



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:22 AM GMT

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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

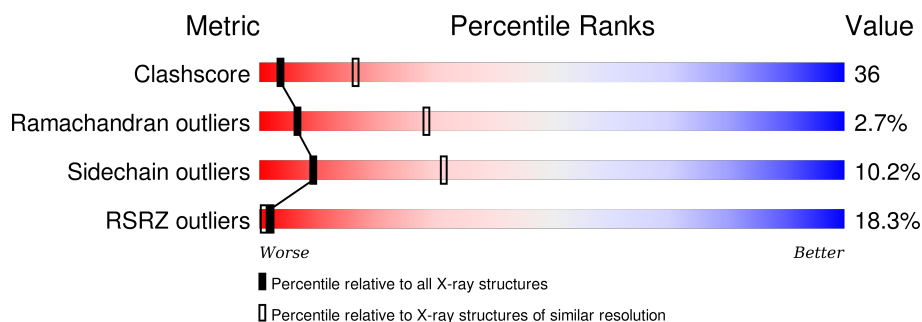
# 1 Overall quality at a glance

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.



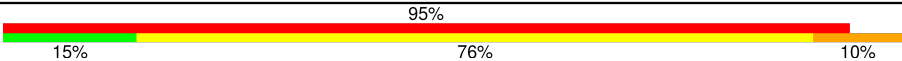
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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. 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	<div> <div>18%</div> <div> <div>55%</div> <div>33%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	502	<div> <div>16%</div> <div> <div>54%</div> <div>33%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	502	<div> <div>15%</div> <div> <div>55%</div> <div>32%</div> <div>6%</div> <div>6%</div> </div> </div>
2	D	462	<div> <div>15%</div> <div> <div>55%</div> <div>37%</div> <div>7%</div> <div>.</div> </div> </div>
2	E	462	<div> <div>7%</div> <div> <div>56%</div> <div>36%</div> <div>7%</div> </div> </div>
2	F	462	<div> <div>11%</div> <div> <div>54%</div> <div>38%</div> <div>7%</div> <div>.</div> </div> </div>
3	G	286	<div> <div>19%</div> <div> <div>9%</div> <div>57%</div> <div>13%</div> <div>.</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	H	135	 <p>A horizontal bar chart showing the quality of chain H. The bar is divided into four segments: green (15%), yellow (76%), red (95%), and orange (10%). The percentages are labeled below the bar segments. The red segment is the largest, followed by yellow, orange, and green.</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			

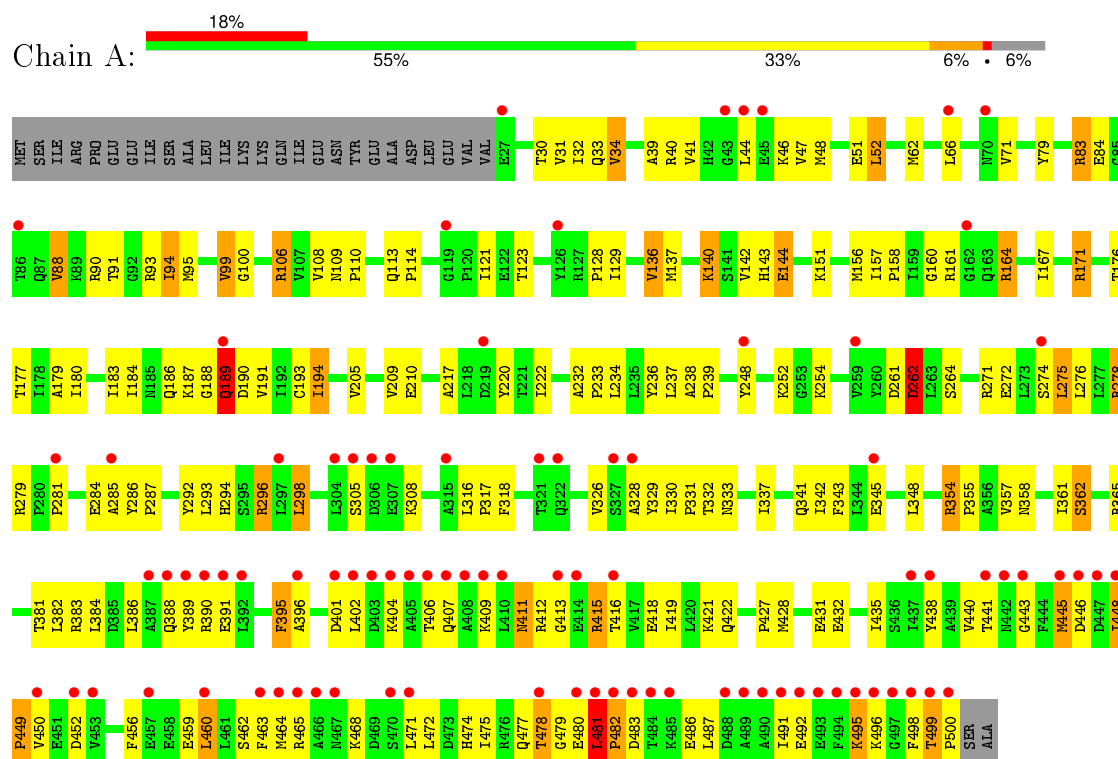
- Molecule 4 is a protein called ATP synthase subunit epsilon.

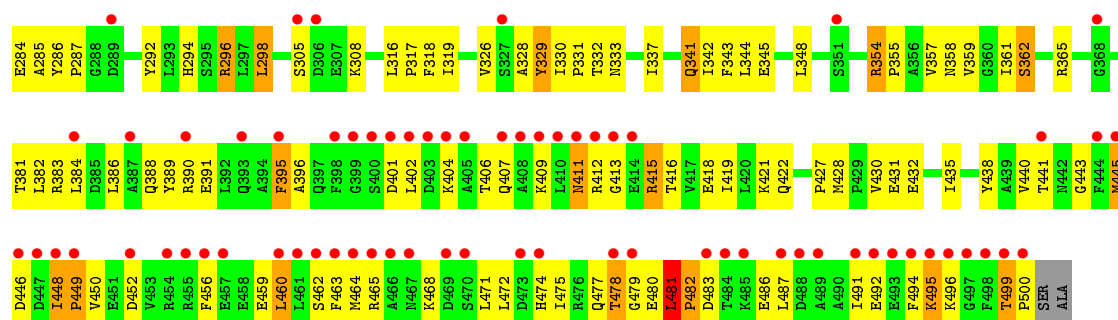
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	135	Total	C	N	O	S	0	135	0
			3150	1974	579	591	6			

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

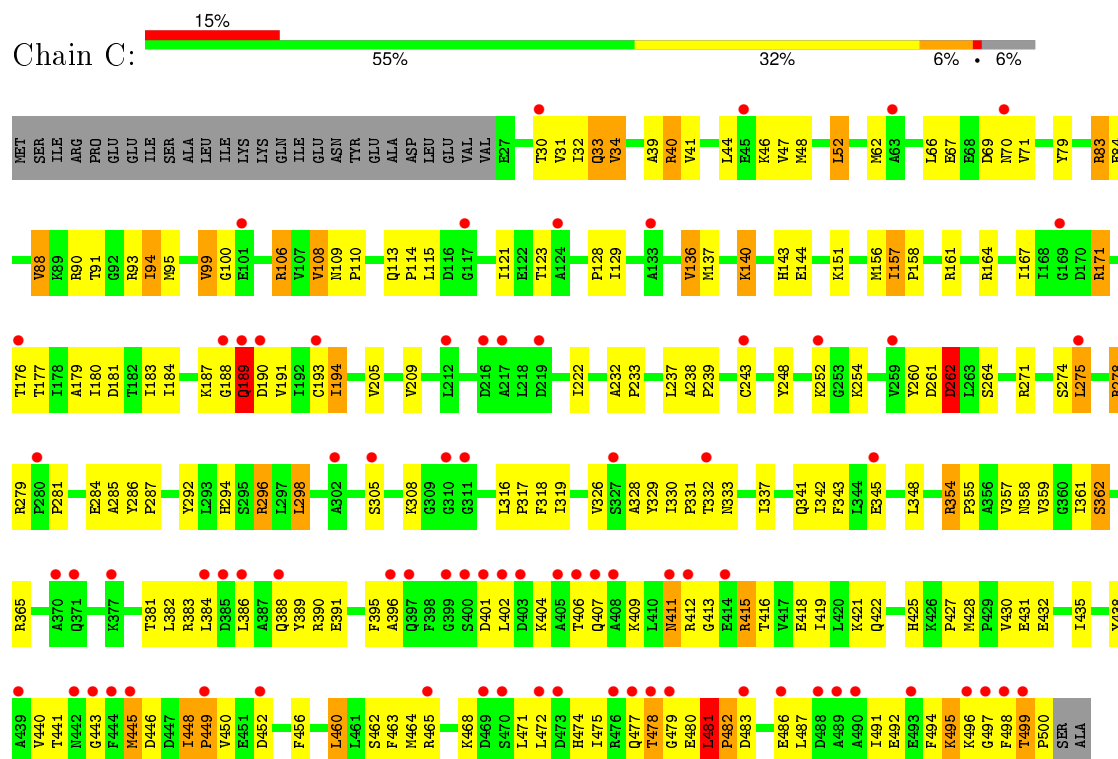
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: ATP synthase subunit alpha

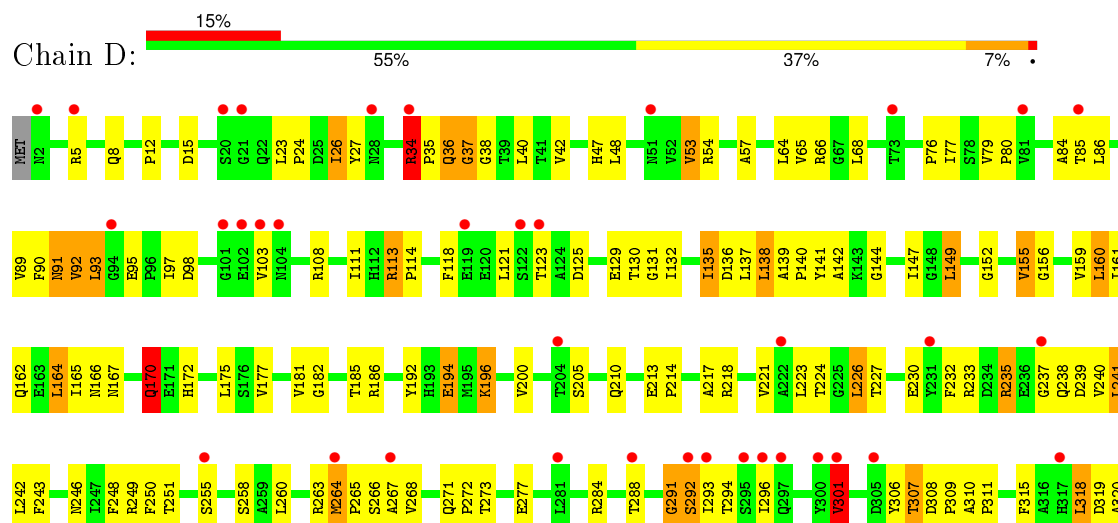


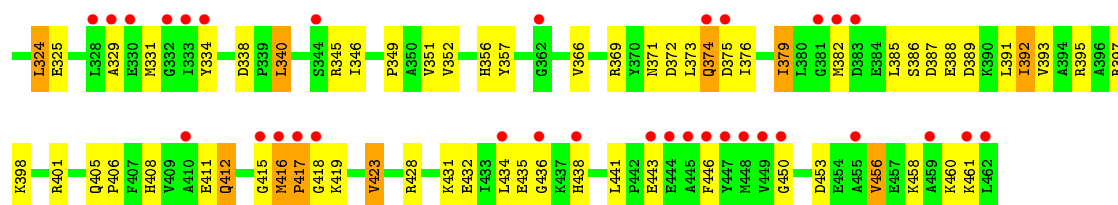


• Molecule 1: ATP synthase subunit alpha

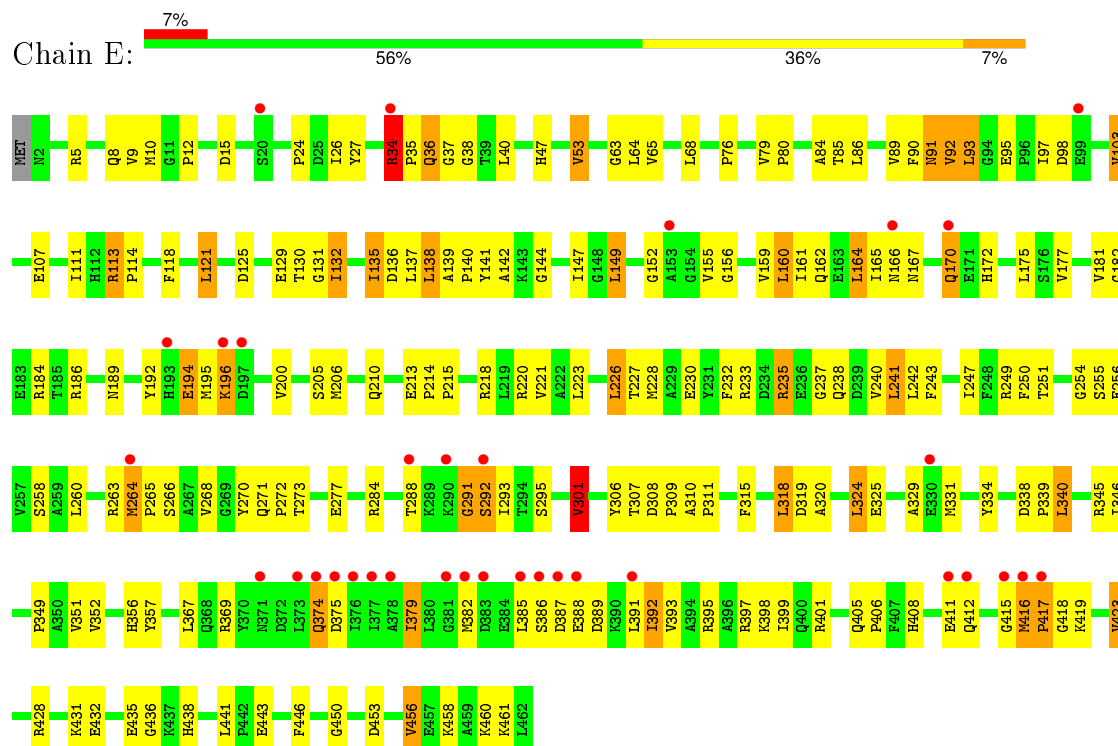


• Molecule 2: ATP synthase subunit beta

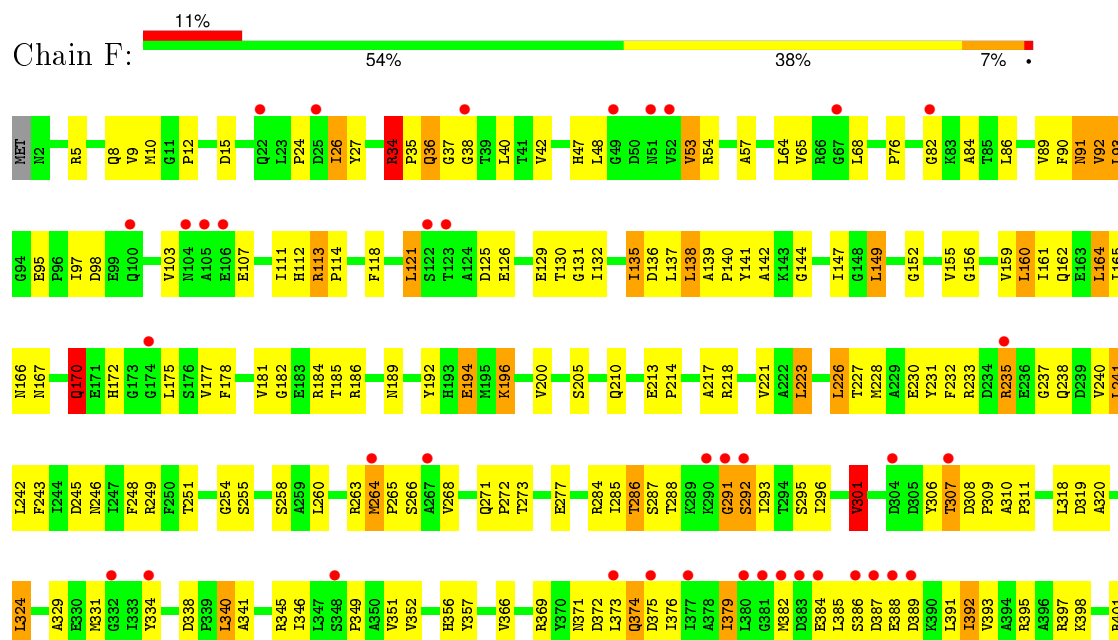




• Molecule 2: ATP synthase subunit beta

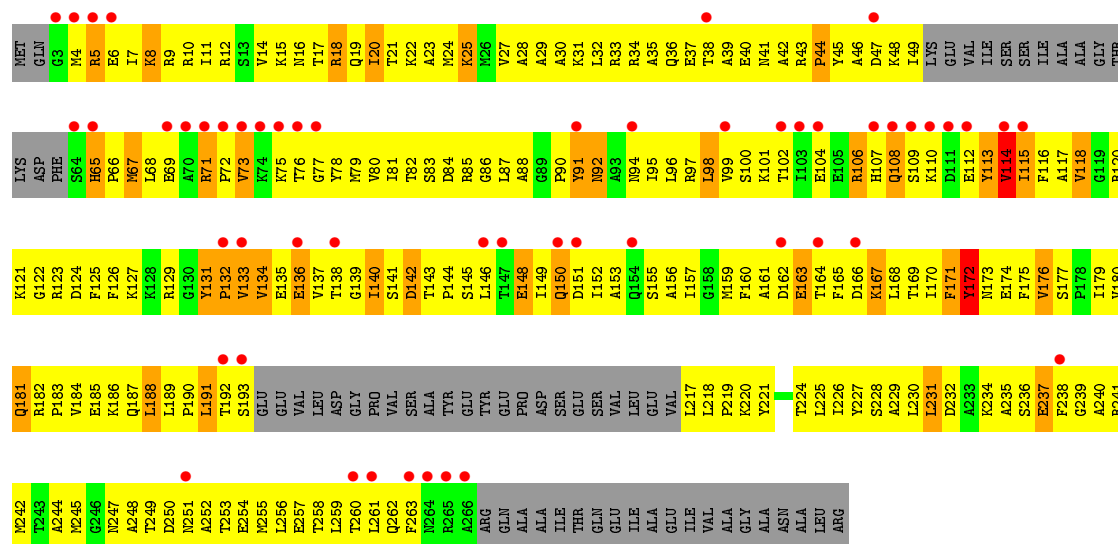
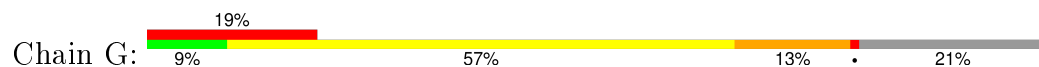


• Molecule 2: ATP synthase subunit beta

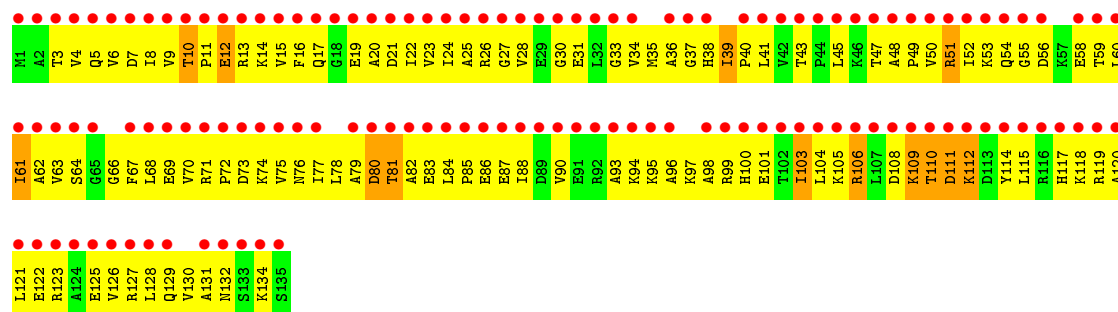




• Molecule 3: ATP synthase subunit gamma



• 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 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
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> )	0.20 , 100.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 103086 reflections	Xtriage
$F_o, F_c$ correlation	0.87	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, 0.375 respectively for untwinned datasets, and 0.333, 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:32[C]:LEU:CB	3:G:238[C]:PHE:HB2	1.90	1.02
3:G:80[A]:VAL:HA	3:G:171[A]:PHE:HB2	1.38	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
3:G:48[C]:LYS:HD3	4:H:78[C]:LEU:HD22	1.46	0.98
1:A:492:GLU:HA	1:A:495:LYS:HB2	1.45	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
4:H:13[B]:ARG:HH11	4:H:13[B]:ARG:HG3	1.27	0.96
1:C:171:ARG:HH11	1:C:171:ARG:CG	1.78	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:C:492:GLU:HA	1:C:495:LYS:HB2	1.44	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:HH11	1:A:171:ARG:HG3	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
3:G:86[C]:GLY:HA2	3:G:241[C]:ARG:HH22	1.31	0.93
1:C:365:ARG:HH21	2:D:186:ARG:NH2	1.65	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:B:83:ARG:HB2	2:E:47:HIS:HE1	1.33	0.92
1:A:284:GLU:HG3	1:A:329:TYR:CG	2.05	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
3:G:162[C]:ASP:HA	3:G:163[C]:GLU:HB2	1.52	0.91
1:B:284:GLU:HG3	1:B:329:TYR:CG	2.06	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
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
1:C:171:ARG:HG3	1:C:171:ARG:HH11	1.33	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
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
2:E:264:MET:CB	2:E:272:PRO:HG3	2.05	0.87
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.39	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
4:H:5[B]:GLN:HA	4:H:19[B]:GLU:HA	1.56	0.87
2:D:268:VAL:HG11	2:D:309:PRO:HG2	1.57	0.87
3:G:38[C]:THR:HA	4:H:13[C]:ARG:HH22	1.36	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
1:C:66:LEU:HB3	2:D:66:ARG:HD3	1.56	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
3:G:72[C]:PRO:HB2	3:G:73[C]:VAL:HG22	1.58	0.85
2:D:34:ARG:HG3	2:D:35:PRO:HA	1.58	0.85
1:A:474:HIS:NE2	1:A:482:PRO:HD2	1.90	0.85
4:H:8[A]:ILE:HA	4:H:77[A]:ILE:HG12	1.60	0.84
2:E:175:LEU:H	2:E:238:GLN:HE21	1.21	0.84
3:G:32[A]:LEU:HD12	3:G:35[A]:ALA:HB2	1.58	0.84
4:H:51[C]:ARG:HG2	4:H:60[C]:LEU:HA	1.57	0.84
2:E:34:ARG:HG3	2:E:35:PRO:HA	1.59	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
4:H:110[C]:THR:C	4:H:112[C]:LYS:HG3	1.98	0.84
2:F:89:VAL:HG22	2:F:98:ASP:HB3	1.58	0.84
1:C:156:MET:HE3	1:C:383:ARG:HA	1.60	0.83
2:F:371:ASN:HB3	3:G:10[B]:ARG:HH11	1.03	0.83
1:B:474:HIS:NE2	1:B:482:PRO:HD2	1.92	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:HG2	1:B:415:ARG:HH11	1.45	0.81
3:G:84[C]:ASP:CB	3:G:120[C]:ARG:H	1.91	0.81
3:G:142[B]:ASP:HA	3:G:234[B]:LYS:NZ	1.95	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:71[A]:ARG:HH11	3:G:71[A]:ARG:HG2	1.45	0.81
2:E:264:MET:HB3	2:E:272:PRO:HG3	1.62	0.81
1:B:275:LEU:CB	2:E:264:MET:HG3	2.11	0.81
2:F:264:MET:CB	2:F:272:PRO:HG3	2.10	0.81
1:C:480:GLU:C	1:C:482:PRO:HD3	2.01	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
4:H:25[B]:ALA:HB2	4:H:50[B]:VAL:HG13	1.61	0.81
1:C:106:ARG:NH1	1:C:106:ARG:HG2	1.80	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
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
1:B:66:LEU:HD12	2:F:9:VAL:HB	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
2:E:130:THR:HG21	2:E:135:ILE:HD11	1.62	0.80
1:C:354:ARG:NH1	1:C:354:ARG:HG3	1.95	0.80
1:B:480:GLU:C	1:B:482:PRO:HD3	2.02	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)
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:B:275:LEU:HB3	2:E:264:MET:SD	2.20	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
3:G:72[C]:PRO:CA	3:G:73[C]:VAL:HG13	2.14	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: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
3:G:65[C]:HIS:CD2	3:G:69[C]:GLU:HB2	2.19	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
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
4:H:110[C]:THR:CB	4:H:112[C]:LYS:HE2	2.13	0.77
1:C:151:LYS:N	1:C:422:GLN:HE22	1.81	0.77
3:G:76[C]:THR:HB	3:G:167[C]:LYS:HG2	1.67	0.77
2:E:264:MET:HE3	2:E:272:PRO:HB3	1.67	0.77
3:G:84[C]:ASP:HB3	3:G:120[C]:ARG:N	1.94	0.77
3:G:87[C]:LEU:H	3:G:241[C]:ARG:NH2	1.83	0.77
3:G:170[C]:ILE:HG13	3:G:188[C]:LEU:HD11	1.66	0.77
1:A:354:ARG:HH11	1:A:354:ARG:HG2	1.50	0.77
1:C:415:ARG:HH11	1:C:415:ARG:HG3	1.49	0.77
1:B:156:MET:HE3	1:B:383:ARG:HA	1.64	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
3:G:72[B]:PRO:CA	3:G:73[B]:VAL:HB	2.15	0.76
1:C:79:TYR:HE1	2:F:26:ILE:HD11	1.49	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
3:G:78[B]:TYR:HD1	3:G:115[B]:ILE:HG22	1.51	0.76
1:A:354:ARG:NH1	1:A:354:ARG:HG3	1.99	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
3:G:81[B]:ILE:HA	3:G:118[B]:VAL:HG13	1.68	0.75
2:E:379:ILE:HD12	3:G:252[A]:ALA:HB2	1.68	0.75
1:B:354:ARG:NH1	1:B:354:ARG:HG3	1.97	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:328:ALA:O	1:B:332:THR:HG23	1.86	0.75
1:B:440:VAL:HA	1:B:445:MET:HG3	1.68	0.75
3:G:25[C]:LYS:HG2	3:G:245[C]:MET:HB2	1.69	0.75
1:C:275:LEU:HG	1:C:278:ARG:HA	1.67	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
3:G:40[B]:GLU:O	3:G:44[B]:PRO:HD3	1.87	0.74
1:A:462:SER:CA	1:A:465:ARG:NH1	2.50	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
2:D:419:LYS:HE2	2:D:450:GLY:HA3	1.69	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
4:H:47[B]:THR:HG21	4:H:122[B]:GLU:HB3	1.68	0.74
2:D:264:MET:HB3	2:D:272:PRO:HG3	1.70	0.74
3:G:91[B]:TYR:CD2	3:G:240[B]:ALA:HB1	2.23	0.73
1:C:481:LEU:N	1:C:482:PRO:HD3	2.02	0.73
3:G:32[C]:LEU:HB2	3:G:238[C]:PHE:HB3	1.69	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
1:B:298:LEU:HD12	1:B:317:PRO:HG3	1.70	0.73
3:G:72[A]:PRO:CA	3:G:73[A]:VAL:HB	2.18	0.73
1:B:79:TYR:HE1	2:E:26:ILE:HD11	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:THR:N	1:B:500:PRO:HD3	2.02	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:354:ARG:HH11	1:B:354:ARG:HG2	1.51	0.73
2:F:255:SER:HA	2:F:271:GLN:HG3	1.70	0.73
1:C:328:ALA:O	1:C:332:THR:HG23	1.88	0.73
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.70	0.73
2:D:175:LEU:HG	2:D:238:GLN:HE22	1.53	0.73
1:C:44:LEU:HB3	1:C:47:VAL:HG13	1.69	0.73
3:G:71[A]:ARG:HH11	3:G:71[A]:ARG:HG3	1.53	0.73
3:G:172[B]:TYR:CE1	3:G:229[B]:ALA:HA	2.24	0.73
1:C:354:ARG:HH11	1:C:354:ARG:HG2	1.53	0.73
2:D:401:ARG:HD3	2:D:443:GLU:O	1.88	0.73
2:D:374:GLN:HA	2:D:374:GLN:HE21	1.54	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
2:F:419:LYS:HE2	2:F:450:GLY:HA3	1.68	0.73
2:E:136:ASP:HB3	2:E:423:VAL:HG13	1.70	0.73
3:G:140[C]:ILE:HD12	3:G:234[C]:LYS:NZ	2.04	0.72
1:C:365:ARG:NH2	2:D:186:ARG:HH22	1.87	0.72
3:G:72[B]:PRO:CB	3:G:73[B]:VAL:HB	2.19	0.72
2:F:264:MET:HB2	2:F:272:PRO:HG3	1.71	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
4:H:103[A]:ILE:HA	4:H:106[A]:ARG:HB2	1.70	0.72
3:G:45[C]:TYR:CB	4:H:11[C]:PRO:HA	2.19	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:172[B]:TYR:HE1	3:G:229[B]:ALA:HA	1.53	0.72
3:G:80[B]:VAL:HB	3:G:171[B]:PHE:HD1	1.54	0.72
4:H:104[C]:LEU:HD13	4:H:118[C]:LYS:HG2	1.70	0.72
3:G:98[C]:LEU:O	3:G:102[C]:THR:HG23	1.89	0.72
2:E:156:GLY:O	2:E:159:VAL:HG12	1.90	0.72
2:D:310:ALA:HB3	2:D:311:PRO:HD3	1.72	0.72
3:G:72[C]:PRO:CB	3:G:73[C]:VAL:HG22	2.19	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
1:C:326:VAL:HG11	1:C:343:PHE:HE2	1.55	0.72
3:G:146[C]:LEU:HA	3:G:227[C]:TYR:HH	1.55	0.72
1:C:390:ARG:HH21	1:C:391:GLU:HG2	1.54	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
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
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
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
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:44:LEU:HB3	1:A:47:VAL:HG13	1.71	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:390:ARG:HH21	1:A:391:GLU:HG2	1.56	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: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
1:B:151:LYS:N	1:B:422:GLN:HE22	1.85	0.71
1:A:342:ILE:HA	1:A:362:SER:OG	1.91	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
3:G:71[B]:ARG:HH21	3:G:163[B]:GLU:HG2	1.54	0.70
2:F:374:GLN:HA	2:F:374:GLN:HE21	1.56	0.70
1:C:462:SER:CA	1:C:465:ARG:NH1	2.53	0.70
1:A:151:LYS:N	1:A:422:GLN:HE22	1.83	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
3:G:32[A]:LEU:HD23	3:G:238[A]:PHE:CD2	2.27	0.70
2:F:401:ARG:HD3	2:F:443:GLU:O	1.92	0.70
3:G:132[C]:PRO:O	3:G:133[C]:VAL:HB	1.91	0.70
2:D:226:LEU:HD11	2:D:284:ARG:HB2	1.74	0.70
1:C:298:LEU:HD12	1:C:317:PRO:HG3	1.72	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
2:D:264:MET:HB2	2:D:272:PRO:HG3	1.74	0.70
1:C:171:ARG:NH1	1:C:171:ARG:CG	2.48	0.70
2:F:301:VAL:HG13	2:F:306:TYR:HE1	1.56	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
4:H:14[B]:LYS:HZ2	4:H:17[B]:GLN:HG2	1.55	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
3:G:77[C]:GLY:HA3	3:G:165[C]:PHE:CZ	2.28	0.69
3:G:48[A]:LYS:HG3	3:G:49[A]:ILE:H	1.56	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
1:B:388:GLN:HG3	1:B:409:LYS:NZ	2.08	0.69
4:H:27[A]:GLY:H	4:H:31[A]:GLU:HA	1.57	0.69
1:A:275:LEU:HB3	2:D:264:MET:HG3	1.74	0.69
2:E:264:MET:HB2	2:E:272:PRO:HG3	1.73	0.69
2:F:264:MET:HB3	2:F:265:PRO:CA	2.22	0.69
1:B:438:TYR:HA	1:B:441:THR:HG22	1.74	0.69
2:E:374:GLN:HA	2:E:374:GLN:HE21	1.57	0.69
3:G:8[B]:LYS:HD2	3:G:263[B]:PHE:CE1	2.28	0.69
4:H:20[A]:ALA:HA	4:H:54[A]:GLN:HB3	1.75	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
1:B:48:MET:CE	1:B:94:ILE:HG23	2.23	0.69
3:G:172[A]:TYR:HD1	3:G:173[A]:ASN:H	1.41	0.69
2:D:398:LYS:HD3	2:D:446:PHE:CE1	2.27	0.69
1:A:48:MET:HB3	2:E:63:GLY:HA2	1.75	0.69
2:E:416:MET:N	2:E:417:PRO:HA	2.08	0.68
2:D:408:HIS:ND1	2:D:418:GLY:HA3	2.08	0.68
1:A:438:TYR:CE1	1:A:487:LEU:HD12	2.27	0.68
3:G:66[C]:PRO:O	3:G:67[C]:MET:HB3	1.92	0.68
2:F:264:MET:HB3	2:F:272:PRO:HG3	1.73	0.68
1:B:164:ARG:HH22	2:F:184:ARG:HD3	1.59	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
3:G:143[A]:THR:H	3:G:144[A]:PRO:HA	1.57	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:172[C]:TYR:HE1	3:G:232[C]:ASP:HB3	1.58	0.68
3:G:176[C]:VAL:HG12	3:G:177[C]:SER:N	2.08	0.68
3:G:80[C]:VAL:HG11	3:G:126[C]:PHE:CE2	2.28	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
3:G:45[C]:TYR:CG	4:H:11[C]:PRO:HA	2.29	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
4:H:24[C]:ILE:HD11	4:H:51[C]:ARG:HB2	1.76	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
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
3:G:253[C]:THR:HG22	3:G:254[C]:GLU:N	2.08	0.68
3:G:68[A]:LEU:HA	3:G:160[A]:PHE:HE2	1.59	0.68
1:B:342:ILE:HA	1:B:362:SER:OG	1.93	0.68
1:B:79:TYR:CE1	2:E:26:ILE:HD11	2.28	0.68
2:D:162:GLN:HE22	2:D:194:GLU:HG2	1.57	0.68
3:G:107[C]:HIS:C	3:G:109[C]:SER:H	1.95	0.68
2:F:398:LYS:HD3	2:F:446:PHE:CE1	2.29	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
3:G:144[A]:PRO:HG2	3:G:230[A]:LEU:CD1	2.24	0.67
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
1:C:48:MET:CE	1:C:94:ILE:HG23	2.24	0.67
1:C:161:ARG:HH12	1:C:190:ASP:HB3	1.59	0.67
2:F:91:ASN:HD21	2:F:95:GLU:H	1.42	0.67
3:G:104[C]:GLU:HA	3:G:107[C]:HIS:HD1	1.60	0.67
1:B:275:LEU:CD2	2:E:264:MET:HA	2.21	0.67
1:B:415:ARG:HG2	1:B:415:ARG:NH1	2.08	0.67
1:A:48:MET:HE3	1:A:94:ILE:HG23	1.76	0.67
1:A:328:ALA:O	1:A:332:THR:HG23	1.94	0.67
4:H:4[B]:VAL:HG21	4:H:37[B]:GLY:H	1.60	0.67
1:B:401:ASP:HB3	1:B:406:THR:HG22	1.74	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:E:135:ILE:HD12	2:E:141:TYR:CZ	2.30	0.67
2:D:152:GLY:H	2:D:155:VAL:CG2	2.08	0.67
2:E:8:GLN:HB2	2:E:15:ASP:HB2	1.75	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
2:F:135:ILE:HD12	2:F:141:TYR:CZ	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:81[B]:THR:HG21	4:H:127[B]:ARG:HH21	1.58	0.67
1:A:440:VAL:HG12	1:A:445:MET:CE	2.24	0.67
1:A:388:GLN:HG3	1:A:409:LYS:NZ	2.10	0.67
2:E:137:LEU:HG	2:E:138:LEU:HD13	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:129:ILE:HD11	1:B:237:LEU:HD22	1.77	0.67
1:A:401:ASP:HB3	1:A:406:THR:HG22	1.76	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
2:F:175:LEU:HG	2:F:238:GLN:HE22	1.59	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
1:B:386:LEU:HD23	1:B:386:LEU:H	1.60	0.66
3:G:86[B]:GLY:HA2	3:G:241[B]:ARG:HH22	1.61	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: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
1:A:151:LYS:H	1:A:422:GLN:NE2	1.86	0.66
2:F:226:LEU:HD11	2:F:284:ARG:HB2	1.76	0.66
2:D:142:ALA:HB2	2:D:346:ILE:HD13	1.76	0.66
3:G:160[C]:PHE:CB	3:G:189[C]:LEU:HD23	2.26	0.66
1:A:83:ARG:HB2	2:D:47:HIS:HE1	1.56	0.66
2:F:416:MET:N	2:F:417:PRO:HA	2.11	0.66
2:D:91:ASN:HD21	2:D:95:GLU:H	1.44	0.66
1:B:52:LEU:O	1:B:91:THR:HB	1.96	0.66
3:G:87[C]:LEU:N	3:G:241[C]:ARG:NH2	2.36	0.66
3:G:80[B]:VAL:HA	3:G:171[B]:PHE:HB2	1.78	0.66
4:H:60[C]:LEU:HB2	4:H:130[C]:VAL:HG13	1.76	0.66
1:C:44:LEU:HB3	1:C:47:VAL:CG1	2.26	0.66
1:B:161:ARG:HH12	1:B:190:ASP:HB3	1.61	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:A:52:LEU:O	1:A:91:THR:HB	1.96	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
3:G:32[B]:LEU:CG	3:G:238[B]:PHE:CB	2.74	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)
1:A:262:ASP:H	1:A:318:PHE:HB2	1.60	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: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
1:A:449:PRO:HB2	1:A:452:ASP:HB2	1.79	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: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
2:D:416:MET:H	2:D:417:PRO:HA	1.60	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:9[C]:VAL:HG21	4:H:14[C]:LYS:HD2	1.78	0.65
4:H:39[A]:ILE:H	4:H:39[A]:ILE:HD13	1.61	0.65
1:C:48:MET:HE3	1:C:94:ILE:HG23	1.77	0.65
1:A:140:LYS:HE2	1:A:143:HIS:CE1	2.31	0.65
1:C:449:PRO:HB2	1:C:452:ASP:HB2	1.78	0.65
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.27	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
4:H:13[B]:ARG:NH1	4:H:13[B]:ARG:HG3	2.08	0.64
1:B:462:SER:CA	1:B:465:ARG:NH1	2.56	0.64
3:G:66[C]:PRO:HD2	3:G:68[C]:LEU:HD23	1.80	0.64
3:G:91[A]:TYR:CD2	3:G:240[A]:ALA:HB1	2.31	0.64
2:F:416:MET:H	2:F:417:PRO:HA	1.60	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
1:A:114:PRO:HG3	1:A:121:ILE:HD12	1.79	0.64
2:E:125:ASP:CG	2:E:345:ARG:HH22	2.01	0.64
4:H:51[B]:ARG:HE	4:H:60[B]:LEU:HD21	1.62	0.64
2:F:162:GLN:HE22	2:F:194:GLU:HG2	1.62	0.64
1:B:438:TYR:CE1	1:B:487:LEU:HD12	2.33	0.64
3:G:91[B]:TYR:CG	3:G:240[B]:ALA:HB1	2.32	0.64
3:G:82[B]:THR:HG22	3:G:95[B]:ILE:HD13	1.78	0.64
2:D:379:ILE:HD11	3:G:17[C]:THR:HG21	1.78	0.64
3:G:146[A]:LEU:HD12	4:H:81[A]:THR:HB	1.78	0.64
1:C:52:LEU:O	1:C:91:THR:HB	1.96	0.64
3:G:184[A]:VAL:HG22	3:G:185[A]:GLU:H	1.61	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
1:A:100:GLY:HA2	1:A:248:TYR:CE2	2.33	0.64
4:H:8[C]:ILE:HG13	4:H:15[C]:VAL:HB	1.78	0.63
4:H:8[B]:ILE:CG1	4:H:15[B]:VAL:HB	2.28	0.63
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
3:G:77[A]:GLY:O	3:G:168[A]:LEU:HA	1.98	0.63
3:G:41[C]:ASN:HB3	4:H:13[C]:ARG:HE	1.63	0.63
3:G:16[C]:ASN:O	3:G:19[C]:GLN:HB2	1.98	0.63
2:D:268:VAL:HG22	2:D:268:VAL:O	1.98	0.63
1:C:156:MET:CE	1:C:383:ARG:HA	2.29	0.63
2:F:65:VAL:O	2:F:68:LEU:HG	1.98	0.63
4:H:41[C]:LEU:HB2	4:H:70[C]:VAL:HB	1.80	0.63
2:D:291:GLY:O	2:D:292:SER:HB2	1.98	0.63
1:C:388:GLN:HG3	1:C:409:LYS:NZ	2.14	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
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
2:F:308:ASP:O	2:F:311:PRO:HD2	1.98	0.63
1:A:161:ARG:HH12	1:A:190:ASP:HB3	1.62	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
1:B:46:LYS:NZ	1:B:46:LYS:HB2	2.14	0.63
4:H:13[C]:ARG:HD2	4:H:13[C]:ARG:N	2.13	0.63
2:F:460:LYS:O	2:F:461:LYS:HD2	1.97	0.63
4:H:21[B]:ASP:HB2	4:H:22[B]:ILE:HD13	1.80	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
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
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: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
4:H:45[A]:LEU:HD21	4:H:68[A]:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:MET:HB3	2:E:265:PRO:CA	2.29	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: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[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
1:C:47:VAL:HG21	1:C:71:VAL:HG21	1.81	0.62
1:C:390:ARG:NH2	1:C:391:GLU:HG2	2.13	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
1:A:46:LYS:HB2	1:A:46:LYS:NZ	2.15	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
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
2:F:395:ARG:NH2	2:F:436:GLY:HA3	2.14	0.62
1:B:358:ASN:O	1:B:362:SER:HB2	1.99	0.62
1:A:386:LEU:H	1:A:386:LEU:HD23	1.63	0.62
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
3:G:221[C]:TYR:CE2	3:G:225[C]:LEU:HD11	2.36	0.61
4:H:84[B]:LEU:HB3	4:H:85[B]:PRO:CD	2.30	0.61
1:C:440:VAL:HG12	1:C:445:MET:CE	2.28	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
2:E:301:VAL:HG13	2:E:306:TYR:CE1	2.36	0.61
3:G:91[A]:TYR:O	3:G:92[A]:ASN:HB2	2.01	0.61
1:B:275:LEU:N	2:E:264:MET:HE1	2.15	0.61
1:A:358:ASN:O	1:A:362:SER:HB2	2.00	0.61
1:B:345:GLU:HG2	1:B:358:ASN:HB2	1.83	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
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:275:LEU:HA	1:B:278:ARG:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:233:ARG:O	2:F:237:GLY:HA2	1.99	0.61
4:H:110[B]:THR:HB	4:H:112[B]:LYS:HG3	1.81	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
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
3:G:135[C]:GLU:OE1	3:G:152[C]:ILE:HG13	2.00	0.61
2:E:375:ASP:O	2:E:379:ILE:HG23	2.01	0.61
3:G:218[C]:LEU:HD23	3:G:218[C]:LEU:O	2.01	0.61
3:G:38[A]:THR:CG2	4:H:13[A]:ARG:HH21	2.13	0.61
1:B:275:LEU:CB	2:E:264:MET:CG	2.72	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
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: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
2:E:125:ASP:OD2	2:E:345:ARG:NH2	2.33	0.61
1:C:386:LEU:H	1:C:386:LEU:HD23	1.65	0.61
3:G:67[C]:MET:C	3:G:69[C]:GLU:H	2.03	0.60
1:C:62:MET:HB2	1:C:95:MET:CE	2.28	0.60
1:C:345:GLU:HG2	1:C:358:ASN:HB2	1.81	0.60
2:F:91:ASN:ND2	2:F:95:GLU:H	1.97	0.60
2:E:401:ARG:HD3	2:E:443:GLU:O	2.01	0.60
1:A:275:LEU:HD13	2:D:264:MET:HG3	1.83	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:390:ARG:NH2	1:A:391:GLU:HG2	2.16	0.60
3:G:255[C]:MET:HA	3:G:258[C]:THR:HG23	1.81	0.60
3:G:175[B]:PHE:HD1	3:G:236[B]:SER:HA	1.65	0.60
3:G:33[B]:ARG:C	3:G:35[B]:ALA:H	2.04	0.60
1:C:440:VAL:HA	1:C:445:MET:CG	2.29	0.60
1:A:41:VAL:HG21	1:A:88:VAL:HG21	1.83	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
4:H:100[C]:HIS:HD2	4:H:117[C]:HIS:HD2	1.50	0.60
1:B:440:VAL:HG12	1:B:445:MET:CE	2.32	0.60
2:F:226:LEU:O	2:F:230:GLU:HG3	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:D:460:LYS:O	2:D:461:LYS:HD2	2.02	0.60
1:B:114:PRO:HG3	1:B:121:ILE:HD12	1.84	0.60
3:G:131[C]:TYR:N	3:G:132[C]:PRO:HA	2.09	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
3:G:17[B]:THR:O	3:G:17[B]:THR:HG22	2.02	0.60
2:D:91:ASN:ND2	2:D:95:GLU:H	1.99	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:A:419:ILE:HG21	1:A:440:VAL:HG11	1.82	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
4:H:121[B]:LEU:HD22	4:H:125[B]:GLU:OE2	2.02	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
2:F:291:GLY:O	2:F:292:SER:HB2	2.02	0.60
1:B:365:ARG:HH21	2:F:186:ARG:HH22	1.47	0.60
3:G:11[A]:ILE:O	3:G:15[A]:LYS:HG3	2.02	0.60
3:G:113[C]:TYR:O	3:G:114[C]:VAL:HG22	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
2:F:213:GLU:HG3	2:F:214:PRO:CD	2.31	0.60
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:B:298:LEU:HD21	1:B:337:ILE:HG21	1.83	0.59
4:H:45[A]:LEU:HD11	4:H:68[A]:LEU:HD21	1.84	0.59
1:A:151:LYS:HE2	1:A:428:MET:HE3	1.84	0.59
1:A:298:LEU:HD21	1:A:337:ILE:HG21	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
1:A:252:LYS:HD3	1:A:254:LYS:HE2	1.84	0.59
2:F:144:GLY:HA2	2:F:293:ILE:O	2.02	0.59
3:G:129[C]:ARG:O	3:G:131[C]:TYR:HD1	1.86	0.59
3:G:15[B]:LYS:HG3	3:G:256[B]:LEU:HD11	1.84	0.59
1:C:358:ASN:O	1:C:362:SER:HB2	2.01	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)
2:D:149:LEU:HD21	2:D:324:LEU:HD22	1.84	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: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:91[A]:TYR:CG	3:G:240[A]:ALA:HB1	2.37	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
1:A:435:ILE:HD12	1:A:472:LEU:HD21	1.84	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: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: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
2:D:266:SER:OG	2:D:268:VAL:HG12	2.03	0.59
1:B:36:ASP:OD2	2:E:263:ARG:HD3	2.01	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: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
1:C:438:TYR:CE1	1:C:487:LEU:HD12	2.37	0.59
1:C:188:GLY:O	1:C:189:GLN:HB2	2.03	0.59
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:F:266:SER:OG	2:F:268:VAL:HG12	2.02	0.58
3:G:18[C]:ARG:NH1	3:G:253[C]:THR:OG1	2.32	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
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
2:E:40:LEU:HD23	2:E:64:LEU:HD11	1.85	0.58
4:H:60[A]:LEU:HD13	4:H:130[A]:VAL:HA	1.84	0.58
2:E:139:ALA:N	2:E:140:PRO:HD3	2.18	0.58
1:C:31:VAL:HG11	1:C:34:VAL:HG22	1.85	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
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

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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
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:188:GLY:O	1:B:189:GLN:HB2	2.04	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:B:382:LEU:O	1:B:386:LEU:HD23	2.03	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:C:275:LEU:H	2:F:264:MET:HE1	1.66	0.58
3:G:84[C]:ASP:CB	3:G:120[C]:ARG:HB3	2.30	0.58
1:A:275:LEU:CB	2:D:264:MET:HG3	2.34	0.58
2:E:40:LEU:CD2	2:E:64:LEU:HD11	2.33	0.58
2:D:395:ARG:NH2	2:D:436:GLY:HA3	2.18	0.58
2:F:90:PHE:HE2	2:F:103:VAL:HG21	1.68	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: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: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: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: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:275:LEU:HB3	2:F:264:MET:HG3	1.85	0.57
2:F:416:MET:HB2	2:F:417:PRO:O	2.04	0.57
2:F:182:GLY:H	2:F:210:GLN:H	1.50	0.57
3:G:81[A]:ILE:HA	3:G:118[A]:VAL:HG13	1.85	0.57
3:G:230[C]:LEU:HD22	3:G:230[C]:LEU:O	2.03	0.57
1:C:499:THR:H	1:C:500:PRO:HD3	1.69	0.57
1:C:412:ARG:NH2	1:C:443:GLY:N	2.53	0.57
2:F:111:ILE:HA	2:F:227:THR:OG1	2.05	0.57
3:G:112[C]:GLU:OE2	3:G:112[C]:GLU:HA	2.03	0.57
2:D:375:ASP:O	2:D:379:ILE:HG23	2.04	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
2:F:301:VAL:HG13	2:F:306:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:188:GLY:O	1:A:189:GLN:HB2	2.04	0.57
2:F:371:ASN:CG	3:G:10[B]:ARG:HH11	1.96	0.57
3:G:261[C]:LEU:HD12	3:G:262[C]:GLN:HG3	1.87	0.57
3:G:92[C]:ASN:ND2	3:G:121[C]:LYS:HB3	2.18	0.57
3:G:80[C]:VAL:HG11	3:G:126[C]:PHE:HE2	1.65	0.57
3:G:86[A]:GLY:O	3:G:87[A]:LEU:HB2	2.03	0.57
4:H:100[B]:HIS:HD2	4:H:117[B]:HIS:CD2	2.23	0.57
1:C:382:LEU:O	1:C:386:LEU:HD23	2.04	0.57
4:H:8[B]:ILE:HA	4:H:77[B]:ILE:HG12	1.87	0.57
1:B:275:LEU:CG	1:B:278:ARG:HA	2.33	0.57
1:A:109:ASN:OD1	1:A:113:GLN:HG2	2.05	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
1:A:136:VAL:O	2:E:189:ASN:HB2	2.05	0.57
4:H:114[C]:TYR:O	4:H:118[C]:LYS:HB2	2.04	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
3:G:91[C]:TYR:CD1	3:G:181[C]:GLN:HG2	2.39	0.57
1:C:79:TYR:CE1	2:F:26:ILE:HD11	2.35	0.57
3:G:4[A]:MET:O	3:G:8[A]:LYS:HE3	2.04	0.56
1:B:462:SER:HB3	1:B:465:ARG:HH12	1.69	0.56
1:A:415:ARG:CG	1:A:415:ARG:NH1	2.49	0.56
2:F:349:PRO:HG3	2:F:357:TYR:CD2	2.40	0.56
2:E:388:GLU:O	2:E:392:ILE:HG23	2.05	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: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:241:LEU:HD23	2:D:243:PHE:CZ	2.40	0.56
2:D:181:VAL:HG22	2:D:221:VAL:HG13	1.86	0.56
3:G:6[B]:GLU:O	3:G:10[B]:ARG:HG3	2.05	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
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

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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
1:B:440:VAL:CA	1:B:445:MET:HG3	2.35	0.56
1:B:298:LEU:H	1:B:298:LEU:CD2	2.19	0.56
2:D:131:GLY:HA3	2:D:167:ASN:ND2	2.21	0.56
2:F:288:THR:HG23	2:F:291:GLY:H	1.70	0.56
1:C:248:TYR:O	1:C:252:LYS:HB2	2.05	0.56
2:F:125:ASP:OD2	2:F:345:ARG:NH2	2.38	0.56
2:E:369:ARG:HG2	2:E:392:ILE:HD11	1.87	0.56
1:C:292:TYR:O	1:C:296:ARG:HB3	2.05	0.56
3:G:104[B]:GLU:HA	3:G:107[B]:HIS:CE1	2.40	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
3:G:80[C]:VAL:CG1	3:G:126[C]:PHE:HE2	2.19	0.56
4:H:119[B]:ARG:HA	4:H:122[B]:GLU:OE1	2.04	0.56
1:A:238:ALA:HB3	1:A:239:PRO:HD3	1.86	0.56
1:B:252:LYS:HD3	1:B:254:LYS:HE2	1.85	0.56
1:A:31:VAL:HG11	1:A:34:VAL:HG22	1.88	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:171:ARG:NH1	1:B:171:ARG:CG	2.55	0.56
3:G:5[A]:ARG:HH11	3:G:5[A]:ARG:HB3	1.70	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:72[C]:PRO:HA	3:G:73[C]:VAL:CG1	2.29	0.56
1:C:495:LYS:O	1:C:496:LYS:HB2	2.06	0.56
2:F:388:GLU:O	2:F:392:ILE:HG23	2.06	0.56
2:E:241:LEU:HD23	2:E:243:PHE:CZ	2.40	0.56
1:B:435:ILE:HD12	1:B:472:LEU:HD21	1.88	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
1:A:294:HIS:O	1:A:298:LEU:HD22	2.05	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
1:B:34:VAL:HG13	1:B:39:ALA:HB2	1.87	0.56
2:E:460:LYS:O	2:E:461:LYS:HD2	2.06	0.56
1:C:129:ILE:HD11	1:C:237:LEU:HD22	1.88	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)
2:F:371:ASN:ND2	3:G:10[B]:ARG:HH11	2.04	0.56
3:G:83[A]:SER:HB3	3:G:237[A]:GLU:HG2	1.88	0.56
3:G:86[C]:GLY:CA	3:G:241[C]:ARG:NH2	2.64	0.56
4:H:86[A]:GLU:HG2	4:H:134[A]:LYS:HB3	1.88	0.56
1:C:435:ILE:HD12	1:C:472:LEU:HD21	1.88	0.56
3:G:17[B]:THR:HA	3:G:20[B]:ILE:HD12	1.87	0.56
2:D:416:MET:HB2	2:D:417:PRO:O	2.06	0.56
1:C:41:VAL:HG21	1:C:88:VAL:HG21	1.87	0.56
1:B:261:ASP:O	1:B:262:ASP:HB2	2.05	0.56
2:F:142:ALA:HB2	2:F:346:ILE:HD13	1.86	0.56
1:A:156:MET:C	1:A:157:ILE:HG13	2.25	0.56
1:A:140:LYS:NZ	1:A:143:HIS:HE1	2.03	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
3:G:5[A]:ARG:H	3:G:5[A]:ARG:HD2	1.70	0.55
3:G:45[B]:TYR:CZ	4:H:11[B]:PRO:HG3	2.41	0.55
4:H:110[C]:THR:C	4:H:112[C]:LYS:HE2	2.26	0.55
4:H:119[B]:ARG:HA	4:H:122[B]:GLU:CD	2.26	0.55
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:172[C]:TYR:HD2	3:G:186[C]:LYS:HG2	1.71	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:152[C]:ILE:N	3:G:152[C]:ILE:HD12	2.21	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:C:114:PRO:HG3	1:C:121:ILE:CD1	2.36	0.55
3:G:21[A]:THR:HG21	3:G:248[A]:ALA:HB3	1.88	0.55
2:D:113:ARG:HD3	2:D:114:PRO:O	2.06	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
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: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: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:495:LYS:HE3	1:B:496:LYS:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:LEU:N	1:B:482:PRO:CD	2.70	0.55
1:C:384:LEU:O	1:C:388:GLN:HG2	2.07	0.55
2:F:395:ARG:HH21	2:F:436:GLY:HA3	1.71	0.55
1:A:382:LEU:HD11	1:A:416:THR:HG23	1.88	0.55
2:F:438:HIS:HB3	2:F:441:LEU:HD22	1.89	0.55
3:G:120[B]:ARG:HG3	3:G:123[B]:ARG:HE	1.71	0.55
3:G:120[C]:ARG:O	3:G:120[C]:ARG:HG2	2.06	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:A:275:LEU:N	2:D:264:MET:HE1	2.22	0.55
1:B:355:PRO:HB2	1:B:357:VAL:HG23	1.87	0.55
3:G:5[B]:ARG:HB2	3:G:5[B]:ARG:NH1	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:456:PHE:HZ	1:B:495:LYS:HD2	1.72	0.55
2:F:397:ARG:O	2:F:401:ARG:HD2	2.07	0.55
1:B:32:ILE:HG12	1:B:40:ARG:O	2.07	0.55
1:C:32:ILE:HG12	1:C:40:ARG:O	2.07	0.55
3:G:77[B]:GLY:O	3:G:168[B]:LEU:HG	2.06	0.55
3:G:234[C]:LYS:O	3:G:235[C]:ALA:C	2.44	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: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:129[B]:ARG:HB2	3:G:131[B]:TYR:HE1	1.71	0.55
3:G:36[B]:GLN:HA	3:G:39[B]:ALA:HB3	1.89	0.55
1:C:495:LYS:HE3	1:C:496:LYS:H	1.72	0.55
1:B:440:VAL:HB	1:B:445:MET:HG3	1.88	0.55
2:D:397:ARG:O	2:D:401:ARG:HD2	2.07	0.55
1:B:129:ILE:CD1	1:B:237:LEU:HD22	2.37	0.55
1:B:41:VAL:HG21	1:B:88:VAL:HG21	1.88	0.55
3:G:260[B]:THR:HG22	3:G:260[B]:THR:O	2.07	0.55
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:9[B]:VAL:HG22	4:H:14[B]:LYS:HD2	1.89	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
1:C:261:ASP:O	1:C:262:ASP:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:69[C]:GLU:OE1	4:H:76[C]:ASN:HB2	2.07	0.54
3:G:4[A]:MET:HG3	3:G:5[A]:ARG:HH11	1.68	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
1:A:275:LEU:HA	1:A:278:ARG:N	2.22	0.54
1:B:157:ILE:HG21	1:B:342:ILE:HG12	1.89	0.54
1:A:384:LEU:O	1:A:388:GLN:HG2	2.07	0.54
2:D:91:ASN:HD22	2:D:91:ASN:C	2.11	0.54
2:D:288:THR:HG23	2:D:291:GLY:H	1.72	0.54
1:A:456:PHE:HZ	1:A:495:LYS:HD2	1.73	0.54
1:C:62:MET:CB	1:C:95:MET:HE1	2.34	0.54
1:A:481:LEU:O	1:A:482:PRO:O	2.25	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
3:G:25[C]:LYS:HG2	3:G:245[C]:MET:CB	2.37	0.54
1:C:275:LEU:CD1	1:C:281:PRO:HD3	2.37	0.54
2:E:12:PRO:HD2	2:E:260:LEU:HD22	1.89	0.54
2:D:453:ASP:O	2:D:456:VAL:HG23	2.07	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
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
1:B:275:LEU:CG	2:E:264:MET:HG3	2.37	0.54
1:B:275:LEU:HB2	2:E:264:MET:SD	2.47	0.54
1:C:284:GLU:HG3	1:C:329:TYR:CB	2.38	0.54
1:B:419:ILE:HD13	1:B:440:VAL:HG11	1.89	0.54
1:B:384:LEU:O	1:B:388:GLN:HG2	2.08	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
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
3:G:122[B]:GLY:O	3:G:126[B]:PHE:HB2	2.07	0.54
2:E:226:LEU:HD11	2:E:284:ARG:CB	2.37	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
3:G:114[C]:VAL:HB	3:G:134[C]:VAL:CG1	2.38	0.54
4:H:10[C]:THR:OG1	4:H:11[C]:PRO:HD2	2.07	0.54
4:H:21[B]:ASP:OD2	4:H:21[B]:ASP:N	2.40	0.54
4:H:63[A]:VAL:HG13	4:H:79[A]:ALA:HB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95[C]:ILE:CD1	3:G:171[C]:PHE:HB3	2.38	0.54
3:G:91[C]:TYR:CD2	3:G:240[C]:ALA:HB1	2.43	0.54
1:A:495:LYS:HE3	1:A:496:LYS:H	1.72	0.54
2:D:26:ILE:O	2:D:27:TYR:HB2	2.08	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:372:ASP:OD2	3:G:9[C]:ARG:NH1	2.39	0.54
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:72[C]:PRO:CB	3:G:73[C]:VAL:HG13	2.37	0.53
1:C:354:ARG:HA	1:C:355:PRO:C	2.28	0.53
1:A:407:GLN:HA	1:A:411:ASN:HB2	1.91	0.53
3:G:244[C]:ALA:O	3:G:248[C]:ALA:HB2	2.07	0.53
1:C:32:ILE:HG13	1:C:33:GLN:HG3	1.90	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
1:B:354:ARG:HA	1:B:355:PRO:C	2.28	0.53
2:D:97:ILE:HG12	2:D:97:ILE:O	2.07	0.53
1:B:499:THR:H	1:B:500:PRO:HD3	1.73	0.53
1:B:262:ASP:H	1:B:318:PHE:HB2	1.73	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:C:47:VAL:HG12	1:C:90:ARG:HG2	1.91	0.53
1:B:140:LYS:NZ	1:B:143:HIS:HE1	2.05	0.53
2:E:393:VAL:O	2:E:397:ARG:HG3	2.07	0.53
2:E:395:ARG:HH21	2:E:436:GLY:HA3	1.74	0.53
1:B:100:GLY:HA2	1:B:248:TYR:CE2	2.42	0.53
2:D:438:HIS:HB3	2:D:441:LEU:HD22	1.89	0.53
2:D:111:ILE:HA	2:D:227:THR:OG1	2.07	0.53
1:A:292:TYR:O	1:A:296:ARG:HB3	2.09	0.53
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
3:G:84[B]:ASP:HB2	3:G:120[B]:ARG:CZ	2.39	0.53
4:H:51[B]:ARG:HG2	4:H:60[B]:LEU:HD23	1.90	0.53
1:B:495:LYS:O	1:B:496:LYS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:109:ASN:HB2	1:B:110:PRO:CD	2.39	0.53
3:G:32[A]:LEU:CB	3:G:238[A]:PHE:HB2	2.37	0.53
1:A:440:VAL:CA	1:A:445:MET:HG3	2.36	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
1:A:449:PRO:HG2	1:A:452:ASP:OD1	2.09	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:271:ARG:NH1	1:A:285:ALA:CB	2.72	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:C:106:ARG:CB	1:C:106:ARG:HH11	2.20	0.53
1:A:456:PHE:O	1:A:460:LEU:HB2	2.09	0.53
1:C:275:LEU:HD12	1:C:281:PRO:HD3	1.91	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
2:D:369:ARG:HG2	2:D:392:ILE:HD11	1.91	0.53
1:C:418:GLU:OE2	1:C:421:LYS:HE2	2.08	0.53
1:B:275:LEU:HA	1:B:278:ARG:CA	2.39	0.53
1:B:415:ARG:NH1	1:B:450:VAL:HG22	2.23	0.53
1:B:284:GLU:HG3	1:B:329:TYR:CB	2.39	0.53
1:A:157:ILE:N	1:A:158:PRO:CD	2.71	0.53
2:F:375:ASP:O	2:F:379:ILE:HG23	2.08	0.53
1:C:46:LYS:NZ	1:C:46:LYS:HB2	2.23	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
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: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
1:A:284:GLU:HG3	1:A:329:TYR:CB	2.39	0.53
1:C:157:ILE:HG21	1:C:342:ILE:HG12	1.90	0.53
1:B:48:MET:HG3	1:B:51:GLU:OE2	2.09	0.53
2:D:398:LYS:HD3	2:D:446:PHE:CZ	2.44	0.53
1:C:109:ASN:OD1	1:C:113:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:419:ILE:HD13	1:C:440:VAL:HG11	1.91	0.53
1:A:47:VAL:HG21	1:A:71:VAL:HG21	1.90	0.53
2:E:315:PHE:HA	2:E:318:LEU:HD22	1.90	0.53
3:G:84[A]:ASP:OD2	3:G:139[A]:GLY:HA2	2.08	0.52
3:G:43[C]:ARG:HB2	3:G:44[C]:PRO:CD	2.39	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
1:A:275:LEU:CD2	2:D:264:MET:HA	2.20	0.52
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
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: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
2:E:264:MET:CE	2:E:272:PRO:HB3	2.38	0.52
2:D:301:VAL:HG22	2:D:301:VAL:O	2.09	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
1:C:440:VAL:HB	1:C:445:MET:HG3	1.91	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
2:F:129:GLU:O	2:F:172:HIS:HE1	1.92	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
1:A:412:ARG:HG3	1:A:446:ASP:OD1	2.09	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:88[B]:ALA:CB	3:G:241[B]:ARG:HA	2.40	0.52
3:G:19[A]:GLN:HA	3:G:22[A]:LYS:HG2	1.91	0.52
3:G:257[C]:GLU:HG2	3:G:257[C]:GLU:O	2.08	0.52
3:G:184[C]:VAL:HG11	3:G:186[C]:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:65[C]:HIS:CD2	3:G:69[C]:GLU:CA	2.93	0.52
1:A:142:VAL:HG22	1:A:161:ARG:O	2.10	0.52
2:E:91:ASN:HD22	2:E:91:ASN:C	2.12	0.52
1:A:271:ARG:NH1	1:A:285:ALA:HB1	2.25	0.52
2:E:382:MET:HG3	2:E:385:LEU:HD22	1.91	0.52
2:F:181:VAL:HG22	2:F:221:VAL:HG13	1.92	0.52
3:G:8[C]:LYS:HA	3:G:11[C]:ILE:HB	1.92	0.52
3:G:67[A]:MET:SD	3:G:161[A]:ALA:HA	2.49	0.52
4:H:118[C]:LYS:HA	4:H:121[C]:LEU:HG	1.92	0.52
1:B:106:ARG:CB	1:B:106:ARG:HH11	2.22	0.52
1:A:171:ARG:NH1	1:A:171:ARG:CG	2.53	0.52
2:D:35:PRO:HD2	2:D:36:GLN:OE1	2.09	0.52
3:G:42[C]:ALA:O	3:G:43[C]:ARG:C	2.47	0.52
1:B:62:MET:CE	1:B:95:MET:HE3	2.40	0.52
1:B:62:MET:CB	1:B:95:MET:HE1	2.29	0.52
1:B:382:LEU:HD11	1:B:416:THR:HG23	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
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:B:275:LEU:HD13	2:E:264:MET:HG3	1.91	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
2:E:91:ASN:ND2	2:E:95:GLU:H	2.08	0.52
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:275:LEU:HD12	1:A:279:ARG:O	2.10	0.51
4:H:12[A]:GLU:C	4:H:13[A]:ARG:HD2	2.31	0.51
1:C:440:VAL:CB	1:C:445:MET:HG3	2.41	0.51
1:A:157:ILE:HG21	1:A:342:ILE:HG12	1.93	0.51
2:E:84:ALA:HB1	2:E:103:VAL:HG12	1.92	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
2:F:386:SER:HB3	2:F:389:ASP:OD1	2.10	0.51
3:G:15[C]:LYS:O	3:G:18[C]:ARG:HB3	2.09	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

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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: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:456:PHE:O	1:C:460:LEU:HB2	2.11	0.51
1:C:275:LEU:HD13	2:F:264:MET:HG3	1.92	0.51
2:F:40:LEU:CD2	2:F:64:LEU:HD11	2.40	0.51
2:D:85:THR:O	2:D:205:SER:HB3	2.11	0.51
4:H:14[B]:LYS:HB3	4:H:14[B]:LYS:NZ	2.25	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
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:C:106:ARG:NH1	1:C:106:ARG:CG	2.48	0.51
1:C:137:MET:HG3	2:D:97:ILE:O	2.11	0.51
1:C:156:MET:C	1:C:157:ILE:HG13	2.30	0.51
2:D:226:LEU:O	2:D:230:GLU:HG3	2.10	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
2:E:453:ASP:O	2:E:456:VAL:HG23	2.11	0.51
1:C:271:ARG:NH1	1:C:285:ALA:CB	2.74	0.51
2:F:113:ARG:HD3	2:F:114:PRO:O	2.11	0.51
2:D:246:ASN:OD1	2:D:248:PHE:HB3	2.11	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
1:B:407:GLN:HA	1:B:411:ASN:HB2	1.92	0.51
1:A:62:MET:CB	1:A:95:MET:HE1	2.33	0.51
2:E:411:GLU:OE2	2:E:417:PRO:HB3	2.11	0.51
1:C:140:LYS:HE2	1:C:143:HIS:ND1	2.26	0.51
2:F:131:GLY:HA3	2:F:167:ASN:HD22	1.76	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
2:E:129:GLU:O	2:E:172:HIS:HE1	1.93	0.51
4:H:8[B]:ILE:HD11	4:H:15[B]:VAL:HB	1.93	0.51
1:A:354:ARG:HA	1:A:355:PRO:C	2.30	0.51
1:C:355:PRO:HB2	1:C:357:VAL:HG23	1.92	0.51
1:A:140:LYS:HE2	1:A:143:HIS:ND1	2.25	0.51
1:B:449:PRO:HG2	1:B:452:ASP:OD1	2.09	0.51
3:G:14[A]:VAL:CG1	3:G:256[A]:LEU:HG	2.41	0.51
3:G:101[C]:LYS:O	3:G:101[C]:LYS:HD2	2.11	0.51
3:G:177[C]:SER:O	3:G:180[C]:VAL:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32[C]:LEU:CD2	3:G:238[C]:PHE:HB2	2.41	0.51
4:H:39[A]:ILE:HB	4:H:40[A]:PRO:CD	2.41	0.51
1:B:164:ARG:NH2	2:F:184:ARG:HD3	2.23	0.51
1:A:184:ILE:HG22	1:A:427:PRO:HG2	1.91	0.51
2:D:139:ALA:N	2:D:140:PRO:HD3	2.25	0.51
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:B:481:LEU:O	1:B:482:PRO:O	2.28	0.50
2:E:131:GLY:HA3	2:E:167:ASN:HD22	1.75	0.50
2:D:428:ARG:O	2:D:432:GLU:HG3	2.12	0.50
3:G:149[C]:ILE:O	3:G:151[C]:ASP:N	2.44	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:E:428:ARG:O	2:E:432:GLU:HG3	2.11	0.50
2:D:129:GLU:O	2:D:172:HIS:HE1	1.94	0.50
1:C:407:GLN:HB3	1:C:411:ASN:HB2	1.93	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
2:D:388:GLU:O	2:D:392:ILE:HG23	2.10	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:462:SER:CB	1:A:465:ARG:HH12	2.23	0.50
1:A:440:VAL:CB	1:A:445:MET:HG3	2.42	0.50
1:C:407:GLN:CA	1:C:411:ASN:HB2	2.42	0.50
1:C:157:ILE:N	1:C:158:PRO:CD	2.74	0.50
1:B:157:ILE:N	1:B:158:PRO:CD	2.75	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
1:C:136:VAL:HG12	2:D:185:THR:HG23	1.92	0.50
3:G:149[B]:ILE:HD11	3:G:227[B]:TYR:CZ	2.47	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:C:449:PRO:HG2	1:C:452:ASP:OD1	2.12	0.50
1:B:32:ILE:HG13	1:B:33:GLN:HG3	1.93	0.50
2:E:273:THR:O	2:E:277:GLU:HG3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:349:PRO:HG3	2:D:357:TYR:CD2	2.46	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:48:MET:CB	2:E:63:GLY:HA2	2.40	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
3:G:96[A]:LEU:HD22	3:G:125[A]:PHE:CD1	2.47	0.50
2:F:264:MET:HG2	2:F:265:PRO:O	2.11	0.50
1:C:481:LEU:O	1:C:482:PRO:O	2.29	0.50
2:F:374:GLN:HA	2:F:374:GLN:NE2	2.23	0.50
1:A:143:HIS:NE2	1:A:144:GLU:HG2	2.27	0.50
2:F:162:GLN:NE2	2:F:194:GLU:HG2	2.27	0.50
1:B:412:ARG:HG3	1:B:446:ASP:OD1	2.11	0.50
2:F:453:ASP:O	2:F:456:VAL:HG23	2.11	0.50
4:H:83[C]:GLU:HB2	4:H:87[C]:GLU:HB3	1.94	0.50
2:E:349:PRO:HG3	2:E:357:TYR:CD2	2.46	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:B:395:PHE:N	1:B:395:PHE:CD2	2.80	0.50
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:48:MET:HG3	1:A:51:GLU:OE2	2.12	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
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:B:275:LEU:CD1	1:B:281:PRO:HD3	2.42	0.49
1:A:48:MET:HB3	2:E:63:GLY:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:308:ASP:O	2:E:311:PRO:HD2	2.12	0.49
2:D:411:GLU:OE2	2:D:417:PRO:HB3	2.12	0.49
2:E:386:SER:HB3	2:E:389:ASP:HB2	1.94	0.49
3:G:220[C]:LYS:HB3	3:G:220[C]:LYS:NZ	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
3:G:95[C]:ILE:HD11	3:G:171[C]:PHE:HB3	1.94	0.49
4:H:26[C]:ARG:HB2	4:H:48[C]:ALA:CB	2.42	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: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:A:415:ARG:NH1	1:A:450:VAL:HG22	2.27	0.49
2:F:398:LYS:HD3	2:F:446:PHE:CZ	2.46	0.49
2:E:431:LYS:HE3	2:E:435:GLU:OE2	2.12	0.49
1:A:205:VAL:O	1:A:209:VAL:HG23	2.13	0.49
2:E:160:LEU:HD22	2:E:164:LEU:HD22	1.95	0.49
4:H:88[B]:ILE:HD13	4:H:130[B]:VAL:HG12	1.94	0.49
1:C:411:ASN:O	1:C:415:ARG:NH1	2.45	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
3:G:118[C]:VAL:HB	3:G:137[C]:VAL:CG1	2.43	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
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
2:E:406:PRO:HB3	2:E:416:MET:HG3	1.94	0.49
1:C:388:GLN:HG3	1:C:409:LYS:HZ1	1.78	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
2:F:268:VAL:CG2	2:F:268:VAL:O	2.59	0.49
3:G:143[C]:THR:HB	3:G:144[C]:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32[C]:LEU:CD2	3:G:238[C]:PHE:CD2	2.94	0.49
3:G:68[C]:LEU:HD12	3:G:189[C]:LEU:HG	1.95	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
3:G:45[C]:TYR:HB3	4:H:11[C]:PRO:HA	1.94	0.49
1:A:419:ILE:HD13	1:A:440:VAL:HG11	1.95	0.49
1:A:499:THR:H	1:A:500:PRO:HD3	1.73	0.49
2:E:346:ILE:HB	2:E:351:VAL:HG11	1.95	0.49
1:B:386:LEU:HD22	1:B:416:THR:HG21	1.94	0.49
3:G:22[C]:LYS:HB3	3:G:249[C]:THR:OG1	2.13	0.49
1:B:286:TYR:HB3	1:B:287:PRO:HD2	1.95	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: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:84[C]:ASP:OD1	3:G:140[C]:ILE:HG12	2.13	0.48
3:G:143[C]:THR:HB	3:G:144[C]:PRO:CA	2.43	0.48
4:H:71[C]:ARG:HB3	4:H:72[C]:PRO:HD2	1.95	0.48
2:D:264:MET:HG2	2:D:265:PRO:O	2.13	0.48
1:A:114:PRO:HG3	1:A:121:ILE:CD1	2.43	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:B:298:LEU:N	1:B:298:LEU:CD2	2.76	0.48
2:F:161:ILE:HG23	2:F:243:PHE:CE1	2.48	0.48
2:F:166:ASN:O	2:F:170:GLN:HB2	2.13	0.48
2:E:113:ARG:HD3	2:E:114:PRO:O	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
2:E:268:VAL:O	2:E:268:VAL:CG2	2.58	0.48
2:F:411:GLU:OE2	2:F:417:PRO:HB3	2.13	0.48
1:C:34:VAL:HG13	1:C:39:ALA:HB2	1.94	0.48
1:C:462:SER:CB	1:C:465:ARG:HH12	2.26	0.48
1:A:471:LEU:HD13	1:A:487:LEU:HD22	1.95	0.48
1:A:411:ASN:O	1:A:415:ARG:NH1	2.46	0.48
2:E:379:ILE:HG13	2:E:379:ILE:O	2.12	0.48
2:D:379:ILE:HA	3:G:251[C]:ASN:HB3	1.95	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:E:166:ASN:O	2:E:170:GLN:HB2	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:456:PHE:CZ	1:B:495:LYS:HD2	2.49	0.48
2:F:97:ILE:O	2:F:97:ILE:HG12	2.13	0.48
2:D:301:VAL:CG1	2:D:306:TYR:HE1	2.23	0.48
2:F:406:PRO:HB3	2:F:416:MET:HG3	1.95	0.48
2:E:397:ARG:O	2:E:401:ARG:HD2	2.13	0.48
1:A:41:VAL:CG2	1:A:88:VAL:HG21	2.42	0.48
1:A:176:THR:O	1:A:180:ILE:HG12	2.13	0.48
2:F:340:LEU:HD12	2:F:340:LEU:HA	1.67	0.48
3:G:31[C]:LYS:HB3	3:G:32[C]:LEU:HD22	1.94	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
1:B:172:GLN:NE2	2:E:345:ARG:HB3	2.28	0.48
2:F:129:GLU:O	2:F:172:HIS:CE1	2.66	0.48
1:B:205:VAL:O	1:B:209:VAL:HG23	2.14	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:C:462:SER:CA	1:C:465:ARG:HH12	2.27	0.48
1:B:284:GLU:HG3	1:B:329:TYR:HB2	1.96	0.48
1:A:62:MET:CE	1:A:95:MET:HE3	2.44	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
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:407:GLN:CA	1:B:411:ASN:HB2	2.43	0.48
1:C:471:LEU:HD13	1:C:487:LEU:HD22	1.95	0.48
2:E:35:PRO:HD2	2:E:36:GLN:OE1	2.14	0.48
1:C:333:ASN:O	1:C:337:ILE:HG13	2.13	0.48
2:D:142:ALA:HB2	2:D:346:ILE:HG21	1.96	0.48
3:G:85[C]:ARG:CA	3:G:120[C]:ARG:NH2	2.77	0.48
3:G:238[C]:PHE:O	3:G:241[C]:ARG:N	2.46	0.48
4:H:90[B]:VAL:HG13	4:H:128[B]:LEU:HD21	1.95	0.48
4:H:22[A]:ILE:HG22	4:H:35[A]:MET:SD	2.54	0.48
1:B:388:GLN:HG3	1:B:409:LYS:HZ2	1.77	0.48
3:G:238[B]:PHE:CD1	3:G:241[B]:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:475:ILE:O	1:C:479:GLY:HA3	2.14	0.47
2:D:356:HIS:CD2	2:D:356:HIS:C	2.88	0.47
2:D:23:LEU:HA	2:D:24:PRO:HD3	1.75	0.47
1:B:65:ASN:HB3	2:F:10:MET:HE3	1.96	0.47
3:G:5[A]:ARG:HG2	3:G:6[A]:GLU:HG2	1.95	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
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:460:LEU:O	1:A:464:MET:HG2	2.14	0.47
1:A:326:VAL:HG12	1:A:326:VAL:O	2.13	0.47
1:C:108:VAL:HG13	1:C:109:ASN:O	2.14	0.47
2:F:369:ARG:HG2	2:F:392:ILE:HD11	1.96	0.47
1:B:431:GLU:HG2	1:B:432:GLU:H	1.77	0.47
2:E:165:ILE:HG21	2:E:200:VAL:HG13	1.95	0.47
3:G:4[A]:MET:HG3	3:G:5[A]:ARG:HH12	1.73	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:87[C]:LEU:HD12	3:G:87[C]:LEU:HA	1.51	0.47
1:A:456:PHE:CZ	1:A:495:LYS:HD2	2.49	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
1:C:298:LEU:CD2	1:C:298:LEU:H	2.27	0.47
1:B:326:VAL:HG11	1:B:343:PHE:CE2	2.44	0.47
1:C:167:ILE:HD11	1:C:316:LEU:HD13	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:B:411:ASN:O	1:B:415:ARG:NH1	2.48	0.47
2:F:233:ARG:HD3	2:F:292:SER:HB3	1.95	0.47
1:A:32:ILE:HG13	1:A:33:GLN:HG3	1.96	0.47
2:F:232:PHE:HB2	2:F:240:VAL:HG21	1.95	0.47
3:G:11[C]:ILE:HG13	3:G:259[C]:LEU:HD12	1.96	0.47
3:G:25[C]:LYS:HD2	3:G:25[C]:LYS:O	2.14	0.47
4:H:96[C]:ALA:CB	4:H:100[C]:HIS:ND1	2.77	0.47
4:H:119[C]:ARG:HA	4:H:122[C]:GLU:OE2	2.15	0.47
1:C:48:MET:HE1	1:C:94:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95[C]:ILE:HD13	3:G:95[C]:ILE:O	2.15	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
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:A:330:ILE:HB	1:A:331:PRO:HD3	1.95	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
2:D:264:MET:CB	2:D:265:PRO:CA	2.92	0.47
1:C:151:LYS:HD2	1:C:419:ILE:O	2.14	0.47
1:B:140:LYS:HE2	1:B:143:HIS:ND1	2.30	0.47
2:E:233:ARG:HD3	2:E:292:SER:HB3	1.97	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
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
2:F:352:VAL:HG21	2:F:356:HIS:CD2	2.49	0.47
1:B:146:LEU:HD21	1:B:257:LEU:HD13	1.96	0.47
1:A:210:GLU:HB2	2:D:123:THR:HB	1.96	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:175[C]:PHE:HB2	3:G:236[C]:SER:OG	2.14	0.47
3:G:168[C]:LEU:HB2	3:G:189[C]:LEU:HB2	1.97	0.47
2:F:254:GLY:HA3	2:F:271:GLN:HE21	1.80	0.47
1:B:471:LEU:HD13	1:B:487:LEU:HD22	1.96	0.47
1:A:99:VAL:CG1	1:A:248:TYR:CD1	2.98	0.47
1:B:31:VAL:CG1	1:B:34:VAL:HG22	2.45	0.47
1:B:271:ARG:NH1	1:B:285:ALA:CB	2.78	0.47
3:G:185[C]:GLU:O	3:G:185[C]:GLU:HG3	2.15	0.47
3:G:168[B]:LEU:H	3:G:190[B]:PRO:HD3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:C	2:E:264:MET:HE2	2.36	0.47
1:C:99:VAL:CG1	1:C:248:TYR:CD1	2.98	0.47
2:E:441:LEU:HD21	2:E:456:VAL:HG13	1.96	0.47
1:C:31:VAL:CG1	1:C:34:VAL:HG22	2.44	0.47
1:C:271:ARG:NH1	1:C:285:ALA:HB1	2.29	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:C:462:SER:HA	1:C:465:ARG:HH12	1.72	0.47
1:C:460:LEU:O	1:C:464:MET:HG2	2.15	0.47
1:C:66:LEU:HD13	2:D:66:ARG:HG3	1.97	0.47
1:B:47:VAL:HG12	1:B:90:ARG:HG2	1.95	0.47
2:F:65:VAL:HB	2:F:68:LEU:HD21	1.97	0.47
1:C:386:LEU:HD22	1:C:416:THR:HG21	1.97	0.47
2:F:84:ALA:HB1	2:F:103:VAL:HG12	1.96	0.47
2:D:48:LEU:HD11	2:D:54:ARG:HB2	1.97	0.47
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: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
2:F:34:ARG:CG	2:F:35:PRO:HA	2.39	0.46
1:C:499:THR:N	1:C:500:PRO:CD	2.76	0.46
2:E:254:GLY:HA3	2:E:271:GLN:NE2	2.30	0.46
2:D:65:VAL:HB	2:D:68:LEU:HD21	1.98	0.46
2:D:129:GLU:O	2:D:172:HIS:CE1	2.67	0.46
1:C:286:TYR:HB3	1:C:287:PRO:HD2	1.96	0.46
2:E:247:ILE:O	2:E:250:PHE:HB3	2.14	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:A:275:LEU:HA	1:A:278:ARG:CA	2.45	0.46
1:C:431:GLU:HG2	1:C:432:GLU:H	1.78	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
3:G:170[A]:ILE:O	3:G:185[A]:GLU:HB2	2.15	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:C:284:GLU:HG3	1:C:329:TYR:CD1	2.48	0.46
3:G:217[A]:LEU:O	3:G:219[A]:PRO:HD3	2.16	0.46
3:G:116[C]:PHE:HE2	3:G:165[C]:PHE:HZ	1.62	0.46
1:A:275:LEU:CB	2:D:264:MET:SD	3.03	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:275:LEU:HA	1:B:278:ARG:HA	1.98	0.46
2:E:97:ILE:O	2:E:97:ILE:HG12	2.14	0.46
2:E:27:TYR:O	2:E:76:PRO:HA	2.15	0.46
2:F:91:ASN:HD22	2:F:91:ASN:C	2.17	0.46
1:B:41:VAL:CG2	1:B:88:VAL:HG21	2.44	0.46
2:E:340:LEU:HD12	2:E:340:LEU:HA	1.62	0.46
4:H:20[C]:ALA:HA	4:H:53[C]:LYS:O	2.16	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
1:B:99:VAL:CG1	1:B:248:TYR:CD1	2.99	0.46
2:D:441:LEU:HD21	2:D:456:VAL:HG13	1.97	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:A:284:GLU:HG3	1:A:329:TYR:HB2	1.97	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
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
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:C:284:GLU:HG3	1:C:329:TYR:CD2	2.48	0.46
1:C:188:GLY:O	1:C:189:GLN:CB	2.64	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
1:C:184:ILE:HG22	1:C:427:PRO:HG2	1.98	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
2:E:264:MET:CB	2:E:265:PRO:CA	2.93	0.46
1:C:438:TYR:CA	1:C:441:THR:HG22	2.42	0.46
2:F:27:TYR:O	2:F:76:PRO:HA	2.15	0.46
1:B:44:LEU:HD23	1:B:44:LEU:HA	1.77	0.46
2:F:301:VAL:HG22	2:F:301:VAL:O	2.16	0.46
2:D:131:GLY:HA3	2:D:167:ASN:HD22	1.77	0.46
2:F:292:SER:OG	2:F:293:ILE:N	2.46	0.46
1:C:395:PHE:CD2	1:C:395:PHE:N	2.82	0.46
1:A:395:PHE:N	1:A:395:PHE:CD2	2.82	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:HG22	1.98	0.46
3:G:75[A]:LYS:HD2	3:G:164[A]:THR:O	2.16	0.46
1:B:388:GLN:HG3	1:B:409:LYS:HZ1	1.78	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:D:416:MET:N	2:D:417:PRO:CA	2.79	0.46
2:F:235:ARG:O	2:F:237:GLY:N	2.48	0.46
1:B:292:TYR:O	1:B:296:ARG:HB3	2.16	0.46
2:F:246:ASN:OD1	2:F:248:PHE:HB3	2.15	0.46
2:D:373:LEU:HA	2:D:376:ILE:HG12	1.98	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
2:E:264:MET:CB	2:E:265:PRO:HA	2.39	0.46
1:A:440:VAL:HG12	1:A:445:MET:HE3	1.97	0.46
2:D:34:ARG:CG	2:D:35:PRO:HA	2.38	0.46
2:E:34:ARG:CG	2:E:35:PRO:HA	2.37	0.46
2:D:346:ILE:HB	2:D:351:VAL:HG11	1.97	0.46
1:A:109:ASN:HD21	1:A:113:GLN:CG	2.29	0.46
2:D:241:LEU:HD12	2:D:241:LEU:HA	1.64	0.46
2:E:458:LYS:C	2:E:460:LYS:H	2.18	0.46
2:E:24:PRO:HD2	2:E:53:VAL:HG11	1.98	0.46
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: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:379:ILE:O	2:D:379:ILE:HG13	2.16	0.45
2:E:65:VAL:HB	2:E:68:LEU:HD21	1.98	0.45
1:A:109:ASN:HB2	1:A:110:PRO:CD	2.46	0.45
2:D:291:GLY:O	2:D:292:SER:CB	2.63	0.45
2:F:12:PRO:HG2	2:F:260:LEU:HD11	1.97	0.45
2:E:195:MET:HE2	2:E:206:MET:SD	2.56	0.45
3:G:220[B]:LYS:HD3	3:G:220[B]:LYS:HA	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:97[C]:LYS:HE3	4:H:128[C]:LEU:CD1	2.42	0.45
1:A:275:LEU:HG	1:A:278:ARG:CA	2.42	0.45
1:A:333:ASN:O	1:A:337:ILE:HG13	2.15	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)
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:A:286:TYR:HB3	1:A:287:PRO:HD2	1.98	0.45
1:C:243:CYS:HB2	1:C:260:TYR:OH	2.16	0.45
2:F:92:VAL:HG21	2:F:217:ALA:HB1	1.98	0.45
4:H:95[C]:LYS:HA	4:H:95[C]:LYS:HD2	1.63	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: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
1:B:93:ARG:HD3	1:B:96:GLU:OE2	2.17	0.45
2:F:160:LEU:HD22	2:F:164:LEU:HD22	1.97	0.45
3:G:86[A]:GLY:CA	3:G:121[A]:LYS:HD2	2.47	0.45
3:G:131[A]:TYR:N	3:G:132[A]:PRO:HA	2.25	0.45
3:G:23[C]:ALA:O	3:G:27[C]:VAL:HG23	2.16	0.45
4:H:88[A]:ILE:HD11	4:H:131[A]:ALA:CA	2.47	0.45
1:C:435:ILE:HD13	1:C:464:MET:CE	2.46	0.45
1:C:275:LEU:CB	2:F:264:MET:HG3	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
3:G:217[C]:LEU:C	3:G:219[C]:PRO:HD3	2.36	0.45
2:F:12:PRO:HD2	2:F:260:LEU:CD2	2.47	0.45
2:F:218:ARG:O	2:F:221:VAL:HG12	2.16	0.45
2:E:387:ASP:O	2:E:391:LEU:HB2	2.17	0.45
3:G:184[C]:VAL:CG1	3:G:186[C]:LYS:HE3	2.47	0.45
2:D:264:MET:CE	2:D:272:PRO:HB3	2.40	0.45
1:B:462:SER:CA	1:B:465:ARG:HH12	2.30	0.45
1:A:492:GLU:CA	1:A:495:LYS:HB2	2.33	0.45
2:F:135:ILE:HD12	2:F:141:TYR:CE2	2.50	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:C:179:ALA:HB2	1:C:318:PHE:HZ	1.82	0.45
2:D:387:ASP:O	2:D:391:LEU:HB2	2.17	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:151:LYS:HE2	1:A:428:MET:CE	2.46	0.45
2:D:135:ILE:HD12	2:D:141:TYR:CE2	2.52	0.45
2:D:419:LYS:CE	2:D:450:GLY:HA3	2.42	0.45
2:F:397:ARG:NH1	2:F:443:GLU:OE2	2.49	0.45
1:B:389:TYR:CD1	1:B:413:GLY:HA3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:VAL:O	1:C:209:VAL:HG23	2.17	0.45
2:D:92:VAL:HG21	2:D:217:ALA:HB1	1.99	0.45
2:D:307:THR:HG23	2:D:307:THR:O	2.16	0.45
2:D:166:ASN:O	2:D:170:GLN:HB2	2.16	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
2:F:35:PRO:HD2	2:F:36:GLN:OE1	2.17	0.45
1:B:232:ALA:N	1:B:233:PRO:CD	2.79	0.45
2:F:416:MET:N	2:F:417:PRO:CA	2.78	0.45
2:F:149:LEU:CD2	2:F:324:LEU:HD22	2.47	0.45
1:B:330:ILE:HB	1:B:331:PRO:HD3	1.99	0.45
1:B:167:ILE:HD11	1:B:316:LEU:HD13	1.99	0.45
2:D:329:ALA:C	2:D:331:MET:H	2.20	0.45
1:C:176:THR:O	1:C:180:ILE:HG12	2.17	0.45
1:C:319:ILE:HA	1:C:319:ILE:HD13	1.75	0.45
1:A:194:ILE:CD1	1:A:222:ILE:HD12	2.46	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: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
1:C:109:ASN:HB3	1:C:115:LEU:HD11	1.99	0.45
2:D:461:LYS:HE2	2:D:461:LYS:HB3	1.71	0.45
2:D:241:LEU:O	2:D:242:LEU:HB3	2.16	0.45
2:E:177:VAL:O	2:E:242:LEU:HA	2.16	0.45
1:B:262:ASP:OD1	1:B:264:SER:HB2	2.17	0.45
2:D:165:ILE:HG21	2:D:200:VAL:HG13	1.99	0.45
3:G:32[C]:LEU:HG	3:G:238[C]:PHE:CB	2.27	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:F:387:ASP:O	2:F:391:LEU:HB2	2.17	0.45
2:D:40:LEU:HD23	2:D:64:LEU:HD11	1.98	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
1:B:275:LEU:HG	1:B:278:ARG:CA	2.43	0.45
1:B:151:LYS:HE2	1:B:428:MET:HE3	1.98	0.45
1:C:480:GLU:HG3	1:C:482:PRO:CD	2.47	0.45
1:A:47:VAL:HG12	1:A:90:ARG:HG2	1.97	0.45
1:A:144:GLU:O	1:A:161:ARG:HG3	2.17	0.45
1:A:121:ILE:HG22	1:A:123:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:157:ILE:N	1:A:158:PRO:HD2	2.32	0.44
1:A:179:ALA:HB2	1:A:318:PHE:HZ	1.82	0.44
1:A:188:GLY:O	1:A:189:GLN:CB	2.64	0.44
2:F:177:VAL:O	2:F:242:LEU:HA	2.17	0.44
1:A:183:ILE:HG12	1:A:193:CYS:HB3	1.99	0.44
2:F:82:GLY:HA2	2:F:231:TYR:CE2	2.52	0.44
3:G:139[C]:GLY:O	3:G:141[C]:SER:N	2.50	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
3:G:71[C]:ARG:NH1	3:G:166[C]:ASP:HA	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
2:F:264:MET:CE	2:F:272:PRO:HB3	2.44	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:E:205:SER:HB2	2:E:228:MET:HE1	1.99	0.44
2:D:79:VAL:HG11	2:D:224:THR:HG23	1.99	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:157:ILE:HG21	1:A:342:ILE:CG1	2.46	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
1:C:183:ILE:HG12	1:C:193:CYS:HB3	1.98	0.44
2:F:285:ILE:HD13	2:F:295:SER:HB2	2.00	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
2:E:264:MET:HG2	2:E:265:PRO:O	2.17	0.44
1:B:462:SER:HA	1:B:465:ARG:HH12	1.75	0.44
1:A:495:LYS:HB3	1:A:496:LYS:H	1.58	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:A:475:ILE:O	1:A:479:GLY:HA3	2.18	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
2:E:419:LYS:CE	2:E:450:GLY:HA3	2.43	0.44
2:F:441:LEU:HD21	2:F:456:VAL:HG13	1.99	0.44
2:F:192:TYR:O	2:F:196:LYS:HB3	2.17	0.44
2:D:315:PHE:HA	2:D:318:LEU:HD22	1.99	0.44
1:C:181:ASP:OD1	1:C:425:HIS:HA	2.17	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:A:298:LEU:HD21	1:A:337:ILE:CG2	2.47	0.44
2:E:411:GLU:CD	2:E:417:PRO:HB3	2.38	0.44
2:D:411:GLU:CD	2:D:417:PRO:HB3	2.38	0.44
1:A:142:VAL:CG1	1:A:160:GLY:HA3	2.48	0.44
2:D:177:VAL:O	2:D:242:LEU:HA	2.18	0.44
1:B:99:VAL:HG11	1:B:248:TYR:HB2	1.99	0.44
2:E:218:ARG:O	2:E:221:VAL:HG12	2.17	0.44
2:E:85:THR:O	2:E:205:SER:HB3	2.17	0.44
1:B:176:THR:O	1:B:180:ILE:HG12	2.17	0.44
2:F:307:THR:HG23	2:F:307:THR:O	2.16	0.44
1:A:232:ALA:N	1:A:233:PRO:CD	2.81	0.44
3:G:11[B]:ILE:HD11	3:G:259[B]:LEU:O	2.18	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
2:D:379:ILE:HD11	3:G:17[C]:THR:HG22	1.96	0.44
2:F:165:ILE:HG21	2:F:200:VAL:HG13	2.00	0.44
1:B:183:ILE:HG12	1:B:193:CYS:HB3	2.00	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:45[A]:TYR:HE1	4:H:9[A]:VAL:HG12	1.83	0.44
3:G:79[B]:MET:HG3	3:G:116[B]:PHE:CB	2.46	0.44
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
1:A:440:VAL:CG2	1:A:441:THR:N	2.81	0.44
1:B:95:MET:O	1:B:128:PRO:HA	2.17	0.44
2:E:288:THR:O	2:E:291:GLY:HA2	2.17	0.44
1:A:448:ILE:HG23	1:A:449:PRO:CD	2.48	0.44
1:A:389:TYR:CD1	1:A:413:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HG12	1:A:84:GLU:HA	1.99	0.44
2:D:12:PRO:HD2	2:D:260:LEU:CD2	2.48	0.44
2:F:329:ALA:C	2:F:331:MET:H	2.20	0.44
2:D:366:VAL:HG21	2:D:434:LEU:CD2	2.48	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:415:ARG:NH1	1:B:415:ARG:CG	2.49	0.44
1:C:71:VAL:HG23	2:D:66:ARG:NH2	2.32	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
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: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:261[C]:LEU:HD12	3:G:262[C]:GLN:N	2.33	0.43
3:G:148[B]:GLU:HG2	3:G:149[B]:ILE:HG23	2.00	0.43
4:H:23[B]:VAL:HG22	4:H:52[B]:ILE:HG22	2.00	0.43
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: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:C:95:MET:O	1:C:128:PRO:HA	2.18	0.43
2:F:419:LYS:CE	2:F:450:GLY:HA3	2.43	0.43
2:E:164:LEU:HD12	2:E:164:LEU:HA	1.82	0.43
3:G:127[C]:LYS:C	3:G:127[C]:LYS:HD3	2.39	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
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:B:462:SER:CB	1:B:465:ARG:HH12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:356:HIS:C	2:E:356:HIS:CD2	2.91	0.43
1:C:194:ILE:HD13	1:C:222:ILE:HD12	2.00	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: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
3:G:5[A]:ARG:HH11	3:G:5[A]:ARG:CB	2.30	0.43
3:G:48[C]:LYS:CD	4:H:78[C]:LEU:HD22	2.34	0.43
1:A:151:LYS:HD2	1:A:419:ILE:O	2.19	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
1:B:114:PRO:HG3	1:B:121:ILE:CD1	2.48	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
4:H:55[C]:GLY:O	4:H:56[C]:ASP:HB2	2.18	0.43
3:G:33[B]:ARG:HG2	3:G:34[B]:ARG:N	2.33	0.43
2:E:264:MET:HB2	2:E:264:MET:HE2	1.75	0.43
1:C:460:LEU:O	1:C:463:PHE:HB3	2.17	0.43
1:B:284:GLU:HG3	1:B:329:TYR:CD2	2.49	0.43
1:B:137:MET:HG3	2:F:98:ASP:HA	1.98	0.43
1:C:113:GLN:HA	1:C:114:PRO:HD3	1.79	0.43
2:F:288:THR:HG23	2:F:291:GLY:N	2.32	0.43
1:B:187:LYS:C	1:B:189:GLN:HG2	2.39	0.43
1:B:431:GLU:HB2	1:B:472:LEU:HD22	2.00	0.43
1:A:271:ARG:HH11	1:A:285:ALA:HB1	1.83	0.43
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.84	0.43
2:F:223:LEU:HD12	2:F:223:LEU:HA	1.79	0.43
2:D:192:TYR:O	2:D:196:LYS:HB3	2.19	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
4:H:96[B]:ALA:HA	4:H:99[B]:ARG:HB2	2.01	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:E:86:LEU:HD11	2:E:175:LEU:HD13	2.00	0.43
2:D:325:GLU:HG3	2:D:338:ASP:HB2	1.99	0.43
2:F:147:ILE:HA	2:F:320:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:132:ILE:HG12	2:E:132:ILE:H	1.47	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:B:95:MET:HB2	1:B:95:MET:HE3	1.76	0.43
1:A:95:MET:O	1:A:128:PRO:HA	2.19	0.43
1:C:480:GLU:HG3	1:C:482:PRO:HD3	2.00	0.43
2:F:254:GLY:HA3	2:F:271:GLN:NE2	2.33	0.43
1:B:233:PRO:O	1:B:237:LEU:HG	2.18	0.43
1:B:144:GLU:O	1:B:161:ARG:HG3	2.19	0.43
1:A:262:ASP:OD1	1:A:264:SER:HB2	2.18	0.43
1:A:113:GLN:HA	1:A:114:PRO:HD3	1.80	0.43
2:F:324:LEU:HD12	2:F:324:LEU:HA	1.81	0.43
1:C:31:VAL:HG12	1:C:84:GLU:HA	2.01	0.43
2:F:373:LEU:HA	2:F:376:ILE:HG12	2.01	0.43
2:F:118:PHE:HA	2:F:121:LEU:HD22	2.01	0.43
2:D:296:ILE:N	2:D:296:ILE:HD12	2.34	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:B:156:MET:SD	1:B:359:VAL:HG11	2.58	0.43
2:E:291:GLY:O	2:E:292:SER:CB	2.65	0.43
2:D:233:ARG:CD	2:D:292:SER:HB3	2.49	0.43
2:F:356:HIS:CD2	2:F:356:HIS:C	2.92	0.43
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.87	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: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
3:G:80[C]:VAL:HG11	3:G:126[C]:PHE:CZ	2.53	0.43
4:H:47[B]:THR:HG21	4:H:122[B]:GLU:CB	2.43	0.43
1:A:491:ILE:HG22	1:A:495:LYS:HG3	2.00	0.43
2:F:26:ILE:O	2:F:27:TYR:HB2	2.19	0.43
1:B:44:LEU:O	1:B:47:VAL:HG22	2.19	0.43
1:A:44:LEU:HA	1:A:44:LEU:HD23	1.78	0.43
1:B:140:LYS:NZ	1:B:143:HIS:CE1	2.87	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
1:A:271:ARG:HH11	1:A:285:ALA:CB	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ALA:HA	2:D:267:ALA:HB3	2.01	0.43
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:B:411:ASN:HD22	1:B:411:ASN:HA	1.59	0.42
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: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: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
2:F:91:ASN:ND2	2:F:91:ASN:H	2.17	0.42
1:C:121:ILE:HG22	1:C:123:THR:HG22	2.02	0.42
2:D:91:ASN:ND2	2:D:91:ASN:H	2.17	0.42
2:D:218:ARG:O	2:D:221:VAL:HG12	2.19	0.42
1:C:46:LYS:HZ2	1:C:46:LYS:HB2	1.85	0.42
2:D:371:ASN:HB3	3:G:10[C]:ARG:HD2	2.02	0.42
3:G:104[C]:GLU:CA	3:G:107[C]:HIS:HD1	2.28	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:462:SER:HA	1:A:465:ARG:HH12	1.69	0.42
1:A:440:VAL:HG22	1:A:441:THR:N	2.34	0.42
1:C:431:GLU:HB2	1:C:472:LEU:HD22	2.02	0.42
1:B:161:ARG:HH12	1:B:190:ASP:CB	2.30	0.42
2:F:288:THR:O	2:F:291:GLY:HA2	2.19	0.42
1:A:194:ILE:HD13	1:A:222:ILE:HD12	2.01	0.42
2:F:372:ASP:O	2:F:376:ILE:HG12	2.19	0.42
2:F:258:SER:OG	2:F:263:ARG:HB2	2.19	0.42
2:E:367:LEU:HD21	2:E:399:ILE:HG22	2.01	0.42
2:E:329:ALA:C	2:E:331:MET:H	2.22	0.42
2:D:258:SER:OG	2:D:263:ARG:HB2	2.18	0.42
3:G:15[B]:LYS:HG3	3:G:256[B]:LEU:CD1	2.47	0.42
3:G:107[C]:HIS:HB2	3:G:113[C]:TYR:CE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:51[B]:ARG:NE	4:H:60[B]:LEU:HD21	2.32	0.42
1:C:419:ILE:HD13	1:C:440:VAL:CG1	2.49	0.42
1:A:480:GLU:HG3	1:A:482:PRO:CD	2.49	0.42
1:B:481:LEU:C	1:B:481:LEU:HD22	2.39	0.42
2:E:142:ALA:CB	2:E:346:ILE:HD13	2.46	0.42
1:C:140:LYS:NZ	1:C:143:HIS:CE1	2.86	0.42
1:A:110:PRO:HG3	1:A:238:ALA:HA	2.01	0.42
1:A:99:VAL:HG13	1:A:248:TYR:CG	2.54	0.42
1:A:189:GLN:HE22	1:A:220:TYR:HB3	1.85	0.42
1:C:194:ILE:CD1	1:C:222:ILE:HD12	2.49	0.42
3:G:18[B]:ARG:HG2	3:G:18[B]:ARG:O	2.18	0.42
3:G:82[A]:THR:HG21	3:G:122[A]:GLY:HA3	2.01	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
2:D:264:MET:HE2	2:D:264:MET:HB2	1.71	0.42
1:B:492:GLU:CA	1:B:495:LYS:HB2	2.33	0.42
1:A:475:ILE:HA	1:A:479:GLY:HA2	2.00	0.42
1:B:66:LEU:HD12	2:F:9:VAL:CB	2.42	0.42
2:F:137:LEU:CG	2:F:138:LEU:HD13	2.47	0.42
2:E:91:ASN:C	2:E:91:ASN:ND2	2.73	0.42
2:F:42:VAL:HG12	2:F:57:ALA:HA	2.02	0.42
3:G:8[B]:LYS:CD	3:G:263[B]:PHE:CE1	3.00	0.42
3:G:78[B]:TYR:O	3:G:116[B]:PHE:HD2	2.02	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:171:ARG:NH1	1:A:171:ARG:HG3	2.13	0.42
1:A:365:ARG:NH2	2:E:186:ARG:HH22	2.01	0.42
1:B:440:VAL:HG12	1:B:445:MET:HE2	2.02	0.42
1:B:471:LEU:HD21	1:B:486:GLU:OE1	2.20	0.42
1:A:91:THR:HG22	1:A:93:ARG:CG	2.49	0.42
1:B:46:LYS:HB2	1:B:46:LYS:HZ3	1.84	0.42
3:G:217[A]:LEU:HG	3:G:218[A]:LEU:N	2.34	0.42
1:B:113:GLN:HA	1:B:114:PRO:HD3	1.85	0.42
2:D:164:LEU:HA	2:D:164:LEU:HD12	1.75	0.42
1:B:194:ILE:CD1	1:B:222:ILE:HD12	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:B:275:LEU:CD1	2:E:264:MET:HG3	2.50	0.42
2:F:89:VAL:HG23	2:F:97:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:411:GLU:CD	2:F:417:PRO:HB3	2.40	0.42
1:B:187:LYS:O	1:B:189:GLN:HG2	2.19	0.42
1:A:271:ARG:NH1	1:A:285:ALA:HB3	2.35	0.42
2:D:93:LEU:HA	2:D:93:LEU:HD12	1.73	0.42
2:F:178:PHE:CZ	2:F:245:ASP:HB2	2.54	0.42
3:G:169[A]:THR:HG23	3:G:186[A]:LYS:O	2.20	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:C:483:ASP:O	1:C:486:GLU:HB3	2.19	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
2:D:235:ARG:O	2:D:237:GLY:N	2.52	0.42
3:G:191[C]:LEU:HD12	3:G:191[C]:LEU:HA	1.86	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:43[C]:ARG:O	3:G:44[C]:PRO:C	2.58	0.42
1:A:480:GLU:HG3	1:A:482:PRO:HD3	2.01	0.42
3:G:249[B]:THR:O	3:G:250[B]:ASP:C	2.57	0.42
2:D:239:ASP:HA	2:D:292:SER:HA	2.02	0.42
1:C:271:ARG:HH11	1:C:285:ALA:CB	2.33	0.42
1:B:271:ARG:NH1	1:B:285:ALA:HB1	2.34	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
1:B:319:ILE:HD13	1:B:319:ILE:HA	1.74	0.42
2:D:412:GLN:HE21	2:D:412:GLN:HB2	1.52	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
2:D:86:LEU:HD11	2:D:175:LEU:HD13	2.02	0.42
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.78	0.42
1:A:499:THR:N	1:A:500:PRO:CD	2.78	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:B:187:LYS:O	1:B:189:GLN:CG	2.68	0.42
1:C:232:ALA:N	1:C:233:PRO:CD	2.83	0.42
2:D:42:VAL:HG12	2:D:57:ALA:HA	2.02	0.42
1:B:166:LEU:HB3	1:B:341:GLN:HB3	2.01	0.42
3:G:81[C]:ILE:HA	3:G:118[C]:VAL:HG13	2.02	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
4:H:117[C]:HIS:HA	4:H:120[C]:ALA:CB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:264:MET:HG2	2:D:265:PRO:C	2.40	0.41
1:B:275:LEU:C	1:B:278:ARG:H	2.24	0.41
1:C:354:ARG:NH1	1:C:354:ARG:HG2	2.23	0.41
1:C:440:VAL:HG22	1:C:441:THR:N	2.35	0.41
3:G:217[B]:LEU:HG	3:G:218[B]:LEU:N	2.35	0.41
2:E:91:ASN:H	2:E:91:ASN:ND2	2.17	0.41
2:E:242:LEU:O	2:E:295:SER:HA	2.20	0.41
1:C:271:ARG:NH1	1:C:285:ALA:HB3	2.35	0.41
1:B:191:VAL:HA	1:B:255:HIS:O	2.20	0.41
3:G:18[C]:ARG:HH12	3:G:253[C]:THR:CB	2.33	0.41
3:G:167[A]:LYS:N	3:G:167[A]:LYS:HD2	2.35	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:B:460:LEU:HG	1:B:494:PHE:CE2	2.55	0.41
1:A:284:GLU:HG3	1:A:329:TYR:CD1	2.52	0.41
1:C:109:ASN:HB2	1:C:110:PRO:CD	2.49	0.41
2:D:233:ARG:HB2	2:D:292:SER:CB	2.50	0.41
1:A:386:LEU:HA	1:A:389:TYR:HB3	2.02	0.41
2:F:107:GLU:CD	2:F:235:ARG:HH12	2.23	0.41
1:C:167:ILE:O	1:C:318:PHE:HA	2.20	0.41
1:A:236:TYR:HE1	1:A:293:LEU:CD1	2.34	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
4:H:22[C]:ILE:CG1	4:H:53[C]:LYS:HD2	2.47	0.41
1:A:275:LEU:HA	1:A:278:ARG:HA	2.02	0.41
1:B:440:VAL:HG12	1:B:445:MET:HE3	2.02	0.41
2:F:423:VAL:O	2:F:424:LYS:C	2.58	0.41
2:F:416:MET:CE	2:F:416:MET:HA	2.50	0.41
2:F:233:ARG:CD	2:F:292:SER:HB3	2.50	0.41
1:B:121:ILE:HG22	1:B:123:THR:HG22	2.02	0.41
1:A:217:ALA:HA	1:A:220:TYR:CE2	2.56	0.41
2:D:24:PRO:HD2	2:D:53:VAL:HG11	2.01	0.41
2:F:93:LEU:HA	2:F:93:LEU:HD12	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HD11	1:A:316:LEU:HD13	2.03	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:275:LEU:C	1:C:278:ARG:H	2.24	0.41
2:F:291:GLY:O	2:F:292:SER:CB	2.68	0.41
2:E:397:ARG:NH1	2:E:443:GLU:OE2	2.53	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
1:B:65:ASN:HB3	2:F:10:MET:CE	2.49	0.41
2:E:93:LEU:HD12	2:E:93:LEU:HA	1.59	0.41
3:G:99[B]:VAL:CG2	3:G:100[B]:SER:N	2.82	0.41
3:G:184[B]:VAL:HG21	3:G:186[B]:LYS:HE3	2.03	0.41
3:G:83[C]:SER:O	3:G:121[C]:LYS:HB2	2.21	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
2:E:270:TYR:CZ	2:E:310:ALA:HB2	2.55	0.41
1:C:330:ILE:HB	1:C:331:PRO:HD3	2.01	0.41
3:G:17[B]:THR:O	3:G:17[B]:THR:CG2	2.67	0.41
1:C:389:TYR:CD1	1:C:413:GLY:HA3	2.54	0.41
2:F:241:LEU:O	2:F:242:LEU:HB3	2.20	0.41
2:E:118:PHE:HA	2:E:121:LEU:HD22	2.02	0.41
1:C:477:GLN:O	1:C:478:THR:C	2.59	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
3:G:79[B]:MET:HB2	3:G:168[B]:LEU:HD21	2.01	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
1:A:464:MET:HE2	1:A:464:MET:HB3	1.90	0.41
1:C:275:LEU:N	2:F:264:MET:HE1	2.34	0.41
1:A:498:PHE:CD1	1:A:499:THR:HG22	2.55	0.41
2:E:411:GLU:HA	2:E:415:GLY:HA2	2.02	0.41
2:E:288:THR:HG23	2:E:291:GLY:N	2.35	0.41
2:D:241:LEU:O	2:D:294:THR:O	2.38	0.41
2:F:241:LEU:HA	2:F:241:LEU:HD12	1.59	0.41
1:C:271:ARG:HH11	1:C:285:ALA:HB1	1.86	0.41
2:F:296:ILE:N	2:F:296:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32[C]:LEU:HD12	3:G:234[C]:LYS:C	2.41	0.41
4:H:109[A]:LYS:HB2	4:H:109[A]:LYS:HE3	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: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
3:G:192[B]:THR:O	3:G:193[B]:SER:C	2.59	0.41
1:C:69:ASP:N	1:C:69:ASP:OD1	2.53	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:275:LEU:CB	2:D:264:MET:CG	2.94	0.41
1:B:459:GLU:HA	1:B:462:SER:OG	2.21	0.41
1:C:460:LEU:HG	1:C:494:PHE:CE2	2.55	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:B:438:TYR:HA	1:B:441:THR:CG2	2.45	0.41
1:A:94:ILE:HG13	1:A:94:ILE:H	1.59	0.41
1:C:140:LYS:HB3	1:C:305:SER:HA	2.03	0.41
2:D:181:VAL:HG22	2:D:221:VAL:CG1	2.49	0.41
2:F:366:VAL:HG21	2:F:434:LEU:CD2	2.51	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
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: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:308:ASP:C	2:D:311:PRO:HD2	2.40	0.41
2:F:308:ASP:C	2:F:311:PRO:HD2	2.41	0.41
1:C:144:GLU:O	1:C:161:ARG:HG3	2.21	0.41
2:D:125:ASP:CG	2:D:345:ARG:NH2	2.72	0.41
2:D:149:LEU:CD2	2:D:324:LEU:HD22	2.51	0.41
2:E:395:ARG:NH2	2:E:436:GLY:CA	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:VAL:HG12	2:D:241:LEU:N	2.36	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:325:GLU:CG	2:E:338:ASP:HB2	2.51	0.41
1:B:206:ALA:HA	2:E:118:PHE:CZ	2.56	0.41
2:E:92:VAL:HG11	2:E:220:ARG:HB2	2.03	0.41
1:A:477:GLN:O	1:A:478:THR:C	2.58	0.41
2:F:338:ASP:HB3	2:F:341:ALA:HB3	2.03	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:B:62:MET:HE3	1:B:95:MET:HE3	2.03	0.41
2:D:268:VAL:CG2	2:D:268:VAL:O	2.67	0.41
2:E:419:LYS:HA	2:E:419:LYS:HD2	1.88	0.41
1:B:91:THR:HG22	1:B:93:ARG:CG	2.50	0.41
1:A:161:ARG:HH12	1:A:190:ASP:CB	2.29	0.41
2:D:77:ILE:O	2:D:111:ILE:HG23	2.20	0.41
3:G:12[B]:ARG:CZ	3:G:12[B]:ARG:CB	2.99	0.41
1:C:497:GLY:O	1:C:498:PHE:CG	2.74	0.41
3:G:261[C]:LEU:CD1	3:G:262[C]:GLN:HG3	2.48	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: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:419:ILE:HD13	1:A:440:VAL:CG1	2.51	0.40
1:C:491:ILE:HG22	1:C:495:LYS:HG3	2.02	0.40
1:C:161:ARG:HH12	1:C:190:ASP:CB	2.30	0.40
2:D:411:GLU:HA	2:D:415:GLY:HA2	2.02	0.40
2:D:319:ASP:OD2	2:D:345:ARG:HD3	2.21	0.40
1:C:386:LEU:HA	1:C:389:TYR:HB3	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: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
1:A:459:GLU:HA	1:A:462:SER:OG	2.20	0.40
1:C:83:ARG:CB	2:F:47:HIS:CE1	2.88	0.40
2:F:86:LEU:HD11	2:F:175:LEU:HD13	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:264:MET:HG2	2:E:265:PRO:C	2.41	0.40
1:A:284:GLU:HG3	1:A:329:TYR:CD2	2.52	0.40
1:C:471:LEU:HD21	1:C:486:GLU:OE1	2.21	0.40
1:B:475:ILE:HA	1:B:479:GLY:HA2	2.03	0.40
2:F:27:TYR:HB3	2:F:112:HIS:CD2	2.57	0.40
2:F:235:ARG:HD3	2:F:235:ARG:HA	1.89	0.40
2:F:319:ASP:OD2	2:F:345:ARG:HD3	2.22	0.40
2:E:79:VAL:HA	2:E:80:PRO:HD3	1.95	0.40
1:B:477:GLN:O	1:B:478:THR:C	2.60	0.40
2:F:431:LYS:HE3	2:F:435:GLU:OE2	2.20	0.40
3:G:255[C]:MET:HA	3:G:258[C]:THR:CG2	2.50	0.40
3:G:176[C]:VAL:CG1	3:G:177[C]:SER:N	2.76	0.40
3:G:179[B]:ILE:HG23	3:G:179[B]:ILE:O	2.21	0.40
3:G:91[B]:TYR:O	3:G:92[B]:ASN:HB2	2.20	0.40
1:A:460:LEU:O	1:A:463:PHE:HB3	2.20	0.40
1:C:450:VAL:C	1:C:452:ASP:H	2.25	0.40
1:C:44:LEU:HA	1:C:44:LEU:HD23	1.79	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
1:B:142:VAL:CG1	1:B:160:GLY:HA3	2.52	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
2:F:264:MET:HG2	2:F:265:PRO:C	2.42	0.40
1:C:481:LEU:C	1:C:481:LEU:HD22	2.42	0.40
1:B:31:VAL:HG12	1:B:84:GLU:HA	2.04	0.40
2:D:273:THR:O	2:D:277:GLU:HG3	2.22	0.40
1:A:483:ASP:O	1:A:486:GLU:HB3	2.21	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%)	9	35
1	B	472/502 (94%)	417 (88%)	44 (9%)	11 (2%)	8	32
1	C	472/502 (94%)	417 (88%)	44 (9%)	11 (2%)	8	32
2	D	459/462 (99%)	406 (88%)	44 (10%)	9 (2%)	9	36
2	E	459/462 (99%)	408 (89%)	43 (9%)	8 (2%)	11	41
2	F	459/462 (99%)	407 (89%)	43 (9%)	9 (2%)	9	36
3	G	663/286 (232%)	468 (71%)	141 (21%)	54 (8%)	1	5
4	H	399/135 (296%)	294 (74%)	78 (20%)	27 (7%)	1	8
All	All	3855/3313 (116%)	3235 (84%)	481 (12%)	139 (4%)	6	22

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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Mol	Chain	Res	Type
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%)	9	32
1	B	388/413 (94%)	347 (89%)	41 (11%)	8	30
1	C	388/413 (94%)	349 (90%)	39 (10%)	9	32
2	D	375/376 (100%)	335 (89%)	40 (11%)	8	30
2	E	375/376 (100%)	336 (90%)	39 (10%)	9	31
2	F	375/376 (100%)	336 (90%)	39 (10%)	9	31
3	G	576/239 (241%)	507 (88%)	69 (12%)	6	23
4	H	339/113 (300%)	324 (96%)	15 (4%)	35	70
All	All	3204/2719 (118%)	2883 (90%)	321 (10%)	9	32

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%)	1.26	89 (18%) 2 0	44, 69, 152, 234	0
1	B	474/502 (94%)	1.10	78 (16%) 2 1	38, 61, 167, 246	0
1	C	474/502 (94%)	1.12	77 (16%) 3 1	45, 67, 128, 185	0
2	D	461/462 (99%)	1.07	69 (14%) 3 1	43, 76, 129, 174	0
2	E	461/462 (99%)	0.64	34 (7%) 17 6	36, 55, 113, 170	0
2	F	461/462 (99%)	0.90	52 (11%) 7 2	40, 62, 124, 173	0
3	G	227/286 (79%)	1.49	53 (23%) 1 0	10, 51, 103, 140	0
4	H	135/135 (100%)	4.80	128 (94%) 0 0	82, 133, 194, 213	0
All	All	3167/3313 (95%)	1.21	580 (18%) 2 1	10, 66, 144, 246	0

All (580) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	LYS	17.8
4	H	47[A]	THR	14.8
4	H	100[A]	HIS	12.6
1	A	497	GLY	12.5
1	A	500	PRO	12.1
2	F	462	LEU	11.8
4	H	59[A]	THR	11.7
1	B	446	ASP	10.8
1	B	497	GLY	10.6
1	B	500	PRO	10.3
1	C	499	THR	10.3
4	H	90[A]	VAL	9.8
4	H	27[A]	GLY	9.2
4	H	70[A]	VAL	8.4
1	C	400	SER	8.0
4	H	99[A]	ARG	8.0

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Mol	Chain	Res	Type	RSRZ
4	H	108[A]	ASP	8.0
3	G	266[A]	ALA	7.7
4	H	132[A]	ASN	7.7
1	A	489	ALA	7.6
1	B	400	SER	7.5
4	H	2[A]	ALA	7.4
4	H	23[A]	VAL	7.3
4	H	93[A]	ALA	7.3
4	H	111[A]	ASP	7.3
1	B	409	LYS	7.2
4	H	5[A]	GLN	7.2
4	H	58[A]	GLU	7.1
4	H	75[A]	VAL	7.1
1	C	188	GLY	7.0
1	A	463	PHE	7.0
4	H	109[A]	LYS	7.0
4	H	124[A]	ALA	6.9
4	H	1[A]	MET	6.8
1	C	490	ALA	6.8
1	A	483	ASP	6.7
4	H	102[A]	THR	6.7
4	H	128[A]	LEU	6.6
1	A	496	LYS	6.6
1	A	447	ASP	6.5
4	H	3[A]	THR	6.3
4	H	101[A]	GLU	6.3
1	A	406	THR	6.3
1	A	482	PRO	6.3
4	H	114[A]	TYR	6.3
4	H	30[A]	GLY	6.2
4	H	54[A]	GLN	6.2
4	H	9[A]	VAL	6.2
1	C	399	GLY	6.2
1	A	452	ASP	6.2
4	H	51[A]	ARG	6.2
4	H	129[A]	GLN	6.1
1	A	408	ALA	6.1
1	A	484	THR	6.1
4	H	84[A]	LEU	6.0
4	H	73[A]	ASP	6.0
3	G	107[A]	HIS	6.0
4	H	60[A]	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
4	H	133[A]	SER	6.0
1	A	495	LYS	6.0
1	A	189	GLN	5.9
4	H	17[A]	GLN	5.9
4	H	126[A]	VAL	5.8
4	H	48[A]	ALA	5.8
2	D	443	GLU	5.8
1	B	387	ALA	5.8
4	H	41[A]	LEU	5.8
4	H	74[A]	LYS	5.8
2	E	387	ASP	5.8
4	H	107[A]	LEU	5.7
4	H	20[A]	ALA	5.7
1	C	408	ALA	5.7
4	H	110[A]	THR	5.6
2	D	416	MET	5.6
4	H	28[A]	VAL	5.6
4	H	103[A]	ILE	5.6
4	H	81[A]	THR	5.5
1	B	465	ARG	5.5
3	G	108[A]	GLN	5.5
3	G	76[A]	THR	5.4
4	H	98[A]	ALA	5.4
4	H	117[A]	HIS	5.4
2	F	446	PHE	5.4
1	A	488	ASP	5.4
4	H	40[A]	PRO	5.3
1	C	498	PHE	5.3
2	F	386	SER	5.3
4	H	131[A]	ALA	5.3
2	E	383	ASP	5.3
4	H	33[A]	GLY	5.2
1	B	410	LEU	5.2
4	H	113[A]	ASP	5.2
2	D	450	GLY	5.2
4	H	29[A]	GLU	5.2
1	C	483	ASP	5.2
1	A	405	ALA	5.1
4	H	65[A]	GLY	5.1
4	H	104[A]	LEU	5.1
1	C	403	ASP	5.1
1	A	457	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
4	H	127[A]	ARG	5.1
4	H	92[A]	ARG	5.0
4	H	134[A]	LYS	5.0
4	H	55[A]	GLY	5.0
4	H	91[A]	GLU	5.0
1	A	306	ASP	5.0
2	D	462	LEU	5.0
4	H	19[A]	GLU	4.9
2	E	382	MET	4.9
1	A	403	ASP	4.9
1	A	387	ALA	4.9
4	H	79[A]	ALA	4.9
1	C	444	PHE	4.9
1	B	448	ILE	4.9
4	H	52[A]	ILE	4.9
3	G	109[A]	SER	4.9
2	D	81	VAL	4.8
1	C	402	LEU	4.8
1	B	368	GLY	4.8
3	G	132[A]	PRO	4.8
4	H	85[A]	PRO	4.8
1	B	399	GLY	4.8
1	C	470	SER	4.8
1	B	449	PRO	4.7
1	B	445	MET	4.7
4	H	121[A]	LEU	4.7
1	B	441	THR	4.7
1	A	404	LYS	4.7
3	G	5[A]	ARG	4.7
1	B	499	THR	4.7
2	F	291	GLY	4.7
1	C	397	GLN	4.6
2	F	267	ALA	4.6
2	E	381	GLY	4.6
4	H	63[A]	VAL	4.6
2	D	21	GLY	4.6
4	H	49[A]	PRO	4.6
4	H	36[A]	ALA	4.5
4	H	64[A]	SER	4.5
4	H	72[A]	PRO	4.5
4	H	87[A]	GLU	4.5
2	E	34	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
4	H	135[A]	SER	4.5
1	C	377	LYS	4.5
1	B	485	LYS	4.5
1	B	455	ARG	4.5
2	D	103	VAL	4.5
1	B	452	ASP	4.5
2	F	383	ASP	4.5
1	B	498	PHE	4.4
1	B	401	ASP	4.4
1	B	447	ASP	4.4
3	G	147[A]	THR	4.4
1	A	492	GLU	4.4
4	H	4[A]	VAL	4.4
4	H	71[A]	ARG	4.4
1	B	403	ASP	4.4
4	H	37[A]	GLY	4.4
4	H	88[A]	ILE	4.4
1	A	442	ASN	4.4
1	A	305	SER	4.4
1	B	495	LYS	4.4
4	H	56[A]	ASP	4.3
3	G	261[A]	LEU	4.3
2	D	34	ARG	4.3
2	E	415	GLY	4.3
4	H	118[A]	LYS	4.3
1	A	443	GLY	4.2
4	H	62[A]	ALA	4.2
2	D	461	LYS	4.2
2	F	380	LEU	4.2
4	H	43[A]	THR	4.2
3	G	4[A]	MET	4.2
2	D	449	VAL	4.2
4	H	11[A]	PRO	4.2
4	H	46[A]	LYS	4.2
1	B	280	PRO	4.2
4	H	106[A]	ARG	4.1
1	B	461	LEU	4.1
2	E	416	MET	4.1
1	A	409	LYS	4.0
1	B	488	ASP	4.0
2	D	102	GLU	4.0
4	H	8[A]	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	453	VAL	4.0
2	D	455	ALA	4.0
2	F	373	LEU	4.0
4	H	82[A]	ALA	4.0
1	A	491	ILE	3.9
4	H	80[A]	ASP	3.9
2	D	292	SER	3.9
1	A	45	GLU	3.9
2	E	417	PRO	3.9
4	H	21[A]	ASP	3.9
1	B	408	ALA	3.9
4	H	115[A]	LEU	3.9
2	F	389	ASP	3.9
1	C	478	THR	3.9
4	H	89[A]	ASP	3.9
3	G	74[A]	LYS	3.9
1	B	444	PHE	3.8
4	H	31[A]	GLU	3.8
1	A	391	GLU	3.8
1	C	489	ALA	3.8
2	F	382	MET	3.8
4	H	76[A]	ASN	3.8
4	H	7[A]	ASP	3.8
2	F	123	THR	3.8
2	D	332	GLY	3.8
1	C	411	ASN	3.7
4	H	105[A]	LYS	3.7
4	H	18[A]	GLY	3.7
2	F	448	MET	3.7
2	F	443	GLU	3.7
2	F	51	ASN	3.7
4	H	26[A]	ARG	3.7
2	F	292	SER	3.7
4	H	24[A]	ILE	3.7
1	B	457	GLU	3.6
2	E	373	LEU	3.6
1	C	385	ASP	3.6
4	H	12[A]	GLU	3.6
2	D	459	ALA	3.6
1	A	407	GLN	3.6
3	G	110[A]	LYS	3.6
4	H	32[A]	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	H	96[A]	ALA	3.6
2	F	384	GLU	3.6
1	C	190	ASP	3.6
2	E	166	ASN	3.6
2	F	334	TYR	3.5
1	B	479	GLY	3.5
1	C	406	THR	3.5
1	C	311	GLY	3.5
4	H	50[A]	VAL	3.5
2	D	381	GLY	3.5
4	H	122[A]	GLU	3.5
2	D	267	ALA	3.5
2	D	444	GLU	3.5
1	A	470	SER	3.5
1	A	464	MET	3.4
4	H	10[A]	THR	3.4
3	G	69[A]	GLU	3.4
1	A	467	ASN	3.4
1	A	413	GLY	3.4
1	B	463	PHE	3.4
4	H	69[A]	GLU	3.4
4	H	13[A]	ARG	3.4
4	H	14[A]	LYS	3.4
1	A	446	ASP	3.4
1	B	466	ALA	3.4
4	H	42[A]	VAL	3.3
4	H	83[A]	GLU	3.3
1	B	489	ALA	3.3
4	H	61[A]	ILE	3.3
1	A	485	LYS	3.3
1	A	460	LEU	3.3
4	H	6[A]	VAL	3.3
2	F	375	ASP	3.3
1	A	70	ASN	3.3
2	D	2	ASN	3.3
1	B	478	THR	3.3
2	D	305	ASP	3.3
2	E	412	GLN	3.3
1	C	442	ASN	3.2
1	C	386	LEU	3.2
2	F	290	LYS	3.2
1	A	392	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	483	ASP	3.2
1	B	305	SER	3.2
1	B	405	ALA	3.2
4	H	125[A]	GLU	3.2
3	G	73[A]	VAL	3.2
1	C	465	ARG	3.2
1	A	119	GLY	3.2
3	G	91[A]	TYR	3.2
1	C	407	GLN	3.2
2	D	297	GLN	3.2
2	E	197	ASP	3.2
2	E	377	ILE	3.2
2	E	378	ALA	3.2
1	C	496	LYS	3.2
1	C	189	GLN	3.1
1	B	456	PHE	3.1
1	B	474	HIS	3.1
2	D	330	GLU	3.1
2	E	388	GLU	3.1
3	G	263[A]	PHE	3.1
2	F	416	MET	3.1
4	H	67[A]	PHE	3.1
1	A	448	ILE	3.1
1	A	490	ALA	3.1
1	C	473	ASP	3.1
2	F	387	ASP	3.1
1	A	402	LEU	3.1
1	C	486	GLU	3.1
2	D	51	ASN	3.1
4	H	120[A]	ALA	3.1
4	H	123[A]	ARG	3.1
1	C	414	GLU	3.0
1	B	45	GLU	3.0
4	H	95[A]	LYS	3.0
1	B	469	ASP	3.0
1	A	478	THR	3.0
2	F	447	TYR	3.0
2	E	170	GLN	3.0
3	G	146[A]	LEU	3.0
2	D	417	PRO	3.0
1	A	410	LEU	3.0
2	D	329	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	382	MET	3.0
4	H	86[A]	GLU	3.0
1	B	493	GLU	3.0
1	A	219	ASP	3.0
2	D	20	SER	2.9
3	G	138[A]	THR	2.9
1	B	351	SER	2.9
1	A	388	GLN	2.9
1	C	449	PRO	2.9
3	G	264[A]	ASN	2.9
1	C	388	GLN	2.9
3	G	75[A]	LYS	2.9
1	B	487	LEU	2.9
1	A	327	SER	2.9
1	B	467	ASN	2.9
3	G	104[A]	GLU	2.9
2	D	94	GLY	2.9
1	B	460	LEU	2.9
1	C	310	GLY	2.9
4	H	77[A]	ILE	2.9
1	C	405	ALA	2.9
2	E	391	LEU	2.9
2	D	300	TYR	2.9
3	G	3[A]	GLY	2.9
2	E	99	GLU	2.8
2	E	385	LEU	2.8
1	A	499	THR	2.8
1	B	411	ASN	2.8
1	C	70	ASN	2.8
2	D	104	ASN	2.8
1	B	413	GLY	2.8
1	B	395	PHE	2.8
1	C	439	ALA	2.8
2	F	388	GLU	2.8
3	G	192[A]	THR	2.8
1	C	371	GLN	2.8
2	D	383	ASP	2.8
1	A	438	TYR	2.8
1	B	491	ILE	2.8
2	D	447	TYR	2.8
2	F	22	GLN	2.8
4	H	68[A]	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	441	THR	2.8
3	G	38[A]	THR	2.8
1	A	493	GLU	2.8
1	B	407	GLN	2.8
4	H	119[A]	ARG	2.8
1	B	398	PHE	2.8
4	H	116[A]	ARG	2.8
4	H	15[A]	VAL	2.7
2	D	5	ARG	2.7
2	D	445	ALA	2.7
2	E	196	LYS	2.7
4	H	34[A]	VAL	2.7
3	G	70[A]	ALA	2.7
2	E	330	GLU	2.7
3	G	112[A]	GLU	2.7
3	G	162[A]	ASP	2.7
1	B	122	GLU	2.7
1	A	66	LEU	2.7
1	B	414	GLU	2.7
1	C	488	ASP	2.7
2	F	377	ILE	2.7
3	G	111[A]	ASP	2.7
1	C	396	ALA	2.7
2	F	381	GLY	2.7
1	C	219	ASP	2.7
1	A	328	ALA	2.7
1	B	101	GLU	2.7
2	D	101	GLY	2.6
1	B	462	SER	2.6
3	G	151[A]	ASP	2.6
4	H	22[A]	ILE	2.6
4	H	94[A]	LYS	2.6
1	A	450	VAL	2.6
1	B	393	GLN	2.6
4	H	25[A]	ALA	2.6
1	C	45	GLU	2.6
1	A	285	ALA	2.6
2	D	328	LEU	2.6
1	C	243	CYS	2.6
3	G	77[A]	GLY	2.6
1	B	484	THR	2.6
2	D	293	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	414	GLU	2.6
2	F	429	GLY	2.6
2	D	333	ILE	2.6
2	E	374	GLN	2.6
2	D	204	THR	2.6
1	B	494	PHE	2.6
1	C	302	ALA	2.5
1	A	471	LEU	2.5
1	A	401	ASP	2.5
1	C	327	SER	2.5
3	G	265[A]	ARG	2.5
1	B	275	LEU	2.5
1	C	443	GLY	2.5
2	D	73	THR	2.5
2	D	438	HIS	2.5
3	G	72[A]	PRO	2.5
1	C	252	LYS	2.5
1	C	401	ASP	2.5
2	F	455	ALA	2.5
1	C	280	PRO	2.5
1	A	396	ALA	2.5
1	B	402	LEU	2.5
1	A	416	THR	2.5
1	C	493	GLU	2.5
2	F	461	LYS	2.5
2	E	153	ALA	2.5
3	G	64[A]	SER	2.5
3	G	193[A]	SER	2.5
2	D	418	GLY	2.5
1	A	390	ARG	2.5
4	H	112[A]	LYS	2.5
2	D	28	ASN	2.5
1	A	466	ALA	2.4
2	F	38	GLY	2.4
1	B	384	LEU	2.4
1	A	27	GLU	2.4
1	A	281	PRO	2.4
2	F	100	GLN	2.4
2	F	304	ASP	2.4
2	D	301	VAL	2.4
2	F	264	MET	2.4
3	G	65[A]	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	235	ARG	2.4
1	C	345	GLU	2.4
1	C	412	ARG	2.4
1	C	117	GLY	2.4
2	D	375	ASP	2.4
1	A	248	TYR	2.4
2	E	292	SER	2.4
2	F	348	SER	2.4
1	B	412	ARG	2.4
1	A	465	ARG	2.4
1	B	473	ASP	2.4
2	D	434	LEU	2.4
2	F	441	LEU	2.4
3	G	150[A]	GLN	2.4
1	B	91	THR	2.3
2	D	264	MET	2.3
1	A	304	LEU	2.3
1	A	162	GLY	2.3
2	F	307	THR	2.3
1	A	315	ALA	2.3
2	E	290	LYS	2.3
2	D	448	MET	2.3
2	E	375	ASP	2.3
2	F	25	ASP	2.3
2	D	122	SER	2.3
2	D	288	THR	2.3
2	F	174	GLY	2.3
2	F	52	VAL	2.3
4	H	53[A]	LYS	2.3
2	D	119	GLU	2.3
1	A	321	THR	2.3
2	F	410	ALA	2.3
1	A	44	LEU	2.3
3	G	47[A]	ASP	2.3
1	A	274	SER	2.3
1	B	390	ARG	2.3
3	G	154[A]	GLN	2.3
4	H	16[A]	PHE	2.3
1	C	384	LEU	2.3
1	B	470	SER	2.3
1	C	30	THR	2.3
2	D	255	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	445	MET	2.3
1	C	212	LEU	2.3
1	C	472	LEU	2.3
2	F	105	ALA	2.3
2	F	409	VAL	2.3
3	G	136[A]	GLU	2.3
2	D	231	TYR	2.3
1	A	494	PHE	2.3
1	C	332	THR	2.3
1	A	307	GLU	2.3
2	E	264	MET	2.3
1	A	481	LEU	2.2
2	F	82	GLY	2.2
3	G	238[A]	PHE	2.2
3	G	133[A]	VAL	2.2
1	C	305	SER	2.2
1	B	306	ASP	2.2
2	D	374	GLN	2.2
1	C	479	GLY	2.2
2	D	222	ALA	2.2
2	F	411	GLU	2.2
1	C	176	THR	2.2
1	A	43	GLY	2.2
1	B	327	SER	2.2
1	A	86	THR	2.2
1	A	297	LEU	2.2
1	B	454	ARG	2.2
2	E	20	SER	2.2
1	B	88	VAL	2.2
1	B	464	MET	2.2
2	D	281	LEU	2.2
2	E	386	SER	2.2
2	D	85	THR	2.2
3	G	99[A]	VAL	2.2
1	A	498	PHE	2.2
3	G	166[A]	ASP	2.2
2	D	446	PHE	2.2
2	F	49	GLY	2.2
2	D	344	SER	2.2
1	B	190	ASP	2.2
1	C	275	LEU	2.2
2	D	334	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	189	GLN	2.2
2	D	237	GLY	2.2
3	G	164[A]	THR	2.2
3	G	94[A]	ASN	2.2
1	B	289	ASP	2.2
1	C	101	GLU	2.1
3	G	103[A]	ILE	2.2
2	E	371	ASN	2.1
1	C	452	ASP	2.1
1	C	469	ASP	2.1
2	E	376	ILE	2.1
1	A	322	GLN	2.1
2	D	295	SER	2.1
2	D	296	ILE	2.1
2	D	415	GLY	2.1
2	F	332	GLY	2.1
4	H	44[A]	PRO	2.1
1	A	259	VAL	2.1
1	B	492	GLU	2.1
3	G	6[A]	GLU	2.1
1	C	124	ALA	2.1
2	F	122	SER	2.1
3	G	102[A]	THR	2.1
1	C	497	GLY	2.1
2	D	410	ALA	2.1
4	H	45[A]	LEU	2.1
1	C	216	ASP	2.1
1	C	217	ALA	2.1
2	D	123	THR	2.1
3	G	251[A]	ASN	2.1
1	C	193	CYS	2.1
4	H	38[A]	HIS	2.1
1	C	133	ALA	2.1
1	C	370	ALA	2.1
1	A	445	MET	2.1
1	C	169	GLY	2.1
2	D	317	HIS	2.1
2	E	193	HIS	2.1
2	F	67	GLY	2.1
1	A	345	GLU	2.1
1	A	389	TYR	2.1
1	A	480	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	404	LYS	2.1
2	F	106	GLU	2.1
1	A	437	ILE	2.0
2	F	444	GLU	2.0
1	C	259	VAL	2.0
1	C	477	GLN	2.0
3	G	71[A]	ARG	2.0
2	E	288	THR	2.0
2	D	436	GLY	2.0
1	C	63	ALA	2.0
1	A	126	TYR	2.0
2	D	362	GLY	2.0
3	G	114[A]	VAL	2.0
2	E	411	GLU	2.0
1	C	476	ARG	2.0
3	G	115[A]	ILE	2.0
2	F	104	ASN	2.0
3	G	260[A]	THR	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.