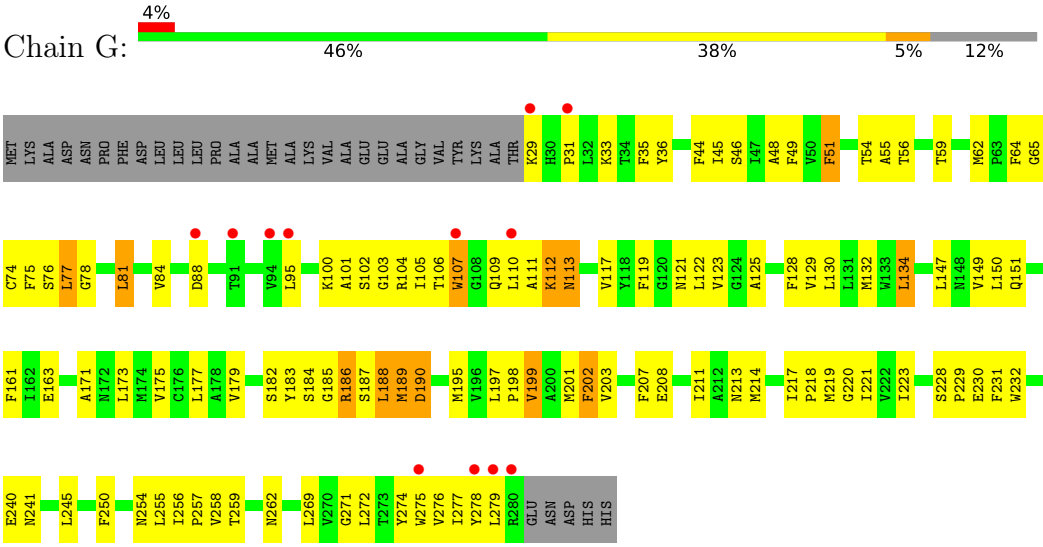
• Molecule 1: Probable formate transporter 1

Chain F:



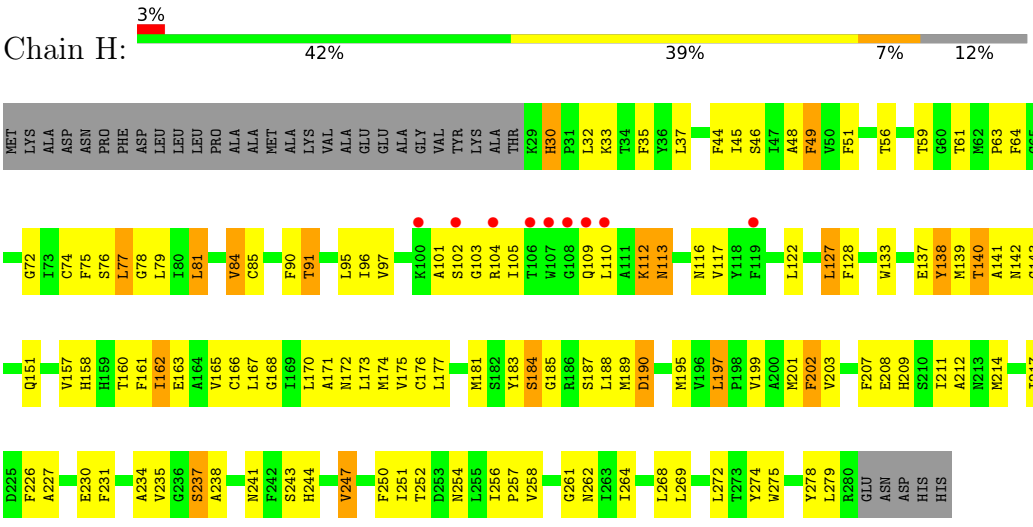
• Molecule 1: Probable formate transporter 1

Chain G:



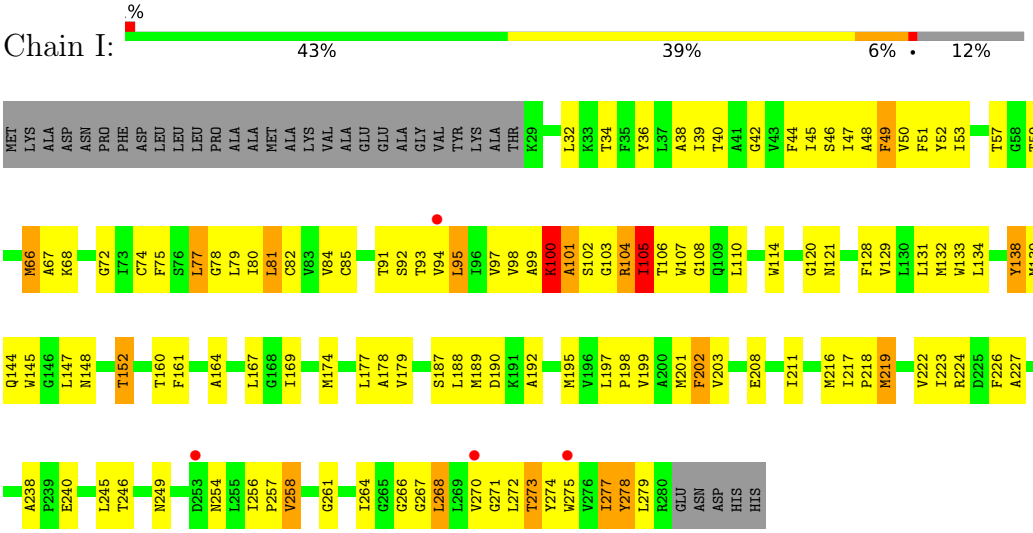
• Molecule 1: Probable formate transporter 1

Chain H:



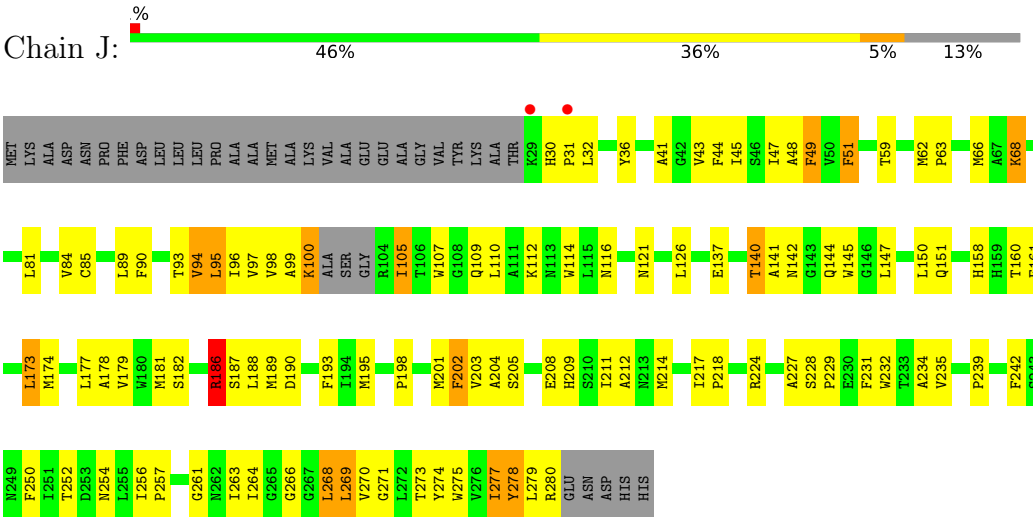
• Molecule 1: Probable formate transporter 1

Chain I:



• Molecule 1: Probable formate transporter 1

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	107.03Å 107.03Å 285.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.61 – 3.20 48.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (48.61-3.20) 99.6 (48.61-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.260 0.195 , 0.259	Depositor DCC
R_{free} test set	3238 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å^2)	84.0	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.027 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19120	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.42	0/1958	0.62	1/2670 (0.0%)
1	B	0.40	0/1958	0.57	0/2670
1	C	0.40	0/1958	0.56	0/2670
1	D	0.38	0/1963	0.57	0/2677
1	E	0.43	0/1968	0.60	0/2684
1	F	0.44	0/1968	0.58	1/2684 (0.0%)
1	G	0.43	0/1968	0.61	0/2684
1	H	0.42	0/1968	0.56	0/2684
1	I	0.46	0/1968	0.70	3/2684 (0.1%)
1	J	0.42	0/1952	0.61	0/2661
All	All	0.42	0/19629	0.60	5/26768 (0.0%)

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	I	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	100	LYS	N-CA-C	11.12	141.04	111.00
1	I	100	LYS	CB-CA-C	-8.88	92.63	110.40
1	I	100	LYS	C-N-CA	6.06	136.84	121.70
1	A	77	LEU	CA-CB-CG	5.48	127.90	115.30
1	F	77	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	100	LYS	Peptide

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	1907	0	1946	128	0
1	B	1907	0	1946	108	0
1	C	1907	0	1946	130	0
1	D	1912	0	1948	168	0
1	E	1917	0	1950	134	0
1	F	1917	0	1950	114	0
1	G	1917	0	1950	129	0
1	H	1917	0	1950	158	0
1	I	1917	0	1950	147	0
1	J	1902	0	1936	114	0
All	All	19120	0	19472	1160	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 30.

All (1160) 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:223:ILE:O	1:C:227:ALA:HB2	1.39	1.23
1:D:101:ALA:O	1:D:104:ARG:HB2	1.45	1.13
1:H:95:LEU:HD21	1:H:269:LEU:HB3	1.37	1.05
1:I:271:GLY:O	1:I:275:TRP:HD1	1.38	1.04
1:C:274:TYR:O	1:C:278:TYR:HB3	1.59	1.02
1:D:98:VAL:HG11	1:D:270:VAL:HG13	1.36	1.02
1:D:264:ILE:O	1:D:268:LEU:HB3	1.61	1.00
1:E:101:ALA:O	1:E:104:ARG:HB2	1.62	0.98
1:C:140:THR:O	1:C:145:TRP:HB2	1.66	0.95
1:C:106:THR:O	1:C:110:LEU:HB2	1.66	0.95
1:A:190:ASP:OD2	1:B:187:SER:HB2	1.68	0.92
1:I:271:GLY:O	1:I:275:TRP:CD1	2.22	0.92
1:G:190:ASP:HB3	1:H:188:LEU:HB3	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LYS:HD2	1:J:280:ARG:HA	1.53	0.90
1:I:268:LEU:O	1:I:272:LEU:HD13	1.70	0.89
1:J:271:GLY:O	1:J:274:TYR:HB3	1.70	0.89
1:C:95:LEU:HD21	1:C:269:LEU:HB3	1.55	0.89
1:E:95:LEU:HD21	1:E:269:LEU:HB3	1.54	0.88
1:D:102:SER:HB2	1:D:104:ARG:HD3	1.56	0.87
1:D:98:VAL:HG21	1:D:270:VAL:CG2	2.04	0.86
1:J:97:VAL:HB	1:J:270:VAL:HG11	1.58	0.85
1:A:190:ASP:HB3	1:B:188:LEU:HB2	1.58	0.84
1:H:264:ILE:O	1:H:268:LEU:HG	1.77	0.84
1:D:264:ILE:O	1:D:268:LEU:CB	2.26	0.83
1:C:223:ILE:O	1:C:227:ALA:CB	2.22	0.83
1:D:186:ARG:HH12	1:H:230:GLU:HG3	1.43	0.82
1:D:275:TRP:HA	1:D:278:TYR:HB3	1.60	0.82
1:G:48:ALA:HB2	1:G:78:GLY:HA3	1.61	0.82
1:F:33:LYS:HB2	1:J:279:LEU:HB2	1.60	0.82
1:H:109:GLN:HA	1:H:112:LYS:HE3	1.62	0.81
1:H:197:LEU:HB3	1:I:77:LEU:HG	1.63	0.81
1:C:274:TYR:O	1:C:278:TYR:CB	2.27	0.81
1:H:95:LEU:HD11	1:H:269:LEU:HD13	1.62	0.81
1:I:201:MET:HA	1:J:51:PHE:CE1	2.16	0.81
1:D:98:VAL:HG21	1:D:270:VAL:HG21	1.64	0.80
1:D:96:ILE:HD12	1:D:96:ILE:H	1.45	0.80
1:D:94:VAL:HG11	1:D:266:GLY:HA2	1.63	0.80
1:G:275:TRP:O	1:G:279:LEU:HB2	1.82	0.80
1:I:94:VAL:HG23	1:I:114:TRP:CZ2	2.17	0.80
1:A:188:LEU:HD23	1:E:190:ASP:HB3	1.64	0.80
1:F:186:ARG:HD3	1:F:187:SER:N	1.97	0.79
1:A:48:ALA:HB2	1:A:78:GLY:HA3	1.62	0.79
1:H:45:ILE:HG21	1:H:211:ILE:HG22	1.63	0.79
1:I:94:VAL:HG23	1:I:114:TRP:HZ2	1.45	0.79
1:A:193:PHE:HZ	1:E:193:PHE:O	1.65	0.79
1:B:101:ALA:HB1	1:B:105:ILE:HB	1.65	0.79
1:I:274:TYR:O	1:I:278:TYR:HB3	1.81	0.78
1:G:101:ALA:O	1:G:104:ARG:HG2	1.83	0.78
1:D:62:MET:HE2	1:D:67:ALA:HB2	1.64	0.78
1:I:177:LEU:HD13	1:J:81:LEU:HD21	1.65	0.78
1:C:271:GLY:O	1:C:274:TYR:HB3	1.84	0.78
1:A:274:TYR:O	1:A:278:TYR:CB	2.32	0.78
1:E:186:ARG:HH11	1:E:186:ARG:HA	1.47	0.77
1:H:122:LEU:HD13	1:H:214:MET:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ILE:HD12	1:C:250:PHE:CD1	2.18	0.77
1:J:256:ILE:HB	1:J:257:PRO:HD3	1.65	0.77
1:B:95:LEU:HD11	1:B:269:LEU:HB3	1.67	0.76
1:C:108:GLY:O	1:C:112:LYS:HG2	1.84	0.76
1:C:94:VAL:HG12	1:C:95:LEU:HD23	1.68	0.75
1:A:63:PRO:HB3	1:B:58:GLY:O	1.87	0.75
1:F:66:MET:HE2	1:F:66:MET:N	2.01	0.75
1:A:163:GLU:O	1:A:167:LEU:HG	1.86	0.74
1:I:66:MET:HE1	1:J:59:THR:HG21	1.68	0.74
1:I:101:ALA:HB2	1:I:110:LEU:CD2	2.18	0.74
1:A:249:ASN:O	1:A:253:ASP:HB2	1.87	0.74
1:C:106:THR:O	1:C:110:LEU:CB	2.35	0.74
1:F:254:ASN:O	1:F:257:PRO:HD2	1.88	0.74
1:A:98:VAL:HG11	1:A:273:THR:HG21	1.68	0.73
1:J:177:LEU:HD21	1:J:269:LEU:HD11	1.70	0.73
1:H:76:SER:HA	1:H:199:VAL:HG11	1.69	0.73
1:J:97:VAL:CB	1:J:270:VAL:HG11	2.19	0.73
1:A:224:ARG:HH21	1:A:243:SER:HA	1.53	0.72
1:C:48:ALA:HB2	1:C:78:GLY:HA3	1.72	0.72
1:D:268:LEU:HD23	1:D:269:LEU:N	2.05	0.72
1:A:274:TYR:O	1:A:278:TYR:HB3	1.90	0.72
1:E:179:VAL:O	1:E:182:SER:HB3	1.88	0.72
1:G:147:LEU:HD22	1:G:235:VAL:HB	1.70	0.72
1:I:238:ALA:HB1	1:I:240:GLU:OE1	1.90	0.72
1:D:94:VAL:HG11	1:D:266:GLY:CA	2.20	0.71
1:E:104:ARG:HD2	1:I:61:THR:HG22	1.71	0.71
1:J:97:VAL:CG1	1:J:270:VAL:HG11	2.20	0.71
1:G:66:MET:HE1	1:H:59:THR:HG22	1.72	0.71
1:C:278:TYR:CE2	1:C:279:LEU:HG	2.25	0.71
1:D:186:ARG:NH1	1:H:230:GLU:HG3	2.05	0.71
1:G:160:THR:OG1	1:G:163:GLU:HG3	1.90	0.71
1:A:186:ARG:HD2	1:A:186:ARG:N	2.06	0.71
1:D:223:ILE:O	1:D:227:ALA:HB2	1.91	0.71
1:C:218:PRO:O	1:C:222:VAL:HG23	1.91	0.71
1:B:197:LEU:HD23	1:C:77:LEU:HB2	1.71	0.70
1:D:250:PHE:CZ	1:D:255:LEU:HD22	2.26	0.70
1:F:138:TYR:CE1	1:F:139:MET:HG2	2.26	0.70
1:E:105:ILE:HG23	1:E:110:LEU:HD11	1.72	0.70
1:E:150:LEU:CD2	1:E:224:ARG:HB2	2.22	0.70
1:B:244:HIS:CD2	1:B:244:HIS:H	2.09	0.70
1:D:123:VAL:O	1:D:127:LEU:HG	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:SER:HB3	1:E:128:PHE:HD2	1.57	0.70
1:F:202:PHE:HB2	1:F:207:PHE:HD2	1.56	0.70
1:B:115:LEU:O	1:B:115:LEU:HD12	1.92	0.70
1:F:48:ALA:HB2	1:F:78:GLY:HA3	1.73	0.69
1:A:185:GLY:HA2	1:B:188:LEU:HD22	1.72	0.69
1:I:279:LEU:HD22	1:J:30:HIS:CE1	2.27	0.69
1:H:211:ILE:HD13	1:H:214:MET:HE1	1.75	0.69
1:G:75:PHE:CD2	1:G:203:VAL:HG21	2.27	0.69
1:D:98:VAL:HG21	1:D:270:VAL:HG22	1.74	0.69
1:I:101:ALA:HB2	1:I:110:LEU:HD21	1.73	0.69
1:C:181:MET:HG2	1:D:84:VAL:HG11	1.72	0.69
1:B:94:VAL:HG12	1:B:95:LEU:HD23	1.75	0.69
1:E:102:SER:HB2	1:E:104:ARG:HD3	1.73	0.69
1:H:103:GLY:C	1:H:105:ILE:H	1.96	0.69
1:I:95:LEU:CD1	1:I:179:VAL:HG12	2.23	0.69
1:D:190:ASP:HB3	1:E:188:LEU:HB3	1.74	0.69
1:I:63:PRO:HB3	1:J:59:THR:HG22	1.73	0.69
1:H:166:CYS:SG	1:I:134:LEU:HB3	2.32	0.69
1:A:187:SER:HA	1:E:186:ARG:HG3	1.76	0.68
1:C:94:VAL:CG1	1:C:270:VAL:HG23	2.24	0.68
1:B:154:ASP:OD1	1:B:244:HIS:CD2	2.47	0.68
1:I:100:LYS:O	1:I:104:ARG:N	2.22	0.68
1:J:161:PHE:CD1	1:J:257:PRO:HG3	2.28	0.68
1:A:98:VAL:HG21	1:A:270:VAL:HG22	1.76	0.67
1:A:81:LEU:O	1:A:85:CYS:HB2	1.93	0.67
1:E:202:PHE:CZ	1:E:203:VAL:HG23	2.28	0.67
1:J:32:LEU:HD23	1:J:32:LEU:O	1.93	0.67
1:J:142:ASN:ND2	1:J:234:ALA:HB1	2.09	0.67
1:C:274:TYR:HD2	1:C:275:TRP:N	1.92	0.67
1:E:186:ARG:HA	1:E:186:ARG:NH1	2.09	0.67
1:G:276:VAL:HG12	1:G:276:VAL:O	1.94	0.67
1:A:274:TYR:O	1:A:278:TYR:HB2	1.95	0.67
1:H:174:MET:SD	1:I:47:ILE:HD13	2.34	0.67
1:A:228:SER:O	1:A:231:PHE:HB3	1.95	0.67
1:E:96:ILE:HG12	1:E:183:TYR:CZ	2.30	0.67
1:F:75:PHE:CD2	1:F:203:VAL:HG21	2.30	0.67
1:A:32:LEU:HD12	1:A:32:LEU:H	1.59	0.67
1:B:154:ASP:HA	1:B:245:LEU:HD21	1.77	0.67
1:H:140:THR:HG22	1:H:145:TRP:HB2	1.76	0.67
1:B:129:VAL:HA	1:B:219:MET:HE1	1.77	0.66
1:D:96:ILE:HD12	1:D:96:ILE:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD13	1:A:242:PHE:CE2	2.30	0.66
1:D:266:GLY:O	1:D:270:VAL:HG23	1.94	0.66
1:A:254:ASN:O	1:A:257:PRO:HD2	1.96	0.66
1:J:274:TYR:CE2	1:J:275:TRP:CD1	2.84	0.66
1:G:190:ASP:OD2	1:H:188:LEU:N	2.26	0.65
1:J:84:VAL:HG11	1:J:188:LEU:HD11	1.78	0.65
1:B:261:GLY:HA2	1:B:264:ILE:HD12	1.78	0.65
1:C:90:PHE:CD2	1:C:91:THR:HG23	2.31	0.65
1:C:276:VAL:HG13	1:D:37:LEU:HD21	1.78	0.65
1:C:217:ILE:HB	1:C:218:PRO:HD3	1.78	0.65
1:D:110:LEU:C	1:D:110:LEU:HD23	2.17	0.65
1:H:48:ALA:HB2	1:H:78:GLY:HA3	1.77	0.65
1:H:256:ILE:HB	1:H:257:PRO:HD3	1.79	0.65
1:D:161:PHE:CE1	1:D:257:PRO:HG3	2.32	0.65
1:E:255:LEU:O	1:E:259:THR:HB	1.97	0.65
1:G:202:PHE:HD1	1:G:207:PHE:HB2	1.62	0.65
1:D:103:GLY:C	1:D:105:ILE:H	1.99	0.65
1:C:93:THR:O	1:C:97:VAL:HG23	1.97	0.64
1:A:279:LEU:HD11	1:B:32:LEU:HB3	1.80	0.64
1:C:145:TRP:O	1:C:149:VAL:HG23	1.97	0.64
1:D:119:PHE:O	1:D:123:VAL:HG23	1.96	0.64
1:I:99:ALA:O	1:I:103:GLY:HA3	1.97	0.64
1:H:101:ALA:HB1	1:H:105:ILE:HB	1.78	0.64
1:I:195:MET:C	1:I:198:PRO:HD2	2.18	0.64
1:E:43:VAL:O	1:E:47:ILE:HG13	1.98	0.64
1:J:43:VAL:O	1:J:47:ILE:HG13	1.97	0.64
1:A:175:VAL:O	1:A:179:VAL:HG23	1.98	0.64
1:C:35:PHE:O	1:C:39:ILE:HG13	1.98	0.64
1:H:46:SER:HB3	1:H:128:PHE:HD2	1.62	0.64
1:H:105:ILE:HG23	1:H:105:ILE:O	1.97	0.64
1:I:208:GLU:HB3	1:I:258:VAL:HG21	1.80	0.64
1:D:45:ILE:O	1:D:48:ALA:HB3	1.98	0.63
1:B:129:VAL:HG22	1:B:219:MET:HE2	1.80	0.63
1:D:101:ALA:HB3	1:D:105:ILE:HB	1.79	0.63
1:D:101:ALA:O	1:D:104:ARG:CB	2.36	0.63
1:H:274:TYR:O	1:H:278:TYR:HB3	1.99	0.63
1:A:187:SER:HB2	1:E:190:ASP:OD2	1.99	0.63
1:D:178:ALA:HB1	1:D:195:MET:HG2	1.81	0.63
1:E:93:THR:HG22	1:E:183:TYR:OH	1.97	0.63
1:I:38:ALA:O	1:I:121:ASN:ND2	2.29	0.63
1:E:48:ALA:HB2	1:E:78:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:HIS:CE1	1:F:32:LEU:HD22	2.34	0.63
1:A:129:VAL:HA	1:A:219:MET:CE	2.29	0.63
1:A:215:PHE:CE1	1:A:219:MET:HE2	2.34	0.63
1:B:35:PHE:HB2	1:B:116:ASN:HD21	1.64	0.63
1:F:46:SER:HB3	1:F:128:PHE:CD2	2.34	0.63
1:B:63:PRO:HB3	1:C:58:GLY:O	1.99	0.62
1:D:102:SER:C	1:D:104:ARG:H	2.02	0.62
1:H:97:VAL:HG12	1:H:110:LEU:HG	1.80	0.62
1:J:137:GLU:O	1:J:140:THR:HB	1.98	0.62
1:A:84:VAL:O	1:A:84:VAL:HG12	1.97	0.62
1:F:109:GLN:HA	1:F:112:LYS:HE3	1.81	0.62
1:H:133:TRP:CZ2	1:H:226:PHE:HB3	2.34	0.62
1:J:277:ILE:HG22	1:J:277:ILE:O	2.00	0.62
1:B:94:VAL:CG1	1:B:270:VAL:HG23	2.29	0.62
1:H:81:LEU:O	1:H:85:CYS:HB2	1.99	0.62
1:I:178:ALA:HB2	1:I:198:PRO:HB2	1.82	0.62
1:A:224:ARG:NH2	1:A:243:SER:HA	2.14	0.62
1:G:147:LEU:HG	1:G:151:GLN:OE1	2.00	0.62
1:A:76:SER:HA	1:A:199:VAL:HG11	1.81	0.62
1:A:77:LEU:HD21	1:E:198:PRO:HG3	1.82	0.62
1:J:177:LEU:CD2	1:J:269:LEU:HD11	2.29	0.62
1:H:217:ILE:HB	1:H:218:PRO:HD3	1.82	0.62
1:A:181:MET:HE3	1:A:194:ILE:HG13	1.81	0.61
1:H:84:VAL:HG12	1:H:84:VAL:O	1.99	0.61
1:J:75:PHE:CD2	1:J:203:VAL:HG21	2.35	0.61
1:C:210:SER:O	1:C:214:MET:HG3	2.00	0.61
1:H:201:MET:HG2	1:I:51:PHE:CD1	2.35	0.61
1:H:75:PHE:CD2	1:H:203:VAL:HG21	2.35	0.61
1:D:186:ARG:HH12	1:H:230:GLU:HA	1.64	0.61
1:F:96:ILE:CD1	1:F:183:TYR:HB2	2.30	0.61
1:F:223:ILE:O	1:F:227:ALA:HB2	2.00	0.61
1:G:95:LEU:HD11	1:G:269:LEU:HB3	1.82	0.61
1:B:83:VAL:HG12	1:B:84:VAL:N	2.14	0.61
1:B:161:PHE:CD1	1:B:257:PRO:HG3	2.35	0.61
1:C:176:CYS:HB2	1:C:269:LEU:HD12	1.82	0.61
1:D:105:ILE:O	1:D:105:ILE:HG23	2.01	0.61
1:H:66:MET:HE1	1:I:59:THR:HG21	1.83	0.61
1:H:189:MET:HG3	1:I:189:MET:CE	2.31	0.61
1:D:186:ARG:HH12	1:H:230:GLU:CG	2.14	0.61
1:J:48:ALA:HB2	1:J:78:GLY:HA3	1.82	0.61
1:I:48:ALA:HB2	1:I:78:GLY:HA3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:O	1:C:100:LYS:HB3	2.00	0.61
1:D:179:VAL:O	1:D:182:SER:HB3	2.01	0.61
1:E:202:PHE:CE2	1:E:203:VAL:HG23	2.36	0.61
1:I:98:VAL:HA	1:I:101:ALA:HB3	1.81	0.61
1:C:256:ILE:HB	1:C:257:PRO:HD3	1.83	0.60
1:E:164:ALA:HA	1:E:167:LEU:HD12	1.82	0.60
1:G:202:PHE:HA	1:G:207:PHE:CD2	2.36	0.60
1:H:189:MET:HG3	1:I:189:MET:HE1	1.83	0.60
1:I:195:MET:O	1:I:198:PRO:HD2	2.01	0.60
1:C:217:ILE:HD12	1:C:254:ASN:HD22	1.66	0.60
1:D:79:LEU:HD21	1:D:175:VAL:HG13	1.84	0.60
1:E:95:LEU:HD21	1:E:269:LEU:CB	2.31	0.60
1:H:166:CYS:O	1:H:170:LEU:HD12	2.00	0.60
1:H:211:ILE:HD13	1:H:214:MET:CE	2.31	0.60
1:B:275:TRP:O	1:B:279:LEU:HB2	2.02	0.60
1:G:189:MET:HG3	1:H:189:MET:HE2	1.82	0.60
1:H:190:ASP:OD2	1:I:188:LEU:N	2.32	0.60
1:I:95:LEU:HD12	1:I:179:VAL:HG12	1.83	0.60
1:E:167:LEU:HA	1:E:170:LEU:HD12	1.83	0.60
1:J:105:ILE:HB	1:J:109:GLN:OE1	2.02	0.60
1:I:197:LEU:HB3	1:J:77:LEU:HD23	1.84	0.60
1:A:132:MET:HB3	1:A:219:MET:HE1	1.84	0.59
1:A:232:TRP:CE3	1:A:238:ALA:HA	2.37	0.59
1:D:149:VAL:HG11	1:D:219:MET:HG3	1.82	0.59
1:F:46:SER:HB3	1:F:128:PHE:HD2	1.67	0.59
1:F:188:LEU:N	1:J:190:ASP:OD2	2.29	0.59
1:B:217:ILE:O	1:B:221:ILE:HG13	2.03	0.59
1:H:252:THR:HA	1:H:256:ILE:HD12	1.82	0.59
1:C:90:PHE:CD1	1:C:118:TYR:HD1	2.20	0.59
1:D:108:GLY:O	1:D:112:LYS:HE3	2.03	0.59
1:C:161:PHE:CE1	1:C:257:PRO:HG3	2.37	0.59
1:F:198:PRO:HG3	1:G:77:LEU:HD21	1.83	0.59
1:J:275:TRP:HZ3	1:J:279:LEU:HD21	1.67	0.59
1:A:83:VAL:HG12	1:A:84:VAL:N	2.17	0.59
1:D:103:GLY:C	1:D:105:ILE:N	2.55	0.59
1:H:224:ARG:NH2	1:H:243:SER:HA	2.16	0.59
1:J:141:ALA:O	1:J:144:GLN:HB2	2.03	0.59
1:C:227:ALA:HB1	1:C:231:PHE:CD2	2.37	0.59
1:C:274:TYR:C	1:C:274:TYR:CD2	2.75	0.59
1:E:60:GLY:C	1:E:62:MET:H	2.05	0.59
1:G:190:ASP:HB3	1:H:188:LEU:CB	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:TRP:HA	1:B:275:TRP:CE3	2.38	0.58
1:G:254:ASN:O	1:G:257:PRO:HD2	2.03	0.58
1:C:75:PHE:CD2	1:C:203:VAL:HG21	2.38	0.58
1:D:98:VAL:HG13	1:D:105:ILE:HG21	1.84	0.58
1:A:129:VAL:HA	1:A:219:MET:HE2	1.83	0.58
1:B:77:LEU:O	1:B:81:LEU:HB2	2.03	0.58
1:D:110:LEU:HD23	1:D:110:LEU:O	2.03	0.58
1:E:178:ALA:HB2	1:E:198:PRO:HB2	1.86	0.58
1:F:52:TYR:O	1:F:56:THR:HG23	2.03	0.58
1:G:155:HIS:C	1:G:155:HIS:HD1	2.06	0.58
1:B:179:VAL:O	1:B:182:SER:HB3	2.03	0.58
1:A:122:LEU:HD13	1:A:214:MET:SD	2.43	0.58
1:D:91:THR:O	1:D:94:VAL:HB	2.03	0.58
1:F:217:ILE:O	1:F:221:ILE:HG13	2.04	0.58
1:H:30:HIS:CE1	1:H:32:LEU:H	2.22	0.58
1:H:72:GLY:HA2	1:H:203:VAL:CG1	2.34	0.58
1:E:179:VAL:HG12	1:E:180:TRP:N	2.18	0.58
1:J:217:ILE:HG21	1:J:250:PHE:HB2	1.86	0.58
1:C:72:GLY:HA2	1:C:203:VAL:CG1	2.34	0.58
1:D:48:ALA:HB2	1:D:78:GLY:HA3	1.85	0.58
1:D:227:ALA:HB1	1:D:231:PHE:CD2	2.39	0.58
1:C:271:GLY:O	1:C:275:TRP:CD1	2.57	0.57
1:D:129:VAL:HA	1:D:219:MET:CE	2.34	0.57
1:B:242:PHE:HA	1:B:244:HIS:NE2	2.18	0.57
1:C:270:VAL:O	1:C:274:TYR:CB	2.52	0.57
1:D:103:GLY:HA2	1:D:105:ILE:HG22	1.84	0.57
1:D:224:ARG:HG3	1:D:242:PHE:HB2	1.86	0.57
1:D:238:ALA:HB1	1:D:240:GLU:OE1	2.04	0.57
1:E:150:LEU:HD21	1:E:224:ARG:HB2	1.85	0.57
1:F:186:ARG:HB3	1:F:190:ASP:OD2	2.03	0.57
1:F:201:MET:HB2	1:G:51:PHE:CE2	2.39	0.57
1:H:168:GLY:HA2	1:H:208:GLU:O	2.04	0.57
1:C:201:MET:HA	1:D:51:PHE:CE1	2.39	0.57
1:D:96:ILE:HG12	1:D:183:TYR:OH	2.05	0.57
1:B:161:PHE:CE1	1:B:257:PRO:HG3	2.39	0.57
1:B:167:LEU:HD23	1:C:135:SER:HB2	1.86	0.57
1:B:242:PHE:HA	1:B:244:HIS:CD2	2.39	0.57
1:D:106:THR:HG22	1:D:109:GLN:HB3	1.86	0.57
1:E:223:ILE:O	1:E:227:ALA:HB2	2.04	0.57
1:G:66:MET:HE1	1:H:59:THR:CG2	2.34	0.57
1:G:66:MET:CE	1:H:59:THR:HG22	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:161:PHE:CE1	1:J:257:PRO:HG3	2.40	0.57
1:B:246:THR:OG1	1:B:249:ASN:ND2	2.37	0.57
1:B:256:ILE:HB	1:B:257:PRO:HD3	1.87	0.57
1:F:187:SER:HB2	1:J:190:ASP:OD2	2.05	0.57
1:H:44:PHE:CD2	1:H:81:LEU:HB3	2.40	0.57
1:E:123:VAL:HG12	1:E:127:LEU:HD12	1.87	0.57
1:B:260:ILE:HG22	1:B:264:ILE:HD11	1.87	0.57
1:H:138:TYR:HD2	1:H:223:ILE:HG23	1.67	0.57
1:I:94:VAL:O	1:I:98:VAL:HG22	2.04	0.57
1:E:46:SER:CB	1:E:128:PHE:CD2	2.88	0.57
1:I:266:GLY:O	1:I:270:VAL:HG23	2.05	0.57
1:F:181:MET:SD	1:G:81:LEU:HD12	2.45	0.57
1:G:101:ALA:HB1	1:G:104:ARG:HG3	1.87	0.57
1:H:237:SER:OG	1:H:241:ASN:ND2	2.36	0.57
1:A:189:MET:HG2	1:B:189:MET:HG2	1.87	0.56
1:D:242:PHE:HB3	1:D:245:LEU:HD12	1.87	0.56
1:E:76:SER:OG	1:E:196:VAL:HG22	2.04	0.56
1:E:161:PHE:CD1	1:E:257:PRO:HG3	2.39	0.56
1:A:185:GLY:CA	1:B:188:LEU:HD22	2.36	0.56
1:B:46:SER:HB3	1:B:128:PHE:CD2	2.40	0.56
1:F:30:HIS:CD2	1:J:279:LEU:HD22	2.41	0.56
1:F:129:VAL:HG13	1:F:219:MET:SD	2.45	0.56
1:I:100:LYS:O	1:I:104:ARG:C	2.43	0.56
1:J:121:ASN:HB3	1:J:211:ILE:HD12	1.86	0.56
1:G:161:PHE:CD1	1:G:257:PRO:HG3	2.40	0.56
1:I:106:THR:O	1:I:110:LEU:HG	2.06	0.56
1:A:171:ALA:O	1:A:175:VAL:HG23	2.05	0.56
1:E:231:PHE:O	1:E:235:VAL:HG22	2.05	0.56
1:G:101:ALA:C	1:G:103:GLY:H	2.08	0.56
1:G:190:ASP:OD2	1:H:187:SER:HB2	2.05	0.56
1:A:128:PHE:O	1:A:132:MET:HB2	2.05	0.56
1:H:66:MET:H	1:H:66:MET:HE2	1.69	0.56
1:I:142:ASN:ND2	1:I:234:ALA:HB1	2.21	0.56
1:A:46:SER:HB3	1:A:128:PHE:CD2	2.41	0.56
1:A:160:THR:OG1	1:A:163:GLU:HG3	2.04	0.56
1:D:249:ASN:O	1:D:253:ASP:HB2	2.06	0.56
1:E:68:LYS:HD2	1:E:68:LYS:N	2.19	0.56
1:H:49:PHE:CE2	1:H:212:ALA:HB1	2.41	0.56
1:I:199:VAL:HG13	1:I:202:PHE:HE2	1.71	0.56
1:A:32:LEU:HD12	1:A:32:LEU:N	2.20	0.56
1:B:76:SER:OG	1:B:196:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ALA:HB1	1:C:231:PHE:HD2	1.71	0.56
1:D:217:ILE:HB	1:D:218:PRO:HD3	1.87	0.56
1:A:259:THR:O	1:A:263:ILE:HG13	2.05	0.55
1:D:95:LEU:HD21	1:D:269:LEU:CB	2.36	0.55
1:I:81:LEU:O	1:I:85:CYS:HB2	2.05	0.55
1:I:101:ALA:HA	1:I:105:ILE:HG22	1.88	0.55
1:F:224:ARG:NH2	1:F:243:SER:HA	2.20	0.55
1:D:95:LEU:HD21	1:D:269:LEU:HB3	1.86	0.55
1:G:76:SER:CB	1:G:199:VAL:HG11	2.36	0.55
1:A:251:ILE:O	1:A:256:ILE:HG13	2.07	0.55
1:G:44:PHE:CD2	1:G:81:LEU:HB3	2.41	0.55
1:G:160:THR:HG23	1:G:163:GLU:OE2	2.06	0.55
1:H:72:GLY:HA2	1:H:203:VAL:HG11	1.87	0.55
1:J:121:ASN:CB	1:J:211:ILE:HD12	2.36	0.55
1:J:274:TYR:HE2	1:J:275:TRP:NE1	2.05	0.55
1:B:81:LEU:O	1:B:85:CYS:HB2	2.06	0.55
1:C:201:MET:CE	1:D:47:ILE:HG23	2.36	0.55
1:D:186:ARG:NH1	1:H:230:GLU:HA	2.21	0.55
1:G:219:MET:O	1:G:223:ILE:HG13	2.07	0.55
1:H:105:ILE:HG23	1:H:110:LEU:HD12	1.86	0.55
1:I:174:MET:SD	1:J:47:ILE:HD13	2.46	0.55
1:I:187:SER:HB3	1:I:190:ASP:H	1.71	0.55
1:A:273:THR:HG22	1:A:274:TYR:N	2.21	0.55
1:G:185:GLY:HA2	1:G:190:ASP:HB2	1.89	0.55
1:D:106:THR:HG22	1:D:109:GLN:CB	2.36	0.55
1:D:123:VAL:HG12	1:D:127:LEU:HD11	1.89	0.55
1:J:95:LEU:O	1:J:98:VAL:HG22	2.06	0.55
1:J:274:TYR:CD2	1:J:275:TRP:CD1	2.94	0.55
1:B:110:LEU:HD23	1:B:110:LEU:O	2.06	0.55
1:B:244:HIS:O	1:B:249:ASN:ND2	2.39	0.55
1:F:140:THR:HG22	1:F:145:TRP:HB2	1.87	0.55
1:F:195:MET:O	1:F:199:VAL:HG23	2.06	0.55
1:G:105:ILE:HG23	1:G:105:ILE:O	2.07	0.55
1:I:278:TYR:CE2	1:I:279:LEU:HD23	2.42	0.55
1:F:249:ASN:O	1:F:253:ASP:HB2	2.07	0.55
1:G:119:PHE:O	1:G:123:VAL:HG23	2.06	0.55
1:C:154:ASP:O	1:C:157:VAL:HG22	2.06	0.55
1:C:164:ALA:CB	1:C:257:PRO:HB2	2.36	0.55
1:I:95:LEU:HD11	1:I:179:VAL:HG12	1.88	0.55
1:E:229:PRO:HD2	1:E:230:GLU:OE2	2.07	0.54
1:I:138:TYR:CE1	1:I:139:MET:HG2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:222:VAL:O	1:I:226:PHE:HB2	2.08	0.54
1:D:109:GLN:HA	1:D:112:LYS:HD2	1.88	0.54
1:B:174:MET:SD	1:C:47:ILE:HD13	2.47	0.54
1:C:50:VAL:HG13	1:C:145:TRP:HZ2	1.72	0.54
1:D:147:LEU:HD22	1:D:235:VAL:HB	1.90	0.54
1:G:76:SER:HA	1:G:199:VAL:HG11	1.88	0.54
1:I:93:THR:C	1:I:95:LEU:N	2.60	0.54
1:A:39:ILE:HA	1:A:120:GLY:O	2.06	0.54
1:A:230:GLU:H	1:A:230:GLU:CD	2.11	0.54
1:B:48:ALA:HB2	1:B:78:GLY:HA3	1.89	0.54
1:C:96:ILE:HG13	1:C:183:TYR:CG	2.43	0.54
1:G:125:ALA:O	1:G:129:VAL:HG23	2.08	0.54
1:I:161:PHE:CE1	1:I:257:PRO:HG3	2.43	0.54
1:E:143:GLY:HA3	1:E:235:VAL:HG13	1.89	0.54
1:H:175:VAL:HG21	1:H:209:HIS:CD2	2.43	0.54
1:C:201:MET:HE2	1:D:47:ILE:HG23	1.89	0.54
1:F:161:PHE:CE1	1:F:257:PRO:HG3	2.43	0.54
1:H:96:ILE:HD12	1:H:96:ILE:N	2.23	0.54
1:I:264:ILE:O	1:I:268:LEU:HB2	2.08	0.54
1:B:94:VAL:HG11	1:B:270:VAL:HG23	1.88	0.54
1:C:97:VAL:HG12	1:C:105:ILE:HD13	1.90	0.54
1:G:130:LEU:HG	1:G:134:LEU:HD12	1.89	0.54
1:G:184:SER:HB2	1:H:188:LEU:HD22	1.90	0.54
1:E:183:TYR:C	1:E:185:GLY:H	2.11	0.54
1:F:147:LEU:O	1:F:151:GLN:HG3	2.07	0.54
1:D:57:THR:OG1	1:D:145:TRP:HA	2.08	0.53
1:D:198:PRO:HG3	1:E:77:LEU:HD21	1.89	0.53
1:E:102:SER:C	1:E:104:ARG:H	2.11	0.53
1:F:181:MET:HE3	1:F:194:ILE:HG13	1.90	0.53
1:H:143:GLY:HA3	1:H:235:VAL:HG12	1.90	0.53
1:H:272:LEU:HD21	1:I:40:THR:OG1	2.08	0.53
1:G:208:GLU:HB3	1:G:258:VAL:HG11	1.90	0.53
1:H:113:ASN:O	1:H:117:VAL:HG23	2.07	0.53
1:F:51:PHE:CD2	1:F:74:CYS:O	2.61	0.53
1:I:44:PHE:HD2	1:I:82:CYS:HA	1.73	0.53
1:J:178:ALA:HB1	1:J:195:MET:HG2	1.89	0.53
1:A:91:THR:HG22	1:A:114:TRP:CZ2	2.44	0.53
1:A:190:ASP:CB	1:B:188:LEU:HB2	2.36	0.53
1:D:35:PHE:HE1	1:D:119:PHE:CD2	2.26	0.53
1:A:46:SER:HB3	1:A:128:PHE:HD2	1.74	0.53
1:B:49:PHE:CE2	1:B:212:ALA:HB1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:O	1:B:167:LEU:HG	2.07	0.53
1:A:100:LYS:C	1:A:102:SER:H	2.11	0.53
1:A:217:ILE:HG21	1:A:250:PHE:CD1	2.44	0.53
1:F:66:MET:HE2	1:F:66:MET:H	1.69	0.53
1:C:63:PRO:HB3	1:D:58:GLY:O	2.09	0.53
1:C:95:LEU:HD11	1:C:269:LEU:HD13	1.91	0.53
1:I:84:VAL:HG12	1:I:84:VAL:O	2.08	0.53
1:D:83:VAL:HG12	1:D:84:VAL:N	2.24	0.53
1:F:38:ALA:O	1:F:121:ASN:ND2	2.42	0.53
1:A:66:MET:SD	1:A:66:MET:N	2.81	0.53
1:E:179:VAL:HG13	1:E:183:TYR:HE2	1.74	0.53
1:D:201:MET:HG3	1:E:51:PHE:HB2	1.90	0.53
1:H:96:ILE:HG21	1:H:183:TYR:OH	2.09	0.53
1:C:94:VAL:HG11	1:C:270:VAL:HG23	1.91	0.52
1:D:103:GLY:CA	1:D:105:ILE:HG22	2.39	0.52
1:D:201:MET:HA	1:E:51:PHE:CE1	2.44	0.52
1:D:254:ASN:O	1:D:257:PRO:HD2	2.08	0.52
1:I:141:ALA:O	1:I:144:GLN:HG2	2.08	0.52
1:I:231:PHE:O	1:I:235:VAL:HG22	2.09	0.52
1:C:140:THR:O	1:C:141:ALA:HB3	2.09	0.52
1:D:39:ILE:HA	1:D:120:GLY:O	2.09	0.52
1:J:81:LEU:O	1:J:85:CYS:HB2	2.09	0.52
1:C:94:VAL:HG13	1:C:270:VAL:HG23	1.92	0.52
1:D:49:PHE:CE2	1:D:212:ALA:HB1	2.44	0.52
1:F:66:MET:HE1	1:G:59:THR:CG2	2.39	0.52
1:H:138:TYR:HE2	1:H:227:ALA:HB1	1.75	0.52
1:C:272:LEU:HD21	1:D:40:THR:OG1	2.09	0.52
1:G:101:ALA:HB1	1:G:104:ARG:CG	2.39	0.52
1:G:250:PHE:CZ	1:G:255:LEU:HD22	2.45	0.52
1:H:96:ILE:HG12	1:H:183:TYR:CE2	2.44	0.52
1:B:45:ILE:HG21	1:B:211:ILE:HG22	1.91	0.52
1:G:217:ILE:HB	1:G:218:PRO:HD3	1.91	0.52
1:J:45:ILE:HG21	1:J:211:ILE:HG22	1.91	0.52
1:B:46:SER:HB3	1:B:128:PHE:HD2	1.75	0.52
1:B:149:VAL:HG11	1:B:219:MET:HG3	1.92	0.52
1:D:93:THR:HB	1:D:96:ILE:HD13	1.92	0.52
1:G:187:SER:HB2	1:G:190:ASP:OD1	2.09	0.52
1:I:101:ALA:HB2	1:I:110:LEU:HD22	1.92	0.52
1:C:176:CYS:HB2	1:C:269:LEU:CD1	2.38	0.52
1:C:190:ASP:OD2	1:D:187:SER:HB2	2.10	0.52
1:C:217:ILE:HG21	1:C:250:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:SER:HB2	1:E:128:PHE:CD2	2.45	0.52
1:H:181:MET:CE	1:I:81:LEU:HD13	2.40	0.52
1:J:217:ILE:HB	1:J:218:PRO:HD3	1.92	0.52
1:H:224:ARG:HH21	1:H:243:SER:HA	1.75	0.52
1:B:270:VAL:O	1:B:273:THR:HB	2.10	0.52
1:H:202:PHE:HB2	1:H:207:PHE:HD2	1.75	0.52
1:D:49:PHE:CD2	1:D:212:ALA:HB1	2.45	0.52
1:G:189:MET:HG3	1:H:189:MET:CE	2.40	0.52
1:I:66:MET:CE	1:J:59:THR:HG21	2.37	0.52
1:I:91:THR:O	1:I:94:VAL:HB	2.10	0.52
1:A:36:TYR:CE2	1:E:279:LEU:HD12	2.46	0.51
1:C:270:VAL:O	1:C:274:TYR:HB3	2.09	0.51
1:I:92:SER:O	1:I:179:VAL:HG11	2.09	0.51
1:C:46:SER:HB3	1:C:128:PHE:CD2	2.45	0.51
1:C:161:PHE:CD1	1:C:257:PRO:HG3	2.46	0.51
1:D:94:VAL:HG23	1:D:114:TRP:HZ2	1.75	0.51
1:E:45:ILE:HG21	1:E:211:ILE:HG22	1.92	0.51
1:G:68:LYS:N	1:G:68:LYS:HD2	2.25	0.51
1:C:181:MET:HG2	1:D:84:VAL:CG1	2.39	0.51
1:D:107:TRP:HE3	1:D:107:TRP:H	1.55	0.51
1:E:108:GLY:C	1:E:110:LEU:H	2.14	0.51
1:H:51:PHE:CD2	1:H:74:CYS:HB3	2.45	0.51
1:A:190:ASP:OD2	1:B:188:LEU:N	2.44	0.51
1:B:225:ASP:O	1:B:226:PHE:CD2	2.63	0.51
1:C:274:TYR:CD2	1:C:275:TRP:N	2.76	0.51
1:F:187:SER:HA	1:J:186:ARG:HG3	1.91	0.51
1:G:76:SER:CA	1:G:199:VAL:HG11	2.41	0.51
1:G:161:PHE:CE1	1:G:257:PRO:HG3	2.45	0.51
1:B:46:SER:CB	1:B:128:PHE:CD2	2.94	0.51
1:E:160:THR:HG23	1:E:163:GLU:OE2	2.10	0.51
1:F:30:HIS:CG	1:J:279:LEU:HD22	2.45	0.51
1:H:35:PHE:HB2	1:H:116:ASN:HD21	1.75	0.51
1:J:158:HIS:NE2	1:J:244:HIS:CD2	2.79	0.51
1:D:96:ILE:O	1:D:100:LYS:HB2	2.11	0.51
1:E:161:PHE:O	1:E:165:VAL:HG23	2.09	0.51
1:A:256:ILE:HB	1:A:257:PRO:HD3	1.91	0.51
1:C:163:GLU:O	1:C:167:LEU:HG	2.11	0.51
1:C:217:ILE:CD1	1:C:254:ASN:ND2	2.74	0.51
1:D:108:GLY:O	1:D:112:LYS:HG2	2.11	0.51
1:H:101:ALA:CB	1:H:105:ILE:HB	2.41	0.51
1:I:201:MET:HG2	1:J:51:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:44:PHE:CD1	1:J:81:LEU:HD23	2.46	0.51
1:C:217:ILE:O	1:C:221:ILE:HG13	2.09	0.51
1:D:193:PHE:HB3	1:E:193:PHE:CZ	2.46	0.51
1:E:111:ALA:O	1:E:112:LYS:C	2.49	0.51
1:F:119:PHE:O	1:F:123:VAL:HG23	2.10	0.51
1:H:183:TYR:C	1:H:185:GLY:H	2.14	0.51
1:C:95:LEU:HD12	1:C:180:TRP:HB2	1.92	0.51
1:D:152:THR:O	1:D:156:LYS:HG3	2.10	0.51
1:B:72:GLY:HA2	1:B:203:VAL:HG11	1.93	0.51
1:D:186:ARG:NH2	1:H:230:GLU:O	2.44	0.51
1:G:105:ILE:O	1:G:105:ILE:CG2	2.59	0.51
1:H:238:ALA:H	1:H:241:ASN:ND2	2.09	0.51
1:I:75:PHE:CD2	1:I:203:VAL:HG21	2.46	0.51
1:A:51:PHE:CD2	1:E:201:MET:HB2	2.46	0.50
1:A:221:ILE:HG12	1:A:245:LEU:O	2.10	0.50
1:B:181:MET:HG2	1:C:84:VAL:CG1	2.42	0.50
1:B:186:ARG:NH1	1:G:240:GLU:HB3	2.27	0.50
1:H:77:LEU:HD22	1:H:81:LEU:HD22	1.93	0.50
1:J:68:LYS:HD2	1:J:68:LYS:N	2.26	0.50
1:A:91:THR:HG22	1:A:114:TRP:CE2	2.47	0.50
1:A:132:MET:HB3	1:A:219:MET:CE	2.41	0.50
1:H:279:LEU:HD11	1:I:36:TYR:HE2	1.77	0.50
1:B:91:THR:HG22	1:B:114:TRP:CZ2	2.46	0.50
1:B:94:VAL:CG2	1:B:114:TRP:HZ2	2.24	0.50
1:B:98:VAL:HG11	1:B:273:THR:HG21	1.92	0.50
1:C:72:GLY:HA2	1:C:203:VAL:HG11	1.93	0.50
1:J:140:THR:HG22	1:J:145:TRP:HB2	1.93	0.50
1:C:35:PHE:CE2	1:C:39:ILE:HD11	2.47	0.50
1:F:190:ASP:HB3	1:G:188:LEU:CB	2.42	0.50
1:G:201:MET:HA	1:H:51:PHE:CE1	2.47	0.50
1:E:147:LEU:HA	1:E:150:LEU:HD12	1.92	0.50
1:E:186:ARG:HB2	1:E:190:ASP:OD2	2.12	0.50
1:C:217:ILE:HD11	1:C:254:ASN:ND2	2.27	0.50
1:E:33:LYS:O	1:E:37:LEU:HG	2.12	0.50
1:I:62:MET:HE2	1:I:67:ALA:HB2	1.93	0.50
1:I:72:GLY:HA2	1:I:203:VAL:HG11	1.92	0.50
1:J:186:ARG:HH11	1:J:186:ARG:HB3	1.75	0.50
1:J:228:SER:O	1:J:231:PHE:HB3	2.11	0.50
1:F:66:MET:HE1	1:G:59:THR:HG21	1.94	0.50
1:H:279:LEU:HD22	1:I:32:LEU:HD23	1.93	0.50
1:C:97:VAL:HG12	1:C:105:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:PHE:O	1:C:235:VAL:HG13	2.11	0.50
1:D:193:PHE:HD1	1:E:193:PHE:CZ	2.30	0.50
1:F:250:PHE:O	1:F:254:ASN:HB3	2.12	0.50
1:D:97:VAL:HG12	1:D:97:VAL:O	2.11	0.50
1:E:132:MET:HB2	1:E:219:MET:HE1	1.94	0.50
1:A:34:THR:HG21	1:A:113:ASN:ND2	2.27	0.49
1:A:140:THR:HG22	1:A:145:TRP:HB2	1.94	0.49
1:C:217:ILE:CD1	1:C:254:ASN:HD22	2.24	0.49
1:D:201:MET:CE	1:E:47:ILE:HG23	2.42	0.49
1:D:223:ILE:O	1:D:227:ALA:CB	2.60	0.49
1:F:186:ARG:HD3	1:F:186:ARG:C	2.32	0.49
1:G:111:ALA:O	1:G:113:ASN:N	2.44	0.49
1:H:138:TYR:HE2	1:H:227:ALA:CB	2.25	0.49
1:I:98:VAL:HG21	1:I:270:VAL:HG22	1.94	0.49
1:J:232:TRP:HZ3	1:J:242:PHE:HE2	1.59	0.49
1:A:198:PRO:HA	1:B:77:LEU:HD11	1.93	0.49
1:C:46:SER:OG	1:C:215:PHE:HB2	2.12	0.49
1:C:164:ALA:HB1	1:C:257:PRO:HB2	1.93	0.49
1:I:44:PHE:CD2	1:I:82:CYS:HA	2.46	0.49
1:A:113:ASN:O	1:A:117:VAL:HG23	2.12	0.49
1:A:229:PRO:HA	1:A:232:TRP:HD1	1.76	0.49
1:A:260:ILE:HG22	1:A:261:GLY:N	2.28	0.49
1:D:201:MET:HE1	1:E:47:ILE:HG23	1.95	0.49
1:H:96:ILE:HD12	1:H:96:ILE:H	1.77	0.49
1:I:98:VAL:HB	1:I:270:VAL:HG22	1.94	0.49
1:I:199:VAL:HG13	1:I:202:PHE:CE2	2.46	0.49
1:D:217:ILE:HD12	1:D:250:PHE:CD1	2.47	0.49
1:E:132:MET:HB2	1:E:219:MET:CE	2.42	0.49
1:A:51:PHE:CE2	1:E:201:MET:HB2	2.48	0.49
1:F:96:ILE:HD11	1:F:183:TYR:HB2	1.94	0.49
1:G:276:VAL:O	1:G:276:VAL:CG1	2.60	0.49
1:H:84:VAL:O	1:H:84:VAL:CG1	2.60	0.49
1:A:84:VAL:O	1:A:84:VAL:CG1	2.61	0.49
1:A:138:TYR:CE1	1:A:139:MET:HG2	2.47	0.49
1:B:112:LYS:HG3	1:B:113:ASN:H	1.78	0.49
1:C:81:LEU:O	1:C:85:CYS:HB2	2.13	0.49
1:E:149:VAL:HG11	1:E:219:MET:HG3	1.93	0.49
1:F:190:ASP:HB3	1:G:188:LEU:HB3	1.95	0.49
1:I:93:THR:O	1:I:95:LEU:N	2.46	0.49
1:F:84:VAL:CG1	1:J:181:MET:HG2	2.42	0.49
1:G:208:GLU:HB3	1:G:258:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:ILE:HG22	1:G:257:PRO:N	2.27	0.49
1:H:138:TYR:CD2	1:H:223:ILE:HG23	2.47	0.49
1:H:247:VAL:O	1:H:251:ILE:HG12	2.12	0.49
1:I:187:SER:HB3	1:I:190:ASP:CG	2.33	0.49
1:I:273:THR:HG23	1:I:277:ILE:HG22	1.94	0.49
1:C:44:PHE:CD2	1:C:82:CYS:HA	2.48	0.49
1:A:210:SER:HB3	1:A:258:VAL:HG12	1.94	0.49
1:B:169:ILE:HG12	1:B:264:ILE:HB	1.94	0.49
1:C:197:LEU:HB3	1:D:77:LEU:HG	1.95	0.49
1:E:275:TRP:CE3	1:E:278:TYR:HB3	2.48	0.49
1:E:165:VAL:O	1:E:261:GLY:HA3	2.13	0.49
1:H:64:PHE:HD2	1:I:57:THR:HG22	1.78	0.49
1:F:51:PHE:HD2	1:F:74:CYS:O	1.96	0.48
1:F:80:ILE:HG12	1:F:192:ALA:HB1	1.95	0.48
1:F:190:ASP:OD2	1:G:188:LEU:N	2.42	0.48
1:G:107:TRP:O	1:G:110:LEU:HB2	2.13	0.48
1:E:179:VAL:HG13	1:E:183:TYR:CE2	2.48	0.48
1:H:161:PHE:CD1	1:H:257:PRO:HG3	2.48	0.48
1:A:31:PRO:HB2	1:A:32:LEU:HD12	1.94	0.48
1:A:202:PHE:CE2	1:A:203:VAL:HG23	2.48	0.48
1:C:49:PHE:CE2	1:C:212:ALA:HB1	2.48	0.48
1:F:240:GLU:N	1:F:240:GLU:CD	2.66	0.48
1:G:59:THR:HB	1:G:62:MET:HB2	1.94	0.48
1:D:98:VAL:HG11	1:D:270:VAL:CG1	2.24	0.48
1:D:267:GLY:HA2	1:D:270:VAL:HB	1.95	0.48
1:G:75:PHE:CG	1:G:203:VAL:HG21	2.48	0.48
1:C:90:PHE:CE2	1:C:91:THR:HG23	2.48	0.48
1:B:222:VAL:O	1:B:226:PHE:HB2	2.13	0.48
1:E:112:LYS:HG3	1:E:113:ASN:N	2.28	0.48
1:F:190:ASP:OD2	1:G:187:SER:HB3	2.13	0.48
1:A:36:TYR:HE2	1:E:279:LEU:HD12	1.78	0.48
1:I:164:ALA:CB	1:I:257:PRO:HB2	2.43	0.48
1:I:246:THR:O	1:I:249:ASN:HB2	2.14	0.48
1:B:154:ASP:O	1:B:157:VAL:HG22	2.13	0.48
1:C:250:PHE:CZ	1:C:255:LEU:HD22	2.49	0.48
1:G:95:LEU:HD21	1:G:269:LEU:HB3	1.95	0.48
1:J:147:LEU:HG	1:J:151:GLN:NE2	2.29	0.48
1:A:50:VAL:HG11	1:A:132:MET:HE1	1.96	0.48
1:B:217:ILE:HB	1:B:218:PRO:HD3	1.96	0.48
1:C:94:VAL:HG13	1:C:270:VAL:CG2	2.44	0.48
1:C:101:ALA:CB	1:C:105:ILE:HB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LEU:C	1:D:173:LEU:HD13	2.34	0.48
1:E:232:TRP:CE2	1:E:239:PRO:HD3	2.49	0.48
1:F:232:TRP:CD2	1:F:239:PRO:HD3	2.49	0.48
1:G:155:HIS:C	1:G:155:HIS:ND1	2.65	0.48
1:C:217:ILE:HD12	1:C:250:PHE:HD1	1.75	0.48
1:G:177:LEU:HD23	1:G:177:LEU:N	2.28	0.48
1:H:173:LEU:HD22	1:H:173:LEU:O	2.14	0.48
1:H:279:LEU:HD13	1:I:32:LEU:HG	1.94	0.48
1:J:30:HIS:CD2	1:J:31:PRO:HD2	2.48	0.48
1:A:130:LEU:HD12	1:A:130:LEU:O	2.13	0.47
1:B:39:ILE:HA	1:B:120:GLY:O	2.14	0.47
1:B:241:ASN:OD1	1:B:241:ASN:N	2.47	0.47
1:C:133:TRP:CZ2	1:C:226:PHE:HB3	2.49	0.47
1:D:102:SER:C	1:D:104:ARG:N	2.67	0.47
1:E:76:SER:HA	1:E:199:VAL:HG11	1.96	0.47
1:E:133:TRP:HZ3	1:E:223:ILE:HG12	1.79	0.47
1:F:123:VAL:O	1:F:127:LEU:HD12	2.13	0.47
1:H:63:PRO:HG2	1:I:62:MET:SD	2.54	0.47
1:J:41:ALA:HA	1:J:44:PHE:HB2	1.95	0.47
1:J:173:LEU:O	1:J:177:LEU:HG	2.14	0.47
1:B:129:VAL:HA	1:B:219:MET:CE	2.44	0.47
1:D:166:CYS:SG	1:E:134:LEU:HB3	2.54	0.47
1:E:96:ILE:HG12	1:E:183:TYR:CE1	2.49	0.47
1:J:227:ALA:HB1	1:J:231:PHE:CD2	2.49	0.47
1:A:35:PHE:HD1	1:A:116:ASN:OD1	1.96	0.47
1:E:248:MET:O	1:E:252:THR:HG23	2.14	0.47
1:G:190:ASP:CB	1:H:188:LEU:HB3	2.33	0.47
1:G:213:ASN:ND2	1:G:254:ASN:HD21	2.12	0.47
1:J:231:PHE:CE1	1:J:235:VAL:HG11	2.49	0.47
1:B:44:PHE:CD2	1:B:82:CYS:HA	2.50	0.47
1:B:259:THR:O	1:B:262:ASN:HB2	2.14	0.47
1:D:109:GLN:HA	1:D:112:LYS:CD	2.45	0.47
1:E:256:ILE:HB	1:E:257:PRO:HD3	1.95	0.47
1:H:173:LEU:HD13	1:H:173:LEU:C	2.34	0.47
1:A:201:MET:HA	1:B:51:PHE:CE1	2.49	0.47
1:D:186:ARG:HH12	1:H:230:GLU:CA	2.28	0.47
1:E:40:THR:HG22	1:E:44:PHE:CE2	2.50	0.47
1:E:129:VAL:HA	1:E:219:MET:CE	2.44	0.47
1:F:66:MET:HE1	1:G:55:ALA:O	2.15	0.47
1:H:66:MET:HE1	1:I:59:THR:CG2	2.44	0.47
1:H:137:GLU:HG3	1:H:137:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:SER:HB2	1:C:195:MET:HG3	1.95	0.47
1:D:169:ILE:HG13	1:D:261:GLY:HA2	1.96	0.47
1:E:41:ALA:HB1	1:E:89:LEU:HD12	1.96	0.47
1:F:115:LEU:HD12	1:F:115:LEU:O	2.15	0.47
1:F:279:LEU:HD13	1:G:33:LYS:HB2	1.97	0.47
1:H:161:PHE:CE1	1:H:257:PRO:HG3	2.50	0.47
1:H:162:ILE:HG22	1:H:163:GLU:N	2.30	0.47
1:I:51:PHE:HD2	1:I:74:CYS:O	1.98	0.47
1:J:100:LYS:HE2	1:J:107:TRP:CE2	2.49	0.47
1:J:266:GLY:O	1:J:270:VAL:HG13	2.14	0.47
1:A:32:LEU:H	1:A:32:LEU:CD1	2.24	0.47
1:A:33:LYS:N	1:E:279:LEU:HD13	2.30	0.47
1:B:150:LEU:O	1:B:154:ASP:HB2	2.14	0.47
1:B:181:MET:HG2	1:C:84:VAL:HG12	1.97	0.47
1:C:129:VAL:CG1	1:C:222:VAL:HG21	2.45	0.47
1:I:94:VAL:O	1:I:98:VAL:HG13	2.15	0.47
1:J:179:VAL:O	1:J:182:SER:HB3	2.14	0.47
1:D:217:ILE:O	1:D:221:ILE:HG13	2.15	0.47
1:H:103:GLY:C	1:H:105:ILE:N	2.66	0.47
1:H:147:LEU:HG	1:H:151:GLN:HE21	1.78	0.47
1:J:110:LEU:C	1:J:110:LEU:HD23	2.35	0.47
1:A:46:SER:CB	1:A:128:PHE:CD2	2.98	0.47
1:B:63:PRO:HB3	1:C:59:THR:HG23	1.97	0.47
1:C:174:MET:SD	1:D:47:ILE:HD13	2.55	0.47
1:D:168:GLY:HA2	1:D:208:GLU:O	2.16	0.47
1:D:197:LEU:HB3	1:E:77:LEU:HD23	1.96	0.47
1:D:230:GLU:H	1:D:230:GLU:CD	2.19	0.47
1:F:47:ILE:HD13	1:J:174:MET:SD	2.54	0.47
1:F:105:ILE:HA	1:F:109:GLN:OE1	2.16	0.47
1:G:149:VAL:HG12	1:G:220:GLY:HA2	1.96	0.47
1:A:178:ALA:HB1	1:A:195:MET:HG2	1.96	0.46
1:B:137:GLU:O	1:B:137:GLU:HG3	2.15	0.46
1:D:186:ARG:HH21	1:H:234:ALA:HB2	1.79	0.46
1:H:197:LEU:HD12	1:H:197:LEU:HA	1.70	0.46
1:J:97:VAL:HG12	1:J:270:VAL:HG11	1.97	0.46
1:J:97:VAL:HG12	1:J:270:VAL:HG21	1.97	0.46
1:J:278:TYR:C	1:J:278:TYR:CD2	2.88	0.46
1:A:75:PHE:CD2	1:A:203:VAL:HG21	2.49	0.46
1:C:197:LEU:HD12	1:C:197:LEU:HA	1.70	0.46
1:F:164:ALA:HB3	1:F:257:PRO:HB2	1.97	0.46
1:H:176:CYS:HB2	1:H:269:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:267:GLY:O	1:I:270:VAL:HB	2.15	0.46
1:A:109:GLN:HG3	1:F:241:ASN:ND2	2.31	0.46
1:B:195:MET:C	1:B:198:PRO:HD2	2.35	0.46
1:F:122:LEU:CD1	1:F:214:MET:HG2	2.45	0.46
1:F:181:MET:HG2	1:G:84:VAL:HG12	1.97	0.46
1:A:193:PHE:CZ	1:E:193:PHE:O	2.56	0.46
1:D:96:ILE:H	1:D:96:ILE:CD1	2.21	0.46
1:D:129:VAL:HA	1:D:219:MET:HE2	1.96	0.46
1:E:217:ILE:HB	1:E:218:PRO:HD3	1.97	0.46
1:I:46:SER:HB3	1:I:128:PHE:HD2	1.80	0.46
1:I:98:VAL:CB	1:I:270:VAL:HG22	2.46	0.46
1:A:138:TYR:HE2	1:A:227:ALA:HB1	1.81	0.46
1:C:154:ASP:O	1:C:156:LYS:N	2.49	0.46
1:D:166:CYS:O	1:D:170:LEU:HD12	2.16	0.46
1:F:65:GLY:HA2	1:G:54:THR:O	2.16	0.46
1:I:169:ILE:HD11	1:I:264:ILE:HD13	1.97	0.46
1:C:133:TRP:HZ2	1:C:226:PHE:HB3	1.81	0.46
1:F:159:HIS:CE1	1:F:167:LEU:HD11	2.50	0.46
1:G:195:MET:C	1:G:198:PRO:HD2	2.36	0.46
1:H:167:LEU:HA	1:H:170:LEU:HD12	1.97	0.46
1:J:45:ILE:O	1:J:48:ALA:HB3	2.15	0.46
1:D:232:TRP:CE2	1:D:239:PRO:HG3	2.51	0.46
1:F:34:THR:HG21	1:F:113:ASN:OD1	2.16	0.46
1:F:76:SER:HA	1:F:199:VAL:HG11	1.98	0.46
1:F:201:MET:HB2	1:G:51:PHE:CD2	2.51	0.46
1:H:56:THR:HA	1:H:59:THR:CG2	2.45	0.46
1:I:104:ARG:O	1:I:105:ILE:CD1	2.64	0.46
1:J:97:VAL:HB	1:J:270:VAL:CG1	2.38	0.46
1:C:219:MET:O	1:C:223:ILE:HG13	2.16	0.46
1:D:96:ILE:CG1	1:D:183:TYR:CE2	2.98	0.46
1:F:99:ALA:HB2	1:F:180:TRP:CH2	2.51	0.46
1:C:201:MET:HE3	1:D:47:ILE:HG12	1.98	0.46
1:C:261:GLY:HA2	1:C:264:ILE:HD12	1.97	0.46
1:E:96:ILE:N	1:E:96:ILE:HD12	2.30	0.46
1:G:121:ASN:HB3	1:G:211:ILE:HG23	1.98	0.46
1:I:98:VAL:CG2	1:I:270:VAL:HG22	2.45	0.46
1:I:106:THR:HG22	1:I:108:GLY:H	1.81	0.46
1:I:208:GLU:CB	1:I:258:VAL:HG21	2.44	0.46
1:J:256:ILE:CB	1:J:257:PRO:HD3	2.41	0.46
1:B:45:ILE:HD12	1:B:45:ILE:HA	1.66	0.46
1:C:275:TRP:HA	1:C:278:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:VAL:O	1:D:219:MET:HE1	2.16	0.46
1:E:259:THR:HG22	1:E:260:ILE:N	2.31	0.46
1:G:100:LYS:C	1:G:102:SER:H	2.19	0.46
1:H:66:MET:HE2	1:H:66:MET:N	2.30	0.46
1:H:176:CYS:CB	1:H:269:LEU:HD12	2.46	0.46
1:I:53:ILE:HG22	1:I:145:TRP:NE1	2.31	0.46
1:F:130:LEU:O	1:F:134:LEU:HG	2.17	0.45
1:F:188:LEU:HD12	1:F:188:LEU:HA	1.67	0.45
1:I:79:LEU:HD21	1:I:179:VAL:HG23	1.98	0.45
1:E:39:ILE:O	1:E:42:GLY:N	2.49	0.45
1:I:142:ASN:CG	1:I:142:ASN:O	2.53	0.45
1:C:94:VAL:HG12	1:C:95:LEU:N	2.31	0.45
1:D:193:PHE:HD1	1:E:193:PHE:CE1	2.35	0.45
1:D:217:ILE:HD12	1:D:250:PHE:CE1	2.51	0.45
1:F:105:ILE:HG23	1:F:105:ILE:O	2.17	0.45
1:F:135:SER:HB2	1:J:167:LEU:CD2	2.46	0.45
1:G:179:VAL:O	1:G:182:SER:HB3	2.16	0.45
1:H:102:SER:C	1:H:104:ARG:H	2.20	0.45
1:H:110:LEU:O	1:H:110:LEU:HD23	2.16	0.45
1:I:49:PHE:O	1:I:52:TYR:N	2.50	0.45
1:J:229:PRO:HA	1:J:232:TRP:HD1	1.80	0.45
1:A:279:LEU:CD1	1:B:32:LEU:HB3	2.46	0.45
1:D:169:ILE:HG12	1:D:264:ILE:HB	1.98	0.45
1:F:189:MET:HB2	1:J:190:ASP:OD1	2.16	0.45
1:H:49:PHE:CD2	1:H:212:ALA:HB1	2.52	0.45
1:H:138:TYR:CE1	1:H:139:MET:HG2	2.52	0.45
1:J:84:VAL:HG12	1:J:84:VAL:O	2.16	0.45
1:J:93:THR:O	1:J:97:VAL:HG23	2.16	0.45
1:F:33:LYS:HB2	1:J:279:LEU:CB	2.38	0.45
1:F:122:LEU:HD13	1:F:214:MET:HG2	1.99	0.45
1:F:123:VAL:HG12	1:F:127:LEU:CD1	2.46	0.45
1:F:194:ILE:HG13	1:F:194:ILE:O	2.14	0.45
1:F:255:LEU:HD12	1:F:255:LEU:HA	1.82	0.45
1:G:107:TRP:HH2	1:G:271:GLY:HA2	1.82	0.45
1:A:38:ALA:O	1:A:121:ASN:ND2	2.50	0.45
1:B:279:LEU:HD23	1:B:279:LEU:HA	1.68	0.45
1:C:110:LEU:O	1:C:110:LEU:HD23	2.16	0.45
1:E:199:VAL:HA	1:E:202:PHE:HD2	1.81	0.45
1:E:213:ASN:ND2	1:E:254:ASN:OD1	2.47	0.45
1:G:29:LYS:O	1:G:31:PRO:HD3	2.16	0.45
1:G:106:THR:HG22	1:G:109:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:TRP:HA	1:G:110:LEU:HD12	1.98	0.45
1:G:274:TYR:O	1:G:278:TYR:HB2	2.16	0.45
1:H:141:ALA:O	1:H:144:GLN:HB2	2.17	0.45
1:I:80:ILE:HD13	1:I:192:ALA:HB1	1.99	0.45
1:J:150:LEU:HD13	1:J:242:PHE:CE2	2.52	0.45
1:C:270:VAL:O	1:C:274:TYR:HB2	2.16	0.45
1:H:139:MET:SD	1:H:231:PHE:HB2	2.56	0.45
1:I:45:ILE:HD12	1:I:45:ILE:HA	1.77	0.45
1:J:202:PHE:O	1:J:202:PHE:CD1	2.69	0.45
1:B:270:VAL:HG12	1:B:271:GLY:N	2.31	0.45
1:D:35:PHE:HD1	1:D:116:ASN:OD1	1.99	0.45
1:D:181:MET:HE3	1:D:194:ILE:HG13	1.98	0.45
1:F:146:GLY:O	1:F:149:VAL:HB	2.17	0.45
1:F:268:LEU:HD23	1:F:268:LEU:HA	1.85	0.45
1:H:275:TRP:HZ3	1:H:278:TYR:CE2	2.35	0.45
1:I:46:SER:CB	1:I:128:PHE:CD2	3.00	0.45
1:B:185:GLY:O	1:B:191:LYS:HE3	2.16	0.45
1:D:44:PHE:HD2	1:D:82:CYS:HA	1.82	0.45
1:D:96:ILE:HG12	1:D:183:TYR:CE2	2.51	0.45
1:D:169:ILE:HA	1:D:261:GLY:O	2.16	0.45
1:D:264:ILE:O	1:D:268:LEU:HB2	2.14	0.45
1:I:77:LEU:O	1:I:81:LEU:HB2	2.17	0.45
1:I:198:PRO:HG3	1:J:77:LEU:HD21	1.99	0.45
1:D:96:ILE:CG1	1:D:183:TYR:HE2	2.29	0.45
1:G:88:ASP:OD2	1:G:117:VAL:HG13	2.17	0.45
1:H:171:ALA:HB2	1:H:207:PHE:CB	2.46	0.45
1:H:231:PHE:CE1	1:H:235:VAL:HG11	2.51	0.45
1:J:214:MET:O	1:J:218:PRO:HG2	2.17	0.45
1:D:75:PHE:CD2	1:D:203:VAL:HG21	2.52	0.44
1:E:39:ILE:HG22	1:E:40:THR:N	2.31	0.44
1:F:54:THR:HG21	1:J:204:ALA:C	2.38	0.44
1:F:174:MET:HE1	1:G:77:LEU:HD11	1.99	0.44
1:H:147:LEU:O	1:H:151:GLN:HG3	2.17	0.44
1:H:202:PHE:HB2	1:H:207:PHE:CD2	2.53	0.44
1:I:164:ALA:HB3	1:I:257:PRO:HB2	1.99	0.44
1:B:150:LEU:CD2	1:B:224:ARG:HB2	2.46	0.44
1:D:84:VAL:HG22	1:D:188:LEU:HD11	1.99	0.44
1:E:53:ILE:HG21	1:E:145:TRP:CE2	2.53	0.44
1:H:68:LYS:O	1:H:69:LEU:C	2.55	0.44
1:H:137:GLU:O	1:H:140:THR:HB	2.17	0.44
1:H:170:LEU:HG	1:I:131:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:MET:O	1:H:199:VAL:HG23	2.17	0.44
1:I:133:TRP:HA	1:I:133:TRP:CE3	2.52	0.44
1:A:118:TYR:O	1:A:121:ASN:HB2	2.18	0.44
1:A:130:LEU:HD12	1:A:130:LEU:C	2.37	0.44
1:D:181:MET:CE	1:D:194:ILE:HG13	2.47	0.44
1:A:232:TRP:HA	1:A:235:VAL:HG22	1.98	0.44
1:B:254:ASN:O	1:B:257:PRO:HD2	2.18	0.44
1:G:221:ILE:HG12	1:G:245:LEU:O	2.17	0.44
1:I:217:ILE:HB	1:I:218:PRO:HD3	1.98	0.44
1:A:30:HIS:HA	1:A:31:PRO:HD3	1.90	0.44
1:A:51:PHE:CE1	1:E:201:MET:HA	2.52	0.44
1:B:79:LEU:N	1:B:79:LEU:HD22	2.32	0.44
1:C:189:MET:HG2	1:D:189:MET:HG2	1.99	0.44
1:D:35:PHE:HE1	1:D:119:PHE:HD2	1.64	0.44
1:G:46:SER:HB2	1:G:128:PHE:CD2	2.53	0.44
1:G:132:MET:HB3	1:G:219:MET:CE	2.47	0.44
1:H:171:ALA:HB2	1:H:207:PHE:HB3	2.00	0.44
1:I:187:SER:HB3	1:I:190:ASP:CB	2.48	0.44
1:A:232:TRP:CZ2	1:A:239:PRO:HG3	2.52	0.44
1:D:77:LEU:HD22	1:D:81:LEU:HD22	1.98	0.44
1:H:183:TYR:O	1:H:185:GLY:N	2.51	0.44
1:I:106:THR:HG22	1:I:107:TRP:N	2.33	0.44
1:I:224:ARG:HD2	1:I:245:LEU:HB2	1.99	0.44
1:I:278:TYR:CD2	1:I:279:LEU:N	2.86	0.44
1:A:72:GLY:HA2	1:A:203:VAL:CG1	2.48	0.44
1:A:72:GLY:HA2	1:A:203:VAL:HG11	2.00	0.44
1:C:217:ILE:HD12	1:C:250:PHE:CE1	2.50	0.44
1:D:96:ILE:HG12	1:D:183:TYR:CZ	2.53	0.44
1:E:269:LEU:HD23	1:E:269:LEU:HA	1.84	0.44
1:G:238:ALA:O	1:G:241:ASN:HB2	2.18	0.44
1:H:172:ASN:HB2	1:H:262:ASN:ND2	2.33	0.44
1:B:192:ALA:C	1:B:194:ILE:H	2.20	0.44
1:C:254:ASN:O	1:C:258:VAL:HG23	2.17	0.44
1:D:211:ILE:O	1:D:214:MET:HB2	2.17	0.44
1:I:49:PHE:CE2	1:I:216:MET:HB2	2.52	0.44
1:J:169:ILE:HG13	1:J:261:GLY:HA2	2.00	0.44
1:D:66:MET:HE2	1:D:66:MET:N	2.33	0.44
1:D:84:VAL:CG2	1:D:188:LEU:HD11	2.48	0.44
1:F:76:SER:OG	1:F:196:VAL:HG22	2.17	0.44
1:F:113:ASN:O	1:F:117:VAL:HG23	2.18	0.44
1:H:105:ILE:CG2	1:H:110:LEU:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:GLY:O	1:I:45:ILE:HG22	2.18	0.44
1:A:149:VAL:HG11	1:A:219:MET:HG3	2.00	0.43
1:A:217:ILE:HB	1:A:218:PRO:HD3	1.99	0.43
1:B:122:LEU:HB2	1:B:214:MET:SD	2.58	0.43
1:D:77:LEU:O	1:D:81:LEU:HB2	2.18	0.43
1:G:35:PHE:CE1	1:G:119:PHE:HD2	2.36	0.43
1:H:214:MET:O	1:H:218:PRO:HG2	2.18	0.43
1:I:46:SER:HB2	1:I:128:PHE:CD2	2.53	0.43
1:I:272:LEU:HD12	1:J:36:TYR:OH	2.17	0.43
1:J:62:MET:HG3	1:J:63:PRO:HD2	1.99	0.43
1:J:168:GLY:HA2	1:J:208:GLU:O	2.17	0.43
1:J:264:ILE:O	1:J:268:LEU:HB2	2.18	0.43
1:A:106:THR:HG21	1:F:241:ASN:OD1	2.16	0.43
1:A:123:VAL:O	1:A:127:LEU:HG	2.17	0.43
1:C:201:MET:HG2	1:D:51:PHE:CD1	2.52	0.43
1:E:183:TYR:C	1:E:185:GLY:N	2.71	0.43
1:E:202:PHE:HD1	1:E:207:PHE:HB2	1.83	0.43
1:G:64:PHE:CD2	1:H:141:ALA:HB2	2.53	0.43
1:A:98:VAL:HG21	1:A:270:VAL:CG2	2.47	0.43
1:A:201:MET:HB2	1:B:51:PHE:CE2	2.53	0.43
1:C:256:ILE:CB	1:C:257:PRO:HD3	2.49	0.43
1:D:95:LEU:HD11	1:D:269:LEU:HD12	1.99	0.43
1:D:132:MET:HB2	1:D:219:MET:CE	2.48	0.43
1:E:72:GLY:O	1:E:75:PHE:HB3	2.17	0.43
1:G:129:VAL:HG13	1:G:219:MET:HA	1.98	0.43
1:H:202:PHE:HD1	1:H:207:PHE:HB2	1.82	0.43
1:B:186:ARG:HD3	1:B:186:ARG:HA	1.74	0.43
1:E:75:PHE:CD2	1:E:203:VAL:HG21	2.53	0.43
1:F:33:LYS:CD	1:J:280:ARG:HA	2.38	0.43
1:G:160:THR:HG23	1:G:163:GLU:CD	2.38	0.43
1:G:171:ALA:O	1:G:175:VAL:HG23	2.18	0.43
1:G:183:TYR:N	1:G:183:TYR:CD2	2.86	0.43
1:J:45:ILE:HD12	1:J:45:ILE:HA	1.77	0.43
1:J:94:VAL:O	1:J:98:VAL:HG13	2.18	0.43
1:D:232:TRP:NE1	1:D:239:PRO:HG3	2.34	0.43
1:E:188:LEU:HD12	1:E:188:LEU:HA	1.82	0.43
1:E:275:TRP:CH2	1:E:278:TYR:CD2	3.06	0.43
1:F:130:LEU:O	1:F:130:LEU:HD12	2.19	0.43
1:G:48:ALA:HB2	1:G:78:GLY:CA	2.42	0.43
1:G:51:PHE:CG	1:G:74:CYS:HB3	2.54	0.43
1:H:46:SER:HB3	1:H:128:PHE:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:MET:HB3	1:I:219:MET:CE	2.48	0.43
1:I:189:MET:HG3	1:J:189:MET:HE1	2.01	0.43
1:B:76:SER:HA	1:B:199:VAL:HG11	2.01	0.43
1:C:96:ILE:HG13	1:C:183:TYR:CD1	2.54	0.43
1:D:95:LEU:HD11	1:D:269:LEU:CD1	2.48	0.43
1:E:171:ALA:HB2	1:E:207:PHE:HB3	2.01	0.43
1:G:84:VAL:CG2	1:G:188:LEU:HD11	2.48	0.43
1:G:109:GLN:HA	1:G:112:LYS:HE3	2.01	0.43
1:H:127:LEU:HD22	1:H:127:LEU:HA	1.53	0.43
1:J:49:PHE:CE2	1:J:212:ALA:HB1	2.54	0.43
1:C:129:VAL:HG22	1:C:219:MET:HB2	2.01	0.43
1:C:169:ILE:O	1:C:173:LEU:HB2	2.18	0.43
1:H:162:ILE:O	1:H:163:GLU:C	2.57	0.43
1:H:250:PHE:O	1:H:254:ASN:HB3	2.19	0.43
1:I:49:PHE:O	1:I:50:VAL:C	2.56	0.43
1:I:72:GLY:HA2	1:I:203:VAL:CG1	2.49	0.43
1:A:33:LYS:HE3	1:E:276:VAL:O	2.18	0.43
1:A:69:LEU:HD21	1:B:74:CYS:SG	2.59	0.43
1:G:122:LEU:HB2	1:G:214:MET:SD	2.59	0.43
1:H:79:LEU:HD11	1:H:175:VAL:HG13	2.01	0.43
1:I:195:MET:O	1:I:199:VAL:HG23	2.19	0.43
1:J:96:ILE:O	1:J:99:ALA:HB3	2.19	0.43
1:J:186:ARG:HB2	1:J:187:SER:H	1.61	0.43
1:D:35:PHE:CE1	1:D:119:PHE:CD2	3.07	0.43
1:E:130:LEU:HG	1:E:134:LEU:HD12	2.01	0.43
1:F:65:GLY:HA3	1:G:55:ALA:O	2.19	0.43
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.76	0.43
1:B:129:VAL:HG22	1:B:219:MET:CE	2.49	0.43
1:C:164:ALA:HB3	1:C:257:PRO:HB2	2.00	0.43
1:D:44:PHE:CD2	1:D:82:CYS:HA	2.53	0.43
1:E:129:VAL:HG22	1:E:215:PHE:CD1	2.54	0.43
1:F:46:SER:CB	1:F:128:PHE:CD2	3.01	0.43
1:F:77:LEU:O	1:F:81:LEU:HB2	2.19	0.43
1:G:259:THR:O	1:G:262:ASN:HB2	2.18	0.43
1:H:81:LEU:HD12	1:H:81:LEU:HA	1.79	0.43
1:I:45:ILE:O	1:I:48:ALA:HB3	2.18	0.43
1:A:49:PHE:CD2	1:A:212:ALA:HB1	2.53	0.42
1:A:186:ARG:HD2	1:A:186:ARG:H	1.84	0.42
1:B:80:ILE:O	1:B:84:VAL:HB	2.18	0.42
1:C:182:SER:C	1:C:184:SER:H	2.22	0.42
1:D:41:ALA:HB1	1:D:89:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LEU:HA	1:D:150:LEU:HD12	2.01	0.42
1:E:118:TYR:CE1	1:E:211:ILE:HD11	2.54	0.42
1:F:35:PHE:O	1:F:38:ALA:N	2.52	0.42
1:H:202:PHE:CE2	1:H:203:VAL:HG23	2.54	0.42
1:I:129:VAL:HG21	1:I:218:PRO:HB2	2.01	0.42
1:I:254:ASN:O	1:I:257:PRO:HD2	2.19	0.42
1:C:181:MET:CG	1:D:84:VAL:HG11	2.46	0.42
1:D:93:THR:CA	1:D:96:ILE:HD13	2.50	0.42
1:D:186:ARG:HH12	1:H:230:GLU:CB	2.32	0.42
1:F:83:VAL:HG12	1:F:84:VAL:N	2.34	0.42
1:F:232:TRP:CZ2	1:F:239:PRO:HG3	2.54	0.42
1:G:105:ILE:HG13	1:G:109:GLN:NE2	2.35	0.42
1:G:183:TYR:N	1:G:183:TYR:HD2	2.16	0.42
1:H:269:LEU:HD23	1:H:269:LEU:HA	1.92	0.42
1:I:39:ILE:HA	1:I:120:GLY:O	2.19	0.42
1:J:232:TRP:CE2	1:J:239:PRO:HD3	2.54	0.42
1:D:94:VAL:HG12	1:D:176:CYS:SG	2.59	0.42
1:F:33:LYS:HD2	1:J:280:ARG:CA	2.38	0.42
1:F:150:LEU:HD21	1:F:223:ILE:HG22	2.00	0.42
1:G:65:GLY:O	1:G:66:MET:C	2.58	0.42
1:G:173:LEU:O	1:G:177:LEU:HG	2.19	0.42
1:H:201:MET:HG2	1:I:51:PHE:CG	2.54	0.42
1:H:201:MET:HA	1:I:51:PHE:CE1	2.55	0.42
1:A:201:MET:HB2	1:B:51:PHE:CD2	2.54	0.42
1:C:79:LEU:HD23	1:C:195:MET:SD	2.60	0.42
1:D:52:TYR:O	1:D:56:THR:HG23	2.20	0.42
1:F:276:VAL:O	1:F:276:VAL:CG1	2.68	0.42
1:G:160:THR:O	1:G:161:PHE:C	2.55	0.42
1:G:214:MET:O	1:G:218:PRO:HG2	2.19	0.42
1:J:232:TRP:CD2	1:J:239:PRO:HD3	2.54	0.42
1:C:153:ALA:HB1	1:C:217:ILE:HA	1.99	0.42
1:D:181:MET:HE3	1:D:181:MET:HB2	1.88	0.42
1:E:49:PHE:O	1:E:52:TYR:HB3	2.20	0.42
1:F:37:LEU:HD23	1:F:37:LEU:HA	1.86	0.42
1:F:94:VAL:CG1	1:F:95:LEU:N	2.81	0.42
1:F:190:ASP:CG	1:G:187:SER:HB3	2.40	0.42
1:F:195:MET:O	1:F:198:PRO:HD2	2.19	0.42
1:G:102:SER:O	1:G:277:ILE:HG21	2.19	0.42
1:H:223:ILE:O	1:H:227:ALA:HB2	2.20	0.42
1:J:248:MET:O	1:J:252:THR:HG23	2.19	0.42
1:J:274:TYR:CE2	1:J:275:TRP:NE1	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:MET:HE1	1:E:59:THR:CG2	2.50	0.42
1:D:202:PHE:CE2	1:D:203:VAL:HG23	2.54	0.42
1:E:30:HIS:HA	1:E:31:PRO:HD3	1.94	0.42
1:E:268:LEU:HD23	1:E:268:LEU:HA	1.86	0.42
1:F:98:VAL:HG23	1:F:110:LEU:HD21	2.01	0.42
1:G:190:ASP:OD1	1:G:190:ASP:N	2.52	0.42
1:G:228:SER:HB2	1:G:229:PRO:HD2	2.01	0.42
1:G:245:LEU:HD23	1:G:245:LEU:HA	1.81	0.42
1:H:91:THR:HB	1:H:172:ASN:HD21	1.84	0.42
1:H:181:MET:HE1	1:I:81:LEU:HD13	2.02	0.42
1:A:39:ILE:HG12	1:A:120:GLY:O	2.20	0.42
1:A:55:ALA:O	1:E:65:GLY:HA3	2.19	0.42
1:C:122:LEU:HD12	1:C:122:LEU:O	2.20	0.42
1:C:214:MET:O	1:C:218:PRO:HG2	2.19	0.42
1:E:44:PHE:CE1	1:E:81:LEU:HG	2.54	0.42
1:E:166:CYS:O	1:E:170:LEU:HD12	2.20	0.42
1:H:63:PRO:HB3	1:I:59:THR:HG22	2.00	0.42
1:J:84:VAL:CG1	1:J:188:LEU:HD11	2.48	0.42
1:B:246:THR:HB	1:B:248:MET:SD	2.60	0.42
1:E:46:SER:HB3	1:E:128:PHE:CD2	2.42	0.42
1:G:106:THR:HG23	1:G:109:GLN:HB3	2.01	0.42
1:I:98:VAL:C	1:I:100:LYS:N	2.70	0.42
1:I:167:LEU:HD23	1:I:167:LEU:HA	1.70	0.42
1:C:195:MET:C	1:C:198:PRO:HD2	2.40	0.42
1:D:195:MET:O	1:D:199:VAL:HG23	2.19	0.42
1:D:201:MET:HG2	1:E:51:PHE:CD1	2.55	0.42
1:E:178:ALA:O	1:E:195:MET:HG2	2.20	0.42
1:G:187:SER:HB3	1:G:189:MET:HB2	2.02	0.42
1:H:56:THR:HA	1:H:59:THR:HG21	2.02	0.42
1:C:165:VAL:O	1:C:169:ILE:HD12	2.20	0.41
1:C:197:LEU:HB2	1:C:198:PRO:HD3	2.02	0.41
1:D:110:LEU:C	1:D:110:LEU:CD2	2.86	0.41
1:D:214:MET:O	1:D:218:PRO:HG2	2.20	0.41
1:E:106:THR:HG22	1:E:109:GLN:HB3	2.01	0.41
1:G:48:ALA:HB1	1:G:75:PHE:O	2.20	0.41
1:G:202:PHE:HA	1:G:207:PHE:HD2	1.81	0.41
1:G:254:ASN:C	1:G:257:PRO:HD2	2.40	0.41
1:G:277:ILE:C	1:G:279:LEU:H	2.23	0.41
1:H:231:PHE:CZ	1:H:235:VAL:HG11	2.55	0.41
1:H:279:LEU:CD1	1:I:36:TYR:HE2	2.33	0.41
1:I:147:LEU:HB2	1:I:235:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HA	1:A:219:MET:HE1	1.98	0.41
1:B:211:ILE:O	1:B:214:MET:HB2	2.20	0.41
1:C:270:VAL:O	1:C:271:GLY:C	2.58	0.41
1:D:256:ILE:HB	1:D:257:PRO:HD3	2.02	0.41
1:F:30:HIS:CB	1:J:279:LEU:HD22	2.50	0.41
1:F:137:GLU:O	1:F:140:THR:HB	2.20	0.41
1:H:33:LYS:O	1:H:37:LEU:HG	2.20	0.41
1:J:112:LYS:O	1:J:116:ASN:HB2	2.20	0.41
1:A:194:ILE:HD12	1:A:194:ILE:HA	1.95	0.41
1:A:237:SER:OG	1:A:241:ASN:ND2	2.50	0.41
1:B:63:PRO:HG2	1:C:62:MET:HG3	2.02	0.41
1:E:246:THR:O	1:E:249:ASN:HB2	2.20	0.41
1:E:259:THR:O	1:E:262:ASN:HB2	2.20	0.41
1:F:135:SER:HB2	1:J:167:LEU:HD23	2.02	0.41
1:H:208:GLU:HB3	1:H:258:VAL:CG2	2.50	0.41
1:I:268:LEU:O	1:I:272:LEU:CD1	2.57	0.41
1:B:189:MET:HE3	1:B:193:PHE:CE2	2.55	0.41
1:C:158:HIS:CE1	1:C:244:HIS:CD2	3.08	0.41
1:E:179:VAL:CG1	1:E:183:TYR:HE2	2.32	0.41
1:E:210:SER:O	1:E:214:MET:HG3	2.20	0.41
1:G:230:GLU:H	1:G:230:GLU:HG3	1.66	0.41
1:H:165:VAL:O	1:H:261:GLY:HA3	2.20	0.41
1:I:227:ALA:HB1	1:I:231:PHE:CD2	2.55	0.41
1:J:195:MET:C	1:J:198:PRO:HD2	2.41	0.41
1:J:277:ILE:O	1:J:277:ILE:CG2	2.67	0.41
1:A:276:VAL:HG12	1:A:276:VAL:O	2.20	0.41
1:B:159:HIS:HB3	1:B:164:ALA:HB2	2.02	0.41
1:B:276:VAL:HG13	1:C:33:LYS:NZ	2.35	0.41
1:D:32:LEU:HA	1:D:32:LEU:HD12	1.85	0.41
1:D:181:MET:SD	1:E:81:LEU:HD12	2.61	0.41
1:D:236:GLY:O	1:D:237:SER:HB2	2.21	0.41
1:I:38:ALA:O	1:I:121:ASN:HA	2.21	0.41
1:C:140:THR:O	1:C:145:TRP:CB	2.54	0.41
1:D:51:PHE:CD2	1:D:74:CYS:HB3	2.56	0.41
1:D:167:LEU:CD2	1:E:135:SER:HB2	2.50	0.41
1:D:254:ASN:C	1:D:257:PRO:HD2	2.40	0.41
1:E:45:ILE:O	1:E:48:ALA:HB3	2.21	0.41
1:E:197:LEU:HD12	1:E:197:LEU:HA	1.75	0.41
1:F:31:PRO:O	1:F:35:PHE:HB2	2.20	0.41
1:F:75:PHE:CG	1:F:203:VAL:HG21	2.56	0.41
1:F:123:VAL:HG12	1:F:127:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:HIS:ND1	1:G:155:HIS:O	2.53	0.41
1:H:165:VAL:HA	1:H:257:PRO:O	2.20	0.41
1:I:197:LEU:HD12	1:I:197:LEU:HA	1.83	0.41
1:I:223:ILE:O	1:I:227:ALA:HB2	2.21	0.41
1:A:279:LEU:HD13	1:B:30:HIS:CE1	2.56	0.41
1:B:44:PHE:HD2	1:B:82:CYS:HA	1.84	0.41
1:E:223:ILE:O	1:E:227:ALA:CB	2.69	0.41
1:F:91:THR:HG22	1:F:114:TRP:CZ2	2.56	0.41
1:G:150:LEU:HD11	1:G:231:PHE:HE2	1.85	0.41
1:A:33:LYS:HB2	1:E:279:LEU:HB3	2.03	0.41
1:A:100:LYS:C	1:A:102:SER:N	2.72	0.41
1:A:264:ILE:O	1:A:268:LEU:HG	2.20	0.41
1:C:108:GLY:C	1:C:110:LEU:H	2.24	0.41
1:E:160:THR:O	1:E:161:PHE:C	2.59	0.41
1:G:45:ILE:HD12	1:G:45:ILE:HA	1.91	0.41
1:H:30:HIS:CE1	1:H:32:LEU:CB	3.03	0.41
1:H:64:PHE:HD2	1:I:57:THR:CG2	2.33	0.41
1:H:101:ALA:O	1:H:104:ARG:HB2	2.21	0.41
1:H:168:GLY:O	1:H:262:ASN:ND2	2.51	0.41
1:I:53:ILE:CG2	1:I:145:TRP:CE2	3.04	0.41
1:J:126:LEU:HD23	1:J:126:LEU:HA	1.87	0.41
1:A:189:MET:CG	1:B:189:MET:HG2	2.50	0.41
1:A:227:ALA:HB1	1:A:231:PHE:CD2	2.56	0.41
1:B:77:LEU:HD22	1:B:81:LEU:HD22	2.03	0.41
1:C:64:PHE:HB3	1:D:57:THR:HG22	2.03	0.41
1:C:90:PHE:CE1	1:C:118:TYR:HD1	2.39	0.41
1:E:44:PHE:CG	1:E:81:LEU:HB3	2.56	0.41
1:E:151:GLN:HE21	1:E:151:GLN:HB2	1.67	0.41
1:G:232:TRP:CZ2	1:G:239:PRO:HG3	2.56	0.41
1:I:46:SER:HB3	1:I:128:PHE:CD2	2.56	0.41
1:I:97:VAL:O	1:I:97:VAL:HG12	2.20	0.41
1:I:102:SER:O	1:I:103:GLY:C	2.59	0.41
1:I:277:ILE:HG23	1:I:277:ILE:O	2.21	0.41
1:B:96:ILE:HD12	1:B:180:TRP:HE3	1.85	0.41
1:H:158:HIS:NE2	1:H:244:HIS:CG	2.88	0.41
1:I:261:GLY:HA2	1:I:264:ILE:HD12	2.02	0.41
1:A:201:MET:HE1	1:B:47:ILE:HG23	2.03	0.40
1:A:254:ASN:C	1:A:257:PRO:HD2	2.41	0.40
1:D:232:TRP:HB3	1:D:237:SER:O	2.21	0.40
1:E:171:ALA:O	1:E:175:VAL:HG23	2.20	0.40
1:F:81:LEU:HD11	1:J:177:LEU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:LEU:HG	1:G:134:LEU:CD1	2.50	0.40
1:G:202:PHE:HB2	1:G:207:PHE:HD2	1.86	0.40
1:I:273:THR:O	1:I:274:TYR:C	2.57	0.40
1:J:209:HIS:HE1	1:J:211:ILE:HB	1.86	0.40
1:A:51:PHE:CD2	1:A:74:CYS:HB3	2.56	0.40
1:B:153:ALA:HB1	1:B:217:ILE:HA	2.03	0.40
1:C:95:LEU:HD11	1:C:269:LEU:HD22	2.03	0.40
1:F:138:TYR:O	1:F:143:GLY:HA2	2.21	0.40
1:F:228:SER:O	1:F:231:PHE:HB3	2.20	0.40
1:H:217:ILE:HG21	1:H:250:PHE:CD1	2.56	0.40
1:I:148:ASN:O	1:I:152:THR:OG1	2.35	0.40
1:B:101:ALA:CB	1:B:105:ILE:HB	2.43	0.40
1:C:30:HIS:ND1	1:C:31:PRO:HD2	2.36	0.40
1:E:201:MET:SD	1:E:201:MET:C	3.00	0.40
1:F:106:THR:HG22	1:F:109:GLN:HG3	2.04	0.40
1:G:130:LEU:O	1:G:134:LEU:HD12	2.21	0.40
1:H:101:ALA:O	1:H:104:ARG:CB	2.69	0.40
1:I:45:ILE:HG21	1:I:211:ILE:HG22	2.04	0.40
1:I:169:ILE:HG12	1:I:264:ILE:HB	2.02	0.40
1:J:211:ILE:O	1:J:214:MET:HB2	2.21	0.40
1:A:98:VAL:CG1	1:A:273:THR:HG21	2.44	0.40
1:A:202:PHE:HB2	1:A:207:PHE:HD2	1.86	0.40
1:D:66:MET:HE2	1:D:66:MET:H	1.86	0.40
1:E:138:TYR:HA	1:E:145:TRP:HE3	1.86	0.40
1:E:168:GLY:HA2	1:E:208:GLU:O	2.22	0.40
1:F:254:ASN:C	1:F:257:PRO:HD2	2.42	0.40
1:G:274:TYR:O	1:G:278:TYR:CB	2.69	0.40
1:H:97:VAL:CG1	1:H:110:LEU:HG	2.50	0.40
1:I:94:VAL:HG21	1:I:266:GLY:HA3	2.03	0.40
1:J:114:TRP:HZ3	1:J:263:ILE:HG23	1.87	0.40
1:J:201:MET:O	1:J:205:SER:HB2	2.21	0.40
1:J:250:PHE:O	1:J:254:ASN:HB3	2.22	0.40
1:A:94:VAL:HG13	1:A:95:LEU:N	2.36	0.40
1:A:190:ASP:HB3	1:B:188:LEU:CB	2.40	0.40
1:E:232:TRP:CZ2	1:E:239:PRO:HD3	2.57	0.40
1:E:254:ASN:O	1:E:257:PRO:HD2	2.21	0.40
1:F:53:ILE:HG22	1:F:145:TRP:CE2	2.57	0.40
1:G:56:THR:O	1:G:59:THR:HG23	2.21	0.40
1:I:256:ILE:HB	1:I:257:PRO:HD3	2.04	0.40
1:J:89:LEU:O	1:J:90:PHE:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/285 (87%)	230 (93%)	15 (6%)	3 (1%)	13	49
1	B	248/285 (87%)	217 (88%)	26 (10%)	5 (2%)	7	38
1	C	248/285 (87%)	220 (89%)	23 (9%)	5 (2%)	7	38
1	D	249/285 (87%)	224 (90%)	20 (8%)	5 (2%)	7	38
1	E	250/285 (88%)	220 (88%)	23 (9%)	7 (3%)	5	29
1	F	250/285 (88%)	234 (94%)	12 (5%)	4 (2%)	9	43
1	G	250/285 (88%)	222 (89%)	25 (10%)	3 (1%)	13	49
1	H	250/285 (88%)	225 (90%)	19 (8%)	6 (2%)	6	34
1	I	250/285 (88%)	218 (87%)	28 (11%)	4 (2%)	9	43
1	J	245/285 (86%)	219 (89%)	22 (9%)	4 (2%)	9	43
All	All	2488/2850 (87%)	2229 (90%)	213 (9%)	46 (2%)	8	41

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	186	ARG
1	G	113	ASN
1	I	95	LEU
1	I	101	ALA
1	J	94	VAL
1	J	268	LEU
1	A	101	ALA
1	B	86	GLY
1	C	155	HIS
1	C	276	VAL
1	D	113	ASN
1	E	61	THR
1	G	112	LYS
1	G	186	ARG

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Mol	Chain	Res	Type
1	H	112	LYS
1	H	184	SER
1	I	104	ARG
1	B	193	PHE
1	E	186	ARG
1	F	104	ARG
1	H	90	PHE
1	B	112	LYS
1	C	90	PHE
1	E	105	ILE
1	E	107	TRP
1	E	184	SER
1	F	90	PHE
1	J	186	ARG
1	A	84	VAL
1	A	90	PHE
1	C	183	TYR
1	C	189	MET
1	D	91	THR
1	D	279	LEU
1	E	104	ARG
1	H	113	ASN
1	I	105	ILE
1	B	221	ILE
1	D	136	GLY
1	F	105	ILE
1	B	236	GLY
1	H	162	ILE
1	E	31	PRO
1	D	83	VAL
1	J	277	ILE
1	H	84	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	203/230 (88%)	183 (90%)	20 (10%)	8 30
1	B	203/230 (88%)	182 (90%)	21 (10%)	7 29
1	C	203/230 (88%)	177 (87%)	26 (13%)	4 20
1	D	203/230 (88%)	186 (92%)	17 (8%)	11 39
1	E	203/230 (88%)	184 (91%)	19 (9%)	8 33
1	F	203/230 (88%)	180 (89%)	23 (11%)	6 25
1	G	203/230 (88%)	186 (92%)	17 (8%)	11 39
1	H	203/230 (88%)	183 (90%)	20 (10%)	8 30
1	I	203/230 (88%)	184 (91%)	19 (9%)	8 33
1	J	202/230 (88%)	184 (91%)	18 (9%)	9 35
All	All	2029/2300 (88%)	1829 (90%)	200 (10%)	8 30

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	PHE
1	A	61	THR
1	A	66	MET
1	A	77	LEU
1	A	81	LEU
1	A	82	CYS
1	A	93	THR
1	A	107	TRP
1	A	130	LEU
1	A	132	MET
1	A	138	TYR
1	A	142	ASN
1	A	157	VAL
1	A	160	THR
1	A	182	SER
1	A	189	MET
1	A	191	LYS
1	A	202	PHE
1	A	224	ARG
1	A	273	THR
1	B	45	ILE
1	B	49	PHE
1	B	51	PHE
1	B	61	THR

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Mol	Chain	Res	Type
1	B	77	LEU
1	B	82	CYS
1	B	94	VAL
1	B	113	ASN
1	B	132	MET
1	B	138	TYR
1	B	160	THR
1	B	182	SER
1	B	183	TYR
1	B	184	SER
1	B	188	LEU
1	B	189	MET
1	B	196	VAL
1	B	241	ASN
1	B	244	HIS
1	B	246	THR
1	B	275	TRP
1	C	45	ILE
1	C	46	SER
1	C	49	PHE
1	C	59	THR
1	C	61	THR
1	C	66	MET
1	C	77	LEU
1	C	81	LEU
1	C	94	VAL
1	C	96	ILE
1	C	104	ARG
1	C	106	THR
1	C	113	ASN
1	C	173	LEU
1	C	183	TYR
1	C	188	LEU
1	C	189	MET
1	C	197	LEU
1	C	201	MET
1	C	202	PHE
1	C	210	SER
1	C	235	VAL
1	C	247	VAL
1	C	274	TYR
1	C	277	ILE

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Mol	Chain	Res	Type
1	C	278	TYR
1	D	45	ILE
1	D	49	PHE
1	D	57	THR
1	D	66	MET
1	D	77	LEU
1	D	81	LEU
1	D	96	ILE
1	D	106	THR
1	D	113	ASN
1	D	138	TYR
1	D	142	ASN
1	D	157	VAL
1	D	202	PHE
1	D	237	SER
1	D	243	SER
1	D	256	ILE
1	D	268	LEU
1	E	49	PHE
1	E	53	ILE
1	E	61	THR
1	E	66	MET
1	E	81	LEU
1	E	93	THR
1	E	127	LEU
1	E	142	ASN
1	E	160	THR
1	E	173	LEU
1	E	179	VAL
1	E	186	ARG
1	E	187	SER
1	E	197	LEU
1	E	202	PHE
1	E	203	VAL
1	E	235	VAL
1	E	259	THR
1	E	276	VAL
1	F	32	LEU
1	F	45	ILE
1	F	49	PHE
1	F	51	PHE
1	F	53	ILE

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Mol	Chain	Res	Type
1	F	66	MET
1	F	77	LEU
1	F	79	LEU
1	F	94	VAL
1	F	107	TRP
1	F	113	ASN
1	F	130	LEU
1	F	138	TYR
1	F	140	THR
1	F	186	ARG
1	F	187	SER
1	F	197	LEU
1	F	202	PHE
1	F	240	GLU
1	F	243	SER
1	F	246	THR
1	F	249	ASN
1	F	274	TYR
1	G	36	TYR
1	G	49	PHE
1	G	51	PHE
1	G	66	MET
1	G	77	LEU
1	G	81	LEU
1	G	107	TRP
1	G	134	LEU
1	G	154	ASP
1	G	186	ARG
1	G	188	LEU
1	G	189	MET
1	G	190	ASP
1	G	197	LEU
1	G	199	VAL
1	G	202	PHE
1	G	272	LEU
1	H	30	HIS
1	H	49	PHE
1	H	61	THR
1	H	66	MET
1	H	77	LEU
1	H	81	LEU
1	H	91	THR

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Mol	Chain	Res	Type
1	H	127	LEU
1	H	138	TYR
1	H	140	THR
1	H	142	ASN
1	H	157	VAL
1	H	160	THR
1	H	177	LEU
1	H	184	SER
1	H	190	ASP
1	H	197	LEU
1	H	202	PHE
1	H	237	SER
1	H	247	VAL
1	I	34	THR
1	I	49	PHE
1	I	61	THR
1	I	66	MET
1	I	68	LYS
1	I	77	LEU
1	I	81	LEU
1	I	100	LYS
1	I	105	ILE
1	I	138	TYR
1	I	152	THR
1	I	160	THR
1	I	202	PHE
1	I	219	MET
1	I	258	VAL
1	I	268	LEU
1	I	273	THR
1	I	277	ILE
1	I	278	TYR
1	J	49	PHE
1	J	51	PHE
1	J	66	MET
1	J	68	LYS
1	J	95	LEU
1	J	100	LYS
1	J	105	ILE
1	J	140	THR
1	J	160	THR
1	J	173	LEU

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Mol	Chain	Res	Type
1	J	186	ARG
1	J	193	PHE
1	J	202	PHE
1	J	224	ARG
1	J	247	VAL
1	J	269	LEU
1	J	273	THR
1	J	278	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	144	GLN
1	A	158	HIS
1	A	241	ASN
1	B	113	ASN
1	B	116	ASN
1	B	142	ASN
1	B	151	GLN
1	B	249	ASN
1	C	113	ASN
1	C	142	ASN
1	C	151	GLN
1	C	158	HIS
1	C	159	HIS
1	C	244	HIS
1	C	254	ASN
1	D	142	ASN
1	D	213	ASN
1	D	244	HIS
1	E	142	ASN
1	E	151	GLN
1	F	142	ASN
1	F	159	HIS
1	F	249	ASN
1	G	113	ASN
1	G	116	ASN
1	G	213	ASN
1	G	241	ASN
1	H	113	ASN
1	H	116	ASN

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Mol	Chain	Res	Type
1	H	151	GLN
1	H	209	HIS
1	H	241	ASN
1	I	142	ASN
1	I	144	GLN
1	I	158	HIS
1	I	244	HIS
1	J	30	HIS
1	J	113	ASN
1	J	142	ASN
1	J	148	ASN
1	J	151	GLN
1	J	241	ASN
1	J	244	HIS
1	J	249	ASN

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 monosaccharides 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

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	250/285 (87%)	-0.35	2 (0%)	86	78	54, 78, 115, 178	0
1	B	250/285 (87%)	-0.33	8 (3%)	47	31	57, 88, 164, 301	0
1	C	250/285 (87%)	-0.07	16 (6%)	19	11	64, 98, 183, 259	0
1	D	251/285 (88%)	-0.15	11 (4%)	34	21	61, 91, 182, 314	0
1	E	252/285 (88%)	-0.12	12 (4%)	30	18	44, 83, 175, 306	0
1	F	252/285 (88%)	-0.27	7 (2%)	53	37	47, 79, 135, 210	0
1	G	252/285 (88%)	-0.10	12 (4%)	30	18	53, 84, 184, 236	0
1	H	252/285 (88%)	-0.15	9 (3%)	42	27	59, 90, 192, 316	0
1	I	252/285 (88%)	-0.28	4 (1%)	72	59	52, 85, 125, 224	0
1	J	249/285 (87%)	-0.28	2 (0%)	86	78	53, 84, 137, 223	0
All	All	2510/2850 (88%)	-0.21	83 (3%)	46	30	44, 86, 166, 316	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	279	LEU	6.5
1	C	110	LEU	6.4
1	G	279	LEU	6.1
1	G	278	TYR	5.8
1	B	110	LEU	5.4
1	D	280	ARG	5.4
1	D	102	SER	5.3
1	H	110	LEU	5.2
1	C	107	TRP	5.1
1	H	109	GLN	4.6
1	D	101	ALA	4.3
1	F	279	LEU	4.2
1	G	280	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	107	TRP	4.1
1	G	29	LYS	4.0
1	F	278	TYR	3.9
1	C	113	ASN	3.8
1	E	31	PRO	3.8
1	C	105	ILE	3.8
1	F	274	TYR	3.7
1	E	32	LEU	3.6
1	H	106	THR	3.5
1	G	94	VAL	3.5
1	I	94	VAL	3.4
1	F	31	PRO	3.3
1	E	95	LEU	3.3
1	D	278	TYR	3.2
1	G	95	LEU	3.2
1	G	88	ASP	3.2
1	E	36	TYR	3.2
1	C	106	THR	3.1
1	G	110	LEU	3.1
1	F	36	TYR	3.0
1	H	100	LYS	3.0
1	C	276	VAL	3.0
1	C	104	ARG	2.9
1	C	111	ALA	2.9
1	E	94	VAL	2.9
1	J	29	LYS	2.9
1	G	107	TRP	2.9
1	D	107	TRP	2.8
1	E	30	HIS	2.8
1	H	104	ARG	2.8
1	D	104	ARG	2.8
1	B	279	LEU	2.8
1	A	278	TYR	2.8
1	C	109	GLN	2.8
1	H	119	PHE	2.8
1	E	29	LYS	2.7
1	I	275	TRP	2.7
1	E	98	VAL	2.7
1	J	31	PRO	2.7
1	A	279	LEU	2.7
1	D	103	GLY	2.6
1	B	109	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	100	LYS	2.4
1	E	102	SER	2.4
1	I	253	ASP	2.3
1	G	31	PRO	2.3
1	C	143	GLY	2.3
1	C	88	ASP	2.3
1	D	274	TYR	2.3
1	B	103	GLY	2.3
1	E	33	LYS	2.3
1	D	275	TRP	2.3
1	I	270	VAL	2.3
1	H	102	SER	2.2
1	B	111	ALA	2.2
1	E	101	ALA	2.2
1	G	91	THR	2.2
1	G	275	TRP	2.2
1	B	252	THR	2.2
1	F	275	TRP	2.2
1	C	273	THR	2.1
1	F	32	LEU	2.1
1	C	30	HIS	2.1
1	E	90	PHE	2.1
1	B	274	TYR	2.1
1	C	277	ILE	2.1
1	H	108	GLY	2.1
1	C	92	SER	2.1
1	C	32	LEU	2.0
1	B	98	VAL	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 monosaccharides 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.