



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:50 am BST

PDB ID : 2QE7  
Title : Crystal structure of the f1-atpase from the thermoalkaliphilic bacterium bacillus sp. ta2.a1  
Authors : Stocker, A.; Keis, S.; Vonck, J.; Cook, G.M.; Dimroth, P.  
Deposited on : 2007-06-25  
Resolution : 3.06 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.

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

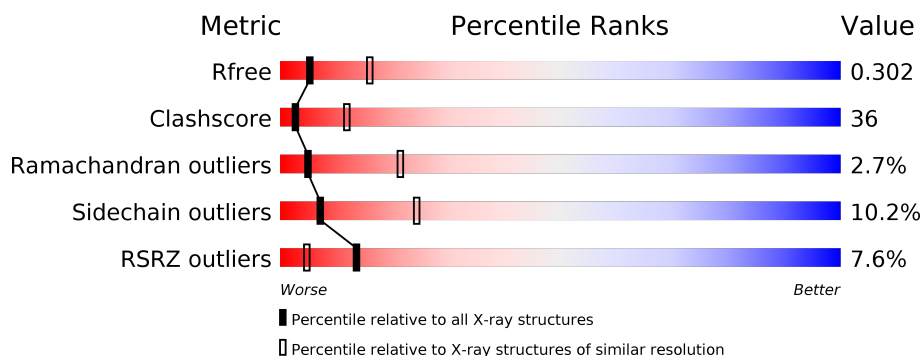
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	502	
1	B	502	
1	C	502	
2	D	462	
2	E	462	
2	F	462	

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Mol	Chain	Length	Quality of chain
3	G	286	<p>12% 9% 57% 13% 21%</p>
4	H	135	<p>80% 15% 76% 10%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30018 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3640	2295	628	703	14			
1	B	474	Total	C	N	O	S	0	0	0
			3640	2295	628	703	14			
1	C	474	Total	C	N	O	S	0	0	0
			3640	2295	628	703	14			

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	461	Total	C	N	O	S	0	0	0
			3522	2218	608	683	13			
2	E	461	Total	C	N	O	S	0	0	0
			3522	2218	608	683	13			
2	F	461	Total	C	N	O	S	0	0	0
			3522	2218	608	683	13			

- Molecule 3 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	227	Total	C	N	O	S	0	227	0
			5382	3396	954	1005	27			

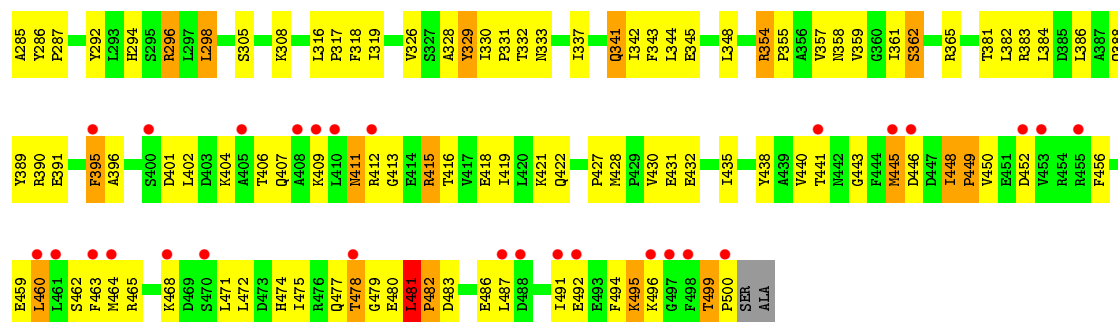
- Molecule 4 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	135	Total	C	N	O	S	0	135	0
			3150	1974	579	591	6			

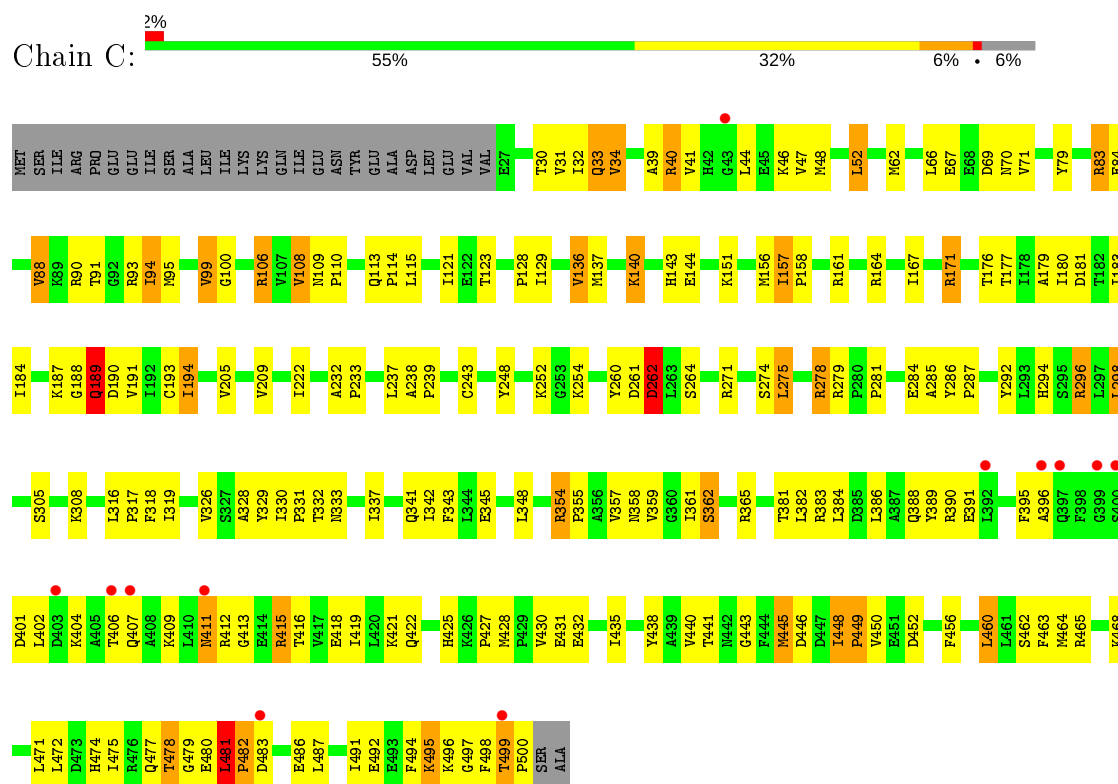
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

- Chain A:

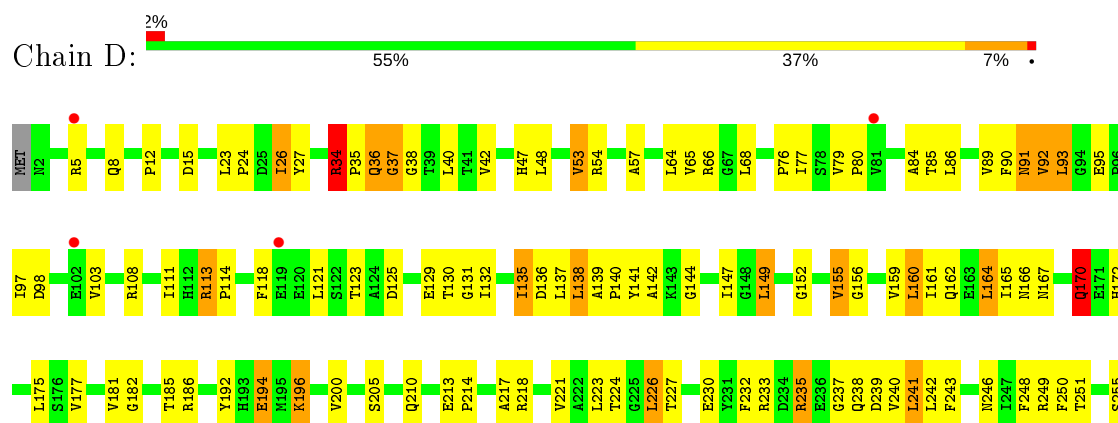
- Chain B:
- 
- 6% 54% 33% 7% 6%
- | Amino Acid | Percentage |
|------------|------------|
| MET        | 6%         |
| SER        | 6%         |
| ILE        | 6%         |
| ARG        | 6%         |
| PRO        | 6%         |
| GLU        | 6%         |
| ILE        | 6%         |
| SER        | 6%         |
| ALA        | 6%         |
| LEU        | 6%         |
| ILE        | 6%         |
| LYS        | 6%         |
| GLN        | 6%         |
| ILE        | 6%         |
| GLU        | 6%         |
| ASN        | 6%         |
| TYR        | 6%         |
| GLU        | 6%         |
| ASP        | 6%         |
| ALA        | 6%         |
| LEU        | 6%         |
| GLU        | 6%         |
| VAL        | 6%         |
| E27        | 6%         |
| T30        | 6%         |
| V31        | 6%         |
| I32        | 6%         |
| Q33        | 6%         |
| V34        | 6%         |
| G35        | 6%         |
| D36        | 6%         |
| A39        | 6%         |
| R40        | 6%         |
| V41        | 6%         |
| L44        | 6%         |
| E45        | 6%         |
| K46        | 6%         |
| V47        | 6%         |
| M48        | 6%         |
| E51        | 6%         |
| L52        | 6%         |
| L53        | 6%         |
| E56        | 6%         |
| M62        | 6%         |
| M65        | 6%         |
| L66        | 6%         |
| V71        | 6%         |
| V70        | 6%         |

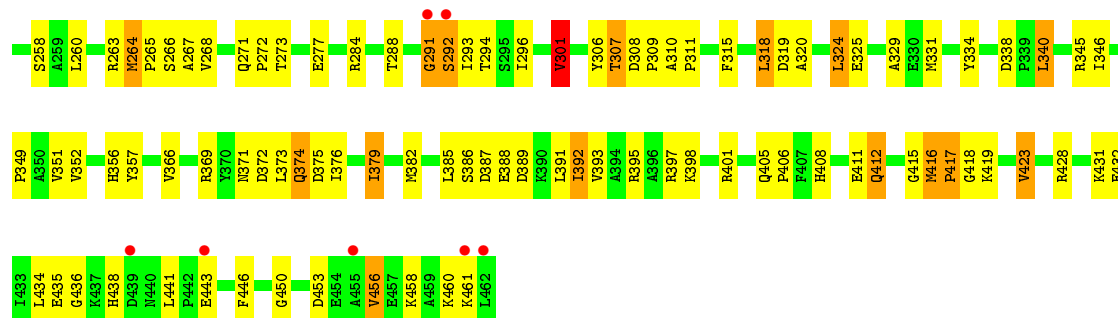


• Molecule 1: ATP synthase subunit alpha

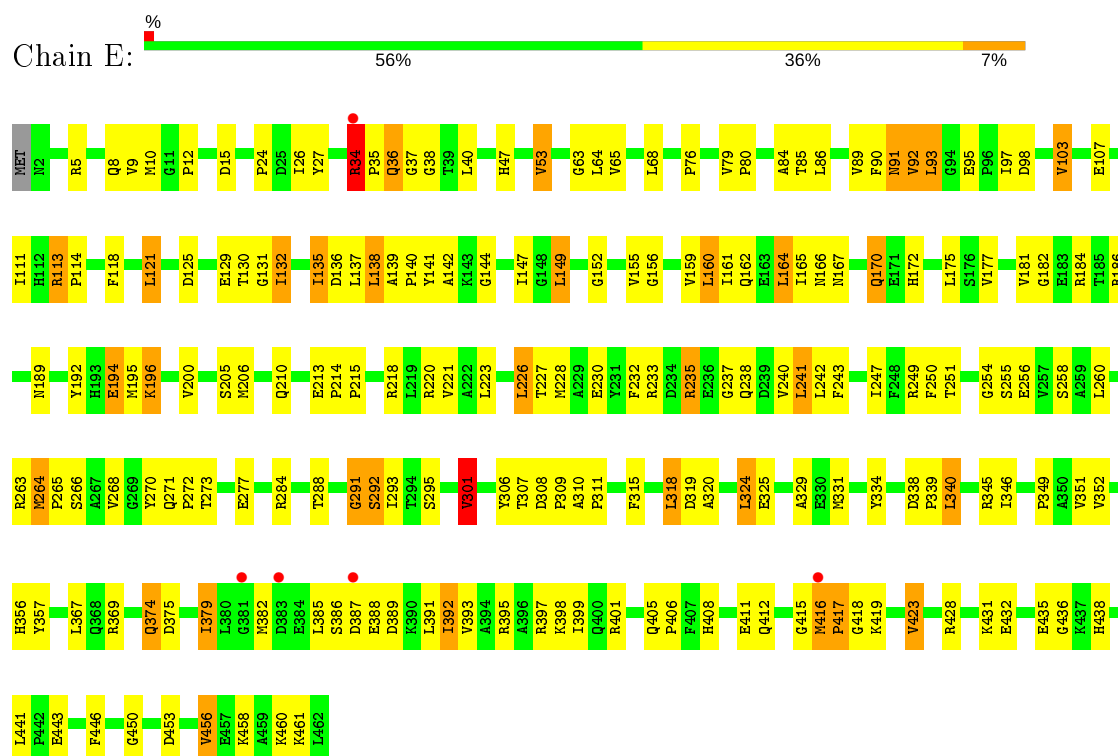


• Molecule 2: ATP synthase subunit beta

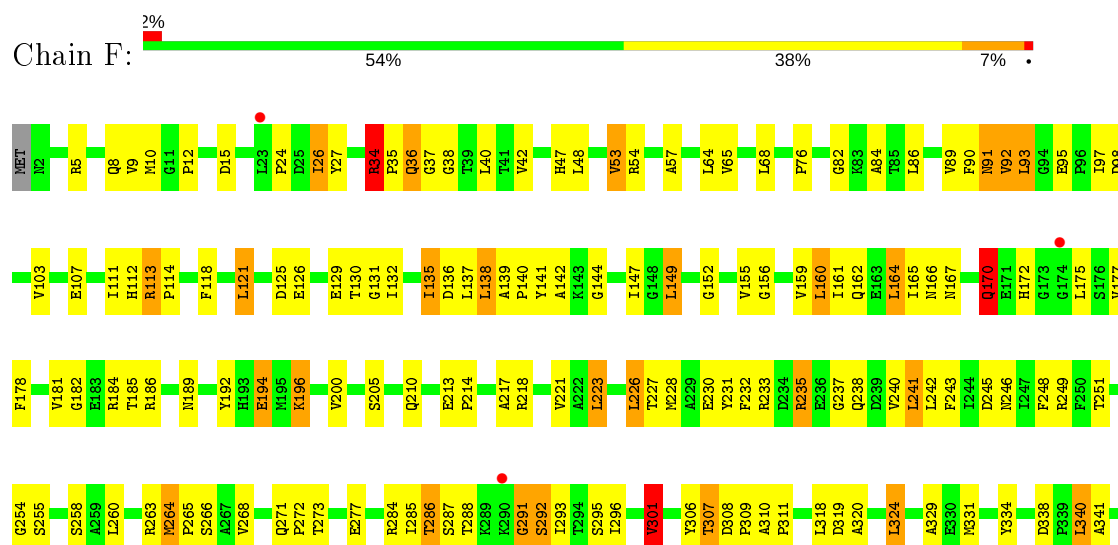


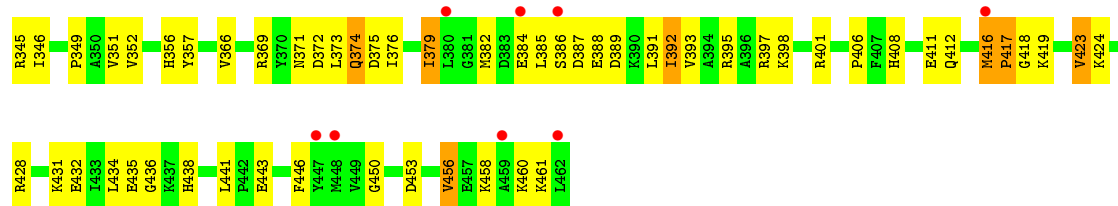


• Molecule 2: ATP synthase subunit beta

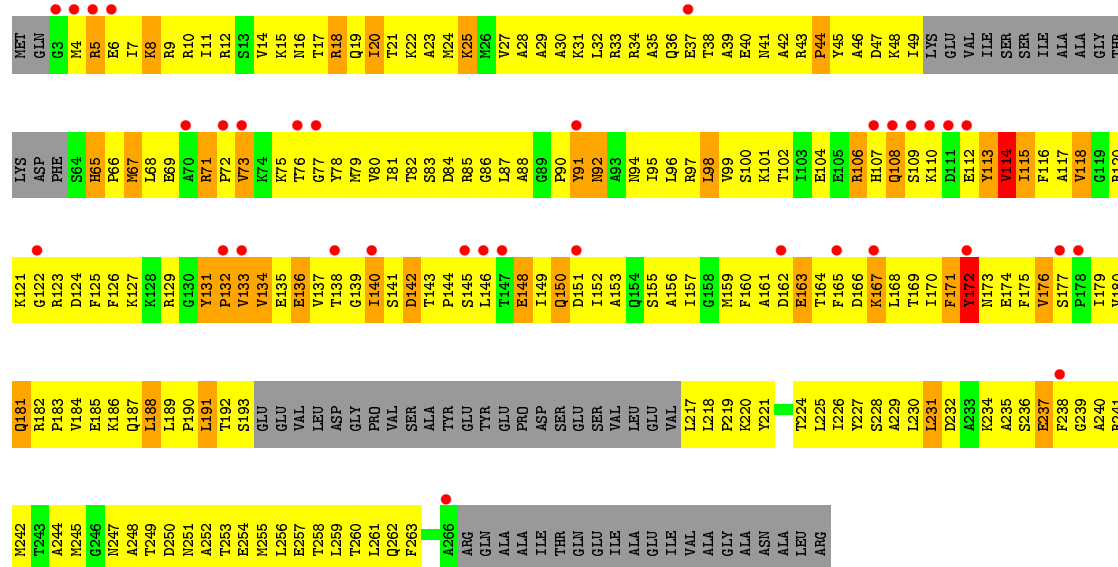
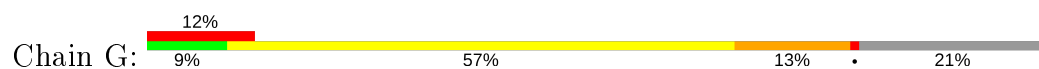


• Molecule 2: ATP synthase subunit beta

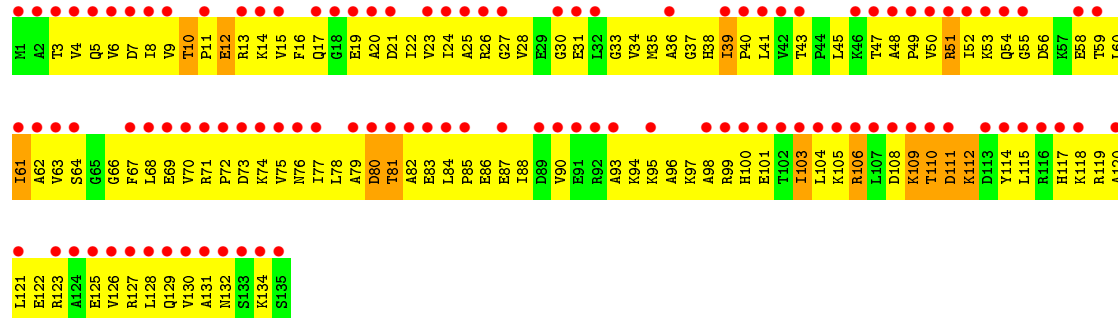
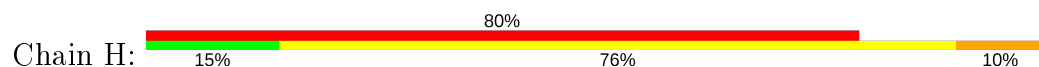




• Molecule 3: ATP synthase subunit gamma



• Molecule 4: ATP synthase subunit epsilon





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.21Å 173.02Å 218.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.06 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.00-3.06) 89.6 (40.00-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.252 , 0.306 0.241 , 0.302	Depositor DCC
$R_{free}$ test set	2577 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 83.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	30018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.48	0/3699	0.64	1/5006 (0.0%)
1	B	0.49	0/3699	0.64	2/5006 (0.0%)
1	C	0.48	0/3699	0.63	1/5006 (0.0%)
2	D	0.46	0/3582	0.62	0/4852
2	E	0.56	0/3582	0.67	0/4852
2	F	0.52	0/3582	0.65	0/4852
3	G	0.24	0/5460	0.49	0/7344
4	H	0.20	0/3183	0.39	0/4287
All	All	0.44	0/30486	0.60	4/41205 (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
2	D	0	1
2	E	0	1
2	F	0	1
3	G	0	2
4	H	0	1
All	All	0	6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	LEU	CA-CB-CG	7.83	133.32	115.30
1	C	481	LEU	CA-CB-CG	7.46	132.46	115.30
1	B	481	LEU	CA-CB-CG	7.34	132.19	115.30
1	B	275	LEU	CA-CB-CG	5.51	127.97	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	334	TYR	Peptide
2	E	334	TYR	Peptide
2	F	334	TYR	Peptide
3	G	171[B]	PHE	Peptide
3	G	171[C]	PHE	Peptide
4	H	111[C]	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3640	0	3675	261	0
1	B	3640	0	3675	267	0
1	C	3640	0	3675	251	0
2	D	3522	0	3530	211	1
2	E	3522	0	3530	210	0
2	F	3522	0	3530	208	0
3	G	5382	0	5529	615	0
4	H	3150	0	3331	283	1
All	All	30018	0	30475	2174	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (2174) 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)
2:F:371:ASN:CB	3:G:10[B]:ARG:NH1	1.78	1.45
2:F:371:ASN:HB3	3:G:10[B]:ARG:NH1	1.03	1.35
1:B:83:ARG:HB2	2:E:47:HIS:CE1	1.64	1.31
3:G:28[C]:ALA:HA	3:G:238[C]:PHE:HD1	1.04	1.17
1:A:275:LEU:HD22	2:D:264:MET:HA	1.28	1.15
4:H:110[C]:THR:O	4:H:112[C]:LYS:HG3	1.45	1.12
1:B:106:ARG:HG2	1:B:106:ARG:HH11	1.03	1.12
1:C:106:ARG:HH11	1:C:106:ARG:HG2	1.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32[C]:LEU:CG	3:G:238[C]:PHE:HB2	1.82	1.09
3:G:71[B]:ARG:HG3	3:G:71[B]:ARG:HH11	1.01	1.09
2:F:371:ASN:CB	3:G:10[B]:ARG:HH12	1.44	1.09
1:B:354:ARG:HH11	1:B:354:ARG:CG	1.68	1.07
3:G:32[C]:LEU:HG	3:G:238[C]:PHE:HB2	1.37	1.06
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.16	1.06
1:A:354:ARG:HH11	1:A:354:ARG:CG	1.69	1.06
3:G:84[C]:ASP:HB3	3:G:120[C]:ARG:H	1.08	1.06
1:B:275:LEU:HB3	2:E:264:MET:CG	1.87	1.05
3:G:28[C]:ALA:HA	3:G:238[C]:PHE:CD1	1.91	1.04
1:A:462:SER:HA	1:A:465:ARG:NH1	1.72	1.04
1:C:354:ARG:CG	1:C:354:ARG:HH11	1.68	1.04
3:G:4[A]:MET:HG3	3:G:5[A]:ARG:NH1	1.73	1.03
4:H:110[C]:THR:HB	4:H:112[C]:LYS:HE2	1.40	1.03
1:B:151:LYS:H	1:B:422:GLN:HE22	1.06	1.03
3:G:32[C]:LEU:HD23	3:G:238[C]:PHE:CG	1.92	1.03
1:B:106:ARG:HH11	1:B:106:ARG:CG	1.71	1.03
1:B:275:LEU:HD22	2:E:264:MET:HA	1.40	1.02
3:G:80[A]:VAL:HA	3:G:171[A]:PHE:HB2	1.38	1.02
3:G:32[C]:LEU:CB	3:G:238[C]:PHE:HB2	1.90	1.02
1:C:462:SER:HA	1:C:465:ARG:NH1	1.73	1.01
1:B:462:SER:HA	1:B:465:ARG:NH1	1.76	1.00
3:G:38[C]:THR:HA	4:H:13[C]:ARG:NH2	1.77	0.99
1:C:354:ARG:HG3	1:C:354:ARG:HH11	1.26	0.99
3:G:32[C]:LEU:HB2	3:G:238[C]:PHE:CB	1.93	0.98
1:B:275:LEU:HB3	2:E:264:MET:HG3	1.43	0.98
1:A:492:GLU:HA	1:A:495:LYS:HB2	1.45	0.98
3:G:48[C]:LYS:HD3	4:H:78[C]:LEU:HD22	1.46	0.98
1:A:151:LYS:H	1:A:422:GLN:HE22	1.03	0.97
1:C:106:ARG:HH11	1:C:106:ARG:CG	1.78	0.97
3:G:71[A]:ARG:HH11	3:G:71[A]:ARG:CG	1.77	0.97
4:H:61[B]:ILE:HG22	4:H:84[B]:LEU:HA	1.43	0.96
1:B:492:GLU:HA	1:B:495:LYS:HB2	1.44	0.96
1:C:171:ARG:HH11	1:C:171:ARG:CG	1.78	0.96
4:H:13[B]:ARG:HH11	4:H:13[B]:ARG:HG3	1.27	0.96
1:C:492:GLU:HA	1:C:495:LYS:HB2	1.44	0.96
3:G:32[C]:LEU:HB2	3:G:238[C]:PHE:HB2	1.43	0.96
3:G:72[C]:PRO:HA	3:G:73[C]:VAL:HG13	1.48	0.96
1:A:415:ARG:CG	1:A:415:ARG:HH11	1.78	0.96
1:B:354:ARG:HH11	1:B:354:ARG:HG3	1.27	0.96
1:C:275:LEU:HD22	2:F:264:MET:HA	1.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:HH11	1:A:354:ARG:HG3	1.30	0.96
1:C:415:ARG:HH11	1:C:415:ARG:CG	1.78	0.95
1:C:137:MET:HG3	2:D:98:ASP:HA	1.48	0.95
1:B:415:ARG:CG	1:B:415:ARG:HH11	1.78	0.95
1:C:83:ARG:HB2	2:F:47:HIS:CE1	1.99	0.95
1:C:284:GLU:HG3	1:C:329:TYR:CG	2.01	0.95
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.30	0.95
1:C:365:ARG:HH21	2:D:186:ARG:HH22	1.14	0.94
3:G:71[B]:ARG:NH1	3:G:71[B]:ARG:HG3	1.79	0.94
3:G:162[A]:ASP:HA	3:G:163[A]:GLU:HB2	1.50	0.94
3:G:87[C]:LEU:N	3:G:241[C]:ARG:HH21	1.64	0.94
2:F:371:ASN:CG	3:G:10[B]:ARG:NH1	2.21	0.94
1:C:365:ARG:HH21	2:D:186:ARG:NH2	1.65	0.93
3:G:86[C]:GLY:HA2	3:G:241[C]:ARG:HH22	1.31	0.93
1:B:62:MET:HB2	1:B:95:MET:HE1	1.47	0.93
3:G:146[C]:LEU:HA	3:G:227[C]:TYR:OH	1.69	0.92
3:G:238[C]:PHE:CE2	3:G:241[C]:ARG:NH1	2.36	0.92
1:A:284:GLU:HG3	1:A:329:TYR:CG	2.05	0.92
1:B:83:ARG:HB2	2:E:47:HIS:HE1	1.33	0.92
3:G:168[A]:LEU:HB3	3:G:189[A]:LEU:HB2	1.50	0.92
1:C:151:LYS:H	1:C:422:GLN:HE22	1.00	0.91
2:D:175:LEU:H	2:D:238:GLN:HE21	1.17	0.91
1:B:284:GLU:HG3	1:B:329:TYR:CG	2.06	0.91
3:G:162[C]:ASP:HA	3:G:163[C]:GLU:HB2	1.52	0.91
4:H:6[C]:VAL:HG21	4:H:23[C]:VAL:HG21	1.51	0.91
3:G:43[A]:ARG:HB2	3:G:44[A]:PRO:HD3	1.52	0.91
1:A:156:MET:HE3	1:A:383:ARG:HA	1.51	0.90
1:A:171:ARG:HH11	1:A:171:ARG:CG	1.83	0.90
1:A:365:ARG:HH21	2:E:186:ARG:HH22	1.20	0.90
1:A:106:ARG:CG	1:A:106:ARG:HH11	1.84	0.90
1:C:171:ARG:HG3	1:C:171:ARG:HH11	1.33	0.90
3:G:32[B]:LEU:HG	3:G:238[B]:PHE:CB	2.01	0.90
3:G:65[C]:HIS:HD2	3:G:69[C]:GLU:HB2	1.37	0.90
2:D:213:GLU:HG3	2:D:214:PRO:HD2	1.54	0.90
3:G:84[C]:ASP:HB2	3:G:120[C]:ARG:HB3	1.54	0.89
3:G:86[C]:GLY:HA2	3:G:241[C]:ARG:NH2	1.85	0.89
2:D:89:VAL:HG22	2:D:98:ASP:HB3	1.54	0.89
3:G:172[C]:TYR:HB3	3:G:184[C]:VAL:HG12	1.52	0.89
4:H:100[A]:HIS:HB2	4:H:121[A]:LEU:HG	1.54	0.89
1:B:171:ARG:HH11	1:B:171:ARG:CG	1.86	0.88
1:A:106:ARG:NH1	1:A:106:ARG:HG2	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:268:VAL:HG11	2:E:309:PRO:HG2	1.54	0.88
1:A:62:MET:HB2	1:A:95:MET:HE1	1.54	0.88
2:F:264:MET:HB3	2:F:265:PRO:HA	1.53	0.88
1:C:62:MET:HB2	1:C:95:MET:HE1	1.56	0.88
1:B:106:ARG:NH1	1:B:106:ARG:HG2	1.73	0.87
1:C:474:HIS:NE2	1:C:482:PRO:HD2	1.89	0.87
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.39	0.87
2:E:264:MET:CB	2:E:272:PRO:HG3	2.05	0.87
3:G:160[A]:PHE:HB2	3:G:189[A]:LEU:HD21	1.55	0.87
4:H:66[C]:GLY:HA3	4:H:79[C]:ALA:HA	1.53	0.87
1:C:83:ARG:HB2	2:F:47:HIS:HE1	1.36	0.87
1:B:83:ARG:CB	2:E:47:HIS:CE1	2.54	0.87
2:D:268:VAL:HG11	2:D:309:PRO:HG2	1.57	0.87
4:H:5[B]:GLN:HA	4:H:19[B]:GLU:HA	1.56	0.87
3:G:38[C]:THR:HA	4:H:13[C]:ARG:HH22	1.36	0.86
1:C:66:LEU:HB3	2:D:66:ARG:HD3	1.56	0.86
2:F:371:ASN:CB	3:G:10[B]:ARG:HH11	1.65	0.86
3:G:131[C]:TYR:H	3:G:132[C]:PRO:HA	1.40	0.86
3:G:29[C]:ALA:HB2	3:G:242[C]:MET:SD	2.14	0.86
4:H:110[C]:THR:HB	4:H:112[C]:LYS:CE	2.05	0.86
2:D:130:THR:HG21	2:D:135:ILE:HD11	1.55	0.86
1:A:83:ARG:HB2	2:D:47:HIS:CE1	2.10	0.86
2:E:89:VAL:HG22	2:E:98:ASP:HB3	1.56	0.86
2:F:175:LEU:H	2:F:238:GLN:HE21	1.21	0.86
1:A:164:ARG:HH22	2:E:184:ARG:HD3	1.38	0.86
2:F:268:VAL:HG11	2:F:309:PRO:HG2	1.57	0.86
2:D:264:MET:HB3	2:D:265:PRO:HA	1.55	0.85
4:H:90[C]:VAL:HG22	4:H:131[C]:ALA:HB1	1.59	0.85
2:F:213:GLU:HG3	2:F:214:PRO:HD2	1.58	0.85
2:D:34:ARG:HG3	2:D:35:PRO:HA	1.58	0.85
3:G:72[C]:PRO:HB2	3:G:73[C]:VAL:HG22	1.58	0.85
1:A:474:HIS:NE2	1:A:482:PRO:HD2	1.90	0.85
2:E:175:LEU:H	2:E:238:GLN:HE21	1.21	0.84
4:H:8[A]:ILE:HA	4:H:77[A]:ILE:HG12	1.60	0.84
3:G:32[A]:LEU:HD12	3:G:35[A]:ALA:HB2	1.58	0.84
2:E:34:ARG:HG3	2:E:35:PRO:HA	1.59	0.84
4:H:51[C]:ARG:HG2	4:H:60[C]:LEU:HA	1.57	0.84
2:E:264:MET:HB3	2:E:265:PRO:HA	1.57	0.84
2:F:130:THR:HG21	2:F:135:ILE:HD11	1.58	0.84
4:H:50[C]:VAL:H	4:H:61[C]:ILE:HG12	1.42	0.84
3:G:32[B]:LEU:HG	3:G:238[B]:PHE:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:45[C]:TYR:HA	3:G:48[C]:LYS:HD2	1.58	0.84
2:F:89:VAL:HG22	2:F:98:ASP:HB3	1.58	0.84
4:H:110[C]:THR:C	4:H:112[C]:LYS:HG3	1.98	0.84
1:C:156:MET:HE3	1:C:383:ARG:HA	1.60	0.83
1:B:474:HIS:NE2	1:B:482:PRO:HD2	1.92	0.83
2:F:371:ASN:HB3	3:G:10[B]:ARG:HH11	1.03	0.83
3:G:148[A]:GLU:HG2	3:G:149[A]:ILE:HG13	1.59	0.83
2:D:175:LEU:H	2:D:238:GLN:NE2	1.76	0.83
2:F:34:ARG:HG3	2:F:35:PRO:HA	1.61	0.83
1:A:79:TYR:HE1	2:D:26:ILE:HD11	1.44	0.83
3:G:188[A]:LEU:HD21	3:G:225[A]:LEU:HB3	1.59	0.83
4:H:103[B]:ILE:HD11	4:H:117[B]:HIS:CD2	2.14	0.83
2:F:371:ASN:CA	3:G:10[B]:ARG:HH12	1.93	0.82
4:H:47[A]:THR:HG21	4:H:122[A]:GLU:HB3	1.62	0.82
2:D:264:MET:CB	2:D:272:PRO:HG3	2.10	0.82
1:B:415:ARG:HH11	1:B:415:ARG:HG2	1.45	0.81
3:G:84[C]:ASP:CB	3:G:120[C]:ARG:H	1.91	0.81
1:A:66:LEU:HD12	2:E:9:VAL:HB	1.63	0.81
2:E:398:LYS:HD3	2:E:446:PHE:CE1	2.14	0.81
3:G:142[B]:ASP:HA	3:G:234[B]:LYS:NZ	1.95	0.81
2:E:264:MET:HB3	2:E:272:PRO:HG3	1.62	0.81
3:G:71[A]:ARG:HH11	3:G:71[A]:ARG:HG2	1.45	0.81
1:B:275:LEU:CB	2:E:264:MET:HG3	2.11	0.81
1:C:480:GLU:C	1:C:482:PRO:HD3	2.01	0.81
2:F:264:MET:CB	2:F:272:PRO:HG3	2.10	0.81
3:G:170[C]:ILE:HD11	3:G:186[C]:LYS:HB2	1.62	0.81
3:G:189[A]:LEU:HB3	3:G:190[A]:PRO:HD3	1.63	0.81
1:C:106:ARG:NH1	1:C:106:ARG:HG2	1.80	0.81
4:H:25[B]:ALA:HB2	4:H:50[B]:VAL:HG13	1.61	0.81
1:A:415:ARG:HH11	1:A:415:ARG:HG2	1.46	0.80
2:F:175:LEU:H	2:F:238:GLN:NE2	1.79	0.80
3:G:72[A]:PRO:HB3	3:G:73[A]:VAL:HB	1.61	0.80
1:B:66:LEU:HD12	2:F:9:VAL:HB	1.62	0.80
3:G:45[C]:TYR:HE2	3:G:224[C]:THR:HG21	1.45	0.80
4:H:26[B]:ARG:HA	4:H:31[B]:GLU:HG2	1.63	0.80
2:E:130:THR:HG21	2:E:135:ILE:HD11	1.62	0.80
3:G:120[B]:ARG:HD3	3:G:123[B]:ARG:HH21	1.44	0.80
4:H:60[C]:LEU:HD12	4:H:130[C]:VAL:HA	1.62	0.80
1:B:480:GLU:C	1:B:482:PRO:HD3	2.02	0.80
1:C:354:ARG:NH1	1:C:354:ARG:HG3	1.95	0.80
1:C:440:VAL:HA	1:C:445:MET:HG3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HB3	2:E:264:MET:SD	2.20	0.80
3:G:120[B]:ARG:CD	3:G:123[B]:ARG:HH21	1.95	0.80
3:G:71[B]:ARG:CG	3:G:71[B]:ARG:HH11	1.91	0.80
1:A:480:GLU:C	1:A:482:PRO:HD3	2.01	0.79
3:G:96[A]:LEU:HA	3:G:99[A]:VAL:HG12	1.64	0.79
3:G:118[C]:VAL:HA	3:G:137[C]:VAL:HG13	1.64	0.79
3:G:220[C]:LYS:O	3:G:224[C]:THR:HG23	1.82	0.79
4:H:110[C]:THR:O	4:H:112[C]:LYS:CG	2.29	0.79
3:G:261[B]:LEU:HD12	3:G:262[B]:GLN:HG3	1.63	0.79
3:G:72[B]:PRO:HB3	3:G:73[B]:VAL:HB	1.64	0.79
4:H:5[A]:GLN:HG2	4:H:19[A]:GLU:HG2	1.62	0.79
1:B:345:GLU:HB2	1:B:348:LEU:HD22	1.65	0.79
4:H:103[B]:ILE:HA	4:H:106[B]:ARG:HG3	1.64	0.79
2:D:264:MET:HE3	2:D:272:PRO:HB3	1.63	0.78
1:A:275:LEU:HG	1:A:278:ARG:HA	1.65	0.78
1:B:48:MET:HE3	1:B:94:ILE:HG23	1.65	0.78
3:G:72[C]:PRO:CA	3:G:73[C]:VAL:HG13	2.14	0.78
3:G:32[A]:LEU:HB2	3:G:238[A]:PHE:HB2	1.63	0.78
3:G:85[C]:ARG:HD2	3:G:85[C]:ARG:O	1.84	0.78
4:H:13[B]:ARG:CG	4:H:13[B]:ARG:HH11	1.96	0.78
1:C:345:GLU:HB2	1:C:348:LEU:HD22	1.63	0.78
1:C:499:THR:N	1:C:500:PRO:HD3	1.99	0.78
3:G:65[C]:HIS:CD2	3:G:69[C]:GLU:HB2	2.19	0.78
2:E:175:LEU:H	2:E:238:GLN:NE2	1.82	0.78
3:G:68[C]:LEU:HD22	3:G:68[C]:LEU:H	1.49	0.78
1:B:83:ARG:HB2	2:E:47:HIS:ND1	1.97	0.78
3:G:71[B]:ARG:NH2	3:G:163[B]:GLU:HG2	1.99	0.78
2:E:213:GLU:HG3	2:E:214:PRO:HD2	1.64	0.77
1:C:151:LYS:N	1:C:422:GLN:HE22	1.81	0.77
4:H:110[C]:THR:CB	4:H:112[C]:LYS:HE2	2.13	0.77
2:E:264:MET:HE3	2:E:272:PRO:HB3	1.67	0.77
3:G:76[C]:THR:HB	3:G:167[C]:LYS:HG2	1.67	0.77
3:G:87[C]:LEU:H	3:G:241[C]:ARG:NH2	1.83	0.77
3:G:84[C]:ASP:HB3	3:G:120[C]:ARG:N	1.94	0.77
1:A:354:ARG:HH11	1:A:354:ARG:HG2	1.50	0.77
3:G:170[C]:ILE:HG13	3:G:188[C]:LEU:HD11	1.66	0.77
1:B:156:MET:HE3	1:B:383:ARG:HA	1.64	0.77
1:C:415:ARG:HH11	1:C:415:ARG:HG3	1.49	0.77
3:G:32[A]:LEU:HB2	3:G:238[A]:PHE:CB	2.16	0.76
4:H:97[C]:LYS:HE3	4:H:128[C]:LEU:HD12	1.67	0.76
2:F:408:HIS:ND1	2:F:418:GLY:HA3	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HG	1:B:278:ARG:HA	1.67	0.76
1:C:79:TYR:HE1	2:F:26:ILE:HD11	1.49	0.76
3:G:72[B]:PRO:CA	3:G:73[B]:VAL:HB	2.15	0.76
2:F:264:MET:HE3	2:F:272:PRO:HB3	1.67	0.76
1:C:415:ARG:HH11	1:C:415:ARG:HG2	1.51	0.76
1:A:354:ARG:NH1	1:A:354:ARG:HG3	1.99	0.76
3:G:78[B]:TYR:HD1	3:G:115[B]:ILE:HG22	1.51	0.76
1:A:275:LEU:HB3	2:D:264:MET:CG	2.16	0.76
1:A:345:GLU:HB2	1:A:348:LEU:HD22	1.68	0.76
3:G:170[B]:ILE:HD11	3:G:186[B]:LYS:HB2	1.67	0.75
2:E:379:ILE:HD12	3:G:252[A]:ALA:HB2	1.68	0.75
3:G:81[B]:ILE:HA	3:G:118[B]:VAL:HG13	1.68	0.75
1:B:354:ARG:NH1	1:B:354:ARG:HG3	1.97	0.75
1:B:328:ALA:O	1:B:332:THR:HG23	1.86	0.75
4:H:117[C]:HIS:HA	4:H:120[C]:ALA:HB3	1.68	0.75
4:H:34[A]:VAL:HA	4:H:38[A]:HIS:CE1	2.22	0.75
1:B:440:VAL:HA	1:B:445:MET:HG3	1.68	0.75
1:C:275:LEU:HG	1:C:278:ARG:HA	1.67	0.75
3:G:25[C]:LYS:HG2	3:G:245[C]:MET:HB2	1.69	0.75
3:G:241[B]:ARG:HB2	3:G:241[B]:ARG:HH11	1.51	0.75
1:B:275:LEU:CB	2:E:264:MET:SD	2.75	0.74
1:A:499:THR:N	1:A:500:PRO:HD3	2.02	0.74
1:A:462:SER:CA	1:A:465:ARG:NH1	2.50	0.74
3:G:40[B]:GLU:O	3:G:44[B]:PRO:HD3	1.87	0.74
2:D:419:LYS:HE2	2:D:450:GLY:HA3	1.69	0.74
3:G:118[C]:VAL:HA	3:G:137[C]:VAL:CG1	2.18	0.74
3:G:65[C]:HIS:HD2	3:G:69[C]:GLU:CB	2.00	0.74
3:G:5[A]:ARG:NH1	3:G:5[A]:ARG:HB3	2.02	0.74
3:G:146[B]:LEU:HA	3:G:227[B]:TYR:OH	1.88	0.74
3:G:87[C]:LEU:H	3:G:241[C]:ARG:HH21	1.34	0.74
1:B:136:VAL:O	2:F:189:ASN:HB2	1.87	0.74
2:D:264:MET:HB3	2:D:272:PRO:HG3	1.70	0.74
4:H:47[B]:THR:HG21	4:H:122[B]:GLU:HB3	1.68	0.74
1:C:481:LEU:N	1:C:482:PRO:HD3	2.02	0.73
3:G:91[B]:TYR:CD2	3:G:240[B]:ALA:HB1	2.23	0.73
1:B:298:LEU:HD12	1:B:317:PRO:HG3	1.70	0.73
1:B:354:ARG:NH1	1:B:354:ARG:CG	2.40	0.73
2:E:310:ALA:HB3	2:E:311:PRO:HD3	1.70	0.73
3:G:32[C]:LEU:HB2	3:G:238[C]:PHE:HB3	1.69	0.73
3:G:72[A]:PRO:CA	3:G:73[A]:VAL:HB	2.18	0.73
1:B:499:THR:N	1:B:500:PRO:HD3	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:TYR:HE1	2:E:26:ILE:HD11	1.51	0.73
1:B:354:ARG:HH11	1:B:354:ARG:HG2	1.51	0.73
3:G:43[C]:ARG:HA	3:G:46[C]:ALA:HB3	1.68	0.73
4:H:100[A]:HIS:CD2	4:H:120[A]:ALA:HB1	2.23	0.73
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.70	0.73
1:C:328:ALA:O	1:C:332:THR:HG23	1.88	0.73
2:F:255:SER:HA	2:F:271:GLN:HG3	1.70	0.73
1:C:44:LEU:HB3	1:C:47:VAL:HG13	1.69	0.73
2:D:175:LEU:HG	2:D:238:GLN:HE22	1.53	0.73
3:G:71[A]:ARG:HH11	3:G:71[A]:ARG:HG3	1.53	0.73
1:C:354:ARG:HH11	1:C:354:ARG:HG2	1.53	0.73
2:D:374:GLN:HA	2:D:374:GLN:HE21	1.54	0.73
2:D:401:ARG:HD3	2:D:443:GLU:O	1.88	0.73
3:G:172[B]:TYR:CE1	3:G:229[B]:ALA:HA	2.24	0.73
2:E:136:ASP:HB3	2:E:423:VAL:HG13	1.70	0.73
2:F:419:LYS:HE2	2:F:450:GLY:HA3	1.68	0.73
3:G:72[A]:PRO:CB	3:G:73[A]:VAL:HB	2.18	0.73
4:H:9[C]:VAL:HG13	4:H:14[C]:LYS:HA	1.71	0.73
1:C:365:ARG:NH2	2:D:186:ARG:HH22	1.87	0.72
3:G:140[C]:ILE:HD12	3:G:234[C]:LYS:NZ	2.04	0.72
2:F:264:MET:HB2	2:F:272:PRO:HG3	1.71	0.72
3:G:72[B]:PRO:CB	3:G:73[B]:VAL:HB	2.19	0.72
2:E:268:VAL:HG22	2:E:268:VAL:O	1.89	0.72
3:G:92[C]:ASN:HD21	3:G:121[C]:LYS:HB3	1.54	0.72
3:G:45[C]:TYR:CB	4:H:11[C]:PRO:HA	2.19	0.72
4:H:103[A]:ILE:HA	4:H:106[A]:ARG:HB2	1.70	0.72
2:D:255:SER:HA	2:D:271:GLN:HG3	1.71	0.72
3:G:149[C]:ILE:C	3:G:151[C]:ASP:H	1.91	0.72
3:G:80[B]:VAL:HB	3:G:171[B]:PHE:HD1	1.54	0.72
3:G:172[B]:TYR:HE1	3:G:229[B]:ALA:HA	1.53	0.72
4:H:104[C]:LEU:HD13	4:H:118[C]:LYS:HG2	1.70	0.72
2:D:310:ALA:HB3	2:D:311:PRO:HD3	1.72	0.72
2:E:156:GLY:O	2:E:159:VAL:HG12	1.90	0.72
3:G:98[C]:LEU:O	3:G:102[C]:THR:HG23	1.89	0.72
1:C:438:TYR:HA	1:C:441:THR:HG22	1.70	0.72
2:D:301:VAL:HG13	2:D:306:TYR:HE1	1.54	0.72
3:G:72[C]:PRO:CB	3:G:73[C]:VAL:HG22	2.19	0.72
1:C:326:VAL:HG11	1:C:343:PHE:HE2	1.55	0.72
1:C:390:ARG:HH21	1:C:391:GLU:HG2	1.54	0.72
3:G:146[C]:LEU:HA	3:G:227[C]:TYR:HH	1.55	0.72
1:A:415:ARG:HG3	1:A:415:ARG:HH11	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ARG:HH11	1:B:415:ARG:HG3	1.54	0.71
2:F:136:ASP:HB3	2:F:423:VAL:HG13	1.71	0.71
1:A:440:VAL:HA	1:A:445:MET:HG3	1.71	0.71
2:E:175:LEU:HG	2:E:238:GLN:HE22	1.54	0.71
3:G:131[A]:TYR:H	3:G:132[A]:PRO:HA	1.54	0.71
3:G:32[A]:LEU:HD23	3:G:238[A]:PHE:CG	2.26	0.71
2:E:142:ALA:HB2	2:E:346:ILE:HD13	1.73	0.71
1:A:275:LEU:H	2:D:264:MET:HE1	1.55	0.71
2:E:301:VAL:HG13	2:E:306:TYR:HE1	1.55	0.71
2:E:416:MET:H	2:E:417:PRO:HA	1.55	0.71
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.71	0.71
3:G:144[B]:PRO:O	3:G:145[B]:SER:HB2	1.90	0.71
3:G:176[C]:VAL:HB	3:G:180[C]:VAL:HG23	1.71	0.71
1:A:390:ARG:HH21	1:A:391:GLU:HG2	1.56	0.71
1:A:438:TYR:HA	1:A:441:THR:HG22	1.72	0.71
2:F:268:VAL:HG22	2:F:268:VAL:O	1.91	0.71
1:A:137:MET:HG3	2:E:98:ASP:HA	1.73	0.71
1:B:298:LEU:H	1:B:298:LEU:HD22	1.56	0.71
2:D:136:ASP:HB3	2:D:423:VAL:HG13	1.73	0.71
3:G:32[B]:LEU:CD2	3:G:238[B]:PHE:HB3	2.20	0.71
4:H:6[B]:VAL:HG11	4:H:23[B]:VAL:HG21	1.72	0.71
1:A:342:ILE:HA	1:A:362:SER:OG	1.91	0.71
1:B:151:LYS:N	1:B:422:GLN:HE22	1.85	0.71
1:C:342:ILE:HA	1:C:362:SER:OG	1.90	0.70
2:E:255:SER:HA	2:E:271:GLN:HG3	1.71	0.70
2:F:374:GLN:HA	2:F:374:GLN:HE21	1.56	0.70
3:G:71[B]:ARG:HH21	3:G:163[B]:GLU:HG2	1.54	0.70
1:A:151:LYS:N	1:A:422:GLN:HE22	1.83	0.70
1:C:462:SER:CA	1:C:465:ARG:NH1	2.53	0.70
3:G:131[B]:TYR:H	3:G:132[B]:PRO:HA	1.56	0.70
3:G:5[A]:ARG:H	3:G:5[A]:ARG:HH11	1.38	0.70
2:F:401:ARG:HD3	2:F:443:GLU:O	1.92	0.70
3:G:32[A]:LEU:HD23	3:G:238[A]:PHE:CD2	2.27	0.70
1:C:298:LEU:HD12	1:C:317:PRO:HG3	1.72	0.70
2:D:226:LEU:HD11	2:D:284:ARG:HB2	1.74	0.70
3:G:132[C]:PRO:O	3:G:133[C]:VAL:HB	1.91	0.70
1:C:171:ARG:NH1	1:C:171:ARG:CG	2.48	0.70
2:D:264:MET:HB2	2:D:272:PRO:HG3	1.74	0.70
2:F:301:VAL:HG13	2:F:306:TYR:HE1	1.56	0.70
4:H:100[B]:HIS:HD2	4:H:117[B]:HIS:HD2	1.40	0.70
4:H:22[C]:ILE:HG13	4:H:53[C]:LYS:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:LEU:HG	2:F:138:LEU:HD13	1.74	0.70
1:B:326:VAL:HG11	1:B:343:PHE:HE2	1.57	0.69
1:A:326:VAL:HG11	1:A:343:PHE:HE2	1.57	0.69
2:F:310:ALA:HB3	2:F:311:PRO:HD3	1.74	0.69
1:A:343:PHE:CD1	1:A:361:ILE:HG13	2.27	0.69
2:D:65:VAL:O	2:D:68:LEU:HG	1.93	0.69
4:H:14[B]:LYS:HZ2	4:H:17[B]:GLN:HG2	1.55	0.69
3:G:77[C]:GLY:HA3	3:G:165[C]:PHE:CZ	2.28	0.69
1:C:343:PHE:CD1	1:C:361:ILE:HG13	2.28	0.69
2:E:419:LYS:HE2	2:E:450:GLY:HA3	1.73	0.69
3:G:48[A]:LYS:HG3	3:G:49[A]:ILE:H	1.56	0.69
1:B:388:GLN:HG3	1:B:409:LYS:NZ	2.08	0.69
1:A:275:LEU:HB3	2:D:264:MET:HG3	1.74	0.69
1:B:438:TYR:HA	1:B:441:THR:HG22	1.74	0.69
2:E:264:MET:HB2	2:E:272:PRO:HG3	1.73	0.69
2:E:374:GLN:HA	2:E:374:GLN:HE21	1.57	0.69
2:F:264:MET:HB3	2:F:265:PRO:CA	2.22	0.69
4:H:27[A]:GLY:H	4:H:31[A]:GLU:HA	1.57	0.69
3:G:8[B]:LYS:HD2	3:G:263[B]:PHE:CE1	2.28	0.69
1:C:151:LYS:H	1:C:422:GLN:NE2	1.84	0.69
1:C:401:ASP:HB3	1:C:406:THR:HG22	1.74	0.69
2:E:408:HIS:ND1	2:E:418:GLY:HA3	2.08	0.69
4:H:20[A]:ALA:HA	4:H:54[A]:GLN:HB3	1.75	0.69
1:B:48:MET:CE	1:B:94:ILE:HG23	2.23	0.69
1:A:48:MET:HB3	2:E:63:GLY:HA2	1.75	0.69
2:D:398:LYS:HD3	2:D:446:PHE:CE1	2.27	0.69
3:G:172[A]:TYR:HD1	3:G:173[A]:ASN:H	1.41	0.69
2:D:408:HIS:ND1	2:D:418:GLY:HA3	2.08	0.68
2:E:416:MET:N	2:E:417:PRO:HA	2.08	0.68
1:A:438:TYR:CE1	1:A:487:LEU:HD12	2.27	0.68
1:B:164:ARG:HH22	2:F:184:ARG:HD3	1.59	0.68
2:F:264:MET:HB3	2:F:272:PRO:HG3	1.73	0.68
3:G:66[C]:PRO:O	3:G:67[C]:MET:HB3	1.92	0.68
3:G:148[C]:GLU:HG2	3:G:149[C]:ILE:HG13	1.75	0.68
4:H:66[C]:GLY:CA	4:H:79[C]:ALA:HA	2.24	0.68
1:A:481:LEU:N	1:A:482:PRO:HD3	2.08	0.68
1:B:390:ARG:HH21	1:B:391:GLU:HG2	1.58	0.68
3:G:143[A]:THR:H	3:G:144[A]:PRO:HA	1.57	0.68
3:G:80[C]:VAL:HG11	3:G:126[C]:PHE:CE2	2.28	0.68
3:G:176[C]:VAL:HG12	3:G:177[C]:SER:N	2.08	0.68
3:G:172[C]:TYR:HE1	3:G:232[C]:ASP:HB3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:9[A]:VAL:HG22	4:H:14[A]:LYS:HE3	1.75	0.68
1:A:415:ARG:NH1	1:A:415:ARG:HG2	2.08	0.68
1:B:481:LEU:N	1:B:482:PRO:HD3	2.09	0.68
3:G:72[B]:PRO:HA	3:G:73[B]:VAL:HB	1.75	0.68
3:G:90[B]:PRO:HB2	3:G:94[B]:ASN:HD22	1.58	0.68
3:G:45[C]:TYR:CG	4:H:11[C]:PRO:HA	2.29	0.68
4:H:24[C]:ILE:HD11	4:H:51[C]:ARG:HB2	1.76	0.68
1:B:275:LEU:H	2:E:264:MET:HE1	1.58	0.68
2:F:8:GLN:HB2	2:F:15:ASP:HB2	1.76	0.68
1:B:342:ILE:HA	1:B:362:SER:OG	1.93	0.68
2:D:162:GLN:HE22	2:D:194:GLU:HG2	1.57	0.68
1:B:79:TYR:CE1	2:E:26:ILE:HD11	2.28	0.68
3:G:68[A]:LEU:HA	3:G:160[A]:PHE:HE2	1.59	0.68
3:G:253[C]:THR:HG22	3:G:254[C]:GLU:N	2.08	0.68
2:D:156:GLY:O	2:D:159:VAL:HG12	1.93	0.68
2:F:156:GLY:O	2:F:159:VAL:HG12	1.94	0.68
2:F:398:LYS:HD3	2:F:446:PHE:CE1	2.29	0.68
3:G:107[C]:HIS:C	3:G:109[C]:SER:H	1.95	0.68
1:A:354:ARG:NH1	1:A:354:ARG:CG	2.40	0.67
2:D:137:LEU:HG	2:D:138:LEU:HD13	1.75	0.67
3:G:144[A]:PRO:HG2	3:G:230[A]:LEU:CD1	2.24	0.67
1:C:161:ARG:HH12	1:C:190:ASP:HB3	1.59	0.67
1:C:48:MET:CE	1:C:94:ILE:HG23	2.24	0.67
2:F:91:ASN:HD21	2:F:95:GLU:H	1.42	0.67
1:B:275:LEU:CD2	2:E:264:MET:HA	2.21	0.67
3:G:104[C]:GLU:HA	3:G:107[C]:HIS:HD1	1.60	0.67
1:A:328:ALA:O	1:A:332:THR:HG23	1.94	0.67
1:A:48:MET:HE3	1:A:94:ILE:HG23	1.76	0.67
1:B:415:ARG:HG2	1:B:415:ARG:NH1	2.08	0.67
1:B:401:ASP:HB3	1:B:406:THR:HG22	1.74	0.67
4:H:4[B]:VAL:HG21	4:H:37[B]:GLY:H	1.60	0.67
2:F:384:GLU:OE2	3:G:87[B]:LEU:HA	1.95	0.67
3:G:123[B]:ARG:HG3	3:G:136[B]:GLU:OE2	1.95	0.67
2:D:152:GLY:H	2:D:155:VAL:CG2	2.08	0.67
2:E:135:ILE:HD12	2:E:141:TYR:CZ	2.30	0.67
2:E:8:GLN:HB2	2:E:15:ASP:HB2	1.75	0.67
2:F:135:ILE:HD12	2:F:141:TYR:CZ	2.29	0.67
3:G:113[B]:TYR:O	3:G:114[B]:VAL:HG22	1.95	0.67
3:G:66[A]:PRO:HD2	3:G:68[A]:LEU:HD23	1.77	0.67
1:A:388:GLN:HG3	1:A:409:LYS:NZ	2.10	0.67
1:A:440:VAL:HG12	1:A:445:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:LEU:HG	2:E:138:LEU:HD13	1.77	0.67
3:G:79[C]:MET:O	3:G:170[C]:ILE:HA	1.95	0.67
3:G:92[A]:ASN:O	3:G:95[A]:ILE:HG22	1.95	0.67
4:H:81[B]:THR:HG21	4:H:127[B]:ARG:HH21	1.58	0.67
1:A:401:ASP:HB3	1:A:406:THR:HG22	1.76	0.67
1:B:129:ILE:HD11	1:B:237:LEU:HD22	1.77	0.67
3:G:96[C]:LEU:HD13	3:G:125[C]:PHE:CD1	2.29	0.67
4:H:24[B]:ILE:HG22	4:H:33[B]:GLY:HA2	1.75	0.67
1:B:44:LEU:HB3	1:B:47:VAL:CG1	2.26	0.66
3:G:85[C]:ARG:HH12	3:G:238[C]:PHE:HZ	1.41	0.66
1:C:114:PRO:HG3	1:C:121:ILE:HD12	1.78	0.66
1:B:386:LEU:HD23	1:B:386:LEU:H	1.60	0.66
1:C:140:LYS:HE2	1:C:143:HIS:CE1	2.30	0.66
2:D:379:ILE:HD11	3:G:17[C]:THR:CG2	2.25	0.66
2:F:175:LEU:HG	2:F:238:GLN:HE22	1.59	0.66
3:G:86[B]:GLY:HA2	3:G:241[B]:ARG:HH22	1.61	0.66
1:B:294:HIS:O	1:B:298:LEU:HD22	1.95	0.66
2:D:308:ASP:O	2:D:311:PRO:HD2	1.96	0.66
3:G:142[B]:ASP:HA	3:G:234[B]:LYS:HZ3	1.61	0.66
3:G:32[C]:LEU:HD23	3:G:238[C]:PHE:CD2	2.29	0.66
1:A:151:LYS:H	1:A:422:GLN:NE2	1.86	0.66
2:D:142:ALA:HB2	2:D:346:ILE:HD13	1.76	0.66
2:F:226:LEU:HD11	2:F:284:ARG:HB2	1.76	0.66
1:B:52:LEU:O	1:B:91:THR:HB	1.96	0.66
1:A:83:ARG:HB2	2:D:47:HIS:HE1	1.56	0.66
2:D:91:ASN:HD21	2:D:95:GLU:H	1.44	0.66
2:F:416:MET:N	2:F:417:PRO:HA	2.11	0.66
3:G:160[C]:PHE:CB	3:G:189[C]:LEU:HD23	2.26	0.66
1:B:161:ARG:HH12	1:B:190:ASP:HB3	1.61	0.66
1:C:44:LEU:HB3	1:C:47:VAL:CG1	2.26	0.66
3:G:80[B]:VAL:HA	3:G:171[B]:PHE:HB2	1.78	0.66
3:G:87[C]:LEU:N	3:G:241[C]:ARG:NH2	2.36	0.66
4:H:60[C]:LEU:HB2	4:H:130[C]:VAL:HG13	1.76	0.66
1:A:52:LEU:O	1:A:91:THR:HB	1.96	0.66
3:G:152[C]:ILE:H	3:G:152[C]:ILE:HD12	1.61	0.66
4:H:22[B]:ILE:HG13	4:H:53[B]:LYS:HD2	1.77	0.66
1:B:275:LEU:HD22	2:E:264:MET:CA	2.22	0.65
1:B:62:MET:HB2	1:B:95:MET:CE	2.22	0.65
1:C:480:GLU:O	1:C:481:LEU:HB3	1.95	0.65
1:A:262:ASP:H	1:A:318:PHE:HB2	1.60	0.65
2:D:264:MET:HB3	2:D:265:PRO:CA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32[B]:LEU:CG	3:G:238[B]:PHE:CB	2.74	0.65
2:E:144:GLY:HA2	2:E:293:ILE:O	1.97	0.65
1:A:298:LEU:HD12	1:A:317:PRO:HG3	1.77	0.65
1:A:449:PRO:HB2	1:A:452:ASP:HB2	1.79	0.65
1:B:343:PHE:CD1	1:B:361:ILE:HG13	2.31	0.65
2:D:8:GLN:HB2	2:D:15:ASP:HB2	1.79	0.65
2:D:416:MET:H	2:D:417:PRO:HA	1.60	0.65
1:A:365:ARG:HH21	2:E:186:ARG:NH2	1.92	0.65
2:E:65:VAL:O	2:E:68:LEU:HG	1.97	0.65
3:G:113[A]:TYR:O	3:G:114[A]:VAL:HG22	1.97	0.65
4:H:14[B]:LYS:NZ	4:H:17[B]:GLN:HG2	2.11	0.65
1:C:48:MET:HE3	1:C:94:ILE:HG23	1.77	0.65
3:G:65[C]:HIS:HD2	3:G:69[C]:GLU:CA	2.10	0.65
3:G:79[B]:MET:HG3	3:G:116[B]:PHE:HB2	1.79	0.65
4:H:39[A]:ILE:H	4:H:39[A]:ILE:HD13	1.61	0.65
4:H:9[C]:VAL:HG21	4:H:14[C]:LYS:HD2	1.78	0.65
1:A:140:LYS:HE2	1:A:143:HIS:CE1	2.31	0.65
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.27	0.65
1:C:449:PRO:HB2	1:C:452:ASP:HB2	1.78	0.65
1:C:419:ILE:HG21	1:C:440:VAL:HG11	1.78	0.65
3:G:32[B]:LEU:CG	3:G:238[B]:PHE:HB2	2.26	0.65
2:D:416:MET:N	2:D:417:PRO:HA	2.11	0.64
1:B:462:SER:CA	1:B:465:ARG:NH1	2.56	0.64
4:H:13[B]:ARG:NH1	4:H:13[B]:ARG:HG3	2.08	0.64
3:G:91[A]:TYR:CD2	3:G:240[A]:ALA:HB1	2.31	0.64
3:G:66[C]:PRO:HD2	3:G:68[C]:LEU:HD23	1.80	0.64
1:A:114:PRO:HG3	1:A:121:ILE:HD12	1.79	0.64
1:B:140:LYS:HE2	1:B:143:HIS:CE1	2.32	0.64
2:E:226:LEU:HD11	2:E:284:ARG:HB2	1.79	0.64
2:F:416:MET:H	2:F:417:PRO:HA	1.60	0.64
2:E:125:ASP:CG	2:E:345:ARG:HH22	2.01	0.64
2:F:162:GLN:HE22	2:F:194:GLU:HG2	1.62	0.64
4:H:51[B]:ARG:HE	4:H:60[B]:LEU:HD21	1.62	0.64
1:B:438:TYR:CE1	1:B:487:LEU:HD12	2.33	0.64
2:D:379:ILE:HD11	3:G:17[C]:THR:HG21	1.78	0.64
3:G:82[B]:THR:HG22	3:G:95[B]:ILE:HD13	1.78	0.64
3:G:91[B]:TYR:CG	3:G:240[B]:ALA:HB1	2.32	0.64
1:C:52:LEU:O	1:C:91:THR:HB	1.96	0.64
3:G:146[A]:LEU:HD12	4:H:81[A]:THR:HB	1.78	0.64
1:A:100:GLY:HA2	1:A:248:TYR:CE2	2.33	0.64
2:D:135:ILE:HD12	2:D:141:TYR:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:162:GLN:HE22	2:E:194:GLU:HG2	1.63	0.64
3:G:184[A]:VAL:HG22	3:G:185[A]:GLU:H	1.61	0.64
1:C:66:LEU:HB3	2:D:66:ARG:CD	2.26	0.63
2:E:291:GLY:O	2:E:292:SER:HB2	1.98	0.63
4:H:8[B]:ILE:CG1	4:H:15[B]:VAL:HB	2.28	0.63
4:H:8[C]:ILE:HG13	4:H:15[C]:VAL:HB	1.78	0.63
3:G:77[A]:GLY:O	3:G:168[A]:LEU:HA	1.98	0.63
3:G:16[C]:ASN:O	3:G:19[C]:GLN:HB2	1.98	0.63
3:G:41[C]:ASN:HB3	4:H:13[C]:ARG:HE	1.63	0.63
1:C:156:MET:CE	1:C:383:ARG:HA	2.29	0.63
2:D:268:VAL:O	2:D:268:VAL:HG22	1.98	0.63
2:F:65:VAL:O	2:F:68:LEU:HG	1.98	0.63
2:D:291:GLY:O	2:D:292:SER:HB2	1.98	0.63
4:H:41[C]:LEU:HB2	4:H:70[C]:VAL:HB	1.80	0.63
1:C:388:GLN:HG3	1:C:409:LYS:NZ	2.14	0.63
1:A:161:ARG:HH12	1:A:190:ASP:HB3	1.62	0.63
1:A:462:SER:HB3	1:A:465:ARG:HH12	1.63	0.63
1:A:62:MET:HB2	1:A:95:MET:CE	2.26	0.63
1:B:156:MET:CE	1:B:383:ARG:HA	2.27	0.63
1:B:46:LYS:NZ	1:B:46:LYS:HB2	2.14	0.63
2:D:90:PHE:HE2	2:D:103:VAL:HG21	1.63	0.63
2:E:152:GLY:H	2:E:155:VAL:CG2	2.12	0.63
2:F:308:ASP:O	2:F:311:PRO:HD2	1.98	0.63
3:G:87[A]:LEU:HG	3:G:245[A]:MET:HE1	1.80	0.63
4:H:45[C]:LEU:HG	4:H:68[C]:LEU:HG	1.80	0.63
2:F:460:LYS:O	2:F:461:LYS:HD2	1.97	0.63
4:H:13[C]:ARG:HD2	4:H:13[C]:ARG:N	2.13	0.63
1:B:136:VAL:HG12	2:F:185:THR:HG23	1.80	0.63
1:C:298:LEU:H	1:C:298:LEU:HD22	1.64	0.63
4:H:21[B]:ASP:HB2	4:H:22[B]:ILE:HD13	1.80	0.63
1:B:449:PRO:HB2	1:B:452:ASP:HB2	1.80	0.62
2:D:125:ASP:CG	2:D:345:ARG:HH22	2.02	0.62
3:G:153[C]:ALA:O	3:G:157[C]:ILE:HD12	1.99	0.62
3:G:238[A]:PHE:CE2	3:G:241[A]:ARG:NH1	2.66	0.62
3:G:32[B]:LEU:HG	3:G:238[B]:PHE:HB3	1.81	0.62
4:H:100[C]:HIS:HD2	4:H:117[C]:HIS:CD2	2.17	0.62
1:B:448:ILE:HG23	1:B:449:PRO:HD2	1.81	0.62
1:C:415:ARG:NH1	1:C:415:ARG:HG2	2.12	0.62
2:D:213:GLU:HG3	2:D:214:PRO:CD	2.28	0.62
2:F:152:GLY:H	2:F:155:VAL:CG2	2.11	0.62
2:E:264:MET:HB3	2:E:265:PRO:CA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:45[A]:LEU:HD21	4:H:68[A]:LEU:HD11	1.80	0.62
1:C:475:ILE:HG12	1:C:481:LEU:HA	1.81	0.62
2:E:90:PHE:HE2	2:E:103:VAL:HG21	1.64	0.62
3:G:104[C]:GLU:HA	3:G:107[C]:HIS:ND1	2.15	0.62
4:H:86[C]:GLU:HG2	4:H:134[C]:LYS:HB3	1.80	0.62
1:A:46:LYS:HB2	1:A:46:LYS:NZ	2.15	0.62
1:C:390:ARG:NH2	1:C:391:GLU:HG2	2.13	0.62
1:C:47:VAL:HG21	1:C:71:VAL:HG21	1.81	0.62
2:D:233:ARG:O	2:D:237:GLY:HA2	1.99	0.62
2:D:125:ASP:OD2	2:D:345:ARG:NH2	2.32	0.62
3:G:104[B]:GLU:HA	3:G:107[B]:HIS:ND1	2.13	0.62
4:H:109[B]:LYS:HB2	4:H:109[B]:LYS:NZ	2.14	0.62
4:H:109[C]:LYS:O	4:H:112[C]:LYS:HE3	2.00	0.62
4:H:4[A]:VAL:HG23	4:H:36[A]:ALA:HA	1.81	0.62
3:G:142[B]:ASP:HA	3:G:234[B]:LYS:HZ1	1.62	0.62
3:G:67[B]:MET:SD	3:G:161[B]:ALA:HA	2.39	0.62
2:F:395:ARG:NH2	2:F:436:GLY:HA3	2.14	0.62
3:G:177[B]:SER:HB3	3:G:180[B]:VAL:HG13	1.81	0.62
3:G:81[A]:ILE:HG21	3:G:230[A]:LEU:HD23	1.82	0.62
4:H:110[C]:THR:HB	4:H:112[C]:LYS:NZ	2.14	0.62
1:A:386:LEU:H	1:A:386:LEU:HD23	1.63	0.62
1:B:358:ASN:O	1:B:362:SER:HB2	1.99	0.62
1:C:440:VAL:HG12	1:C:445:MET:CE	2.28	0.61
3:G:221[C]:TYR:CE2	3:G:225[C]:LEU:HD11	2.36	0.61
3:G:15[B]:LYS:HZ3	3:G:256[B]:LEU:HD21	1.64	0.61
3:G:5[A]:ARG:HH11	3:G:5[A]:ARG:N	1.97	0.61
4:H:84[B]:LEU:HB3	4:H:85[B]:PRO:CD	2.30	0.61
2:E:301:VAL:HG13	2:E:306:TYR:CE1	2.36	0.61
3:G:112[C]:GLU:O	3:G:114[C]:VAL:N	2.33	0.61
3:G:176[C]:VAL:HG12	3:G:177[C]:SER:H	1.65	0.61
4:H:84[B]:LEU:HB3	4:H:85[B]:PRO:HD2	1.81	0.61
1:A:358:ASN:O	1:A:362:SER:HB2	2.00	0.61
1:B:275:LEU:N	2:E:264:MET:HE1	2.15	0.61
1:B:345:GLU:HG2	1:B:358:ASN:HB2	1.83	0.61
3:G:91[A]:TYR:O	3:G:92[A]:ASN:HB2	2.01	0.61
3:G:168[B]:LEU:HB3	3:G:189[B]:LEU:HB2	1.82	0.61
4:H:108[C]:ASP:O	4:H:112[C]:LYS:HE3	2.00	0.61
1:A:345:GLU:HG2	1:A:358:ASN:HB2	1.83	0.61
1:A:448:ILE:HG23	1:A:449:PRO:HD2	1.82	0.61
1:B:275:LEU:HA	1:B:278:ARG:N	2.16	0.61
2:F:233:ARG:O	2:F:237:GLY:HA2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:116[C]:PHE:HD1	3:G:152[C]:ILE:HG23	1.65	0.61
3:G:28[A]:ALA:HA	3:G:238[A]:PHE:CD1	2.35	0.61
3:G:71[A]:ARG:NH1	3:G:71[A]:ARG:HG3	2.15	0.61
1:B:440:VAL:HA	1:B:445:MET:CG	2.31	0.61
1:C:100:GLY:HA2	1:C:248:TYR:CE2	2.36	0.61
1:C:462:SER:HB3	1:C:465:ARG:HH12	1.65	0.61
2:E:398:LYS:HD3	2:E:446:PHE:CZ	2.36	0.61
4:H:110[B]:THR:HB	4:H:112[B]:LYS:HG3	1.81	0.61
2:E:375:ASP:O	2:E:379:ILE:HG23	2.01	0.61
3:G:135[C]:GLU:OE1	3:G:152[C]:ILE:HG13	2.00	0.61
3:G:218[C]:LEU:HD23	3:G:218[C]:LEU:O	2.01	0.61
1:A:475:ILE:HG12	1:A:481:LEU:HA	1.83	0.61
1:A:79:TYR:CE1	2:D:26:ILE:HD11	2.31	0.61
1:B:275:LEU:CB	2:E:264:MET:CG	2.72	0.61
3:G:38[A]:THR:CG2	4:H:13[A]:ARG:HH21	2.13	0.61
1:A:480:GLU:O	1:A:481:LEU:HB3	2.00	0.61
1:B:475:ILE:HG12	1:B:481:LEU:HA	1.82	0.61
1:C:386:LEU:H	1:C:386:LEU:HD23	1.65	0.61
2:E:125:ASP:OD2	2:E:345:ARG:NH2	2.33	0.61
3:G:72[A]:PRO:HA	3:G:73[A]:VAL:HB	1.80	0.61
4:H:40[C]:PRO:HA	4:H:70[C]:VAL:O	2.00	0.61
1:C:345:GLU:HG2	1:C:358:ASN:HB2	1.81	0.60
1:C:62:MET:HB2	1:C:95:MET:CE	2.28	0.60
2:E:401:ARG:HD3	2:E:443:GLU:O	2.01	0.60
2:F:91:ASN:ND2	2:F:95:GLU:H	1.97	0.60
3:G:67[C]:MET:C	3:G:69[C]:GLU:H	2.03	0.60
1:A:275:LEU:HD13	2:D:264:MET:HG3	1.83	0.60
1:A:390:ARG:NH2	1:A:391:GLU:HG2	2.16	0.60
1:C:354:ARG:CG	1:C:354:ARG:NH1	2.40	0.60
1:C:481:LEU:N	1:C:482:PRO:CD	2.65	0.60
1:A:41:VAL:HG21	1:A:88:VAL:HG21	1.83	0.60
1:C:440:VAL:HA	1:C:445:MET:CG	2.29	0.60
3:G:175[B]:PHE:HD1	3:G:236[B]:SER:HA	1.65	0.60
3:G:255[C]:MET:HA	3:G:258[C]:THR:HG23	1.81	0.60
3:G:33[B]:ARG:C	3:G:35[B]:ALA:H	2.04	0.60
1:C:294:HIS:O	1:C:298:LEU:HD22	2.00	0.60
2:F:149:LEU:HD21	2:F:324:LEU:HD22	1.84	0.60
3:G:68[C]:LEU:N	3:G:68[C]:LEU:HD22	2.15	0.60
1:B:114:PRO:HG3	1:B:121:ILE:HD12	1.84	0.60
1:B:440:VAL:HG12	1:B:445:MET:CE	2.32	0.60
2:D:460:LYS:O	2:D:461:LYS:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:ASN:HD21	2:E:95:GLU:H	1.48	0.60
2:F:226:LEU:O	2:F:230:GLU:HG3	2.02	0.60
4:H:100[C]:HIS:HD2	4:H:117[C]:HIS:HD2	1.50	0.60
1:B:419:ILE:HG21	1:B:440:VAL:HG11	1.82	0.60
1:B:47:VAL:HG21	1:B:71:VAL:HG21	1.84	0.60
2:D:91:ASN:ND2	2:D:95:GLU:H	1.99	0.60
3:G:131[C]:TYR:N	3:G:132[C]:PRO:HA	2.09	0.60
3:G:17[B]:THR:O	3:G:17[B]:THR:HG22	2.02	0.60
1:A:140:LYS:CE	1:A:143:HIS:CE1	2.85	0.60
1:A:143:HIS:CD2	1:A:144:GLU:HG2	2.37	0.60
1:A:419:ILE:HG21	1:A:440:VAL:HG11	1.82	0.60
3:G:78[B]:TYR:CD1	3:G:115[B]:ILE:HG22	2.37	0.60
4:H:49[B]:PRO:HG3	4:H:130[B]:VAL:HG22	1.84	0.60
1:C:275:LEU:HB3	2:F:264:MET:CG	2.32	0.60
1:C:440:VAL:CA	1:C:445:MET:HG3	2.32	0.60
2:D:144:GLY:HA2	2:D:293:ILE:O	2.02	0.60
1:B:365:ARG:HH21	2:F:186:ARG:HH22	1.47	0.60
2:F:291:GLY:O	2:F:292:SER:HB2	2.02	0.60
4:H:121[B]:LEU:HD22	4:H:125[B]:GLU:OE2	2.02	0.60
2:F:213:GLU:HG3	2:F:214:PRO:CD	2.31	0.60
3:G:113[C]:TYR:O	3:G:114[C]:VAL:HG22	2.02	0.60
3:G:11[A]:ILE:O	3:G:15[A]:LYS:HG3	2.02	0.60
3:G:120[B]:ARG:HD3	3:G:123[B]:ARG:NH2	2.14	0.60
4:H:100[C]:HIS:CD2	4:H:117[C]:HIS:HD2	2.20	0.60
1:B:298:LEU:HD21	1:B:337:ILE:HG21	1.83	0.59
3:G:149[C]:ILE:C	3:G:151[C]:ASP:N	2.55	0.59
3:G:28[C]:ALA:HB3	3:G:242[C]:MET:HB3	1.83	0.59
3:G:31[A]:LYS:HG2	3:G:32[A]:LEU:HD22	1.83	0.59
4:H:23[C]:VAL:HB	4:H:34[C]:VAL:HB	1.84	0.59
1:A:252:LYS:HD3	1:A:254:LYS:HE2	1.84	0.59
1:A:298:LEU:HD21	1:A:337:ILE:HG21	1.84	0.59
1:A:151:LYS:HE2	1:A:428:MET:HE3	1.84	0.59
1:B:390:ARG:NH2	1:B:391:GLU:HG2	2.17	0.59
1:C:140:LYS:CE	1:C:143:HIS:CE1	2.85	0.59
2:F:144:GLY:HA2	2:F:293:ILE:O	2.02	0.59
4:H:45[A]:LEU:HD11	4:H:68[A]:LEU:HD21	1.84	0.59
3:G:129[C]:ARG:O	3:G:131[C]:TYR:HD1	1.86	0.59
1:C:358:ASN:O	1:C:362:SER:HB2	2.01	0.59
2:D:149:LEU:HD21	2:D:324:LEU:HD22	1.84	0.59
2:E:416:MET:HB2	2:E:417:PRO:O	2.02	0.59
2:E:438:HIS:HB3	2:E:441:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:15[B]:LYS:HG3	3:G:256[B]:LEU:HD11	1.84	0.59
1:A:412:ARG:NH2	1:A:443:GLY:N	2.50	0.59
2:E:395:ARG:NH2	2:E:436:GLY:HA3	2.17	0.59
3:G:107[C]:HIS:C	3:G:109[C]:SER:N	2.54	0.59
4:H:22[A]:ILE:HD11	4:H:53[A]:LYS:HD2	1.83	0.59
1:A:435:ILE:HD12	1:A:472:LEU:HD21	1.84	0.59
3:G:241[C]:ARG:O	3:G:245[C]:MET:HG2	2.02	0.59
3:G:48[C]:LYS:HD3	4:H:78[C]:LEU:CD2	2.27	0.59
3:G:91[A]:TYR:CG	3:G:240[A]:ALA:HB1	2.37	0.59
1:A:164:ARG:NH2	2:E:184:ARG:HD3	2.12	0.59
2:F:125:ASP:CG	2:F:345:ARG:HH22	2.05	0.59
3:G:256[B]:LEU:HD23	3:G:256[B]:LEU:O	2.03	0.59
4:H:111[C]:ASP:O	4:H:112[C]:LYS:HB2	2.03	0.59
1:B:36:ASP:OD2	2:E:263:ARG:HD3	2.01	0.59
2:D:266:SER:OG	2:D:268:VAL:HG12	2.03	0.59
3:G:177[C]:SER:OG	3:G:180[C]:VAL:HG22	2.03	0.59
3:G:144[C]:PRO:HG2	3:G:230[C]:LEU:HD13	1.85	0.59
4:H:110[C]:THR:CA	4:H:112[C]:LYS:HE2	2.33	0.59
1:A:156:MET:CE	1:A:383:ARG:HA	2.29	0.59
2:D:182:GLY:H	2:D:210:GLN:H	1.51	0.59
3:G:29[A]:ALA:HB2	3:G:242[A]:MET:SD	2.43	0.59
4:H:8[B]:ILE:HG13	4:H:15[B]:VAL:HB	1.85	0.59
1:C:188:GLY:O	1:C:189:GLN:HB2	2.03	0.59
1:C:438:TYR:CE1	1:C:487:LEU:HD12	2.37	0.59
2:F:266:SER:OG	2:F:268:VAL:HG12	2.02	0.58
3:G:123[B]:ARG:HD2	3:G:124[B]:ASP:OD2	2.03	0.58
3:G:71[C]:ARG:NH2	3:G:163[C]:GLU:HG3	2.18	0.58
2:E:40:LEU:HD23	2:E:64:LEU:HD11	1.85	0.58
3:G:114[C]:VAL:HB	3:G:134[C]:VAL:HG13	1.84	0.58
3:G:160[C]:PHE:HB3	3:G:189[C]:LEU:HD23	1.85	0.58
3:G:18[C]:ARG:NH1	3:G:253[C]:THR:OG1	2.32	0.58
4:H:34[A]:VAL:HG13	4:H:38[A]:HIS:ND1	2.19	0.58
4:H:51[C]:ARG:CG	4:H:60[C]:LEU:HA	2.31	0.58
1:C:31:VAL:HG11	1:C:34:VAL:HG22	1.85	0.58
2:E:139:ALA:N	2:E:140:PRO:HD3	2.18	0.58
4:H:60[A]:LEU:HD13	4:H:130[A]:VAL:HA	1.84	0.58
2:D:301:VAL:HG13	2:D:306:TYR:CE1	2.36	0.58
2:F:226:LEU:HD11	2:F:284:ARG:CB	2.33	0.58
3:G:45[C]:TYR:CE2	3:G:224[C]:THR:HG21	2.33	0.58
3:G:28[A]:ALA:HA	3:G:238[A]:PHE:HD1	1.68	0.58
4:H:49[A]:PRO:HA	4:H:61[A]:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:NH2	1:B:443:GLY:N	2.51	0.58
1:B:188:GLY:O	1:B:189:GLN:HB2	2.04	0.58
3:G:189[B]:LEU:HB3	3:G:190[B]:PRO:HD3	1.85	0.58
3:G:95[B]:ILE:O	3:G:99[B]:VAL:HG13	2.04	0.58
4:H:103[B]:ILE:HD11	4:H:117[B]:HIS:NE2	2.19	0.58
1:B:382:LEU:O	1:B:386:LEU:HD23	2.03	0.58
3:G:126[B]:PHE:HB3	3:G:132[B]:PRO:O	2.04	0.58
3:G:177[B]:SER:CB	3:G:180[B]:VAL:HG13	2.34	0.58
1:C:275:LEU:H	2:F:264:MET:HE1	1.66	0.58
3:G:94[C]:ASN:HB3	3:G:97[C]:ARG:NH1	2.19	0.58
4:H:50[B]:VAL:HG23	4:H:63[B]:VAL:HG21	1.85	0.58
1:A:275:LEU:CB	2:D:264:MET:HG3	2.34	0.58
2:D:395:ARG:NH2	2:D:436:GLY:HA3	2.18	0.58
2:E:40:LEU:CD2	2:E:64:LEU:HD11	2.33	0.58
2:F:90:PHE:HE2	2:F:103:VAL:HG21	1.68	0.58
3:G:84[C]:ASP:CB	3:G:120[C]:ARG:HB3	2.30	0.58
1:A:382:LEU:O	1:A:386:LEU:HD23	2.04	0.58
2:D:232:PHE:HB2	2:D:240:VAL:HG21	1.86	0.58
3:G:140[C]:ILE:HD12	3:G:234[C]:LYS:HZ3	1.68	0.58
3:G:76[A]:THR:HA	3:G:167[A]:LYS:HD3	1.86	0.58
1:B:140:LYS:CE	1:B:143:HIS:CE1	2.87	0.57
1:B:31:VAL:HG11	1:B:34:VAL:HG22	1.86	0.57
3:G:68[B]:LEU:HD13	3:G:160[B]:PHE:CE2	2.38	0.57
3:G:43[C]:ARG:CA	3:G:46[C]:ALA:HB3	2.34	0.57
4:H:108[C]:ASP:C	4:H:109[C]:LYS:HD2	2.24	0.57
1:C:275:LEU:HB3	2:F:264:MET:HG3	1.85	0.57
2:F:182:GLY:H	2:F:210:GLN:H	1.50	0.57
2:F:416:MET:HB2	2:F:417:PRO:O	2.04	0.57
3:G:144[C]:PRO:HG2	3:G:230[C]:LEU:CD1	2.34	0.57
3:G:78[B]:TYR:OH	3:G:106[B]:ARG:HD2	2.04	0.57
1:C:412:ARG:NH2	1:C:443:GLY:N	2.53	0.57
1:C:499:THR:H	1:C:500:PRO:HD3	1.69	0.57
2:F:111:ILE:HA	2:F:227:THR:OG1	2.05	0.57
3:G:230[C]:LEU:HD22	3:G:230[C]:LEU:O	2.03	0.57
3:G:81[A]:ILE:HA	3:G:118[A]:VAL:HG13	1.85	0.57
2:D:375:ASP:O	2:D:379:ILE:HG23	2.04	0.57
3:G:112[C]:GLU:OE2	3:G:112[C]:GLU:HA	2.03	0.57
2:F:301:VAL:HG13	2:F:306:TYR:CE1	2.39	0.57
3:G:149[B]:ILE:HD12	3:G:150[B]:GLN:N	2.19	0.57
3:G:85[B]:ARG:NH2	3:G:241[B]:ARG:HH21	2.03	0.57
3:G:86[A]:GLY:HA3	3:G:121[A]:LYS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLY:O	1:A:189:GLN:HB2	2.04	0.57
1:C:275:LEU:CG	1:C:278:ARG:HA	2.34	0.57
2:E:131:GLY:HA3	2:E:167:ASN:ND2	2.19	0.57
3:G:38[A]:THR:HG21	4:H:13[A]:ARG:HH21	1.70	0.57
4:H:49[B]:PRO:HG3	4:H:130[B]:VAL:CG2	2.33	0.57
1:C:382:LEU:O	1:C:386:LEU:HD23	2.04	0.57
2:F:371:ASN:CG	3:G:10[B]:ARG:HH11	1.96	0.57
3:G:80[C]:VAL:HG11	3:G:126[C]:PHE:HE2	1.65	0.57
3:G:261[C]:LEU:HD12	3:G:262[C]:GLN:HG3	1.87	0.57
3:G:86[A]:GLY:O	3:G:87[A]:LEU:HB2	2.03	0.57
3:G:92[C]:ASN:ND2	3:G:121[C]:LYS:HB3	2.18	0.57
4:H:100[B]:HIS:HD2	4:H:117[B]:HIS:CD2	2.23	0.57
1:A:109:ASN:OD1	1:A:113:GLN:HG2	2.05	0.57
1:A:136:VAL:O	2:E:189:ASN:HB2	2.05	0.57
1:B:275:LEU:CG	1:B:278:ARG:HA	2.33	0.57
1:C:252:LYS:HD3	1:C:254:LYS:HE2	1.87	0.57
2:F:131:GLY:HA3	2:F:167:ASN:ND2	2.19	0.57
4:H:8[B]:ILE:HA	4:H:77[B]:ILE:HG12	1.87	0.57
1:A:275:LEU:CG	1:A:278:ARG:HA	2.33	0.57
1:A:440:VAL:HA	1:A:445:MET:CG	2.34	0.57
4:H:114[C]:TYR:O	4:H:118[C]:LYS:HB2	2.04	0.57
1:C:79:TYR:CE1	2:F:26:ILE:HD11	2.35	0.57
3:G:91[C]:TYR:CD1	3:G:181[C]:GLN:HG2	2.39	0.57
1:A:415:ARG:CG	1:A:415:ARG:NH1	2.49	0.56
1:B:462:SER:HB3	1:B:465:ARG:HH12	1.69	0.56
2:E:388:GLU:O	2:E:392:ILE:HG23	2.05	0.56
2:F:349:PRO:HG3	2:F:357:TYR:CD2	2.40	0.56
3:G:4[A]:MET:O	3:G:8[A]:LYS:HE3	2.04	0.56
1:B:480:GLU:O	1:B:481:LEU:HB3	2.02	0.56
1:C:140:LYS:NZ	1:C:143:HIS:HE1	2.02	0.56
2:D:181:VAL:HG22	2:D:221:VAL:HG13	1.86	0.56
2:D:241:LEU:HD23	2:D:243:PHE:CZ	2.40	0.56
3:G:140[B]:ILE:O	3:G:141[B]:SER:HB3	2.05	0.56
3:G:140[C]:ILE:HD12	3:G:234[C]:LYS:HZ1	1.71	0.56
4:H:117[C]:HIS:O	4:H:121[C]:LEU:HG	2.05	0.56
4:H:5[A]:GLN:HB2	4:H:74[A]:LYS:HG2	1.87	0.56
1:B:298:LEU:H	1:B:298:LEU:CD2	2.19	0.56
1:B:440:VAL:CA	1:B:445:MET:HG3	2.35	0.56
1:C:248:TYR:O	1:C:252:LYS:HB2	2.05	0.56
1:C:292:TYR:O	1:C:296:ARG:HB3	2.05	0.56
2:D:131:GLY:HA3	2:D:167:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:213:GLU:HG3	2:E:214:PRO:CD	2.35	0.56
2:E:369:ARG:HG2	2:E:392:ILE:HD11	1.87	0.56
2:F:288:THR:HG23	2:F:291:GLY:H	1.70	0.56
3:G:149[B]:ILE:HD11	3:G:227[B]:TYR:CE2	2.40	0.56
4:H:13[B]:ARG:CG	4:H:13[B]:ARG:NH1	2.60	0.56
2:F:125:ASP:OD2	2:F:345:ARG:NH2	2.38	0.56
3:G:6[B]:GLU:O	3:G:10[B]:ARG:HG3	2.05	0.56
3:G:126[B]:PHE:HD1	3:G:131[B]:TYR:CD1	2.23	0.56
4:H:49[A]:PRO:HG3	4:H:126[A]:VAL:HG13	1.87	0.56
1:A:238:ALA:HB3	1:A:239:PRO:HD3	1.86	0.56
1:A:31:VAL:HG11	1:A:34:VAL:HG22	1.88	0.56
1:B:252:LYS:HD3	1:B:254:LYS:HE2	1.85	0.56
3:G:104[B]:GLU:HA	3:G:107[B]:HIS:CE1	2.40	0.56
3:G:80[C]:VAL:CG1	3:G:126[C]:PHE:HE2	2.19	0.56
3:G:143[B]:THR:HB	3:G:144[B]:PRO:C	2.25	0.56
3:G:41[C]:ASN:O	3:G:44[C]:PRO:HD2	2.06	0.56
4:H:119[B]:ARG:HA	4:H:122[B]:GLU:OE1	2.04	0.56
1:B:171:ARG:NH1	1:B:171:ARG:CG	2.55	0.56
3:G:230[B]:LEU:O	3:G:234[B]:LYS:HB2	2.05	0.56
3:G:31[B]:LYS:C	3:G:32[B]:LEU:HD22	2.26	0.56
3:G:43[C]:ARG:HB2	3:G:44[C]:PRO:HD3	1.88	0.56
3:G:95[B]:ILE:HG23	3:G:96[B]:LEU:N	2.20	0.56
4:H:93[B]:ALA:HB3	4:H:128[B]:LEU:HG	1.88	0.56
1:B:435:ILE:HD12	1:B:472:LEU:HD21	1.88	0.56
1:C:495:LYS:O	1:C:496:LYS:HB2	2.06	0.56
2:E:241:LEU:HD23	2:E:243:PHE:CZ	2.40	0.56
2:F:388:GLU:O	2:F:392:ILE:HG23	2.06	0.56
3:G:148[C]:GLU:OE1	3:G:148[C]:GLU:N	2.38	0.56
3:G:170[C]:ILE:H	3:G:170[C]:ILE:HD12	1.70	0.56
3:G:5[A]:ARG:HH11	3:G:5[A]:ARG:HB3	1.70	0.56
3:G:72[C]:PRO:HA	3:G:73[C]:VAL:CG1	2.29	0.56
1:A:294:HIS:O	1:A:298:LEU:HD22	2.05	0.56
1:B:34:VAL:HG13	1:B:39:ALA:HB2	1.87	0.56
1:C:129:ILE:HD11	1:C:237:LEU:HD22	1.88	0.56
2:D:226:LEU:HD11	2:D:284:ARG:CB	2.35	0.56
2:E:233:ARG:O	2:E:237:GLY:HA2	2.05	0.56
2:E:460:LYS:O	2:E:461:LYS:HD2	2.06	0.56
3:G:146[B]:LEU:HA	3:G:227[B]:TYR:HH	1.71	0.56
4:H:103[B]:ILE:HD11	4:H:117[B]:HIS:CG	2.41	0.56
4:H:24[C]:ILE:HA	4:H:33[C]:GLY:HA2	1.86	0.56
2:D:352:VAL:HG21	2:D:356:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASP:O	1:B:262:ASP:HB2	2.05	0.56
1:C:41:VAL:HG21	1:C:88:VAL:HG21	1.87	0.56
1:C:435:ILE:HD12	1:C:472:LEU:HD21	1.88	0.56
2:D:416:MET:HB2	2:D:417:PRO:O	2.06	0.56
2:F:142:ALA:HB2	2:F:346:ILE:HD13	1.86	0.56
2:F:371:ASN:ND2	3:G:10[B]:ARG:HH11	2.04	0.56
3:G:17[B]:THR:HA	3:G:20[B]:ILE:HD12	1.87	0.56
3:G:86[C]:GLY:CA	3:G:241[C]:ARG:NH2	2.64	0.56
3:G:83[A]:SER:HB3	3:G:237[A]:GLU:HG2	1.88	0.56
4:H:86[A]:GLU:HG2	4:H:134[A]:LYS:HB3	1.88	0.56
1:A:140:LYS:NZ	1:A:143:HIS:HE1	2.03	0.56
1:A:156:MET:C	1:A:157:ILE:HG13	2.25	0.56
1:A:431:GLU:HG2	1:A:432:GLU:H	1.71	0.56
1:B:305:SER:OG	1:B:308:LYS:HG2	2.06	0.56
1:A:129:ILE:HD11	1:A:237:LEU:HD22	1.86	0.55
2:E:182:GLY:H	2:E:210:GLN:H	1.53	0.55
3:G:5[A]:ARG:H	3:G:5[A]:ARG:HD2	1.70	0.55
4:H:110[C]:THR:C	4:H:112[C]:LYS:HE2	2.26	0.55
3:G:45[B]:TYR:CZ	4:H:11[B]:PRO:HG3	2.41	0.55
4:H:119[B]:ARG:HA	4:H:122[B]:GLU:CD	2.26	0.55
1:B:106:ARG:NH1	1:B:106:ARG:CG	2.44	0.55
1:C:262:ASP:H	1:C:318:PHE:HB2	1.71	0.55
3:G:172[C]:TYR:HD2	3:G:186[C]:LYS:HG2	1.71	0.55
1:C:114:PRO:HG3	1:C:121:ILE:CD1	2.36	0.55
2:D:113:ARG:HD3	2:D:114:PRO:O	2.06	0.55
3:G:152[C]:ILE:N	3:G:152[C]:ILE:HD12	2.21	0.55
3:G:21[A]:THR:HG21	3:G:248[A]:ALA:HB3	1.88	0.55
4:H:39[A]:ILE:HB	4:H:40[A]:PRO:HD2	1.87	0.55
4:H:68[B]:LEU:HD23	4:H:77[B]:ILE:HG22	1.88	0.55
4:H:88[A]:ILE:HD11	4:H:131[A]:ALA:HA	1.88	0.55
1:A:481:LEU:N	1:A:482:PRO:CD	2.70	0.55
1:C:298:LEU:HD21	1:C:337:ILE:HG21	1.86	0.55
3:G:17[B]:THR:HA	3:G:20[B]:ILE:CD1	2.37	0.55
1:C:156:MET:SD	1:C:359:VAL:HG11	2.47	0.55
2:D:12:PRO:HD2	2:D:260:LEU:HD22	1.89	0.55
3:G:96[C]:LEU:HD11	3:G:122[C]:GLY:HA2	1.88	0.55
4:H:47[B]:THR:CG2	4:H:122[B]:GLU:HB3	2.36	0.55
1:A:382:LEU:HD11	1:A:416:THR:HG23	1.88	0.55
1:B:481:LEU:N	1:B:482:PRO:CD	2.70	0.55
1:B:495:LYS:HE3	1:B:496:LYS:H	1.72	0.55
1:C:384:LEU:O	1:C:388:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:395:ARG:HH21	2:F:436:GLY:HA3	1.71	0.55
2:F:438:HIS:HB3	2:F:441:LEU:HD22	1.89	0.55
3:G:104[C]:GLU:HA	3:G:107[C]:HIS:CE1	2.41	0.55
3:G:39[B]:ALA:HA	3:G:231[B]:LEU:HD21	1.88	0.55
4:H:100[A]:HIS:CB	4:H:121[A]:LEU:HG	2.31	0.55
1:B:355:PRO:HB2	1:B:357:VAL:HG23	1.87	0.55
1:A:275:LEU:N	2:D:264:MET:HE1	2.22	0.55
3:G:120[C]:ARG:O	3:G:120[C]:ARG:HG2	2.06	0.55
3:G:120[B]:ARG:HG3	3:G:123[B]:ARG:HE	1.71	0.55
3:G:170[B]:ILE:HD12	3:G:186[B]:LYS:H	1.70	0.55
3:G:84[C]:ASP:HB2	3:G:120[C]:ARG:CB	2.33	0.55
1:B:32:ILE:HG12	1:B:40:ARG:O	2.07	0.55
1:B:456:PHE:HZ	1:B:495:LYS:HD2	1.72	0.55
1:C:32:ILE:HG12	1:C:40:ARG:O	2.07	0.55
2:F:397:ARG:O	2:F:401:ARG:HD2	2.07	0.55
3:G:5[B]:ARG:NH1	3:G:5[B]:ARG:HB2	2.22	0.55
3:G:68[C]:LEU:CD2	3:G:68[C]:LEU:H	2.17	0.55
4:H:6[B]:VAL:HG12	4:H:75[B]:VAL:HB	1.89	0.55
1:B:365:ARG:HH21	2:F:186:ARG:NH2	2.04	0.55
1:A:272:GLU:CD	2:D:273:THR:HG22	2.27	0.55
3:G:234[C]:LYS:O	3:G:235[C]:ALA:C	2.44	0.55
3:G:77[B]:GLY:O	3:G:168[B]:LEU:HG	2.06	0.55
3:G:96[B]:LEU:O	3:G:99[B]:VAL:HG22	2.06	0.55
3:G:94[A]:ASN:HB3	3:G:97[A]:ARG:NH1	2.22	0.55
4:H:108[A]:ASP:HA	4:H:114[A]:TYR:HE1	1.72	0.55
4:H:93[A]:ALA:HB3	4:H:128[A]:LEU:HD21	1.89	0.55
1:B:129:ILE:CD1	1:B:237:LEU:HD22	2.37	0.55
1:B:440:VAL:HB	1:B:445:MET:HG3	1.88	0.55
1:B:41:VAL:HG21	1:B:88:VAL:HG21	1.88	0.55
1:C:495:LYS:HE3	1:C:496:LYS:H	1.72	0.55
2:D:397:ARG:O	2:D:401:ARG:HD2	2.07	0.55
3:G:129[B]:ARG:HB2	3:G:131[B]:TYR:HE1	1.71	0.55
3:G:260[B]:THR:HG22	3:G:260[B]:THR:O	2.07	0.55
3:G:36[B]:GLN:HA	3:G:39[B]:ALA:HB3	1.89	0.55
1:C:261:ASP:O	1:C:262:ASP:HB2	2.06	0.54
2:E:266:SER:OG	2:E:268:VAL:HG12	2.07	0.54
2:E:374:GLN:HA	2:E:374:GLN:NE2	2.22	0.54
3:G:101[C]:LYS:C	3:G:101[C]:LYS:HD2	2.27	0.54
3:G:170[C]:ILE:HG13	3:G:188[C]:LEU:HD21	1.87	0.54
3:G:221[C]:TYR:O	3:G:225[C]:LEU:HG	2.07	0.54
4:H:69[C]:GLU:OE1	4:H:76[C]:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:9[B]:VAL:HG22	4:H:14[B]:LYS:HD2	1.89	0.54
1:A:275:LEU:HA	1:A:278:ARG:N	2.22	0.54
1:A:384:LEU:O	1:A:388:GLN:HG2	2.07	0.54
1:B:157:ILE:HG21	1:B:342:ILE:HG12	1.89	0.54
2:D:288:THR:HG23	2:D:291:GLY:H	1.72	0.54
2:D:91:ASN:HD22	2:D:91:ASN:C	2.11	0.54
3:G:116[B]:PHE:HZ	3:G:159[B]:MET:HG3	1.72	0.54
3:G:79[A]:MET:HE3	3:G:226[A]:ILE:HG23	1.88	0.54
3:G:4[A]:MET:HG3	3:G:5[A]:ARG:HH11	1.68	0.54
1:A:456:PHE:HZ	1:A:495:LYS:HD2	1.73	0.54
1:A:481:LEU:O	1:A:482:PRO:O	2.25	0.54
1:C:62:MET:CB	1:C:95:MET:HE1	2.34	0.54
2:D:393:VAL:O	2:D:397:ARG:HG3	2.06	0.54
3:G:17[C]:THR:O	3:G:21[C]:THR:HG23	2.07	0.54
1:C:275:LEU:CD1	1:C:281:PRO:HD3	2.37	0.54
2:D:453:ASP:O	2:D:456:VAL:HG23	2.07	0.54
2:E:12:PRO:HD2	2:E:260:LEU:HD22	1.89	0.54
3:G:25[C]:LYS:HG2	3:G:245[C]:MET:CB	2.37	0.54
1:A:495:LYS:O	1:A:496:LYS:HB2	2.08	0.54
1:C:171:ARG:HG3	1:C:171:ARG:NH1	2.13	0.54
1:C:262:ASP:OD1	1:C:264:SER:HB2	2.07	0.54
1:B:275:LEU:HB2	2:E:264:MET:SD	2.47	0.54
1:B:384:LEU:O	1:B:388:GLN:HG2	2.08	0.54
1:B:419:ILE:HD13	1:B:440:VAL:HG11	1.89	0.54
1:C:284:GLU:HG3	1:C:329:TYR:CB	2.38	0.54
1:B:275:LEU:CG	2:E:264:MET:HG3	2.37	0.54
3:G:255[A]:MET:HG3	3:G:259[A]:LEU:HD23	1.90	0.54
3:G:41[B]:ASN:O	3:G:44[B]:PRO:HD2	2.08	0.54
2:E:319:ASP:OD2	2:E:345:ARG:HD3	2.07	0.54
2:E:352:VAL:HG21	2:E:356:HIS:CD2	2.43	0.54
2:F:371:ASN:HB3	3:G:10[B]:ARG:HH12	1.02	0.54
3:G:117[A]:ALA:O	3:G:136[A]:GLU:HA	2.07	0.54
3:G:77[B]:GLY:HA3	3:G:165[B]:PHE:CE2	2.42	0.54
1:B:248:TYR:O	1:B:252:LYS:HB2	2.08	0.54
1:B:418:GLU:OE2	1:B:421:LYS:HE2	2.08	0.54
2:E:226:LEU:HD11	2:E:284:ARG:CB	2.37	0.54
3:G:122[B]:GLY:O	3:G:126[B]:PHE:HB2	2.07	0.54
1:B:275:LEU:HA	1:B:278:ARG:H	1.72	0.54
1:C:305:SER:OG	1:C:308:LYS:HG2	2.07	0.54
2:F:40:LEU:HD23	2:F:64:LEU:HD11	1.89	0.54
3:G:114[C]:VAL:HB	3:G:134[C]:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:10[C]:THR:OG1	4:H:11[C]:PRO:HD2	2.07	0.54
4:H:21[B]:ASP:N	4:H:21[B]:ASP:OD2	2.40	0.54
4:H:63[A]:VAL:HG13	4:H:79[A]:ALA:HB1	1.88	0.54
1:A:495:LYS:HE3	1:A:496:LYS:H	1.72	0.54
1:B:156:MET:C	1:B:157:ILE:HG13	2.28	0.54
1:C:382:LEU:HD11	1:C:416:THR:HG23	1.90	0.54
2:D:26:ILE:O	2:D:27:TYR:HB2	2.08	0.54
2:D:372:ASP:OD2	3:G:9[C]:ARG:NH1	2.39	0.54
3:G:91[C]:TYR:CD2	3:G:240[C]:ALA:HB1	2.43	0.54
3:G:95[C]:ILE:CD1	3:G:171[C]:PHE:HB3	2.38	0.54
1:A:407:GLN:HA	1:A:411:ASN:HB2	1.91	0.53
1:C:32:ILE:HG13	1:C:33:GLN:HG3	1.90	0.53
1:C:354:ARG:HA	1:C:355:PRO:C	2.28	0.53
2:E:111:ILE:HA	2:E:227:THR:OG1	2.08	0.53
2:F:139:ALA:N	2:F:140:PRO:HD3	2.23	0.53
3:G:132[C]:PRO:O	3:G:133[C]:VAL:CB	2.56	0.53
3:G:32[C]:LEU:CD2	3:G:238[C]:PHE:CG	2.80	0.53
3:G:244[C]:ALA:O	3:G:248[C]:ALA:HB2	2.07	0.53
3:G:72[C]:PRO:CB	3:G:73[C]:VAL:HG13	2.37	0.53
1:B:262:ASP:H	1:B:318:PHE:HB2	1.73	0.53
1:B:354:ARG:HA	1:B:355:PRO:C	2.28	0.53
1:B:499:THR:H	1:B:500:PRO:HD3	1.73	0.53
2:D:97:ILE:HG12	2:D:97:ILE:O	2.07	0.53
1:A:292:TYR:O	1:A:296:ARG:HB3	2.09	0.53
1:B:140:LYS:NZ	1:B:143:HIS:HE1	2.05	0.53
1:B:100:GLY:HA2	1:B:248:TYR:CE2	2.42	0.53
1:C:47:VAL:HG12	1:C:90:ARG:HG2	1.91	0.53
2:D:111:ILE:HA	2:D:227:THR:OG1	2.07	0.53
2:D:438:HIS:HB3	2:D:441:LEU:HD22	1.89	0.53
2:E:395:ARG:HH21	2:E:436:GLY:HA3	1.74	0.53
2:E:393:VAL:O	2:E:397:ARG:HG3	2.07	0.53
2:F:384:GLU:HG2	3:G:121[B]:LYS:NZ	2.24	0.53
3:G:143[B]:THR:HB	3:G:144[B]:PRO:CA	2.39	0.53
3:G:68[A]:LEU:HA	3:G:160[A]:PHE:CE2	2.41	0.53
4:H:100[A]:HIS:CD2	4:H:120[A]:ALA:CB	2.90	0.53
4:H:51[C]:ARG:HG2	4:H:60[C]:LEU:CA	2.34	0.53
1:B:109:ASN:HB2	1:B:110:PRO:CD	2.39	0.53
1:B:495:LYS:O	1:B:496:LYS:HB2	2.09	0.53
1:C:275:LEU:HA	1:C:278:ARG:N	2.23	0.53
2:E:288:THR:HG23	2:E:291:GLY:H	1.74	0.53
3:G:84[B]:ASP:HB2	3:G:120[B]:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:170[C]:ILE:HD11	3:G:188[C]:LEU:HD21	1.90	0.53
3:G:188[C]:LEU:HD23	3:G:188[C]:LEU:N	2.24	0.53
4:H:51[B]:ARG:HG2	4:H:60[B]:LEU:HD23	1.90	0.53
1:A:271:ARG:NH1	1:A:285:ALA:CB	2.72	0.53
1:A:34:VAL:HG13	1:A:39:ALA:HB2	1.90	0.53
1:A:418:GLU:OE2	1:A:421:LYS:HE2	2.08	0.53
1:A:440:VAL:CA	1:A:445:MET:HG3	2.36	0.53
1:A:449:PRO:HG2	1:A:452:ASP:OD1	2.09	0.53
1:C:456:PHE:HZ	1:C:495:LYS:HD2	1.73	0.53
2:F:393:VAL:O	2:F:397:ARG:HG3	2.08	0.53
3:G:32[A]:LEU:CB	3:G:238[A]:PHE:HB2	2.37	0.53
1:A:298:LEU:HD22	1:A:298:LEU:H	1.72	0.53
1:A:388:GLN:HG3	1:A:409:LYS:HZ1	1.71	0.53
1:A:456:PHE:O	1:A:460:LEU:HB2	2.09	0.53
1:C:106:ARG:CB	1:C:106:ARG:HH11	2.20	0.53
1:C:275:LEU:HD12	1:C:281:PRO:HD3	1.91	0.53
1:C:418:GLU:OE2	1:C:421:LYS:HE2	2.08	0.53
2:D:369:ARG:HG2	2:D:392:ILE:HD11	1.91	0.53
3:G:118[C]:VAL:HB	3:G:137[C]:VAL:HG11	1.89	0.53
3:G:166[C]:ASP:C	3:G:167[C]:LYS:HD2	2.29	0.53
3:G:43[C]:ARG:O	3:G:47[C]:ASP:N	2.42	0.53
1:A:157:ILE:N	1:A:158:PRO:CD	2.71	0.53
1:B:275:LEU:HA	1:B:278:ARG:CA	2.39	0.53
1:B:284:GLU:HG3	1:B:329:TYR:CB	2.39	0.53
1:B:415:ARG:NH1	1:B:450:VAL:HG22	2.23	0.53
1:C:46:LYS:NZ	1:C:46:LYS:HB2	2.23	0.53
2:F:375:ASP:O	2:F:379:ILE:HG23	2.08	0.53
2:D:374:GLN:HA	2:D:374:GLN:NE2	2.21	0.53
2:D:382:MET:HG3	2:D:385:LEU:HD22	1.90	0.53
3:G:7[B]:ILE:HA	3:G:10[B]:ARG:HB2	1.91	0.53
3:G:131[B]:TYR:N	3:G:132[B]:PRO:HA	2.21	0.53
3:G:238[C]:PHE:HA	3:G:241[C]:ARG:HB3	1.90	0.53
3:G:72[C]:PRO:HB3	3:G:73[C]:VAL:HG13	1.91	0.53
4:H:97[A]:LYS:NZ	4:H:125[A]:GLU:HG2	2.23	0.53
1:A:284:GLU:HG3	1:A:329:TYR:CB	2.39	0.53
1:B:48:MET:HG3	1:B:51:GLU:OE2	2.09	0.53
1:C:109:ASN:OD1	1:C:113:GLN:HG2	2.09	0.53
1:C:157:ILE:HG21	1:C:342:ILE:HG12	1.90	0.53
2:D:398:LYS:HD3	2:D:446:PHE:CZ	2.44	0.53
3:G:129[B]:ARG:HB2	3:G:131[B]:TYR:CE1	2.44	0.53
3:G:75[C]:LYS:HB2	3:G:75[C]:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG21	1:A:71:VAL:HG21	1.90	0.53
1:C:419:ILE:HD13	1:C:440:VAL:HG11	1.91	0.53
2:E:315:PHE:HA	2:E:318:LEU:HD22	1.90	0.53
3:G:238[A]:PHE:O	3:G:242[A]:MET:HB3	2.08	0.53
3:G:94[C]:ASN:HA	3:G:97[C]:ARG:HB3	1.90	0.53
4:H:110[C]:THR:O	4:H:112[C]:LYS:HE2	2.09	0.53
4:H:88[B]:ILE:HD11	4:H:131[B]:ALA:HA	1.91	0.53
1:A:440:VAL:HG12	1:A:445:MET:HE2	1.91	0.52
1:C:171:ARG:HH11	1:C:171:ARG:HG2	1.69	0.52
1:C:407:GLN:HA	1:C:411:ASN:HB2	1.91	0.52
2:D:162:GLN:NE2	2:D:194:GLU:HG2	2.24	0.52
1:A:275:LEU:CD2	2:D:264:MET:HA	2.20	0.52
2:D:395:ARG:HH21	2:D:436:GLY:HA3	1.74	0.52
2:F:241:LEU:HD23	2:F:243:PHE:CZ	2.44	0.52
2:F:428:ARG:O	2:F:432:GLU:HG3	2.09	0.52
3:G:43[C]:ARG:HB2	3:G:44[C]:PRO:CD	2.39	0.52
3:G:84[A]:ASP:OD2	3:G:139[A]:GLY:HA2	2.08	0.52
4:H:109[C]:LYS:O	4:H:112[C]:LYS:CE	2.58	0.52
4:H:12[C]:GLU:C	4:H:13[C]:ARG:HD2	2.30	0.52
2:D:301:VAL:O	2:D:301:VAL:HG22	2.09	0.52
2:E:264:MET:CE	2:E:272:PRO:HB3	2.38	0.52
3:G:15[B]:LYS:NZ	3:G:256[B]:LEU:HD21	2.24	0.52
3:G:71[B]:ARG:NH1	3:G:71[B]:ARG:CG	2.57	0.52
1:C:440:VAL:HB	1:C:445:MET:HG3	1.91	0.52
3:G:159[B]:MET:HB3	3:G:165[B]:PHE:CD1	2.44	0.52
3:G:38[C]:THR:HA	4:H:13[C]:ARG:HH21	1.71	0.52
3:G:79[A]:MET:HA	3:G:115[A]:ILE:O	2.08	0.52
2:F:129:GLU:O	2:F:172:HIS:HE1	1.92	0.52
3:G:131[B]:TYR:H	3:G:132[B]:PRO:CA	2.22	0.52
3:G:77[C]:GLY:HA3	3:G:165[C]:PHE:CE2	2.45	0.52
3:G:170[C]:ILE:CG1	3:G:188[C]:LEU:HD21	2.39	0.52
1:A:412:ARG:HG3	1:A:446:ASP:OD1	2.09	0.52
1:B:456:PHE:O	1:B:460:LEU:HB2	2.09	0.52
1:C:275:LEU:HD12	1:C:279:ARG:O	2.09	0.52
2:D:84:ALA:HB1	2:D:103:VAL:HG12	1.91	0.52
2:F:12:PRO:HD2	2:F:260:LEU:HD22	1.91	0.52
3:G:187[C]:GLN:C	3:G:188[C]:LEU:HD23	2.29	0.52
3:G:19[A]:GLN:HA	3:G:22[A]:LYS:HG2	1.91	0.52
3:G:88[B]:ALA:CB	3:G:241[B]:ARG:HA	2.40	0.52
1:A:142:VAL:HG22	1:A:161:ARG:O	2.10	0.52
1:A:271:ARG:NH1	1:A:285:ALA:HB1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:382:MET:HG3	2:E:385:LEU:HD22	1.91	0.52
2:E:91:ASN:HD22	2:E:91:ASN:C	2.12	0.52
2:F:181:VAL:HG22	2:F:221:VAL:HG13	1.92	0.52
3:G:184[C]:VAL:HG11	3:G:186[C]:LYS:HE3	1.92	0.52
3:G:257[C]:GLU:HG2	3:G:257[C]:GLU:O	2.08	0.52
3:G:65[C]:HIS:CD2	3:G:69[C]:GLU:CA	2.93	0.52
1:A:171:ARG:NH1	1:A:171:ARG:CG	2.53	0.52
1:B:106:ARG:CB	1:B:106:ARG:HH11	2.22	0.52
2:D:35:PRO:HD2	2:D:36:GLN:OE1	2.09	0.52
3:G:67[A]:MET:SD	3:G:161[A]:ALA:HA	2.49	0.52
3:G:8[C]:LYS:HA	3:G:11[C]:ILE:HB	1.92	0.52
4:H:118[C]:LYS:HA	4:H:121[C]:LEU:HG	1.92	0.52
1:A:305:SER:OG	1:A:308:LYS:HG2	2.10	0.52
1:B:238:ALA:HB3	1:B:239:PRO:HD3	1.92	0.52
1:B:382:LEU:HD11	1:B:416:THR:HG23	1.92	0.52
1:B:62:MET:CB	1:B:95:MET:HE1	2.29	0.52
1:B:62:MET:CE	1:B:95:MET:HE3	2.40	0.52
3:G:42[C]:ALA:O	3:G:43[C]:ARG:C	2.47	0.52
1:A:462:SER:CA	1:A:465:ARG:HH12	2.21	0.52
1:B:440:VAL:CB	1:B:445:MET:HG3	2.40	0.52
1:B:275:LEU:HD13	2:E:264:MET:HG3	1.91	0.52
2:E:91:ASN:ND2	2:E:95:GLU:H	2.08	0.52
3:G:148[B]:GLU:CD	3:G:149[B]:ILE:HG13	2.30	0.52
3:G:47[C]:ASP:O	3:G:48[C]:LYS:C	2.47	0.52
3:G:68[A]:LEU:HD22	3:G:68[A]:LEU:H	1.75	0.52
4:H:3[C]:THR:OG1	4:H:19[C]:GLU:HB3	2.10	0.52
1:A:275:LEU:HD12	1:A:279:ARG:O	2.10	0.51
3:G:85[C]:ARG:O	3:G:85[C]:ARG:CD	2.57	0.51
4:H:7[C]:ASP:HA	4:H:16[C]:PHE:O	2.10	0.51
4:H:53[A]:LYS:HE2	4:H:58[A]:GLU:HG2	1.92	0.51
1:A:157:ILE:HG21	1:A:342:ILE:HG12	1.93	0.51
1:B:108:VAL:HG13	1:B:109:ASN:O	2.10	0.51
1:C:41:VAL:CG2	1:C:88:VAL:HG21	2.40	0.51
1:C:440:VAL:CB	1:C:445:MET:HG3	2.41	0.51
2:E:84:ALA:HB1	2:E:103:VAL:HG12	1.92	0.51
2:F:386:SER:HB3	2:F:389:ASP:OD1	2.10	0.51
4:H:12[A]:GLU:C	4:H:13[A]:ARG:HD2	2.31	0.51
1:A:440:VAL:HB	1:A:445:MET:HG3	1.90	0.51
1:C:238:ALA:HB3	1:C:239:PRO:HD3	1.93	0.51
2:F:382:MET:HG3	2:F:385:LEU:HD22	1.92	0.51
3:G:15[C]:LYS:O	3:G:18[C]:ARG:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LEU:HD13	2:F:264:MET:HG3	1.92	0.51
1:C:456:PHE:O	1:C:460:LEU:HB2	2.11	0.51
2:D:85:THR:O	2:D:205:SER:HB3	2.11	0.51
2:F:40:LEU:CD2	2:F:64:LEU:HD11	2.40	0.51
3:G:32[B]:LEU:CG	3:G:238[B]:PHE:HB3	2.37	0.51
3:G:86[A]:GLY:HA2	3:G:241[A]:ARG:NH2	2.26	0.51
4:H:114[C]:TYR:HB3	4:H:118[C]:LYS:HE2	1.93	0.51
4:H:63[C]:VAL:HG13	4:H:79[C]:ALA:HB1	1.93	0.51
1:C:143:HIS:CD2	1:C:144:GLU:HG2	2.46	0.51
2:E:226:LEU:O	2:E:230:GLU:HG3	2.11	0.51
4:H:14[B]:LYS:HB3	4:H:14[B]:LYS:NZ	2.25	0.51
1:A:261:ASP:O	1:A:262:ASP:HB2	2.11	0.51
1:B:109:ASN:OD1	1:B:113:GLN:HG2	2.10	0.51
1:C:106:ARG:NH1	1:C:106:ARG:CG	2.48	0.51
1:C:156:MET:C	1:C:157:ILE:HG13	2.30	0.51
1:C:271:ARG:NH1	1:C:285:ALA:CB	2.74	0.51
2:D:226:LEU:O	2:D:230:GLU:HG3	2.10	0.51
2:D:246:ASN:OD1	2:D:248:PHE:HB3	2.11	0.51
1:C:137:MET:HG3	2:D:97:ILE:O	2.11	0.51
2:E:453:ASP:O	2:E:456:VAL:HG23	2.11	0.51
2:F:113:ARG:HD3	2:F:114:PRO:O	2.11	0.51
3:G:115[C]:ILE:HD11	3:G:133[C]:VAL:HB	1.92	0.51
3:G:155[B]:SER:O	3:G:159[B]:MET:HG2	2.10	0.51
1:A:62:MET:CB	1:A:95:MET:HE1	2.33	0.51
1:B:407:GLN:HA	1:B:411:ASN:HB2	1.92	0.51
1:C:140:LYS:HE2	1:C:143:HIS:ND1	2.26	0.51
2:E:411:GLU:OE2	2:E:417:PRO:HB3	2.11	0.51
2:F:131:GLY:HA3	2:F:167:ASN:HD22	1.76	0.51
3:G:77[B]:GLY:HA3	3:G:165[B]:PHE:CZ	2.46	0.51
3:G:170[C]:ILE:CD1	3:G:188[C]:LEU:HD21	2.41	0.51
2:E:129:GLU:O	2:E:172:HIS:HE1	1.93	0.51
4:H:48[B]:ALA:O	4:H:63[B]:VAL:HB	2.10	0.51
4:H:8[B]:ILE:HD13	4:H:61[B]:ILE:HD12	1.92	0.51
1:A:140:LYS:HE2	1:A:143:HIS:ND1	2.25	0.51
1:A:354:ARG:HA	1:A:355:PRO:C	2.30	0.51
1:B:449:PRO:HG2	1:B:452:ASP:OD1	2.09	0.51
1:C:355:PRO:HB2	1:C:357:VAL:HG23	1.92	0.51
4:H:8[B]:ILE:HD11	4:H:15[B]:VAL:HB	1.93	0.51
1:A:184:ILE:HG22	1:A:427:PRO:HG2	1.91	0.51
1:B:164:ARG:NH2	2:F:184:ARG:HD3	2.23	0.51
2:D:139:ALA:N	2:D:140:PRO:HD3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:101[C]:LYS:HD2	3:G:101[C]:LYS:O	2.11	0.51
3:G:177[C]:SER:O	3:G:180[C]:VAL:O	2.29	0.51
3:G:32[C]:LEU:CD2	3:G:238[C]:PHE:HB2	2.41	0.51
3:G:14[A]:VAL:CG1	3:G:256[A]:LEU:HG	2.41	0.51
4:H:39[A]:ILE:HB	4:H:40[A]:PRO:CD	2.41	0.51
1:B:481:LEU:O	1:B:482:PRO:O	2.28	0.50
2:D:428:ARG:O	2:D:432:GLU:HG3	2.12	0.50
2:E:131:GLY:HA3	2:E:167:ASN:HD22	1.75	0.50
3:G:104[C]:GLU:CD	3:G:107[C]:HIS:HE1	2.15	0.50
3:G:48[C]:LYS:NZ	4:H:9[C]:VAL:HB	2.26	0.50
1:A:275:LEU:HA	1:A:278:ARG:H	1.77	0.50
1:A:407:GLN:CA	1:A:411:ASN:HB2	2.42	0.50
1:A:48:MET:CE	1:A:94:ILE:HG23	2.39	0.50
2:D:129:GLU:O	2:D:172:HIS:HE1	1.94	0.50
2:E:428:ARG:O	2:E:432:GLU:HG3	2.11	0.50
3:G:149[C]:ILE:O	3:G:151[C]:ASP:N	2.44	0.50
1:C:407:GLN:HB3	1:C:411:ASN:HB2	1.93	0.50
2:D:388:GLU:O	2:D:392:ILE:HG23	2.10	0.50
2:E:26:ILE:O	2:E:27:TYR:HB2	2.10	0.50
2:F:301:VAL:CG1	2:F:306:TYR:HE1	2.24	0.50
1:A:440:VAL:CB	1:A:445:MET:HG3	2.42	0.50
1:A:462:SER:CB	1:A:465:ARG:HH12	2.23	0.50
1:B:157:ILE:N	1:B:158:PRO:CD	2.75	0.50
1:C:157:ILE:N	1:C:158:PRO:CD	2.74	0.50
1:C:407:GLN:CA	1:C:411:ASN:HB2	2.42	0.50
1:C:136:VAL:HG12	2:D:185:THR:HG23	1.92	0.50
2:E:301:VAL:CG1	2:E:306:TYR:HE1	2.21	0.50
2:E:386:SER:HB3	2:E:389:ASP:OD1	2.11	0.50
3:G:113[C]:TYR:O	3:G:114[C]:VAL:HG13	2.10	0.50
4:H:50[C]:VAL:H	4:H:61[C]:ILE:CG1	2.21	0.50
4:H:68[C]:LEU:HD23	4:H:77[C]:ILE:HG22	1.93	0.50
1:A:355:PRO:HB2	1:A:357:VAL:HG23	1.92	0.50
1:B:151:LYS:H	1:B:422:GLN:NE2	1.89	0.50
1:B:32:ILE:HG13	1:B:33:GLN:HG3	1.93	0.50
1:C:449:PRO:HG2	1:C:452:ASP:OD1	2.12	0.50
2:D:386:SER:HB3	2:D:389:ASP:OD1	2.11	0.50
2:E:181:VAL:HG22	2:E:221:VAL:HG13	1.94	0.50
2:E:273:THR:O	2:E:277:GLU:HG3	2.12	0.50
3:G:149[B]:ILE:HD11	3:G:227[B]:TYR:CZ	2.47	0.50
1:C:448:ILE:HG23	1:C:449:PRO:HD2	1.93	0.50
2:D:160:LEU:HD22	2:D:164:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:PRO:HG3	2:D:357:TYR:CD2	2.46	0.50
3:G:132[C]:PRO:CG	3:G:133[C]:VAL:H	2.25	0.50
3:G:155[C]:SER:O	3:G:159[C]:MET:HG3	2.12	0.50
3:G:182[A]:ARG:NE	3:G:182[A]:ARG:HA	2.27	0.50
3:G:80[B]:VAL:HB	3:G:171[B]:PHE:CD1	2.39	0.50
4:H:114[C]:TYR:HA	4:H:118[C]:LYS:HG3	1.93	0.50
4:H:10[A]:THR:HA	4:H:79[A]:ALA:O	2.12	0.50
1:A:248:TYR:O	1:A:252:LYS:HB2	2.11	0.50
2:D:161:ILE:HG23	2:D:243:PHE:CE1	2.47	0.50
2:D:325:GLU:CG	2:D:338:ASP:HB2	2.42	0.50
1:A:48:MET:CB	2:E:63:GLY:HA2	2.40	0.50
3:G:107[C]:HIS:HB2	3:G:113[C]:TYR:OH	2.11	0.50
3:G:174[A]:GLU:HA	3:G:232[A]:ASP:OD2	2.11	0.50
1:A:143:HIS:NE2	1:A:144:GLU:HG2	2.27	0.50
1:B:412:ARG:HG3	1:B:446:ASP:OD1	2.11	0.50
1:C:481:LEU:O	1:C:482:PRO:O	2.29	0.50
2:E:349:PRO:HG3	2:E:357:TYR:CD2	2.46	0.50
2:F:162:GLN:NE2	2:F:194:GLU:HG2	2.27	0.50
2:F:264:MET:HG2	2:F:265:PRO:O	2.11	0.50
2:F:374:GLN:HA	2:F:374:GLN:NE2	2.23	0.50
2:F:453:ASP:O	2:F:456:VAL:HG23	2.11	0.50
3:G:96[A]:LEU:HD22	3:G:125[A]:PHE:CD1	2.47	0.50
4:H:83[C]:GLU:HB2	4:H:87[C]:GLU:HB3	1.94	0.50
1:B:395:PHE:N	1:B:395:PHE:CD2	2.80	0.50
1:C:438:TYR:HA	1:C:441:THR:CG2	2.39	0.50
2:E:241:LEU:O	2:E:242:LEU:HB3	2.12	0.50
2:F:386:SER:HB3	2:F:389:ASP:HB2	1.94	0.50
4:H:28[B]:VAL:C	4:H:30[B]:GLY:H	2.15	0.50
1:A:48:MET:HG3	1:A:51:GLU:OE2	2.12	0.49
3:G:10[C]:ARG:HB3	3:G:259[C]:LEU:HD11	1.93	0.49
3:G:172[A]:TYR:HD1	3:G:173[A]:ASN:N	2.09	0.49
4:H:9[C]:VAL:HA	4:H:15[C]:VAL:HG23	1.94	0.49
4:H:47[C]:THR:HA	4:H:64[C]:SER:HA	1.93	0.49
1:A:275:LEU:CD1	1:A:281:PRO:HD3	2.41	0.49
1:A:275:LEU:HD12	1:A:281:PRO:HD3	1.94	0.49
1:A:48:MET:HB3	2:E:63:GLY:CA	2.42	0.49
1:B:275:LEU:CD1	1:B:281:PRO:HD3	2.42	0.49
3:G:96[A]:LEU:HD13	3:G:125[A]:PHE:CG	2.47	0.49
4:H:7[B]:ASP:HA	4:H:16[B]:PHE:O	2.12	0.49
4:H:50[C]:VAL:N	4:H:61[C]:ILE:HG12	2.20	0.49
4:H:79[B]:ALA:HB3	4:H:82[B]:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:411:GLU:OE2	2:D:417:PRO:HB3	2.12	0.49
2:E:308:ASP:O	2:E:311:PRO:HD2	2.12	0.49
2:E:386:SER:HB3	2:E:389:ASP:HB2	1.94	0.49
3:G:27[A]:VAL:O	3:G:31[A]:LYS:HB2	2.11	0.49
4:H:118[C]:LYS:HA	4:H:121[C]:LEU:HB2	1.93	0.49
4:H:62[A]:ALA:N	4:H:130[A]:VAL:HG21	2.27	0.49
4:H:86[A]:GLU:HG2	4:H:134[A]:LYS:HD3	1.94	0.49
1:B:275:LEU:HD12	1:B:279:ARG:O	2.13	0.49
1:C:275:LEU:HA	1:C:278:ARG:CA	2.41	0.49
2:D:147:ILE:HA	2:D:320:ALA:O	2.12	0.49
3:G:95[C]:ILE:HD11	3:G:171[C]:PHE:HB3	1.94	0.49
3:G:220[C]:LYS:NZ	3:G:220[C]:LYS:HB3	2.28	0.49
3:G:236[A]:SER:O	3:G:240[A]:ALA:N	2.37	0.49
3:G:32[C]:LEU:HD23	3:G:238[C]:PHE:CB	2.41	0.49
4:H:26[C]:ARG:HB2	4:H:48[C]:ALA:CB	2.42	0.49
1:A:205:VAL:O	1:A:209:VAL:HG23	2.13	0.49
1:A:415:ARG:NH1	1:A:450:VAL:HG22	2.27	0.49
2:E:160:LEU:HD22	2:E:164:LEU:HD22	1.95	0.49
2:E:431:LYS:HE3	2:E:435:GLU:OE2	2.12	0.49
2:F:398:LYS:HD3	2:F:446:PHE:CZ	2.46	0.49
3:G:107[C]:HIS:C	3:G:107[C]:HIS:CD2	2.86	0.49
3:G:38[B]:THR:HG22	4:H:13[B]:ARG:HE	1.77	0.49
4:H:94[B]:LYS:HG3	4:H:128[B]:LEU:HD11	1.92	0.49
1:C:411:ASN:O	1:C:415:ARG:NH1	2.45	0.49
4:H:88[B]:ILE:HD13	4:H:130[B]:VAL:HG12	1.94	0.49
1:A:275:LEU:HB3	2:D:264:MET:SD	2.52	0.49
1:A:407:GLN:HB3	1:A:411:ASN:HB2	1.94	0.49
1:B:407:GLN:HB3	1:B:411:ASN:HB2	1.95	0.49
1:C:388:GLN:HG3	1:C:409:LYS:HZ1	1.78	0.49
2:E:406:PRO:HB3	2:E:416:MET:HG3	1.94	0.49
3:G:118[C]:VAL:HB	3:G:137[C]:VAL:CG1	2.43	0.49
3:G:14[A]:VAL:HG12	3:G:256[A]:LEU:HG	1.95	0.49
3:G:7[C]:ILE:HD12	3:G:262[C]:GLN:HB3	1.95	0.49
4:H:119[B]:ARG:O	4:H:122[B]:GLU:HB2	2.13	0.49
4:H:120[B]:ALA:C	4:H:122[B]:GLU:H	2.16	0.49
2:F:268:VAL:CG2	2:F:268:VAL:O	2.59	0.49
3:G:32[B]:LEU:HA	3:G:35[B]:ALA:HB2	1.93	0.49
3:G:45[B]:TYR:O	3:G:49[B]:ILE:HG12	2.12	0.49
4:H:103[B]:ILE:HD11	4:H:117[B]:HIS:CE1	2.48	0.49
4:H:43[C]:THR:H	4:H:68[C]:LEU:HB2	1.78	0.49
1:A:419:ILE:HD13	1:A:440:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:THR:H	1:A:500:PRO:HD3	1.73	0.49
1:B:286:TYR:HB3	1:B:287:PRO:HD2	1.95	0.49
1:B:386:LEU:HD22	1:B:416:THR:HG21	1.94	0.49
2:E:346:ILE:HB	2:E:351:VAL:HG11	1.95	0.49
3:G:143[C]:THR:HB	3:G:144[C]:PRO:HA	1.94	0.49
3:G:68[C]:LEU:HD12	3:G:189[C]:LEU:HG	1.95	0.49
3:G:22[C]:LYS:HB3	3:G:249[C]:THR:OG1	2.13	0.49
3:G:32[C]:LEU:CD2	3:G:238[C]:PHE:CD2	2.94	0.49
3:G:45[C]:TYR:HB3	4:H:11[C]:PRO:HA	1.94	0.49
3:G:79[B]:MET:HA	3:G:115[B]:ILE:O	2.13	0.49
4:H:103[A]:ILE:HD13	4:H:103[A]:ILE:H	1.78	0.49
1:C:62:MET:CE	1:C:95:MET:HE3	2.43	0.49
2:D:130:THR:CG2	2:D:135:ILE:HD11	2.36	0.49
2:F:379:ILE:O	2:F:379:ILE:HG13	2.13	0.49
3:G:96[A]:LEU:CA	3:G:99[A]:VAL:HG12	2.40	0.49
4:H:101[A]:GLU:HG2	4:H:104[A]:LEU:HD12	1.94	0.49
4:H:64[B]:SER:HB2	4:H:123[B]:ARG:HG2	1.95	0.49
4:H:63[A]:VAL:HG12	4:H:64[A]:SER:N	2.28	0.49
4:H:66[C]:GLY:HA3	4:H:79[C]:ALA:CA	2.35	0.49
1:A:114:PRO:HG3	1:A:121:ILE:CD1	2.43	0.48
2:D:264:MET:HG2	2:D:265:PRO:O	2.13	0.48
3:G:143[C]:THR:HB	3:G:144[C]:PRO:CA	2.43	0.48
3:G:84[C]:ASP:OD1	3:G:140[C]:ILE:HG12	2.13	0.48
4:H:71[C]:ARG:HB3	4:H:72[C]:PRO:HD2	1.95	0.48
1:B:298:LEU:N	1:B:298:LEU:CD2	2.76	0.48
2:E:113:ARG:HD3	2:E:114:PRO:O	2.13	0.48
2:F:166:ASN:O	2:F:170:GLN:HB2	2.13	0.48
2:F:161:ILE:HG23	2:F:243:PHE:CE1	2.48	0.48
3:G:132[C]:PRO:CD	3:G:133[C]:VAL:H	2.25	0.48
3:G:35[C]:ALA:HA	3:G:38[C]:THR:OG1	2.13	0.48
1:C:34:VAL:HG13	1:C:39:ALA:HB2	1.94	0.48
2:E:268:VAL:CG2	2:E:268:VAL:O	2.58	0.48
2:F:411:GLU:OE2	2:F:417:PRO:HB3	2.13	0.48
3:G:32[B]:LEU:HD21	3:G:238[B]:PHE:HB3	1.93	0.48
3:G:94[A]:ASN:HA	3:G:97[A]:ARG:HB3	1.95	0.48
4:H:62[A]:ALA:O	4:H:82[A]:ALA:HA	2.13	0.48
1:A:411:ASN:O	1:A:415:ARG:NH1	2.46	0.48
1:A:471:LEU:HD13	1:A:487:LEU:HD22	1.95	0.48
1:C:462:SER:CB	1:C:465:ARG:HH12	2.26	0.48
2:E:166:ASN:O	2:E:170:GLN:HB2	2.13	0.48
2:E:379:ILE:HG13	2:E:379:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:458:LYS:C	2:F:460:LYS:H	2.16	0.48
2:F:48:LEU:HD11	2:F:54:ARG:HB2	1.95	0.48
3:G:12[B]:ARG:HB3	3:G:12[B]:ARG:NH1	2.28	0.48
2:D:379:ILE:HA	3:G:251[C]:ASN:HB3	1.95	0.48
1:A:176:THR:O	1:A:180:ILE:HG12	2.13	0.48
1:A:41:VAL:CG2	1:A:88:VAL:HG21	2.42	0.48
1:B:456:PHE:CZ	1:B:495:LYS:HD2	2.49	0.48
2:D:301:VAL:CG1	2:D:306:TYR:HE1	2.23	0.48
2:E:397:ARG:O	2:E:401:ARG:HD2	2.13	0.48
2:F:340:LEU:HD12	2:F:340:LEU:HA	1.67	0.48
2:F:406:PRO:HB3	2:F:416:MET:HG3	1.95	0.48
2:F:97:ILE:O	2:F:97:ILE:HG12	2.13	0.48
3:G:255[B]:MET:C	3:G:257[B]:GLU:H	2.16	0.48
3:G:27[C]:VAL:HA	3:G:30[C]:ALA:HB3	1.96	0.48
3:G:37[C]:GLU:C	3:G:39[C]:ALA:H	2.15	0.48
1:B:172:GLN:NE2	2:E:345:ARG:HB3	2.28	0.48
1:C:326:VAL:HG11	1:C:343:PHE:CE2	2.42	0.48
2:E:416:MET:N	2:E:417:PRO:CA	2.76	0.48
2:F:129:GLU:O	2:F:172:HIS:CE1	2.66	0.48
3:G:31[C]:LYS:HB3	3:G:32[C]:LEU:HD22	1.94	0.48
1:B:205:VAL:O	1:B:209:VAL:HG23	2.14	0.48
1:A:62:MET:CE	1:A:95:MET:HE3	2.44	0.48
1:B:284:GLU:HG3	1:B:329:TYR:HB2	1.96	0.48
1:C:462:SER:CA	1:C:465:ARG:HH12	2.27	0.48
2:D:386:SER:HB3	2:D:389:ASP:HB2	1.95	0.48
2:E:232:PHE:HB2	2:E:240:VAL:HG21	1.94	0.48
1:B:83:ARG:CB	2:E:47:HIS:HE1	2.12	0.48
4:H:88[C]:ILE:HD12	4:H:131[C]:ALA:HA	1.95	0.48
1:B:407:GLN:CA	1:B:411:ASN:HB2	2.43	0.48
1:C:333:ASN:O	1:C:337:ILE:HG13	2.13	0.48
1:C:471:LEU:HD13	1:C:487:LEU:HD22	1.95	0.48
2:D:142:ALA:HB2	2:D:346:ILE:HG21	1.96	0.48
2:E:35:PRO:HD2	2:E:36:GLN:OE1	2.14	0.48
3:G:167[C]:LYS:N	3:G:167[C]:LYS:HD2	2.28	0.48
4:H:101[B]:GLU:CD	4:H:121[B]:LEU:HD21	2.34	0.48
1:B:388:GLN:HG3	1:B:409:LYS:HZ2	1.77	0.48
3:G:238[C]:PHE:O	3:G:241[C]:ARG:N	2.46	0.48
3:G:85[C]:ARG:CA	3:G:120[C]:ARG:NH2	2.77	0.48
4:H:22[A]:ILE:HG22	4:H:35[A]:MET:SD	2.54	0.48
4:H:90[B]:VAL:HG13	4:H:128[B]:LEU:HD21	1.95	0.48
1:B:65:ASN:HB3	2:F:10:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ILE:O	1:C:479:GLY:HA3	2.14	0.47
2:D:23:LEU:HA	2:D:24:PRO:HD3	1.75	0.47
2:D:356:HIS:CD2	2:D:356:HIS:C	2.88	0.47
3:G:238[B]:PHE:CD1	3:G:241[B]:ARG:HD2	2.49	0.47
3:G:31[B]:LYS:HG2	3:G:32[B]:LEU:HD22	1.95	0.47
3:G:65[B]:HIS:HB3	3:G:68[B]:LEU:HB2	1.96	0.47
1:A:326:VAL:HG12	1:A:326:VAL:O	2.13	0.47
1:A:460:LEU:O	1:A:464:MET:HG2	2.14	0.47
1:B:431:GLU:HG2	1:B:432:GLU:H	1.77	0.47
1:C:108:VAL:HG13	1:C:109:ASN:O	2.14	0.47
2:E:165:ILE:HG21	2:E:200:VAL:HG13	1.95	0.47
2:F:369:ARG:HG2	2:F:392:ILE:HD11	1.96	0.47
3:G:86[C]:GLY:C	3:G:241[C]:ARG:HH21	2.15	0.47
3:G:27[B]:VAL:HG12	3:G:28[B]:ALA:N	2.28	0.47
3:G:5[A]:ARG:HG2	3:G:6[A]:GLU:HG2	1.95	0.47
4:H:14[B]:LYS:HB3	4:H:14[B]:LYS:HZ2	1.79	0.47
4:H:49[B]:PRO:HA	4:H:61[B]:ILE:O	2.14	0.47
1:A:456:PHE:CZ	1:A:495:LYS:HD2	2.49	0.47
1:B:326:VAL:HG11	1:B:343:PHE:CE2	2.44	0.47
1:C:298:LEU:CD2	1:C:298:LEU:H	2.27	0.47
1:C:167:ILE:HD11	1:C:316:LEU:HD13	1.95	0.47
1:C:415:ARG:NH1	1:C:450:VAL:HG22	2.29	0.47
2:E:301:VAL:HG22	2:E:301:VAL:O	2.13	0.47
3:G:153[B]:ALA:O	3:G:157[B]:ILE:HG12	2.13	0.47
3:G:160[C]:PHE:HA	3:G:165[C]:PHE:HB2	1.95	0.47
3:G:168[B]:LEU:CB	3:G:189[B]:LEU:HB2	2.43	0.47
3:G:4[A]:MET:HG3	3:G:5[A]:ARG:HH12	1.73	0.47
3:G:87[C]:LEU:HD12	3:G:87[C]:LEU:HA	1.51	0.47
1:A:32:ILE:HG13	1:A:33:GLN:HG3	1.96	0.47
1:B:411:ASN:O	1:B:415:ARG:NH1	2.48	0.47
2:F:232:PHE:HB2	2:F:240:VAL:HG21	1.95	0.47
2:F:233:ARG:HD3	2:F:292:SER:HB3	1.95	0.47
3:G:14[B]:VAL:HG12	3:G:256[B]:LEU:HD12	1.96	0.47
4:H:100[B]:HIS:CD2	4:H:117[B]:HIS:HD2	2.28	0.47
4:H:126[C]:VAL:O	4:H:130[C]:VAL:HB	2.14	0.47
4:H:4[B]:VAL:HG21	4:H:36[B]:ALA:HA	1.96	0.47
1:C:48:MET:HE1	1:C:94:ILE:HG23	1.95	0.47
2:E:149:LEU:HD21	2:E:324:LEU:HD22	1.95	0.47
3:G:108[B]:GLN:H	3:G:108[B]:GLN:NE2	2.12	0.47
3:G:11[C]:ILE:HG13	3:G:259[C]:LEU:HD12	1.96	0.47
3:G:25[C]:LYS:O	3:G:25[C]:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:119[C]:ARG:HA	4:H:122[C]:GLU:OE2	2.15	0.47
4:H:96[C]:ALA:CB	4:H:100[C]:HIS:ND1	2.77	0.47
1:A:330:ILE:HB	1:A:331:PRO:HD3	1.95	0.47
1:A:386:LEU:HD22	1:A:416:THR:HG21	1.97	0.47
1:B:179:ALA:HB2	1:B:318:PHE:HZ	1.79	0.47
1:C:275:LEU:HG	1:C:278:ARG:CA	2.42	0.47
2:F:264:MET:CB	2:F:265:PRO:CA	2.90	0.47
3:G:95[C]:ILE:HD13	3:G:95[C]:ILE:O	2.15	0.47
1:A:46:LYS:HB2	1:A:46:LYS:HZ3	1.80	0.47
1:A:431:GLU:HB2	1:A:472:LEU:HD22	1.97	0.47
1:B:140:LYS:HE2	1:B:143:HIS:ND1	2.30	0.47
1:B:146:LEU:HD21	1:B:257:LEU:HD13	1.96	0.47
1:C:151:LYS:HD2	1:C:419:ILE:O	2.14	0.47
1:A:210:GLU:HB2	2:D:123:THR:HB	1.96	0.47
2:D:264:MET:CB	2:D:265:PRO:CA	2.92	0.47
2:D:406:PRO:HB3	2:D:416:MET:HG3	1.97	0.47
2:E:125:ASP:CG	2:E:345:ARG:NH2	2.68	0.47
2:E:233:ARG:HD3	2:E:292:SER:HB3	1.97	0.47
2:F:352:VAL:HG21	2:F:356:HIS:CD2	2.49	0.47
3:G:168[C]:LEU:HD22	3:G:189[C]:LEU:HD22	1.97	0.47
3:G:72[B]:PRO:HA	3:G:73[B]:VAL:CB	2.41	0.47
3:G:95[C]:ILE:O	3:G:99[C]:VAL:HG13	2.15	0.47
4:H:119[C]:ARG:HA	4:H:122[C]:GLU:CD	2.34	0.47
3:G:181[A]:GLN:O	3:G:183[A]:PRO:HD3	2.15	0.47
3:G:85[C]:ARG:HA	3:G:120[C]:ARG:NH2	2.30	0.47
4:H:101[B]:GLU:HB3	4:H:121[B]:LEU:HD21	1.97	0.47
4:H:60[A]:LEU:HB2	4:H:130[A]:VAL:HG13	1.96	0.47
4:H:41[C]:LEU:HD12	4:H:70[C]:VAL:HG11	1.96	0.47
1:A:99:VAL:CG1	1:A:248:TYR:CD1	2.98	0.47
1:B:271:ARG:NH1	1:B:285:ALA:CB	2.78	0.47
1:B:31:VAL:CG1	1:B:34:VAL:HG22	2.45	0.47
1:B:471:LEU:HD13	1:B:487:LEU:HD22	1.96	0.47
2:F:254:GLY:HA3	2:F:271:GLN:HE21	1.80	0.47
3:G:150[B]:GLN:O	3:G:150[B]:GLN:HG2	2.15	0.47
3:G:71[C]:ARG:HH22	3:G:163[C]:GLU:HG3	1.79	0.47
3:G:168[C]:LEU:HB2	3:G:189[C]:LEU:HB2	1.97	0.47
3:G:175[C]:PHE:HB2	3:G:236[C]:SER:OG	2.14	0.47
1:B:275:LEU:C	2:E:264:MET:HE2	2.36	0.47
1:C:271:ARG:NH1	1:C:285:ALA:HB1	2.29	0.47
1:C:31:VAL:CG1	1:C:34:VAL:HG22	2.44	0.47
1:C:99:VAL:CG1	1:C:248:TYR:CD1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:441:LEU:HD21	2:E:456:VAL:HG13	1.96	0.47
3:G:168[B]:LEU:H	3:G:190[B]:PRO:HD3	1.80	0.47
3:G:185[C]:GLU:O	3:G:185[C]:GLU:HG3	2.15	0.47
4:H:85[A]:PRO:HA	4:H:130[A]:VAL:HG12	1.97	0.47
4:H:9[C]:VAL:HG22	4:H:14[C]:LYS:HA	1.96	0.47
1:B:47:VAL:HG12	1:B:90:ARG:HG2	1.95	0.47
1:C:386:LEU:HD22	1:C:416:THR:HG21	1.97	0.47
1:C:460:LEU:O	1:C:464:MET:HG2	2.15	0.47
1:C:462:SER:HA	1:C:465:ARG:HH12	1.72	0.47
1:C:66:LEU:HD13	2:D:66:ARG:HG3	1.97	0.47
2:D:48:LEU:HD11	2:D:54:ARG:HB2	1.97	0.47
2:F:65:VAL:HB	2:F:68:LEU:HD21	1.97	0.47
2:F:84:ALA:HB1	2:F:103:VAL:HG12	1.96	0.47
4:H:123[B]:ARG:O	4:H:127[B]:ARG:HG3	2.14	0.47
4:H:4[A]:VAL:HG13	4:H:73[A]:ASP:O	2.15	0.47
3:G:48[C]:LYS:HZ1	4:H:9[C]:VAL:CG1	2.26	0.47
1:A:106:ARG:CG	1:A:106:ARG:NH1	2.55	0.46
1:A:337:ILE:O	2:E:184:ARG:NE	2.47	0.46
1:C:286:TYR:HB3	1:C:287:PRO:HD2	1.96	0.46
1:C:499:THR:N	1:C:500:PRO:CD	2.76	0.46
2:D:129:GLU:O	2:D:172:HIS:CE1	2.67	0.46
2:D:65:VAL:HB	2:D:68:LEU:HD21	1.98	0.46
2:E:247:ILE:O	2:E:250:PHE:HB3	2.14	0.46
2:E:254:GLY:HA3	2:E:271:GLN:NE2	2.30	0.46
2:F:34:ARG:CG	2:F:35:PRO:HA	2.39	0.46
3:G:140[C]:ILE:HG13	3:G:141[C]:SER:N	2.31	0.46
3:G:95[B]:ILE:HG23	3:G:96[B]:LEU:H	1.80	0.46
1:A:275:LEU:HA	1:A:278:ARG:CA	2.45	0.46
1:B:143:HIS:CD2	1:B:144:GLU:HG2	2.50	0.46
1:B:184:ILE:HG22	1:B:427:PRO:HG2	1.96	0.46
1:C:431:GLU:HG2	1:C:432:GLU:H	1.78	0.46
3:G:29[B]:ALA:HA	3:G:242[B]:MET:SD	2.55	0.46
3:G:32[C]:LEU:CG	3:G:238[C]:PHE:CB	2.75	0.46
1:C:284:GLU:HG3	1:C:329:TYR:CD1	2.48	0.46
3:G:170[A]:ILE:O	3:G:185[A]:GLU:HB2	2.15	0.46
3:G:217[A]:LEU:O	3:G:219[A]:PRO:HD3	2.16	0.46
3:G:68[A]:LEU:N	3:G:68[A]:LEU:HD22	2.30	0.46
4:H:8[C]:ILE:HG13	4:H:8[C]:ILE:O	2.15	0.46
1:A:275:LEU:CB	2:D:264:MET:SD	3.03	0.46
1:B:275:LEU:HA	1:B:278:ARG:HA	1.98	0.46
1:B:354:ARG:NH1	1:B:354:ARG:HG2	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:VAL:CG2	1:B:88:VAL:HG21	2.44	0.46
2:E:27:TYR:O	2:E:76:PRO:HA	2.15	0.46
2:E:340:LEU:HD12	2:E:340:LEU:HA	1.62	0.46
2:E:97:ILE:O	2:E:97:ILE:HG12	2.14	0.46
2:F:91:ASN:HD22	2:F:91:ASN:C	2.17	0.46
3:G:116[C]:PHE:HE2	3:G:165[C]:PHE:HZ	1.62	0.46
1:B:99:VAL:CG1	1:B:248:TYR:CD1	2.99	0.46
1:C:456:PHE:CZ	1:C:495:LYS:HD2	2.50	0.46
2:D:233:ARG:HD3	2:D:292:SER:HB3	1.98	0.46
2:D:441:LEU:HD21	2:D:456:VAL:HG13	1.97	0.46
4:H:20[C]:ALA:HA	4:H:53[C]:LYS:O	2.16	0.46
1:A:284:GLU:HG3	1:A:329:TYR:HB2	1.97	0.46
1:A:31:VAL:CG1	1:A:34:VAL:HG22	2.46	0.46
1:A:209:VAL:HG21	2:D:118:PHE:HZ	1.80	0.46
2:E:175:LEU:HG	2:E:238:GLN:NE2	2.27	0.46
2:E:162:GLN:NE2	2:E:194:GLU:HG2	2.29	0.46
3:G:88[B]:ALA:HB1	3:G:241[B]:ARG:HA	1.96	0.46
4:H:9[A]:VAL:HG13	4:H:14[A]:LYS:HE3	1.97	0.46
1:C:184:ILE:HG22	1:C:427:PRO:HG2	1.98	0.46
1:C:188:GLY:O	1:C:189:GLN:CB	2.64	0.46
1:C:284:GLU:HG3	1:C:329:TYR:CD2	2.48	0.46
2:E:241:LEU:HD12	2:E:241:LEU:HA	1.70	0.46
2:F:346:ILE:HB	2:F:351:VAL:HG11	1.98	0.46
3:G:170[B]:ILE:HD12	3:G:170[B]:ILE:O	2.14	0.46
3:G:76[C]:THR:HB	3:G:167[C]:LYS:CG	2.40	0.46
1:A:395:PHE:N	1:A:395:PHE:CD2	2.82	0.46
1:B:44:LEU:HD23	1:B:44:LEU:HA	1.77	0.46
1:C:395:PHE:CD2	1:C:395:PHE:N	2.82	0.46
1:C:438:TYR:CA	1:C:441:THR:HG22	2.42	0.46
2:D:131:GLY:HA3	2:D:167:ASN:HD22	1.77	0.46
2:E:264:MET:CB	2:E:265:PRO:CA	2.93	0.46
2:F:292:SER:OG	2:F:293:ILE:N	2.46	0.46
2:F:301:VAL:HG22	2:F:301:VAL:O	2.16	0.46
2:F:27:TYR:O	2:F:76:PRO:HA	2.15	0.46
3:G:175[B]:PHE:HA	3:G:236[B]:SER:HB2	1.98	0.46
3:G:238[C]:PHE:C	3:G:241[C]:ARG:H	2.19	0.46
3:G:65[C]:HIS:CD2	3:G:69[C]:GLU:HA	2.51	0.46
1:B:292:TYR:O	1:B:296:ARG:HB3	2.16	0.46
1:B:388:GLN:HG3	1:B:409:LYS:HZ1	1.78	0.46
2:D:373:LEU:HA	2:D:376:ILE:HG12	1.98	0.46
2:D:416:MET:N	2:D:417:PRO:CA	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:292:SER:OG	2:E:293:ILE:N	2.46	0.46
2:F:235:ARG:O	2:F:237:GLY:N	2.48	0.46
2:F:246:ASN:OD1	2:F:248:PHE:HB3	2.15	0.46
3:G:102[B]:THR:C	3:G:104[B]:GLU:H	2.19	0.46
3:G:75[A]:LYS:HD2	3:G:164[A]:THR:O	2.16	0.46
3:G:75[A]:LYS:HD2	3:G:164[A]:THR:HG22	1.98	0.46
1:A:109:ASN:HD21	1:A:113:GLN:CG	2.29	0.46
1:A:440:VAL:HG12	1:A:445:MET:HE3	1.97	0.46
2:D:241:LEU:HD12	2:D:241:LEU:HA	1.64	0.46
2:D:346:ILE:HB	2:D:351:VAL:HG11	1.97	0.46
2:D:34:ARG:CG	2:D:35:PRO:HA	2.38	0.46
2:E:24:PRO:HD2	2:E:53:VAL:HG11	1.98	0.46
2:E:264:MET:CB	2:E:265:PRO:HA	2.39	0.46
2:E:34:ARG:CG	2:E:35:PRO:HA	2.37	0.46
2:E:458:LYS:C	2:E:460:LYS:H	2.18	0.46
3:G:152[C]:ILE:CD1	3:G:152[C]:ILE:H	2.28	0.46
3:G:189[A]:LEU:HB3	3:G:190[A]:PRO:CD	2.40	0.46
3:G:38[C]:THR:O	3:G:231[C]:LEU:HD21	2.15	0.46
3:G:76[A]:THR:HB	3:G:78[A]:TYR:CE1	2.51	0.46
4:H:38[B]:HIS:NE2	4:H:41[B]:LEU:CD1	2.79	0.46
4:H:49[C]:PRO:HB3	4:H:61[C]:ILE:H	1.81	0.46
1:A:109:ASN:HB2	1:A:110:PRO:CD	2.46	0.45
1:A:354:ARG:NH1	1:A:354:ARG:HG2	2.20	0.45
1:B:275:LEU:HD12	1:B:281:PRO:HD3	1.97	0.45
1:C:298:LEU:HD12	1:C:317:PRO:CG	2.44	0.45
2:D:291:GLY:O	2:D:292:SER:CB	2.63	0.45
2:D:379:ILE:O	2:D:379:ILE:HG13	2.16	0.45
2:E:195:MET:HE2	2:E:206:MET:SD	2.56	0.45
2:E:65:VAL:HB	2:E:68:LEU:HD21	1.98	0.45
2:F:12:PRO:HG2	2:F:260:LEU:HD11	1.97	0.45
3:G:164[C]:THR:O	3:G:165[C]:PHE:HD1	1.99	0.45
3:G:189[C]:LEU:HD12	3:G:189[C]:LEU:HA	1.12	0.45
4:H:114[C]:TYR:HD2	4:H:118[C]:LYS:HD3	1.81	0.45
4:H:64[C]:SER:OG	4:H:81[C]:THR:HG23	2.16	0.45
1:A:275:LEU:HG	1:A:278:ARG:CA	2.42	0.45
1:A:286:TYR:HB3	1:A:287:PRO:HD2	1.98	0.45
1:A:333:ASN:O	1:A:337:ILE:HG13	2.15	0.45
1:B:188:GLY:O	1:B:189:GLN:CB	2.65	0.45
1:C:233:PRO:O	1:C:237:LEU:HG	2.16	0.45
1:C:243:CYS:HB2	1:C:260:TYR:OH	2.16	0.45
2:D:27:TYR:O	2:D:76:PRO:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:VAL:HG21	2:F:217:ALA:HB1	1.98	0.45
3:G:220[B]:LYS:HA	3:G:220[B]:LYS:HD3	1.72	0.45
3:G:49[B]:ILE:HG13	3:G:49[B]:ILE:O	2.15	0.45
3:G:86[B]:GLY:CA	3:G:241[B]:ARG:HH22	2.26	0.45
4:H:95[C]:LYS:HA	4:H:95[C]:LYS:HD2	1.63	0.45
4:H:97[C]:LYS:HE3	4:H:128[C]:LEU:CD1	2.42	0.45
1:B:93:ARG:HD3	1:B:96:GLU:OE2	2.17	0.45
1:C:284:GLU:HG3	1:C:329:TYR:HB2	1.98	0.45
2:E:89:VAL:HG23	2:E:97:ILE:CG2	2.46	0.45
2:F:160:LEU:HD22	2:F:164:LEU:HD22	1.97	0.45
3:G:123[C]:ARG:CG	3:G:136[C]:GLU:HB2	2.45	0.45
4:H:100[A]:HIS:HB2	4:H:121[A]:LEU:CG	2.36	0.45
1:C:435:ILE:HD13	1:C:464:MET:CE	2.46	0.45
2:E:135:ILE:HD12	2:E:141:TYR:CE2	2.51	0.45
2:E:254:GLY:HA3	2:E:271:GLN:HE21	1.81	0.45
2:E:387:ASP:O	2:E:391:LEU:HB2	2.17	0.45
2:F:218:ARG:O	2:F:221:VAL:HG12	2.16	0.45
2:F:12:PRO:HD2	2:F:260:LEU:CD2	2.47	0.45
1:C:275:LEU:CB	2:F:264:MET:HG3	2.46	0.45
3:G:131[A]:TYR:N	3:G:132[A]:PRO:HA	2.25	0.45
3:G:217[C]:LEU:C	3:G:219[C]:PRO:HD3	2.36	0.45
3:G:23[C]:ALA:O	3:G:27[C]:VAL:HG23	2.16	0.45
3:G:86[A]:GLY:CA	3:G:121[A]:LYS:HD2	2.47	0.45
4:H:88[A]:ILE:HD11	4:H:131[A]:ALA:CA	2.47	0.45
1:A:492:GLU:CA	1:A:495:LYS:HB2	2.33	0.45
1:B:157:ILE:HG21	1:B:342:ILE:CG1	2.46	0.45
1:B:419:ILE:HD13	1:B:440:VAL:CG1	2.47	0.45
1:B:448:ILE:HG23	1:B:449:PRO:CD	2.47	0.45
1:B:462:SER:CA	1:B:465:ARG:HH12	2.30	0.45
1:C:179:ALA:HB2	1:C:318:PHE:HZ	1.82	0.45
2:D:264:MET:CE	2:D:272:PRO:HB3	2.40	0.45
2:D:387:ASP:O	2:D:391:LEU:HB2	2.17	0.45
2:F:135:ILE:HD12	2:F:141:TYR:CE2	2.50	0.45
3:G:184[C]:VAL:CG1	3:G:186[C]:LYS:HE3	2.47	0.45
1:A:151:LYS:HE2	1:A:428:MET:CE	2.46	0.45
1:B:389:TYR:CD1	1:B:413:GLY:HA3	2.51	0.45
1:C:205:VAL:O	1:C:209:VAL:HG23	2.17	0.45
2:D:135:ILE:HD12	2:D:141:TYR:CE2	2.52	0.45
2:D:166:ASN:O	2:D:170:GLN:HB2	2.16	0.45
2:D:307:THR:HG23	2:D:307:THR:O	2.16	0.45
2:D:419:LYS:CE	2:D:450:GLY:HA3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:VAL:HG21	2:D:217:ALA:HB1	1.99	0.45
2:F:397:ARG:NH1	2:F:443:GLU:OE2	2.49	0.45
4:H:96[C]:ALA:HB1	4:H:100[C]:HIS:ND1	2.31	0.45
3:G:48[C]:LYS:HZ3	4:H:9[C]:VAL:HB	1.81	0.45
1:A:194:ILE:CD1	1:A:222:ILE:HD12	2.46	0.45
1:B:167:ILE:HD11	1:B:316:LEU:HD13	1.99	0.45
1:B:232:ALA:N	1:B:233:PRO:CD	2.79	0.45
1:B:330:ILE:HB	1:B:331:PRO:HD3	1.99	0.45
1:C:176:THR:O	1:C:180:ILE:HG12	2.17	0.45
1:C:319:ILE:HD13	1:C:319:ILE:HA	1.75	0.45
2:D:329:ALA:C	2:D:331:MET:H	2.20	0.45
2:F:149:LEU:CD2	2:F:324:LEU:HD22	2.47	0.45
2:F:35:PRO:HD2	2:F:36:GLN:OE1	2.17	0.45
2:F:416:MET:N	2:F:417:PRO:CA	2.78	0.45
3:G:31[B]:LYS:HE3	3:G:142[B]:ASP:CG	2.36	0.45
4:H:8[B]:ILE:CD1	4:H:15[B]:VAL:HB	2.46	0.45
1:B:262:ASP:OD1	1:B:264:SER:HB2	2.17	0.45
1:C:109:ASN:HB3	1:C:115:LEU:HD11	1.99	0.45
1:C:151:LYS:HE2	1:C:428:MET:HE3	1.98	0.45
1:C:440:VAL:HG12	1:C:445:MET:HE3	1.97	0.45
2:D:165:ILE:HG21	2:D:200:VAL:HG13	1.99	0.45
2:D:241:LEU:O	2:D:242:LEU:HB3	2.16	0.45
2:D:461:LYS:HE2	2:D:461:LYS:HB3	1.71	0.45
2:E:177:VAL:O	2:E:242:LEU:HA	2.16	0.45
3:G:255[C]:MET:CA	3:G:258[C]:THR:HG23	2.46	0.45
4:H:97[C]:LYS:HG3	4:H:128[C]:LEU:HD11	1.99	0.45
1:A:326:VAL:HG11	1:A:343:PHE:CE2	2.45	0.45
1:C:412:ARG:HG3	1:C:446:ASP:OD1	2.17	0.45
2:D:40:LEU:HD23	2:D:64:LEU:HD11	1.98	0.45
2:F:387:ASP:O	2:F:391:LEU:HB2	2.17	0.45
3:G:32[C]:LEU:HG	3:G:238[C]:PHE:CB	2.27	0.45
1:A:121:ILE:HG22	1:A:123:THR:HG22	1.99	0.45
1:A:144:GLU:O	1:A:161:ARG:HG3	2.17	0.45
1:A:47:VAL:HG12	1:A:90:ARG:HG2	1.97	0.45
1:B:151:LYS:HE2	1:B:428:MET:HE3	1.98	0.45
1:B:275:LEU:HG	1:B:278:ARG:CA	2.43	0.45
1:C:480:GLU:HG3	1:C:482:PRO:CD	2.47	0.45
3:G:96[C]:LEU:HD13	3:G:125[C]:PHE:CG	2.52	0.45
3:G:144[C]:PRO:HD3	3:G:231[C]:LEU:CD1	2.47	0.45
3:G:234[C]:LYS:HA	3:G:234[C]:LYS:HD2	1.61	0.45
4:H:71[B]:ARG:HB2	4:H:74[B]:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:N	1:A:158:PRO:HD2	2.32	0.44
1:A:183:ILE:HG12	1:A:193:CYS:HB3	1.99	0.44
1:A:188:GLY:O	1:A:189:GLN:CB	2.64	0.44
1:A:179:ALA:HB2	1:A:318:PHE:HZ	1.82	0.44
1:A:495:LYS:HE3	1:A:495:LYS:HB3	1.45	0.44
1:C:275:LEU:HA	1:C:278:ARG:H	1.82	0.44
2:F:82:GLY:HA2	2:F:231:TYR:CE2	2.52	0.44
2:F:177:VAL:O	2:F:242:LEU:HA	2.17	0.44
3:G:132[C]:PRO:HD2	3:G:133[C]:VAL:H	1.81	0.44
3:G:114[B]:VAL:HB	3:G:134[B]:VAL:HG13	2.00	0.44
3:G:65[C]:HIS:CD2	3:G:68[C]:LEU:O	2.69	0.44
3:G:82[C]:THR:HG21	3:G:96[C]:LEU:HD21	1.98	0.44
4:H:35[A]:MET:H	4:H:38[A]:HIS:CE1	2.34	0.44
1:C:48:MET:HA	2:D:65:VAL:HG22	2.00	0.44
2:D:288:THR:HG23	2:D:291:GLY:N	2.32	0.44
2:D:79:VAL:HG11	2:D:224:THR:HG23	1.99	0.44
2:E:205:SER:HB2	2:E:228:MET:HE1	1.99	0.44
2:F:264:MET:CE	2:F:272:PRO:HB3	2.44	0.44
3:G:139[C]:GLY:O	3:G:141[C]:SER:N	2.50	0.44
3:G:71[C]:ARG:NH1	3:G:166[C]:ASP:HA	2.32	0.44
3:G:48[A]:LYS:CG	3:G:49[A]:ILE:H	2.26	0.44
3:G:68[B]:LEU:N	3:G:68[B]:LEU:HD22	2.32	0.44
4:H:125[A]:GLU:O	4:H:129[A]:GLN:HG3	2.17	0.44
4:H:8[A]:ILE:HG13	4:H:16[A]:PHE:H	1.83	0.44
4:H:8[C]:ILE:O	4:H:15[C]:VAL:HB	2.17	0.44
1:A:157:ILE:HG21	1:A:342:ILE:CG1	2.46	0.44
1:C:183:ILE:HG12	1:C:193:CYS:HB3	1.98	0.44
2:E:161:ILE:HG23	2:E:243:PHE:CE1	2.53	0.44
2:F:273:THR:O	2:F:277:GLU:HG3	2.18	0.44
2:F:285:ILE:HD13	2:F:295:SER:HB2	2.00	0.44
3:G:131[A]:TYR:HB2	3:G:132[A]:PRO:O	2.18	0.44
3:G:141[B]:SER:OG	3:G:144[B]:PRO:HA	2.17	0.44
3:G:159[A]:MET:HB3	3:G:165[A]:PHE:CG	2.52	0.44
3:G:33[B]:ARG:C	3:G:35[B]:ALA:N	2.70	0.44
3:G:72[B]:PRO:CA	3:G:73[B]:VAL:CB	2.89	0.44
1:A:475:ILE:O	1:A:479:GLY:HA3	2.18	0.44
1:A:495:LYS:HB3	1:A:496:LYS:H	1.58	0.44
1:B:462:SER:HA	1:B:465:ARG:HH12	1.75	0.44
1:B:480:GLU:HG3	1:B:482:PRO:HD3	1.99	0.44
1:B:499:THR:N	1:B:500:PRO:CD	2.78	0.44
1:C:275:LEU:HA	1:C:278:ARG:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASP:OD1	1:C:425:HIS:HA	2.17	0.44
2:D:315:PHE:HA	2:D:318:LEU:HD22	1.99	0.44
2:E:264:MET:HG2	2:E:265:PRO:O	2.17	0.44
2:E:419:LYS:CE	2:E:450:GLY:HA3	2.43	0.44
2:F:192:TYR:O	2:F:196:LYS:HB3	2.17	0.44
2:F:441:LEU:HD21	2:F:456:VAL:HG13	1.99	0.44
3:G:170[C]:ILE:HD12	3:G:170[C]:ILE:N	2.33	0.44
3:G:177[B]:SER:HB3	3:G:180[B]:VAL:CG1	2.47	0.44
1:A:142:VAL:CG1	1:A:160:GLY:HA3	2.48	0.44
1:A:232:ALA:N	1:A:233:PRO:CD	2.81	0.44
1:A:298:LEU:HD21	1:A:337:ILE:CG2	2.47	0.44
1:B:176:THR:O	1:B:180:ILE:HG12	2.17	0.44
1:B:99:VAL:HG11	1:B:248:TYR:HB2	1.99	0.44
2:D:177:VAL:O	2:D:242:LEU:HA	2.18	0.44
2:D:411:GLU:CD	2:D:417:PRO:HB3	2.38	0.44
2:E:218:ARG:O	2:E:221:VAL:HG12	2.17	0.44
2:E:411:GLU:CD	2:E:417:PRO:HB3	2.38	0.44
2:E:85:THR:O	2:E:205:SER:HB3	2.17	0.44
2:F:307:THR:HG23	2:F:307:THR:O	2.16	0.44
3:G:174[B]:GLU:HG3	3:G:174[B]:GLU:O	2.17	0.44
3:G:86[A]:GLY:HA3	3:G:121[A]:LYS:CD	2.48	0.44
1:B:183:ILE:HG12	1:B:193:CYS:HB3	2.00	0.44
2:F:165:ILE:HG21	2:F:200:VAL:HG13	2.00	0.44
3:G:11[B]:ILE:HD11	3:G:259[B]:LEU:O	2.18	0.44
2:D:379:ILE:HD11	3:G:17[C]:THR:HG22	1.96	0.44
3:G:184[A]:VAL:HG22	3:G:185[A]:GLU:N	2.29	0.44
3:G:49[C]:ILE:HD13	3:G:49[C]:ILE:HA	1.68	0.44
4:H:93[A]:ALA:HA	4:H:96[A]:ALA:HB3	1.99	0.44
1:A:389:TYR:CD1	1:A:413:GLY:HA3	2.53	0.44
1:A:440:VAL:CG2	1:A:441:THR:N	2.81	0.44
1:A:448:ILE:HG23	1:A:449:PRO:CD	2.48	0.44
1:A:31:VAL:HG12	1:A:84:GLU:HA	1.99	0.44
1:B:95:MET:O	1:B:128:PRO:HA	2.17	0.44
2:D:12:PRO:HD2	2:D:260:LEU:CD2	2.48	0.44
2:D:366:VAL:HG21	2:D:434:LEU:CD2	2.48	0.44
2:E:288:THR:O	2:E:291:GLY:HA2	2.17	0.44
2:F:329:ALA:C	2:F:331:MET:H	2.20	0.44
3:G:132[C]:PRO:CD	3:G:133[C]:VAL:N	2.80	0.44
3:G:28[C]:ALA:CA	3:G:238[C]:PHE:HD1	1.98	0.44
3:G:36[B]:GLN:HA	3:G:39[B]:ALA:CB	2.47	0.44
3:G:79[B]:MET:HG3	3:G:116[B]:PHE:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:117[B]:HIS:O	4:H:120[B]:ALA:HB3	2.18	0.44
4:H:9[C]:VAL:CG2	4:H:14[C]:LYS:HD2	2.47	0.44
4:H:52[A]:ILE:HD11	4:H:59[A]:THR:HB	2.00	0.44
3:G:45[A]:TYR:HE1	4:H:9[A]:VAL:HG12	1.83	0.44
1:B:415:ARG:CG	1:B:415:ARG:NH1	2.49	0.44
1:B:94:ILE:HD12	1:B:94:ILE:O	2.18	0.44
1:C:91:THR:HG22	1:C:93:ARG:CG	2.48	0.44
2:D:340:LEU:HA	2:D:340:LEU:HD12	1.67	0.44
1:C:71:VAL:HG23	2:D:66:ARG:NH2	2.32	0.44
3:G:102[A]:THR:O	3:G:106[A]:ARG:HB2	2.18	0.44
3:G:149[B]:ILE:O	3:G:153[B]:ALA:HB3	2.18	0.44
3:G:172[A]:TYR:HB2	3:G:185[A]:GLU:HA	1.99	0.44
4:H:80[C]:ASP:HB3	4:H:81[C]:THR:H	1.60	0.44
1:B:460:LEU:O	1:B:463:PHE:HB3	2.18	0.44
1:B:480:GLU:HG3	1:B:482:PRO:CD	2.47	0.44
2:E:107:GLU:CD	2:E:235:ARG:HH12	2.22	0.44
3:G:101[C]:LYS:NZ	3:G:102[C]:THR:HG22	2.33	0.44
3:G:85[B]:ARG:HH22	3:G:241[B]:ARG:HE	1.66	0.44
4:H:71[C]:ARG:HB3	4:H:72[C]:PRO:CD	2.48	0.44
1:A:438:TYR:HA	1:A:441:THR:CG2	2.44	0.43
1:C:171:ARG:NH1	1:C:171:ARG:HG2	2.27	0.43
1:C:328:ALA:HB3	1:C:331:PRO:HG2	2.00	0.43
2:D:458:LYS:C	2:D:460:LYS:H	2.20	0.43
2:E:147:ILE:HA	2:E:320:ALA:O	2.17	0.43
2:E:338:ASP:HA	2:E:339:PRO:HD3	1.92	0.43
3:G:148[B]:GLU:HG2	3:G:149[B]:ILE:HG23	2.00	0.43
3:G:261[C]:LEU:HD12	3:G:262[C]:GLN:N	2.33	0.43
4:H:23[B]:VAL:HG22	4:H:52[B]:ILE:HG22	2.00	0.43
1:C:95:MET:O	1:C:128:PRO:HA	2.18	0.43
2:E:164:LEU:HD12	2:E:164:LEU:HA	1.82	0.43
2:F:419:LYS:CE	2:F:450:GLY:HA3	2.43	0.43
3:G:127[C]:LYS:C	3:G:127[C]:LYS:HD3	2.39	0.43
3:G:143[A]:THR:HB	3:G:144[A]:PRO:CA	2.48	0.43
4:H:104[C]:LEU:HD21	4:H:117[C]:HIS:HB2	1.99	0.43
1:B:462:SER:CB	1:B:465:ARG:HH12	2.31	0.43
1:C:194:ILE:HD13	1:C:222:ILE:HD12	2.00	0.43
2:D:91:ASN:ND2	2:D:91:ASN:C	2.71	0.43
2:E:258:SER:OG	2:E:263:ARG:HB2	2.19	0.43
2:E:356:HIS:C	2:E:356:HIS:CD2	2.91	0.43
3:G:162[A]:ASP:CA	3:G:163[A]:GLU:HB2	2.35	0.43
3:G:41[B]:ASN:C	3:G:44[B]:PRO:HD2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:94[B]:ASN:OD1	3:G:183[B]:PRO:HG3	2.18	0.43
4:H:117[A]:HIS:HA	4:H:120[A]:ALA:CB	2.48	0.43
1:A:186:GLN:HB2	1:A:220:TYR:CE1	2.54	0.43
2:E:192:TYR:O	2:E:196:LYS:HB3	2.17	0.43
2:F:24:PRO:HD2	2:F:53:VAL:HG11	1.99	0.43
2:F:371:ASN:ND2	3:G:10[B]:ARG:NH1	2.64	0.43
3:G:79[C]:MET:HE2	3:G:226[C]:ILE:HG21	1.99	0.43
4:H:59[B]:THR:HB	4:H:85[B]:PRO:HG2	2.00	0.43
4:H:51[C]:ARG:NE	4:H:60[C]:LEU:CD2	2.81	0.43
3:G:218[C]:LEU:HD12	4:H:67[C]:PHE:CE1	2.53	0.43
1:A:151:LYS:HD2	1:A:419:ILE:O	2.19	0.43
1:B:114:PRO:HG3	1:B:121:ILE:CD1	2.48	0.43
1:B:460:LEU:O	1:B:464:MET:HG2	2.17	0.43
2:D:292:SER:OG	2:D:293:ILE:N	2.47	0.43
2:E:129:GLU:O	2:E:172:HIS:CE1	2.70	0.43
2:F:286:THR:OG1	2:F:287:SER:N	2.51	0.43
3:G:5[A]:ARG:CB	3:G:5[A]:ARG:HH11	2.30	0.43
4:H:55[C]:GLY:O	4:H:56[C]:ASP:HB2	2.18	0.43
3:G:48[C]:LYS:CD	4:H:78[C]:LEU:HD22	2.34	0.43
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.84	0.43
1:A:271:ARG:HH11	1:A:285:ALA:HB1	1.83	0.43
1:B:187:LYS:C	1:B:189:GLN:HG2	2.39	0.43
1:B:284:GLU:HG3	1:B:329:TYR:CD2	2.49	0.43
1:B:431:GLU:HB2	1:B:472:LEU:HD22	2.00	0.43
1:C:113:GLN:HA	1:C:114:PRO:HD3	1.79	0.43
1:C:460:LEU:O	1:C:463:PHE:HB3	2.17	0.43
2:D:192:TYR:O	2:D:196:LYS:HB3	2.19	0.43
2:E:264:MET:HB2	2:E:264:MET:HE2	1.75	0.43
2:F:223:LEU:HD12	2:F:223:LEU:HA	1.79	0.43
2:F:288:THR:HG23	2:F:291:GLY:N	2.32	0.43
1:B:137:MET:HG3	2:F:98:ASP:HA	1.98	0.43
3:G:33[B]:ARG:HG2	3:G:34[B]:ARG:N	2.33	0.43
1:A:106:ARG:CB	1:A:106:ARG:HH11	2.29	0.43
1:B:171:ARG:NH1	1:B:171:ARG:HG3	2.19	0.43
2:D:325:GLU:HG3	2:D:338:ASP:HB2	1.99	0.43
2:E:132:ILE:HG12	2:E:132:ILE:H	1.47	0.43
2:E:86:LEU:HD11	2:E:175:LEU:HD13	2.00	0.43
2:F:147:ILE:HA	2:F:320:ALA:O	2.18	0.43
3:G:120[B]:ARG:HG2	3:G:120[B]:ARG:O	2.19	0.43
3:G:87[A]:LEU:N	3:G:241[A]:ARG:HH21	2.15	0.43
4:H:123[A]:ARG:O	4:H:127[A]:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:96[B]:ALA:HA	4:H:99[B]:ARG:HB2	2.01	0.43
1:A:113:GLN:HA	1:A:114:PRO:HD3	1.80	0.43
1:A:95:MET:O	1:A:128:PRO:HA	2.19	0.43
1:A:262:ASP:OD1	1:A:264:SER:HB2	2.18	0.43
1:B:144:GLU:O	1:B:161:ARG:HG3	2.19	0.43
1:B:233:PRO:O	1:B:237:LEU:HG	2.18	0.43
1:B:95:MET:HE3	1:B:95:MET:HB2	1.76	0.43
1:C:480:GLU:HG3	1:C:482:PRO:HD3	2.00	0.43
1:C:31:VAL:HG12	1:C:84:GLU:HA	2.01	0.43
2:D:296:ILE:N	2:D:296:ILE:HD12	2.34	0.43
2:F:118:PHE:HA	2:F:121:LEU:HD22	2.01	0.43
2:F:254:GLY:HA3	2:F:271:GLN:NE2	2.33	0.43
2:F:324:LEU:HD12	2:F:324:LEU:HA	1.81	0.43
2:F:373:LEU:HA	2:F:376:ILE:HG12	2.01	0.43
3:G:144[A]:PRO:O	3:G:145[A]:SER:HB2	2.18	0.43
4:H:51[C]:ARG:NE	4:H:60[C]:LEU:HD22	2.33	0.43
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.87	0.43
1:B:156:MET:SD	1:B:359:VAL:HG11	2.58	0.43
2:D:233:ARG:CD	2:D:292:SER:HB3	2.49	0.43
2:E:291:GLY:O	2:E:292:SER:CB	2.65	0.43
2:F:356:HIS:CD2	2:F:356:HIS:C	2.92	0.43
3:G:144[C]:PRO:O	3:G:145[C]:SER:HB2	2.19	0.43
3:G:162[C]:ASP:HA	3:G:163[C]:GLU:CB	2.33	0.43
3:G:241[A]:ARG:O	3:G:245[A]:MET:HG2	2.19	0.43
3:G:67[C]:MET:C	3:G:69[C]:GLU:N	2.71	0.43
4:H:85[C]:PRO:O	4:H:134[C]:LYS:HG2	2.18	0.43
1:A:271:ARG:HH11	1:A:285:ALA:CB	2.31	0.43
1:A:285:ALA:HA	2:D:267:ALA:HB3	2.01	0.43
1:A:44:LEU:HA	1:A:44:LEU:HD23	1.78	0.43
1:A:491:ILE:HG22	1:A:495:LYS:HG3	2.00	0.43
1:B:140:LYS:NZ	1:B:143:HIS:CE1	2.87	0.43
1:B:44:LEU:O	1:B:47:VAL:HG22	2.19	0.43
1:C:91:THR:HG22	1:C:93:ARG:H	1.84	0.43
2:F:142:ALA:HB2	2:F:346:ILE:HG21	2.01	0.43
2:F:26:ILE:O	2:F:27:TYR:HB2	2.19	0.43
3:G:107[C]:HIS:O	3:G:107[C]:HIS:CD2	2.72	0.43
3:G:115[A]:ILE:HD13	3:G:115[A]:ILE:N	2.33	0.43
3:G:80[C]:VAL:HG11	3:G:126[C]:PHE:CZ	2.53	0.43
3:G:133[B]:VAL:HG22	3:G:134[B]:VAL:N	2.34	0.43
3:G:148[B]:GLU:OE1	3:G:149[B]:ILE:HG13	2.19	0.43
3:G:151[C]:ASP:O	3:G:155[C]:SER:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:47[B]:THR:HG21	4:H:122[B]:GLU:CB	2.43	0.43
1:B:333:ASN:O	1:B:337:ILE:HG13	2.20	0.42
1:B:386:LEU:HA	1:B:389:TYR:HB3	2.01	0.42
1:B:411:ASN:HA	1:B:411:ASN:HD22	1.59	0.42
1:C:99:VAL:HG13	1:C:248:TYR:CG	2.54	0.42
2:D:388:GLU:O	2:D:391:LEU:HB3	2.19	0.42
2:E:205:SER:HB2	2:E:228:MET:CE	2.48	0.42
3:G:144[B]:PRO:HG2	3:G:230[B]:LEU:CD1	2.48	0.42
3:G:225[C]:LEU:O	3:G:228[C]:SER:HB2	2.19	0.42
4:H:26[A]:ARG:HA	4:H:31[A]:GLU:HB3	2.01	0.42
4:H:40[B]:PRO:HA	4:H:70[B]:VAL:HB	2.00	0.42
1:C:121:ILE:HG22	1:C:123:THR:HG22	2.02	0.42
1:C:46:LYS:HZ2	1:C:46:LYS:HB2	1.85	0.42
2:D:218:ARG:O	2:D:221:VAL:HG12	2.19	0.42
2:D:91:ASN:ND2	2:D:91:ASN:H	2.17	0.42
2:F:91:ASN:ND2	2:F:91:ASN:H	2.17	0.42
3:G:32[B]:LEU:CD1	3:G:238[B]:PHE:HB2	2.49	0.42
4:H:8[A]:ILE:HD11	4:H:15[A]:VAL:HB	2.00	0.42
1:A:194:ILE:HD13	1:A:222:ILE:HD12	2.01	0.42
1:A:440:VAL:HG22	1:A:441:THR:N	2.34	0.42
1:A:462:SER:HA	1:A:465:ARG:HH12	1.69	0.42
1:B:161:ARG:HH12	1:B:190:ASP:CB	2.30	0.42
1:C:431:GLU:HB2	1:C:472:LEU:HD22	2.02	0.42
2:D:258:SER:OG	2:D:263:ARG:HB2	2.18	0.42
2:E:329:ALA:C	2:E:331:MET:H	2.22	0.42
2:E:367:LEU:HD21	2:E:399:ILE:HG22	2.01	0.42
2:F:258:SER:OG	2:F:263:ARG:HB2	2.19	0.42
2:F:288:THR:O	2:F:291:GLY:HA2	2.19	0.42
2:F:372:ASP:O	2:F:376:ILE:HG12	2.19	0.42
3:G:104[C]:GLU:CA	3:G:107[C]:HIS:HD1	2.28	0.42
2:D:371:ASN:HB3	3:G:10[C]:ARG:HD2	2.02	0.42
3:G:24[C]:MET:HE1	3:G:87[C]:LEU:HD23	2.00	0.42
4:H:114[A]:TYR:O	4:H:118[A]:LYS:HE2	2.20	0.42
4:H:61[B]:ILE:O	4:H:63[B]:VAL:HG23	2.20	0.42
1:A:189:GLN:HE22	1:A:220:TYR:HB3	1.85	0.42
1:A:110:PRO:HG3	1:A:238:ALA:HA	2.01	0.42
1:A:480:GLU:HG3	1:A:482:PRO:CD	2.49	0.42
1:A:99:VAL:HG13	1:A:248:TYR:CG	2.54	0.42
1:B:481:LEU:C	1:B:481:LEU:HD22	2.39	0.42
1:C:140:LYS:NZ	1:C:143:HIS:CE1	2.86	0.42
1:C:194:ILE:CD1	1:C:222:ILE:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ILE:HD13	1:C:440:VAL:CG1	2.49	0.42
2:E:142:ALA:CB	2:E:346:ILE:HD13	2.46	0.42
3:G:107[C]:HIS:HB2	3:G:113[C]:TYR:CE1	2.54	0.42
3:G:15[B]:LYS:HG3	3:G:256[B]:LEU:CD1	2.47	0.42
3:G:179[A]:ILE:HG23	3:G:180[A]:VAL:HG13	2.02	0.42
3:G:225[A]:LEU:HA	3:G:225[A]:LEU:HD23	1.95	0.42
3:G:32[C]:LEU:HD13	3:G:35[C]:ALA:HB2	2.01	0.42
3:G:39[C]:ALA:O	3:G:42[C]:ALA:N	2.50	0.42
4:H:110[C]:THR:O	4:H:112[C]:LYS:CD	2.66	0.42
4:H:51[B]:ARG:NE	4:H:60[B]:LEU:HD21	2.32	0.42
1:A:475:ILE:HA	1:A:479:GLY:HA2	2.00	0.42
1:B:492:GLU:CA	1:B:495:LYS:HB2	2.33	0.42
1:B:66:LEU:HD12	2:F:9:VAL:CB	2.42	0.42
2:D:264:MET:HE2	2:D:264:MET:HB2	1.71	0.42
2:E:91:ASN:C	2:E:91:ASN:ND2	2.73	0.42
2:F:137:LEU:CG	2:F:138:LEU:HD13	2.47	0.42
2:F:42:VAL:HG12	2:F:57:ALA:HA	2.02	0.42
3:G:82[A]:THR:HG21	3:G:122[A]:GLY:HA3	2.01	0.42
3:G:18[B]:ARG:HG2	3:G:18[B]:ARG:O	2.18	0.42
3:G:245[B]:MET:C	3:G:247[B]:ASN:H	2.21	0.42
3:G:65[A]:HIS:HD2	3:G:69[A]:GLU:OE2	2.02	0.42
4:H:97[A]:LYS:HZ3	4:H:125[A]:GLU:HG2	1.84	0.42
1:A:171:ARG:NH1	1:A:171:ARG:HG3	2.13	0.42
1:A:91:THR:HG22	1:A:93:ARG:CG	2.49	0.42
1:B:113:GLN:HA	1:B:114:PRO:HD3	1.85	0.42
1:B:194:ILE:CD1	1:B:222:ILE:HD12	2.50	0.42
1:B:440:VAL:HG12	1:B:445:MET:HE2	2.02	0.42
1:B:46:LYS:HB2	1:B:46:LYS:HZ3	1.84	0.42
1:B:471:LEU:HD21	1:B:486:GLU:OE1	2.20	0.42
2:D:164:LEU:HA	2:D:164:LEU:HD12	1.75	0.42
1:A:365:ARG:NH2	2:E:186:ARG:HH22	2.01	0.42
3:G:78[B]:TYR:O	3:G:116[B]:PHE:HD2	2.02	0.42
3:G:217[A]:LEU:HG	3:G:218[A]:LEU:N	2.34	0.42
3:G:8[B]:LYS:CD	3:G:263[B]:PHE:CE1	3.00	0.42
3:G:43[B]:ARG:N	3:G:44[B]:PRO:CD	2.83	0.42
3:G:82[B]:THR:CG2	3:G:95[B]:ILE:HD13	2.48	0.42
4:H:111[C]:ASP:OD2	4:H:115[C]:LEU:HD11	2.20	0.42
1:A:271:ARG:NH1	1:A:285:ALA:HB3	2.35	0.42
1:B:187:LYS:O	1:B:189:GLN:HG2	2.19	0.42
2:D:93:LEU:HA	2:D:93:LEU:HD12	1.73	0.42
1:B:275:LEU:CD1	2:E:264:MET:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:178:PHE:CZ	2:F:245:ASP:HB2	2.54	0.42
2:F:411:GLU:CD	2:F:417:PRO:HB3	2.40	0.42
2:F:89:VAL:HG23	2:F:97:ILE:CG2	2.50	0.42
4:H:10[A]:THR:HG23	4:H:13[A]:ARG:O	2.19	0.42
4:H:22[B]:ILE:HG22	4:H:35[B]:MET:SD	2.59	0.42
1:A:140:LYS:HB3	1:A:305:SER:HA	2.01	0.42
1:A:99:VAL:HG11	1:A:248:TYR:HB2	2.01	0.42
1:C:483:ASP:O	1:C:486:GLU:HB3	2.19	0.42
2:D:235:ARG:O	2:D:237:GLY:N	2.52	0.42
3:G:169[A]:THR:HG23	3:G:186[A]:LYS:O	2.20	0.42
3:G:191[C]:LEU:HD12	3:G:191[C]:LEU:HA	1.86	0.42
3:G:32[C]:LEU:HD12	3:G:235[C]:ALA:N	2.34	0.42
4:H:115[B]:LEU:O	4:H:119[B]:ARG:HG3	2.20	0.42
4:H:90[B]:VAL:HA	4:H:128[B]:LEU:HD21	2.02	0.42
1:A:480:GLU:HG3	1:A:482:PRO:HD3	2.01	0.42
1:B:271:ARG:NH1	1:B:285:ALA:HB1	2.34	0.42
1:B:319:ILE:HD13	1:B:319:ILE:HA	1.74	0.42
1:C:271:ARG:HH11	1:C:285:ALA:CB	2.33	0.42
2:D:239:ASP:HA	2:D:292:SER:HA	2.02	0.42
2:D:412:GLN:HE21	2:D:412:GLN:HB2	1.52	0.42
2:D:80:PRO:HG3	2:D:108:ARG:NH1	2.35	0.42
2:F:205:SER:HB2	2:F:228:MET:CE	2.50	0.42
3:G:148[C]:GLU:CG	3:G:149[C]:ILE:HG13	2.47	0.42
3:G:175[B]:PHE:CD1	3:G:236[B]:SER:HA	2.48	0.42
3:G:249[B]:THR:O	3:G:250[B]:ASP:C	2.57	0.42
3:G:43[C]:ARG:O	3:G:44[C]:PRO:C	2.58	0.42
1:A:499:THR:N	1:A:500:PRO:CD	2.78	0.42
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.78	0.42
1:B:187:LYS:O	1:B:189:GLN:CG	2.68	0.42
1:B:166:LEU:HB3	1:B:341:GLN:HB3	2.01	0.42
1:B:483:ASP:O	1:B:486:GLU:HB3	2.20	0.42
1:B:52:LEU:O	1:B:53:LEU:HD23	2.19	0.42
1:C:232:ALA:N	1:C:233:PRO:CD	2.83	0.42
2:D:86:LEU:HD11	2:D:175:LEU:HD13	2.02	0.42
2:D:42:VAL:HG12	2:D:57:ALA:HA	2.02	0.42
3:G:45[B]:TYR:CE2	3:G:49[B]:ILE:HD11	2.55	0.42
4:H:109[C]:LYS:O	4:H:110[C]:THR:OG1	2.36	0.42
1:B:191:VAL:HA	1:B:255:HIS:O	2.20	0.41
1:B:275:LEU:C	1:B:278:ARG:H	2.24	0.41
1:C:271:ARG:NH1	1:C:285:ALA:HB3	2.35	0.41
1:C:354:ARG:NH1	1:C:354:ARG:HG2	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:VAL:HG22	1:C:441:THR:N	2.35	0.41
2:D:264:MET:HG2	2:D:265:PRO:C	2.40	0.41
2:E:242:LEU:O	2:E:295:SER:HA	2.20	0.41
2:E:91:ASN:H	2:E:91:ASN:ND2	2.17	0.41
3:G:143[A]:THR:N	3:G:144[A]:PRO:HA	2.25	0.41
3:G:182[A]:ARG:NH2	3:G:183[A]:PRO:HD2	2.35	0.41
3:G:217[B]:LEU:HG	3:G:218[B]:LEU:N	2.35	0.41
3:G:81[C]:ILE:HA	3:G:118[C]:VAL:HG13	2.02	0.41
4:H:117[C]:HIS:HA	4:H:120[C]:ALA:CB	2.46	0.41
4:H:130[B]:VAL:C	4:H:132[B]:ASN:H	2.24	0.41
4:H:22[B]:ILE:CG1	4:H:53[B]:LYS:HD2	2.46	0.41
1:A:284:GLU:HG3	1:A:329:TYR:CD1	2.52	0.41
1:A:236:TYR:HE1	1:A:293:LEU:CD1	2.34	0.41
1:A:386:LEU:HA	1:A:389:TYR:HB3	2.02	0.41
1:B:460:LEU:HG	1:B:494:PHE:CE2	2.55	0.41
1:C:109:ASN:HB2	1:C:110:PRO:CD	2.49	0.41
1:C:167:ILE:O	1:C:318:PHE:HA	2.20	0.41
2:D:233:ARG:HB2	2:D:292:SER:CB	2.50	0.41
2:F:107:GLU:CD	2:F:235:ARG:HH12	2.23	0.41
3:G:167[A]:LYS:N	3:G:167[A]:LYS:HD2	2.35	0.41
3:G:18[C]:ARG:HH12	3:G:253[C]:THR:CB	2.33	0.41
3:G:239[B]:GLY:O	3:G:242[B]:MET:HG2	2.21	0.41
3:G:72[A]:PRO:HA	3:G:73[A]:VAL:CB	2.44	0.41
3:G:79[A]:MET:HB3	3:G:170[A]:ILE:HB	2.01	0.41
4:H:4[B]:VAL:CG2	4:H:36[B]:ALA:HA	2.50	0.41
1:A:217:ALA:HA	1:A:220:TYR:CE2	2.56	0.41
1:A:275:LEU:HA	1:A:278:ARG:HA	2.02	0.41
1:A:167:ILE:HD11	1:A:316:LEU:HD13	2.03	0.41
1:B:121:ILE:HG22	1:B:123:THR:HG22	2.02	0.41
1:B:440:VAL:HG12	1:B:445:MET:HE3	2.02	0.41
2:D:24:PRO:HD2	2:D:53:VAL:HG11	2.01	0.41
2:F:233:ARG:CD	2:F:292:SER:HB3	2.50	0.41
2:F:416:MET:HA	2:F:416:MET:CE	2.50	0.41
2:F:423:VAL:O	2:F:424:LYS:C	2.58	0.41
2:F:93:LEU:HA	2:F:93:LEU:HD12	1.72	0.41
3:G:115[A]:ILE:HD11	3:G:126[A]:PHE:CE1	2.55	0.41
3:G:84[A]:ASP:OD1	3:G:140[A]:ILE:HG12	2.20	0.41
3:G:27[C]:VAL:O	3:G:28[C]:ALA:C	2.59	0.41
3:G:79[C]:MET:HG3	3:G:116[C]:PHE:HB2	2.03	0.41
4:H:38[B]:HIS:NE2	4:H:41[B]:LEU:HD12	2.35	0.41
4:H:27[C]:GLY:HA2	4:H:45[C]:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:22[C]:ILE:CG1	4:H:53[C]:LYS:HD2	2.47	0.41
1:B:65:ASN:HB3	2:F:10:MET:CE	2.49	0.41
1:C:275:LEU:C	1:C:278:ARG:H	2.24	0.41
2:D:12:PRO:HG2	2:D:260:LEU:HD11	2.03	0.41
2:E:218:ARG:HH11	2:E:218:ARG:HD2	1.74	0.41
2:E:397:ARG:NH1	2:E:443:GLU:OE2	2.53	0.41
2:E:93:LEU:HD12	2:E:93:LEU:HA	1.59	0.41
2:F:291:GLY:O	2:F:292:SER:CB	2.68	0.41
3:G:168[B]:LEU:HD23	3:G:169[B]:THR:N	2.36	0.41
3:G:188[A]:LEU:CD2	3:G:225[A]:LEU:HB3	2.41	0.41
3:G:71[B]:ARG:HA	3:G:72[B]:PRO:HD3	1.87	0.41
3:G:98[A]:LEU:HA	3:G:98[A]:LEU:HD22	1.83	0.41
4:H:9[C]:VAL:HG11	4:H:14[C]:LYS:HD3	2.02	0.41
1:C:330:ILE:HB	1:C:331:PRO:HD3	2.01	0.41
1:C:389:TYR:CD1	1:C:413:GLY:HA3	2.54	0.41
1:C:477:GLN:O	1:C:478:THR:C	2.59	0.41
2:E:118:PHE:HA	2:E:121:LEU:HD22	2.02	0.41
2:E:270:TYR:CZ	2:E:310:ALA:HB2	2.55	0.41
2:F:241:LEU:O	2:F:242:LEU:HB3	2.20	0.41
3:G:99[B]:VAL:CG2	3:G:100[B]:SER:N	2.82	0.41
3:G:83[C]:SER:O	3:G:121[C]:LYS:HB2	2.21	0.41
3:G:17[B]:THR:O	3:G:17[B]:THR:CG2	2.67	0.41
3:G:184[B]:VAL:HG21	3:G:186[B]:LYS:HE3	2.03	0.41
4:H:86[A]:GLU:CG	4:H:134[A]:LYS:HB3	2.51	0.41
4:H:5[B]:GLN:HG2	4:H:19[B]:GLU:HG2	2.01	0.41
4:H:59[C]:THR:OG1	4:H:85[C]:PRO:HB3	2.21	0.41
4:H:8[C]:ILE:HD13	4:H:61[C]:ILE:HD12	2.02	0.41
1:A:464:MET:HE2	1:A:464:MET:HB3	1.90	0.41
1:A:498:PHE:CD1	1:A:499:THR:HG22	2.55	0.41
1:C:271:ARG:HH11	1:C:285:ALA:HB1	1.86	0.41
2:D:241:LEU:O	2:D:294:THR:O	2.38	0.41
2:E:288:THR:HG23	2:E:291:GLY:N	2.35	0.41
2:E:411:GLU:HA	2:E:415:GLY:HA2	2.02	0.41
2:F:241:LEU:HA	2:F:241:LEU:HD12	1.59	0.41
1:C:275:LEU:N	2:F:264:MET:HE1	2.34	0.41
2:F:296:ILE:N	2:F:296:ILE:HD12	2.36	0.41
3:G:79[B]:MET:HB2	3:G:168[B]:LEU:HD21	2.01	0.41
3:G:5[C]:ARG:O	3:G:8[C]:LYS:HB2	2.20	0.41
3:G:71[C]:ARG:HA	3:G:72[C]:PRO:HD3	1.81	0.41
4:H:9[A]:VAL:HG13	4:H:14[A]:LYS:CD	2.51	0.41
4:H:38[B]:HIS:CD2	4:H:39[B]:ILE:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:CG1	1:A:248:TYR:HB2	2.51	0.41
1:C:67:GLU:HB2	1:C:70:ASN:O	2.19	0.41
1:C:69:ASP:N	1:C:69:ASP:OD1	2.53	0.41
3:G:114[A]:VAL:HB	3:G:134[A]:VAL:HG13	2.02	0.41
3:G:120[C]:ARG:O	3:G:120[C]:ARG:CG	2.67	0.41
3:G:79[A]:MET:H	3:G:170[A]:ILE:HA	1.85	0.41
3:G:192[B]:THR:O	3:G:193[B]:SER:C	2.59	0.41
3:G:32[C]:LEU:HD12	3:G:234[C]:LYS:C	2.41	0.41
4:H:109[A]:LYS:HE3	4:H:109[A]:LYS:HB2	1.94	0.41
4:H:48[A]:ALA:HA	4:H:49[A]:PRO:HD3	1.98	0.41
4:H:71[B]:ARG:C	4:H:73[B]:ASP:H	2.24	0.41
4:H:6[B]:VAL:HA	4:H:75[B]:VAL:O	2.20	0.41
1:A:94:ILE:HG13	1:A:94:ILE:H	1.59	0.41
1:B:438:TYR:HA	1:B:441:THR:CG2	2.45	0.41
1:B:459:GLU:HA	1:B:462:SER:OG	2.21	0.41
1:C:140:LYS:HB3	1:C:305:SER:HA	2.03	0.41
1:C:278:ARG:HE	1:C:278:ARG:HB3	1.68	0.41
1:C:411:ASN:HA	1:C:411:ASN:HD22	1.60	0.41
1:C:460:LEU:HG	1:C:494:PHE:CE2	2.55	0.41
2:D:181:VAL:HG22	2:D:221:VAL:CG1	2.49	0.41
1:A:275:LEU:CB	2:D:264:MET:CG	2.94	0.41
2:F:366:VAL:HG21	2:F:434:LEU:CD2	2.51	0.41
3:G:116[C]:PHE:HE2	3:G:165[C]:PHE:CZ	2.38	0.41
3:G:160[B]:PHE:HB2	3:G:189[B]:LEU:HD21	2.03	0.41
3:G:80[A]:VAL:HG11	3:G:126[A]:PHE:CZ	2.55	0.41
3:G:86[B]:GLY:O	3:G:87[B]:LEU:HB2	2.19	0.41
1:A:477:GLN:O	1:A:478:THR:C	2.58	0.41
1:B:206:ALA:HA	2:E:118:PHE:CZ	2.56	0.41
1:B:491:ILE:HG22	1:B:495:LYS:HG3	2.02	0.41
1:B:495:LYS:HB3	1:B:496:LYS:H	1.58	0.41
2:D:125:ASP:CG	2:D:345:ARG:NH2	2.72	0.41
2:D:240:VAL:HG12	2:D:241:LEU:N	2.36	0.41
2:D:308:ASP:C	2:D:311:PRO:HD2	2.40	0.41
2:D:325:GLU:HG2	2:D:338:ASP:HB2	2.02	0.41
2:D:40:LEU:CD2	2:D:64:LEU:HD11	2.50	0.41
2:E:92:VAL:HG11	2:E:220:ARG:HB2	2.03	0.41
2:F:338:ASP:HB3	2:F:341:ALA:HB3	2.03	0.41
3:G:234[C]:LYS:O	3:G:237[C]:GLU:N	2.52	0.41
3:G:91[A]:TYR:O	3:G:92[A]:ASN:CB	2.66	0.41
4:H:103[B]:ILE:HG22	4:H:106[B]:ARG:NE	2.36	0.41
4:H:39[B]:ILE:CG2	4:H:40[B]:PRO:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:O	1:C:161:ARG:HG3	2.21	0.41
2:D:149:LEU:CD2	2:D:324:LEU:HD22	2.51	0.41
2:E:325:GLU:CG	2:E:338:ASP:HB2	2.51	0.41
2:E:395:ARG:NH2	2:E:436:GLY:CA	2.83	0.41
2:F:308:ASP:C	2:F:311:PRO:HD2	2.41	0.41
3:G:175[B]:PHE:CZ	3:G:177[B]:SER:O	2.74	0.41
3:G:38[B]:THR:O	3:G:231[B]:LEU:HD21	2.21	0.41
4:H:128[C]:LEU:HD23	4:H:128[C]:LEU:HA	1.91	0.41
1:A:161:ARG:HH12	1:A:190:ASP:CB	2.29	0.41
1:B:91:THR:HG22	1:B:93:ARG:CG	2.50	0.41
1:B:62:MET:HE3	1:B:95:MET:HE3	2.03	0.41
1:C:497:GLY:O	1:C:498:PHE:CG	2.74	0.41
2:D:268:VAL:O	2:D:268:VAL:CG2	2.67	0.41
2:D:77:ILE:O	2:D:111:ILE:HG23	2.20	0.41
2:E:419:LYS:HA	2:E:419:LYS:HD2	1.88	0.41
3:G:12[B]:ARG:CZ	3:G:12[B]:ARG:CB	2.99	0.41
3:G:65[C]:HIS:C	3:G:67[C]:MET:N	2.73	0.41
3:G:83[B]:SER:HB3	3:G:92[B]:ASN:ND2	2.35	0.41
1:A:419:ILE:HD13	1:A:440:VAL:CG1	2.51	0.40
1:C:161:ARG:HH12	1:C:190:ASP:CB	2.30	0.40
1:C:386:LEU:HA	1:C:389:TYR:HB3	2.02	0.40
1:C:491:ILE:HG22	1:C:495:LYS:HG3	2.02	0.40
2:D:319:ASP:OD2	2:D:345:ARG:HD3	2.21	0.40
2:D:411:GLU:HA	2:D:415:GLY:HA2	2.02	0.40
2:D:431:LYS:HE3	2:D:435:GLU:OE2	2.20	0.40
2:E:215:PRO:HB3	2:E:256:GLU:HB2	2.03	0.40
3:G:132[C]:PRO:HD2	3:G:133[C]:VAL:N	2.37	0.40
3:G:156[C]:ALA:HB1	3:G:168[C]:LEU:HD11	2.04	0.40
3:G:261[C]:LEU:CD1	3:G:262[C]:GLN:HG3	2.48	0.40
3:G:75[A]:LYS:CD	3:G:164[A]:THR:HG22	2.51	0.40
4:H:45[C]:LEU:HD11	4:H:68[C]:LEU:HD21	2.02	0.40
1:A:459:GLU:HA	1:A:462:SER:OG	2.20	0.40
1:B:271:ARG:HH11	1:B:285:ALA:CB	2.34	0.40
1:B:56:GLU:HG3	1:B:87:GLN:HB2	2.03	0.40
2:F:86:LEU:HD11	2:F:175:LEU:HD13	2.03	0.40
1:C:83:ARG:CB	2:F:47:HIS:CE1	2.88	0.40
3:G:165[A]:PHE:HE2	3:G:168[A]:LEU:HD13	1.86	0.40
4:H:101[B]:GLU:HB3	4:H:121[B]:LEU:HG	2.02	0.40
4:H:111[C]:ASP:N	4:H:112[C]:LYS:HG3	2.35	0.40
4:H:15[C]:VAL:HG12	4:H:16[C]:PHE:CD1	2.57	0.40
4:H:64[C]:SER:HB2	4:H:123[C]:ARG:HE	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:HG3	1:A:329:TYR:CD2	2.52	0.40
1:B:475:ILE:HA	1:B:479:GLY:HA2	2.03	0.40
1:B:477:GLN:O	1:B:478:THR:C	2.60	0.40
1:C:471:LEU:HD21	1:C:486:GLU:OE1	2.21	0.40
2:E:264:MET:HG2	2:E:265:PRO:C	2.41	0.40
2:E:79:VAL:HA	2:E:80:PRO:HD3	1.95	0.40
2:F:27:TYR:HB3	2:F:112:HIS:CD2	2.57	0.40
2:F:235:ARG:HA	2:F:235:ARG:HD3	1.89	0.40
2:F:319:ASP:OD2	2:F:345:ARG:HD3	2.22	0.40
2:F:431:LYS:HE3	2:F:435:GLU:OE2	2.20	0.40
3:G:32[A]:LEU:HB2	3:G:238[A]:PHE:HB3	2.00	0.40
4:H:100[B]:HIS:HB3	4:H:120[B]:ALA:HB3	2.03	0.40
4:H:50[A]:VAL:HG23	4:H:63[A]:VAL:HG21	2.04	0.40
1:A:460:LEU:O	1:A:463:PHE:HB3	2.20	0.40
1:B:142:VAL:CG1	1:B:160:GLY:HA3	2.52	0.40
1:C:44:LEU:HA	1:C:44:LEU:HD23	1.79	0.40
1:C:450:VAL:C	1:C:452:ASP:H	2.25	0.40
2:D:167:ASN:OD1	2:D:408:HIS:HD2	2.04	0.40
2:E:233:ARG:CG	2:E:292:SER:HB3	2.51	0.40
2:E:318:LEU:HA	2:E:318:LEU:HD12	1.87	0.40
3:G:176[C]:VAL:CG1	3:G:177[C]:SER:N	2.76	0.40
3:G:179[B]:ILE:O	3:G:179[B]:ILE:HG23	2.21	0.40
3:G:255[C]:MET:HA	3:G:258[C]:THR:CG2	2.50	0.40
3:G:91[B]:TYR:O	3:G:92[B]:ASN:HB2	2.20	0.40
1:A:483:ASP:O	1:A:486:GLU:HB3	2.21	0.40
1:B:31:VAL:HG12	1:B:84:GLU:HA	2.04	0.40
1:C:481:LEU:C	1:C:481:LEU:HD22	2.42	0.40
2:D:273:THR:O	2:D:277:GLU:HG3	2.22	0.40
2:F:264:MET:HG2	2:F:265:PRO:C	2.42	0.40
3:G:179[C]:ILE:HG22	3:G:180[C]:VAL:HG13	2.04	0.40
4:H:110[C]:THR:C	4:H:112[C]:LYS:CG	2.81	0.40
4:H:38[C]:HIS:O	4:H:72[C]:PRO:HA	2.22	0.40
4:H:90[B]:VAL:O	4:H:128[B]:LEU:HD21	2.21	0.40
3:G:45[A]:TYR:CE1	4:H:9[A]:VAL:HG12	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:GLY:O	4:H:111[C]:ASP:O[2_454]	2.11	0.09



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	472/502 (94%)	418 (89%)	44 (9%)	10 (2%)	7	26
1	B	472/502 (94%)	417 (88%)	44 (9%)	11 (2%)	6	24
1	C	472/502 (94%)	417 (88%)	44 (9%)	11 (2%)	6	24
2	D	459/462 (99%)	406 (88%)	44 (10%)	9 (2%)	7	27
2	E	459/462 (99%)	408 (89%)	43 (9%)	8 (2%)	9	32
2	F	459/462 (99%)	407 (89%)	43 (9%)	9 (2%)	7	27
3	G	663/286 (232%)	468 (71%)	141 (21%)	54 (8%)	1	4
4	H	399/135 (296%)	294 (74%)	78 (20%)	27 (7%)	1	6
All	All	3855/3313 (116%)	3235 (84%)	481 (12%)	139 (4%)	5	16

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	396	ALA
1	A	404	LYS
1	A	481	LEU
1	A	482	PRO
1	B	189	GLN
1	B	262	ASP
1	B	396	ALA
1	B	404	LYS
1	B	481	LEU
1	B	482	PRO
1	C	189	GLN
1	C	262	ASP
1	C	396	ALA
1	C	404	LYS
1	C	481	LEU
1	C	482	PRO

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Mol	Chain	Res	Type
2	D	264	MET
2	D	292	SER
2	E	264	MET
2	E	292	SER
2	F	264	MET
2	F	292	SER
3	G	67[A]	MET
3	G	67[B]	MET
3	G	67[C]	MET
3	G	73[A]	VAL
3	G	73[B]	VAL
3	G	73[C]	VAL
3	G	92[A]	ASN
3	G	92[B]	ASN
3	G	92[C]	ASN
3	G	106[A]	ARG
3	G	106[B]	ARG
3	G	106[C]	ARG
3	G	132[A]	PRO
3	G	132[B]	PRO
3	G	132[C]	PRO
3	G	133[A]	VAL
3	G	133[B]	VAL
3	G	133[C]	VAL
3	G	138[A]	THR
3	G	138[B]	THR
3	G	138[C]	THR
3	G	140[A]	ILE
3	G	140[B]	ILE
3	G	140[C]	ILE
3	G	150[A]	GLN
3	G	150[B]	GLN
3	G	150[C]	GLN
3	G	163[A]	GLU
3	G	163[B]	GLU
3	G	163[C]	GLU
3	G	172[A]	TYR
3	G	172[B]	TYR
3	G	172[C]	TYR
3	G	176[A]	VAL
3	G	176[B]	VAL
3	G	176[C]	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	H	105[A]	LYS
4	H	105[B]	LYS
4	H	105[C]	LYS
4	H	112[A]	LYS
4	H	112[B]	LYS
4	H	112[C]	LYS
1	A	262	ASP
1	A	495	LYS
1	B	495	LYS
1	C	449	PRO
1	C	495	LYS
3	G	113[A]	TYR
3	G	113[B]	TYR
3	G	113[C]	TYR
3	G	114[A]	VAL
3	G	114[B]	VAL
3	G	114[C]	VAL
4	H	51[A]	ARG
4	H	51[B]	ARG
4	H	51[C]	ARG
4	H	80[A]	ASP
4	H	80[B]	ASP
4	H	80[C]	ASP
4	H	106[A]	ARG
4	H	106[B]	ARG
4	H	106[C]	ARG
4	H	109[A]	LYS
4	H	109[B]	LYS
4	H	109[C]	LYS
1	A	449	PRO
1	B	449	PRO
3	G	44[A]	PRO
3	G	44[B]	PRO
3	G	44[C]	PRO
3	G	131[A]	TYR
3	G	131[B]	TYR
3	G	131[C]	TYR
4	H	110[A]	THR
4	H	110[B]	THR
4	H	110[C]	THR
1	A	402	LEU
1	A	478	THR

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Mol	Chain	Res	Type
1	B	402	LEU
1	B	478	THR
1	C	402	LEU
1	C	478	THR
2	D	38	GLY
2	D	170	GLN
2	D	301	VAL
2	E	301	VAL
2	F	170	GLN
2	F	301	VAL
2	D	37	GLY
3	G	191[A]	LEU
3	G	191[B]	LEU
3	G	191[C]	LEU
4	H	98[A]	ALA
4	H	98[B]	ALA
4	H	98[C]	ALA
1	B	329	TYR
2	E	34	ARG
2	E	38	GLY
2	F	34	ARG
4	H	12[A]	GLU
4	H	12[B]	GLU
4	H	12[C]	GLU
1	C	157	ILE
2	D	34	ARG
2	E	37	GLY
2	D	291	GLY
2	F	37	GLY
2	F	291	GLY
3	G	65[A]	HIS
3	G	65[B]	HIS
3	G	65[C]	HIS
2	E	291	GLY
2	F	38	GLY
2	F	417	PRO
2	D	417	PRO
2	E	417	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/413 (94%)	349 (90%)	39 (10%)	7	25
1	B	388/413 (94%)	347 (89%)	41 (11%)	6	23
1	C	388/413 (94%)	349 (90%)	39 (10%)	7	25
2	D	375/376 (100%)	335 (89%)	40 (11%)	6	23
2	E	375/376 (100%)	336 (90%)	39 (10%)	7	24
2	F	375/376 (100%)	336 (90%)	39 (10%)	7	24
3	G	576/239 (241%)	507 (88%)	69 (12%)	5	18
4	H	339/113 (300%)	324 (96%)	15 (4%)	28	58
All	All	3204/2719 (118%)	2883 (90%)	321 (10%)	7	25

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	34	VAL
1	A	40	ARG
1	A	52	LEU
1	A	83	ARG
1	A	88	VAL
1	A	94	ILE
1	A	99	VAL
1	A	106	ARG
1	A	108	VAL
1	A	136	VAL
1	A	140	LYS
1	A	144	GLU
1	A	164	ARG
1	A	171	ARG
1	A	177	THR
1	A	187	LYS
1	A	189	GLN
1	A	191	VAL

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Mol	Chain	Res	Type
1	A	194	ILE
1	A	262	ASP
1	A	274	SER
1	A	275	LEU
1	A	278	ARG
1	A	296	ARG
1	A	298	LEU
1	A	341	GLN
1	A	354	ARG
1	A	362	SER
1	A	381	THR
1	A	395	PHE
1	A	411	ASN
1	A	415	ARG
1	A	445	MET
1	A	448	ILE
1	A	460	LEU
1	A	468	LYS
1	A	481	LEU
1	A	499	THR
1	B	30	THR
1	B	34	VAL
1	B	40	ARG
1	B	52	LEU
1	B	80	THR
1	B	83	ARG
1	B	87	GLN
1	B	88	VAL
1	B	94	ILE
1	B	99	VAL
1	B	106	ARG
1	B	108	VAL
1	B	136	VAL
1	B	164	ARG
1	B	171	ARG
1	B	177	THR
1	B	187	LYS
1	B	189	GLN
1	B	191	VAL
1	B	194	ILE
1	B	262	ASP
1	B	274	SER

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Mol	Chain	Res	Type
1	B	275	LEU
1	B	278	ARG
1	B	296	ARG
1	B	298	LEU
1	B	341	GLN
1	B	344	LEU
1	B	354	ARG
1	B	362	SER
1	B	381	THR
1	B	395	PHE
1	B	411	ASN
1	B	415	ARG
1	B	430	VAL
1	B	445	MET
1	B	448	ILE
1	B	460	LEU
1	B	468	LYS
1	B	481	LEU
1	B	499	THR
1	C	30	THR
1	C	33	GLN
1	C	34	VAL
1	C	40	ARG
1	C	52	LEU
1	C	83	ARG
1	C	88	VAL
1	C	94	ILE
1	C	99	VAL
1	C	106	ARG
1	C	108	VAL
1	C	136	VAL
1	C	140	LYS
1	C	164	ARG
1	C	171	ARG
1	C	177	THR
1	C	187	LYS
1	C	189	GLN
1	C	191	VAL
1	C	194	ILE
1	C	262	ASP
1	C	274	SER
1	C	275	LEU

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Mol	Chain	Res	Type
1	C	278	ARG
1	C	296	ARG
1	C	298	LEU
1	C	341	GLN
1	C	354	ARG
1	C	362	SER
1	C	381	THR
1	C	411	ASN
1	C	415	ARG
1	C	430	VAL
1	C	445	MET
1	C	448	ILE
1	C	460	LEU
1	C	468	LYS
1	C	481	LEU
1	C	499	THR
2	D	5	ARG
2	D	26	ILE
2	D	34	ARG
2	D	36	GLN
2	D	53	VAL
2	D	91	ASN
2	D	92	VAL
2	D	93	LEU
2	D	113	ARG
2	D	121	LEU
2	D	132	ILE
2	D	135	ILE
2	D	138	LEU
2	D	149	LEU
2	D	155	VAL
2	D	160	LEU
2	D	164	LEU
2	D	170	GLN
2	D	194	GLU
2	D	196	LYS
2	D	223	LEU
2	D	226	LEU
2	D	235	ARG
2	D	241	LEU
2	D	249	ARG
2	D	250	PHE

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Mol	Chain	Res	Type
2	D	251	THR
2	D	301	VAL
2	D	307	THR
2	D	318	LEU
2	D	324	LEU
2	D	340	LEU
2	D	374	GLN
2	D	379	ILE
2	D	392	ILE
2	D	405	GLN
2	D	412	GLN
2	D	416	MET
2	D	423	VAL
2	D	456	VAL
2	E	5	ARG
2	E	10	MET
2	E	34	ARG
2	E	36	GLN
2	E	53	VAL
2	E	91	ASN
2	E	92	VAL
2	E	93	LEU
2	E	103	VAL
2	E	113	ARG
2	E	121	LEU
2	E	132	ILE
2	E	135	ILE
2	E	138	LEU
2	E	149	LEU
2	E	160	LEU
2	E	164	LEU
2	E	170	GLN
2	E	194	GLU
2	E	196	LYS
2	E	223	LEU
2	E	226	LEU
2	E	235	ARG
2	E	241	LEU
2	E	249	ARG
2	E	251	THR
2	E	301	VAL
2	E	307	THR

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Mol	Chain	Res	Type
2	E	318	LEU
2	E	324	LEU
2	E	340	LEU
2	E	374	GLN
2	E	379	ILE
2	E	392	ILE
2	E	405	GLN
2	E	412	GLN
2	E	416	MET
2	E	423	VAL
2	E	456	VAL
2	F	5	ARG
2	F	26	ILE
2	F	34	ARG
2	F	36	GLN
2	F	53	VAL
2	F	91	ASN
2	F	92	VAL
2	F	93	LEU
2	F	113	ARG
2	F	121	LEU
2	F	126	GLU
2	F	132	ILE
2	F	135	ILE
2	F	138	LEU
2	F	149	LEU
2	F	160	LEU
2	F	164	LEU
2	F	170	GLN
2	F	194	GLU
2	F	196	LYS
2	F	223	LEU
2	F	226	LEU
2	F	235	ARG
2	F	241	LEU
2	F	249	ARG
2	F	251	THR
2	F	286	THR
2	F	301	VAL
2	F	307	THR
2	F	318	LEU
2	F	324	LEU

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Mol	Chain	Res	Type
2	F	340	LEU
2	F	374	GLN
2	F	379	ILE
2	F	392	ILE
2	F	412	GLN
2	F	416	MET
2	F	423	VAL
2	F	456	VAL
3	G	5[A]	ARG
3	G	5[B]	ARG
3	G	5[C]	ARG
3	G	8[A]	LYS
3	G	8[B]	LYS
3	G	8[C]	LYS
3	G	18[A]	ARG
3	G	18[B]	ARG
3	G	18[C]	ARG
3	G	20[A]	ILE
3	G	20[B]	ILE
3	G	20[C]	ILE
3	G	25[A]	LYS
3	G	25[B]	LYS
3	G	25[C]	LYS
3	G	71[A]	ARG
3	G	71[B]	ARG
3	G	71[C]	ARG
3	G	91[A]	TYR
3	G	91[B]	TYR
3	G	91[C]	TYR
3	G	98[A]	LEU
3	G	98[B]	LEU
3	G	98[C]	LEU
3	G	108[A]	GLN
3	G	108[B]	GLN
3	G	108[C]	GLN
3	G	110[A]	LYS
3	G	110[B]	LYS
3	G	110[C]	LYS
3	G	114[A]	VAL
3	G	114[B]	VAL
3	G	114[C]	VAL
3	G	115[A]	ILE

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Mol	Chain	Res	Type
3	G	115[B]	ILE
3	G	115[C]	ILE
3	G	118[A]	VAL
3	G	118[B]	VAL
3	G	118[C]	VAL
3	G	134[A]	VAL
3	G	134[B]	VAL
3	G	134[C]	VAL
3	G	136[A]	GLU
3	G	136[B]	GLU
3	G	136[C]	GLU
3	G	142[A]	ASP
3	G	142[B]	ASP
3	G	142[C]	ASP
3	G	148[A]	GLU
3	G	148[B]	GLU
3	G	148[C]	GLU
3	G	167[A]	LYS
3	G	167[B]	LYS
3	G	167[C]	LYS
3	G	172[A]	TYR
3	G	172[B]	TYR
3	G	172[C]	TYR
3	G	181[A]	GLN
3	G	181[B]	GLN
3	G	181[C]	GLN
3	G	188[A]	LEU
3	G	188[B]	LEU
3	G	188[C]	LEU
3	G	231[A]	LEU
3	G	231[B]	LEU
3	G	231[C]	LEU
3	G	237[A]	GLU
3	G	237[B]	GLU
3	G	237[C]	GLU
4	H	10[A]	THR
4	H	10[B]	THR
4	H	10[C]	THR
4	H	39[A]	ILE
4	H	39[B]	ILE
4	H	39[C]	ILE
4	H	61[A]	ILE

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Mol	Chain	Res	Type
4	H	61[B]	ILE
4	H	61[C]	ILE
4	H	81[A]	THR
4	H	81[B]	THR
4	H	81[C]	THR
4	H	103[A]	ILE
4	H	103[B]	ILE
4	H	103[C]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	87	GLN
1	A	143	HIS
1	A	147	GLN
1	A	189	GLN
1	A	200	GLN
1	A	215	HIS
1	A	333	ASN
1	A	341	GLN
1	A	411	ASN
1	A	422	GLN
1	B	64	GLN
1	B	87	GLN
1	B	143	HIS
1	B	147	GLN
1	B	189	GLN
1	B	215	HIS
1	B	333	ASN
1	B	341	GLN
1	B	411	ASN
1	B	422	GLN
1	C	64	GLN
1	C	87	GLN
1	C	143	HIS
1	C	147	GLN
1	C	189	GLN
1	C	215	HIS
1	C	333	ASN
1	C	341	GLN
1	C	411	ASN

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Mol	Chain	Res	Type
1	C	422	GLN
2	D	8	GLN
2	D	91	ASN
2	D	162	GLN
2	D	166	ASN
2	D	172	HIS
2	D	238	GLN
2	D	280	GLN
2	D	323	ASN
2	D	356	HIS
2	D	374	GLN
2	D	408	HIS
2	D	412	GLN
2	D	438	HIS
2	E	2	ASN
2	E	91	ASN
2	E	162	GLN
2	E	166	ASN
2	E	172	HIS
2	E	238	GLN
2	E	280	GLN
2	E	323	ASN
2	E	356	HIS
2	E	374	GLN
2	E	408	HIS
2	E	412	GLN
2	E	438	HIS
2	F	91	ASN
2	F	162	GLN
2	F	166	ASN
2	F	172	HIS
2	F	238	GLN
2	F	252	GLN
2	F	280	GLN
2	F	323	ASN
2	F	356	HIS
2	F	374	GLN
2	F	408	HIS
2	F	412	GLN
2	F	438	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	474/502 (94%)	0.00	33 (6%) 16 6	44, 69, 152, 234	0
1	B	474/502 (94%)	-0.11	28 (5%) 22 9	38, 61, 167, 246	0
1	C	474/502 (94%)	-0.14	12 (2%) 57 32	45, 67, 128, 185	0
2	D	461/462 (99%)	-0.14	11 (2%) 59 34	43, 76, 129, 174	0
2	E	461/462 (99%)	-0.38	5 (1%) 80 60	36, 55, 113, 170	0
2	F	461/462 (99%)	-0.22	11 (2%) 59 34	40, 62, 124, 173	0
3	G	227/286 (79%)	1.33	34 (14%) 2 1	10, 51, 103, 140	0
4	H	135/135 (100%)	3.28	108 (80%) 0 0	82, 133, 194, 213	0
All	All	3167/3313 (95%)	0.09	242 (7%) 13 5	10, 66, 144, 246	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	1[A]	MET	10.8
1	B	496	LYS	8.8
4	H	54[A]	GLN	8.2
4	H	5[A]	GLN	8.0
4	H	132[A]	ASN	6.8
3	G	266[A]	ALA	6.4
4	H	55[A]	GLY	6.4
4	H	129[A]	GLN	6.4
4	H	47[A]	THR	6.3
4	H	103[A]	ILE	6.3
2	F	462	LEU	6.2
1	A	405	ALA	6.2
4	H	100[A]	HIS	6.0
1	B	500	PRO	5.9
4	H	128[A]	LEU	5.9
4	H	2[A]	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	499	THR	5.7
4	H	126[A]	VAL	5.5
3	G	109[A]	SER	5.4
4	H	75[A]	VAL	5.3
4	H	73[A]	ASP	5.2
4	H	70[A]	VAL	5.2
4	H	90[A]	VAL	5.2
1	B	446	ASP	5.1
1	B	497	GLY	5.1
4	H	99[A]	ARG	5.0
1	A	497	GLY	5.0
4	H	59[A]	THR	5.0
4	H	58[A]	GLU	4.9
4	H	9[A]	VAL	4.9
4	H	74[A]	LYS	4.9
4	H	41[A]	LEU	4.8
1	A	452	ASP	4.8
2	D	455	ALA	4.8
1	A	500	PRO	4.7
4	H	91[A]	GLU	4.7
1	A	189	GLN	4.7
4	H	104[A]	LEU	4.6
1	A	495	LYS	4.5
1	C	399	GLY	4.5
1	A	496	LYS	4.5
4	H	26[A]	ARG	4.5
4	H	92[A]	ARG	4.4
1	A	457	GLU	4.4
4	H	102[A]	THR	4.4
1	B	409	LYS	4.4
1	C	396	ALA	4.3
4	H	25[A]	ALA	4.2
1	B	460	LEU	4.2
4	H	84[A]	LEU	4.2
1	B	445	MET	4.2
4	H	52[A]	ILE	4.2
4	H	17[A]	GLN	4.2
4	H	81[A]	THR	4.1
4	H	106[A]	ARG	4.1
4	H	50[A]	VAL	4.1
1	B	405	ALA	4.0
4	H	6[A]	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
4	H	134[A]	LYS	4.0
4	H	89[A]	ASP	4.0
4	H	133[A]	SER	4.0
4	H	124[A]	ALA	4.0
1	B	491	ILE	4.0
4	H	82[A]	ALA	4.0
3	G	91[A]	TYR	3.9
1	A	453	VAL	3.9
4	H	40[A]	PRO	3.9
3	G	132[A]	PRO	3.9
4	H	80[A]	ASP	3.9
4	H	69[A]	GLU	3.9
3	G	147[A]	THR	3.9
4	H	117[A]	HIS	3.9
1	B	455	ARG	3.8
1	A	403	ASP	3.8
2	D	292	SER	3.8
4	H	62[A]	ALA	3.8
4	H	64[A]	SER	3.8
4	H	3[A]	THR	3.8
1	A	404	LYS	3.7
4	H	114[A]	TYR	3.7
3	G	4[A]	MET	3.7
4	H	110[A]	THR	3.7
1	A	460	LEU	3.7
4	H	123[A]	ARG	3.6
4	H	113[A]	ASP	3.6
4	H	30[A]	GLY	3.5
1	B	463	PHE	3.5
4	H	61[A]	ILE	3.5
2	D	119	GLU	3.5
4	H	4[A]	VAL	3.5
4	H	109[A]	LYS	3.5
4	H	48[A]	ALA	3.4
1	A	463	PHE	3.4
2	F	386	SER	3.4
4	H	27[A]	GLY	3.4
4	H	43[A]	THR	3.4
1	A	446	ASP	3.3
4	H	36[A]	ALA	3.3
2	D	81	VAL	3.3
4	H	23[A]	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	447	ASP	3.2
4	H	115[A]	LEU	3.2
4	H	131[A]	ALA	3.2
4	H	107[A]	LEU	3.1
4	H	98[A]	ALA	3.1
2	E	416	MET	3.1
4	H	19[A]	GLU	3.1
4	H	121[A]	LEU	3.1
1	B	488	ASP	3.1
1	A	470	SER	3.1
4	H	7[A]	ASP	3.1
1	B	410	LEU	3.0
4	H	95[A]	LYS	3.0
1	B	461	LEU	3.0
4	H	53[A]	LYS	3.0
3	G	107[A]	HIS	3.0
1	B	492	GLU	3.0
2	F	459	ALA	3.0
1	B	464	MET	3.0
3	G	112[A]	GLU	3.0
4	H	13[A]	ARG	3.0
4	H	108[A]	ASP	2.9
1	A	443	GLY	2.9
1	C	407	GLN	2.9
3	G	110[A]	LYS	2.9
2	F	174	GLY	2.9
4	H	63[A]	VAL	2.9
3	G	76[A]	THR	2.9
4	H	116[A]	ARG	2.9
4	H	42[A]	VAL	2.8
1	A	491	ILE	2.8
2	E	383	ASP	2.8
3	G	111[A]	ASP	2.8
4	H	135[A]	SER	2.8
1	A	483	ASP	2.8
3	G	6[A]	GLU	2.7
1	B	400	SER	2.7
3	G	70[A]	ALA	2.7
1	A	492	GLU	2.7
2	D	102	GLU	2.7
4	H	76[A]	ASN	2.7
4	H	125[A]	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	387	ASP	2.7
4	H	79[A]	ALA	2.7
1	C	411	ASN	2.7
4	H	111[A]	ASP	2.7
3	G	5[A]	ARG	2.7
1	A	406	THR	2.7
4	H	21[A]	ASP	2.7
1	C	43	GLY	2.7
1	A	409	LYS	2.7
4	H	127[A]	ARG	2.7
3	G	162[A]	ASP	2.7
4	H	83[A]	GLU	2.6
3	G	73[A]	VAL	2.6
2	E	34	ARG	2.6
4	H	77[A]	ILE	2.6
4	H	130[A]	VAL	2.6
4	H	49[A]	PRO	2.6
4	H	20[A]	ALA	2.5
1	A	408	ALA	2.5
2	D	462	LEU	2.5
1	B	498	PHE	2.5
4	H	68[A]	LEU	2.5
1	C	483	ASP	2.5
4	H	24[A]	ILE	2.5
1	B	478	THR	2.5
1	A	488	ASP	2.5
1	B	468	LYS	2.5
3	G	140[A]	ILE	2.5
4	H	11[A]	PRO	2.5
4	H	31[A]	GLU	2.5
3	G	146[A]	LEU	2.4
4	H	105[A]	LYS	2.4
1	C	403	ASP	2.4
3	G	77[A]	GLY	2.4
3	G	145[A]	SER	2.4
3	G	172[A]	TYR	2.4
1	A	444	PHE	2.4
4	H	72[A]	PRO	2.4
1	B	408	ALA	2.4
2	E	381	GLY	2.4
3	G	37[A]	GLU	2.4
3	G	167[A]	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	400	SER	2.4
2	F	448	MET	2.4
1	A	387	ALA	2.3
2	F	290	LYS	2.3
4	H	51[A]	ARG	2.3
1	B	452	ASP	2.3
1	C	397	GLN	2.3
2	D	443	GLU	2.3
4	H	93[A]	ALA	2.3
1	A	456	PHE	2.3
4	H	15[A]	VAL	2.3
1	B	487	LEU	2.3
2	D	461	LYS	2.3
2	D	291	GLY	2.3
2	F	384	GLU	2.3
3	G	138[A]	THR	2.3
4	H	18[A]	GLY	2.2
1	A	307	GLU	2.2
4	H	120[A]	ALA	2.2
4	H	46[A]	LYS	2.2
2	F	416	MET	2.2
2	D	5	ARG	2.2
1	B	453	VAL	2.2
4	H	14[A]	LYS	2.2
3	G	108[A]	GLN	2.2
4	H	39[A]	ILE	2.2
3	G	178[A]	PRO	2.2
3	G	238[A]	PHE	2.2
1	B	412	ARG	2.2
4	H	67[A]	PHE	2.2
4	H	118[A]	LYS	2.2
4	H	8[A]	ILE	2.1
1	B	441	THR	2.1
1	A	87	GLN	2.1
4	H	85[A]	PRO	2.1
1	A	478	THR	2.1
1	C	406	THR	2.1
3	G	177[A]	SER	2.1
1	A	306	ASP	2.1
3	G	165[A]	PHE	2.1
3	G	72[A]	PRO	2.1
1	C	392	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	392	LEU	2.1
2	F	23	LEU	2.1
4	H	101[A]	GLU	2.1
2	D	439	ASP	2.1
1	B	395	PHE	2.1
4	H	87[A]	GLU	2.1
1	B	470	SER	2.1
4	H	71[A]	ARG	2.1
2	F	380	LEU	2.1
2	F	447	TYR	2.0
3	G	133[A]	VAL	2.0
4	H	32[A]	LEU	2.0
3	G	3[A]	GLY	2.0
3	G	122[A]	GLY	2.0
3	G	151[A]	ASP	2.0
1	A	482	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.