



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 12:55 PM EDT

PDB ID : 3RQC  
Title : Crystal structure of the catalytic core of the 2-oxoacid dehydrogenase multienzyme complex from *Thermoplasma acidophilum*  
Authors : Marrott, N.L.; Crennell, S.J.; Hough, D.W.; Danson, M.J.; van den Elsen, J.M.H.  
Deposited on : 2011-04-28  
Resolution : 4.01 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

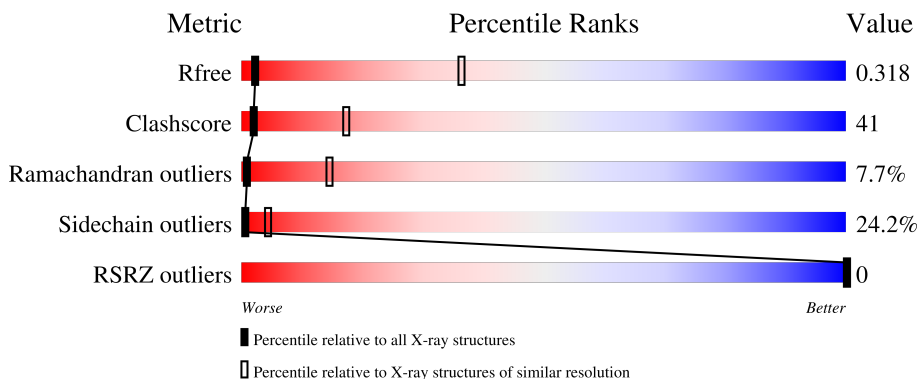
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.01 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.




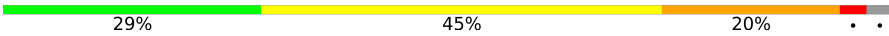
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1098 (4.34-3.70)
Clashscore	141614	1159 (4.34-3.70)
Ramachandran outliers	138981	1118 (4.34-3.70)
Sidechain outliers	138945	1108 (4.34-3.70)
RSRZ outliers	127900	1034 (4.38-3.66)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	
1	C	224	
1	D	224	
1	E	224	

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Mol	Chain	Length	Quality of chain
1	F	224	 31% 50% 13% . .
1	G	224	 29% 45% 20% . .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12157 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 lipoamide acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	Total 1733	C 1105	N 297	O 322	S 9	0	0	0
1	B	218	Total 1744	C 1111	N 301	O 323	S 9	0	0	0
1	C	220	Total 1755	C 1118	N 303	O 325	S 9	0	0	0
1	D	218	Total 1744	C 1111	N 301	O 323	S 9	0	0	0
1	E	217	Total 1733	C 1105	N 297	O 322	S 9	0	0	0
1	F	215	Total 1715	C 1095	N 295	O 316	S 9	0	0	0
1	G	217	Total 1733	C 1105	N 297	O 322	S 9	0	0	0

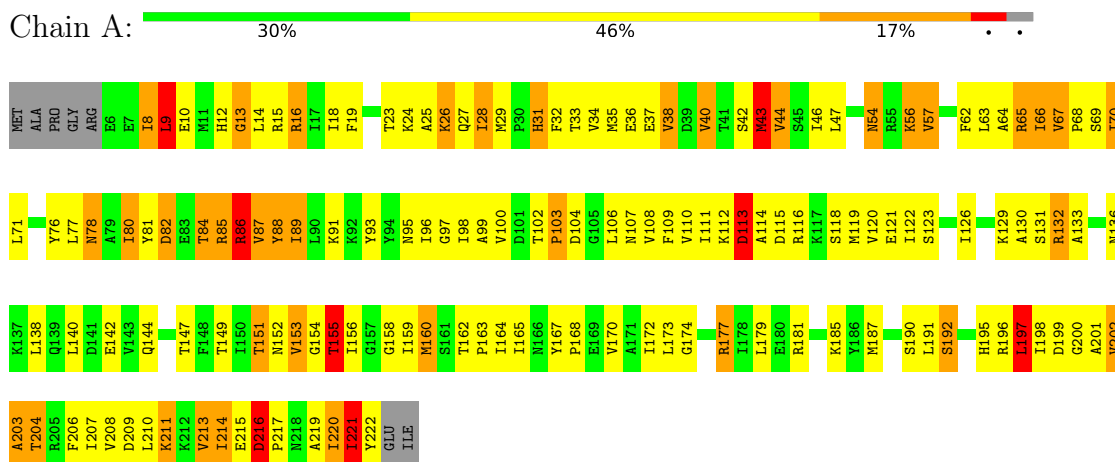
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9HIA5
B	1	MET	-	expression tag	UNP Q9HIA5
C	1	MET	-	expression tag	UNP Q9HIA5
D	1	MET	-	expression tag	UNP Q9HIA5
E	1	MET	-	expression tag	UNP Q9HIA5
F	1	MET	-	expression tag	UNP Q9HIA5
G	1	MET	-	expression tag	UNP Q9HIA5

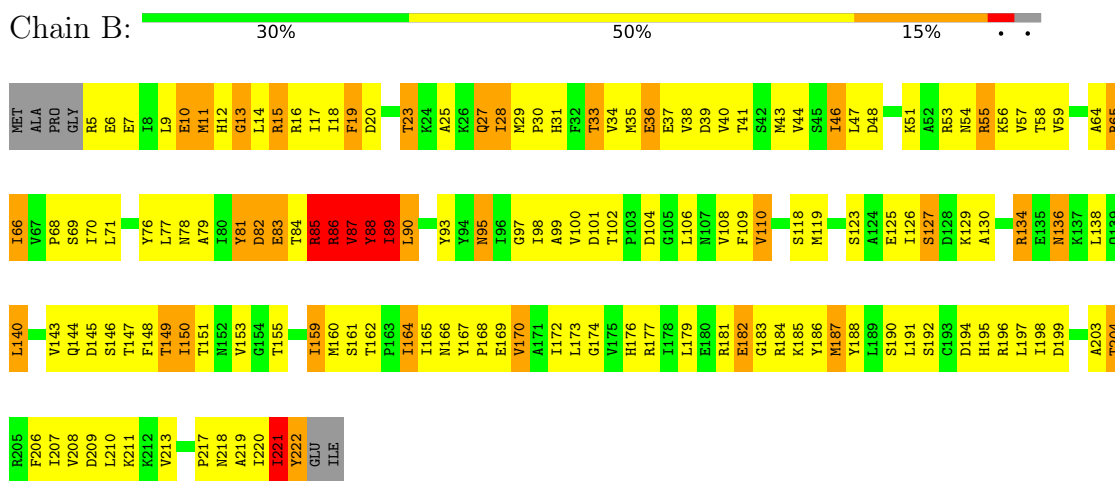
### 3 Residue-property plots [i](#)

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.

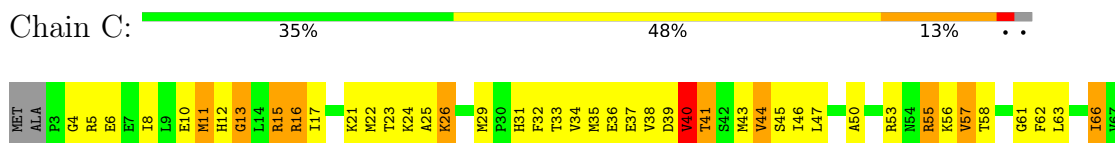
- Molecule 1: Probable lipamide acyltransferase

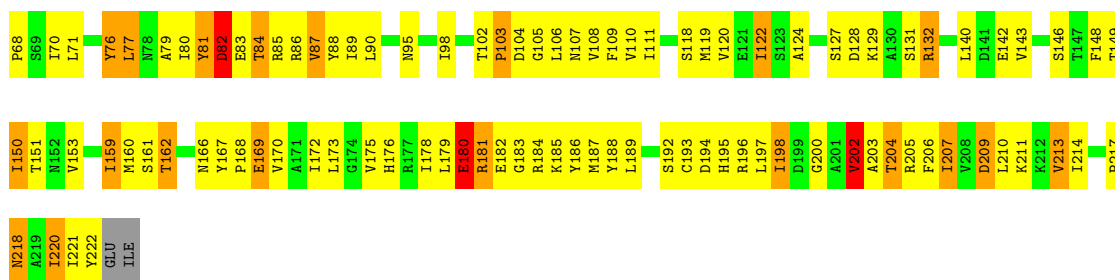


- Molecule 1: Probable lipamide acyltransferase



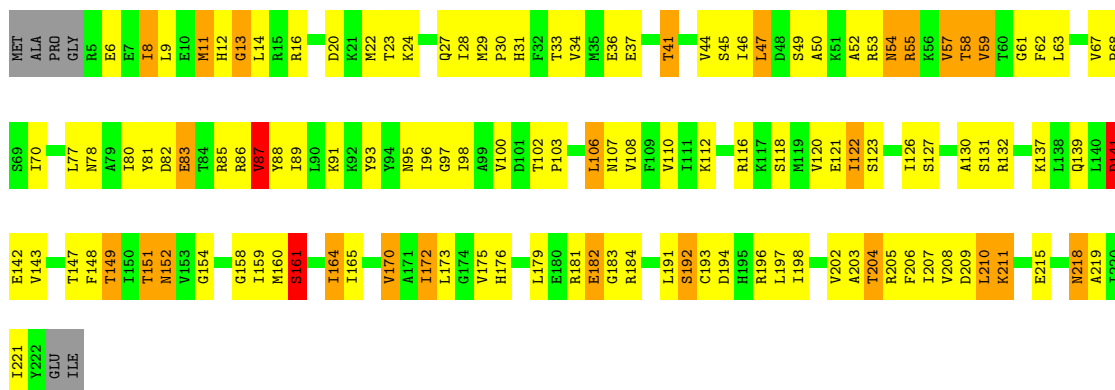
- Molecule 1: Probable lipamide acyltransferase





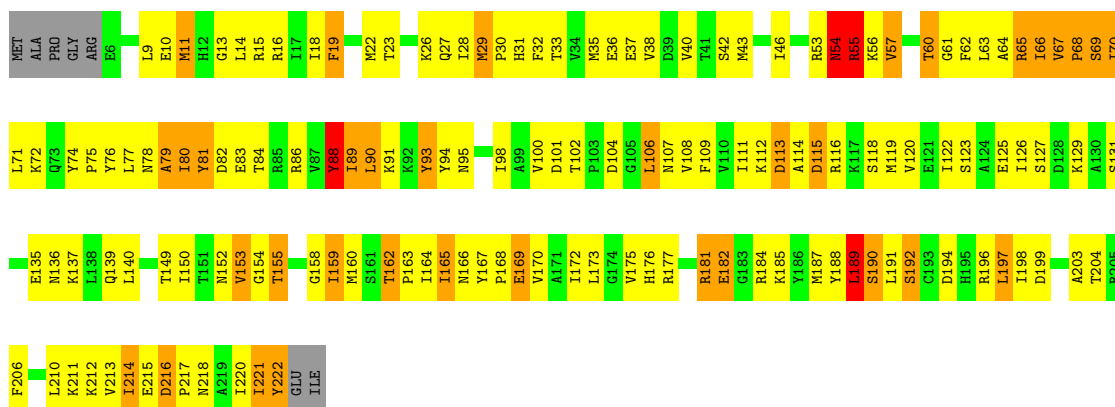
- Molecule 1: Probable lipamide acyltransferase

Chain D: 42% 43% 11% ..



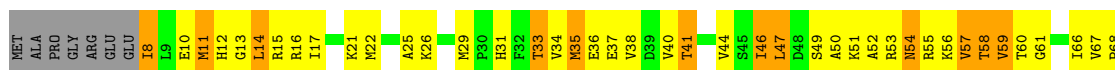
- Molecule 1: Probable lipamide acyltransferase

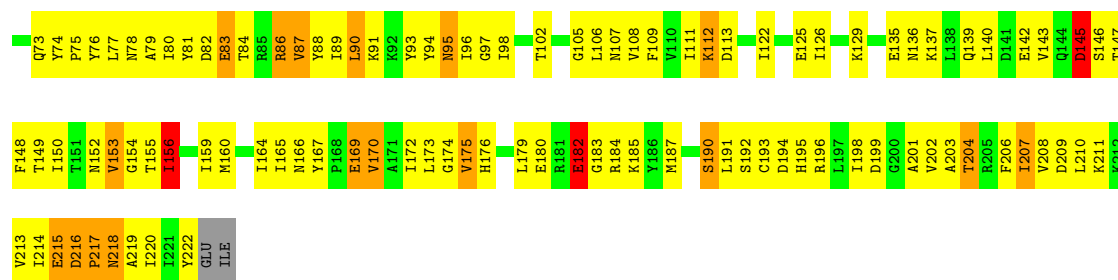
Chain E: 31% 48% 16% ..



- Molecule 1: Probable lipamide acyltransferase

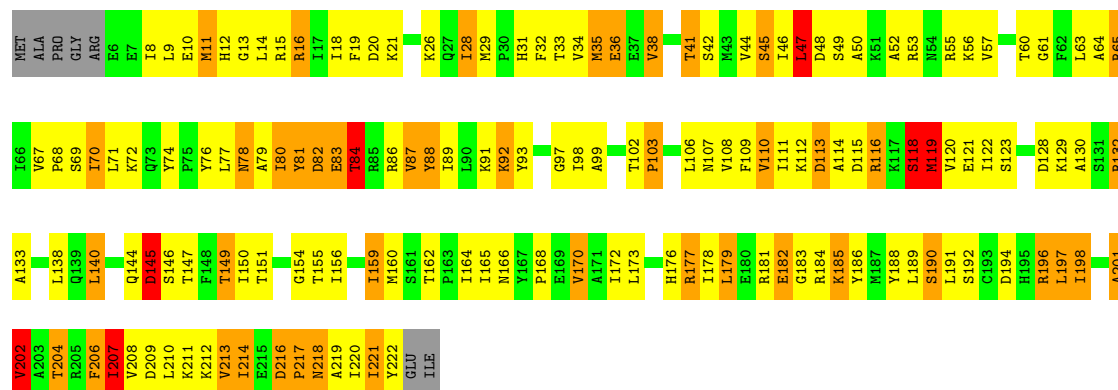
Chain F: 31% 50% 13% ..





- Molecule 1: Probable lipoamide acyltransferase

Chain G: 29% 45% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.84Å 204.84Å 441.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.95 – 4.01 44.95 – 4.01	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.95-4.01) 97.9 (44.95-4.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 4.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.253 , 0.328 0.246 , 0.318	Depositor DCC
$R_{free}$ test set	1504 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.8	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 17.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.76	0/1759	0.93	2/2375 (0.1%)
1	B	0.74	0/1770	0.88	2/2389 (0.1%)
1	C	0.75	1/1782 (0.1%)	0.86	0/2405
1	D	0.63	0/1770	0.78	1/2389 (0.0%)
1	E	0.68	0/1759	0.85	2/2375 (0.1%)
1	F	0.69	0/1741	0.83	0/2351
1	G	0.76	1/1759 (0.1%)	0.95	3/2375 (0.1%)
All	All	0.72	2/12340 (0.0%)	0.87	10/16659 (0.1%)

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	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	G	0	2
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	GLU	CB-CG	8.07	1.67	1.52
1	G	119	MET	CB-CG	5.08	1.67	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	LEU	CA-CB-CG	6.89	131.15	115.30
1	A	9	LEU	CA-CB-CG	6.63	130.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	179	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	90	LEU	CA-CB-CG	5.54	128.03	115.30
1	D	87	VAL	N-CA-C	5.54	125.95	111.00
1	E	189	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	88	TYR	N-CA-C	5.24	125.15	111.00
1	G	84	THR	N-CA-C	5.23	125.12	111.00
1	E	88	TYR	N-CA-C	5.20	125.04	111.00
1	G	47	LEU	CB-CG-CD2	5.15	119.76	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	81	TYR	Peptide
1	B	85	ARG	Peptide
1	C	11	MET	Peptide
1	C	81	TYR	Peptide
1	D	118	SER	Peptide
1	D	83	GLU	Peptide
1	E	81	TYR	Peptide
1	E	83	GLU	Peptide
1	G	118	SER	Peptide
1	G	140	LEU	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	1733	0	1795	207	0
1	B	1744	0	1808	164	0
1	C	1755	0	1819	178	0
1	D	1744	0	1808	107	0
1	E	1733	0	1795	170	0
1	F	1715	0	1783	140	0
1	G	1733	0	1795	163	0
All	All	12157	0	12603	1004	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 41.

All (1004) 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:222:TYR:HA	1:G:119:MET:HB3	1.19	1.18
1:B:56:LYS:HB3	1:B:57:VAL:HA	1.18	1.16
1:B:30:PRO:HA	1:C:26:LYS:HD3	1.30	1.12
1:C:82:ASP:HB2	1:C:87:VAL:HG23	1.30	1.12
1:G:76:TYR:HD1	1:G:197:LEU:HD21	1.13	1.10
1:A:43:MET:O	1:A:46:ILE:HG22	1.51	1.09
1:E:30:PRO:HA	1:F:26:LYS:HE2	1.15	1.09
1:G:11:MET:HG2	1:G:15:ARG:HG3	1.20	1.09
1:G:159:ILE:O	1:G:159:ILE:HD12	1.52	1.08
1:A:221:ILE:HA	1:G:220:ILE:HD11	1.36	1.07
1:A:153:VAL:HG11	1:C:204:THR:HG21	1.36	1.06
1:D:67:VAL:HG23	1:D:68:PRO:HD3	1.36	1.06
1:C:119:MET:HG3	1:E:221:ILE:HD12	1.37	1.06
1:C:38:VAL:HG23	1:C:40:VAL:HG12	1.34	1.05
1:C:12:HIS:O	1:C:16:ARG:HB2	1.58	1.03
1:A:111:ILE:HD12	1:A:111:ILE:O	1.59	1.02
1:C:221:ILE:HG22	1:E:119:MET:HG3	1.43	1.01
1:E:76:TYR:CD1	1:E:197:LEU:HD21	1.95	1.00
1:B:41:THR:HG21	1:B:184:ARG:HE	1.24	1.00
1:D:41:THR:HG21	1:D:184:ARG:HH21	1.28	0.99
1:E:181:ARG:O	1:E:182:GLU:HB3	1.61	0.99
1:G:76:TYR:HD1	1:G:197:LEU:CD2	1.76	0.99
1:B:33:THR:HB	1:B:192:SER:OG	1.63	0.98
1:G:29:MET:HE2	1:G:194:ASP:HB2	1.47	0.96
1:F:98:ILE:HD11	1:F:126:ILE:HG21	1.44	0.96
1:A:86:ARG:HH22	1:B:11:MET:HB2	1.29	0.96
1:G:71:LEU:HD22	1:G:78:ASN:HB3	1.48	0.95
1:G:182:GLU:N	1:G:183:GLY:HA2	1.80	0.94
1:A:221:ILE:HD13	1:G:220:ILE:HG13	1.47	0.94
1:G:76:TYR:CD1	1:G:197:LEU:HD21	2.02	0.93
1:B:35:MET:HG3	1:B:190:SER:HB3	1.51	0.93
1:A:82:ASP:OD2	1:A:87:VAL:HG23	1.69	0.93
1:C:62:PHE:HA	1:C:119:MET:HE1	1.51	0.92
1:G:150:ILE:HG22	1:G:173:LEU:HB3	1.49	0.92
1:C:222:TYR:HB3	1:E:119:MET:HB2	1.52	0.92
1:C:82:ASP:HB2	1:C:87:VAL:CG2	1.99	0.91
1:F:165:ILE:HA	1:F:172:ILE:HG13	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TYR:HE1	1:C:159:ILE:HD12	1.36	0.91
1:F:98:ILE:HD11	1:F:126:ILE:CG2	2.00	0.91
1:G:11:MET:HG2	1:G:15:ARG:CG	2.01	0.90
1:E:80:ILE:HD13	1:E:168:PRO:HG2	1.53	0.90
1:G:82:ASP:O	1:G:83:GLU:HG2	1.70	0.89
1:G:99:ALA:HB2	1:G:108:VAL:HG13	1.54	0.89
1:B:217:PRO:HA	1:B:220:ILE:HG23	1.55	0.89
1:A:98:ILE:HD11	1:A:126:ILE:HG22	1.53	0.89
1:A:62:PHE:CD2	1:A:119:MET:SD	2.66	0.89
1:B:56:LYS:CB	1:B:57:VAL:HA	2.03	0.88
1:B:11:MET:CE	1:B:19:PHE:HD1	1.86	0.88
1:A:221:ILE:HD13	1:G:220:ILE:CG1	2.03	0.88
1:A:33:THR:H	1:B:162:THR:HG22	1.39	0.88
1:G:162:THR:HG23	1:G:162:THR:O	1.72	0.88
1:A:71:LEU:HD13	1:A:78:ASN:HB3	1.55	0.87
1:A:119:MET:HE2	1:G:221:ILE:HG22	1.56	0.87
1:A:85:ARG:O	1:A:86:ARG:HB2	1.74	0.87
1:C:62:PHE:HA	1:C:119:MET:CE	2.05	0.87
1:A:86:ARG:HA	1:A:86:ARG:HH11	1.37	0.87
1:B:56:LYS:HB3	1:B:57:VAL:CA	2.02	0.86
1:B:88:TYR:CZ	1:B:197:LEU:HG	2.10	0.86
1:A:77:LEU:HD12	1:A:198:ILE:HD12	1.58	0.86
1:F:219:ALA:O	1:F:222:TYR:HB2	1.76	0.86
1:G:79:ALA:HB1	1:G:89:ILE:O	1.75	0.86
1:A:15:ARG:NH1	1:C:196:ARG:O	2.10	0.85
1:A:222:TYR:CA	1:G:119:MET:HB3	2.05	0.85
1:E:181:ARG:O	1:E:182:GLU:CB	2.24	0.84
1:A:82:ASP:OD2	1:A:84:THR:O	1.94	0.84
1:G:211:LYS:HA	1:G:214:ILE:HD12	1.58	0.84
1:B:78:ASN:HD21	1:B:147:THR:HB	1.43	0.84
1:A:153:VAL:HG11	1:C:204:THR:CG2	2.08	0.84
1:E:95:ASN:ND2	1:E:113:ASP:H	1.76	0.83
1:C:77:LEU:HG	1:C:198:ILE:HD11	1.62	0.82
1:F:96:ILE:HG22	1:F:148:PHE:HB3	1.61	0.82
1:A:114:ALA:O	1:A:116:ARG:N	2.12	0.82
1:B:11:MET:HE1	1:B:19:PHE:HD1	1.45	0.82
1:C:128:ASP:O	1:C:132:ARG:NH1	2.13	0.82
1:D:6:GLU:HG2	1:F:91:LYS:HD2	1.61	0.82
1:D:58:THR:HG22	1:D:123:SER:HB2	1.62	0.82
1:D:182:GLU:N	1:D:183:GLY:HA2	1.94	0.82
1:G:159:ILE:HD12	1:G:159:ILE:C	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:HG23	1:C:161:SER:HB3	1.62	0.81
1:D:11:MET:HB2	1:D:16:ARG:HD3	1.62	0.81
1:G:53:ARG:O	1:G:55:ARG:HD2	1.80	0.81
1:F:77:LEU:HG	1:F:198:ILE:HD11	1.61	0.81
1:F:145:ASP:OD1	1:F:145:ASP:O	1.98	0.81
1:A:98:ILE:CD1	1:A:126:ILE:HG22	2.10	0.81
1:F:216:ASP:HB2	1:F:217:PRO:HD2	1.61	0.81
1:A:31:HIS:CE1	1:A:165:ILE:HD12	2.15	0.81
1:D:41:THR:HG21	1:D:184:ARG:NH2	1.96	0.81
1:F:152:ASN:HA	1:F:175:VAL:HG23	1.61	0.80
1:E:166:ASN:H	1:E:172:ILE:HD11	1.45	0.80
1:A:8:ILE:HG22	1:C:88:TYR:HB2	1.62	0.80
1:A:80:ILE:O	1:A:88:TYR:O	2.00	0.80
1:C:38:VAL:HG23	1:C:40:VAL:CG1	2.13	0.79
1:F:165:ILE:HA	1:F:172:ILE:CG1	2.13	0.79
1:G:81:TYR:HA	1:G:88:TYR:HB3	1.65	0.79
1:E:100:VAL:HG12	1:E:101:ASP:H	1.47	0.79
1:A:77:LEU:CD1	1:A:198:ILE:HD12	2.14	0.78
1:B:30:PRO:HA	1:C:26:LYS:CD	2.12	0.78
1:B:217:PRO:O	1:B:220:ILE:HG12	1.83	0.78
1:A:86:ARG:HH22	1:B:11:MET:CB	1.97	0.78
1:C:40:VAL:HG11	1:C:187:MET:HB3	1.66	0.78
1:B:41:THR:HG22	1:B:185:LYS:H	1.49	0.78
1:A:65:ARG:O	1:A:65:ARG:HD3	1.84	0.78
1:D:67:VAL:CG2	1:D:68:PRO:HD3	2.11	0.78
1:A:47:LEU:HD23	1:A:57:VAL:HG23	1.64	0.77
1:B:33:THR:HG23	1:C:162:THR:CG2	2.15	0.77
1:A:164:ILE:HD11	1:C:31:HIS:O	1.83	0.77
1:D:87:VAL:HG12	1:E:10:GLU:HA	1.64	0.77
1:F:95:ASN:O	1:F:147:THR:HG22	1.85	0.77
1:A:16:ARG:HH22	1:C:85:ARG:HH12	1.30	0.77
1:C:119:MET:HB2	1:E:222:TYR:HD1	1.49	0.77
1:D:80:ILE:HD11	1:D:89:ILE:HD12	1.67	0.76
1:C:179:LEU:O	1:C:180:GLU:HB2	1.84	0.76
1:D:211:LYS:O	1:D:215:GLU:HG3	1.84	0.76
1:D:164:ILE:HD11	1:F:195:HIS:CD2	2.21	0.75
1:G:97:GLY:HA3	1:G:149:THR:CG2	2.16	0.75
1:C:167:TYR:CD1	1:C:168:PRO:HA	2.21	0.75
1:G:11:MET:CG	1:G:15:ARG:HG3	2.11	0.75
1:E:74:TYR:HD2	1:E:206:PHE:HD1	1.35	0.75
1:E:95:ASN:HD22	1:E:113:ASP:H	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:O	1:A:89:ILE:HG13	1.84	0.75
1:A:16:ARG:HH22	1:C:85:ARG:NH1	1.84	0.75
1:C:70:ILE:HG22	1:C:206:PHE:CE1	2.21	0.75
1:D:182:GLU:H	1:D:183:GLY:HA2	1.52	0.75
1:G:76:TYR:CD1	1:G:197:LEU:CD2	2.65	0.74
1:E:165:ILE:HA	1:E:172:ILE:CG1	2.18	0.74
1:E:66:ILE:HG21	1:E:220:ILE:HD11	1.70	0.74
1:E:81:TYR:CD1	1:E:88:TYR:CE1	2.75	0.74
1:A:86:ARG:NH2	1:B:11:MET:HB2	2.00	0.74
1:D:97:GLY:HA3	1:D:149:THR:HG22	1.68	0.74
1:G:80:ILE:O	1:G:88:TYR:HB2	1.88	0.73
1:A:9:LEU:O	1:C:88:TYR:CD2	2.42	0.73
1:E:79:ALA:HB1	1:E:89:ILE:HG22	1.69	0.73
1:B:10:GLU:O	1:B:11:MET:HG3	1.89	0.73
1:B:86:ARG:NH1	1:B:86:ARG:HA	2.03	0.73
1:D:198:ILE:HG23	1:D:202:VAL:HG13	1.70	0.73
1:G:162:THR:O	1:G:162:THR:CG2	2.36	0.73
1:B:182:GLU:N	1:B:183:GLY:HA2	2.03	0.72
1:F:149:THR:HB	1:F:172:ILE:HD13	1.71	0.72
1:G:41:THR:HG22	1:G:185:LYS:H	1.53	0.72
1:A:16:ARG:NH2	1:C:85:ARG:HH12	1.88	0.72
1:A:162:THR:HG22	1:C:33:THR:HB	1.70	0.72
1:G:70:ILE:HG22	1:G:206:PHE:CE1	2.24	0.72
1:G:204:THR:O	1:G:208:VAL:HG23	1.90	0.72
1:E:215:GLU:O	1:E:217:PRO:HD3	1.90	0.72
1:B:66:ILE:O	1:B:69:SER:HB3	1.89	0.72
1:F:35:MET:SD	1:F:35:MET:N	2.62	0.72
1:F:77:LEU:HG	1:F:198:ILE:CD1	2.20	0.72
1:F:98:ILE:CD1	1:F:126:ILE:HG21	2.19	0.72
1:B:167:TYR:CD1	1:B:168:PRO:HA	2.24	0.72
1:C:32:PHE:CD1	1:C:195:HIS:CD2	2.78	0.71
1:C:34:VAL:HG21	1:C:204:THR:HG22	1.71	0.71
1:B:41:THR:HG21	1:B:184:ARG:NE	2.03	0.71
1:E:94:TYR:HB2	1:E:115:ASP:OD2	1.91	0.71
1:B:76:TYR:HD1	1:B:197:LEU:HD22	1.56	0.71
1:E:221:ILE:HD12	1:E:221:ILE:O	1.89	0.70
1:C:39:ASP:C	1:C:41:THR:H	1.94	0.70
1:D:165:ILE:HA	1:D:172:ILE:HD12	1.73	0.70
1:F:91:LYS:HE3	1:F:93:TYR:OH	1.91	0.70
1:A:9:LEU:HB3	1:C:88:TYR:CZ	2.26	0.70
1:E:188:TYR:CE1	1:F:159:ILE:HD11	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HG21	1:A:109:PHE:CE2	2.26	0.70
1:B:97:GLY:HA3	1:B:149:THR:HG22	1.74	0.70
1:G:118:SER:HB3	1:G:121:GLU:H	1.56	0.70
1:E:40:VAL:HG22	1:E:185:LYS:O	1.91	0.70
1:C:81:TYR:O	1:C:81:TYR:CD2	2.46	0.69
1:A:62:PHE:HD2	1:A:119:MET:SD	2.13	0.69
1:E:165:ILE:HA	1:E:172:ILE:HG13	1.73	0.69
1:A:9:LEU:HB3	1:C:88:TYR:CE1	2.28	0.69
1:E:31:HIS:NE2	1:E:165:ILE:HG12	2.06	0.69
1:G:159:ILE:HD11	1:G:188:TYR:CD2	2.27	0.69
1:D:204:THR:HG21	1:E:153:VAL:HB	1.74	0.69
1:G:15:ARG:O	1:G:18:ILE:HG22	1.93	0.69
1:G:84:THR:HB	1:G:87:VAL:CG2	2.22	0.69
1:C:221:ILE:CG2	1:E:119:MET:HG3	2.19	0.69
1:E:166:ASN:N	1:E:172:ILE:HD11	2.08	0.68
1:G:36:GLU:HB2	1:G:207:ILE:HD13	1.75	0.68
1:A:23:THR:O	1:A:27:GLN:HB2	1.94	0.68
1:E:61:GLY:O	1:E:64:ALA:N	2.26	0.68
1:E:74:TYR:HD2	1:E:206:PHE:CD1	2.11	0.68
1:C:39:ASP:O	1:C:41:THR:N	2.27	0.68
1:E:158:GLY:O	1:E:176:HIS:HB3	1.93	0.68
1:E:188:TYR:HE1	1:F:159:ILE:HD11	1.59	0.68
1:A:77:LEU:HD12	1:A:198:ILE:CD1	2.23	0.68
1:B:100:VAL:HG12	1:B:109:PHE:HE2	1.58	0.68
1:G:78:ASN:HD22	1:G:147:THR:HB	1.59	0.67
1:E:26:LYS:HE3	1:E:31:HIS:HB2	1.76	0.67
1:B:150:ILE:CG2	1:B:173:LEU:HB3	2.23	0.67
1:C:221:ILE:HG12	1:E:220:ILE:HG21	1.76	0.67
1:B:71:LEU:HD13	1:B:78:ASN:HB2	1.75	0.67
1:D:67:VAL:HG23	1:D:96:ILE:HD13	1.76	0.67
1:A:64:ALA:HA	1:A:67:VAL:CG2	2.24	0.67
1:D:70:ILE:HD13	1:D:210:LEU:HA	1.77	0.67
1:G:81:TYR:HB2	1:G:88:TYR:HD1	1.60	0.67
1:E:74:TYR:O	1:E:76:TYR:N	2.28	0.67
1:G:194:ASP:OD2	1:G:196:ARG:NH1	2.28	0.67
1:A:98:ILE:HG13	1:A:109:PHE:CE1	2.30	0.66
1:E:81:TYR:OH	1:E:194:ASP:OD2	2.03	0.66
1:F:11:MET:HB3	1:F:16:ARG:HG2	1.77	0.66
1:F:93:TYR:HD1	1:F:95:ASN:OD1	1.77	0.66
1:E:54:ASN:C	1:E:55:ARG:HG2	2.15	0.66
1:A:47:LEU:HD23	1:A:57:VAL:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ILE:O	1:G:88:TYR:CB	2.44	0.66
1:C:62:PHE:HD1	1:C:119:MET:HE1	1.60	0.66
1:G:26:LYS:HG3	1:G:164:ILE:CD1	2.25	0.66
1:C:149:THR:HG23	1:C:172:ILE:HG13	1.78	0.66
1:A:36:GLU:HA	1:A:36:GLU:OE1	1.96	0.66
1:E:188:TYR:HE1	1:F:159:ILE:CD1	2.09	0.66
1:F:44:VAL:HG21	1:F:185:LYS:HD2	1.78	0.66
1:C:119:MET:HG3	1:E:221:ILE:O	1.97	0.65
1:D:67:VAL:HG23	1:D:68:PRO:CD	2.19	0.65
1:G:102:THR:HB	1:G:103:PRO:HD2	1.79	0.65
1:E:91:LYS:HE3	1:E:93:TYR:CE1	2.31	0.65
1:B:11:MET:CE	1:B:19:PHE:CD1	2.75	0.65
1:D:161:SER:HB3	1:F:34:VAL:HG23	1.78	0.65
1:E:30:PRO:HA	1:F:26:LYS:CE	2.09	0.65
1:G:98:ILE:HG21	1:G:111:ILE:HG12	1.77	0.65
1:F:111:ILE:HD11	1:F:125:GLU:O	1.97	0.65
1:A:197:LEU:O	1:B:15:ARG:NH2	2.30	0.65
1:C:119:MET:HG3	1:E:221:ILE:CD1	2.22	0.65
1:E:62:PHE:CD2	1:E:119:MET:CE	2.80	0.65
1:A:46:ILE:HD11	1:G:221:ILE:HD12	1.77	0.64
1:A:119:MET:CE	1:G:221:ILE:HG22	2.27	0.64
1:A:162:THR:O	1:A:162:THR:HG23	1.95	0.64
1:A:63:LEU:O	1:A:67:VAL:HG22	1.97	0.64
1:D:194:ASP:OD1	1:D:196:ARG:HG3	1.98	0.64
1:C:32:PHE:HD1	1:C:195:HIS:HD2	1.44	0.64
1:A:40:VAL:O	1:A:43:MET:HB3	1.96	0.64
1:A:86:ARG:NH2	1:B:16:ARG:HG3	2.11	0.64
1:B:33:THR:HG23	1:C:162:THR:HG21	1.80	0.64
1:C:62:PHE:CD1	1:C:119:MET:HE1	2.32	0.64
1:F:80:ILE:O	1:F:88:TYR:HA	1.97	0.64
1:B:88:TYR:CE2	1:B:197:LEU:HG	2.32	0.64
1:C:76:TYR:HD1	1:C:197:LEU:O	1.81	0.64
1:C:81:TYR:CD1	1:C:197:LEU:HD11	2.33	0.64
1:D:120:VAL:HG13	1:D:121:GLU:HG3	1.80	0.64
1:C:43:MET:O	1:C:46:ILE:HG22	1.98	0.64
1:C:41:THR:HG21	1:C:184:ARG:HD2	1.78	0.64
1:E:98:ILE:HG22	1:E:150:ILE:HB	1.80	0.64
1:A:78:ASN:ND2	1:A:147:THR:HB	2.14	0.63
1:D:191:LEU:HG	1:D:192:SER:N	2.12	0.63
1:D:8:ILE:HG12	1:D:9:LEU:N	2.13	0.63
1:A:33:THR:N	1:B:162:THR:HG22	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:MET:HE1	1:B:19:PHE:CD1	2.32	0.63
1:D:77:LEU:HG	1:D:198:ILE:HD13	1.80	0.63
1:B:41:THR:HG21	1:B:184:ARG:HB3	1.80	0.63
1:D:12:HIS:HD2	1:D:14:LEU:H	1.45	0.63
1:E:66:ILE:CG2	1:E:220:ILE:HD11	2.29	0.63
1:C:32:PHE:CD1	1:C:195:HIS:HD2	2.16	0.63
1:F:14:LEU:HD22	1:F:105:GLY:HA3	1.81	0.63
1:C:62:PHE:CA	1:C:119:MET:HE1	2.25	0.63
1:G:128:ASP:O	1:G:132:ARG:HB2	1.99	0.63
1:A:76:TYR:HD1	1:A:197:LEU:HD13	1.63	0.62
1:G:31:HIS:NE2	1:G:165:ILE:HG13	2.13	0.62
1:G:63:LEU:O	1:G:67:VAL:HG23	2.00	0.62
1:A:8:ILE:CG2	1:C:88:TYR:HB2	2.29	0.62
1:C:81:TYR:HD1	1:C:197:LEU:HD11	1.65	0.62
1:E:123:SER:O	1:E:126:ILE:HG13	1.98	0.62
1:F:204:THR:O	1:F:208:VAL:HG23	1.98	0.62
1:B:31:HIS:NE2	1:B:165:ILE:HG12	2.14	0.62
1:E:15:ARG:O	1:E:18:ILE:HG22	1.99	0.62
1:A:37:GLU:N	1:B:159:ILE:HD11	2.14	0.62
1:A:130:ALA:O	1:A:133:ALA:N	2.33	0.62
1:E:38:VAL:HG12	1:E:215:GLU:HG3	1.81	0.62
1:E:70:ILE:HD13	1:E:210:LEU:HB2	1.81	0.62
1:G:109:PHE:CE1	1:G:129:LYS:HB2	2.33	0.62
1:B:79:ALA:O	1:B:170:VAL:HB	1.99	0.62
1:B:100:VAL:HG22	1:B:101:ASP:N	2.15	0.62
1:B:150:ILE:HG22	1:B:173:LEU:HB3	1.82	0.61
1:D:159:ILE:HG22	1:F:36:GLU:HA	1.81	0.61
1:F:193:CYS:HB2	1:F:198:ILE:HD12	1.82	0.61
1:A:114:ALA:C	1:A:116:ARG:H	2.04	0.61
1:B:16:ARG:O	1:B:20:ASP:OD2	2.18	0.61
1:B:219:ALA:HB1	1:B:222:TYR:HE2	1.66	0.61
1:E:31:HIS:CE1	1:E:165:ILE:HG12	2.34	0.61
1:C:198:ILE:HG22	1:C:198:ILE:O	1.99	0.61
1:E:95:ASN:HB3	1:E:112:LYS:HA	1.82	0.61
1:G:81:TYR:HE1	1:G:196:ARG:HH12	1.47	0.61
1:A:82:ASP:OD1	1:A:87:VAL:O	2.18	0.61
1:C:36:GLU:HB2	1:C:207:ILE:HD11	1.82	0.61
1:F:36:GLU:HA	1:F:36:GLU:OE1	2.00	0.61
1:G:97:GLY:HA3	1:G:149:THR:HG22	1.83	0.61
1:A:119:MET:HE2	1:G:221:ILE:O	2.01	0.61
1:A:221:ILE:CA	1:G:220:ILE:HD11	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:PRO:HB3	1:C:26:LYS:HG2	1.82	0.60
1:B:78:ASN:ND2	1:B:147:THR:HB	2.13	0.60
1:B:167:TYR:CG	1:B:168:PRO:HA	2.36	0.60
1:C:36:GLU:HB2	1:C:207:ILE:CD1	2.30	0.60
1:D:41:THR:CG2	1:D:184:ARG:HH21	2.09	0.60
1:G:97:GLY:HA3	1:G:149:THR:HG23	1.82	0.60
1:C:193:CYS:HB2	1:C:198:ILE:HD13	1.84	0.60
1:D:12:HIS:HD2	1:D:13:GLY:H	1.49	0.60
1:G:46:ILE:O	1:G:47:LEU:C	2.39	0.60
1:D:97:GLY:HA3	1:D:149:THR:CG2	2.31	0.60
1:C:77:LEU:N	1:C:77:LEU:HD12	2.17	0.60
1:A:78:ASN:OD1	1:A:78:ASN:O	2.19	0.60
1:C:119:MET:CG	1:E:221:ILE:HD12	2.22	0.60
1:G:160:MET:HA	1:G:176:HIS:CD2	2.37	0.60
1:B:130:ALA:O	1:B:134:ARG:HG2	2.02	0.60
1:E:60:THR:CG2	1:E:152:ASN:HB2	2.32	0.60
1:E:67:VAL:HG21	1:E:150:ILE:HD11	1.84	0.60
1:B:76:TYR:CD1	1:B:197:LEU:HD22	2.37	0.59
1:C:38:VAL:HG12	1:C:211:LYS:HG3	1.83	0.59
1:E:30:PRO:CA	1:F:26:LYS:HE2	2.09	0.59
1:E:67:VAL:N	1:E:68:PRO:HD2	2.16	0.59
1:G:26:LYS:HG3	1:G:164:ILE:HD13	1.84	0.59
1:C:66:ILE:C	1:C:68:PRO:HD2	2.22	0.59
1:E:173:LEU:HD21	1:E:189:LEU:HD13	1.84	0.59
1:G:81:TYR:HD2	1:G:81:TYR:C	2.05	0.59
1:B:93:TYR:HD2	1:B:95:ASN:OD1	1.84	0.59
1:C:39:ASP:C	1:C:41:THR:N	2.53	0.59
1:C:221:ILE:HG22	1:E:119:MET:CG	2.25	0.59
1:F:102:THR:HG21	1:F:107:ASN:HD22	1.67	0.59
1:D:130:ALA:C	1:D:132:ARG:H	2.04	0.59
1:C:32:PHE:HD1	1:C:195:HIS:CD2	2.20	0.59
1:G:112:LYS:O	1:G:113:ASP:O	2.20	0.59
1:C:11:MET:HG2	1:C:16:ARG:HG3	1.85	0.59
1:C:79:ALA:HB2	1:C:90:LEU:HA	1.85	0.59
1:G:159:ILE:CD1	1:G:188:TYR:CD2	2.86	0.59
1:D:170:VAL:O	1:D:193:CYS:HA	2.03	0.59
1:E:40:VAL:HB	1:E:43:MET:HE1	1.84	0.59
1:E:67:VAL:HG23	1:E:68:PRO:HD2	1.85	0.58
1:F:12:HIS:CE1	1:F:15:ARG:HG3	2.38	0.58
1:G:130:ALA:O	1:G:133:ALA:N	2.36	0.58
1:F:12:HIS:CD2	1:F:13:GLY:H	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:MET:HA	1:F:176:HIS:CE1	2.38	0.58
1:F:220:ILE:C	1:F:222:TYR:H	2.05	0.58
1:B:56:LYS:CB	1:B:57:VAL:HG12	2.34	0.58
1:C:173:LEU:HD21	1:C:189:LEU:HD22	1.85	0.58
1:E:40:VAL:HG11	1:E:187:MET:HB3	1.85	0.58
1:F:80:ILE:HB	1:F:89:ILE:HB	1.84	0.58
1:F:213:VAL:C	1:F:215:GLU:H	2.06	0.58
1:E:14:LEU:HD13	1:E:104:ASP:HB3	1.85	0.58
1:A:26:LYS:HD3	1:A:164:ILE:CD1	2.33	0.58
1:F:139:GLN:HB2	1:F:142:GLU:HG2	1.85	0.58
1:G:18:ILE:HD11	1:G:106:LEU:HD23	1.85	0.58
1:A:162:THR:CG2	1:C:33:THR:HB	2.33	0.58
1:A:93:TYR:O	1:A:93:TYR:CD2	2.56	0.58
1:A:208:VAL:O	1:A:211:LYS:HB3	2.04	0.58
1:D:126:ILE:HG13	1:D:127:SER:N	2.19	0.58
1:F:154:GLY:HA3	1:F:176:HIS:O	2.04	0.58
1:C:43:MET:O	1:C:46:ILE:N	2.32	0.58
1:E:62:PHE:HD2	1:E:119:MET:CE	2.17	0.58
1:A:36:GLU:HA	1:B:159:ILE:CD1	2.32	0.58
1:A:98:ILE:CD1	1:A:126:ILE:CG2	2.82	0.58
1:G:35:MET:HB3	1:G:190:SER:HB3	1.85	0.57
1:A:80:ILE:HD12	1:A:81:TYR:N	2.19	0.57
1:E:91:LYS:HE3	1:E:93:TYR:HE1	1.69	0.57
1:B:29:MET:CE	1:B:81:TYR:HB2	2.35	0.57
1:D:141:ASP:HB3	1:D:142:GLU:HG3	1.85	0.57
1:F:159:ILE:HD12	1:F:160:MET:CG	2.33	0.57
1:G:81:TYR:C	1:G:81:TYR:CD2	2.78	0.57
1:E:95:ASN:HD22	1:E:113:ASP:N	2.01	0.57
1:B:11:MET:HE2	1:B:19:PHE:HD1	1.66	0.57
1:G:45:SER:HA	1:G:48:ASP:HB2	1.87	0.57
1:B:56:LYS:HB2	1:B:57:VAL:HG12	1.87	0.57
1:E:163:PRO:HG2	1:E:192:SER:HB2	1.86	0.57
1:F:95:ASN:ND2	1:F:145:ASP:OD1	2.38	0.57
1:C:86:ARG:CG	1:C:86:ARG:O	2.51	0.57
1:G:219:ALA:HA	1:G:222:TYR:CE2	2.40	0.56
1:B:41:THR:O	1:B:44:VAL:HG12	2.04	0.56
1:D:67:VAL:CG2	1:D:96:ILE:HD13	2.35	0.56
1:E:78:ASN:ND2	1:E:91:LYS:HB3	2.20	0.56
1:E:198:ILE:HG22	1:E:203:ALA:HB2	1.87	0.56
1:C:84:THR:O	1:C:84:THR:OG1	2.20	0.56
1:D:58:THR:HG22	1:D:123:SER:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASN:O	1:E:79:ALA:HB2	2.06	0.56
1:F:159:ILE:HD12	1:F:160:MET:HG2	1.87	0.56
1:G:97:GLY:CA	1:G:149:THR:HA	2.35	0.56
1:A:76:TYR:CD1	1:A:197:LEU:HD13	2.40	0.56
1:B:95:ASN:OD1	1:B:95:ASN:N	2.39	0.56
1:E:64:ALA:HA	1:E:67:VAL:CG2	2.35	0.56
1:G:216:ASP:CG	1:G:219:ALA:HB3	2.26	0.56
1:B:33:THR:CB	1:B:192:SER:OG	2.47	0.56
1:B:118:SER:O	1:B:119:MET:C	2.44	0.56
1:C:82:ASP:CB	1:C:87:VAL:CG2	2.80	0.56
1:C:221:ILE:CG1	1:E:220:ILE:HG21	2.35	0.56
1:A:213:VAL:O	1:A:215:GLU:N	2.39	0.56
1:D:12:HIS:CD2	1:D:14:LEU:H	2.24	0.56
1:F:182:GLU:O	1:F:184:ARG:N	2.37	0.56
1:G:32:PHE:O	1:G:192:SER:HA	2.06	0.56
1:A:213:VAL:C	1:A:215:GLU:H	2.10	0.55
1:G:217:PRO:O	1:G:219:ALA:N	2.40	0.55
1:A:37:GLU:N	1:B:159:ILE:CD1	2.69	0.55
1:A:56:LYS:O	1:A:57:VAL:HG22	2.07	0.55
1:A:99:ALA:HA	1:A:107:ASN:O	2.06	0.55
1:F:149:THR:HB	1:F:172:ILE:CD1	2.35	0.55
1:A:34:VAL:HG11	1:A:204:THR:HG23	1.87	0.55
1:A:213:VAL:C	1:A:215:GLU:N	2.59	0.55
1:F:112:LYS:O	1:F:113:ASP:C	2.45	0.55
1:F:216:ASP:HB2	1:F:217:PRO:CD	2.34	0.55
1:G:151:THR:HG23	1:G:151:THR:O	2.06	0.55
1:A:95:ASN:HB3	1:A:113:ASP:HA	1.87	0.55
1:B:93:TYR:CD1	1:C:4:GLY:HA3	2.42	0.55
1:D:160:MET:O	1:D:176:HIS:CE1	2.59	0.55
1:D:196:ARG:HG2	1:E:19:PHE:HB2	1.89	0.55
1:G:114:ALA:O	1:G:116:ARG:N	2.40	0.55
1:D:67:VAL:CG2	1:D:68:PRO:CD	2.83	0.55
1:E:88:TYR:O	1:E:89:ILE:HB	2.07	0.55
1:G:77:LEU:HD12	1:G:206:PHE:CD1	2.42	0.55
1:E:40:VAL:HB	1:E:43:MET:CE	2.36	0.55
1:F:148:PHE:HE2	1:F:150:ILE:HG13	1.71	0.55
1:G:33:THR:HA	1:G:191:LEU:O	2.07	0.55
1:G:118:SER:HB2	1:G:121:GLU:HB2	1.89	0.55
1:A:8:ILE:HG23	1:C:89:ILE:H	1.72	0.55
1:B:170:VAL:HG21	1:B:197:LEU:HD12	1.88	0.55
1:C:98:ILE:HD11	1:C:111:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ILE:C	1:G:222:TYR:H	2.11	0.55
1:A:162:THR:O	1:A:162:THR:CG2	2.55	0.54
1:E:36:GLU:OE2	1:F:159:ILE:HG23	2.07	0.54
1:G:29:MET:HE1	1:G:170:VAL:HA	1.89	0.54
1:A:33:THR:H	1:B:162:THR:CG2	2.15	0.54
1:A:67:VAL:HG23	1:A:68:PRO:HD3	1.89	0.54
1:A:95:ASN:HB3	1:A:113:ASP:N	2.22	0.54
1:B:143:VAL:HG12	1:B:143:VAL:O	2.08	0.54
1:D:97:GLY:HA2	1:D:110:VAL:HG22	1.89	0.54
1:A:159:ILE:CD1	1:C:188:TYR:HE1	2.20	0.54
1:C:12:HIS:HB3	1:C:15:ARG:HB2	1.89	0.54
1:C:24:LYS:HE3	1:C:167:TYR:HE2	1.73	0.54
1:D:98:ILE:CD1	1:D:126:ILE:HG22	2.38	0.54
1:G:172:ILE:HG22	1:G:192:SER:HB2	1.89	0.54
1:A:38:VAL:HG13	1:A:211:LYS:HG2	1.90	0.54
1:D:106:LEU:HG	1:D:106:LEU:O	2.01	0.54
1:D:160:MET:HB3	1:F:35:MET:HE1	1.88	0.54
1:E:54:ASN:O	1:E:55:ARG:HG2	2.07	0.54
1:F:46:ILE:HG13	1:F:47:LEU:N	2.22	0.54
1:F:79:ALA:HB2	1:F:90:LEU:HA	1.89	0.54
1:A:15:ARG:HD3	1:A:18:ILE:HD11	1.89	0.54
1:B:38:VAL:HG13	1:B:40:VAL:HG13	1.89	0.54
1:D:33:THR:HB	1:E:162:THR:CG2	2.38	0.53
1:B:204:THR:O	1:B:208:VAL:HG23	2.08	0.53
1:D:46:ILE:HD12	1:D:47:LEU:N	2.23	0.53
1:D:78:ASN:HD21	1:D:147:THR:HB	1.72	0.53
1:G:181:ARG:C	1:G:183:GLY:HA2	2.28	0.53
1:A:78:ASN:ND2	1:A:147:THR:CB	2.71	0.53
1:B:29:MET:HE1	1:B:81:TYR:HB2	1.90	0.53
1:C:41:THR:HB	1:C:184:ARG:NH1	2.23	0.53
1:E:111:ILE:HG21	1:E:122:ILE:HG23	1.91	0.53
1:C:81:TYR:O	1:C:81:TYR:HD2	1.90	0.53
1:G:159:ILE:HD11	1:G:188:TYR:CG	2.43	0.53
1:A:152:ASN:OD1	1:A:155:THR:HG22	2.08	0.53
1:D:154:GLY:HA3	1:D:176:HIS:HA	1.91	0.53
1:C:84:THR:HG23	1:C:87:VAL:HG21	1.91	0.53
1:D:16:ARG:HH21	1:F:86:ARG:HH22	1.55	0.53
1:E:165:ILE:HA	1:E:172:ILE:HG12	1.91	0.53
1:G:211:LYS:HA	1:G:214:ILE:CD1	2.36	0.53
1:A:35:MET:HG3	1:A:190:SER:HB3	1.91	0.53
1:A:68:PRO:O	1:A:71:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASP:O	1:A:216:ASP:OD2	2.26	0.53
1:F:98:ILE:HD11	1:F:126:ILE:HG22	1.84	0.53
1:A:36:GLU:C	1:B:159:ILE:HD11	2.29	0.53
1:A:159:ILE:HG23	1:C:36:GLU:HA	1.90	0.53
1:G:10:GLU:O	1:G:11:MET:HG3	2.08	0.53
1:E:154:GLY:HA3	1:E:176:HIS:C	2.29	0.52
1:F:191:LEU:HG	1:F:192:SER:N	2.23	0.52
1:G:65:ARG:HD2	1:G:119:MET:H	1.73	0.52
1:G:81:TYR:HE1	1:G:196:ARG:NH1	2.05	0.52
1:G:81:TYR:O	1:G:82:ASP:O	2.26	0.52
1:A:86:ARG:HA	1:A:86:ARG:NH1	2.16	0.52
1:A:109:PHE:CD2	1:A:129:LYS:HB3	2.43	0.52
1:A:158:GLY:O	1:A:177:ARG:HB3	2.10	0.52
1:C:63:LEU:HA	1:C:66:ILE:HD12	1.91	0.52
1:F:94:TYR:HA	1:F:147:THR:HG21	1.92	0.52
1:B:28:ILE:O	1:B:30:PRO:HD3	2.09	0.52
1:E:79:ALA:HB1	1:E:89:ILE:O	2.10	0.52
1:G:110:VAL:HG21	1:G:144:GLN:O	2.10	0.52
1:A:122:ILE:O	1:A:126:ILE:HG23	2.10	0.52
1:B:109:PHE:CE1	1:B:129:LYS:CB	2.93	0.52
1:D:24:LYS:HG2	1:D:28:ILE:HD12	1.90	0.52
1:F:216:ASP:CB	1:F:217:PRO:HD2	2.34	0.52
1:A:13:GLY:O	1:A:16:ARG:HB3	2.10	0.52
1:C:70:ILE:HD13	1:C:210:LEU:HA	1.91	0.52
1:C:119:MET:HB2	1:E:222:TYR:CD1	2.37	0.52
1:C:214:ILE:O	1:C:217:PRO:HD3	2.10	0.52
1:B:150:ILE:HG23	1:B:173:LEU:HB3	1.90	0.52
1:C:110:VAL:HG22	1:C:142:GLU:O	2.10	0.52
1:B:39:ASP:OD1	1:B:184:ARG:NH2	2.43	0.52
1:D:160:MET:HE1	1:F:160:MET:SD	2.50	0.52
1:E:60:THR:HG21	1:E:152:ASN:HB2	1.92	0.52
1:F:219:ALA:C	1:F:222:TYR:HB2	2.30	0.52
1:G:26:LYS:HG3	1:G:164:ILE:HD11	1.90	0.52
1:G:98:ILE:CG2	1:G:111:ILE:HG12	2.39	0.52
1:G:106:LEU:HG	1:G:107:ASN:N	2.25	0.52
1:A:222:TYR:CE1	1:G:50:ALA:HB2	2.44	0.52
1:B:218:ASN:O	1:B:221:ILE:HG12	2.09	0.52
1:E:77:LEU:HD21	1:E:191:LEU:HD21	1.92	0.52
1:F:93:TYR:HE1	1:F:95:ASN:HD21	1.57	0.52
1:B:41:THR:CG2	1:B:184:ARG:HB3	2.40	0.52
1:B:188:TYR:CE1	1:C:159:ILE:HD12	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HD12	1:B:210:LEU:HD13	1.92	0.51
1:C:56:LYS:HG3	1:C:57:VAL:H	1.75	0.51
1:C:127:SER:O	1:C:131:SER:HB3	2.10	0.51
1:E:74:TYR:CE2	1:E:206:PHE:HA	2.46	0.51
1:G:38:VAL:HG11	1:G:189:LEU:HD12	1.91	0.51
1:G:41:THR:CG2	1:G:185:LYS:H	2.20	0.51
1:B:194:ASP:OD2	1:B:196:ARG:HD3	2.09	0.51
1:C:32:PHE:HE2	1:C:34:VAL:HB	1.75	0.51
1:D:95:ASN:HB3	1:D:112:LYS:HA	1.92	0.51
1:A:66:ILE:C	1:A:68:PRO:HD2	2.31	0.51
1:A:80:ILE:HB	1:A:168:PRO:O	2.11	0.51
1:A:120:VAL:HG13	1:A:121:GLU:H	1.76	0.51
1:C:29:MET:SD	1:C:194:ASP:HB2	2.50	0.51
1:E:166:ASN:ND2	1:E:169:GLU:OE2	2.42	0.51
1:G:29:MET:CE	1:G:194:ASP:HB2	2.31	0.51
1:G:97:GLY:O	1:G:149:THR:HA	2.10	0.51
1:B:33:THR:HB	1:B:192:SER:CB	2.40	0.51
1:D:152:ASN:C	1:D:152:ASN:HD22	2.14	0.51
1:F:93:TYR:CD1	1:F:95:ASN:OD1	2.60	0.51
1:B:81:TYR:CZ	1:B:196:ARG:NH2	2.75	0.51
1:C:22:MET:O	1:C:23:THR:C	2.49	0.51
1:E:29:MET:HE1	1:E:170:VAL:HG23	1.93	0.51
1:F:59:VAL:HG23	1:F:60:THR:H	1.75	0.51
1:A:195:HIS:O	1:A:195:HIS:ND1	2.43	0.51
1:D:181:ARG:HG3	1:E:181:ARG:HH22	1.75	0.51
1:E:76:TYR:HD1	1:E:197:LEU:HD21	1.63	0.51
1:A:64:ALA:HA	1:A:67:VAL:HG21	1.90	0.51
1:A:132:ARG:NH2	1:A:142:GLU:OE1	2.44	0.51
1:E:135:GLU:O	1:E:137:LYS:N	2.43	0.51
1:A:56:LYS:HE3	1:A:56:LYS:HA	1.91	0.51
1:E:213:VAL:O	1:E:215:GLU:N	2.44	0.51
1:A:216:ASP:O	1:A:216:ASP:CG	2.50	0.51
1:B:162:THR:HG23	1:B:162:THR:O	2.11	0.51
1:B:219:ALA:HB1	1:B:222:TYR:CE2	2.46	0.51
1:D:122:ILE:O	1:D:126:ILE:HG23	2.11	0.51
1:D:160:MET:O	1:D:176:HIS:NE2	2.44	0.51
1:E:42:SER:O	1:E:46:ILE:HG23	2.11	0.51
1:G:34:VAL:HG13	1:G:34:VAL:O	2.09	0.51
1:E:65:ARG:HG3	1:E:119:MET:HA	1.93	0.50
1:E:79:ALA:HB2	1:E:90:LEU:HA	1.93	0.50
1:A:219:ALA:O	1:A:220:ILE:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:O	1:A:132:ARG:N	2.44	0.50
1:C:56:LYS:HE2	1:C:124:ALA:HA	1.93	0.50
1:G:56:LYS:HD3	1:G:56:LYS:N	2.27	0.50
1:F:51:LYS:C	1:F:53:ARG:H	2.14	0.50
1:C:37:GLU:HB3	1:C:188:TYR:CE1	2.47	0.50
1:C:62:PHE:HD1	1:C:119:MET:CE	2.25	0.50
1:D:97:GLY:CA	1:D:149:THR:HG22	2.41	0.50
1:G:56:LYS:HB3	1:G:57:VAL:HA	1.93	0.50
1:D:158:GLY:O	1:D:176:HIS:HB3	2.11	0.50
1:C:43:MET:O	1:C:45:SER:N	2.45	0.50
1:C:109:PHE:CE1	1:C:129:LYS:HB2	2.47	0.50
1:F:194:ASP:O	1:F:198:ILE:HB	2.12	0.50
1:E:198:ILE:CG2	1:E:203:ALA:HB2	2.42	0.50
1:F:37:GLU:O	1:F:211:LYS:HE2	2.12	0.50
1:F:204:THR:O	1:F:207:ILE:HG13	2.11	0.50
1:D:12:HIS:CD2	1:D:13:GLY:H	2.29	0.50
1:G:166:ASN:H	1:G:172:ILE:HD12	1.75	0.50
1:A:98:ILE:HD11	1:A:109:PHE:HE1	1.77	0.49
1:C:41:THR:HG23	1:C:185:LYS:H	1.77	0.49
1:D:36:GLU:HB2	1:D:207:ILE:HD12	1.94	0.49
1:D:70:ILE:CD1	1:D:210:LEU:HA	2.42	0.49
1:E:62:PHE:HD2	1:E:119:MET:SD	2.35	0.49
1:G:154:GLY:HA3	1:G:177:ARG:N	2.27	0.49
1:A:173:LEU:HD11	1:A:210:LEU:CD2	2.42	0.49
1:E:191:LEU:HD23	1:E:203:ALA:HB1	1.93	0.49
1:G:31:HIS:CD2	1:G:165:ILE:HG13	2.47	0.49
1:G:108:VAL:HG11	1:G:149:THR:CG2	2.42	0.49
1:B:100:VAL:CG2	1:B:101:ASP:N	2.75	0.49
1:B:109:PHE:CE1	1:B:129:LYS:HB2	2.47	0.49
1:D:154:GLY:CA	1:D:176:HIS:HA	2.42	0.49
1:E:88:TYR:OH	1:E:197:LEU:HB2	2.13	0.49
1:F:40:VAL:HG11	1:F:187:MET:HB3	1.94	0.49
1:F:79:ALA:HA	1:F:89:ILE:O	2.12	0.49
1:F:172:ILE:O	1:F:191:LEU:HA	2.12	0.49
1:B:82:ASP:OD1	1:B:82:ASP:N	2.45	0.49
1:C:166:ASN:O	1:C:169:GLU:HB2	2.12	0.49
1:D:33:THR:HB	1:E:162:THR:HG23	1.95	0.49
1:E:106:LEU:HG	1:E:107:ASN:N	2.26	0.49
1:A:35:MET:O	1:B:159:ILE:HG12	2.11	0.49
1:E:35:MET:HE2	1:E:160:MET:SD	2.52	0.49
1:E:63:LEU:O	1:E:67:VAL:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:VAL:HG12	1:F:68:PRO:HD3	1.95	0.49
1:F:67:VAL:CG1	1:F:68:PRO:HD3	2.43	0.49
1:F:137:LYS:O	1:F:137:LYS:HG3	2.12	0.49
1:G:97:GLY:HA3	1:G:149:THR:HA	1.94	0.49
1:A:119:MET:HB2	1:G:221:ILE:O	2.12	0.49
1:B:110:VAL:HG11	1:B:146:SER:HA	1.95	0.49
1:F:173:LEU:HA	1:F:190:SER:O	2.13	0.49
1:A:89:ILE:HA	1:B:7:GLU:O	2.12	0.49
1:A:102:THR:HG21	1:A:107:ASN:HD22	1.77	0.49
1:B:109:PHE:CD1	1:B:129:LYS:HB3	2.48	0.49
1:F:91:LYS:HE3	1:F:93:TYR:CZ	2.48	0.49
1:A:84:THR:HB	1:A:87:VAL:CG2	2.42	0.49
1:C:217:PRO:O	1:C:220:ILE:N	2.39	0.49
1:A:71:LEU:HD13	1:A:78:ASN:CB	2.36	0.49
1:B:41:THR:HG22	1:B:185:LYS:N	2.25	0.49
1:C:149:THR:HG22	1:C:169:GLU:OE1	2.12	0.49
1:E:74:TYR:O	1:E:75:PRO:C	2.51	0.49
1:A:14:LEU:O	1:A:14:LEU:HD23	2.11	0.48
1:A:26:LYS:HD3	1:A:164:ILE:HD12	1.95	0.48
1:A:36:GLU:CA	1:B:159:ILE:HD11	2.42	0.48
1:A:163:PRO:HD2	1:A:192:SER:OG	2.13	0.48
1:B:70:ILE:HD13	1:B:210:LEU:HA	1.94	0.48
1:B:100:VAL:HG22	1:B:101:ASP:H	1.78	0.48
1:G:210:LEU:O	1:G:211:LYS:C	2.52	0.48
1:E:113:ASP:O	1:E:115:ASP:N	2.46	0.48
1:G:84:THR:HB	1:G:87:VAL:HG23	1.94	0.48
1:B:97:GLY:CA	1:B:149:THR:HG22	2.43	0.48
1:C:50:ALA:CB	1:E:222:TYR:OH	2.62	0.48
1:C:86:ARG:O	1:C:86:ARG:HG2	2.12	0.48
1:D:62:PHE:HD2	1:D:63:LEU:HD12	1.78	0.48
1:F:135:GLU:O	1:F:137:LYS:N	2.45	0.48
1:G:74:TYR:CE2	1:G:206:PHE:HA	2.48	0.48
1:G:84:THR:HB	1:G:87:VAL:HG21	1.94	0.48
1:A:160:MET:CE	1:B:160:MET:SD	3.02	0.48
1:F:201:ALA:O	1:F:204:THR:N	2.47	0.48
1:C:39:ASP:OD1	1:C:184:ARG:NH1	2.46	0.48
1:A:9:LEU:CB	1:C:88:TYR:CE1	2.97	0.48
1:F:31:HIS:CE1	1:F:165:ILE:HD12	2.49	0.48
1:F:213:VAL:C	1:F:215:GLU:N	2.67	0.48
1:A:44:VAL:HG21	1:A:185:LYS:HE2	1.94	0.48
1:C:83:GLU:C	1:C:85:ARG:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:HIS:HE1	1:E:190:SER:OG	1.97	0.48
1:A:217:PRO:O	1:A:220:ILE:HG23	2.14	0.48
1:C:77:LEU:CG	1:C:198:ILE:HD11	2.40	0.48
1:E:22:MET:SD	1:E:164:ILE:HG21	2.54	0.48
1:C:82:ASP:HB3	1:C:87:VAL:HB	1.96	0.48
1:A:201:ALA:O	1:A:202:VAL:C	2.52	0.47
1:B:13:GLY:O	1:B:17:ILE:HG12	2.14	0.47
1:E:213:VAL:C	1:E:215:GLU:N	2.65	0.47
1:F:8:ILE:HG12	1:F:8:ILE:O	2.13	0.47
1:F:36:GLU:HG3	1:F:37:GLU:N	2.28	0.47
1:F:213:VAL:O	1:F:215:GLU:N	2.47	0.47
1:F:219:ALA:O	1:F:222:TYR:CB	2.57	0.47
1:A:33:THR:OG1	1:A:192:SER:HB3	2.14	0.47
1:E:67:VAL:HG23	1:E:68:PRO:CD	2.43	0.47
1:E:74:TYR:HE2	1:E:206:PHE:HA	1.80	0.47
1:G:77:LEU:HD21	1:G:198:ILE:HG21	1.96	0.47
1:A:12:HIS:O	1:A:13:GLY:C	2.52	0.47
1:A:32:PHE:CE2	1:A:34:VAL:HG13	2.49	0.47
1:F:79:ALA:CB	1:F:90:LEU:HA	2.45	0.47
1:A:36:GLU:HA	1:B:159:ILE:HD11	1.96	0.47
1:B:86:ARG:HA	1:B:86:ARG:CZ	2.44	0.47
1:F:95:ASN:C	1:F:147:THR:HG22	2.35	0.47
1:G:97:GLY:O	1:G:150:ILE:N	2.46	0.47
1:A:28:ILE:HG22	1:A:29:MET:N	2.29	0.47
1:A:152:ASN:OD1	1:A:154:GLY:N	2.48	0.47
1:B:11:MET:HE2	1:B:19:PHE:CD1	2.46	0.47
1:C:56:LYS:O	1:C:57:VAL:HB	2.14	0.47
1:E:81:TYR:OH	1:E:196:ARG:CZ	2.62	0.47
1:F:36:GLU:HG3	1:F:37:GLU:H	1.77	0.47
1:G:11:MET:CE	1:G:19:PHE:HB2	2.44	0.47
1:A:37:GLU:H	1:B:159:ILE:CD1	2.28	0.47
1:B:56:LYS:CB	1:B:57:VAL:CA	2.79	0.47
1:B:98:ILE:O	1:B:98:ILE:HG13	2.14	0.47
1:E:28:ILE:HG22	1:E:196:ARG:HH22	1.79	0.47
1:E:64:ALA:HA	1:E:67:VAL:HG22	1.95	0.47
1:E:199:ASP:HB3	1:F:106:LEU:HD13	1.97	0.47
1:F:41:THR:HG23	1:F:185:LYS:H	1.79	0.47
1:F:203:ALA:O	1:F:206:PHE:HB3	2.15	0.47
1:B:97:GLY:HA3	1:B:149:THR:CG2	2.43	0.47
1:B:100:VAL:CG2	1:B:101:ASP:H	2.28	0.47
1:B:109:PHE:CE1	1:B:129:LYS:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLU:HB2	1:D:184:ARG:H	1.79	0.47
1:F:153:VAL:O	1:F:156:ILE:HD12	2.14	0.47
1:F:49:SER:C	1:F:51:LYS:H	2.18	0.47
1:B:165:ILE:HA	1:B:172:ILE:HB	1.97	0.47
1:E:32:PHE:O	1:E:192:SER:HA	2.15	0.47
1:D:80:ILE:HG13	1:D:89:ILE:HB	1.97	0.47
1:B:30:PRO:CA	1:C:26:LYS:HD3	2.22	0.46
1:B:98:ILE:HG22	1:B:150:ILE:HG13	1.96	0.46
1:A:133:ALA:HA	1:A:138:LEU:HD11	1.97	0.46
1:C:81:TYR:HD1	1:C:197:LEU:CD1	2.27	0.46
1:E:81:TYR:CD1	1:E:88:TYR:HE1	2.30	0.46
1:G:206:PHE:O	1:G:207:ILE:C	2.52	0.46
1:C:119:MET:CG	1:E:221:ILE:O	2.62	0.46
1:C:159:ILE:HG22	1:C:160:MET:HG2	1.97	0.46
1:C:194:ASP:OD2	1:C:196:ARG:NH2	2.30	0.46
1:D:130:ALA:C	1:D:132:ARG:N	2.69	0.46
1:E:19:PHE:HA	1:E:22:MET:HB2	1.97	0.46
1:E:62:PHE:CD2	1:E:119:MET:HE1	2.50	0.46
1:A:26:LYS:CD	1:A:164:ILE:CD1	2.93	0.46
1:B:66:ILE:H	1:B:66:ILE:HG12	1.58	0.46
1:G:80:ILE:HA	1:G:168:PRO:O	2.15	0.46
1:B:64:ALA:O	1:B:68:PRO:HD2	2.15	0.46
1:F:17:ILE:O	1:F:21:LYS:HB2	2.16	0.46
1:A:46:ILE:HD11	1:G:221:ILE:CD1	2.44	0.46
1:A:174:GLY:N	1:A:190:SER:O	2.43	0.46
1:A:221:ILE:HG23	1:G:220:ILE:HG12	1.98	0.46
1:B:104:ASP:OD2	1:B:136:ASN:ND2	2.48	0.46
1:D:37:GLU:H	1:E:159:ILE:HD11	1.81	0.46
1:F:166:ASN:O	1:F:169:GLU:HB2	2.16	0.46
1:G:80:ILE:HD12	1:G:81:TYR:N	2.31	0.46
1:C:95:ASN:O	1:C:146:SER:HA	2.15	0.46
1:D:54:ASN:C	1:D:55:ARG:HG2	2.35	0.46
1:A:221:ILE:HD13	1:G:220:ILE:HG12	1.94	0.46
1:A:33:THR:HA	1:A:191:LEU:O	2.16	0.46
1:C:12:HIS:CG	1:C:13:GLY:N	2.84	0.46
1:C:55:ARG:CZ	1:C:55:ARG:H	2.28	0.46
1:C:110:VAL:CG1	1:C:146:SER:HB3	2.45	0.46
1:D:61:GLY:O	1:D:62:PHE:C	2.54	0.46
1:F:166:ASN:HB3	1:F:169:GLU:CD	2.37	0.46
1:G:56:LYS:CB	1:G:57:VAL:HA	2.46	0.46
1:G:154:GLY:HA3	1:G:177:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG23	1:A:187:MET:O	2.14	0.46
1:A:65:ARG:HD3	1:A:65:ARG:C	2.31	0.46
1:C:77:LEU:HG	1:C:198:ILE:CD1	2.38	0.46
1:D:81:TYR:HD1	1:D:88:TYR:CE1	2.34	0.46
1:F:74:TYR:CE2	1:F:206:PHE:HA	2.51	0.46
1:F:75:PRO:HD2	1:F:76:TYR:CD2	2.51	0.46
1:A:67:VAL:N	1:A:68:PRO:HD2	2.31	0.45
1:A:210:LEU:O	1:A:213:VAL:HG23	2.16	0.45
1:B:89:ILE:HA	1:C:8:ILE:HA	1.98	0.45
1:D:46:ILE:H	1:D:46:ILE:HG13	1.64	0.45
1:D:58:THR:HG21	1:D:126:ILE:HD11	1.98	0.45
1:E:173:LEU:HD11	1:E:210:LEU:HD22	1.98	0.45
1:F:173:LEU:HD23	1:F:174:GLY:N	2.31	0.45
1:G:20:ASP:O	1:G:21:LYS:C	2.53	0.45
1:A:36:GLU:OE1	1:B:159:ILE:HD13	2.16	0.45
1:A:64:ALA:HA	1:A:67:VAL:HG22	1.96	0.45
1:A:106:LEU:HG	1:A:107:ASN:H	1.82	0.45
1:B:23:THR:O	1:B:27:GLN:HB2	2.16	0.45
1:B:77:LEU:N	1:B:77:LEU:HD12	2.31	0.45
1:C:38:VAL:C	1:C:40:VAL:H	2.18	0.45
1:G:26:LYS:CG	1:G:164:ILE:HD13	2.45	0.45
1:G:176:HIS:NE2	1:G:190:SER:OG	2.45	0.45
1:A:159:ILE:HG13	1:A:160:MET:HB2	1.97	0.45
1:B:36:GLU:HB2	1:B:207:ILE:HD12	1.99	0.45
1:C:182:GLU:HA	1:C:183:GLY:HA2	1.73	0.45
1:E:95:ASN:CB	1:E:112:LYS:HA	2.46	0.45
1:F:58:THR:O	1:F:61:GLY:N	2.49	0.45
1:G:111:ILE:HG22	1:G:114:ALA:HB2	1.98	0.45
1:A:181:ARG:HH12	1:B:181:ARG:HD3	1.81	0.45
1:E:63:LEU:O	1:E:66:ILE:HG13	2.16	0.45
1:E:100:VAL:HG12	1:E:101:ASP:N	2.24	0.45
1:B:85:ARG:HB3	1:B:86:ARG:H	1.59	0.45
1:C:102:THR:O	1:C:105:GLY:N	2.50	0.45
1:E:56:LYS:O	1:E:57:VAL:HB	2.16	0.45
1:F:78:ASN:CG	1:F:147:THR:HG1	2.20	0.45
1:F:97:GLY:O	1:F:149:THR:HA	2.17	0.45
1:F:217:PRO:HB2	1:F:218:ASN:H	1.59	0.45
1:G:214:ILE:H	1:G:214:ILE:HG13	1.46	0.45
1:E:162:THR:O	1:E:162:THR:OG1	2.35	0.45
1:F:220:ILE:C	1:F:222:TYR:N	2.69	0.45
1:D:218:ASN:O	1:D:221:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:PRO:O	1:E:69:SER:C	2.54	0.45
1:E:74:TYR:CD2	1:E:206:PHE:HD1	2.22	0.45
1:A:9:LEU:C	1:C:88:TYR:CD2	2.90	0.45
1:B:56:LYS:CB	1:B:57:VAL:CG1	2.95	0.45
1:B:140:LEU:HD23	1:B:140:LEU:H	1.81	0.45
1:C:50:ALA:HB2	1:E:222:TYR:OH	2.17	0.45
1:E:125:GLU:HG2	1:E:129:LYS:HE2	1.98	0.45
1:F:38:VAL:HG11	1:F:214:ILE:HB	1.97	0.45
1:A:40:VAL:C	1:A:43:MET:HB3	2.36	0.45
1:B:199:ASP:HB3	1:C:106:LEU:HB2	1.99	0.45
1:F:26:LYS:HB3	1:F:26:LYS:HE3	1.67	0.45
1:F:111:ILE:HD13	1:F:111:ILE:HA	1.86	0.45
1:G:206:PHE:O	1:G:208:VAL:N	2.50	0.45
1:A:87:VAL:HA	1:B:10:GLU:HA	1.98	0.45
1:A:98:ILE:CG1	1:A:109:PHE:CE1	2.98	0.45
1:A:149:THR:O	1:A:172:ILE:HG13	2.17	0.45
1:B:174:GLY:N	1:B:190:SER:O	2.41	0.45
1:C:221:ILE:HG13	1:E:220:ILE:CG2	2.47	0.45
1:F:38:VAL:HG22	1:F:211:LYS:HG3	1.98	0.45
1:F:139:GLN:HB2	1:F:142:GLU:CG	2.47	0.45
1:C:82:ASP:CB	1:C:87:VAL:HB	2.48	0.44
1:C:181:ARG:HH11	1:C:181:ARG:HG2	1.82	0.44
1:E:165:ILE:HG12	1:E:165:ILE:H	1.59	0.44
1:E:213:VAL:C	1:E:215:GLU:H	2.21	0.44
1:E:216:ASP:OD1	1:E:218:ASN:HB2	2.17	0.44
1:F:194:ASP:OD1	1:F:196:ARG:N	2.50	0.44
1:G:80:ILE:CG1	1:G:89:ILE:HD12	2.48	0.44
1:G:210:LEU:O	1:G:213:VAL:N	2.51	0.44
1:B:30:PRO:HD2	1:B:196:ARG:HD2	1.99	0.44
1:C:143:VAL:HG12	1:C:143:VAL:O	2.16	0.44
1:F:201:ALA:O	1:F:202:VAL:C	2.54	0.44
1:A:130:ALA:C	1:A:132:ARG:N	2.70	0.44
1:B:14:LEU:O	1:B:17:ILE:N	2.50	0.44
1:A:9:LEU:C	1:C:88:TYR:CE2	2.91	0.44
1:F:165:ILE:HA	1:F:172:ILE:HG12	1.95	0.44
1:A:195:HIS:CG	1:B:164:ILE:HD11	2.52	0.44
1:E:62:PHE:CD2	1:E:119:MET:HE3	2.53	0.44
1:F:51:LYS:O	1:F:53:ARG:N	2.50	0.44
1:F:83:GLU:HB2	1:F:84:THR:H	1.51	0.44
1:B:56:LYS:HB3	1:B:57:VAL:HG12	1.98	0.44
1:D:122:ILE:HD12	1:D:123:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:MET:HB3	1:F:35:MET:CE	2.47	0.44
1:A:81:TYR:HD2	1:A:82:ASP:H	1.65	0.44
1:C:175:VAL:CG1	1:C:176:HIS:N	2.81	0.44
1:C:220:ILE:HG23	1:C:220:ILE:O	2.18	0.44
1:E:62:PHE:CE2	1:E:119:MET:HE3	2.52	0.44
1:E:126:ILE:O	1:E:127:SER:C	2.56	0.44
1:E:54:ASN:HD22	1:E:54:ASN:HA	1.66	0.44
1:E:182:GLU:HB3	1:E:184:ARG:H	1.83	0.44
1:A:36:GLU:HA	1:B:159:ILE:HD13	2.00	0.44
1:D:123:SER:HA	1:D:126:ILE:HG12	2.00	0.44
1:E:159:ILE:O	1:E:188:TYR:HB2	2.18	0.44
1:F:47:LEU:CD2	1:F:57:VAL:HG12	2.48	0.44
1:G:80:ILE:O	1:G:88:TYR:HB3	2.17	0.44
1:A:95:ASN:HB3	1:A:113:ASP:CA	2.48	0.43
1:D:50:ALA:HB1	1:D:57:VAL:HG21	2.00	0.43
1:D:78:ASN:ND2	1:D:147:THR:HB	2.33	0.43
1:D:211:LYS:HE2	1:E:177:ARG:HH12	1.82	0.43
1:E:149:THR:OG1	1:E:169:GLU:OE1	2.32	0.43
1:G:211:LYS:O	1:G:212:LYS:C	2.57	0.43
1:A:29:MET:HG3	1:A:167:TYR:HE1	1.83	0.43
1:A:120:VAL:HG13	1:A:121:GLU:N	2.32	0.43
1:D:122:ILE:H	1:D:122:ILE:HG13	1.62	0.43
1:F:29:MET:HE3	1:F:167:TYR:HD1	1.82	0.43
1:G:130:ALA:C	1:G:132:ARG:H	2.21	0.43
1:G:210:LEU:O	1:G:214:ILE:HG13	2.18	0.43
1:B:88:TYR:O	1:B:88:TYR:HD1	2.01	0.43
1:C:47:LEU:HD23	1:C:57:VAL:HG12	1.99	0.43
1:G:91:LYS:HD2	1:G:93:TYR:CE1	2.53	0.43
1:E:38:VAL:HG11	1:E:214:ILE:HB	2.00	0.43
1:E:210:LEU:O	1:E:211:LYS:C	2.56	0.43
1:F:111:ILE:HG22	1:F:111:ILE:O	2.18	0.43
1:G:201:ALA:O	1:G:202:VAL:C	2.56	0.43
1:A:68:PRO:HG2	1:A:69:SER:H	1.83	0.43
1:B:11:MET:HE2	1:B:19:PHE:HB2	2.00	0.43
1:C:217:PRO:O	1:C:220:ILE:HG22	2.19	0.43
1:D:98:ILE:HD13	1:D:126:ILE:HG22	2.01	0.43
1:E:33:THR:HG23	1:E:191:LEU:O	2.18	0.43
1:A:70:ILE:HB	1:A:206:PHE:CE1	2.53	0.43
1:B:12:HIS:HD2	1:B:14:LEU:N	2.16	0.43
1:B:187:MET:O	1:B:187:MET:HG3	2.19	0.43
1:C:13:GLY:O	1:C:17:ILE:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ILE:O	1:C:188:TYR:HB2	2.17	0.43
1:D:58:THR:HG23	1:D:61:GLY:HA3	2.00	0.43
1:G:16:ARG:HD2	1:G:16:ARG:HA	1.82	0.43
1:G:35:MET:HB3	1:G:190:SER:HA	2.00	0.43
1:A:159:ILE:HD11	1:C:188:TYR:HE1	1.83	0.43
1:B:54:ASN:O	1:B:55:ARG:HB2	2.19	0.43
1:A:33:THR:N	1:B:162:THR:CG2	2.80	0.43
1:B:221:ILE:HG12	1:B:221:ILE:H	1.68	0.43
1:C:178:ILE:H	1:C:178:ILE:HG13	1.49	0.43
1:D:22:MET:SD	1:D:164:ILE:HD13	2.59	0.43
1:D:31:HIS:CE1	1:D:164:ILE:HG22	2.54	0.43
1:D:78:ASN:O	1:D:91:LYS:HB2	2.19	0.43
1:E:36:GLU:HG3	1:E:37:GLU:N	2.34	0.43
1:E:188:TYR:CE1	1:F:159:ILE:CD1	2.93	0.43
1:F:33:THR:HA	1:F:191:LEU:O	2.19	0.43
1:F:109:PHE:CE1	1:F:129:LYS:HB2	2.53	0.43
1:G:130:ALA:C	1:G:132:ARG:N	2.71	0.43
1:B:86:ARG:O	1:B:87:VAL:HG22	2.19	0.43
1:E:71:LEU:O	1:E:72:LYS:C	2.56	0.43
1:G:65:ARG:HD2	1:G:119:MET:N	2.32	0.43
1:A:130:ALA:C	1:A:132:ARG:H	2.23	0.43
1:D:8:ILE:HD11	1:F:87:VAL:HG11	2.00	0.43
1:D:34:VAL:HG22	1:D:207:ILE:HD11	2.01	0.43
1:G:118:SER:O	1:G:120:VAL:N	2.51	0.43
1:A:88:TYR:CE1	1:A:197:LEU:HD23	2.54	0.42
1:C:81:TYR:CD1	1:C:82:ASP:OD1	2.72	0.42
1:C:102:THR:O	1:C:103:PRO:C	2.58	0.42
1:D:132:ARG:HD2	1:D:137:LYS:O	2.19	0.42
1:G:35:MET:C	1:G:35:MET:HE2	2.40	0.42
1:A:67:VAL:HG23	1:A:68:PRO:CD	2.49	0.42
1:A:88:TYR:OH	1:A:196:ARG:NH1	2.50	0.42
1:A:181:ARG:HD2	1:C:181:ARG:NH1	2.34	0.42
1:B:207:ILE:O	1:B:211:LYS:N	2.39	0.42
1:E:23:THR:O	1:E:27:GLN:HB2	2.19	0.42
1:E:33:THR:HA	1:E:191:LEU:O	2.19	0.42
1:F:36:GLU:CG	1:F:37:GLU:H	2.32	0.42
1:A:80:ILE:HA	1:A:168:PRO:O	2.19	0.42
1:A:159:ILE:HD13	1:C:188:TYR:HE1	1.83	0.42
1:B:78:ASN:ND2	1:B:147:THR:O	2.53	0.42
1:C:132:ARG:HH11	1:C:132:ARG:HB2	1.84	0.42
1:E:149:THR:CB	1:E:169:GLU:OE1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:ASN:CA	1:F:175:VAL:HG23	2.42	0.42
1:A:70:ILE:CD1	1:A:210:LEU:HA	2.49	0.42
1:A:158:GLY:HA2	1:C:36:GLU:HG2	2.00	0.42
1:B:46:ILE:HG22	1:B:47:LEU:N	2.33	0.42
1:D:28:ILE:HG22	1:D:29:MET:N	2.35	0.42
1:E:109:PHE:CD1	1:E:129:LYS:HD2	2.54	0.42
1:F:12:HIS:CG	1:F:13:GLY:H	2.37	0.42
1:F:77:LEU:HD12	1:F:77:LEU:N	2.34	0.42
1:G:74:TYR:HD2	1:G:206:PHE:HD1	1.67	0.42
1:A:100:VAL:CG2	1:A:109:PHE:CE2	3.01	0.42
1:B:12:HIS:HD2	1:B:14:LEU:H	1.66	0.42
1:B:65:ARG:HH11	1:B:65:ARG:HB3	1.84	0.42
1:C:181:ARG:HG2	1:C:181:ARG:NH1	2.35	0.42
1:C:218:ASN:HD22	1:C:218:ASN:HA	1.65	0.42
1:E:61:GLY:O	1:E:62:PHE:C	2.55	0.42
1:G:61:GLY:O	1:G:64:ALA:HB3	2.20	0.42
1:B:83:GLU:HB2	1:B:84:THR:H	1.69	0.42
1:B:84:THR:O	1:B:87:VAL:CG2	2.68	0.42
1:C:76:TYR:CD1	1:C:197:LEU:O	2.68	0.42
1:C:209:ASP:O	1:C:213:VAL:HG23	2.20	0.42
1:D:203:ALA:O	1:D:206:PHE:N	2.46	0.42
1:G:49:SER:O	1:G:52:ALA:HB3	2.20	0.42
1:G:67:VAL:N	1:G:68:PRO:HD2	2.35	0.42
1:G:114:ALA:C	1:G:116:ARG:N	2.71	0.42
1:A:67:VAL:O	1:A:71:LEU:HG	2.20	0.42
1:A:95:ASN:CB	1:A:113:ASP:N	2.82	0.42
1:A:119:MET:CE	1:G:221:ILE:CG2	2.98	0.42
1:C:71:LEU:HD21	1:C:148:PHE:CE1	2.55	0.42
1:C:150:ILE:H	1:C:150:ILE:HG12	1.73	0.42
1:D:151:THR:O	1:D:151:THR:CG2	2.66	0.42
1:F:150:ILE:HG12	1:F:173:LEU:HB3	2.02	0.42
1:A:32:PHE:CZ	1:A:34:VAL:HG13	2.54	0.42
1:A:220:ILE:O	1:A:222:TYR:N	2.53	0.42
1:C:118:SER:O	1:C:122:ILE:HG23	2.20	0.42
1:D:182:GLU:N	1:D:183:GLY:CA	2.74	0.42
1:F:80:ILE:CG2	1:F:81:TYR:N	2.82	0.42
1:F:160:MET:HE2	1:F:160:MET:HB3	1.28	0.42
1:G:11:MET:HE2	1:G:19:PHE:HB2	2.01	0.42
1:G:217:PRO:O	1:G:218:ASN:C	2.58	0.42
1:A:34:VAL:HG12	1:B:161:SER:HB3	2.01	0.42
1:B:99:ALA:HB2	1:B:108:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ILE:HD12	1:B:127:SER:N	2.35	0.42
1:B:203:ALA:O	1:B:206:PHE:HB3	2.19	0.42
1:B:213:VAL:CG1	1:B:220:ILE:HG22	2.50	0.42
1:E:210:LEU:HG	1:E:214:ILE:HD11	2.02	0.42
1:F:160:MET:CA	1:F:176:HIS:CE1	3.02	0.42
1:A:221:ILE:H	1:A:221:ILE:HG12	1.62	0.42
1:C:41:THR:CB	1:C:184:ARG:NH1	2.82	0.42
1:E:56:LYS:HB2	1:E:120:VAL:HG23	2.02	0.42
1:E:79:ALA:O	1:E:170:VAL:HB	2.20	0.42
1:F:170:VAL:O	1:F:193:CYS:HA	2.20	0.42
1:A:97:GLY:HA2	1:A:110:VAL:HA	2.01	0.41
1:A:106:LEU:HG	1:A:107:ASN:N	2.34	0.41
1:B:12:HIS:CE1	1:B:15:ARG:HB2	2.55	0.41
1:E:79:ALA:CB	1:E:89:ILE:O	2.68	0.41
1:E:81:TYR:OH	1:E:196:ARG:NE	2.52	0.41
1:G:29:MET:CE	1:G:170:VAL:HA	2.50	0.41
1:C:70:ILE:CG2	1:C:206:PHE:CE1	3.00	0.41
1:D:34:VAL:HG21	1:D:204:THR:HG23	2.02	0.41
1:E:167:TYR:HA	1:E:168:PRO:HA	1.78	0.41
1:F:47:LEU:HD21	1:F:57:VAL:HG12	2.02	0.41
1:F:173:LEU:HD11	1:F:210:LEU:HD21	2.02	0.41
1:G:77:LEU:CD1	1:G:206:PHE:CD1	3.03	0.41
1:A:43:MET:O	1:A:44:VAL:C	2.59	0.41
1:C:46:ILE:HG23	1:C:47:LEU:N	2.34	0.41
1:C:178:ILE:HA	1:C:187:MET:HB2	2.03	0.41
1:E:38:VAL:CG1	1:E:215:GLU:HG3	2.50	0.41
1:G:145:ASP:O	1:G:145:ASP:CG	2.59	0.41
1:A:26:LYS:CD	1:A:164:ILE:HD12	2.50	0.41
1:A:159:ILE:HD11	1:C:188:TYR:CE1	2.55	0.41
1:B:43:MET:O	1:B:46:ILE:HB	2.20	0.41
1:B:77:LEU:HG	1:B:198:ILE:HD12	2.02	0.41
1:D:30:PRO:HB3	1:E:26:LYS:HB3	2.02	0.41
1:G:33:THR:O	1:G:35:MET:HG3	2.20	0.41
1:A:65:ARG:HG3	1:A:119:MET:HG3	2.02	0.41
1:B:161:SER:OG	1:B:176:HIS:HE1	2.04	0.41
1:E:204:THR:C	1:E:206:PHE:N	2.74	0.41
1:F:31:HIS:CD2	1:F:165:ILE:HG13	2.56	0.41
1:G:29:MET:HG2	1:G:194:ASP:OD2	2.20	0.41
1:C:46:ILE:CG2	1:C:47:LEU:N	2.83	0.41
1:C:55:ARG:HA	1:C:56:LYS:HA	1.78	0.41
1:E:43:MET:O	1:E:46:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ILE:HG22	1:E:188:TYR:HD2	1.86	0.41
1:A:153:VAL:CG1	1:C:204:THR:HG21	2.25	0.41
1:C:162:THR:O	1:C:162:THR:HG23	2.20	0.41
1:D:67:VAL:N	1:D:68:PRO:HD2	2.36	0.41
1:E:176:HIS:HB3	1:E:177:ARG:H	1.66	0.41
1:G:91:LYS:O	1:G:92:LYS:HE2	2.20	0.41
1:A:111:ILE:HD12	1:A:111:ILE:C	2.37	0.41
1:A:204:THR:HA	1:A:207:ILE:HG22	2.03	0.41
1:B:64:ALA:O	1:B:68:PRO:CD	2.69	0.41
1:B:78:ASN:HD21	1:B:147:THR:CB	2.22	0.41
1:C:172:ILE:HG22	1:C:192:SER:HB2	2.02	0.41
1:A:18:ILE:HG13	1:A:19:PHE:N	2.36	0.41
1:A:62:PHE:CD1	1:A:62:PHE:C	2.94	0.41
1:A:70:ILE:HD13	1:A:210:LEU:HA	2.03	0.41
1:A:86:ARG:HH21	1:B:16:ARG:NE	2.19	0.41
1:A:103:PRO:O	1:A:104:ASP:C	2.59	0.41
1:A:201:ALA:O	1:A:203:ALA:N	2.54	0.41
1:A:213:VAL:O	1:A:214:ILE:C	2.59	0.41
1:B:86:ARG:O	1:B:87:VAL:HG13	2.21	0.41
1:B:93:TYR:CD2	1:B:95:ASN:OD1	2.70	0.41
1:C:56:LYS:CE	1:C:124:ALA:HA	2.51	0.41
1:D:102:THR:HG21	1:D:107:ASN:ND2	2.36	0.41
1:G:63:LEU:HD23	1:G:63:LEU:HA	1.98	0.41
1:G:118:SER:C	1:G:120:VAL:N	2.75	0.41
1:C:21:LYS:O	1:C:25:ALA:HB2	2.20	0.41
1:C:62:PHE:CB	1:C:119:MET:HE1	2.51	0.41
1:C:202:VAL:CG1	1:C:203:ALA:N	2.83	0.41
1:D:33:THR:HG22	1:D:34:VAL:N	2.36	0.41
1:D:33:THR:HG22	1:D:34:VAL:H	1.87	0.41
1:D:49:SER:HA	1:D:52:ALA:HB3	2.03	0.41
1:E:167:TYR:CG	1:E:168:PRO:HA	2.56	0.41
1:F:214:ILE:H	1:F:214:ILE:HG13	1.75	0.41
1:A:112:LYS:O	1:A:113:ASP:C	2.60	0.40
1:A:162:THR:HG22	1:C:33:THR:CB	2.46	0.40
1:B:68:PRO:O	1:B:69:SER:C	2.59	0.40
1:C:38:VAL:O	1:C:186:TYR:HD1	2.04	0.40
1:C:57:VAL:HG23	1:C:120:VAL:HG22	2.04	0.40
1:D:126:ILE:HG13	1:D:127:SER:H	1.85	0.40
1:D:173:LEU:HD23	1:D:175:VAL:HG23	2.03	0.40
1:F:150:ILE:O	1:F:150:ILE:HG22	2.21	0.40
1:G:38:VAL:HB	1:G:211:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:THR:O	1:G:206:PHE:N	2.54	0.40
1:G:207:ILE:O	1:G:210:LEU:HB3	2.22	0.40
1:A:78:ASN:HB2	1:A:147:THR:O	2.20	0.40
1:A:151:THR:HG23	1:A:173:LEU:O	2.21	0.40
1:B:81:TYR:CD2	1:B:82:ASP:N	2.83	0.40
1:C:34:VAL:HG21	1:C:204:THR:CG2	2.44	0.40
1:D:29:MET:HA	1:D:30:PRO:HD2	1.94	0.40
1:D:181:ARG:HG3	1:E:181:ARG:HH12	1.86	0.40
1:E:11:MET:SD	1:E:19:PHE:HE2	2.44	0.40
1:G:10:GLU:HB2	1:G:11:MET:H	1.73	0.40
1:G:204:THR:C	1:G:206:PHE:N	2.74	0.40
1:B:100:VAL:HG12	1:B:109:PHE:CE2	2.47	0.40
1:D:218:ASN:OD1	1:D:218:ASN:N	2.50	0.40
1:G:173:LEU:HD23	1:G:173:LEU:O	2.20	0.40
1:B:123:SER:C	1:B:125:GLU:H	2.24	0.40
1:C:61:GLY:HA2	1:C:122:ILE:HD11	2.02	0.40
1:D:62:PHE:CD2	1:D:63:LEU:HD12	2.57	0.40
1:E:166:ASN:HD22	1:E:169:GLU:CD	2.25	0.40
1:F:193:CYS:SG	1:F:198:ILE:HG21	2.62	0.40
1:G:74:TYR:HE2	1:G:206:PHE:HA	1.86	0.40
1:G:184:ARG:HB2	1:G:186:TYR:CE1	2.57	0.40
1:C:33:THR:OG1	1:C:192:SER:OG	2.40	0.40
1:F:36:GLU:CG	1:F:37:GLU:N	2.85	0.40
1:F:81:TYR:CD2	1:F:82:ASP:N	2.89	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	215/224 (96%)	161 (75%)	35 (16%)	19 (9%)	<a href="#">1</a> <a href="#">12</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	216/224 (96%)	164 (76%)	37 (17%)	15 (7%)	1	16
1	C	218/224 (97%)	168 (77%)	36 (16%)	14 (6%)	1	18
1	D	216/224 (96%)	173 (80%)	28 (13%)	15 (7%)	1	16
1	E	215/224 (96%)	166 (77%)	33 (15%)	16 (7%)	1	15
1	F	213/224 (95%)	152 (71%)	44 (21%)	17 (8%)	1	14
1	G	215/224 (96%)	156 (73%)	39 (18%)	20 (9%)	0	11
All	All	1508/1568 (96%)	1140 (76%)	252 (17%)	116 (8%)	1	14

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	89	ILE
1	A	113	ASP
1	A	115	ASP
1	A	216	ASP
1	A	221	ILE
1	B	10	GLU
1	B	85	ARG
1	B	87	VAL
1	B	145	ASP
1	C	10	GLU
1	C	40	VAL
1	C	44	VAL
1	C	82	ASP
1	C	169	GLU
1	C	180	GLU
1	D	58	THR
1	D	86	ARG
1	D	87	VAL
1	E	13	GLY
1	E	54	ASN
1	E	136	ASN
1	E	182	GLU
1	F	10	GLU
1	F	59	VAL
1	F	83	GLU
1	F	136	ASN
1	F	169	GLU
1	F	170	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	183	GLY
1	F	217	PRO
1	G	13	GLY
1	G	41	THR
1	G	82	ASP
1	G	84	THR
1	G	113	ASP
1	G	119	MET
1	G	177	ARG
1	G	201	ALA
1	G	217	PRO
1	G	218	ASN
1	A	13	GLY
1	A	57	VAL
1	A	86	ARG
1	A	131	SER
1	A	199	ASP
1	A	214	ILE
1	B	9	LEU
1	B	86	ARG
1	B	144	GLN
1	B	148	PHE
1	C	13	GLY
1	C	170	VAL
1	C	202	VAL
1	D	131	SER
1	D	141	ASP
1	E	114	ALA
1	F	25	ALA
1	F	54	ASN
1	G	115	ASP
1	G	202	VAL
1	G	206	PHE
1	A	103	PRO
1	A	203	ALA
1	B	169	GLU
1	C	57	VAL
1	C	103	PRO
1	C	181	ARG
1	D	55	ARG
1	D	57	VAL
1	D	148	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	9	LEU
1	E	55	ARG
1	E	79	ALA
1	E	155	THR
1	E	214	ILE
1	F	50	ALA
1	F	52	ALA
1	F	145	ASP
1	G	83	GLU
1	G	103	PRO
1	G	145	ASP
1	G	221	ILE
1	A	43	MET
1	A	200	GLY
1	B	13	GLY
1	D	13	GLY
1	D	59	VAL
1	D	85	ARG
1	D	103	PRO
1	E	68	PRO
1	E	89	ILE
1	E	181	ARG
1	F	156	ILE
1	F	182	GLU
1	A	25	ALA
1	A	155	THR
1	B	19	PHE
1	B	25	ALA
1	B	53	ARG
1	B	221	ILE
1	D	54	ASN
1	D	161	SER
1	E	57	VAL
1	F	55	ARG
1	F	57	VAL
1	G	8	ILE
1	C	200	GLY
1	C	220	ILE
1	D	219	ALA
1	G	28	ILE
1	B	89	ILE
1	E	221	ILE

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Mol	Chain	Res	Type
1	A	44	VAL
1	E	216	ASP
1	G	207	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	193/198 (98%)	139 (72%)	54 (28%)	0 3
1	B	194/198 (98%)	139 (72%)	55 (28%)	0 2
1	C	195/198 (98%)	157 (80%)	38 (20%)	1 8
1	D	194/198 (98%)	154 (79%)	40 (21%)	1 7
1	E	193/198 (98%)	150 (78%)	43 (22%)	1 6
1	F	191/198 (96%)	150 (78%)	41 (22%)	1 6
1	G	193/198 (98%)	137 (71%)	56 (29%)	0 2
All	All	1353/1386 (98%)	1026 (76%)	327 (24%)	0 4

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	LEU
1	A	10	GLU
1	A	16	ARG
1	A	24	LYS
1	A	26	LYS
1	A	28	ILE
1	A	31	HIS
1	A	38	VAL
1	A	40	VAL
1	A	42	SER
1	A	43	MET
1	A	54	ASN
1	A	56	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	65	ARG
1	A	66	ILE
1	A	67	VAL
1	A	70	ILE
1	A	78	ASN
1	A	80	ILE
1	A	82	ASP
1	A	84	THR
1	A	85	ARG
1	A	86	ARG
1	A	87	VAL
1	A	88	TYR
1	A	91	LYS
1	A	96	ILE
1	A	108	VAL
1	A	113	ASP
1	A	118	SER
1	A	123	SER
1	A	132	ARG
1	A	136	ASN
1	A	140	LEU
1	A	144	GLN
1	A	151	THR
1	A	153	VAL
1	A	155	THR
1	A	156	ILE
1	A	160	MET
1	A	170	VAL
1	A	177	ARG
1	A	179	LEU
1	A	192	SER
1	A	197	LEU
1	A	202	VAL
1	A	204	THR
1	A	209	ASP
1	A	211	LYS
1	A	213	VAL
1	A	216	ASP
1	A	220	ILE
1	A	221	ILE
1	B	5	ARG
1	B	6	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	11	MET
1	B	15	ARG
1	B	18	ILE
1	B	23	THR
1	B	27	GLN
1	B	28	ILE
1	B	33	THR
1	B	36	GLU
1	B	37	GLU
1	B	46	ILE
1	B	48	ASP
1	B	51	LYS
1	B	55	ARG
1	B	58	THR
1	B	59	VAL
1	B	65	ARG
1	B	66	ILE
1	B	82	ASP
1	B	83	GLU
1	B	86	ARG
1	B	87	VAL
1	B	88	TYR
1	B	89	ILE
1	B	90	LEU
1	B	95	ASN
1	B	102	THR
1	B	106	LEU
1	B	110	VAL
1	B	127	SER
1	B	134	ARG
1	B	136	ASN
1	B	138	LEU
1	B	140	LEU
1	B	149	THR
1	B	150	ILE
1	B	151	THR
1	B	153	VAL
1	B	155	THR
1	B	159	ILE
1	B	164	ILE
1	B	166	ASN
1	B	170	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	177	ARG
1	B	179	LEU
1	B	182	GLU
1	B	186	TYR
1	B	187	MET
1	B	191	LEU
1	B	195	HIS
1	B	204	THR
1	B	209	ASP
1	B	221	ILE
1	B	222	TYR
1	C	5	ARG
1	C	15	ARG
1	C	16	ARG
1	C	26	LYS
1	C	35	MET
1	C	40	VAL
1	C	41	THR
1	C	44	VAL
1	C	53	ARG
1	C	55	ARG
1	C	58	THR
1	C	66	ILE
1	C	76	TYR
1	C	77	LEU
1	C	80	ILE
1	C	82	ASP
1	C	84	THR
1	C	87	VAL
1	C	104	ASP
1	C	107	ASN
1	C	108	VAL
1	C	122	ILE
1	C	132	ARG
1	C	140	LEU
1	C	150	ILE
1	C	151	THR
1	C	153	VAL
1	C	159	ILE
1	C	162	THR
1	C	180	GLU
1	C	198	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	202	VAL
1	C	204	THR
1	C	205	ARG
1	C	207	ILE
1	C	209	ASP
1	C	213	VAL
1	C	218	ASN
1	D	8	ILE
1	D	11	MET
1	D	20	ASP
1	D	23	THR
1	D	27	GLN
1	D	41	THR
1	D	44	VAL
1	D	45	SER
1	D	47	LEU
1	D	53	ARG
1	D	59	VAL
1	D	82	ASP
1	D	83	GLU
1	D	93	TYR
1	D	100	VAL
1	D	106	LEU
1	D	108	VAL
1	D	116	ARG
1	D	122	ILE
1	D	139	GLN
1	D	141	ASP
1	D	143	VAL
1	D	149	THR
1	D	151	THR
1	D	152	ASN
1	D	161	SER
1	D	164	ILE
1	D	170	VAL
1	D	172	ILE
1	D	179	LEU
1	D	182	GLU
1	D	192	SER
1	D	197	LEU
1	D	204	THR
1	D	205	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	208	VAL
1	D	209	ASP
1	D	210	LEU
1	D	211	LYS
1	D	218	ASN
1	E	11	MET
1	E	16	ARG
1	E	19	PHE
1	E	29	MET
1	E	53	ARG
1	E	54	ASN
1	E	55	ARG
1	E	60	THR
1	E	65	ARG
1	E	66	ILE
1	E	67	VAL
1	E	69	SER
1	E	70	ILE
1	E	80	ILE
1	E	82	ASP
1	E	84	THR
1	E	86	ARG
1	E	88	TYR
1	E	90	LEU
1	E	93	TYR
1	E	102	THR
1	E	106	LEU
1	E	108	VAL
1	E	113	ASP
1	E	115	ASP
1	E	116	ARG
1	E	118	SER
1	E	131	SER
1	E	139	GLN
1	E	140	LEU
1	E	153	VAL
1	E	155	THR
1	E	159	ILE
1	E	162	THR
1	E	165	ILE
1	E	169	GLU
1	E	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	189	LEU
1	E	190	SER
1	E	192	SER
1	E	197	LEU
1	E	212	LYS
1	E	222	TYR
1	F	8	ILE
1	F	11	MET
1	F	14	LEU
1	F	22	MET
1	F	33	THR
1	F	35	MET
1	F	41	THR
1	F	46	ILE
1	F	47	LEU
1	F	54	ASN
1	F	56	LYS
1	F	58	THR
1	F	66	ILE
1	F	73	GLN
1	F	86	ARG
1	F	87	VAL
1	F	90	LEU
1	F	95	ASN
1	F	108	VAL
1	F	112	LYS
1	F	122	ILE
1	F	140	LEU
1	F	143	VAL
1	F	145	ASP
1	F	146	SER
1	F	153	VAL
1	F	155	THR
1	F	156	ILE
1	F	164	ILE
1	F	175	VAL
1	F	179	LEU
1	F	180	GLU
1	F	182	GLU
1	F	190	SER
1	F	199	ASP
1	F	204	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	207	ILE
1	F	209	ASP
1	F	215	GLU
1	F	216	ASP
1	F	218	ASN
1	G	9	LEU
1	G	11	MET
1	G	12	HIS
1	G	14	LEU
1	G	16	ARG
1	G	28	ILE
1	G	35	MET
1	G	36	GLU
1	G	38	VAL
1	G	42	SER
1	G	44	VAL
1	G	45	SER
1	G	47	LEU
1	G	60	THR
1	G	65	ARG
1	G	69	SER
1	G	70	ILE
1	G	72	LYS
1	G	78	ASN
1	G	80	ILE
1	G	81	TYR
1	G	84	THR
1	G	86	ARG
1	G	87	VAL
1	G	88	TYR
1	G	92	LYS
1	G	110	VAL
1	G	116	ARG
1	G	118	SER
1	G	122	ILE
1	G	123	SER
1	G	132	ARG
1	G	138	LEU
1	G	140	LEU
1	G	145	ASP
1	G	146	SER
1	G	149	THR

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Mol	Chain	Res	Type
1	G	155	THR
1	G	156	ILE
1	G	159	ILE
1	G	170	VAL
1	G	178	ILE
1	G	179	LEU
1	G	182	GLU
1	G	185	LYS
1	G	190	SER
1	G	196	ARG
1	G	197	LEU
1	G	198	ILE
1	G	202	VAL
1	G	204	THR
1	G	207	ILE
1	G	209	ASP
1	G	213	VAL
1	G	214	ILE
1	G	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	107	ASN
1	B	12	HIS
1	B	78	ASN
1	B	136	ASN
1	B	176	HIS
1	B	195	HIS
1	C	176	HIS
1	C	195	HIS
1	C	218	ASN
1	D	12	HIS
1	D	78	ASN
1	D	152	ASN
1	E	54	ASN
1	E	95	ASN
1	E	107	ASN
1	F	12	HIS
1	F	95	ASN
1	F	107	ASN

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Mol	Chain	Res	Type
1	F	195	HIS
1	G	12	HIS
1	G	78	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	217/224 (96%)	-0.87	0 100 100	46, 72, 111, 169	0
1	B	218/224 (97%)	-0.77	0 100 100	54, 90, 137, 153	0
1	C	220/224 (98%)	-0.82	0 100 100	49, 82, 135, 234	0
1	D	218/224 (97%)	-0.69	0 100 100	68, 112, 175, 245	0
1	E	217/224 (96%)	-0.68	0 100 100	61, 97, 169, 229	0
1	F	215/224 (95%)	-0.70	0 100 100	65, 101, 164, 213	0
1	G	217/224 (96%)	-0.79	0 100 100	49, 85, 146, 190	0
All	All	1522/1568 (97%)	-0.76	0 100 100	46, 89, 153, 245	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no 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.