



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:30 am BST

PDB ID : 1OHH  
Title : BOVINE MITOCHONDRIAL F1-ATPASE complexed with the inhibitor protein IF1  
Authors : Cabezon, E.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2003-05-27  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

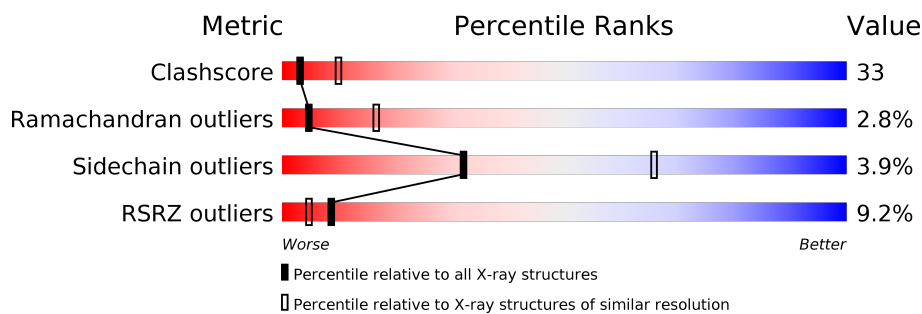
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	1-A	510	
1	1-B	510	
1	1-C	510	
1	2-A	510	
1	2-B	510	
1	2-C	510	
2	1-D	482	

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Mol	Chain	Length	Quality of chain
2	1-E	482	<div><div><div>18%</div><div>48%</div><div>45%</div><div></div><div></div></div></div>
2	1-F	482	<div><div><div>10%</div><div>49%</div><div>45%</div><div></div><div></div></div></div>
2	2-D	482	<div><div><div>9%</div><div>54%</div><div>39%</div><div></div><div></div></div></div>
2	2-E	482	<div><div><div>18%</div><div>48%</div><div>45%</div><div></div><div></div></div></div>
2	2-F	482	<div><div><div>10%</div><div>51%</div><div>43%</div><div></div><div></div></div></div>
3	1-G	272	<div><div><div>12%</div><div>18%</div><div>15%</div><div></div><div>65%</div></div></div>
3	2-G	272	<div><div><div>11%</div><div>22%</div><div>12%</div><div></div><div>65%</div></div></div>
4	1-H	84	<div><div><div>21%</div><div>11%</div><div>25%</div><div>8%</div><div>56%</div></div></div>
4	2-H	84	<div><div><div>27%</div><div>15%</div><div>33%</div><div></div><div>48%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45703 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	2-A	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	1-B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	2-B	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	1-C	488	Total	C	N	O	S	0	0	0
			3718	2341	656	709	12			
1	2-C	480	Total	C	N	O	S	0	0	0
			3661	2304	648	697	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-D	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			
2	2-D	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	1-E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	2-E	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	1-F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2-F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

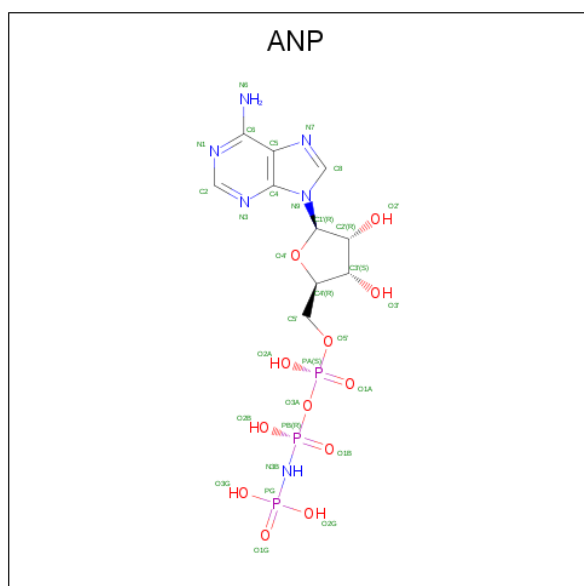
- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1-G	94	Total	C	N	O	S	0	0	0
			709	437	130	136	6			
3	2-G	94	Total	C	N	O	S	0	0	0
			717	444	129	138	6			

- Molecule 4 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	1-H	37	Total	C	N	O	0	0	0
			283	167	59	57			
4	2-H	44	Total	C	N	O	0	0	0
			336	202	69	65			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	1-A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	2-A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

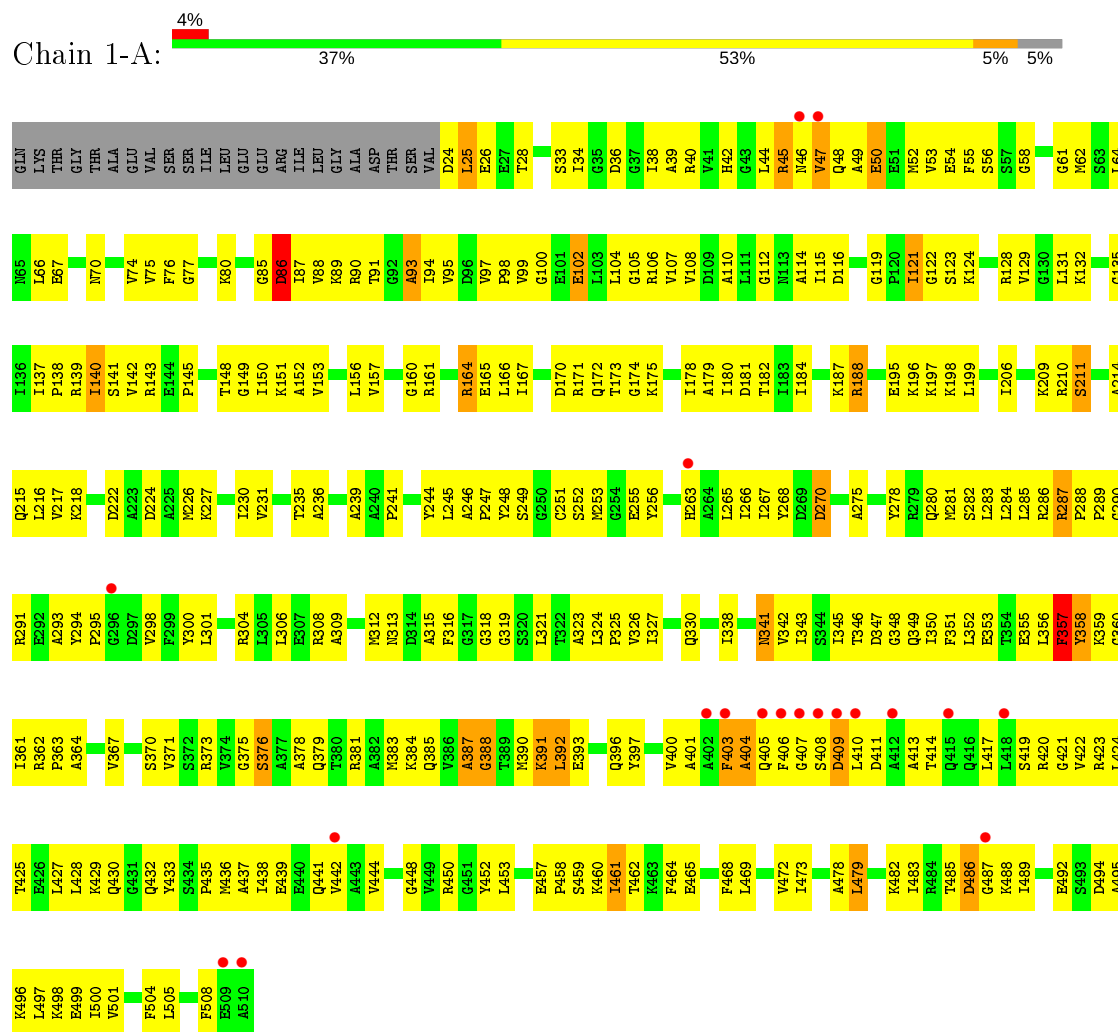
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-D	1	Total	Mg	0	0
			1	1		
6	2-F	1	Total	Mg	0	0
			1	1		
6	1-B	1	Total	Mg	0	0
			1	1		
6	1-C	1	Total	Mg	0	0
			1	1		
6	2-D	1	Total	Mg	0	0
			1	1		
6	2-C	1	Total	Mg	0	0
			1	1		
6	1-A	1	Total	Mg	0	0
			1	1		
6	2-B	1	Total	Mg	0	0
			1	1		
6	2-A	1	Total	Mg	0	0
			1	1		
6	1-F	1	Total	Mg	0	0
			1	1		

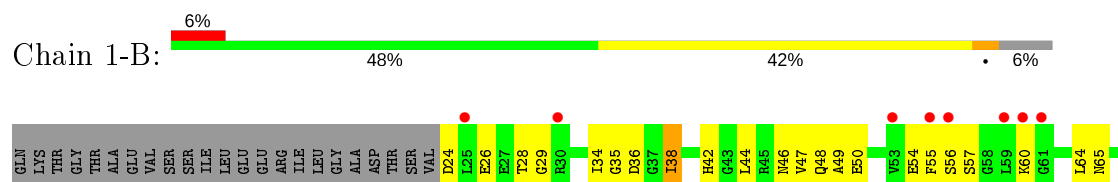
### 3 Residue-property plots

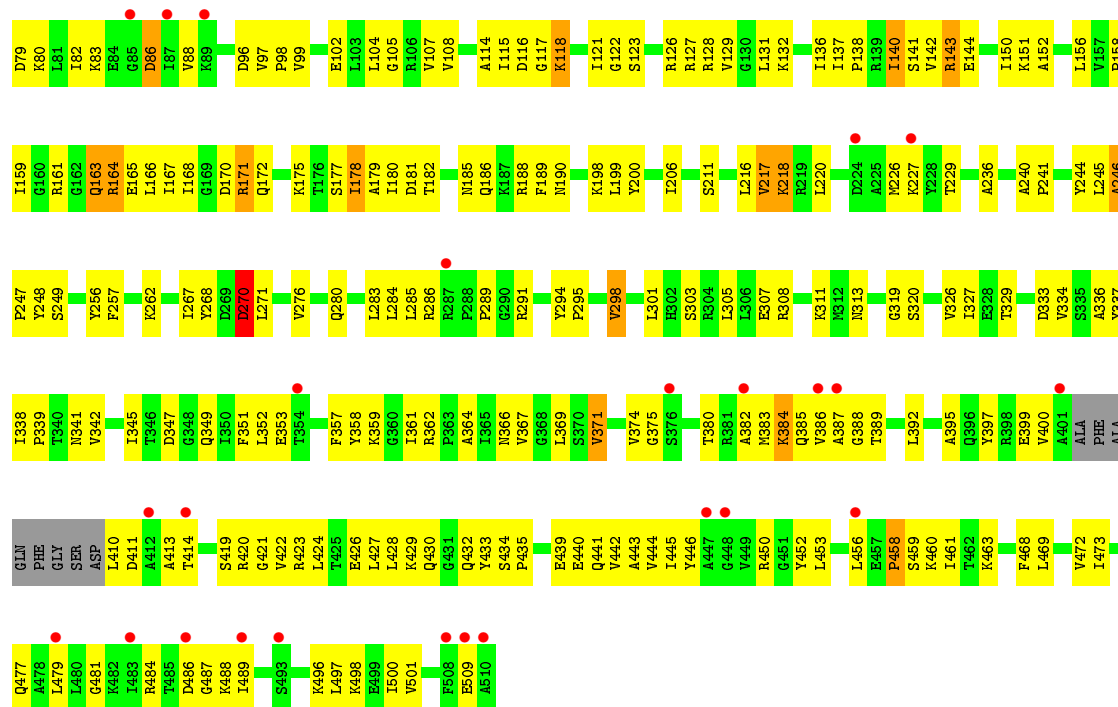
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

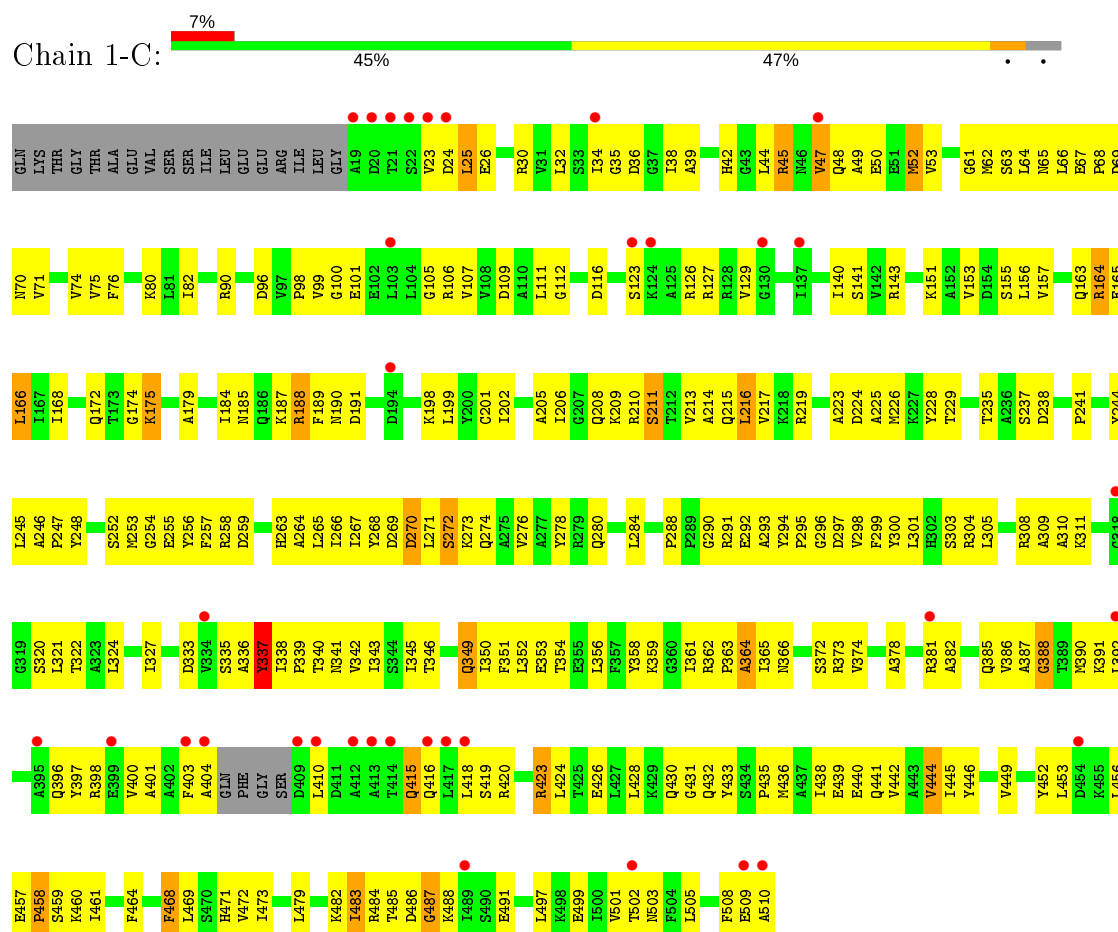


- Molecule 1: ATP synthase subunit alpha, mitochondrial



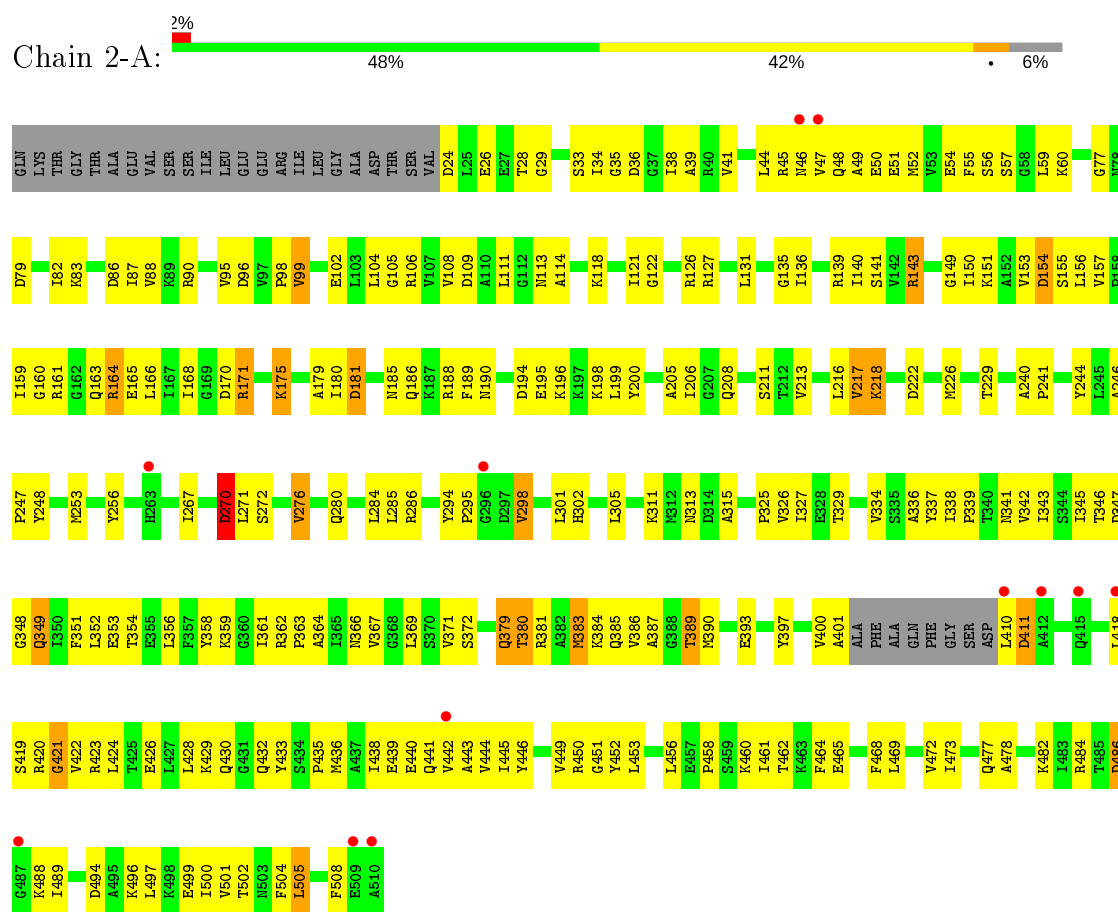


• Molecule 1: ATP synthase subunit alpha, mitochondrial

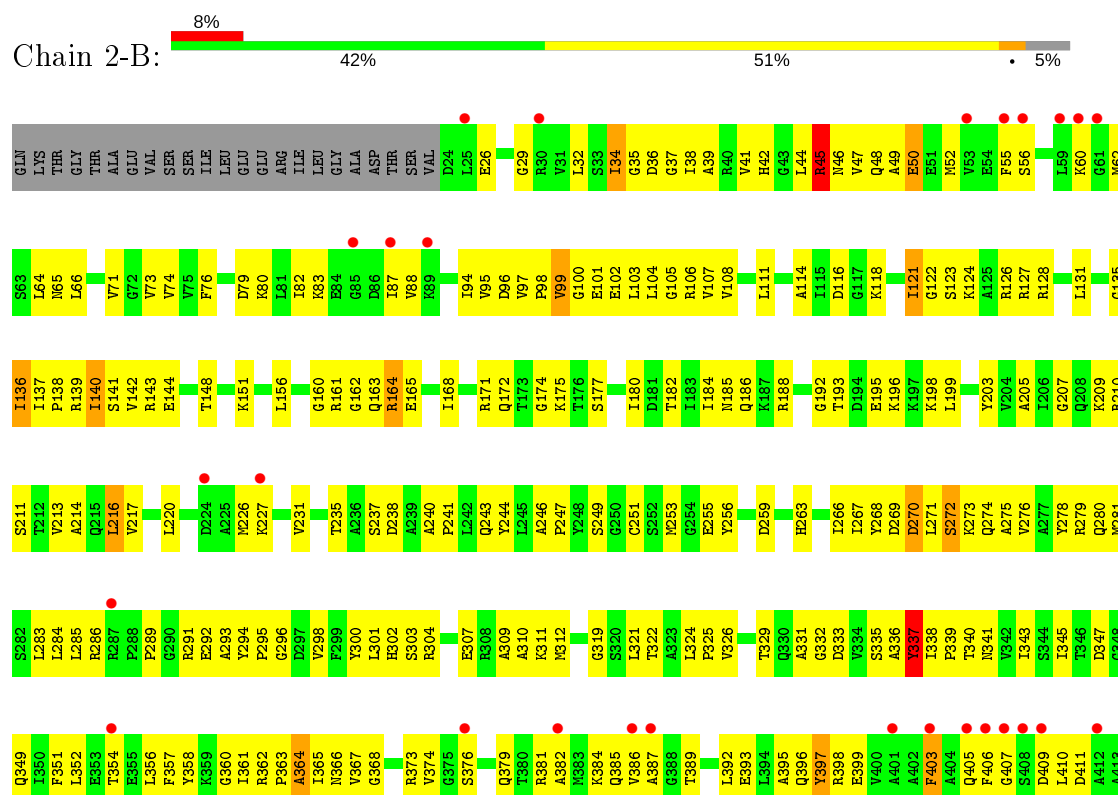


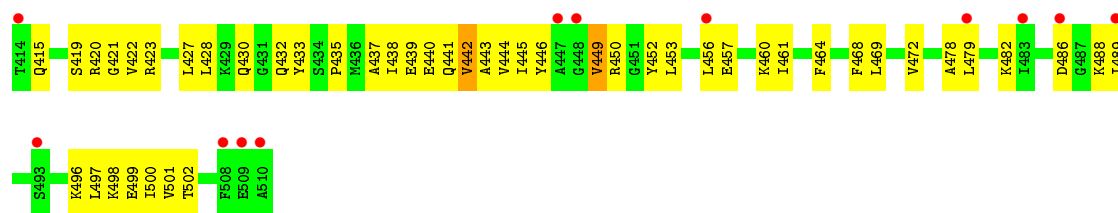
• Molecule 1: ATP synthase subunit alpha, mitochondrial



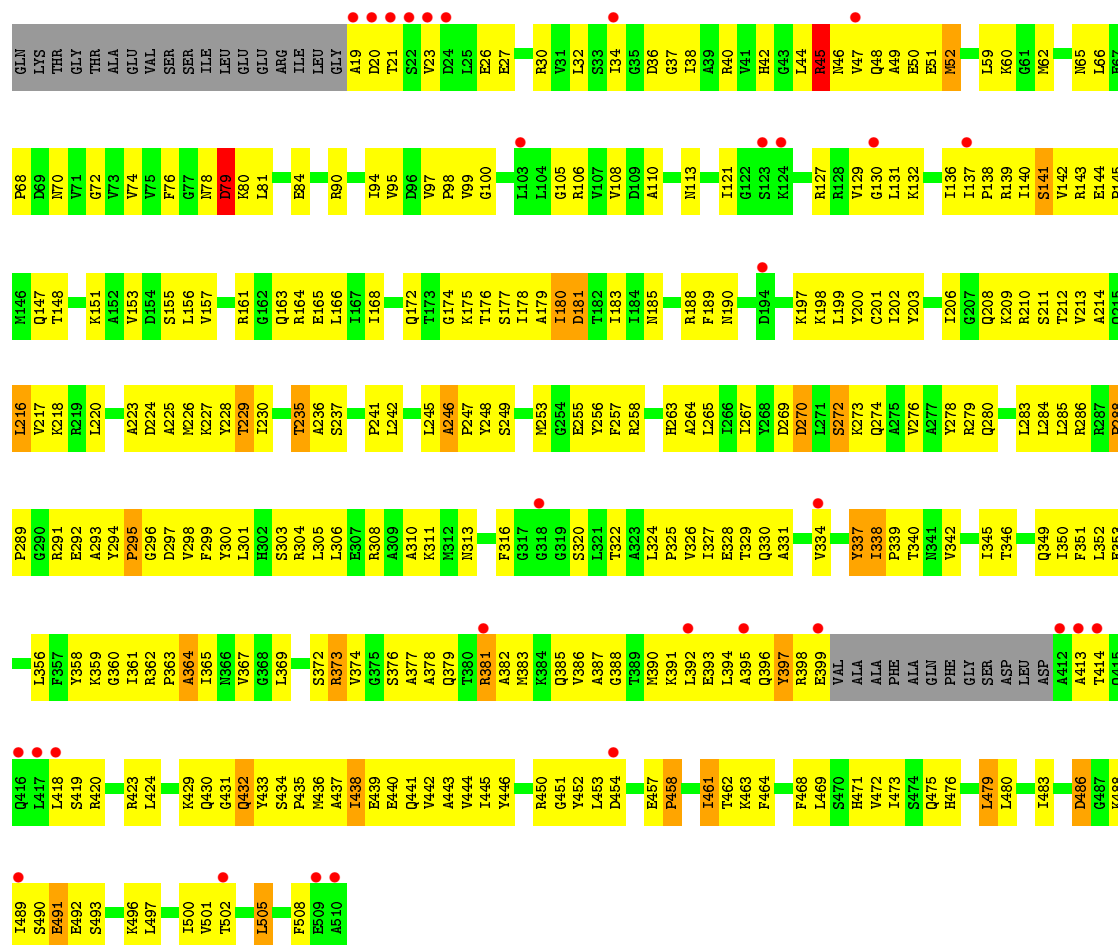


- Molecule 1: ATP synthase subunit alpha, mitochondrial

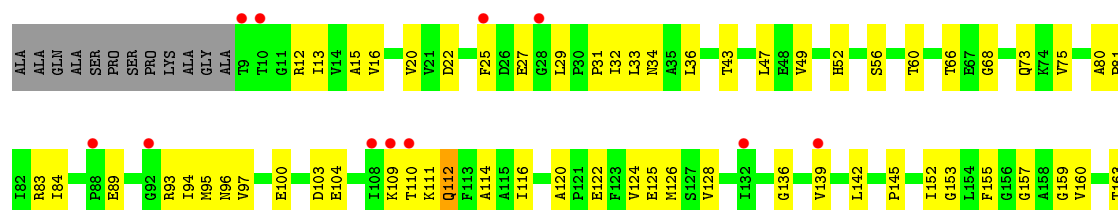


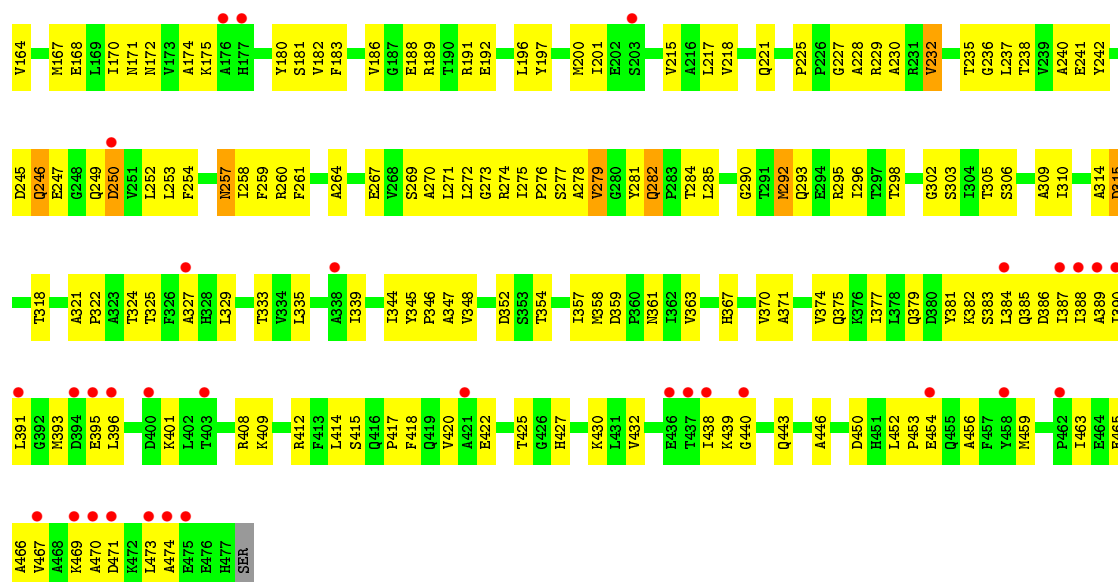


• Molecule 1: ATP synthase subunit alpha, mitochondrial

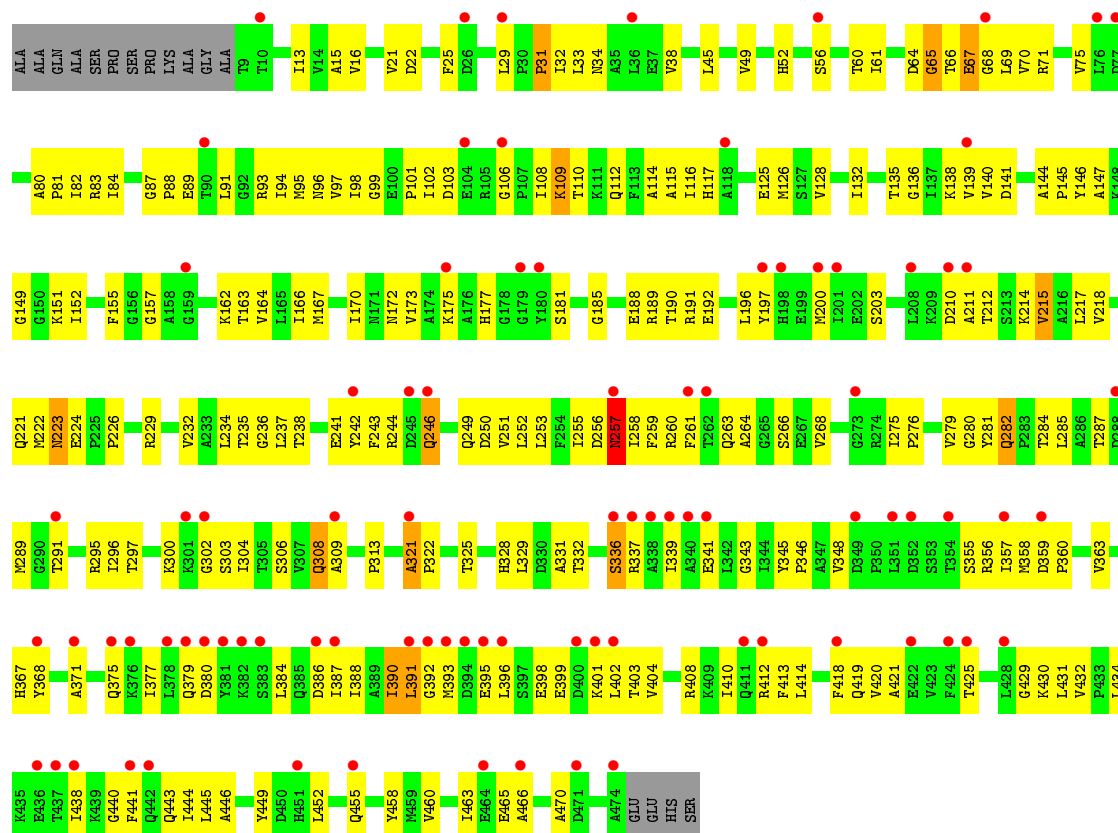


• Molecule 2: ATP synthase subunit beta, mitochondrial



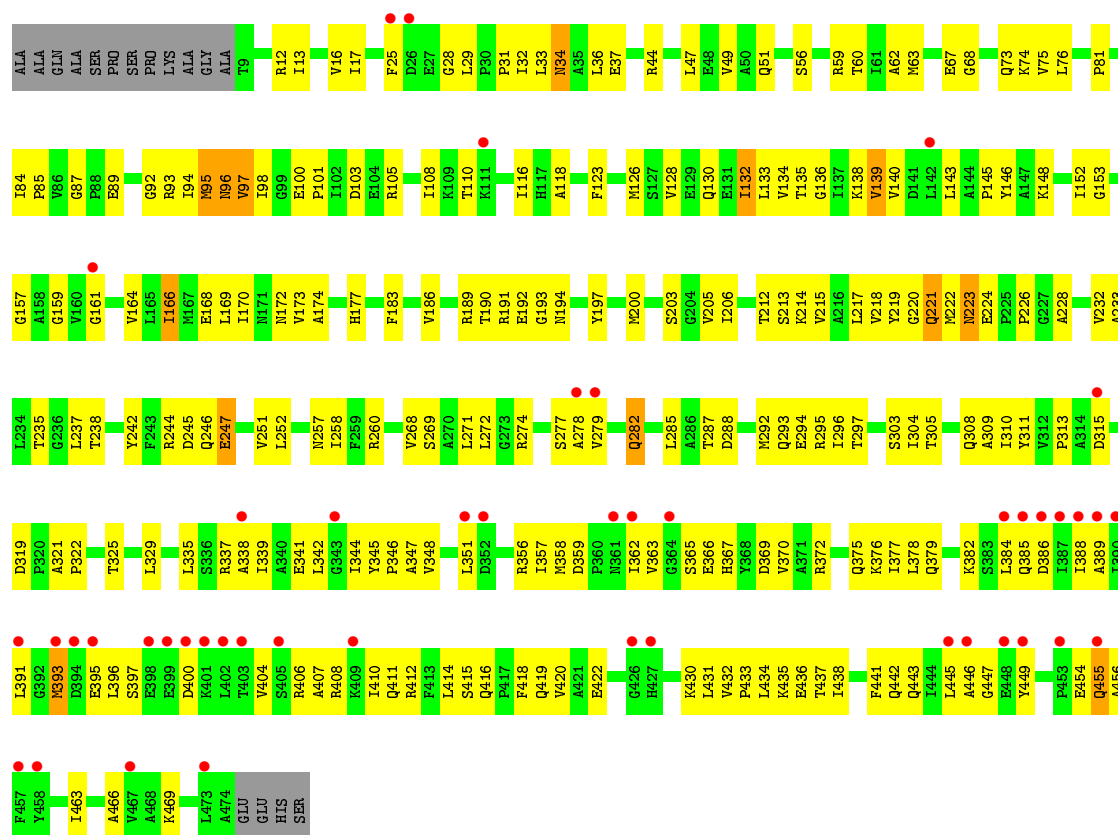


• Molecule 2: ATP synthase subunit beta, mitochondrial

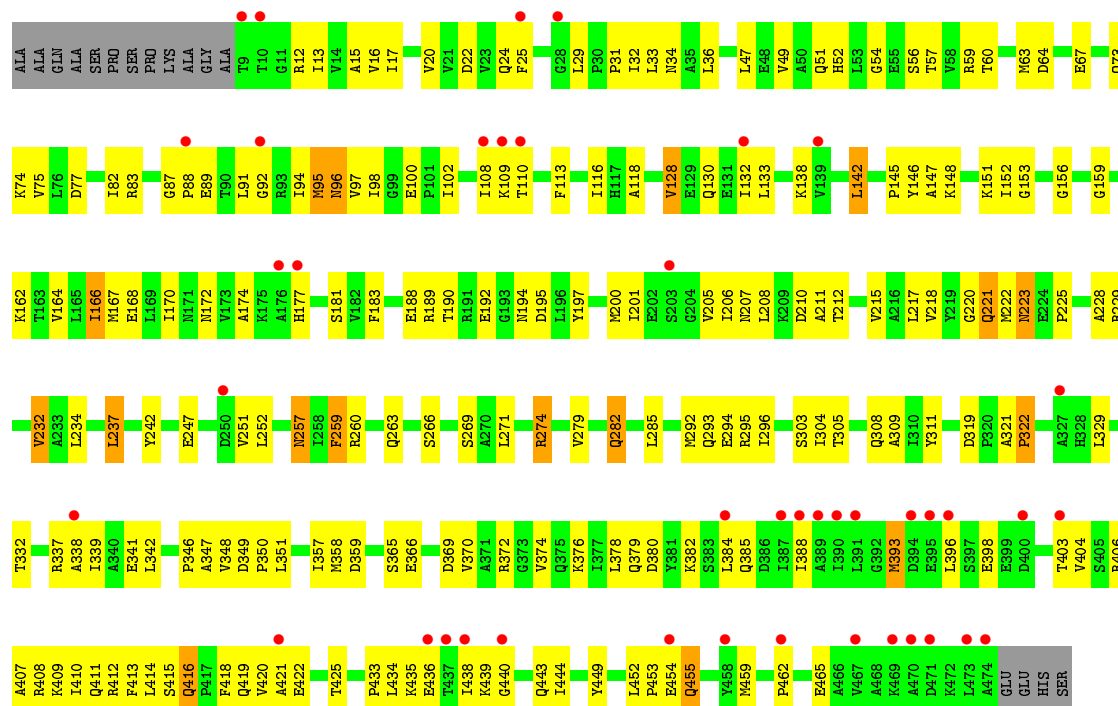


• Molecule 2: ATP synthase subunit beta, mitochondrial



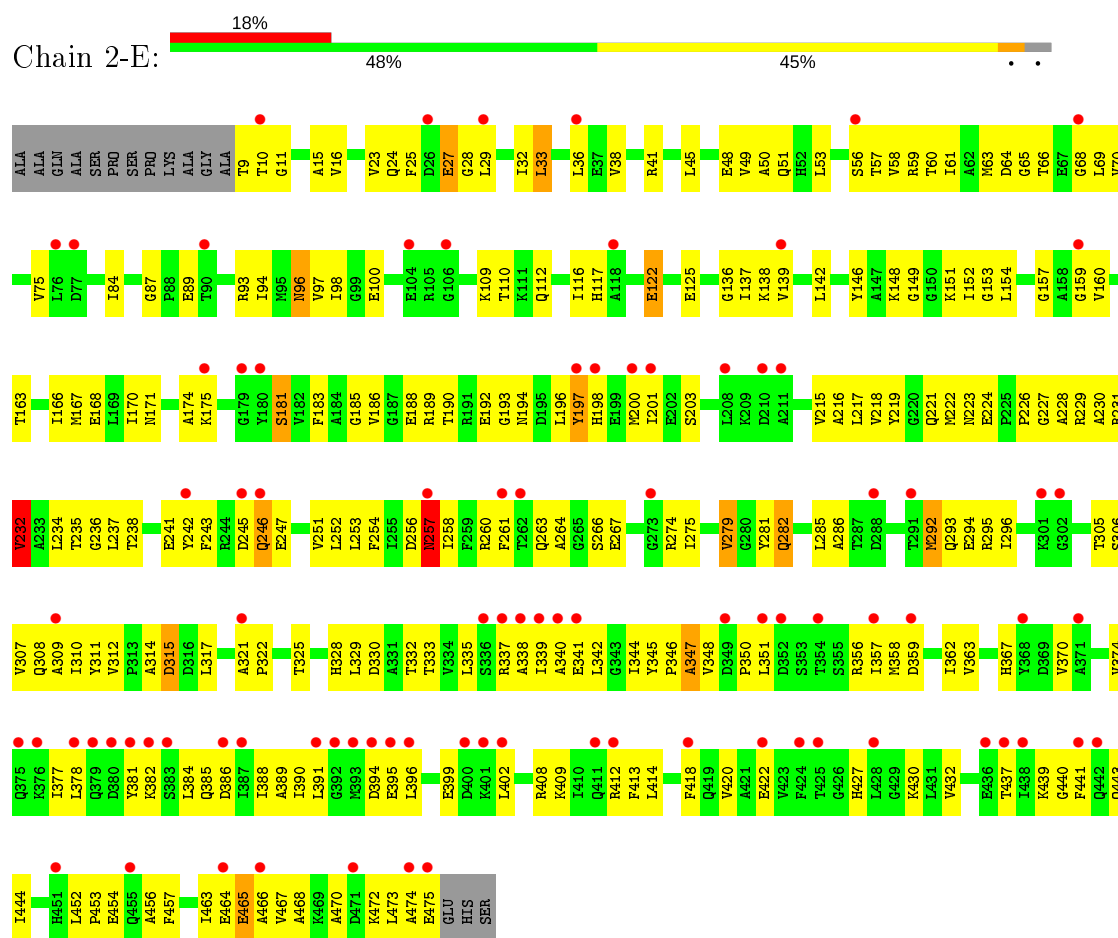


- Molecule 2: ATP synthase subunit beta, mitochondrial



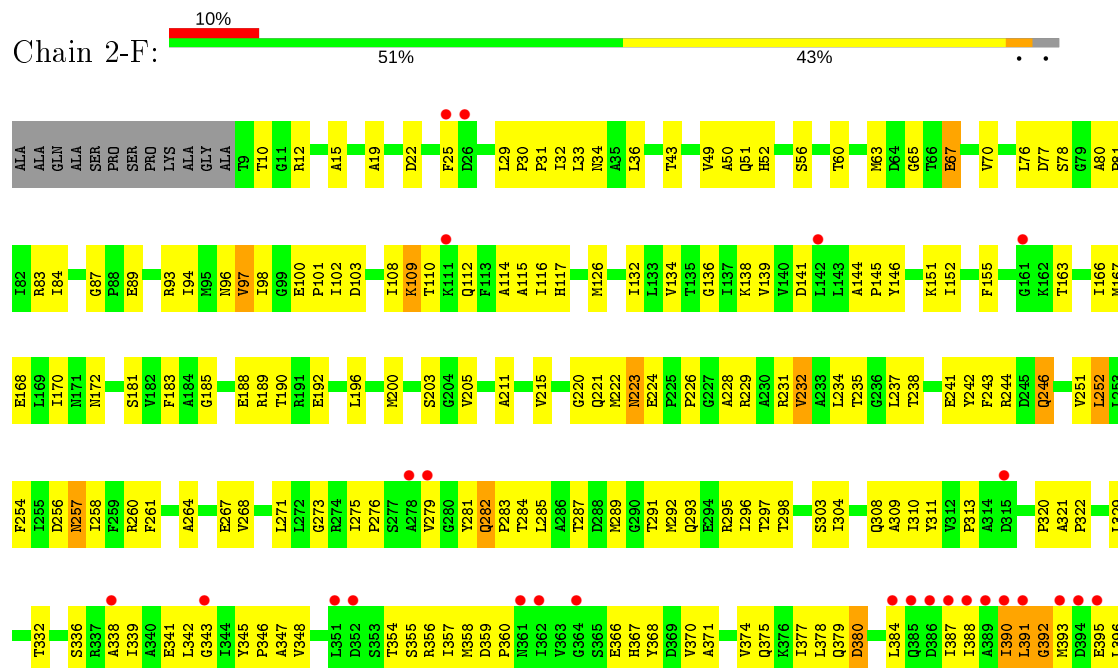
- Molecule 2: ATP synthase subunit beta, mitochondrial

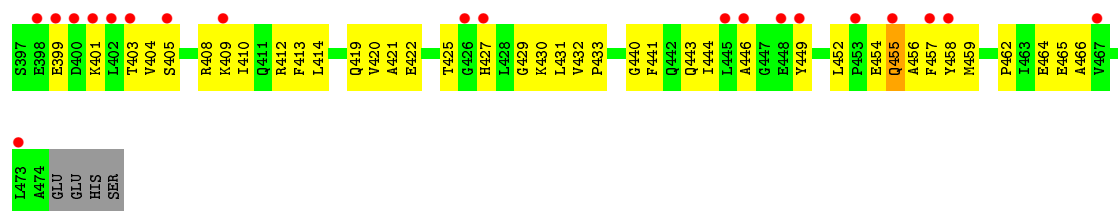
Chain 2-E:



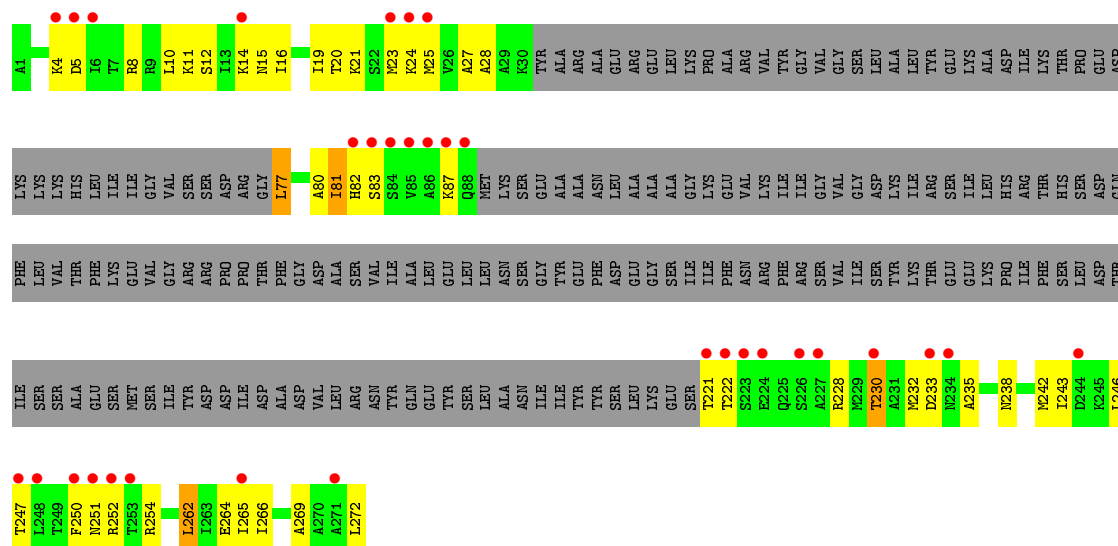
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain 2-F:

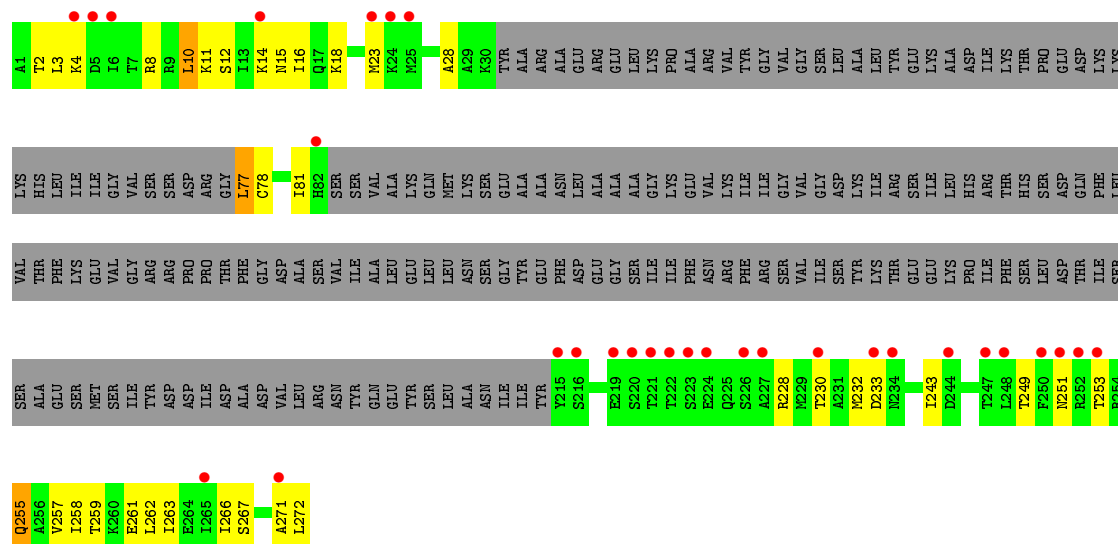




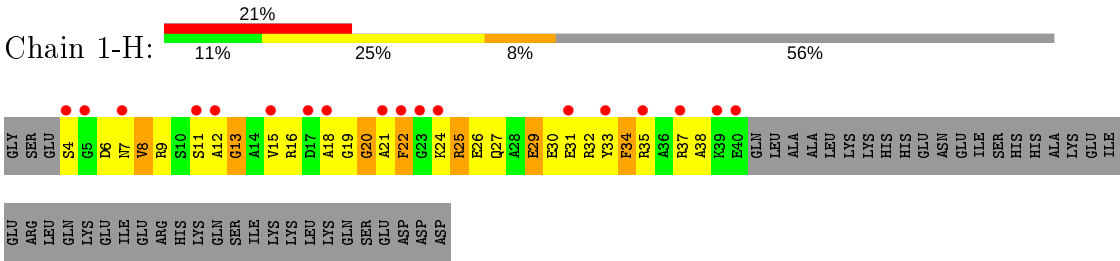
• Molecule 3: ATP synthase subunit gamma, mitochondrial



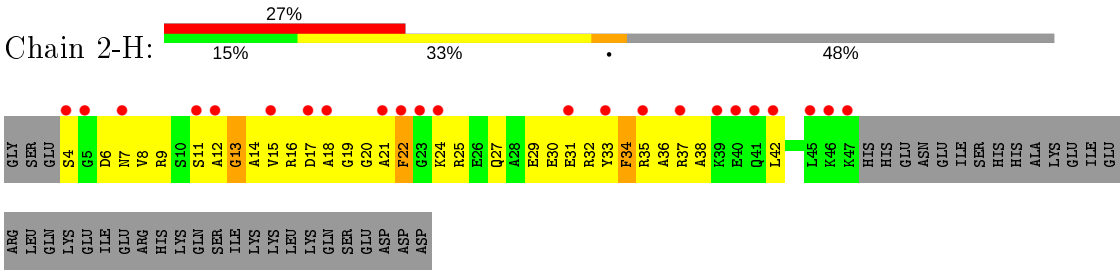
• Molecule 3: ATP synthase subunit gamma, mitochondrial



• Molecule 4: ATPase inhibitor, mitochondrial



● Molecule 4: ATPase inhibitor, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	272.30 Å   107.20 Å   152.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.50 – 2.80 39.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.50-2.80) 99.0 (39.48-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 ,   0.280 0.228 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	45703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	1-A	0.37	0/3766	0.65	0/5080
1	1-B	0.38	0/3704	0.67	0/4995
1	1-C	0.43	0/3767	0.71	0/5082
1	2-A	0.39	0/3704	0.66	0/4995
1	2-B	0.38	0/3766	0.65	0/5080
1	2-C	0.41	0/3709	0.65	0/5002
2	1-D	0.38	0/3616	0.65	0/4906
2	1-E	0.35	0/3587	0.63	0/4867
2	1-F	0.42	0/3587	0.71	0/4867
2	2-D	0.39	0/3587	0.66	0/4867
2	2-E	0.37	0/3596	0.64	0/4879
2	2-F	0.38	0/3587	0.65	0/4867
3	1-G	0.41	0/708	0.67	0/941
3	2-G	0.40	0/717	0.65	0/953
4	1-H	0.48	0/285	0.68	0/376
4	2-H	0.57	0/338	0.67	0/446
All	All	0.39	0/46024	0.66	0/62203

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1-A	3715	0	3814	342	0
1	1-B	3656	0	3766	233	0
1	1-C	3718	0	3818	305	0
1	2-A	3656	0	3765	304	0
1	2-B	3715	0	3814	266	0
1	2-C	3661	0	3766	299	0
2	1-D	3558	0	3605	236	0
2	1-E	3530	0	3587	245	0
2	1-F	3530	0	3586	216	0
2	2-D	3530	0	3586	196	0
2	2-E	3539	0	3592	245	0
2	2-F	3530	0	3587	233	0
3	1-G	709	0	771	57	0
3	2-G	717	0	775	47	0
4	1-H	283	0	265	63	0
4	2-H	336	0	331	71	0
5	1-A	31	0	13	4	0
5	1-B	31	0	13	4	0
5	1-C	31	0	13	3	0
5	1-D	31	0	13	5	0
5	1-F	31	0	13	3	0
5	2-A	31	0	13	6	0
5	2-B	31	0	13	4	0
5	2-C	31	0	13	5	0
5	2-D	31	0	13	4	0
5	2-F	31	0	13	4	0
6	1-A	1	0	0	0	0
6	1-B	1	0	0	0	0
6	1-C	1	0	0	0	0
6	1-D	1	0	0	0	0
6	1-F	1	0	0	0	0
6	2-A	1	0	0	0	0
6	2-B	1	0	0	0	0
6	2-C	1	0	0	0	0
6	2-D	1	0	0	0	0
6	2-F	1	0	0	0	0
All	All	45703	0	46558	3080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (3080) 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:282:GLN:HE21	2:F:282:GLN:N	1.40	1.19
2:D:473:LEU:HB3	4:H:34:PHE:CZ	1.80	1.16
2:F:282:GLN:NE2	2:F:282:GLN:H	1.43	1.15
2:E:282:GLN:H	2:E:282:GLN:NE2	1.46	1.12
2:D:282:GLN:HE21	2:D:282:GLN:N	1.45	1.12
1:A:150:ILE:HA	1:A:430:GLN:HE22	1.11	1.11
2:D:282:GLN:H	2:D:282:GLN:NE2	1.48	1.11
1:A:270:ASP:H	1:A:326:VAL:HB	1.11	1.10
1:C:188:ARG:HH12	1:C:435:PRO:HB2	1.14	1.08
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.35	1.08
1:C:218:LYS:HD2	2:D:128:VAL:HG21	1.31	1.08
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.33	1.08
2:E:282:GLN:NE2	2:E:282:GLN:H	1.50	1.07
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.36	1.07
2:D:257:ASN:H	2:D:309:ALA:HB3	0.97	1.07
1:A:151:LYS:HE3	1:A:436:MET:SD	1.95	1.05
2:E:282:GLN:N	2:E:282:GLN:HE21	1.52	1.05
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.21	1.05
2:D:388:ILE:HD11	2:D:396:LEU:HD11	1.37	1.05
2:E:473:LEU:HB3	4:H:34:PHE:CZ	1.91	1.04
2:E:282:GLN:HE21	2:E:282:GLN:N	1.55	1.04
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.39	1.03
1:B:158:PRO:O	1:B:375:GLY:HA3	1.58	1.03
2:F:246:GLN:HA	2:F:246:GLN:HE21	1.25	1.00
2:F:203:SER:HB2	2:F:420:VAL:HG13	1.45	0.98
2:E:246:GLN:HE21	2:E:246:GLN:HA	1.29	0.98
1:B:38:ILE:HG13	1:B:285:LEU:HD21	1.47	0.97
2:D:282:GLN:HE21	2:D:282:GLN:N	1.59	0.97
2:D:282:GLN:H	2:D:282:GLN:NE2	1.59	0.97
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.47	0.97
1:B:270:ASP:HA	1:B:326:VAL:O	1.64	0.97
1:A:381:ARG:HB3	1:A:487:GLY:O	1.62	0.96
2:D:473:LEU:HB3	4:H:34:PHE:HZ	1.29	0.96
1:A:38:ILE:HG13	1:A:285:LEU:HD21	1.43	0.96
1:C:423:ARG:HH11	1:C:423:ARG:HG2	1.31	0.95
2:E:257:ASN:HD22	2:E:260:ARG:CZ	1.78	0.95
2:D:257:ASN:N	2:D:309:ALA:HB3	1.81	0.94
1:A:379:GLN:HG2	1:A:380:THR:H	1.32	0.94
4:H:29:GLU:O	4:H:32:ARG:HB3	1.68	0.94
3:G:14:LYS:HG2	3:G:243:ILE:HD13	1.46	0.94
1:A:99:VAL:HG23	1:A:253:MET:HA	1.50	0.94
1:A:362:ARG:O	1:A:430:GLN:N	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD13	1:B:121:ILE:H	1.32	0.93
1:C:442:VAL:HG11	1:C:489:ILE:HD11	1.50	0.92
2:F:223:ASN:HD22	2:F:223:ASN:H	1.17	0.92
2:D:252:LEU:HD23	2:D:305:THR:HB	1.52	0.92
3:G:11:LYS:HB3	4:H:7:ASN:ND2	1.83	0.92
2:E:391:LEU:HD21	3:G:23:MET:SD	2.09	0.92
2:D:408:ARG:HH11	4:H:26:GLU:HG3	1.35	0.92
2:F:293:GLN:HE22	2:F:308:GLN:HE22	1.08	0.92
3:G:21:LYS:O	3:G:24:LYS:HG2	1.70	0.92
2:D:282:GLN:H	2:D:282:GLN:HE21	0.92	0.92
3:G:23:MET:SD	3:G:232:MET:HE1	2.10	0.92
2:F:449:TYR:HB3	2:F:452:LEU:HD12	1.52	0.91
1:B:136:ILE:HD12	2:F:190:THR:HG23	1.52	0.91
1:C:338:ILE:HD12	1:C:338:ILE:H	1.36	0.91
1:A:149:GLY:O	1:A:436:MET:N	2.03	0.90
1:A:171:ARG:NH2	2:F:356:ARG:HH21	1.69	0.90
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.52	0.90
2:E:49:VAL:HA	2:E:60:THR:HG22	1.54	0.90
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.51	0.90
2:F:282:GLN:H	2:F:282:GLN:HE21	0.90	0.89
2:D:321:ALA:HB3	2:D:322:PRO:HD3	1.55	0.89
2:F:200:MET:HE1	2:F:215:VAL:HG21	1.55	0.89
1:A:140:ILE:HG12	1:A:143:ARG:HH12	1.38	0.89
1:C:78:ASN:ND2	1:C:80:LYS:HD3	1.88	0.89
2:E:203:SER:HB2	2:E:420:VAL:HG13	1.55	0.89
1:A:171:ARG:HH22	2:F:356:ARG:NH2	1.71	0.88
1:C:101:GLU:HG2	1:C:257:PHE:HE2	1.38	0.88
2:F:282:GLN:N	2:F:282:GLN:HE21	1.71	0.88
1:A:121:ILE:H	1:A:121:ILE:HD13	1.39	0.88
2:E:393:MET:HG3	2:E:396:LEU:HD11	1.55	0.88
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.37	0.88
1:A:356:LEU:HD22	1:A:361:ILE:HG21	1.53	0.88
1:C:217:VAL:HG11	2:F:123:PHE:HZ	1.39	0.88
1:B:171:ARG:HH22	2:E:356:ARG:HH21	1.18	0.88
1:B:142:VAL:HG11	1:B:160:GLY:HA3	1.56	0.87
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.55	0.87
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.57	0.87
1:C:188:ARG:NH1	1:C:435:PRO:HB2	1.89	0.87
1:C:299:PHE:HB3	2:D:267:GLU:OE1	1.74	0.87
1:A:49:ALA:O	1:A:50:GLU:HB2	1.74	0.87
1:A:171:ARG:HH22	2:F:356:ARG:HH21	0.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASP:HA	1:A:326:VAL:O	1.74	0.87
1:C:423:ARG:CG	1:C:423:ARG:HH11	1.88	0.87
1:C:156:LEU:HB3	1:C:391:LYS:HE2	1.56	0.86
1:B:108:VAL:HG12	1:B:114:ALA:HA	1.58	0.85
1:A:361:ILE:HA	1:A:429:LYS:HD3	1.56	0.85
1:C:151:LYS:HB3	1:C:428:LEU:HD22	1.57	0.85
2:F:252:LEU:HD23	2:F:305:THR:HB	1.56	0.85
1:C:99:VAL:HG12	1:C:100:GLY:H	1.38	0.85
1:C:270:ASP:H	1:C:326:VAL:HB	1.41	0.85
1:A:347:ASP:HA	1:A:373:ARG:HH12	1.41	0.84
2:D:133:LEU:HD13	2:D:148:LYS:HG2	1.60	0.84
2:F:257:ASN:H	2:F:309:ALA:HB3	1.43	0.84
2:F:282:GLN:H	2:F:282:GLN:NE2	1.73	0.84
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.57	0.84
2:E:181:SER:OG	2:E:252:LEU:HB2	1.77	0.84
2:E:404:VAL:O	2:E:408:ARG:HG3	1.78	0.84
2:E:388:ILE:HG23	2:E:393:MET:HB2	1.59	0.84
1:A:406:PHE:CE2	3:G:23:MET:HG2	2.13	0.84
1:B:44:LEU:O	1:B:47:VAL:HG23	1.77	0.84
1:C:237:SER:HB3	2:D:294:GLU:HG3	1.60	0.84
1:C:99:VAL:HG13	1:C:253:MET:HA	1.60	0.84
1:C:423:ARG:HD3	1:C:461:ILE:HD11	1.60	0.84
2:D:408:ARG:HH21	2:D:412:ARG:NH2	1.75	0.84
1:A:270:ASP:N	1:A:326:VAL:HB	1.92	0.84
1:B:140:ILE:HG12	1:B:143:ARG:HH12	1.41	0.83
1:A:441:GLN:O	1:A:444:VAL:HG22	1.78	0.83
1:C:362:ARG:NH2	2:F:372:ARG:HD2	1.92	0.83
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.58	0.83
1:A:270:ASP:H	1:A:326:VAL:HB	1.44	0.83
2:D:384:LEU:O	2:D:388:ILE:HG12	1.78	0.83
2:F:170:ILE:HD13	2:F:215:VAL:HG21	1.60	0.83
1:A:420:ARG:HH21	1:A:451:GLY:HA2	1.43	0.83
1:A:47:VAL:HG12	1:A:90:ARG:HG2	1.59	0.83
1:B:44:LEU:O	1:B:47:VAL:HG22	1.78	0.83
1:B:270:ASP:H	1:B:326:VAL:HB	1.42	0.83
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.59	0.83
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.61	0.82
1:B:338:ILE:HD12	1:B:338:ILE:H	1.43	0.82
1:B:28:THR:HG22	1:B:29:GLY:H	1.42	0.82
2:D:401:LYS:HD2	4:H:25:ARG:NH2	1.94	0.82
1:C:296:GLY:O	2:D:267:GLU:HG2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:14:LYS:HA	3:G:243:ILE:HD11	1.62	0.82
2:E:282:GLN:HE21	2:E:282:GLN:H	0.86	0.82
2:D:388:ILE:HD12	2:D:393:MET:HG2	1.61	0.82
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.61	0.82
1:C:439:GLU:HG2	1:C:440:GLU:H	1.41	0.82
1:C:413:ALA:HB2	4:H:31:GLU:CD	1.99	0.82
1:B:283:LEU:HD21	1:B:289:PRO:HB3	1.59	0.82
2:E:237:LEU:HD13	2:E:296:ILE:HG12	1.61	0.82
1:B:148:THR:HA	1:B:182:THR:HG23	1.61	0.81
1:C:483:ILE:HD13	1:C:489:ILE:HG12	1.62	0.81
2:D:390:ILE:HD11	3:G:16:ILE:HG12	1.61	0.81
1:C:381:ARG:O	1:C:385:GLN:HG3	1.80	0.81
1:A:150:ILE:HA	1:A:430:GLN:NE2	1.94	0.81
1:C:127:ARG:HE	1:C:131:LEU:HD12	1.45	0.81
1:C:218:LYS:HD2	2:D:128:VAL:CG2	2.10	0.81
1:A:172:GLN:HA	5:A:1511:ANP:HNB1	1.44	0.81
1:C:68:PRO:HD3	2:E:15:ALA:HB2	1.62	0.81
2:F:293:GLN:NE2	2:F:308:GLN:HE22	1.78	0.81
1:C:296:GLY:O	2:E:267:GLU:HG2	1.79	0.81
2:D:164:VAL:HG23	5:D:1478:ANP:O1A	1.80	0.81
4:H:9:ARG:HD2	4:H:15:VAL:HG13	1.62	0.81
1:A:278:TYR:HA	1:A:281:MET:HE3	1.61	0.81
1:A:155:SER:HB2	1:A:383:MET:SD	2.21	0.81
1:C:367:VAL:CG1	1:C:391:LYS:HG3	2.10	0.81
1:C:210:ARG:HG2	1:C:235:THR:HG21	1.61	0.81
2:E:242:TYR:CE1	2:E:246:GLN:HG3	2.16	0.81
2:D:257:ASN:HA	2:D:309:ALA:O	1.81	0.81
1:C:291:ARG:HB3	1:C:337:TYR:CE2	2.16	0.80
2:E:145:PRO:HB2	2:E:357:ILE:HD11	1.61	0.80
1:A:347:ASP:HA	1:A:373:ARG:NH1	1.96	0.80
1:C:358:TYR:CD2	2:F:375:GLN:HB3	2.15	0.80
2:D:96:ASN:HD22	2:D:96:ASN:C	1.83	0.80
1:B:453:LEU:HD13	1:B:461:ILE:HD12	1.63	0.80
1:B:140:ILE:HG12	1:B:143:ARG:NH1	1.96	0.80
1:A:149:GLY:HA2	1:A:436:MET:O	1.82	0.80
1:A:496:LYS:O	1:A:500:ILE:HG13	1.82	0.80
1:C:338:ILE:HD12	1:C:338:ILE:H	1.45	0.80
2:E:181:SER:HB2	2:E:215:VAL:HG13	1.61	0.80
2:F:221:GLN:HB2	2:F:223:ASN:HD21	1.47	0.80
1:B:44:LEU:HD22	1:B:47:VAL:HG22	1.62	0.79
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:HG2	1:B:60:LYS:HZ2	1.45	0.79
2:E:387:ILE:HD12	2:E:387:ILE:H	1.45	0.79
2:E:97:VAL:HG22	2:E:232:VAL:HG13	1.62	0.79
2:E:390:ILE:HG21	3:G:28:ALA:HB1	1.64	0.79
2:F:412:ARG:HG3	2:F:412:ARG:HH11	1.48	0.79
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.61	0.79
1:A:497:LEU:O	1:A:501:VAL:HG22	1.83	0.79
1:B:196:LYS:H	1:B:196:LYS:HD2	1.45	0.79
1:B:107:VAL:HG22	1:B:231:VAL:HB	1.64	0.79
1:C:327:ILE:HD11	1:C:342:VAL:HG21	1.63	0.79
1:A:154:ASP:HB3	1:A:438:ILE:HD13	1.65	0.79
1:A:422:VAL:O	1:A:426:GLU:HG2	1.82	0.79
1:A:26:GLU:OE2	1:A:45:ARG:HD2	1.83	0.78
1:C:132:LYS:HE3	2:E:223:ASN:HD21	1.48	0.78
2:D:186:VAL:HG12	2:D:260:ARG:HB2	1.65	0.78
2:F:49:VAL:HA	2:F:60:THR:HG22	1.64	0.78
2:E:172:ASN:ND2	2:E:431:LEU:HD13	1.98	0.78
1:C:414:THR:HG21	4:H:24:LYS:HA	1.63	0.78
2:D:171:ASN:HA	2:D:175:LYS:HE3	1.66	0.78
1:B:206:ILE:HD11	1:B:247:PRO:HG3	1.65	0.78
1:A:383:MET:HG2	1:A:438:ILE:HD11	1.63	0.78
2:E:185:GLY:HA3	2:E:188:GLU:HG3	1.65	0.78
1:A:166:LEU:HD11	1:A:327:ILE:HG12	1.64	0.78
2:E:34:ASN:O	2:E:49:VAL:HG23	1.82	0.78
1:B:74:VAL:HG11	1:B:241:PRO:HB3	1.65	0.78
4:H:29:GLU:O	4:H:32:ARG:HB3	1.83	0.78
1:A:379:GLN:CG	1:A:380:THR:H	1.95	0.78
1:A:347:ASP:O	1:A:373:ARG:HG3	1.83	0.78
2:E:223:ASN:HD22	2:E:223:ASN:N	1.78	0.78
2:E:282:GLN:H	2:E:282:GLN:HE21	0.82	0.78
1:C:246:ALA:HB3	1:C:247:PRO:HD3	1.63	0.78
2:F:293:GLN:HE22	2:F:308:GLN:NE2	1.81	0.78
1:C:47:VAL:HG13	1:C:90:ARG:HG2	1.66	0.77
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.66	0.77
1:B:175:LYS:HE3	5:B:1511:ANP:O1B	1.84	0.77
1:C:44:LEU:O	1:C:47:VAL:HG22	1.85	0.77
2:D:391:LEU:HD21	3:G:23:MET:SD	2.25	0.77
2:F:360:PRO:HG3	2:F:368:TYR:CD2	2.20	0.77
1:A:206:ILE:HD11	1:A:247:PRO:HG3	1.64	0.77
1:B:87:ILE:H	1:B:87:ILE:HD12	1.49	0.77
1:B:45:ARG:HH11	1:B:45:ARG:HG2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.14	0.77
1:C:362:ARG:NH2	2:D:372:ARG:HD2	2.00	0.77
4:H:18:ALA:O	4:H:22:PHE:HB2	1.85	0.77
1:B:142:VAL:CG1	1:B:160:GLY:HA3	2.15	0.76
1:B:376:SER:HB3	1:B:384:LYS:HE2	1.66	0.76
2:F:172:ASN:ND2	2:F:431:LEU:HD13	1.99	0.76
1:C:172:GLN:HA	5:C:1511:ANP:HNB1	1.51	0.76
1:A:479:LEU:O	1:A:479:LEU:HD22	1.84	0.76
1:B:76:PHE:HD2	1:B:111:LEU:HD11	1.50	0.76
1:A:379:GLN:NE2	1:A:383:MET:HG3	1.99	0.76
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.67	0.76
1:A:151:LYS:HG2	1:A:441:GLN:HG2	1.66	0.76
1:B:76:PHE:CD2	1:B:111:LEU:HD11	2.21	0.76
1:B:419:SER:O	1:B:423:ARG:HD3	1.86	0.76
1:B:338:ILE:HA	1:B:341:ASN:HD22	1.50	0.76
1:A:361:ILE:HD13	1:A:429:LYS:CE	2.16	0.76
1:A:367:VAL:HG21	1:A:428:LEU:HD13	1.67	0.76
2:D:200:MET:HB3	2:D:205:VAL:HG22	1.66	0.76
2:D:51:GLN:HG2	2:D:59:ARG:HB3	1.67	0.76
1:A:270:ASP:HA	1:A:326:VAL:O	1.86	0.76
2:E:49:VAL:HA	2:E:60:THR:HG22	1.68	0.76
2:D:200:MET:HB3	2:D:205:VAL:CG2	2.16	0.76
4:H:31:GLU:HA	4:H:34:PHE:HB2	1.66	0.76
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.68	0.76
2:F:49:VAL:HA	2:F:60:THR:HG22	1.68	0.76
2:D:257:ASN:HA	2:D:309:ALA:O	1.86	0.76
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.16	0.76
1:A:157:VAL:HG11	1:A:350:ILE:HG12	1.68	0.76
1:C:400:VAL:HG12	1:C:418:LEU:HD13	1.67	0.76
1:B:94:ILE:HG12	1:B:95:VAL:H	1.50	0.75
2:E:257:ASN:HA	2:E:309:ALA:O	1.85	0.75
2:F:319:ASP:O	2:F:322:PRO:HD2	1.86	0.75
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.68	0.75
2:E:89:GLU:CG	2:E:110:THR:HG22	2.16	0.75
1:A:170:ASP:O	1:A:175:LYS:HE2	1.86	0.75
2:F:237:LEU:CD1	2:F:296:ILE:HG12	2.16	0.75
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.68	0.75
1:A:52:MET:HG2	1:A:95:VAL:HG22	1.69	0.75
1:A:155:SER:HA	1:A:383:MET:HG3	1.68	0.75
2:D:147:ALA:HB2	2:D:357:ILE:HG13	1.69	0.75
4:H:18:ALA:O	4:H:22:PHE:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:GLY:HA3	2:D:329:LEU:HD13	1.69	0.75
1:A:140:ILE:HG13	1:A:143:ARG:HH22	1.51	0.75
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.69	0.75
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.69	0.75
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.69	0.74
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.68	0.74
1:C:446:TYR:CE2	1:C:497:LEU:HB3	2.22	0.74
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.01	0.74
1:B:379:GLN:O	1:B:384:LYS:HE3	1.87	0.74
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.15	0.74
1:A:127:ARG:CZ	1:A:131:LEU:HD12	2.17	0.74
2:E:153:GLY:HA3	2:E:329:LEU:HD13	1.69	0.74
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.50	0.74
1:C:209:LYS:HE3	1:C:211:SER:OG	1.86	0.74
1:C:394:LEU:O	1:C:398:ARG:HG3	1.88	0.74
1:A:151:LYS:HG3	1:A:436:MET:SD	2.27	0.74
2:D:163:THR:O	2:D:167:MET:HG2	1.87	0.74
2:D:25:PHE:HB2	2:D:29:LEU:HD12	1.69	0.74
1:A:419:SER:O	1:A:423:ARG:HG2	1.86	0.74
1:C:286:ARG:O	1:C:288:PRO:HD3	1.87	0.74
2:D:366:GLU:O	2:D:370:VAL:HG23	1.87	0.74
2:F:145:PRO:HB2	2:F:357:ILE:HD11	1.70	0.74
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.23	0.74
1:C:297:ASP:HA	2:E:267:GLU:OE1	1.88	0.74
1:B:342:VAL:HA	1:B:345:ILE:HD12	1.69	0.74
2:D:314:ALA:O	2:D:315:ASP:HB2	1.86	0.74
1:B:44:LEU:HD22	1:B:47:VAL:CG2	2.18	0.74
2:D:130:GLN:HB3	2:D:357:ILE:CD1	2.18	0.74
2:E:391:LEU:CD2	3:G:23:MET:SD	2.76	0.74
3:G:77:LEU:HD12	3:G:228:ARG:HH12	1.53	0.74
2:D:196:LEU:O	2:D:200:MET:HG3	1.87	0.73
4:H:35:ARG:O	4:H:38:ALA:HB3	1.88	0.73
2:E:336:SER:OG	2:E:339:ILE:HG12	1.88	0.73
1:C:461:ILE:O	1:C:464:PHE:HB3	1.88	0.73
2:E:173:VAL:HG21	2:E:252:LEU:CD1	2.19	0.73
1:A:363:PRO:CD	1:A:430:GLN:HB3	2.17	0.73
2:F:257:ASN:HD22	2:F:260:ARG:CZ	2.01	0.73
1:C:399:GLU:OE2	4:H:19:GLY:HA3	1.88	0.73
1:A:389:THR:HB	1:A:449:VAL:CG1	2.19	0.73
2:E:390:ILE:HD11	3:G:16:ILE:HG12	1.68	0.73
1:A:38:ILE:HG23	1:A:285:LEU:HD23	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:VAL:HG13	2:D:232:VAL:HG13	1.71	0.73
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.24	0.73
1:C:137:ILE:HB	1:C:138:PRO:HD3	1.70	0.73
2:E:186:VAL:HG12	2:E:260:ARG:HB2	1.70	0.73
2:F:89:GLU:H	2:F:89:GLU:CD	1.89	0.73
1:A:381:ARG:HD2	1:A:488:LYS:HB3	1.70	0.73
1:B:165:GLU:O	1:B:325:PRO:HD2	1.88	0.73
2:E:335:LEU:HA	2:E:347:ALA:O	1.89	0.73
2:F:172:ASN:HD22	2:F:431:LEU:HD13	1.52	0.73
1:A:199:LEU:HD12	1:A:263:HIS:O	1.89	0.73
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.70	0.73
2:F:185:GLY:HA3	2:F:188:GLU:HG3	1.71	0.72
1:A:36:ASP:HB3	1:A:284:LEU:HD13	1.71	0.72
1:C:248:TYR:OH	1:C:301:LEU:HD12	1.89	0.72
1:C:69:ASP:O	1:C:70:ASN:HB3	1.89	0.72
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.24	0.72
2:F:130:GLN:HB3	2:F:357:ILE:CD1	2.19	0.72
1:C:362:ARG:HH22	2:F:372:ARG:HD2	1.52	0.72
1:B:28:THR:HG22	1:B:29:GLY:N	2.03	0.72
1:B:196:LYS:N	1:B:196:LYS:HD2	2.05	0.72
2:E:160:VAL:HG23	2:E:335:LEU:HD23	1.71	0.72
2:F:159:GLY:H	5:F:1478:ANP:HNB1	1.37	0.72
2:E:388:ILE:HG21	2:E:396:LEU:HD11	1.71	0.72
1:A:156:LEU:HD21	1:A:390:MET:SD	2.30	0.72
1:A:381:ARG:HG2	1:A:488:LYS:HD2	1.71	0.72
2:D:170:ILE:O	2:D:174:ALA:HB3	1.89	0.72
1:A:129:VAL:HG12	1:A:249:SER:HA	1.70	0.72
2:D:159:GLY:H	5:D:1478:ANP:HNB1	1.37	0.72
1:C:213:VAL:O	1:C:216:LEU:HB3	1.89	0.72
1:C:246:ALA:HB3	1:C:247:PRO:HD3	1.72	0.72
2:F:221:GLN:HE21	2:F:221:GLN:CA	2.03	0.72
2:F:51:GLN:HG3	2:F:59:ARG:HB3	1.71	0.72
1:B:270:ASP:N	1:B:326:VAL:HB	2.05	0.72
2:F:391:LEU:HB3	2:F:395:GLU:HG3	1.71	0.72
1:B:100:GLY:HA2	1:B:256:TYR:CE2	2.25	0.72
1:B:140:ILE:CG1	1:B:143:ARG:HH12	2.03	0.72
2:D:97:VAL:HG21	2:D:228:ALA:HB1	1.72	0.72
1:C:295:PRO:HD2	1:C:298:VAL:HG22	1.71	0.72
2:F:139:VAL:HG13	2:F:414:LEU:HD22	1.71	0.72
1:C:440:GLU:HB3	1:C:469:LEU:HD11	1.72	0.71
1:C:352:LEU:HA	1:C:364:ALA:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ARG:HB2	1:C:487:GLY:O	1.90	0.71
1:A:420:ARG:HH21	1:A:451:GLY:CA	2.03	0.71
1:B:41:VAL:HG11	1:B:44:LEU:HD12	1.71	0.71
1:C:362:ARG:HH22	2:D:372:ARG:HD2	1.54	0.71
2:E:159:GLY:N	5:F:1478:ANP:HNB1	1.88	0.71
1:A:361:ILE:HD12	1:A:425:THR:HG21	1.73	0.71
2:E:221:GLN:CB	2:E:223:ASN:HD21	2.03	0.71
2:E:257:ASN:ND2	2:E:260:ARG:CZ	2.53	0.71
2:F:223:ASN:H	2:F:223:ASN:ND2	1.88	0.71
2:F:382:LYS:HA	2:F:385:GLN:NE2	2.04	0.71
1:A:151:LYS:HD2	1:A:444:VAL:HG21	1.72	0.71
2:D:393:MET:SD	2:D:404:VAL:HG11	2.30	0.71
2:E:252:LEU:HD23	2:E:305:THR:HB	1.71	0.71
1:C:413:ALA:HB2	4:H:31:GLU:OE1	1.90	0.71
2:D:89:GLU:CG	2:D:110:THR:HG22	2.21	0.71
1:C:303:SER:HB2	2:E:222:MET:HB3	1.73	0.71
1:A:478:ALA:O	1:A:482:LYS:HG3	1.89	0.71
1:C:44:LEU:O	1:C:47:VAL:HG22	1.91	0.71
2:D:237:LEU:O	2:D:241:GLU:HG3	1.90	0.71
1:B:358:TYR:C	1:B:360:GLY:H	1.92	0.71
1:C:439:GLU:HG2	1:C:440:GLU:N	2.04	0.71
1:A:422:VAL:HG23	1:A:423:ARG:HD2	1.72	0.71
1:C:482:LYS:O	1:C:484:ARG:N	2.22	0.71
2:F:279:VAL:HG12	2:F:279:VAL:O	1.90	0.71
1:A:389:THR:HB	1:A:449:VAL:HG11	1.73	0.71
1:A:24:ASP:O	1:A:28:THR:HB	1.90	0.71
1:C:237:SER:HB3	2:F:294:GLU:HG3	1.71	0.71
1:B:270:ASP:H	1:B:326:VAL:HB	1.56	0.71
2:F:440:GLY:O	2:F:444:ILE:HG12	1.91	0.71
1:C:219:ARG:HD2	1:C:433:TYR:CE2	2.26	0.71
1:A:186:GLN:HG3	1:A:199:LEU:HD23	1.72	0.70
1:C:127:ARG:HE	1:C:131:LEU:CD1	2.03	0.70
2:D:96:ASN:ND2	2:D:96:ASN:C	2.45	0.70
1:A:411:ASP:OD2	1:A:413:ALA:HB3	1.91	0.70
1:B:456:LEU:HD23	1:B:461:ILE:HD13	1.71	0.70
2:E:139:VAL:HG12	2:E:414:LEU:HD22	1.73	0.70
2:F:237:LEU:HD11	2:F:296:ILE:HG12	1.73	0.70
2:E:159:GLY:H	5:F:1478:ANP:HNB1	1.37	0.70
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.73	0.70
1:A:44:LEU:O	1:A:47:VAL:HG22	1.91	0.70
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:HD13	1:B:429:LYS:HE2	1.73	0.70
2:D:408:ARG:HD2	4:H:22:PHE:CZ	2.26	0.70
1:A:287:ARG:HB3	1:A:288:PRO:HD2	1.74	0.70
1:A:345:ILE:HA	2:E:222:MET:SD	2.31	0.70
1:B:172:GLN:HA	5:B:1511:ANP:HNB1	1.57	0.70
2:D:388:ILE:HD11	2:D:396:LEU:CD1	2.19	0.70
2:F:200:MET:HB3	2:F:205:VAL:HG23	1.74	0.70
1:C:188:ARG:HH12	1:C:435:PRO:CB	1.98	0.70
1:C:356:LEU:HD11	1:C:366:ASN:HB2	1.74	0.70
1:A:157:VAL:HG12	1:A:372:SER:HB2	1.72	0.70
4:H:12:ALA:O	4:H:15:VAL:N	2.25	0.70
1:A:405:GLN:NE2	2:D:384:LEU:HD21	2.05	0.70
1:C:432:GLN:NE2	1:C:433:TYR:OH	2.24	0.70
1:A:424:LEU:O	1:A:428:LEU:HG	1.91	0.70
1:A:496:LYS:O	1:A:500:ILE:HG13	1.91	0.70
2:D:337:ARG:HG2	2:D:341:GLU:OE2	1.91	0.70
1:A:140:ILE:CG1	1:A:143:ARG:HH22	2.04	0.70
1:A:140:ILE:HG12	1:A:143:ARG:NH1	2.06	0.70
1:B:422:VAL:O	1:B:426:GLU:HG2	1.91	0.70
1:B:307:GLU:OE1	2:F:223:ASN:HB3	1.92	0.70
1:A:206:ILE:CD1	1:A:247:PRO:HG3	2.21	0.70
1:A:334:VAL:HG11	1:A:351:PHE:CD2	2.27	0.70
2:F:139:VAL:HG12	2:F:414:LEU:HD22	1.74	0.70
1:B:80:LYS:HD2	2:E:33:LEU:HD12	1.74	0.70
3:G:11:LYS:HB3	4:H:7:ASN:CG	2.12	0.70
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.56	0.70
1:C:132:LYS:HE3	2:E:223:ASN:ND2	2.06	0.70
1:C:99:VAL:HG12	1:C:100:GLY:N	2.05	0.70
1:C:395:ALA:HA	1:C:398:ARG:HD2	1.73	0.69
1:A:403:PHE:N	1:A:403:PHE:HD2	1.90	0.69
1:A:151:LYS:HA	1:A:441:GLN:CD	2.11	0.69
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.74	0.69
2:D:181:SER:O	2:D:215:VAL:HA	1.91	0.69
1:A:28:THR:HG22	1:A:29:GLY:N	2.07	0.69
4:H:9:ARG:HA	4:H:15:VAL:HG22	1.74	0.69
1:A:107:VAL:HG13	1:A:231:VAL:HG12	1.72	0.69
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.07	0.69
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.73	0.69
4:H:11:SER:C	4:H:15:VAL:HG21	2.11	0.69
2:D:139:VAL:HG22	2:D:414:LEU:HB3	1.74	0.69
2:D:351:LEU:HD13	2:D:379:GLN:OE1	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:HA	1:A:198:LYS:HG2	1.75	0.69
1:A:166:LEU:HD13	1:A:342:VAL:HG11	1.73	0.69
1:A:460:LYS:HD2	1:A:460:LYS:N	2.07	0.69
1:C:457:GLU:HB3	1:C:460:LYS:HG3	1.75	0.69
2:D:285:LEU:HD23	2:D:285:LEU:C	2.13	0.69
1:A:403:PHE:N	1:A:403:PHE:CD2	2.57	0.69
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.74	0.69
2:D:242:TYR:CE1	2:D:246:GLN:HG3	2.26	0.69
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.75	0.69
2:E:25:PHE:O	2:E:56:SER:HB3	1.91	0.69
2:F:388:ILE:HG23	2:F:393:MET:HB2	1.75	0.69
1:C:175:LYS:HE3	5:C:1511:ANP:O1B	1.91	0.69
2:D:409:LYS:HE2	2:D:452:LEU:O	1.93	0.69
1:B:446:TYR:CE2	1:B:497:LEU:HB3	2.28	0.68
2:E:244:ARG:HD3	2:E:304:ILE:HG13	1.75	0.68
1:B:87:ILE:HD12	1:B:87:ILE:N	2.08	0.68
2:E:84:ILE:HD13	2:E:235:THR:HG23	1.76	0.68
1:A:166:LEU:HD22	1:A:342:VAL:HG12	1.75	0.68
2:F:257:ASN:HA	2:F:309:ALA:O	1.93	0.68
1:A:108:VAL:HG12	1:A:114:ALA:HA	1.76	0.68
3:G:11:LYS:HB3	4:H:7:ASN:ND2	2.09	0.68
2:D:49:VAL:HA	2:D:60:THR:HG22	1.74	0.68
2:F:170:ILE:O	2:F:174:ALA:HB3	1.94	0.68
2:D:419:GLN:O	2:D:422:GLU:HG3	1.94	0.68
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.74	0.68
1:A:323:ALA:O	1:A:324:LEU:HD23	1.94	0.68
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.75	0.68
2:D:412:ARG:HG3	2:D:412:ARG:HH11	1.59	0.68
2:F:163:THR:O	2:F:167:MET:HG3	1.93	0.68
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.74	0.68
1:A:149:GLY:HA3	1:A:435:PRO:HB2	1.75	0.68
2:F:287:THR:O	2:F:291:THR:HG23	1.94	0.68
2:E:393:MET:HG3	2:E:396:LEU:CD1	2.22	0.68
2:D:408:ARG:HD2	4:H:22:PHE:CE2	2.29	0.68
1:B:143:ARG:HG3	1:B:143:ARG:HH11	1.59	0.68
1:B:188:ARG:HE	1:B:437:ALA:HB2	1.59	0.68
2:E:251:VAL:HG12	2:E:252:LEU:N	2.09	0.68
1:B:347:ASP:HA	1:B:373:ARG:NH1	2.09	0.67
4:H:8:VAL:O	4:H:15:VAL:HG22	1.94	0.67
1:A:175:LYS:HE3	5:A:1511:ANP:O1B	1.94	0.67
1:A:114:ALA:HB2	1:A:121:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HB3	1:A:287:ARG:NH2	2.08	0.67
2:F:223:ASN:HD22	2:F:224:GLU:N	1.93	0.67
1:A:38:ILE:CG2	1:A:285:LEU:HD23	2.24	0.67
1:C:153:VAL:HA	1:C:157:VAL:CG2	2.23	0.67
1:A:390:MET:CE	1:A:445:ILE:HG23	2.25	0.67
1:C:201:CYS:HB2	1:C:229:THR:HG23	1.74	0.67
1:C:156:LEU:HD13	1:C:391:LYS:HG3	1.74	0.67
1:B:266:ILE:HG22	1:B:322:THR:O	1.94	0.67
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.76	0.67
1:A:151:LYS:HE3	1:A:427:LEU:O	1.94	0.67
2:D:453:PRO:HG2	4:H:34:PHE:CE2	2.29	0.67
1:B:338:ILE:N	1:B:338:ILE:HD12	2.09	0.67
2:D:12:ARG:HE	2:D:74:LYS:CE	2.08	0.67
1:A:166:LEU:HB2	1:A:346:THR:HG21	1.76	0.67
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.29	0.67
2:D:382:LYS:HA	2:D:385:GLN:NE2	2.09	0.67
2:E:251:VAL:HG12	2:E:252:LEU:H	1.60	0.67
1:A:363:PRO:HD2	1:A:430:GLN:CB	2.24	0.67
1:B:338:ILE:CD1	1:B:338:ILE:H	2.08	0.67
2:E:381:TYR:OH	4:H:22:PHE:HE2	1.78	0.67
1:A:151:LYS:CE	1:A:436:MET:SD	2.79	0.67
1:B:105:GLY:HA2	1:B:226:MET:O	1.95	0.67
2:E:25:PHE:O	2:E:56:SER:HB3	1.95	0.67
1:A:100:GLY:HA2	1:A:256:TYR:CE2	2.30	0.67
1:A:381:ARG:CD	1:A:488:LYS:HB3	2.24	0.67
1:B:419:SER:O	1:B:423:ARG:HG2	1.95	0.67
1:C:74:VAL:HG12	1:C:241:PRO:HG2	1.76	0.67
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.76	0.67
1:B:442:VAL:O	1:B:446:TYR:HB2	1.95	0.67
1:C:38:ILE:HG13	1:C:284:LEU:HB3	1.76	0.67
1:B:478:ALA:O	1:B:482:LYS:HG3	1.96	0.66
2:D:282:GLN:H	2:D:282:GLN:HE21	0.74	0.66
1:A:150:ILE:HA	1:A:430:GLN:OE1	1.96	0.66
2:E:203:SER:HB2	2:E:420:VAL:CG1	2.24	0.66
2:E:255:ILE:HD12	2:E:308:GLN:HE21	1.60	0.66
1:A:438:ILE:O	1:A:441:GLN:HB2	1.94	0.66
3:G:23:MET:SD	3:G:232:MET:HE1	2.35	0.66
1:C:413:ALA:HB2	4:H:31:GLU:OE2	1.96	0.66
2:D:191:ARG:HG2	2:D:191:ARG:HH11	1.59	0.66
1:C:156:LEU:HD22	1:C:391:LYS:CB	2.25	0.66
1:C:151:LYS:HD2	1:C:428:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:ILE:HD11	2:F:292:MET:SD	2.36	0.66
2:F:378:LEU:HD21	2:F:411:GLN:HG2	1.77	0.66
2:F:419:GLN:O	2:F:422:GLU:HG3	1.96	0.66
1:B:438:ILE:O	1:B:442:VAL:HG12	1.96	0.66
1:A:362:ARG:O	1:A:429:LYS:HA	1.96	0.66
1:C:166:LEU:O	1:C:166:LEU:HG	1.95	0.66
1:A:469:LEU:O	1:A:472:VAL:HG22	1.95	0.66
1:C:249:SER:O	1:C:253:MET:HG3	1.94	0.66
1:C:300:TYR:CZ	1:C:304:ARG:HD3	2.31	0.66
1:B:406:PHE:HE1	2:E:395:GLU:HB3	1.60	0.66
1:A:407:GLY:HA3	1:A:410:LEU:HG	1.77	0.66
1:B:206:ILE:CD1	1:B:247:PRO:HG3	2.24	0.66
2:E:255:ILE:HD12	2:E:308:GLN:NE2	2.10	0.66
2:F:96:ASN:HD21	2:F:100:GLU:H	1.44	0.66
1:B:62:MET:CE	1:B:64:LEU:HD21	2.25	0.66
2:F:141:ASP:O	2:F:145:PRO:HG3	1.96	0.66
1:B:327:ILE:HD11	1:B:342:VAL:HG21	1.78	0.66
2:F:359:ASP:HB3	2:F:362:ILE:HD12	1.76	0.66
1:A:367:VAL:HG21	1:A:428:LEU:CD1	2.26	0.66
2:E:340:ALA:HB2	2:E:347:ALA:HB2	1.77	0.66
2:F:279:VAL:CG2	3:G:255:GLN:HG2	2.26	0.66
2:D:252:LEU:CD2	2:D:305:THR:HB	2.24	0.66
1:A:155:SER:CB	1:A:383:MET:SD	2.84	0.66
1:B:203:TYR:HE2	1:B:205:ALA:HB2	1.60	0.66
1:A:406:PHE:CZ	3:G:23:MET:HG2	2.31	0.66
1:B:218:LYS:HG3	2:E:128:VAL:HG21	1.76	0.66
2:E:164:VAL:HG12	2:E:418:PHE:HD1	1.61	0.66
4:H:35:ARG:O	4:H:38:ALA:HB3	1.96	0.66
2:E:395:GLU:OE1	2:E:395:GLU:HA	1.96	0.66
1:C:132:LYS:HE3	2:E:224:GLU:OE2	1.95	0.66
2:E:473:LEU:HB3	4:H:34:PHE:CE2	2.31	0.66
2:F:371:ALA:O	2:F:375:GLN:HG3	1.96	0.66
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.77	0.66
1:A:420:ARG:HH11	1:A:420:ARG:HG3	1.61	0.65
1:A:151:LYS:HE2	1:A:465:GLU:OE2	1.97	0.65
1:B:99:VAL:CG2	1:B:253:MET:HA	2.25	0.65
1:C:136:ILE:HG23	2:E:194:ASN:HA	1.77	0.65
1:C:352:LEU:HA	1:C:364:ALA:O	1.96	0.65
1:C:65:ASN:OD1	1:C:285:LEU:HD22	1.96	0.65
1:B:452:TYR:O	1:B:453:LEU:HD23	1.97	0.65
1:C:172:GLN:HA	5:C:1511:ANP:HNB1	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ARG:HG2	1:C:423:ARG:NH1	2.07	0.65
1:A:363:PRO:HD2	1:A:430:GLN:HB3	1.76	0.65
2:E:146:TYR:O	2:E:357:ILE:HD11	1.97	0.65
1:C:153:VAL:HG13	1:C:157:VAL:HG23	1.78	0.65
1:C:294:TYR:CB	1:C:298:VAL:HG21	2.25	0.65
2:E:83:ARG:HA	2:E:114:ALA:O	1.96	0.65
2:E:237:LEU:O	2:E:241:GLU:HG3	1.97	0.65
1:B:175:LYS:HE3	5:B:1511:ANP:O1B	1.97	0.65
1:B:468:PHE:CZ	1:B:501:VAL:HG12	2.31	0.65
1:C:206:ILE:N	1:C:206:ILE:HD12	2.11	0.65
2:D:359:ASP:O	2:D:363:VAL:HG22	1.97	0.65
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.27	0.65
1:C:381:ARG:HD2	1:C:381:ARG:H	1.61	0.65
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.31	0.65
2:D:346:PRO:O	2:D:348:VAL:N	2.29	0.65
1:A:251:CYS:O	1:A:255:GLU:HG3	1.97	0.65
1:A:280:GLN:CD	2:D:284:THR:HG22	2.17	0.65
2:E:258:ILE:O	2:E:261:PHE:HB3	1.97	0.65
2:E:452:LEU:HD22	2:E:470:ALA:CB	2.27	0.65
1:B:423:ARG:HG2	1:B:453:LEU:O	1.96	0.65
1:C:209:LYS:O	1:C:212:THR:N	2.30	0.65
1:C:27:GLU:O	1:C:90:ARG:HG3	1.96	0.65
2:E:171:ASN:HA	2:E:175:LYS:HE3	1.77	0.65
1:C:156:LEU:HA	1:C:391:LYS:HD2	1.78	0.65
2:E:96:ASN:ND2	2:E:98:ILE:HG12	2.11	0.65
2:D:221:GLN:HB2	2:D:223:ASN:ND2	2.12	0.65
2:F:377:ILE:HG21	2:F:410:ILE:HD12	1.79	0.65
1:B:141:SER:O	1:B:143:ARG:HD2	1.97	0.65
3:G:14:LYS:HA	3:G:243:ILE:HD11	1.79	0.65
1:A:36:ASP:O	1:A:284:LEU:HD13	1.97	0.65
1:C:440:GLU:OE1	1:C:473:ILE:HD11	1.97	0.65
1:C:80:LYS:HD2	2:F:33:LEU:HD12	1.77	0.65
1:C:110:ALA:HB3	1:C:242:LEU:HD22	1.79	0.64
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.77	0.64
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.79	0.64
2:E:246:GLN:NE2	2:E:246:GLN:HA	2.06	0.64
1:B:48:GLN:HB3	2:F:68:GLY:HA2	1.78	0.64
2:E:384:LEU:O	2:E:388:ILE:HG12	1.97	0.64
2:F:279:VAL:HG21	3:G:255:GLN:HG2	1.78	0.64
2:E:363:VAL:O	2:E:367:HIS:HB3	1.97	0.64
2:F:151:LYS:HE3	2:F:296:ILE:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASP:O	1:C:26:GLU:N	2.27	0.64
1:A:154:ASP:HB2	1:A:441:GLN:HE22	1.61	0.64
1:A:104:LEU:HD23	1:A:230:ILE:HG13	1.80	0.64
1:A:36:ASP:HB3	1:A:284:LEU:CD1	2.27	0.64
1:A:458:PRO:O	1:A:461:ILE:HG12	1.98	0.64
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.78	0.64
3:G:4:LYS:O	3:G:8:ARG:HG3	1.97	0.64
1:A:363:PRO:HD3	1:A:430:GLN:HB3	1.80	0.64
1:B:331:ALA:O	1:B:333:ASP:N	2.31	0.64
2:D:25:PHE:O	2:D:56:SER:HB3	1.98	0.64
1:A:149:GLY:HA3	1:A:435:PRO:HB2	1.79	0.64
1:A:47:VAL:CG1	1:A:90:ARG:HG2	2.28	0.64
2:D:122:GLU:HG2	2:D:125:GLU:OE2	1.97	0.64
2:F:96:ASN:HD21	2:F:98:ILE:HG12	1.61	0.64
4:H:4:SER:HA	4:H:7:ASN:HD21	1.61	0.64
1:A:478:ALA:O	1:A:482:LYS:HG3	1.98	0.64
2:D:159:GLY:N	5:D:1478:ANP:HNB1	1.95	0.64
2:D:363:VAL:HB	2:D:367:HIS:ND1	2.12	0.64
1:B:298:VAL:O	1:B:301:LEU:HB3	1.98	0.64
1:C:26:GLU:O	1:C:46:ASN:HB2	1.98	0.64
1:C:479:LEU:HD21	1:C:493:SER:HB3	1.79	0.64
1:C:501:VAL:HG23	1:C:502:THR:H	1.63	0.64
1:B:349:GLN:HB2	1:B:351:PHE:CE1	2.32	0.64
2:E:473:LEU:CB	4:H:34:PHE:CZ	2.75	0.64
2:D:453:PRO:HG2	4:H:34:PHE:CD2	2.33	0.64
2:E:223:ASN:H	2:E:223:ASN:ND2	1.94	0.64
2:E:223:ASN:ND2	2:E:223:ASN:N	2.45	0.64
1:B:49:ALA:O	1:B:50:GLU:HB2	1.96	0.64
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.79	0.64
2:F:282:GLN:HE21	2:F:282:GLN:H	0.71	0.64
1:B:251:CYS:O	1:B:255:GLU:HG3	1.98	0.64
1:C:338:ILE:HD12	1:C:338:ILE:N	2.10	0.64
2:D:237:LEU:CD1	2:D:296:ILE:HG12	2.28	0.64
1:A:83:LYS:HD3	2:F:31:PRO:HB3	1.79	0.64
2:D:412:ARG:HG3	2:D:412:ARG:HH11	1.63	0.64
1:B:172:GLN:H	5:B:1511:ANP:HNB1	1.46	0.63
1:B:334:VAL:HG11	1:B:351:PHE:CE2	2.33	0.63
1:A:164:ARG:HD3	1:A:164:ARG:N	2.14	0.63
1:B:403:PHE:CD2	1:B:403:PHE:N	2.66	0.63
1:C:336:ALA:O	1:C:340:THR:HG23	1.99	0.63
4:H:30:GLU:O	4:H:34:PHE:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:CG1	1:A:372:SER:HB2	2.28	0.63
1:B:358:TYR:C	1:B:360:GLY:N	2.52	0.63
1:C:381:ARG:H	1:C:381:ARG:CD	2.12	0.63
2:F:152:ILE:HD12	2:F:152:ILE:N	2.13	0.63
1:C:175:LYS:HB2	5:C:1511:ANP:O1B	1.99	0.63
1:C:392:LEU:O	1:C:396:GLN:HG2	1.97	0.63
2:F:396:LEU:HD13	2:F:400:ASP:HB3	1.79	0.63
2:D:166:ILE:HG22	2:D:167:MET:N	2.13	0.63
2:E:221:GLN:HB3	2:E:223:ASN:HD21	1.62	0.63
2:E:257:ASN:HD22	2:E:260:ARG:NE	1.97	0.63
2:D:252:LEU:CD2	2:D:305:THR:HB	2.28	0.63
2:D:32:ILE:O	2:D:33:LEU:HB2	1.97	0.63
2:E:257:ASN:H	2:E:309:ALA:HB3	1.64	0.63
2:F:257:ASN:N	2:F:309:ALA:HB3	2.12	0.63
1:C:213:VAL:O	1:C:217:VAL:HG12	1.99	0.63
1:B:296:GLY:O	2:F:267:GLU:HG2	1.99	0.63
1:A:74:VAL:HG11	1:A:241:PRO:HB3	1.80	0.63
1:A:87:ILE:N	1:A:87:ILE:HD12	2.13	0.63
1:B:166:LEU:HD13	1:B:342:VAL:HG11	1.80	0.63
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.79	0.63
2:D:221:GLN:HA	2:D:221:GLN:HE21	1.62	0.63
2:D:257:ASN:OD1	2:D:259:PHE:HB3	1.99	0.63
2:E:246:GLN:HE21	2:E:246:GLN:CA	2.08	0.63
2:F:433:PRO:HD2	2:F:436:GLU:HG3	1.79	0.63
1:A:151:LYS:CG	1:A:441:GLN:HG2	2.28	0.63
2:E:116:ILE:HA	2:E:238:THR:OG1	1.97	0.63
1:A:355:GLU:O	1:A:359:LYS:HG3	1.99	0.63
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.80	0.63
1:A:34:ILE:HD11	1:A:79:ASP:HB2	1.81	0.62
2:D:64:ASP:HA	2:D:225:PRO:HG3	1.81	0.62
2:F:116:ILE:HA	2:F:238:THR:OG1	1.99	0.62
3:G:77:LEU:HD12	3:G:228:ARG:NH1	2.14	0.62
1:C:188:ARG:HH22	1:C:435:PRO:C	2.02	0.62
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.82	0.62
2:E:181:SER:OG	2:E:252:LEU:HD12	1.99	0.62
1:C:23:VAL:O	1:C:23:VAL:HG12	1.99	0.62
1:A:339:PRO:O	1:A:343:ILE:HG13	1.99	0.62
1:A:458:PRO:HA	1:A:461:ILE:HG12	1.80	0.62
1:C:206:ILE:HD11	1:C:247:PRO:HG3	1.81	0.62
2:F:237:LEU:HD21	2:F:295:ARG:HD3	1.81	0.62
1:A:77:GLY:H	1:A:239:ALA:CB	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:PRO:HG2	2:E:34:ASN:OD1	2.00	0.62
1:A:383:MET:HE2	1:A:442:VAL:CG1	2.29	0.62
1:B:45:ARG:NH1	1:B:45:ARG:HG2	2.13	0.62
1:B:26:GLU:O	1:B:46:ASN:HB2	1.98	0.62
2:E:422:GLU:HG2	2:E:427:HIS:O	2.00	0.62
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.82	0.62
1:C:105:GLY:HA2	1:C:226:MET:O	1.98	0.62
4:H:11:SER:C	4:H:15:VAL:HG21	2.20	0.62
1:A:154:ASP:HB2	1:A:441:GLN:NE2	2.15	0.62
1:A:361:ILE:HD13	1:A:429:LYS:CD	2.29	0.62
1:C:163:GLN:HG2	1:C:164:ARG:H	1.64	0.62
2:D:443:GLN:HE21	2:D:449:TYR:HE1	1.48	0.62
1:A:180:ILE:O	1:A:184:ILE:HG12	1.99	0.62
1:A:461:ILE:O	1:A:464:PHE:HB3	1.99	0.62
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.81	0.62
2:E:223:ASN:H	2:E:223:ASN:HD22	1.43	0.62
1:A:390:MET:HG3	1:A:424:LEU:HD13	1.79	0.62
1:B:186:GLN:HG3	1:B:199:LEU:HD23	1.80	0.62
2:D:434:LEU:O	2:D:438:ILE:HG12	1.99	0.62
2:E:245:ASP:C	2:E:247:GLU:H	2.01	0.62
1:A:361:ILE:HD13	1:A:429:LYS:HE2	1.81	0.62
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.81	0.62
1:C:32:LEU:HD21	1:C:42:HIS:HB2	1.80	0.62
1:C:381:ARG:HD2	1:C:381:ARG:N	2.15	0.62
2:E:292:MET:HE2	2:E:293:GLN:HA	1.81	0.62
1:A:164:ARG:HG2	1:A:164:ARG:HH11	1.64	0.62
1:A:430:GLN:HE22	1:A:435:PRO:HA	1.64	0.62
2:F:12:ARG:HG2	2:F:74:LYS:HD3	1.82	0.62
1:C:483:ILE:CD1	1:C:489:ILE:HG12	2.30	0.62
2:F:10:THR:HG23	2:F:76:LEU:HD23	1.82	0.62
1:A:400:VAL:HG21	1:A:417:LEU:HD12	1.82	0.62
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.35	0.62
1:C:166:LEU:HD11	1:C:168:ILE:HB	1.82	0.62
1:C:294:TYR:CE1	1:C:338:ILE:HD11	2.35	0.62
2:D:159:GLY:HA2	5:D:1478:ANP:HNB1	1.65	0.62
2:F:32:ILE:O	2:F:33:LEU:HB2	2.00	0.62
1:C:386:VAL:HG23	1:C:387:ALA:H	1.64	0.62
2:F:257:ASN:HD22	2:F:260:ARG:NE	1.97	0.62
1:C:151:LYS:HE3	1:C:428:LEU:O	1.98	0.62
1:C:472:VAL:HG23	1:C:473:ILE:N	2.15	0.62
2:F:335:LEU:HA	2:F:347:ALA:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:GLU:HG3	1:C:480:LEU:HB3	1.82	0.61
1:A:472:VAL:HG23	1:A:473:ILE:N	2.14	0.61
1:A:52:MET:CG	1:A:95:VAL:HG22	2.30	0.61
1:B:441:GLN:O	1:B:445:ILE:HG12	2.00	0.61
2:F:387:ILE:HD12	2:F:387:ILE:H	1.65	0.61
1:A:151:LYS:CE	1:A:427:LEU:O	2.48	0.61
2:D:182:VAL:HG21	2:D:240:ALA:HB2	1.82	0.61
2:E:125:GLU:HA	2:E:300:LYS:HE3	1.82	0.61
2:D:89:GLU:CD	2:D:89:GLU:H	2.02	0.61
2:E:218:VAL:HG21	2:E:236:GLY:HA2	1.81	0.61
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.82	0.61
1:C:453:LEU:HD23	1:C:505:LEU:HG	1.81	0.61
1:A:367:VAL:CG2	1:A:428:LEU:HD13	2.30	0.61
1:B:286:ARG:HH12	3:G:272:LEU:HD13	1.66	0.61
1:B:420:ARG:O	1:B:424:LEU:HG	2.01	0.61
2:D:157:GLY:HA3	2:D:315:ASP:OD1	2.00	0.61
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.82	0.61
2:E:170:ILE:HD13	2:E:215:VAL:HG21	1.80	0.61
2:E:31:PRO:HG2	2:E:34:ASN:CG	2.21	0.61
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.82	0.61
2:F:32:ILE:O	2:F:33:LEU:HB2	2.01	0.61
2:E:381:TYR:OH	4:H:22:PHE:CE2	2.54	0.61
1:A:400:VAL:HG11	1:A:414:THR:HB	1.83	0.61
1:B:171:ARG:HH11	1:B:171:ARG:HB2	1.65	0.61
2:F:374:VAL:O	2:F:378:LEU:HG	2.00	0.61
1:A:196:LYS:HD2	1:A:196:LYS:N	2.15	0.61
1:B:410:LEU:O	1:B:411:ASP:HB3	1.99	0.61
1:B:54:GLU:HG2	1:B:60:LYS:NZ	2.14	0.61
1:C:278:TYR:CD2	1:C:301:LEU:HD22	2.35	0.61
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.83	0.61
2:E:390:ILE:CG2	3:G:28:ALA:HB1	2.30	0.61
2:F:434:LEU:O	2:F:438:ILE:HG12	2.01	0.61
1:B:442:VAL:HB	1:B:489:ILE:HD11	1.83	0.61
1:A:159:ILE:HD11	1:A:165:GLU:HG2	1.83	0.61
2:F:264:ALA:O	2:F:268:VAL:HG23	2.00	0.61
1:A:355:GLU:HG2	1:A:359:LYS:HE3	1.82	0.61
1:A:210:ARG:NH1	2:D:120:ALA:HB3	2.15	0.61
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.30	0.61
2:F:140:VAL:HG11	2:F:146:TYR:CZ	2.36	0.61
1:A:35:GLY:O	1:A:36:ASP:HB2	2.01	0.61
1:A:390:MET:HE3	1:A:445:ILE:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HD13	1:A:178:ILE:HD12	1.82	0.61
2:E:136:GLY:HA2	2:E:432:VAL:O	2.00	0.61
2:F:31:PRO:O	2:F:34:ASN:HB2	2.01	0.61
1:C:132:LYS:HG3	2:E:223:ASN:HD22	1.66	0.61
1:C:19:ALA:O	1:C:21:THR:HG23	2.01	0.61
2:F:96:ASN:ND2	2:F:98:ILE:HG12	2.16	0.61
1:A:36:ASP:CB	1:A:284:LEU:HD13	2.31	0.61
2:D:345:TYR:HA	2:D:346:PRO:C	2.21	0.61
1:B:218:LYS:HG3	2:E:128:VAL:CG2	2.31	0.61
1:B:186:GLN:OE1	1:B:199:LEU:HD23	2.01	0.60
1:C:279:ARG:HD3	1:C:294:TYR:CD2	2.36	0.60
2:E:279:VAL:O	2:E:279:VAL:HG12	2.01	0.60
2:F:170:ILE:HD13	2:F:215:VAL:CG2	2.29	0.60
1:A:313:ASN:OD1	1:A:315:ALA:HB3	2.00	0.60
1:A:430:GLN:NE2	1:A:435:PRO:HA	2.15	0.60
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.83	0.60
2:E:32:ILE:O	2:E:33:LEU:HB2	1.99	0.60
2:D:92:GLY:HA2	2:D:206:ILE:HD12	1.83	0.60
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.16	0.60
2:F:220:GLY:HA3	2:F:232:VAL:HG21	1.83	0.60
1:C:66:LEU:HB2	2:D:16:VAL:HB	1.82	0.60
1:A:439:GLU:OE1	1:A:484:ARG:HG3	2.00	0.60
2:F:228:ALA:O	2:F:232:VAL:HG22	2.01	0.60
2:F:237:LEU:O	2:F:241:GLU:HG3	2.00	0.60
2:F:390:ILE:O	2:F:392:GLY:N	2.34	0.60
1:C:327:ILE:CD1	1:C:342:VAL:HG21	2.31	0.60
3:G:10:LEU:O	3:G:14:LYS:HG3	2.01	0.60
2:D:16:VAL:C	2:D:17:ILE:HD12	2.22	0.60
2:E:452:LEU:HD21	4:H:37:ARG:NH1	2.16	0.60
4:H:25:ARG:O	4:H:29:GLU:HG2	2.02	0.60
1:B:486:ASP:C	1:B:488:LYS:H	2.04	0.60
2:D:136:GLY:HA2	2:D:432:VAL:O	2.01	0.60
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.82	0.60
2:D:181:SER:OG	2:D:252:LEU:HB2	2.02	0.60
2:D:389:ALA:CB	4:H:8:VAL:HG11	2.32	0.60
1:A:44:LEU:O	1:A:47:VAL:HG22	2.01	0.60
1:B:184:ILE:HD11	1:B:220:LEU:HD23	1.83	0.60
1:B:71:VAL:O	1:B:73:VAL:HG23	2.01	0.60
2:E:381:TYR:O	2:E:385:GLN:HG2	2.00	0.60
1:A:422:VAL:CG2	1:A:423:ARG:HH11	2.14	0.60
1:C:66:LEU:O	2:D:15:ALA:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:173:VAL:HG21	2:E:252:LEU:HD12	1.81	0.60
2:E:371:ALA:O	2:E:375:GLN:HG3	2.02	0.60
2:F:412:ARG:HG3	2:F:412:ARG:NH1	2.15	0.60
2:D:223:ASN:H	2:D:223:ASN:HD22	1.48	0.60
2:E:96:ASN:HB2	2:E:100:GLU:O	2.02	0.60
2:E:456:ALA:HB1	2:E:466:ALA:O	2.01	0.60
1:B:292:GLU:HA	3:G:261:GLU:OE2	2.02	0.60
1:A:188:ARG:HH11	1:A:188:ARG:HG3	1.66	0.60
1:B:152:ALA:HA	1:B:428:LEU:HD22	1.83	0.60
1:C:382:ALA:HA	1:C:385:GLN:OE1	2.01	0.60
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.84	0.60
1:A:286:ARG:HA	2:F:275:ILE:HD12	1.84	0.60
1:A:106:ARG:NH1	1:A:121:ILE:HG22	2.17	0.60
1:C:294:TYR:HB3	1:C:298:VAL:CG2	2.30	0.60
1:B:334:VAL:HG11	1:B:351:PHE:HE2	1.67	0.60
1:B:498:LYS:O	1:B:501:VAL:HG22	2.02	0.60
2:D:381:TYR:O	2:D:385:GLN:HG2	2.01	0.60
2:D:96:ASN:HB2	2:D:100:GLU:O	2.02	0.60
1:A:336:ALA:HB3	1:A:339:PRO:HG2	1.84	0.60
1:B:439:GLU:O	1:B:442:VAL:HG13	2.02	0.60
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.02	0.60
1:B:79:ASP:N	1:B:79:ASP:OD2	2.35	0.60
2:D:36:LEU:HD23	2:D:77:ASP:HA	1.84	0.60
2:F:404:VAL:O	2:F:408:ARG:HG3	2.01	0.60
1:A:210:ARG:HG3	1:A:235:THR:HG21	1.83	0.60
1:A:155:SER:HA	1:A:383:MET:CG	2.32	0.60
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.36	0.60
1:B:381:ARG:HD2	1:B:488:LYS:HB3	1.84	0.59
2:D:257:ASN:H	2:D:309:ALA:CB	1.91	0.59
1:B:386:VAL:HG23	1:B:387:ALA:N	2.17	0.59
1:C:153:VAL:HA	1:C:157:VAL:HG23	1.82	0.59
1:C:469:LEU:O	1:C:472:VAL:HG22	2.01	0.59
2:E:191:ARG:HH12	2:E:192:GLU:HG2	1.67	0.59
1:A:419:SER:O	1:A:422:VAL:HG22	2.02	0.59
1:C:430:GLN:NE2	1:C:436:MET:HG3	2.18	0.59
2:F:164:VAL:HG23	5:F:1478:ANP:O1A	2.01	0.59
1:A:140:ILE:HG13	1:A:143:ARG:NH1	2.17	0.59
2:E:32:ILE:O	2:E:33:LEU:HB2	2.01	0.59
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.02	0.59
1:B:395:ALA:O	1:B:399:GLU:HG3	2.01	0.59
1:B:54:GLU:CD	1:B:60:LYS:HZ1	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:GLY:CA	5:D:1478:ANP:HNB1	2.15	0.59
2:F:189:ARG:HB2	2:F:192:GLU:HG3	1.84	0.59
1:C:49:ALA:O	1:C:50:GLU:HB2	2.02	0.59
2:F:298:THR:HG23	2:F:303:SER:HB3	1.84	0.59
2:F:139:VAL:CG1	2:F:414:LEU:HD22	2.32	0.59
1:B:24:ASP:O	1:B:28:THR:HB	2.01	0.59
1:B:276:VAL:HG13	1:B:279:ARG:HH21	1.67	0.59
1:B:486:ASP:C	1:B:488:LYS:N	2.54	0.59
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.83	0.59
1:A:379:GLN:HE21	1:A:383:MET:HG3	1.65	0.59
1:A:468:PHE:O	1:A:472:VAL:HG13	2.02	0.59
1:B:244:TYR:O	1:B:247:PRO:HD2	2.02	0.59
1:C:156:LEU:HD22	1:C:391:LYS:HB2	1.85	0.59
1:C:237:SER:CB	2:F:294:GLU:HG3	2.32	0.59
1:C:188:ARG:NH2	1:C:436:MET:CA	2.66	0.59
2:D:470:ALA:HA	2:D:473:LEU:HD12	1.84	0.59
2:D:474:ALA:HB2	4:H:37:ARG:HG2	1.82	0.59
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.38	0.59
1:A:49:ALA:O	2:E:67:GLU:HA	2.02	0.59
1:A:80:LYS:HG2	1:A:80:LYS:O	2.02	0.59
1:C:295:PRO:O	1:C:298:VAL:HG23	2.02	0.59
2:F:17:ILE:HG21	2:F:271:LEU:HD22	1.83	0.59
1:A:181:ASP:OD1	1:A:433:TYR:HA	2.03	0.59
1:A:361:ILE:HD13	1:A:429:LYS:HD3	1.85	0.59
1:B:291:ARG:HG3	3:G:258:ILE:HG23	1.84	0.59
1:A:166:LEU:HD13	1:A:325:PRO:HG2	1.85	0.59
1:C:199:LEU:HD21	1:C:265:LEU:HB2	1.84	0.59
2:E:173:VAL:HG21	2:E:252:LEU:HD11	1.84	0.59
3:G:80:ALA:HA	3:G:83:SER:OG	2.01	0.59
1:A:175:LYS:HE3	5:A:1511:ANP:O1B	2.03	0.59
1:A:381:ARG:CZ	1:A:488:LYS:HZ3	2.16	0.59
2:E:245:ASP:O	2:E:247:GLU:N	2.35	0.59
2:E:348:VAL:O	2:E:350:PRO:HD3	2.03	0.59
2:F:399:GLU:O	2:F:403:THR:HG23	2.03	0.59
1:B:286:ARG:NH1	3:G:272:LEU:HD13	2.18	0.59
1:C:184:ILE:HG23	1:C:223:ALA:HB1	1.85	0.59
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.85	0.59
2:F:174:ALA:O	2:F:177:HIS:HB3	2.03	0.59
2:F:96:ASN:HD22	2:F:96:ASN:C	2.05	0.59
4:H:24:LYS:O	4:H:27:GLN:HB3	2.03	0.59
1:A:166:LEU:HD22	1:A:342:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:HG11	1:A:351:PHE:CE2	2.38	0.59
1:C:263:HIS:HD2	1:C:320:SER:OG	1.86	0.59
1:C:330:GLN:O	1:C:331:ALA:HB3	2.03	0.59
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.33	0.59
1:C:156:LEU:HB3	1:C:391:LYS:CE	2.31	0.59
4:H:4:SER:HA	4:H:7:ASN:OD1	2.03	0.59
1:B:108:VAL:HG12	1:B:114:ALA:HA	1.85	0.58
1:A:187:LYS:O	1:A:188:ARG:C	2.40	0.58
1:C:25:LEU:HD13	1:C:42:HIS:CD2	2.38	0.58
1:C:468:PHE:O	1:C:471:HIS:HB3	2.02	0.58
2:D:139:VAL:CG2	2:D:414:LEU:HB3	2.33	0.58
2:E:387:ILE:CD1	2:E:387:ILE:H	2.13	0.58
2:F:244:ARG:NH1	2:F:297:THR:O	2.36	0.58
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.68	0.58
1:B:34:ILE:HG13	1:B:35:GLY:N	2.17	0.58
1:B:497:LEU:O	1:B:501:VAL:HG22	2.04	0.58
2:E:337:ARG:HG3	2:E:337:ARG:HH11	1.68	0.58
2:E:97:VAL:HG21	2:E:228:ALA:HB1	1.85	0.58
4:H:20:GLY:O	4:H:22:PHE:N	2.36	0.58
1:A:140:ILE:CG1	1:A:143:ARG:HH12	2.14	0.58
1:B:34:ILE:CG2	2:E:52:HIS:HB2	2.33	0.58
2:E:166:ILE:O	2:E:170:ILE:HG13	2.02	0.58
1:B:286:ARG:HH11	2:E:275:ILE:HD11	1.68	0.58
2:E:387:ILE:HD12	2:E:387:ILE:N	2.17	0.58
2:E:168:GLU:OE1	2:E:418:PHE:HB3	2.03	0.58
3:G:11:LYS:HE2	4:H:7:ASN:CG	2.23	0.58
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.84	0.58
1:A:80:LYS:HE3	2:D:33:LEU:HD12	1.84	0.58
2:E:380:ASP:O	2:E:384:LEU:HG	2.02	0.58
1:A:390:MET:HE1	1:A:445:ILE:HD12	1.85	0.58
1:A:423:ARG:HG3	1:A:423:ARG:HH11	1.68	0.58
1:A:432:GLN:HG2	1:A:433:TYR:CG	2.37	0.58
1:C:390:MET:O	1:C:394:LEU:HG	2.03	0.58
1:C:99:VAL:HG12	1:C:100:GLY:N	2.18	0.58
2:E:243:PHE:O	2:E:251:VAL:CG2	2.51	0.58
2:F:95:MET:HG2	2:F:218:VAL:HG22	1.86	0.58
1:B:195:GLU:HA	1:B:198:LYS:HG3	1.84	0.58
1:A:211:SER:HA	2:D:126:MET:HE3	1.86	0.58
1:A:266:ILE:C	1:A:267:ILE:HD12	2.24	0.58
1:A:352:LEU:HA	1:A:364:ALA:O	2.04	0.58
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ILE:HA	2:D:49:VAL:HG12	1.84	0.58
2:E:191:ARG:NH1	2:E:192:GLU:HG2	2.18	0.58
1:A:168:ILE:HD11	1:A:329:THR:CG2	2.33	0.58
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.84	0.58
2:D:32:ILE:O	2:D:33:LEU:HB2	2.02	0.58
2:F:287:THR:O	2:F:288:ASP:C	2.42	0.58
2:F:366:GLU:O	2:F:370:VAL:HG23	2.04	0.58
1:A:465:GLU:O	1:A:469:LEU:HB2	2.03	0.58
1:A:59:LEU:HD11	1:A:77:GLY:HA3	1.84	0.58
1:B:180:ILE:HD11	1:B:216:LEU:HD11	1.85	0.58
2:D:294:GLU:HA	2:D:294:GLU:OE1	2.03	0.58
2:E:149:GLY:N	2:E:305:THR:OG1	2.29	0.58
2:F:183:PHE:HB3	2:F:217:LEU:CD2	2.34	0.58
1:A:140:ILE:CG2	1:A:311:LYS:HG3	2.34	0.58
1:B:257:PHE:HB3	1:B:262:LYS:HB2	1.85	0.58
2:E:93:ARG:NH2	2:E:106:GLY:O	2.36	0.58
2:E:38:VAL:HG21	2:E:45:LEU:HG	1.86	0.58
1:A:49:ALA:HB3	2:E:66:THR:O	2.03	0.58
2:D:408:ARG:CD	4:H:22:PHE:CE2	2.87	0.58
1:B:62:MET:HE2	1:B:64:LEU:HD21	1.85	0.58
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.04	0.58
2:D:189:ARG:HB2	2:D:192:GLU:HG3	1.85	0.58
1:A:47:VAL:CG1	1:A:90:ARG:HG2	2.30	0.58
1:B:136:ILE:HG22	1:B:137:ILE:N	2.19	0.58
2:F:244:ARG:HD3	2:F:304:ILE:HG13	1.86	0.58
3:G:3:LEU:CD1	3:G:257:VAL:HG21	2.34	0.58
1:A:265:LEU:HD11	1:A:324:LEU:HG	1.85	0.58
1:C:141:SER:HB2	1:C:143:ARG:HE	1.69	0.58
1:C:156:LEU:HD22	1:C:391:LYS:HG3	1.86	0.58
1:C:491:GLU:CD	1:C:491:GLU:H	2.06	0.58
2:E:89:GLU:H	2:E:89:GLU:CD	2.07	0.58
4:H:8:VAL:O	4:H:15:VAL:HG22	2.03	0.58
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.86	0.57
1:C:74:VAL:HG11	1:C:241:PRO:HG3	1.86	0.57
2:D:346:PRO:HD3	2:D:418:PHE:CZ	2.39	0.57
1:A:190:ASN:O	1:A:198:LYS:HE2	2.04	0.57
1:A:294:TYR:HB3	1:A:298:VAL:HG21	1.85	0.57
2:D:393:MET:CE	2:D:404:VAL:HG11	2.34	0.57
2:F:387:ILE:HG23	2:F:391:LEU:HB2	1.86	0.57
3:G:11:LYS:HB3	4:H:7:ASN:CG	2.24	0.57
2:F:169:LEU:O	2:F:173:VAL:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:VAL:HB	1:B:116:ASP:HB3	1.86	0.57
1:B:403:PHE:HD2	1:B:403:PHE:N	2.00	0.57
1:B:74:VAL:CG1	1:B:241:PRO:HB3	2.34	0.57
1:C:47:VAL:HG12	1:C:90:ARG:HG2	1.86	0.57
2:D:221:GLN:HE21	2:D:221:GLN:CA	2.17	0.57
2:D:411:GLN:O	2:D:414:LEU:HB2	2.04	0.57
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.87	0.57
1:A:206:ILE:N	1:A:206:ILE:HD12	2.20	0.57
1:A:224:ASP:OD1	1:A:227:LYS:HD3	2.03	0.57
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.87	0.57
1:A:102:GLU:HG3	1:A:122:GLY:C	2.25	0.57
1:A:272:SER:O	1:A:276:VAL:HG13	2.04	0.57
1:A:386:VAL:HG23	1:A:387:ALA:N	2.20	0.57
1:B:104:LEU:HB3	1:B:227:LYS:O	2.04	0.57
1:B:102:GLU:CD	1:B:124:LYS:HG3	2.25	0.57
1:B:127:ARG:NH2	1:B:259:ASP:OD2	2.37	0.57
2:E:374:VAL:O	2:E:378:LEU:HG	2.04	0.57
2:F:81:PRO:HG2	2:F:115:ALA:HB1	1.87	0.57
4:H:4:SER:HA	4:H:7:ASN:ND2	2.18	0.57
1:A:75:VAL:O	1:A:241:PRO:HG3	2.03	0.57
1:A:442:VAL:HG21	1:A:483:ILE:HG21	1.85	0.57
1:C:187:LYS:HG2	1:C:191:ASP:OD2	2.03	0.57
1:A:26:GLU:HB3	1:A:46:ASN:ND2	2.19	0.57
2:F:166:ILE:HG23	2:F:254:PHE:CE2	2.40	0.57
1:A:142:VAL:CG1	1:A:160:GLY:HA3	2.34	0.57
1:C:96:ASP:OD2	1:C:126:ARG:NE	2.32	0.57
2:D:393:MET:CB	4:H:25:ARG:HG3	2.35	0.57
2:D:388:ILE:HG21	2:D:396:LEU:HD11	1.87	0.57
2:E:264:ALA:O	2:E:268:VAL:HG23	2.04	0.57
2:F:351:LEU:HD13	2:F:379:GLN:OE1	2.03	0.57
2:F:420:VAL:O	2:F:420:VAL:HG12	2.04	0.57
3:G:27:ALA:HB2	3:G:228:ARG:CD	2.35	0.57
1:B:98:PRO:HD3	1:B:126:ARG:HH21	1.69	0.57
2:F:336:SER:HB3	2:F:339:ILE:HG12	1.86	0.57
1:C:151:LYS:HB3	1:C:428:LEU:CD2	2.30	0.57
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.31	0.57
1:B:393:GLU:OE2	1:B:420:ARG:HD2	2.05	0.57
1:C:99:VAL:CG1	1:C:100:GLY:N	2.67	0.57
2:F:89:GLU:CG	2:F:110:THR:HG22	2.31	0.57
1:B:286:ARG:HH12	3:G:272:LEU:CD1	2.18	0.57
1:A:195:GLU:HG2	1:A:198:LYS:NZ	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:PHE:CD2	1:C:241:PRO:HB2	2.40	0.57
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.29	0.57
1:C:505:LEU:HD22	1:C:505:LEU:O	2.04	0.57
2:D:285:LEU:C	2:D:285:LEU:HD23	2.24	0.57
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.70	0.57
1:C:127:ARG:NH2	1:C:259:ASP:OD2	2.38	0.57
2:E:221:GLN:HB2	2:E:223:ASN:HD21	1.68	0.57
1:C:432:GLN:HB3	1:C:433:TYR:CD1	2.40	0.57
1:C:94:ILE:HD11	2:E:68:GLY:HA2	1.87	0.57
2:F:172:ASN:ND2	2:F:431:LEU:HD13	2.19	0.57
3:G:20:THR:HA	3:G:232:MET:CE	2.35	0.57
1:A:362:ARG:O	1:A:430:GLN:O	2.23	0.56
1:C:151:LYS:HG2	1:C:441:GLN:HG2	1.85	0.56
2:E:452:LEU:HD11	2:E:467:VAL:HG22	1.87	0.56
2:F:101:PRO:HB3	2:F:108:ILE:HD11	1.87	0.56
2:F:223:ASN:HD22	2:F:224:GLU:H	1.51	0.56
1:B:226:MET:HA	1:B:229:THR:HB	1.87	0.56
1:C:174:GLY:O	1:C:175:LYS:C	2.43	0.56
1:C:44:LEU:HB3	1:C:47:VAL:CG2	2.35	0.56
2:D:401:LYS:HD2	4:H:25:ARG:CZ	2.35	0.56
2:E:64:ASP:O	2:E:65:GLY:O	2.23	0.56
1:C:363:PRO:O	1:C:365:ILE:N	2.39	0.56
2:D:12:ARG:HG2	2:D:74:LYS:HD3	1.86	0.56
2:E:157:GLY:O	2:E:160:VAL:HG13	2.04	0.56
1:A:188:ARG:NH2	1:A:436:MET:HA	2.20	0.56
1:B:186:GLN:HA	1:B:189:PHE:HD1	1.70	0.56
1:B:105:GLY:HA2	1:B:226:MET:O	2.05	0.56
1:C:141:SER:HB2	1:C:143:ARG:NE	2.20	0.56
1:C:98:PRO:HD2	1:C:112:GLY:HA3	1.87	0.56
2:E:170:ILE:HG21	2:E:215:VAL:CG2	2.35	0.56
3:G:20:THR:HG23	3:G:232:MET:CE	2.35	0.56
1:B:267:ILE:N	1:B:267:ILE:HD12	2.20	0.56
1:C:383:MET:HA	1:C:442:VAL:HG22	1.88	0.56
2:F:31:PRO:O	2:F:34:ASN:HB2	2.05	0.56
1:B:300:TYR:CZ	1:B:304:ARG:HD3	2.40	0.56
1:C:40:ARG:HD2	1:C:70:ASN:OD1	2.06	0.56
1:C:444:VAL:HG23	1:C:445:ILE:N	2.20	0.56
1:C:163:GLN:OE1	1:C:374:VAL:HG21	2.05	0.56
1:C:74:VAL:CG1	1:C:241:PRO:HG3	2.36	0.56
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.87	0.56
2:D:381:TYR:OH	4:H:22:PHE:CZ	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:VAL:HG23	1:A:473:ILE:H	1.71	0.56
1:B:188:ARG:HH11	1:B:188:ARG:HG2	1.70	0.56
2:E:389:ALA:CB	4:H:18:ALA:HB2	2.36	0.56
1:C:298:VAL:O	1:C:301:LEU:HB3	2.06	0.56
2:E:322:PRO:O	2:E:325:THR:N	2.38	0.56
2:F:134:VAL:HG22	2:F:434:LEU:HD22	1.88	0.56
1:A:379:GLN:CG	1:A:380:THR:N	2.64	0.56
1:A:151:LYS:CD	1:A:444:VAL:HG21	2.34	0.56
1:B:196:LYS:CD	1:B:196:LYS:H	2.16	0.56
2:D:97:VAL:HG21	2:D:228:ALA:CB	2.35	0.56
2:E:198:HIS:HA	2:E:201:ILE:HD12	1.87	0.56
1:A:479:LEU:HG	1:A:496:LYS:HG2	1.86	0.56
1:B:432:GLN:HG2	1:B:433:TYR:CD1	2.40	0.56
2:E:257:ASN:H	2:E:309:ALA:HB3	1.69	0.56
2:F:233:ALA:O	2:F:237:LEU:HB2	2.05	0.56
2:F:391:LEU:HB3	2:F:395:GLU:CG	2.35	0.56
1:A:271:LEU:HB3	1:A:302:HIS:CE1	2.41	0.56
1:A:353:GLU:HB2	1:A:356:LEU:HD12	1.86	0.56
1:B:184:ILE:CD1	1:B:220:LEU:HD23	2.35	0.56
1:B:278:TYR:CD2	1:B:295:PRO:HG3	2.40	0.56
1:B:278:TYR:CE2	1:B:295:PRO:HG3	2.41	0.56
1:C:37:GLY:HA2	1:C:79:ASP:CG	2.26	0.56
4:H:20:GLY:C	4:H:22:PHE:H	2.09	0.56
1:A:74:VAL:CG1	1:A:241:PRO:HB3	2.34	0.56
1:C:155:SER:C	1:C:156:LEU:HD23	2.26	0.56
1:C:74:VAL:HG12	1:C:241:PRO:CG	2.35	0.56
2:E:32:ILE:HA	2:E:49:VAL:CG1	2.35	0.56
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.19	0.56
2:F:292:MET:HE3	2:F:293:GLN:HE21	1.69	0.56
4:H:12:ALA:HB1	4:H:16:ARG:CZ	2.36	0.56
1:B:102:GLU:HG3	1:B:122:GLY:C	2.25	0.56
2:E:196:LEU:O	2:E:200:MET:HG3	2.05	0.56
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.86	0.56
2:D:146:TYR:CD1	2:D:152:ILE:HD13	2.41	0.56
2:D:337:ARG:O	2:D:341:GLU:HG3	2.05	0.56
2:D:433:PRO:HD2	2:D:436:GLU:HG3	1.86	0.56
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.88	0.56
1:C:165:GLU:O	1:C:324:LEU:HA	2.06	0.56
2:D:168:GLU:HG3	2:D:172:ASN:ND2	2.21	0.56
1:B:496:LYS:O	1:B:500:ILE:HG13	2.06	0.56
1:C:496:LYS:O	1:C:500:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:ARG:HE	2:D:74:LYS:HE2	1.70	0.56
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.36	0.56
2:E:419:GLN:HA	2:E:429:GLY:HA3	1.87	0.56
2:D:389:ALA:HB1	4:H:8:VAL:HG11	1.87	0.56
1:A:361:ILE:HG23	1:A:429:LYS:HG2	1.88	0.56
1:C:501:VAL:HG23	1:C:502:THR:N	2.21	0.56
1:A:298:VAL:O	1:A:301:LEU:HB3	2.06	0.56
1:C:156:LEU:HD22	1:C:391:LYS:CG	2.36	0.56
1:C:258:ARG:HG2	1:C:258:ARG:O	2.06	0.56
1:C:38:ILE:HG13	1:C:284:LEU:CB	2.35	0.56
1:C:432:GLN:NE2	1:C:433:TYR:CZ	2.73	0.56
1:C:185:ASN:OD1	1:C:435:PRO:HB3	2.06	0.56
2:D:116:ILE:HA	2:D:238:THR:OG1	2.06	0.56
2:D:80:ALA:HB1	2:D:81:PRO:CD	2.36	0.56
2:F:285:LEU:C	2:F:285:LEU:HD23	2.26	0.56
2:F:252:LEU:CD2	2:F:305:THR:HB	2.33	0.56
2:E:412:ARG:HH11	2:E:412:ARG:HG3	1.71	0.55
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.35	0.55
1:A:287:ARG:HB3	1:A:288:PRO:CD	2.35	0.55
1:C:188:ARG:NH2	1:C:436:MET:HA	2.21	0.55
1:C:438:ILE:O	1:C:442:VAL:HG23	2.06	0.55
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.87	0.55
3:G:83:SER:O	3:G:87:LYS:HG3	2.06	0.55
1:A:446:TYR:OH	1:A:450:ARG:NH1	2.38	0.55
1:B:121:ILE:H	1:B:121:ILE:CD1	2.10	0.55
1:C:47:VAL:CG1	1:C:90:ARG:HG2	2.37	0.55
1:C:358:TYR:CD1	2:D:351:LEU:HD22	2.41	0.55
2:E:149:GLY:H	2:E:305:THR:HG1	1.50	0.55
2:E:166:ILE:CG2	2:E:167:MET:N	2.69	0.55
1:B:80:LYS:HE2	2:E:33:LEU:HD12	1.89	0.55
2:F:246:GLN:HA	2:F:246:GLN:NE2	2.08	0.55
1:A:224:ASP:O	1:A:227:LYS:HE2	2.07	0.55
1:C:64:LEU:HD22	1:C:64:LEU:N	2.20	0.55
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.36	0.55
1:B:34:ILE:HD12	1:B:39:ALA:HB2	1.88	0.55
2:F:282:GLN:HG2	2:F:285:LEU:N	2.22	0.55
1:A:44:LEU:HD21	1:A:88:VAL:O	2.05	0.55
1:B:295:PRO:O	1:B:298:VAL:HG22	2.06	0.55
2:D:469:LYS:O	2:D:473:LEU:HG	2.06	0.55
2:E:84:ILE:HD13	2:E:235:THR:HG23	1.88	0.55
2:F:189:ARG:O	2:F:192:GLU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG23	1:B:253:MET:HA	1.88	0.55
1:C:367:VAL:HG13	1:C:391:LYS:HG3	1.88	0.55
1:A:164:ARG:HD3	1:A:164:ARG:N	2.22	0.55
1:B:426:GLU:O	1:B:429:LYS:HB2	2.06	0.55
2:F:363:VAL:HB	2:F:367:HIS:ND1	2.21	0.55
2:F:382:LYS:HA	2:F:385:GLN:HE21	1.70	0.55
1:C:172:GLN:CA	5:C:1511:ANP:HNB1	2.17	0.55
2:D:415:SER:O	2:D:416:GLN:HB2	2.06	0.55
2:E:370:VAL:O	2:E:374:VAL:HG23	2.07	0.55
3:G:230:THR:O	3:G:233:ASP:HB3	2.07	0.55
1:C:99:VAL:CG1	1:C:253:MET:HA	2.34	0.55
2:F:221:GLN:HB2	2:F:223:ASN:ND2	2.21	0.55
1:A:35:GLY:O	1:A:36:ASP:CB	2.54	0.55
2:D:206:ILE:HD11	2:D:215:VAL:HB	1.87	0.55
2:E:338:ALA:O	2:E:341:GLU:HB3	2.07	0.55
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.07	0.55
1:B:34:ILE:HG21	1:B:82:ILE:O	2.05	0.55
1:C:342:VAL:O	1:C:345:ILE:HB	2.06	0.55
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.88	0.55
4:H:12:ALA:O	4:H:15:VAL:N	2.37	0.55
1:A:171:ARG:HB2	1:A:171:ARG:NH1	2.21	0.55
2:D:252:LEU:HD23	2:D:305:THR:HB	1.87	0.55
2:F:462:PRO:HD2	2:F:465:GLU:OE2	2.06	0.55
1:A:306:LEU:HD12	1:A:345:ILE:HG21	1.89	0.55
1:B:347:ASP:OD1	2:F:191:ARG:NH2	2.37	0.55
1:B:34:ILE:HG22	2:E:52:HIS:HB2	1.89	0.55
1:B:472:VAL:HG23	1:B:473:ILE:N	2.21	0.55
2:D:463:ILE:O	2:D:466:ALA:HB3	2.06	0.55
1:B:143:ARG:NH1	1:B:143:ARG:HG3	2.20	0.55
1:C:363:PRO:O	1:C:365:ILE:HG13	2.06	0.55
2:E:243:PHE:O	2:E:251:VAL:HG21	2.06	0.55
1:C:423:ARG:CG	1:C:423:ARG:NH1	2.58	0.55
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.36	0.55
2:E:50:ALA:C	2:E:51:GLN:CG	2.75	0.55
2:E:389:ALA:HA	4:H:18:ALA:HB2	1.88	0.55
1:A:171:ARG:HH22	2:D:352:ASP:CG	2.08	0.55
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.71	0.55
1:B:28:THR:CG2	1:B:29:GLY:H	2.17	0.55
1:B:481:GLY:HA2	1:B:484:ARG:NH1	2.21	0.55
1:C:423:ARG:HA	1:C:461:ILE:CD1	2.37	0.55
2:E:375:GLN:O	2:E:379:GLN:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:ILE:HA	3:G:19:ILE:HD13	1.89	0.55
1:A:381:ARG:CZ	1:A:488:LYS:NZ	2.69	0.55
1:B:300:TYR:HA	1:B:303:SER:OG	2.07	0.55
2:E:312:VAL:HG11	2:E:317:LEU:HD23	1.89	0.55
2:E:38:VAL:HG23	2:E:45:LEU:O	2.06	0.55
2:F:97:VAL:HG21	2:F:228:ALA:HB1	1.89	0.55
1:A:407:GLY:CA	1:A:410:LEU:HG	2.36	0.55
1:C:99:VAL:HG11	1:C:256:TYR:HB2	1.89	0.55
2:E:399:GLU:O	2:E:403:THR:HG23	2.07	0.55
2:F:228:ALA:O	2:F:232:VAL:HG23	2.07	0.55
1:A:458:PRO:HA	1:A:461:ILE:CG1	2.36	0.54
1:C:148:THR:HG21	1:C:153:VAL:HG11	1.90	0.54
3:G:14:LYS:HA	3:G:243:ILE:CD1	2.33	0.54
1:B:159:ILE:HD11	1:B:165:GLU:HG2	1.89	0.54
1:C:501:VAL:CG2	1:C:502:THR:N	2.70	0.54
1:C:358:TYR:HD2	2:F:375:GLN:HB3	1.67	0.54
1:B:468:PHE:O	1:B:472:VAL:HG13	2.07	0.54
1:C:213:VAL:O	1:C:216:LEU:CB	2.54	0.54
1:C:278:TYR:CD2	1:C:301:LEU:HD13	2.42	0.54
1:C:351:PHE:CD2	1:C:369:LEU:HD12	2.43	0.54
2:D:83:ARG:NH2	2:D:113:PHE:HB2	2.23	0.54
1:B:405:GLN:NE2	2:E:384:LEU:HD21	2.23	0.54
2:F:196:LEU:O	2:F:200:MET:HG3	2.06	0.54
2:F:387:ILE:N	2:F:387:ILE:HD12	2.23	0.54
3:G:10:LEU:HD22	3:G:14:LYS:HE3	1.89	0.54
1:A:248:TYR:OH	1:A:301:LEU:HD12	2.06	0.54
1:C:456:LEU:HD22	1:C:505:LEU:HD21	1.88	0.54
2:E:80:ALA:HB1	2:E:81:PRO:CD	2.35	0.54
2:F:12:ARG:HE	2:F:74:LYS:HE3	1.71	0.54
2:F:34:ASN:O	2:F:49:VAL:HG23	2.07	0.54
1:B:180:ILE:O	1:B:184:ILE:HG12	2.08	0.54
1:C:163:GLN:HG2	1:C:164:ARG:N	2.22	0.54
2:E:9:THR:HB	2:E:27:GLU:OE1	2.08	0.54
2:E:381:TYR:HE1	4:H:22:PHE:CZ	2.26	0.54
1:A:36:ASP:HB2	1:A:284:LEU:HD22	1.88	0.54
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.22	0.54
1:C:501:VAL:HG23	1:C:502:THR:N	2.21	0.54
2:E:152:ILE:HD12	2:E:152:ILE:N	2.21	0.54
1:A:383:MET:HE2	1:A:442:VAL:HG12	1.89	0.54
1:A:286:ARG:HH11	2:F:275:ILE:HD11	1.73	0.54
1:B:400:VAL:HG11	1:B:414:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:ILE:HA	2:E:238:THR:OG1	2.07	0.54
2:E:173:VAL:HA	2:E:177:HIS:HD2	1.73	0.54
1:A:106:ARG:NH2	1:A:118:LYS:HB2	2.23	0.54
1:A:361:ILE:CD1	1:A:429:LYS:HE2	2.37	0.54
1:A:151:LYS:HA	1:A:441:GLN:CG	2.37	0.54
1:A:99:VAL:HG13	1:A:256:TYR:HB2	1.89	0.54
1:B:415:GLN:O	1:B:415:GLN:HG2	2.07	0.54
1:C:288:PRO:HG3	3:G:271:ALA:CB	2.38	0.54
1:A:145:PRO:HA	1:A:378:ALA:HB1	1.87	0.54
1:A:38:ILE:HG23	1:A:285:LEU:CD2	2.36	0.54
1:B:26:GLU:O	1:B:46:ASN:HB2	2.08	0.54
1:B:486:ASP:O	1:B:488:LYS:N	2.41	0.54
2:D:253:LEU:HD23	2:D:296:ILE:HG23	1.89	0.54
2:D:145:PRO:HG2	2:D:357:ILE:HG13	1.89	0.54
2:E:263:GLN:HE21	2:E:281:TYR:HE2	1.55	0.54
2:F:134:VAL:CG2	2:F:434:LEU:HD22	2.38	0.54
1:C:440:GLU:OE1	1:C:473:ILE:HD11	2.07	0.54
2:D:407:ALA:O	2:D:411:GLN:HG3	2.08	0.54
4:H:20:GLY:C	4:H:22:PHE:N	2.60	0.54
2:E:398:GLU:O	2:E:402:LEU:HD13	2.08	0.54
2:F:63:MET:CE	2:F:97:VAL:HG11	2.37	0.54
2:D:153:GLY:HA3	2:D:329:LEU:HD13	1.90	0.54
2:E:287:THR:O	2:E:291:THR:HG23	2.07	0.54
2:F:132:ILE:HG13	2:F:145:PRO:HB2	1.88	0.54
2:D:473:LEU:CB	4:H:34:PHE:CZ	2.73	0.54
1:A:52:MET:SD	1:A:95:VAL:HG22	2.47	0.54
1:C:34:ILE:HG22	2:D:52:HIS:HB2	1.90	0.54
2:E:238:THR:O	2:E:241:GLU:HB2	2.07	0.54
2:E:473:LEU:CB	4:H:34:PHE:CE2	2.90	0.54
2:F:390:ILE:C	2:F:392:GLY:H	2.11	0.54
1:A:285:LEU:O	1:A:286:ARG:HB2	2.08	0.54
1:C:215:GLN:HE21	2:F:128:VAL:HA	1.72	0.54
1:B:271:LEU:HB3	1:B:302:HIS:CE1	2.43	0.54
1:C:36:ASP:OD2	2:D:274:ARG:HD2	2.08	0.54
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.88	0.54
2:F:132:ILE:CD1	2:F:145:PRO:HB3	2.38	0.54
2:F:396:LEU:HB2	2:F:401:LYS:HG2	1.90	0.54
1:B:164:ARG:N	1:B:164:ARG:HD3	2.23	0.54
1:C:438:ILE:HA	1:C:441:GLN:NE2	2.23	0.54
2:F:13:ILE:HD12	2:F:73:GLN:HB3	1.90	0.54
2:D:159:GLY:H	5:D:1478:ANP:HNB1	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:PRO:O	2:D:34:ASN:HB2	2.07	0.54
2:D:435:LYS:HG3	2:D:436:GLU:N	2.22	0.54
2:E:61:ILE:HG13	2:E:61:ILE:O	2.07	0.54
1:A:438:ILE:O	1:A:442:VAL:HG13	2.08	0.54
2:D:371:ALA:O	2:D:375:GLN:HG3	2.08	0.54
2:F:25:PHE:O	2:F:56:SER:HB3	2.08	0.54
4:H:20:GLY:O	4:H:21:ALA:C	2.46	0.54
2:D:408:ARG:NH1	4:H:26:GLU:HG3	2.14	0.54
1:B:188:ARG:NE	1:B:437:ALA:HB2	2.23	0.53
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.38	0.53
1:C:139:ARG:NH1	1:C:310:ALA:CB	2.71	0.53
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.73	0.53
2:E:170:ILE:O	2:E:174:ALA:HB3	2.08	0.53
2:F:292:MET:CE	2:F:293:GLN:NE2	2.71	0.53
2:E:390:ILE:HD13	3:G:16:ILE:HG23	1.90	0.53
1:A:357:PHE:O	1:A:359:LYS:N	2.41	0.53
1:C:338:ILE:O	1:C:341:ASN:N	2.41	0.53
2:E:181:SER:CB	2:E:215:VAL:HG13	2.35	0.53
2:F:166:ILE:O	2:F:170:ILE:HG13	2.08	0.53
1:B:240:ALA:N	1:B:241:PRO:HD2	2.23	0.53
1:C:177:SER:O	1:C:178:ILE:C	2.46	0.53
1:C:295:PRO:O	1:C:298:VAL:HG23	2.09	0.53
2:E:97:VAL:HG22	2:E:232:VAL:CG1	2.35	0.53
1:A:280:GLN:OE1	2:D:284:THR:HA	2.08	0.53
2:F:133:LEU:HD13	2:F:148:LYS:HG2	1.90	0.53
2:F:16:VAL:C	2:F:17:ILE:HD12	2.29	0.53
1:A:443:ALA:O	1:A:446:TYR:HB3	2.08	0.53
1:C:360:GLY:O	1:C:362:ARG:HG3	2.08	0.53
2:D:251:VAL:O	2:D:304:ILE:HA	2.09	0.53
2:E:183:PHE:HA	2:E:254:PHE:O	2.08	0.53
2:E:200:MET:HA	2:E:203:SER:OG	2.09	0.53
2:E:63:MET:HE1	2:E:231:ARG:HB2	1.91	0.53
1:A:492:GLU:O	1:A:495:ALA:HB3	2.08	0.53
1:B:98:PRO:HG3	1:B:126:ARG:HH12	1.71	0.53
1:B:200:TYR:H	1:B:200:TYR:HD1	1.57	0.53
1:C:215:GLN:NE2	2:F:128:VAL:HA	2.22	0.53
1:A:453:LEU:HD21	1:A:464:PHE:CE2	2.43	0.53
1:B:486:ASP:C	1:B:488:LYS:H	2.12	0.53
1:C:106:ARG:NH1	1:C:121:ILE:HD13	2.24	0.53
2:D:156:GLY:O	2:D:162:LYS:HD3	2.08	0.53
2:E:382:LYS:HB3	4:H:6:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:PRO:HB3	2:F:77:ASP:OD2	2.09	0.53
1:A:390:MET:HE3	1:A:424:LEU:HD22	1.89	0.53
2:F:101:PRO:HB3	2:F:108:ILE:HD11	1.90	0.53
2:F:118:ALA:O	2:F:295:ARG:HD2	2.08	0.53
1:A:151:LYS:HA	1:A:441:GLN:HG2	1.91	0.53
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.43	0.53
2:F:251:VAL:HG12	2:F:252:LEU:N	2.24	0.53
1:A:164:ARG:NE	1:A:347:ASP:OD2	2.37	0.53
1:A:263:HIS:HE1	1:A:318:GLY:O	1.92	0.53
1:B:333:ASP:HB2	3:G:252:ARG:NH2	2.23	0.53
1:B:380:THR:HG22	1:B:487:GLY:O	2.09	0.53
1:C:358:TYR:HB3	2:F:375:GLN:O	2.09	0.53
3:G:19:ILE:O	3:G:23:MET:HG3	2.08	0.53
1:C:189:PHE:N	1:C:189:PHE:CD2	2.76	0.53
1:A:218:LYS:HG2	1:A:222:ASP:OD2	2.09	0.53
1:A:99:VAL:CG2	1:A:253:MET:HA	2.30	0.53
1:B:156:LEU:HD11	1:B:428:LEU:HD11	1.91	0.53
1:B:241:PRO:HA	1:B:244:TYR:HB3	1.90	0.53
1:B:35:GLY:O	1:B:36:ASP:HB2	2.09	0.53
1:B:446:TYR:CD2	1:B:497:LEU:HG	2.43	0.53
2:D:155:PHE:O	2:D:335:LEU:HD13	2.07	0.53
2:D:258:ILE:O	2:D:261:PHE:HB3	2.09	0.53
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.24	0.53
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.90	0.53
1:A:423:ARG:HE	1:A:458:PRO:HG3	1.74	0.53
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.90	0.53
2:E:329:LEU:O	2:E:356:ARG:CZ	2.57	0.53
2:E:443:GLN:O	2:E:446:ALA:N	2.42	0.53
2:E:61:ILE:HG13	2:E:61:ILE:O	2.08	0.53
1:A:456:LEU:HD23	1:A:461:ILE:HD13	1.91	0.53
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.91	0.53
2:D:168:GLU:OE1	2:D:418:PHE:HB3	2.08	0.53
2:E:98:ILE:HG13	2:E:100:GLU:HG3	1.91	0.53
2:E:197:TYR:O	2:E:201:ILE:HG13	2.09	0.53
2:E:188:GLU:HG3	2:E:256:ASP:OD1	2.09	0.53
2:E:408:ARG:NE	4:H:22:PHE:CE2	2.77	0.53
2:F:170:ILE:HG21	2:F:215:VAL:CG2	2.39	0.53
1:C:430:GLN:HG2	1:C:431:GLY:N	2.24	0.53
2:D:168:GLU:OE1	2:D:420:VAL:HG23	2.08	0.53
2:F:411:GLN:O	2:F:414:LEU:HB2	2.08	0.53
1:A:87:ILE:HD12	1:A:87:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:MET:HG2	1:B:64:LEU:HD21	1.90	0.53
1:C:423:ARG:HA	1:C:461:ILE:CD1	2.38	0.53
2:D:350:PRO:HG2	2:D:378:LEU:HD13	1.92	0.53
2:E:216:ALA:O	2:E:217:LEU:HD23	2.09	0.53
1:B:237:SER:HB3	2:E:294:GLU:HG3	1.91	0.53
1:B:366:ASN:ND2	1:B:369:LEU:HD12	2.23	0.53
2:D:142:LEU:HD21	2:D:374:VAL:HG21	1.90	0.53
2:D:422:GLU:HG2	2:D:427:HIS:O	2.07	0.53
2:E:221:GLN:HB3	2:E:223:ASN:ND2	2.23	0.53
1:A:127:ARG:NE	1:A:131:LEU:HD12	2.23	0.52
1:C:220:LEU:HB2	1:C:226:MET:HG2	1.90	0.52
1:C:351:PHE:HD2	1:C:369:LEU:HD12	1.74	0.52
2:F:311:TYR:O	2:F:313:PRO:HD3	2.08	0.52
2:F:387:ILE:HG13	2:F:391:LEU:HD12	1.91	0.52
4:H:4:SER:HA	4:H:7:ASN:OD1	2.09	0.52
1:A:419:SER:O	1:A:423:ARG:HD3	2.09	0.52
1:B:127:ARG:NE	1:B:131:LEU:HD12	2.24	0.52
1:B:129:VAL:O	1:B:308:ARG:NH1	2.33	0.52
1:B:170:ASP:O	1:B:175:LYS:HE2	2.09	0.52
2:D:111:LYS:HB2	2:D:112:GLN:OE1	2.09	0.52
2:D:170:ILE:O	2:D:174:ALA:HB3	2.09	0.52
2:E:387:ILE:HG23	2:E:391:LEU:HB2	1.90	0.52
2:F:89:GLU:CG	2:F:110:THR:HG22	2.25	0.52
2:F:221:GLN:NE2	2:F:221:GLN:CA	2.66	0.52
2:F:407:ALA:O	2:F:411:GLN:HG3	2.09	0.52
1:C:176:THR:O	1:C:179:ALA:HB3	2.09	0.52
1:C:206:ILE:HG21	1:C:274:GLN:HB2	1.91	0.52
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.75	0.52
1:C:219:ARG:HD2	1:C:433:TYR:CD2	2.45	0.52
2:D:191:ARG:NH1	2:D:191:ARG:HG2	2.23	0.52
2:D:374:VAL:O	2:D:377:ILE:HG22	2.09	0.52
1:A:33:SER:HB2	2:D:52:HIS:O	2.10	0.52
2:D:80:ALA:HB1	2:D:81:PRO:HD2	1.90	0.52
2:E:242:TYR:O	2:E:246:GLN:HB2	2.09	0.52
1:B:214:ALA:O	1:B:217:VAL:HG22	2.10	0.52
1:A:282:SER:OG	1:A:295:PRO:HG3	2.09	0.52
1:B:349:GLN:OE1	1:B:351:PHE:HE1	1.93	0.52
1:C:300:TYR:OH	2:D:225:PRO:HG3	2.10	0.52
2:D:249:GLN:HG2	2:D:250:ASP:N	2.25	0.52
2:D:258:ILE:HD11	2:D:292:MET:SD	2.49	0.52
2:E:266:SER:OG	2:E:282:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:PRO:HG2	2:F:34:ASN:OD1	2.08	0.52
4:H:11:SER:H	4:H:15:VAL:HG21	1.74	0.52
1:A:154:ASP:CB	1:A:438:ILE:HD13	2.38	0.52
1:B:34:ILE:HD13	1:B:82:ILE:HG21	1.90	0.52
1:C:156:LEU:HB3	1:C:391:LYS:HD2	1.91	0.52
1:C:206:ILE:CD1	1:C:247:PRO:HG3	2.40	0.52
1:C:142:VAL:HG22	1:C:311:LYS:HB2	1.91	0.52
1:C:338:ILE:CD1	1:C:338:ILE:H	2.10	0.52
2:D:96:ASN:ND2	2:D:100:GLU:H	2.06	0.52
2:E:185:GLY:C	2:E:221:GLN:NE2	2.63	0.52
2:E:53:LEU:HD11	2:E:59:ARG:HB2	1.91	0.52
3:G:78:CYS:SG	3:G:228:ARG:NH2	2.82	0.52
1:B:129:VAL:HG12	1:B:249:SER:HA	1.89	0.52
2:D:31:PRO:O	2:D:34:ASN:HB2	2.08	0.52
4:H:31:GLU:HA	4:H:34:PHE:HB2	1.91	0.52
2:D:36:LEU:HB2	2:D:47:LEU:HB2	1.91	0.52
2:E:399:GLU:O	2:E:402:LEU:HB3	2.09	0.52
1:B:373:ARG:NH2	2:F:189:ARG:NH2	2.58	0.52
2:F:375:GLN:O	2:F:379:GLN:HG3	2.10	0.52
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.45	0.52
1:B:171:ARG:NH2	2:E:356:ARG:HH21	1.98	0.52
2:E:421:ALA:HB1	2:E:425:THR:CG2	2.39	0.52
1:A:161:ARG:NH1	1:A:198:LYS:O	2.36	0.52
1:C:419:SER:O	1:C:423:ARG:HG2	2.10	0.52
2:D:260:ARG:NH1	2:D:263:GLN:OE1	2.36	0.52
2:E:32:ILE:O	2:E:33:LEU:CB	2.57	0.52
2:F:456:ALA:O	2:F:466:ALA:HA	2.09	0.52
1:B:411:ASP:OD2	1:B:413:ALA:HB3	2.09	0.52
1:C:101:GLU:HG2	1:C:257:PHE:CE2	2.30	0.52
1:C:74:VAL:CG1	1:C:241:PRO:CG	2.88	0.52
2:E:440:GLY:O	2:E:444:ILE:HG12	2.08	0.52
4:H:9:ARG:HD2	4:H:15:VAL:HG13	1.91	0.52
1:B:267:ILE:HG13	1:B:324:LEU:HB2	1.91	0.52
1:B:62:MET:HG2	1:B:64:LEU:CD2	2.39	0.52
1:C:166:LEU:HB2	1:C:346:THR:HG21	1.92	0.52
1:C:300:TYR:CE2	1:C:304:ARG:HD3	2.45	0.52
1:C:337:TYR:HB3	1:C:338:ILE:HD12	1.91	0.52
2:E:453:PRO:HG2	4:H:34:PHE:CD2	2.44	0.52
1:A:293:ALA:N	3:G:265:ILE:HD13	2.24	0.52
1:A:66:LEU:HD12	2:E:16:VAL:HB	1.91	0.52
1:B:190:ASN:OD1	1:B:198:LYS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:O	1:C:50:GLU:HB2	2.10	0.52
2:D:229:ARG:NH2	2:D:267:GLU:OE2	2.42	0.52
1:A:361:ILE:HA	1:A:429:LYS:CD	2.34	0.52
1:C:180:ILE:O	1:C:181:ASP:C	2.48	0.52
1:C:294:TYR:CB	1:C:298:VAL:HG21	2.23	0.52
1:C:434:SER:N	1:C:435:PRO:HD3	2.25	0.52
2:D:25:PHE:HB2	2:D:29:LEU:HD12	1.92	0.52
3:G:4:LYS:O	3:G:8:ARG:HG3	2.10	0.52
1:A:414:THR:O	1:A:417:LEU:N	2.43	0.52
1:B:26:GLU:HB3	1:B:46:ASN:ND2	2.24	0.52
1:C:187:LYS:HE3	1:C:224:ASP:OD2	2.10	0.52
1:C:247:PRO:HG2	1:C:274:GLN:HG3	1.92	0.52
1:A:160:GLY:O	1:A:163:GLN:HB3	2.10	0.52
1:B:396:GLN:O	1:B:399:GLU:N	2.42	0.52
1:B:407:GLY:HA3	1:B:410:LEU:CD1	2.39	0.52
1:C:140:ILE:HB	1:C:313:ASN:HB3	1.92	0.52
2:F:355:SER:OG	2:F:357:ILE:HG12	2.10	0.52
2:F:430:LYS:HE3	2:F:465:GLU:OE1	2.09	0.52
1:A:370:SER:O	1:A:371:VAL:CG1	2.58	0.52
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.91	0.52
2:D:285:LEU:CD2	2:D:285:LEU:C	2.77	0.52
2:F:136:GLY:HA2	2:F:432:VAL:O	2.09	0.52
4:H:29:GLU:OE2	4:H:32:ARG:NH1	2.43	0.52
1:A:362:ARG:C	1:A:430:GLN:H	2.07	0.52
1:C:66:LEU:HD12	2:E:16:VAL:HB	1.92	0.52
2:F:366:GLU:O	2:F:370:VAL:HG23	2.10	0.52
1:A:47:VAL:HG12	1:A:90:ARG:HG2	1.92	0.52
2:E:408:ARG:O	2:E:412:ARG:HG3	2.10	0.52
1:B:352:LEU:HA	1:B:364:ALA:O	2.09	0.51
1:C:155:SER:O	1:C:379:GLN:NE2	2.43	0.51
4:H:34:PHE:O	4:H:37:ARG:HB3	2.11	0.51
1:A:38:ILE:HD12	1:A:285:LEU:HG	1.91	0.51
1:B:283:LEU:CD2	1:B:289:PRO:HB3	2.38	0.51
1:B:407:GLY:HA3	1:B:410:LEU:HD11	1.92	0.51
2:D:416:GLN:H	2:D:459:MET:HE2	1.75	0.51
2:F:292:MET:CE	2:F:293:GLN:HE21	2.24	0.51
2:F:310:ILE:CD1	2:F:329:LEU:HD11	2.40	0.51
1:C:338:ILE:CD1	1:C:338:ILE:H	2.18	0.51
2:D:139:VAL:HG22	2:D:414:LEU:HD22	1.93	0.51
2:D:314:ALA:O	2:D:315:ASP:CB	2.58	0.51
2:E:155:PHE:HE1	2:E:332:THR:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:ILE:HG22	2:F:33:LEU:HG	1.91	0.51
2:F:377:ILE:HG21	2:F:410:ILE:HD12	1.92	0.51
2:F:89:GLU:H	2:F:89:GLU:CD	2.14	0.51
3:G:20:THR:HG23	3:G:232:MET:HE3	1.92	0.51
1:B:163:GLN:OE1	1:B:374:VAL:HG21	2.10	0.51
1:C:225:ALA:HA	1:C:228:TYR:CZ	2.45	0.51
2:D:228:ALA:O	2:D:232:VAL:HG22	2.11	0.51
2:E:258:ILE:O	2:E:261:PHE:HB3	2.10	0.51
3:G:3:LEU:HD11	3:G:257:VAL:HG21	1.91	0.51
1:A:357:PHE:CE2	1:A:362:ARG:HD3	2.45	0.51
1:B:383:MET:SD	1:B:387:ALA:HB2	2.50	0.51
1:C:404:ALA:HB2	1:C:418:LEU:HD21	1.92	0.51
2:D:32:ILE:HA	2:D:49:VAL:CG1	2.39	0.51
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.11	0.51
2:E:221:GLN:CB	2:E:223:ASN:ND2	2.71	0.51
2:D:393:MET:HB2	4:H:25:ARG:HG3	1.93	0.51
1:A:140:ILE:HG22	1:A:311:LYS:HG3	1.92	0.51
1:B:136:ILE:HD12	2:F:190:THR:CG2	2.33	0.51
1:C:188:ARG:HE	1:C:437:ALA:CB	2.23	0.51
1:C:62:MET:HB2	1:C:76:PHE:HE1	1.76	0.51
2:D:293:GLN:HE22	2:D:308:GLN:HE22	1.58	0.51
2:E:409:LYS:HG2	2:E:454:GLU:HG2	1.91	0.51
1:B:137:ILE:HB	1:B:138:PRO:HD3	1.93	0.51
1:C:333:ASP:C	1:C:335:SER:N	2.63	0.51
2:D:89:GLU:CG	2:D:110:THR:HG22	2.39	0.51
2:E:88:PRO:O	2:E:91:LEU:HD12	2.11	0.51
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.93	0.51
2:F:311:TYR:CE2	2:F:313:PRO:HA	2.46	0.51
1:C:399:GLU:OE2	4:H:19:GLY:CA	2.59	0.51
2:D:95:MET:HG2	2:D:218:VAL:HG22	1.93	0.51
2:F:221:GLN:NE2	2:F:224:GLU:OE2	2.43	0.51
3:G:11:LYS:HE2	4:H:7:ASN:OD1	2.10	0.51
1:A:54:GLU:O	1:A:88:VAL:HA	2.11	0.51
1:B:280:GLN:O	1:B:284:LEU:HG	2.11	0.51
1:C:300:TYR:CE1	1:C:304:ARG:HB2	2.44	0.51
2:D:20:VAL:HG21	2:D:271:LEU:HB3	1.92	0.51
1:A:28:THR:CG2	1:A:29:GLY:N	2.73	0.51
2:E:359:ASP:O	2:E:363:VAL:HG22	2.11	0.51
1:A:211:SER:HA	2:F:126:MET:HE2	1.93	0.51
1:A:275:ALA:HB1	1:A:294:TYR:HE2	1.75	0.51
1:A:356:LEU:HA	1:A:359:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:HB	1:C:116:ASP:HB3	1.91	0.51
1:C:338:ILE:N	1:C:338:ILE:HD12	2.18	0.51
1:C:352:LEU:CD2	1:C:365:ILE:HG12	2.40	0.51
1:C:410:LEU:HB3	1:C:415:GLN:HG3	1.93	0.51
2:D:335:LEU:N	2:D:335:LEU:HD12	2.25	0.51
2:D:31:PRO:HG2	2:D:34:ASN:OD1	2.11	0.51
2:E:96:ASN:HD22	2:E:98:ILE:HG12	1.75	0.51
1:A:338:ILE:HB	1:A:339:PRO:HD3	1.93	0.51
1:A:363:PRO:HD2	1:A:430:GLN:N	2.26	0.51
1:A:501:VAL:HG23	1:A:502:THR:N	2.25	0.51
1:C:203:TYR:OH	1:C:269:ASP:OD2	2.25	0.51
2:F:136:GLY:HA2	2:F:432:VAL:O	2.11	0.51
2:F:258:ILE:O	2:F:261:PHE:HB3	2.10	0.51
1:A:278:TYR:HA	1:A:281:MET:CE	2.35	0.51
1:A:390:MET:CE	1:A:424:LEU:HD22	2.40	0.51
1:A:393:GLU:OE2	1:A:420:ARG:NH1	2.43	0.51
1:B:172:GLN:N	5:B:1511:ANP:HNB1	2.07	0.51
1:B:382:ALA:HB1	1:B:442:VAL:HG11	1.92	0.51
1:B:496:LYS:O	1:B:500:ILE:HG13	2.10	0.51
1:C:505:LEU:O	1:C:508:PHE:HB3	2.11	0.51
2:E:337:ARG:O	2:E:341:GLU:HG3	2.11	0.51
2:F:388:ILE:HD11	2:F:396:LEU:HD11	1.92	0.51
3:G:230:THR:O	3:G:233:ASP:HB2	2.10	0.51
4:H:7:ASN:O	4:H:8:VAL:C	2.49	0.51
1:A:181:ASP:HB3	1:A:435:PRO:HB3	1.93	0.51
1:A:439:GLU:O	1:A:442:VAL:HG22	2.11	0.51
1:B:29:GLY:O	1:B:88:VAL:N	2.41	0.51
1:B:422:VAL:HG23	1:B:423:ARG:N	2.25	0.51
1:B:96:ASP:OD2	1:B:126:ARG:HD3	2.11	0.51
2:E:260:ARG:NH1	2:E:263:GLN:OE1	2.39	0.51
2:E:337:ARG:O	2:E:341:GLU:HB2	2.11	0.51
1:C:153:VAL:HA	1:C:157:VAL:HG22	1.93	0.51
1:C:32:LEU:HD21	1:C:42:HIS:HB2	1.93	0.51
1:C:430:GLN:HG2	1:C:431:GLY:H	1.76	0.51
2:D:359:ASP:OD1	2:D:361:ASN:N	2.36	0.51
1:A:28:THR:HG22	1:A:29:GLY:H	1.73	0.51
2:D:183:PHE:HB3	2:D:217:LEU:HD23	1.93	0.51
2:E:340:ALA:HB2	2:E:347:ALA:CB	2.41	0.51
2:E:89:GLU:CG	2:E:110:THR:HG22	2.40	0.51
2:E:98:ILE:HD11	2:E:100:GLU:OE1	2.10	0.51
1:A:76:PHE:CE1	1:A:241:PRO:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG13	1:A:90:ARG:HG2	1.93	0.51
1:B:386:VAL:HG23	1:B:387:ALA:H	1.74	0.51
1:C:109:ASP:C	1:C:109:ASP:OD2	2.48	0.51
1:C:36:ASP:OD2	2:F:274:ARG:HD2	2.11	0.51
2:E:138:LYS:NZ	2:E:413:PHE:O	2.42	0.51
2:F:388:ILE:HD12	2:F:393:MET:SD	2.51	0.51
4:H:9:ARG:HA	4:H:15:VAL:HG13	1.93	0.51
1:A:211:SER:CA	2:F:126:MET:HE2	2.40	0.51
1:A:379:GLN:HG2	1:A:380:THR:N	2.12	0.51
2:E:452:LEU:HD22	2:E:470:ALA:CB	2.41	0.51
1:A:241:PRO:HA	1:A:244:TYR:HB3	1.94	0.51
1:A:99:VAL:HG21	1:A:256:TYR:HB2	1.92	0.51
1:C:288:PRO:HB2	2:D:270:ALA:HB1	1.92	0.51
1:C:62:MET:SD	1:C:64:LEU:HD11	2.51	0.51
1:C:279:ARG:HG3	1:C:294:TYR:HA	1.93	0.50
1:C:51:GLU:OE2	1:C:90:ARG:HB3	2.11	0.50
2:E:257:ASN:OD1	2:E:311:TYR:HB2	2.11	0.50
2:E:53:LEU:HD11	2:E:59:ARG:HE	1.77	0.50
2:F:146:TYR:CD1	2:F:152:ILE:HG12	2.46	0.50
2:F:185:GLY:CA	2:F:188:GLU:HG3	2.39	0.50
2:F:281:TYR:CD1	2:F:320:PRO:HB2	2.46	0.50
1:B:200:TYR:CD1	1:B:200:TYR:N	2.79	0.50
1:B:336:ALA:HB3	1:B:339:PRO:HG2	1.93	0.50
1:A:151:LYS:HG2	1:A:441:GLN:HA	1.93	0.50
1:C:188:ARG:HE	1:C:437:ALA:HB2	1.77	0.50
1:C:161:ARG:HA	1:C:322:THR:OG1	2.11	0.50
1:C:329:THR:HG21	1:C:334:VAL:HG12	1.93	0.50
2:D:257:ASN:OD1	2:D:311:TYR:N	2.44	0.50
2:E:310:ILE:HD13	2:E:325:THR:HG21	1.92	0.50
1:A:407:GLY:HA3	1:A:410:LEU:CG	2.42	0.50
1:C:99:VAL:HG21	1:C:127:ARG:HB2	1.93	0.50
2:D:197:TYR:O	2:D:201:ILE:HG13	2.10	0.50
2:D:310:ILE:HD13	2:D:325:THR:HG21	1.92	0.50
2:E:89:GLU:HG2	2:E:110:THR:CG2	2.32	0.50
1:A:151:LYS:HD3	1:A:436:MET:CE	2.41	0.50
1:C:105:GLY:HA2	1:C:226:MET:O	2.10	0.50
2:E:285:LEU:HD23	2:E:285:LEU:C	2.31	0.50
1:A:306:LEU:HD12	1:A:345:ILE:CG2	2.41	0.50
1:C:274:GLN:NE2	1:C:301:LEU:HD11	2.26	0.50
1:C:361:ILE:O	1:C:364:ALA:HA	2.11	0.50
2:D:36:LEU:HB3	2:D:75:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:435:LYS:HE2	2:F:436:GLU:OE2	2.12	0.50
2:D:454:GLU:HB2	4:H:30:GLU:OE2	2.12	0.50
4:H:4:SER:HA	4:H:7:ASN:HD21	1.76	0.50
1:A:383:MET:HE2	1:A:442:VAL:HG13	1.93	0.50
1:A:486:ASP:OD1	1:A:486:ASP:N	2.44	0.50
1:B:358:TYR:HE1	2:E:351:LEU:O	1.93	0.50
1:B:446:TYR:O	1:B:450:ARG:HG2	2.10	0.50
1:C:141:SER:HB2	1:C:143:ARG:NH2	2.26	0.50
2:E:36:LEU:HB3	2:E:75:VAL:CG1	2.41	0.50
2:F:183:PHE:CZ	2:F:256:ASP:HB2	2.46	0.50
1:C:414:THR:HG21	4:H:24:LYS:HG3	1.93	0.50
4:H:31:GLU:CA	4:H:34:PHE:HB2	2.39	0.50
1:A:107:VAL:HG13	1:A:231:VAL:CG1	2.39	0.50
1:A:107:VAL:HG22	1:A:231:VAL:HB	1.94	0.50
1:B:211:SER:HA	2:E:126:MET:HE2	1.93	0.50
2:D:245:ASP:C	2:D:247:GLU:H	2.14	0.50
2:D:382:LYS:HD3	4:H:6:ASP:OD1	2.12	0.50
2:E:13:ILE:HG13	2:E:75:VAL:HG21	1.93	0.50
2:F:132:ILE:HG12	2:F:133:LEU:N	2.26	0.50
2:F:36:LEU:HB3	2:F:75:VAL:HG12	1.92	0.50
3:G:27:ALA:HB2	3:G:228:ARG:HD2	1.93	0.50
1:A:181:ASP:OD2	1:A:435:PRO:HD3	2.11	0.50
1:A:149:GLY:C	1:A:436:MET:H	2.10	0.50
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.26	0.50
1:B:423:ARG:NH2	1:B:456:LEU:O	2.45	0.50
1:B:453:LEU:HD21	1:B:464:PHE:CE2	2.47	0.50
1:B:498:LYS:O	1:B:502:THR:HG23	2.11	0.50
2:F:223:ASN:ND2	2:F:223:ASN:N	2.58	0.50
1:A:295:PRO:HG2	1:A:298:VAL:HG13	1.93	0.50
1:C:144:GLU:O	1:C:161:ARG:HG3	2.11	0.50
1:A:164:ARG:NH1	1:A:164:ARG:HG2	2.26	0.50
1:A:424:LEU:O	1:A:427:LEU:HB2	2.12	0.50
1:B:163:GLN:HG3	1:B:164:ARG:N	2.26	0.50
1:C:201:CYS:O	1:C:229:THR:HA	2.11	0.50
1:C:100:GLY:HA2	1:C:256:TYR:CE2	2.46	0.50
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.94	0.50
1:B:162:GLY:HA2	1:B:321:LEU:O	2.11	0.50
1:B:36:ASP:OD1	2:E:274:ARG:NH2	2.45	0.50
2:E:473:LEU:HD13	4:H:34:PHE:HZ	1.77	0.50
1:B:171:ARG:HH22	2:E:356:ARG:NH2	1.99	0.50
2:F:337:ARG:O	2:F:341:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ALA:N	1:B:66:LEU:HD11	2.26	0.50
1:C:166:LEU:HD13	1:C:342:VAL:HG11	1.94	0.50
1:C:164:ARG:HH22	2:E:189:ARG:HD3	1.76	0.50
2:F:231:ARG:HD2	2:F:234:LEU:HD12	1.94	0.50
2:F:96:ASN:ND2	2:F:98:ILE:H	2.09	0.50
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.41	0.50
1:A:38:ILE:HD12	1:A:285:LEU:CD2	2.41	0.50
2:D:408:ARG:NE	4:H:22:PHE:CE2	2.80	0.50
2:E:145:PRO:HD2	2:E:358:MET:HG2	1.92	0.50
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.93	0.50
2:F:269:SER:CB	2:F:282:GLN:HB3	2.42	0.50
1:A:432:GLN:OE1	5:A:1511:ANP:H2'	2.12	0.50
1:A:432:GLN:NE2	5:A:1511:ANP:H2'	2.27	0.50
1:B:151:LYS:HE3	1:B:427:LEU:O	2.12	0.50
1:B:266:ILE:C	1:B:267:ILE:HD12	2.32	0.50
1:B:393:GLU:OE1	1:B:420:ARG:NH1	2.45	0.50
1:C:84:GLU:OE1	2:D:54:GLY:HA2	2.11	0.50
2:D:188:GLU:OE2	2:D:257:ASN:ND2	2.44	0.50
2:E:238:THR:HA	2:E:241:GLU:OE2	2.11	0.50
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.92	0.50
1:C:445:ILE:O	1:C:449:VAL:HG23	2.11	0.50
1:C:472:VAL:CG2	1:C:473:ILE:N	2.75	0.50
2:F:435:LYS:HG3	2:F:436:GLU:N	2.27	0.50
1:C:353:GLU:HB2	1:C:356:LEU:HD12	1.93	0.49
2:D:63:MET:HE2	2:D:97:VAL:HG11	1.94	0.49
2:E:50:ALA:C	2:E:51:GLN:HG3	2.32	0.49
2:F:89:GLU:HG3	2:F:109:LYS:O	2.11	0.49
1:A:97:VAL:HG11	1:A:249:SER:CB	2.39	0.49
1:A:54:GLU:OE2	1:A:58:GLY:HA2	2.12	0.49
1:C:258:ARG:HG3	1:C:320:SER:HA	1.94	0.49
1:C:403:PHE:CZ	4:H:21:ALA:N	2.80	0.49
1:B:41:VAL:CG1	1:B:44:LEU:HD12	2.39	0.49
1:C:224:ASP:OD1	1:C:227:LYS:HD3	2.12	0.49
2:F:221:GLN:HB2	2:F:223:ASN:ND2	2.22	0.49
2:F:242:TYR:CE1	2:F:246:GLN:HG3	2.46	0.49
1:A:24:ASP:C	1:A:26:GLU:H	2.14	0.49
2:D:97:VAL:HG21	2:D:228:ALA:HB1	1.94	0.49
2:D:409:LYS:NZ	2:D:450:ASP:HA	2.27	0.49
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.94	0.49
1:A:420:ARG:HG3	1:A:420:ARG:NH1	2.27	0.49
1:C:463:LYS:HE3	1:C:508:PHE:HZ	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:MET:SD	1:C:60:LYS:HD3	2.52	0.49
2:E:122:GLU:HG2	2:E:125:GLU:OE2	2.12	0.49
2:E:188:GLU:O	2:E:221:GLN:HB3	2.12	0.49
2:F:267:GLU:O	2:F:271:LEU:HG	2.11	0.49
2:F:414:LEU:HD23	2:F:441:PHE:CZ	2.48	0.49
1:A:87:ILE:N	1:A:87:ILE:CD1	2.75	0.49
2:E:444:ILE:HD13	2:E:449:TYR:HD1	1.76	0.49
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.77	0.49
1:B:341:ASN:O	1:B:345:ILE:HG13	2.13	0.49
1:C:397:TYR:HD1	1:C:418:LEU:HD23	1.78	0.49
2:D:439:LYS:HE2	2:D:443:GLN:OE1	2.12	0.49
2:D:96:ASN:HD21	2:D:98:ILE:HG13	1.77	0.49
2:E:97:VAL:HG13	2:E:232:VAL:HG13	1.94	0.49
2:F:83:ARG:HA	2:F:114:ALA:O	2.12	0.49
2:F:289:MET:HG3	2:F:293:GLN:HG3	1.94	0.49
2:E:81:PRO:CG	2:E:115:ALA:HB1	2.41	0.49
2:E:296:ILE:O	2:E:297:THR:HG23	2.12	0.49
2:F:445:LEU:C	2:F:447:GLY:H	2.15	0.49
1:A:286:ARG:HH12	3:G:272:LEU:HB3	1.77	0.49
1:A:439:GLU:HG2	1:A:440:GLU:H	1.77	0.49
1:B:48:GLN:HG2	2:F:70:VAL:CG2	2.42	0.49
1:C:300:TYR:CE2	1:C:304:ARG:NH1	2.80	0.49
1:A:309:ALA:HB1	1:A:321:LEU:O	2.13	0.49
1:A:358:TYR:OH	2:D:354:THR:HG22	2.12	0.49
1:B:248:TYR:OH	1:B:301:LEU:HD12	2.13	0.49
1:B:80:LYS:HD2	2:E:33:LEU:CD1	2.42	0.49
1:C:483:ILE:O	1:C:487:GLY:CA	2.60	0.49
1:C:483:ILE:O	1:C:487:GLY:N	2.45	0.49
2:D:188:GLU:HB2	2:D:221:GLN:OE1	2.11	0.49
2:E:38:VAL:CG2	2:E:45:LEU:HG	2.43	0.49
2:E:81:PRO:HG2	2:E:115:ALA:CB	2.40	0.49
2:F:138:LYS:HD3	2:F:432:VAL:HG21	1.94	0.49
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.37	0.49
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.26	0.49
1:A:432:GLN:CD	5:A:1511:ANP:H2'	2.33	0.49
1:A:151:LYS:HA	1:A:441:GLN:OE1	2.11	0.49
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.43	0.49
1:C:367:VAL:HG12	1:C:391:LYS:HG3	1.94	0.49
1:C:383:MET:HB2	1:C:438:ILE:HD11	1.95	0.49
2:F:84:ILE:HG21	2:F:235:THR:HG23	1.94	0.49
1:A:246:ALA:HA	1:A:249:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASP:O	1:C:24:ASP:CG	2.50	0.49
2:D:197:TYR:CE2	2:D:201:ILE:HD11	2.47	0.49
2:E:250:ASP:HA	2:E:303:SER:O	2.12	0.49
1:B:303:SER:HB2	2:F:222:MET:HB3	1.94	0.49
1:B:427:LEU:HD22	1:B:444:VAL:HG23	1.95	0.49
1:C:452:TYR:O	1:C:453:LEU:HD23	2.13	0.49
2:D:181:SER:O	2:D:215:VAL:HA	2.13	0.49
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.93	0.49
2:F:50:ALA:O	2:F:51:GLN:HG3	2.12	0.49
2:F:25:PHE:O	2:F:56:SER:HB3	2.12	0.49
1:B:469:LEU:O	1:B:472:VAL:HG22	2.12	0.49
1:C:217:VAL:HG11	2:F:123:PHE:CZ	2.31	0.49
1:C:446:TYR:CE2	1:C:497:LEU:CB	2.93	0.49
1:B:144:GLU:O	1:B:161:ARG:HG3	2.12	0.49
1:C:78:ASN:C	1:C:80:LYS:H	2.16	0.49
2:D:63:MET:CE	2:D:97:VAL:HG11	2.42	0.49
1:C:299:PHE:CZ	2:E:260:ARG:NH1	2.80	0.49
2:E:154:LEU:HA	2:E:333:THR:O	2.13	0.49
2:F:387:ILE:CD1	2:F:387:ILE:H	2.25	0.49
1:A:427:LEU:HD11	1:A:448:GLY:HA3	1.94	0.49
1:B:104:LEU:HB3	1:B:227:LYS:O	2.11	0.49
1:C:482:LYS:O	1:C:483:ILE:C	2.50	0.49
1:C:48:GLN:HB3	2:D:68:GLY:CA	2.35	0.49
2:E:243:PHE:HB3	2:E:249:GLN:OE1	2.12	0.49
1:A:155:SER:OG	1:A:156:LEU:N	2.43	0.49
1:C:66:LEU:O	2:E:15:ALA:HA	2.13	0.49
1:A:252:SER:O	1:A:255:GLU:N	2.46	0.49
1:A:290:GLY:O	1:A:293:ALA:N	2.46	0.49
1:A:290:GLY:O	1:A:291:ARG:C	2.51	0.49
1:A:301:LEU:HA	1:A:304:ARG:NH1	2.28	0.49
1:A:351:PHE:N	1:A:370:SER:OG	2.45	0.49
1:B:108:VAL:HG12	1:B:114:ALA:CA	2.38	0.49
1:C:382:ALA:O	1:C:385:GLN:HB2	2.12	0.49
2:E:185:GLY:CA	2:E:188:GLU:HG3	2.39	0.49
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.43	0.49
2:F:37:GLU:OE2	2:F:44:ARG:NE	2.44	0.49
3:G:10:LEU:HD21	3:G:246:LEU:HB2	1.94	0.49
1:B:270:ASP:N	1:B:326:VAL:HB	2.27	0.49
1:B:339:PRO:O	1:B:343:ILE:HG13	2.13	0.49
1:C:265:LEU:HD12	1:C:322:THR:O	2.13	0.49
1:C:139:ARG:NH1	1:C:310:ALA:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:PHE:O	1:C:472:VAL:HG13	2.13	0.49
2:D:36:LEU:HB3	2:D:75:VAL:CG1	2.43	0.49
2:E:253:LEU:O	2:E:306:SER:HA	2.12	0.49
2:E:339:ILE:O	2:E:342:LEU:N	2.43	0.49
2:E:409:LYS:CG	2:E:454:GLU:HG2	2.43	0.49
1:A:116:ASP:C	2:D:124:VAL:HG12	2.33	0.49
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.93	0.49
1:A:166:LEU:HD12	1:A:325:PRO:O	2.13	0.49
2:D:186:VAL:O	2:D:260:ARG:HG3	2.13	0.49
2:F:191:ARG:O	2:F:194:ASN:HB3	2.13	0.49
2:F:455:GLN:O	2:F:469:LYS:HE2	2.13	0.49
2:F:47:LEU:HD23	2:F:62:ALA:HA	1.94	0.49
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.47	0.49
1:C:436:MET:HE1	1:C:469:LEU:HD13	1.95	0.48
2:D:293:GLN:NE2	2:D:308:GLN:HE22	2.11	0.48
2:D:36:LEU:HD12	2:D:60:THR:HG21	1.94	0.48
2:F:155:PHE:CE1	2:F:332:THR:HB	2.48	0.48
2:F:310:ILE:HD11	2:F:329:LEU:HD11	1.95	0.48
2:F:63:MET:CE	2:F:228:ALA:HA	2.43	0.48
4:H:24:LYS:O	4:H:27:GLN:HB3	2.14	0.48
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.93	0.48
1:B:357:PHE:HD2	1:B:358:TYR:CE1	2.31	0.48
1:C:98:PRO:CD	1:C:112:GLY:HA3	2.43	0.48
2:F:338:ALA:O	2:F:342:LEU:HG	2.12	0.48
2:D:190:THR:HA	2:D:221:GLN:HG3	1.94	0.48
2:D:279:VAL:O	2:D:279:VAL:HG12	2.13	0.48
2:D:349:ASP:OD1	2:D:351:LEU:N	2.45	0.48
1:C:373:ARG:NH1	5:F:1478:ANP:O3G	2.37	0.48
1:A:172:GLN:HA	5:A:1511:ANP:N3B	2.22	0.48
1:A:25:LEU:HD13	1:A:42:HIS:NE2	2.28	0.48
1:A:469:LEU:O	1:A:472:VAL:HG22	2.12	0.48
1:C:339:PRO:O	1:C:343:ILE:HG13	2.12	0.48
2:D:181:SER:O	2:D:215:VAL:HG13	2.13	0.48
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.96	0.48
2:D:25:PHE:O	2:D:56:SER:HB3	2.13	0.48
2:E:13:ILE:HG13	2:E:75:VAL:CG2	2.43	0.48
2:E:167:MET:O	2:E:170:ILE:HB	2.13	0.48
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.48	0.48
2:E:94:ILE:HG22	2:E:102:ILE:HD11	1.94	0.48
1:A:218:LYS:HE2	1:A:222:ASP:OD2	2.13	0.48
1:B:97:VAL:HG11	1:B:249:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ARG:HG2	2:E:41:ARG:HH11	1.78	0.48
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.44	0.48
1:C:235:THR:N	1:C:238:ASP:OD2	2.47	0.48
1:C:457:GLU:HB3	1:C:460:LYS:CG	2.40	0.48
1:C:461:ILE:O	1:C:464:PHE:HB3	2.13	0.48
2:F:159:GLY:N	5:F:1478:ANP:HNB1	2.06	0.48
1:A:501:VAL:CG2	1:A:502:THR:N	2.76	0.48
1:B:186:GLN:CD	1:B:199:LEU:HD23	2.33	0.48
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.48
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.43	0.48
2:D:365:SER:O	2:D:369:ASP:OD2	2.31	0.48
2:E:196:LEU:HG	2:E:200:MET:HE2	1.94	0.48
2:E:139:VAL:HG22	2:E:414:LEU:HB3	1.96	0.48
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.94	0.48
1:A:99:VAL:CG2	1:A:256:TYR:HB2	2.42	0.48
1:B:468:PHE:O	1:B:472:VAL:HG13	2.14	0.48
1:B:479:LEU:C	1:B:479:LEU:HD13	2.34	0.48
1:C:392:LEU:O	1:C:396:GLN:CG	2.61	0.48
1:C:403:PHE:CZ	4:H:20:GLY:C	2.86	0.48
1:C:65:ASN:HD22	1:C:67:GLU:CG	2.26	0.48
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.49	0.48
2:F:251:VAL:O	2:F:304:ILE:HA	2.13	0.48
1:A:248:TYR:CE2	1:A:305:LEU:HB2	2.48	0.48
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.48	0.48
1:C:141:SER:O	1:C:143:ARG:HG3	2.13	0.48
1:C:386:VAL:HG23	1:C:387:ALA:N	2.29	0.48
2:D:380:ASP:O	2:D:384:LEU:HG	2.14	0.48
2:F:420:VAL:HG12	2:F:420:VAL:O	2.12	0.48
1:A:64:LEU:HB3	1:A:287:ARG:HH22	1.76	0.48
1:A:91:THR:C	1:A:93:ALA:H	2.17	0.48
1:C:456:LEU:HD12	1:C:457:GLU:H	1.78	0.48
1:C:486:ASP:O	1:C:488:LYS:N	2.47	0.48
1:A:389:THR:HB	1:A:449:VAL:HG13	1.94	0.48
1:B:101:GLU:C	1:B:103:LEU:H	2.16	0.48
1:B:102:GLU:HG3	1:B:122:GLY:O	2.13	0.48
1:B:168:ILE:HG12	1:B:329:THR:HG23	1.95	0.48
1:C:189:PHE:HB3	1:C:197:LYS:O	2.13	0.48
2:D:118:ALA:O	2:D:295:ARG:HD2	2.13	0.48
2:E:440:GLY:HA2	2:E:463:ILE:HB	1.96	0.48
2:F:189:ARG:HH11	2:F:189:ARG:HG3	1.79	0.48
4:H:14:ALA:O	4:H:17:ASP:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:HD11	1:B:216:LEU:HD11	1.95	0.48
1:C:184:ILE:HD13	1:C:433:TYR:HD2	1.79	0.48
1:A:293:ALA:CB	2:D:277:SER:HA	2.44	0.48
2:F:93:ARG:NH1	2:F:108:ILE:HG12	2.29	0.48
2:F:437:THR:O	2:F:441:PHE:HD1	1.96	0.48
2:F:443:GLN:HE21	2:F:449:TYR:HE1	1.60	0.48
2:F:443:GLN:NE2	2:F:449:TYR:HE1	2.12	0.48
1:B:102:GLU:HG3	1:B:122:GLY:C	2.33	0.48
1:B:352:LEU:CD2	1:B:365:ILE:HG12	2.43	0.48
1:B:373:ARG:HH22	2:F:189:ARG:HH21	1.60	0.48
1:B:456:LEU:HD21	1:B:464:PHE:HB2	1.96	0.48
1:C:166:LEU:HD13	1:C:342:VAL:CG1	2.43	0.48
2:E:10:THR:HG22	2:E:11:GLY:N	2.29	0.48
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.95	0.48
2:E:189:ARG:HB2	2:E:192:GLU:HG3	1.96	0.48
2:F:276:PRO:HD2	3:G:266:ILE:HD11	1.94	0.48
1:B:177:SER:O	1:B:178:ILE:C	2.51	0.48
2:D:471:ASP:OD1	4:H:37:ARG:NH2	2.41	0.48
2:E:32:ILE:HA	2:E:49:VAL:HG12	1.95	0.48
2:F:365:SER:O	2:F:369:ASP:OD2	2.32	0.48
1:B:395:ALA:HA	1:B:398:ARG:NH2	2.28	0.48
2:D:159:GLY:N	5:D:1478:ANP:HNB1	2.11	0.48
2:D:221:GLN:NE2	2:D:221:GLN:CA	2.76	0.48
1:C:237:SER:CB	2:D:294:GLU:HG3	2.38	0.48
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.96	0.48
2:E:152:ILE:HD12	2:E:152:ILE:N	2.29	0.48
4:H:33:TYR:O	4:H:36:ALA:HB3	2.13	0.48
1:B:156:LEU:HD13	1:B:367:VAL:CG1	2.43	0.48
1:C:436:MET:HE1	1:C:469:LEU:CD1	2.44	0.48
1:C:471:HIS:C	1:C:473:ILE:H	2.16	0.48
2:D:222:MET:HA	2:D:229:ARG:HD3	1.95	0.48
2:F:189:ARG:O	2:F:190:THR:C	2.51	0.48
2:F:393:MET:HG3	2:F:396:LEU:HD11	1.96	0.48
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.96	0.48
1:C:353:GLU:CD	1:C:366:ASN:HD22	2.17	0.48
2:D:228:ALA:O	2:D:232:VAL:HG22	2.14	0.48
2:E:145:PRO:CB	2:E:357:ILE:HD11	2.39	0.48
2:F:12:ARG:CG	2:F:74:LYS:HD3	2.44	0.48
1:A:135:GLY:O	1:A:139:ARG:HD2	2.14	0.48
1:B:156:LEU:HD11	1:B:428:LEU:HD11	1.96	0.48
1:C:300:TYR:HE2	1:C:304:ARG:HH11	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:101:PRO:HB3	2:E:108:ILE:HD11	1.95	0.48
2:E:96:ASN:CG	2:E:97:VAL:H	2.16	0.48
1:A:166:LEU:HA	1:A:325:PRO:HG2	1.96	0.47
1:B:356:LEU:HB3	1:B:361:ILE:HB	1.95	0.47
1:B:52:MET:HE1	1:B:60:LYS:HD3	1.96	0.47
1:C:129:VAL:HG23	1:C:130:GLY:N	2.29	0.47
1:C:278:TYR:CE2	1:C:295:PRO:HG3	2.49	0.47
1:C:396:GLN:O	1:C:399:GLU:N	2.47	0.47
1:C:288:PRO:HG3	3:G:271:ALA:HB3	1.96	0.47
1:A:214:ALA:HA	1:A:217:VAL:HG22	1.95	0.47
1:A:275:ALA:HB1	1:A:294:TYR:CE2	2.49	0.47
1:C:106:ARG:NH2	1:C:116:ASP:OD1	2.47	0.47
1:A:104:LEU:HD11	1:A:200:TYR:CD2	2.50	0.47
1:A:451:GLY:O	1:A:453:LEU:N	2.47	0.47
1:A:497:LEU:O	1:A:500:ILE:N	2.47	0.47
1:A:54:GLU:HG2	1:A:60:LYS:HZ2	1.79	0.47
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.96	0.47
2:E:185:GLY:C	2:E:221:GLN:HE22	2.17	0.47
2:F:390:ILE:CG2	3:G:28:ALA:HB1	2.44	0.47
4:H:27:GLN:O	4:H:31:GLU:HG3	2.14	0.47
1:A:379:GLN:O	1:A:384:LYS:HG3	2.15	0.47
1:A:464:PHE:O	1:A:465:GLU:C	2.52	0.47
1:A:77:GLY:H	1:A:239:ALA:HB3	1.79	0.47
1:B:303:SER:HB2	2:F:222:MET:SD	2.54	0.47
1:C:382:ALA:N	1:C:487:GLY:O	2.39	0.47
2:D:386:ASP:OD1	4:H:6:ASP:HA	2.14	0.47
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.44	0.47
2:F:135:THR:HG21	2:F:146:TYR:CD1	2.49	0.47
2:F:292:MET:HE1	2:F:293:GLN:HG2	1.96	0.47
1:A:106:ARG:NH1	1:A:121:ILE:HD13	2.29	0.47
1:B:272:SER:O	1:B:275:ALA:HB3	2.14	0.47
1:C:139:ARG:HH12	1:C:310:ALA:HB2	1.79	0.47
1:C:34:ILE:CG2	2:D:52:HIS:HB2	2.44	0.47
2:D:378:LEU:HD21	2:D:411:GLN:HG2	1.95	0.47
2:E:381:TYR:HE1	4:H:22:PHE:HZ	1.60	0.47
1:A:505:LEU:O	1:A:508:PHE:N	2.45	0.47
1:B:248:TYR:CD2	1:B:305:LEU:HD13	2.49	0.47
1:B:392:LEU:O	1:B:395:ALA:HB3	2.14	0.47
2:D:425:THR:HG21	2:D:459:MET:CE	2.44	0.47
2:E:420:VAL:O	2:E:420:VAL:HG12	2.14	0.47
3:G:221:THR:O	3:G:222:THR:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLU:HB3	1:B:294:TYR:HE1	1.79	0.47
1:C:172:GLN:N	5:C:1511:ANP:HNB1	2.12	0.47
1:C:491:GLU:H	1:C:491:GLU:CD	2.18	0.47
2:D:378:LEU:HD21	2:D:411:GLN:CG	2.44	0.47
2:F:96:ASN:HB2	2:F:102:ILE:CG2	2.44	0.47
1:A:166:LEU:HD11	1:A:327:ILE:CG1	2.41	0.47
1:A:489:ILE:HG22	1:A:494:ASP:HB2	1.95	0.47
1:B:439:GLU:O	1:B:442:VAL:HG22	2.14	0.47
2:E:396:LEU:HB2	2:E:401:LYS:HG2	1.97	0.47
2:E:434:LEU:O	2:E:438:ILE:HG12	2.15	0.47
1:C:188:ARG:HG3	1:C:188:ARG:HH11	1.80	0.47
2:E:181:SER:O	2:E:215:VAL:HA	2.14	0.47
2:F:408:ARG:O	2:F:412:ARG:HG3	2.13	0.47
2:E:388:ILE:HD11	4:H:22:PHE:CE1	2.49	0.47
1:A:106:ARG:HH11	1:A:106:ARG:HG3	1.79	0.47
1:C:75:VAL:HG21	1:C:82:ILE:HD12	1.95	0.47
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.95	0.47
3:G:5:ASP:C	3:G:5:ASP:OD1	2.53	0.47
1:B:312:MET:HG2	1:B:319:GLY:O	2.14	0.47
1:C:45:ARG:NH2	1:C:68:PRO:O	2.41	0.47
2:D:251:VAL:HB	2:D:304:ILE:HG12	1.97	0.47
2:D:338:ALA:O	2:D:342:LEU:HG	2.14	0.47
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.47
2:D:298:THR:HG23	2:D:303:SER:HA	1.96	0.47
2:E:173:VAL:O	2:E:177:HIS:HB2	2.13	0.47
2:F:277:SER:OG	2:F:278:ALA:N	2.47	0.47
3:G:25:MET:O	3:G:28:ALA:HB3	2.15	0.47
4:H:25:ARG:HD3	4:H:29:GLU:HG2	1.95	0.47
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.96	0.47
2:E:168:GLU:HA	2:E:420:VAL:HG21	1.95	0.47
2:F:151:LYS:HD2	2:F:151:LYS:N	2.30	0.47
2:F:258:ILE:HD11	2:F:292:MET:HE1	1.96	0.47
1:C:248:TYR:CE2	1:C:305:LEU:HB2	2.49	0.47
1:C:372:SER:C	1:C:374:VAL:H	2.18	0.47
2:E:190:THR:O	2:E:193:GLY:N	2.48	0.47
2:E:430:LYS:NZ	2:E:465:GLU:OE1	2.46	0.47
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.96	0.47
2:F:257:ASN:H	2:F:309:ALA:HB3	1.79	0.47
2:F:92:GLY:HA2	2:F:206:ILE:CD1	2.45	0.47
1:A:151:LYS:N	1:A:430:GLN:OE1	2.43	0.47
1:A:479:LEU:O	1:A:483:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLU:CD	1:B:102:GLU:H	2.18	0.47
1:B:140:ILE:HB	1:B:313:ASN:HB3	1.97	0.47
1:B:268:TYR:CE2	1:B:305:LEU:HD21	2.50	0.47
1:C:116:ASP:C	1:C:116:ASP:OD1	2.53	0.47
1:C:499:GLU:O	1:C:503:ASN:ND2	2.47	0.47
1:A:210:ARG:HH12	2:D:120:ALA:HB3	1.79	0.47
2:E:302:GLY:O	2:E:303:SER:HB3	2.14	0.47
2:E:89:GLU:HG3	2:E:109:LYS:O	2.14	0.47
2:F:408:ARG:HE	2:F:454:GLU:CD	2.18	0.47
3:G:20:THR:HA	3:G:232:MET:HE2	1.96	0.47
3:G:10:LEU:CD2	3:G:246:LEU:HB2	2.44	0.47
1:A:153:VAL:O	1:A:155:SER:N	2.48	0.47
1:A:348:GLY:HA2	1:A:349:GLN:NE2	2.29	0.47
1:A:36:ASP:O	1:A:284:LEU:HD13	2.14	0.47
1:B:151:LYS:CE	1:B:427:LEU:O	2.63	0.47
1:C:486:ASP:N	1:C:486:ASP:OD1	2.48	0.47
2:E:94:ILE:HA	2:E:217:LEU:HB2	1.96	0.47
2:F:96:ASN:HB2	2:F:102:ILE:HG23	1.96	0.47
2:F:443:GLN:O	2:F:446:ALA:N	2.48	0.47
4:H:9:ARG:O	4:H:9:ARG:HG3	2.15	0.47
1:A:161:ARG:NH2	1:A:197:LYS:O	2.40	0.47
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.45	0.47
1:C:333:ASP:C	1:C:335:SER:H	2.18	0.47
2:D:84:ILE:CD1	2:D:235:THR:HG23	2.45	0.47
2:D:335:LEU:N	2:D:335:LEU:CD1	2.78	0.47
2:E:151:LYS:HD2	2:E:151:LYS:N	2.30	0.47
4:H:4:SER:HA	4:H:7:ASN:ND2	2.30	0.47
1:A:186:GLN:CG	1:A:199:LEU:HD23	2.44	0.47
1:C:142:VAL:HG13	1:C:161:ARG:O	2.15	0.47
1:C:48:GLN:HB3	2:E:68:GLY:HA2	1.96	0.47
1:C:476:HIS:CE1	1:C:500:ILE:HG12	2.50	0.47
1:A:136:ILE:HG23	2:D:194:ASN:N	2.29	0.47
2:F:132:ILE:HD11	2:F:145:PRO:HB3	1.96	0.47
2:F:296:ILE:HG23	2:F:304:ILE:HG22	1.97	0.47
1:C:151:LYS:HD2	1:C:428:LEU:HA	1.97	0.47
1:C:482:LYS:O	1:C:485:THR:N	2.48	0.47
1:A:36:ASP:OD1	2:D:274:ARG:NH2	2.48	0.47
2:E:96:ASN:CG	2:E:97:VAL:N	2.68	0.47
1:C:215:GLN:HG3	2:F:356:ARG:HH12	1.78	0.47
1:A:105:GLY:HA2	1:A:226:MET:O	2.14	0.47
1:A:436:MET:CE	1:A:469:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLN:H	5:C:1511:ANP:HNB1	1.63	0.47
1:C:265:LEU:HD11	1:C:324:LEU:HG	1.95	0.47
1:C:166:LEU:HA	1:C:325:PRO:HG2	1.97	0.47
2:E:142:LEU:HD22	2:E:441:PHE:CD1	2.50	0.47
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.95	0.47
2:F:146:TYR:CE1	2:F:152:ILE:HG21	2.50	0.47
2:F:390:ILE:HG23	3:G:28:ALA:HB1	1.97	0.47
1:A:408:SER:O	1:A:409:ASP:HB2	2.14	0.47
1:A:436:MET:HG3	1:A:441:GLN:CG	2.46	0.47
1:A:98:PRO:HD2	1:A:112:GLY:HA3	1.96	0.47
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.96	0.47
1:C:373:ARG:NH1	2:D:189:ARG:NH2	2.63	0.47
2:D:84:ILE:HD12	2:D:95:MET:CE	2.45	0.47
2:E:261:PHE:O	2:E:264:ALA:HB3	2.15	0.47
2:F:190:THR:HA	2:F:221:GLN:HG3	1.96	0.47
2:F:17:ILE:CG2	2:F:271:LEU:HD22	2.45	0.47
2:F:415:SER:O	2:F:416:GLN:HB2	2.15	0.47
1:A:349:GLN:OE1	1:A:351:PHE:HE1	1.99	0.46
1:A:432:GLN:HB2	5:A:1511:ANP:C6	2.45	0.46
1:B:210:ARG:HG3	1:B:235:THR:HG21	1.96	0.46
1:C:153:VAL:O	1:C:157:VAL:C	2.53	0.46
2:E:146:TYR:O	2:E:357:ILE:CD1	2.63	0.46
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.45	0.46
1:A:267:ILE:N	1:A:267:ILE:HD12	2.30	0.46
1:A:401:ALA:O	1:A:404:ALA:HB2	2.15	0.46
1:A:381:ARG:CG	1:A:488:LYS:HB3	2.45	0.46
2:E:112:GLN:N	2:E:112:GLN:OE1	2.48	0.46
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.98	0.46
1:C:382:ALA:O	1:C:385:GLN:HB2	2.15	0.46
2:D:406:ARG:O	2:D:410:ILE:HG13	2.15	0.46
2:E:27:GLU:HB2	2:E:28:GLY:H	1.58	0.46
2:E:351:LEU:HD12	2:E:382:LYS:CE	2.44	0.46
2:E:452:LEU:HD22	2:E:470:ALA:HB1	1.96	0.46
1:A:304:ARG:O	1:A:308:ARG:HG3	2.14	0.46
1:C:374:VAL:CG1	1:C:378:ALA:HB2	2.45	0.46
1:C:410:LEU:HD13	1:C:415:GLN:HA	1.97	0.46
1:C:436:MET:HE1	1:C:441:GLN:HA	1.97	0.46
2:D:237:LEU:HD21	2:D:295:ARG:CB	2.45	0.46
1:A:80:LYS:CE	2:D:33:LEU:HD12	2.46	0.46
2:D:36:LEU:HB2	2:D:47:LEU:HB2	1.96	0.46
1:A:438:ILE:HG23	1:A:439:GLU:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:SER:HA	1:B:345:ILE:HD13	1.96	0.46
1:B:362:ARG:HA	1:B:363:PRO:C	2.34	0.46
1:C:147:GLN:O	1:C:185:ASN:ND2	2.48	0.46
2:D:20:VAL:HG21	2:D:271:LEU:HB2	1.97	0.46
2:F:138:LYS:NZ	2:F:413:PHE:O	2.45	0.46
1:B:114:ALA:HB2	1:B:121:ILE:CD1	2.28	0.46
1:B:171:ARG:NH1	1:B:171:ARG:HB2	2.29	0.46
1:C:338:ILE:O	1:C:341:ASN:HB2	2.15	0.46
1:C:483:ILE:O	1:C:487:GLY:HA2	2.15	0.46
2:D:285:LEU:HD23	2:D:285:LEU:O	2.16	0.46
2:D:452:LEU:HD22	2:D:470:ALA:HB1	1.98	0.46
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.51	0.46
2:F:103:ASP:O	2:F:105:ARG:HG3	2.14	0.46
1:A:140:ILE:CG1	1:A:143:ARG:NH1	2.78	0.46
1:A:179:ALA:HB1	1:A:267:ILE:CD1	2.25	0.46
1:A:338:ILE:O	1:A:341:ASN:HB2	2.15	0.46
1:A:390:MET:HE1	1:A:445:ILE:CD1	2.45	0.46
1:A:473:ILE:O	1:A:477:GLN:NE2	2.48	0.46
1:B:270:ASP:OD1	1:B:273:LYS:HB2	2.16	0.46
1:C:272:SER:O	1:C:276:VAL:HG23	2.15	0.46
1:C:74:VAL:HG11	1:C:241:PRO:HG3	1.95	0.46
2:D:210:ASP:O	2:D:212:THR:N	2.42	0.46
2:F:345:TYR:HA	2:F:346:PRO:C	2.35	0.46
4:H:12:ALA:HB1	4:H:16:ARG:NE	2.31	0.46
1:A:381:ARG:HG2	1:A:488:LYS:HB3	1.96	0.46
1:A:387:ALA:O	1:A:388:GLY:C	2.54	0.46
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.80	0.46
2:F:101:PRO:HB3	2:F:108:ILE:CD1	2.45	0.46
2:F:226:PRO:HB2	2:F:268:VAL:HG13	1.96	0.46
2:F:463:ILE:O	2:F:466:ALA:HB3	2.14	0.46
1:B:271:LEU:O	1:B:274:GLN:HB3	2.16	0.46
2:D:49:VAL:HA	2:D:60:THR:HG22	1.98	0.46
2:F:112:GLN:NE2	2:F:242:TYR:OH	2.49	0.46
1:A:357:PHE:C	1:A:359:LYS:N	2.69	0.46
1:B:151:LYS:HZ1	1:B:430:GLN:HB2	1.79	0.46
1:B:83:LYS:HD3	2:E:31:PRO:HB3	1.97	0.46
1:C:300:TYR:O	1:C:304:ARG:HB3	2.16	0.46
1:B:286:ARG:NH1	2:E:275:ILE:HD11	2.31	0.46
2:E:341:GLU:C	2:E:343:GLY:H	2.18	0.46
2:F:143:LEU:HD22	2:F:375:GLN:HG3	1.98	0.46
1:A:205:ALA:HA	1:A:208:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLU:OE1	1:A:449:VAL:HG13	2.16	0.46
1:B:396:GLN:O	1:B:397:TYR:C	2.54	0.46
1:C:269:ASP:O	1:C:270:ASP:CB	2.63	0.46
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.96	0.46
2:F:167:MET:HE3	2:F:203:SER:HB3	1.97	0.46
2:F:281:TYR:CE1	2:F:320:PRO:HB2	2.51	0.46
1:A:167:ILE:HG22	1:A:175:LYS:HG2	1.98	0.46
1:A:357:PHE:C	1:A:359:LYS:H	2.19	0.46
1:C:76:PHE:HD2	1:C:241:PRO:HB2	1.80	0.46
2:D:270:ALA:O	2:D:273:GLY:N	2.43	0.46
2:E:144:ALA:N	2:E:145:PRO:HD3	2.31	0.46
2:F:183:PHE:HB3	2:F:217:LEU:HD23	1.97	0.46
1:A:386:VAL:HG23	1:A:387:ALA:H	1.81	0.46
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.16	0.46
1:C:183:ILE:HD11	1:C:267:ILE:HD12	1.97	0.46
1:C:306:LEU:HD12	1:C:345:ILE:HG21	1.98	0.46
1:C:80:LYS:HG2	1:C:81:LEU:HG	1.98	0.46
2:D:12:ARG:HE	2:D:74:LYS:HE3	1.79	0.46
2:F:292:MET:C	2:F:292:MET:SD	2.94	0.46
4:H:9:ARG:CA	4:H:15:VAL:HG22	2.45	0.46
1:A:45:ARG:HA	2:E:71:ARG:NH2	2.31	0.46
1:A:460:LYS:O	1:A:461:ILE:C	2.54	0.46
1:B:441:GLN:O	1:B:444:VAL:HG22	2.15	0.46
1:C:65:ASN:ND2	1:C:67:GLU:OE2	2.49	0.46
2:D:12:ARG:HG3	2:D:12:ARG:HH11	1.81	0.46
2:E:147:ALA:HB2	2:E:357:ILE:HG21	1.98	0.46
2:E:276:PRO:HD2	3:G:266:ILE:CD1	2.46	0.46
1:B:132:LYS:NZ	2:F:224:GLU:OE1	2.48	0.46
1:C:284:LEU:HD21	2:F:274:ARG:HG2	1.96	0.46
2:D:276:PRO:HG2	3:G:265:ILE:HA	1.97	0.46
1:A:156:LEU:HD11	1:A:428:LEU:HD21	1.98	0.46
1:B:37:GLY:O	1:B:38:ILE:HD13	2.15	0.46
2:F:151:LYS:C	2:F:152:ILE:HD12	2.36	0.46
1:B:159:ILE:HD12	1:B:165:GLU:HB2	1.98	0.46
1:B:248:TYR:CE2	1:B:305:LEU:HB2	2.50	0.46
1:C:65:ASN:O	1:C:71:VAL:HA	2.16	0.46
2:D:279:VAL:HG12	2:D:279:VAL:O	2.15	0.46
2:E:140:VAL:HG13	2:E:146:TYR:CE1	2.51	0.46
1:B:137:ILE:HB	1:B:138:PRO:HD3	1.98	0.46
1:B:164:ARG:HH11	1:B:164:ARG:HG2	1.79	0.46
1:B:244:TYR:CD2	1:B:281:MET:HE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:THR:O	1:B:393:GLU:HG3	2.16	0.46
2:E:154:LEU:HD11	2:E:307:VAL:HG12	1.97	0.46
1:A:122:GLY:O	1:A:124:LYS:N	2.48	0.46
1:A:486:ASP:C	1:A:488:LYS:H	2.20	0.46
1:B:268:TYR:CB	1:B:271:LEU:HD21	2.46	0.46
2:D:94:ILE:HA	2:D:217:LEU:HB2	1.98	0.46
2:E:355:SER:OG	2:E:357:ILE:HG12	2.15	0.46
1:B:367:VAL:O	1:B:367:VAL:HG12	2.16	0.46
1:C:223:ALA:O	1:C:224:ASP:HB3	2.16	0.46
1:C:267:ILE:HG12	1:C:324:LEU:HB2	1.97	0.46
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.51	0.46
2:E:363:VAL:HB	2:E:367:HIS:ND1	2.31	0.46
1:B:136:ILE:CD1	2:F:190:THR:HA	2.47	0.46
1:A:188:ARG:NH1	1:A:188:ARG:HG3	2.31	0.46
1:C:353:GLU:OE2	1:C:366:ASN:ND2	2.49	0.46
1:C:400:VAL:HG11	1:C:418:LEU:HB2	1.96	0.46
2:D:160:VAL:HG23	2:D:335:LEU:HD23	1.97	0.46
2:E:452:LEU:HD22	2:E:470:ALA:HB1	1.97	0.46
1:C:211:SER:HA	2:F:126:MET:HE2	1.98	0.46
2:F:358:MET:HG3	2:F:372:ARG:NH2	2.31	0.46
2:F:96:ASN:ND2	2:F:100:GLU:H	2.09	0.46
2:F:31:PRO:HG2	2:F:34:ASN:OD1	2.16	0.45
2:F:380:ASP:O	2:F:384:LEU:HG	2.16	0.45
1:A:388:GLY:O	1:A:391:LYS:HB3	2.16	0.45
1:C:497:LEU:O	1:C:501:VAL:HG13	2.16	0.45
2:E:218:VAL:HG21	2:E:236:GLY:HA2	1.97	0.45
2:F:85:PRO:HD2	2:F:95:MET:HE1	1.96	0.45
1:A:111:LEU:HB2	1:A:113:ASN:ND2	2.31	0.45
1:A:170:ASP:O	1:A:175:LYS:HE2	2.16	0.45
1:A:379:GLN:CD	1:A:383:MET:HB3	2.37	0.45
1:B:103:LEU:O	1:B:106:ARG:HB2	2.17	0.45
1:B:140:ILE:HG13	1:B:141:SER:N	2.30	0.45
1:B:99:VAL:HG22	1:B:253:MET:HA	1.97	0.45
1:C:255:GLU:OE2	1:C:258:ARG:NH1	2.49	0.45
3:G:12:SER:HB2	4:H:8:VAL:HA	1.97	0.45
2:D:83:ARG:HA	2:D:114:ALA:O	2.16	0.45
2:D:237:LEU:O	2:D:237:LEU:HD12	2.16	0.45
2:E:170:ILE:CG2	2:E:215:VAL:HG22	2.44	0.45
1:A:501:VAL:O	1:A:504:PHE:HB3	2.17	0.45
1:B:432:GLN:HG2	1:B:433:TYR:CD1	2.51	0.45
2:D:17:ILE:N	2:D:17:ILE:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:LEU:HA	2:D:453:PRO:HD3	1.81	0.45
1:C:48:GLN:HB3	2:E:68:GLY:O	2.16	0.45
2:F:234:LEU:O	2:F:237:LEU:HB3	2.16	0.45
1:A:306:LEU:HD13	1:A:346:THR:CG2	2.45	0.45
1:A:40:ARG:NH2	1:A:285:LEU:O	2.50	0.45
1:B:127:ARG:CZ	1:B:131:LEU:HD12	2.46	0.45
1:B:291:ARG:NH2	2:F:319:ASP:OD2	2.49	0.45
1:B:497:LEU:O	1:B:501:VAL:HG13	2.15	0.45
2:E:200:MET:HA	2:E:203:SER:OG	2.17	0.45
2:E:226:PRO:N	2:E:229:ARG:NH1	2.64	0.45
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.97	0.45
2:F:116:ILE:HA	2:F:238:THR:OG1	2.16	0.45
1:A:108:VAL:HG12	1:A:114:ALA:HA	1.97	0.45
1:B:382:ALA:HA	1:B:488:LYS:HA	1.98	0.45
1:C:273:LYS:O	1:C:276:VAL:HB	2.17	0.45
1:C:376:SER:C	1:C:378:ALA:H	2.20	0.45
1:C:440:GLU:O	1:C:443:ALA:HB3	2.16	0.45
2:E:152:ILE:HB	2:E:307:VAL:HA	1.99	0.45
2:E:266:SER:HB3	2:E:282:GLN:HE22	1.82	0.45
1:A:438:ILE:HG22	1:A:439:GLU:OE2	2.17	0.45
1:B:107:VAL:HB	1:B:116:ASP:HB3	1.98	0.45
1:B:294:TYR:CD2	1:B:298:VAL:HG11	2.52	0.45
1:C:199:LEU:HD12	1:C:263:HIS:O	2.15	0.45
2:D:139:VAL:HG23	2:D:414:LEU:O	2.16	0.45
2:D:32:ILE:O	2:D:33:LEU:CB	2.64	0.45
1:A:353:GLU:HG3	1:A:366:ASN:HB2	1.99	0.45
1:A:432:GLN:OE1	1:A:433:TYR:CE1	2.70	0.45
1:C:174:GLY:HA2	5:C:1511:ANP:PA	2.56	0.45
1:C:165:GLU:OE1	1:C:350:ILE:HG13	2.17	0.45
1:C:292:GLU:O	1:C:293:ALA:HB3	2.17	0.45
2:D:293:GLN:HE22	2:D:308:GLN:NE2	2.15	0.45
2:D:32:ILE:O	2:D:33:LEU:CB	2.64	0.45
1:A:195:GLU:HG2	1:A:198:LYS:CE	2.46	0.45
1:C:153:VAL:HG22	1:C:350:ILE:HD13	1.99	0.45
1:C:225:ALA:HA	1:C:228:TYR:CE2	2.52	0.45
1:C:290:GLY:O	1:C:293:ALA:N	2.43	0.45
1:C:392:LEU:O	1:C:396:GLN:N	2.50	0.45
2:D:238:THR:O	2:D:241:GLU:HB2	2.17	0.45
3:G:247:THR:O	3:G:250:PHE:HB3	2.16	0.45
3:G:27:ALA:CB	3:G:228:ARG:HD2	2.47	0.45
1:A:241:PRO:HA	1:A:244:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.47	0.45
1:C:164:ARG:HD3	1:C:306:LEU:O	2.17	0.45
1:C:393:GLU:O	1:C:397:TYR:HB3	2.16	0.45
2:E:311:TYR:CG	2:E:312:VAL:N	2.85	0.45
3:G:12:SER:CB	4:H:8:VAL:HA	2.46	0.45
1:A:128:ARG:HB2	1:A:131:LEU:HG	1.99	0.45
1:A:459:SER:C	1:A:460:LYS:HD2	2.37	0.45
1:A:53:VAL:HG22	1:A:61:GLY:O	2.16	0.45
1:B:34:ILE:HG23	2:E:52:HIS:HB2	1.99	0.45
1:B:388:GLY:O	1:B:392:LEU:HG	2.16	0.45
1:C:188:ARG:CZ	1:C:436:MET:C	2.84	0.45
1:B:213:VAL:O	1:B:217:VAL:HG13	2.17	0.45
1:B:270:ASP:HA	1:B:326:VAL:O	2.16	0.45
1:C:129:VAL:O	1:C:308:ARG:NH1	2.50	0.45
1:C:200:TYR:O	1:C:264:ALA:HA	2.17	0.45
2:E:252:LEU:CD2	2:E:305:THR:HB	2.46	0.45
2:F:234:LEU:O	2:F:237:LEU:N	2.49	0.45
2:F:63:MET:HE1	2:F:228:ALA:HA	1.99	0.45
3:G:259:THR:O	3:G:263:ILE:HG13	2.16	0.45
1:B:156:LEU:HD13	1:B:367:VAL:HG21	1.99	0.45
1:B:440:GLU:O	1:B:443:ALA:HB3	2.16	0.45
1:B:55:PHE:CE2	1:B:82:ILE:HD13	2.52	0.45
1:B:56:SER:OG	1:B:86:ASP:OD2	2.31	0.45
1:C:452:TYR:HD1	1:C:501:VAL:HG21	1.82	0.45
2:F:337:ARG:HH11	2:F:337:ARG:HG3	1.80	0.45
2:F:389:ALA:O	3:G:238:ASN:HB3	2.16	0.45
1:A:153:VAL:C	1:A:155:SER:H	2.19	0.45
1:A:313:ASN:OD1	1:A:315:ALA:HB3	2.17	0.45
1:B:279:ARG:HG3	1:B:293:ALA:O	2.17	0.45
1:B:185:ASN:HB2	1:B:435:PRO:HB2	1.98	0.45
1:B:479:LEU:C	1:B:479:LEU:HD13	2.37	0.45
2:D:319:ASP:O	2:D:322:PRO:HD2	2.16	0.45
2:E:292:MET:CE	2:E:293:GLN:HE21	2.29	0.45
2:E:159:GLY:CA	5:F:1478:ANP:HNB1	2.30	0.45
1:A:283:LEU:CD2	1:A:289:PRO:HB3	2.46	0.45
1:B:28:THR:CG2	1:B:29:GLY:N	2.73	0.45
1:C:163:GLN:O	1:C:322:THR:HG23	2.17	0.45
1:C:268:TYR:O	1:C:270:ASP:N	2.49	0.45
1:C:291:ARG:HA	3:G:264:GLU:OE1	2.17	0.45
1:C:65:ASN:HD22	1:C:67:GLU:CD	2.19	0.45
2:E:421:ALA:HB1	2:E:425:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.46	0.45
3:G:23:MET:HB2	3:G:232:MET:CE	2.47	0.45
1:A:151:LYS:CG	1:A:436:MET:SD	3.02	0.45
1:B:148:THR:O	1:B:182:THR:HA	2.17	0.45
1:C:439:GLU:CG	1:C:440:GLU:N	2.79	0.45
2:D:221:GLN:HB2	2:D:223:ASN:HD22	1.81	0.45
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.98	0.45
2:E:386:ASP:OD2	4:H:6:ASP:HA	2.16	0.45
1:A:211:SER:N	2:F:126:MET:HE2	2.32	0.45
2:F:338:ALA:O	2:F:342:LEU:HG	2.17	0.45
4:H:38:ALA:O	4:H:42:LEU:HB2	2.17	0.45
1:A:85:GLY:O	1:A:86:ASP:C	2.56	0.45
1:B:29:GLY:CA	1:B:42:HIS:O	2.65	0.45
1:B:34:ILE:HG23	1:B:34:ILE:O	2.16	0.45
1:C:356:LEU:CD1	1:C:366:ASN:HB2	2.46	0.45
2:D:103:ASP:O	2:D:104:GLU:HB2	2.16	0.45
2:F:189:ARG:HB2	2:F:192:GLU:CG	2.47	0.45
1:C:359:LYS:O	2:F:376:LYS:HE2	2.17	0.45
1:A:151:LYS:CD	1:A:436:MET:SD	3.05	0.45
1:B:135:GLY:O	1:B:138:PRO:HD2	2.16	0.45
1:B:177:SER:OG	1:B:432:GLN:NE2	2.47	0.45
1:B:52:MET:HG2	1:B:95:VAL:HG22	1.99	0.45
1:C:209:LYS:O	1:C:210:ARG:C	2.55	0.45
1:C:23:VAL:O	1:C:23:VAL:HG12	2.17	0.45
2:D:133:LEU:HB2	2:D:148:LYS:HG3	1.98	0.45
2:F:89:GLU:CD	2:F:89:GLU:N	2.63	0.45
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.99	0.45
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.50	0.45
1:B:166:LEU:HD13	1:B:342:VAL:CG1	2.47	0.45
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.99	0.45
1:C:140:ILE:HG23	1:C:311:LYS:HG3	1.98	0.45
2:D:164:VAL:HG23	5:D:1478:ANP:O1A	2.17	0.45
1:A:213:VAL:O	1:A:216:LEU:HB3	2.17	0.44
1:B:127:ARG:HG2	1:B:131:LEU:HD11	1.98	0.44
1:B:268:TYR:HB2	1:B:325:PRO:HA	1.98	0.44
1:B:489:ILE:HG22	1:B:489:ILE:O	2.17	0.44
2:D:82:ILE:HD12	2:D:116:ILE:HD11	1.98	0.44
2:E:315:ASP:OD1	2:E:337:ARG:NH2	2.42	0.44
1:A:306:LEU:HD13	1:A:346:THR:HG23	1.99	0.44
1:A:362:ARG:HA	1:A:363:PRO:C	2.36	0.44
1:A:485:THR:C	1:A:487:GLY:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:CG2	2:D:52:HIS:HB2	2.48	0.44
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.52	0.44
2:E:419:GLN:CA	2:E:429:GLY:HA3	2.46	0.44
2:E:82:ILE:O	2:E:116:ILE:HG23	2.17	0.44
2:F:36:LEU:HB3	2:F:75:VAL:CG1	2.47	0.44
2:F:420:VAL:O	2:F:420:VAL:CG1	2.64	0.44
2:F:96:ASN:ND2	2:F:96:ASN:C	2.70	0.44
2:D:391:LEU:CD2	3:G:23:MET:SD	3.02	0.44
1:A:432:GLN:HG2	1:A:433:TYR:CD2	2.53	0.44
1:B:294:TYR:CE1	1:B:338:ILE:HD11	2.52	0.44
1:B:357:PHE:HA	1:B:361:ILE:O	2.17	0.44
1:C:359:LYS:O	2:D:376:LYS:HG3	2.17	0.44
2:E:285:LEU:HD23	2:E:286:ALA:N	2.33	0.44
2:E:330:ASP:OD1	2:E:356:ARG:NE	2.50	0.44
1:A:137:ILE:N	1:A:138:PRO:CD	2.80	0.44
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.98	0.44
1:A:387:ALA:O	1:A:390:MET:N	2.51	0.44
1:B:49:ALA:O	1:B:50:GLU:HB2	2.16	0.44
1:C:343:ILE:C	1:C:345:ILE:H	2.20	0.44
1:A:405:GLN:HE22	2:D:384:LEU:HD21	1.82	0.44
2:F:94:ILE:HD11	2:F:197:TYR:CD1	2.52	0.44
1:A:180:ILE:HD11	1:A:216:LEU:HD11	1.99	0.44
1:A:338:ILE:N	1:A:339:PRO:CD	2.79	0.44
1:B:366:ASN:OD1	1:B:368:GLY:N	2.48	0.44
1:C:201:CYS:O	1:C:229:THR:HA	2.18	0.44
1:C:300:TYR:HA	1:C:303:SER:OG	2.17	0.44
2:F:292:MET:HE1	2:F:293:GLN:NE2	2.32	0.44
2:F:377:ILE:HG21	2:F:410:ILE:CD1	2.45	0.44
2:F:94:ILE:HB	2:F:103:ASP:HB3	1.98	0.44
4:H:12:ALA:O	4:H:13:GLY:C	2.55	0.44
1:A:357:PHE:O	1:A:360:GLY:N	2.41	0.44
2:D:408:ARG:CD	4:H:22:PHE:CZ	3.00	0.44
1:A:301:LEU:HD23	1:A:302:HIS:CD2	2.52	0.44
1:A:341:ASN:O	1:A:345:ILE:HG13	2.17	0.44
1:A:352:LEU:HA	1:A:364:ALA:O	2.17	0.44
1:B:203:TYR:CE2	1:B:205:ALA:HB2	2.47	0.44
1:B:311:LYS:HE3	1:B:312:MET:O	2.17	0.44
1:C:213:VAL:HA	1:C:216:LEU:HB2	1.99	0.44
1:C:220:LEU:CB	1:C:226:MET:HG2	2.47	0.44
2:D:357:ILE:HG22	2:D:357:ILE:O	2.17	0.44
2:F:97:VAL:HG22	2:F:232:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:2:THR:O	3:G:3:LEU:C	2.54	0.44
1:A:179:ALA:HB1	1:A:267:ILE:HG12	2.00	0.44
1:A:75:VAL:O	1:A:241:PRO:CG	2.65	0.44
1:A:359:LYS:HG2	1:A:359:LYS:O	2.17	0.44
1:A:400:VAL:HG12	1:A:418:LEU:HD21	2.00	0.44
1:C:203:TYR:CE1	1:C:269:ASP:HB2	2.52	0.44
1:C:37:GLY:O	1:C:38:ILE:HD13	2.17	0.44
1:C:59:LEU:HD12	1:C:60:LYS:H	1.83	0.44
2:E:185:GLY:O	2:E:221:GLN:NE2	2.51	0.44
2:E:381:TYR:CE1	4:H:22:PHE:CZ	3.05	0.44
2:F:341:GLU:C	2:F:343:GLY:H	2.20	0.44
2:F:367:HIS:CD2	2:F:367:HIS:C	2.91	0.44
2:E:390:ILE:CD1	3:G:16:ILE:HG12	2.44	0.44
1:C:414:THR:HG22	4:H:27:GLN:OE1	2.18	0.44
1:A:121:ILE:CD1	1:A:121:ILE:H	2.17	0.44
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.99	0.44
1:B:179:ALA:O	1:B:182:THR:HB	2.17	0.44
1:C:266:ILE:C	1:C:267:ILE:HD12	2.38	0.44
1:A:280:GLN:NE2	2:D:284:THR:HG22	2.33	0.44
2:E:149:GLY:HA2	2:E:304:ILE:O	2.18	0.44
2:F:377:ILE:HD11	2:F:406:ARG:HB2	1.99	0.44
4:H:12:ALA:O	4:H:13:GLY:C	2.55	0.44
1:A:155:SER:HA	1:A:383:MET:SD	2.58	0.44
1:A:451:GLY:C	1:A:453:LEU:H	2.20	0.44
1:C:78:ASN:OD1	1:C:80:LYS:HB3	2.17	0.44
2:D:220:GLY:HA3	2:D:232:VAL:HG21	1.99	0.44
2:E:292:MET:HE1	2:E:296:ILE:HD12	1.99	0.44
2:E:474:ALA:O	2:E:475:GLU:HB2	2.18	0.44
2:F:421:ALA:HB1	2:F:425:THR:CG2	2.48	0.44
1:A:26:GLU:O	1:A:46:ASN:HB2	2.18	0.44
1:A:371:VAL:HG23	1:A:371:VAL:O	2.17	0.44
1:A:44:LEU:HB3	1:A:47:VAL:HG22	1.99	0.44
1:C:351:PHE:CE2	1:C:353:GLU:HG2	2.52	0.44
1:C:351:PHE:CE2	1:C:353:GLU:OE2	2.71	0.44
1:C:185:ASN:HA	1:C:435:PRO:HG2	2.00	0.44
2:D:408:ARG:CZ	4:H:22:PHE:CE2	3.01	0.44
1:A:127:ARG:CZ	1:A:131:LEU:CD1	2.93	0.44
2:D:266:SER:OG	2:D:282:GLN:NE2	2.50	0.44
2:E:167:MET:CE	2:E:196:LEU:HD13	2.47	0.44
2:E:439:LYS:O	2:E:443:GLN:HG3	2.18	0.44
2:E:457:PHE:CD1	2:E:457:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:405:SER:O	2:F:409:LYS:HG3	2.17	0.44
1:A:115:ILE:O	2:D:124:VAL:HG13	2.18	0.44
1:A:164:ARG:HE	1:A:347:ASP:CG	2.17	0.44
1:B:185:ASN:CG	1:B:188:ARG:HH12	2.21	0.44
1:C:156:LEU:HB3	1:C:391:LYS:HG3	1.98	0.44
1:C:34:ILE:HD13	1:C:39:ALA:HB2	1.98	0.44
2:D:200:MET:HE2	2:D:217:LEU:HD21	1.98	0.44
2:D:324:THR:O	2:D:324:THR:HG22	2.17	0.44
1:C:403:PHE:CZ	4:H:24:LYS:HB2	2.53	0.44
1:B:283:LEU:HD22	2:E:275:ILE:HG21	1.99	0.44
1:C:52:MET:HE2	1:C:60:LYS:HB3	1.99	0.44
2:E:163:THR:O	2:E:166:ILE:HG22	2.18	0.44
3:G:253:THR:O	3:G:257:VAL:HG23	2.18	0.44
4:H:8:VAL:O	4:H:15:VAL:CG2	2.64	0.44
1:B:177:SER:O	1:B:179:ALA:N	2.51	0.44
1:B:129:VAL:HG21	1:B:245:LEU:HD11	2.00	0.44
1:B:181:ASP:O	1:B:435:PRO:HG2	2.18	0.44
1:B:473:ILE:O	1:B:477:GLN:NE2	2.50	0.44
1:C:215:GLN:NE2	2:F:128:VAL:CA	2.80	0.44
1:C:216:LEU:HD22	1:C:216:LEU:HA	1.86	0.44
1:C:309:ALA:O	1:C:310:ALA:HB2	2.18	0.44
1:C:363:PRO:O	1:C:365:ILE:N	2.50	0.44
1:C:352:LEU:HD21	1:C:365:ILE:HG12	2.00	0.44
1:C:457:GLU:O	1:C:458:PRO:C	2.56	0.44
2:D:438:ILE:O	2:D:439:LYS:C	2.56	0.44
1:C:49:ALA:HB3	2:D:66:THR:O	2.18	0.44
2:F:268:VAL:O	2:F:272:LEU:HG	2.17	0.44
1:A:440:GLU:CD	1:A:473:ILE:HD11	2.39	0.44
2:D:237:LEU:HD11	2:D:296:ILE:HG12	1.97	0.44
2:D:439:LYS:CE	2:D:443:GLN:OE1	2.66	0.44
2:E:339:ILE:CG2	2:E:344:ILE:HB	2.48	0.44
1:C:48:GLN:HA	2:E:70:VAL:HG22	1.99	0.44
2:F:367:HIS:O	2:F:367:HIS:HD2	2.01	0.44
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.53	0.44
1:A:427:LEU:HD21	1:A:453:LEU:HD11	1.99	0.44
1:A:479:LEU:HD22	1:A:479:LEU:C	2.36	0.44
1:B:188:ARG:NH1	1:B:188:ARG:HG2	2.32	0.44
1:C:292:GLU:O	1:C:293:ALA:HB3	2.18	0.44
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.53	0.43
1:B:139:ARG:HD3	1:B:310:ALA:HB1	2.00	0.43
1:B:207:GLY:HA3	1:B:273:LYS:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ILE:HB	1:C:339:PRO:CD	2.45	0.43
1:C:381:ARG:N	1:C:381:ARG:CD	2.76	0.43
1:C:490:SER:O	1:C:492:GLU:N	2.51	0.43
2:D:384:LEU:O	2:D:388:ILE:HG12	2.18	0.43
2:D:419:GLN:O	2:D:421:ALA:N	2.51	0.43
2:E:440:GLY:O	2:E:444:ILE:HG13	2.19	0.43
1:A:245:LEU:O	1:A:248:TYR:N	2.51	0.43
1:A:342:VAL:O	1:A:343:ILE:C	2.56	0.43
1:C:263:HIS:HD2	1:C:320:SER:OG	2.01	0.43
2:E:175:LYS:NZ	2:E:214:LYS:NZ	2.66	0.43
2:F:384:LEU:O	2:F:388:ILE:HG12	2.17	0.43
2:F:454:GLU:O	2:F:456:ALA:N	2.51	0.43
1:A:441:GLN:O	1:A:444:VAL:HG22	2.18	0.43
1:B:286:ARG:NH1	3:G:272:LEU:CD1	2.79	0.43
1:B:392:LEU:O	1:B:395:ALA:N	2.51	0.43
1:C:44:LEU:O	1:C:46:ASN:N	2.51	0.43
2:D:462:PRO:HG2	2:D:465:GLU:HG3	2.00	0.43
1:B:283:LEU:HD22	2:E:275:ILE:CG2	2.49	0.43
2:F:152:ILE:CD1	2:F:152:ILE:N	2.81	0.43
1:A:148:THR:HG21	1:A:153:VAL:HG11	1.99	0.43
1:B:98:PRO:HG3	1:B:126:ARG:NH1	2.34	0.43
1:B:190:ASN:HA	1:B:198:LYS:HG2	2.00	0.43
1:C:268:TYR:HB3	1:C:271:LEU:HD21	1.98	0.43
1:C:273:LYS:O	1:C:276:VAL:HB	2.18	0.43
1:C:444:VAL:CG2	1:C:445:ILE:N	2.81	0.43
2:F:186:VAL:O	2:F:260:ARG:HG3	2.17	0.43
2:F:372:ARG:NH1	2:F:375:GLN:OE1	2.41	0.43
3:G:23:MET:HB2	3:G:232:MET:HE2	2.00	0.43
4:H:8:VAL:O	4:H:15:VAL:CG2	2.66	0.43
1:A:171:ARG:HH11	1:A:171:ARG:CB	2.32	0.43
1:B:65:ASN:OD1	1:B:285:LEU:HD22	2.18	0.43
2:D:151:LYS:HE3	2:D:296:ILE:O	2.19	0.43
1:A:136:ILE:CG2	2:D:194:ASN:HA	2.48	0.43
2:D:220:GLY:HA3	2:D:232:VAL:HG11	2.00	0.43
1:C:358:TYR:CG	2:D:351:LEU:HD22	2.53	0.43
2:D:398:GLU:HA	2:D:398:GLU:OE2	2.18	0.43
2:E:282:GLN:HG2	2:E:285:LEU:N	2.34	0.43
2:F:189:ARG:NH1	2:F:192:GLU:OE1	2.49	0.43
2:E:390:ILE:CD1	3:G:16:ILE:HG23	2.48	0.43
1:A:300:TYR:O	1:A:304:ARG:HG2	2.18	0.43
1:A:370:SER:C	1:A:371:VAL:HG13	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:VAL:O	1:B:400:VAL:HG12	2.17	0.43
1:C:209:LYS:HE2	1:C:209:LYS:HB3	1.80	0.43
1:C:30:ARG:HG2	1:C:30:ARG:NH1	2.32	0.43
1:C:426:GLU:HB2	1:C:461:ILE:HD12	2.00	0.43
2:D:425:THR:HG21	2:D:459:MET:HE2	1.99	0.43
2:E:189:ARG:HG3	2:E:189:ARG:HH11	1.84	0.43
2:E:234:LEU:O	2:E:237:LEU:HB3	2.18	0.43
2:F:345:TYR:HA	2:F:346:PRO:C	2.39	0.43
2:F:37:GLU:CD	2:F:44:ARG:HE	2.20	0.43
2:D:453:PRO:HB3	4:H:30:GLU:HB3	2.01	0.43
1:A:159:ILE:HD12	1:A:165:GLU:HB2	2.00	0.43
1:A:164:ARG:HE	1:A:347:ASP:CG	2.22	0.43
1:A:397:TYR:CE1	1:A:401:ALA:HB2	2.54	0.43
1:A:432:GLN:CD	1:A:433:TYR:CE1	2.92	0.43
1:B:127:ARG:HG2	1:B:131:LEU:CD1	2.48	0.43
1:B:105:GLY:CA	1:B:226:MET:O	2.65	0.43
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.01	0.43
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.34	0.43
1:C:179:ALA:HB1	1:C:267:ILE:HD13	2.01	0.43
1:C:34:ILE:O	1:C:34:ILE:HG23	2.18	0.43
1:C:486:ASP:C	1:C:488:LYS:N	2.72	0.43
2:D:329:LEU:HD12	2:D:332:THR:HG22	2.00	0.43
2:D:403:THR:O	2:D:404:VAL:C	2.57	0.43
2:D:433:PRO:HB2	2:D:436:GLU:CG	2.48	0.43
2:E:245:ASP:C	2:E:247:GLU:N	2.69	0.43
2:E:351:LEU:HD12	2:E:382:LYS:HE3	2.00	0.43
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.43
2:E:467:VAL:O	2:E:468:ALA:C	2.56	0.43
1:A:47:VAL:O	2:E:70:VAL:HG22	2.19	0.43
1:A:52:MET:HG2	1:A:95:VAL:CG2	2.42	0.43
1:B:452:TYR:CD1	1:B:452:TYR:N	2.86	0.43
2:E:164:VAL:HG12	2:E:418:PHE:CD1	2.49	0.43
2:E:386:ASP:HB2	2:E:387:ILE:HD12	2.01	0.43
2:F:393:MET:SD	2:F:404:VAL:HG11	2.58	0.43
1:A:432:GLN:HB2	5:A:1511:ANP:C5	2.48	0.43
1:A:383:MET:O	1:A:384:LYS:C	2.56	0.43
1:A:149:GLY:C	1:A:436:MET:N	2.69	0.43
1:B:136:ILE:CG2	1:B:137:ILE:N	2.81	0.43
1:B:174:GLY:N	5:B:1511:ANP:O3A	2.51	0.43
1:B:280:GLN:O	1:B:281:MET:C	2.57	0.43
1:B:452:TYR:HE2	1:B:502:THR:HG22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HG12	1:B:95:VAL:N	2.26	0.43
2:D:174:ALA:O	2:D:177:HIS:HB3	2.18	0.43
2:E:138:LYS:NZ	2:E:413:PHE:O	2.42	0.43
2:F:155:PHE:HE1	2:F:332:THR:HB	1.83	0.43
1:A:313:ASN:OD1	1:A:313:ASN:C	2.56	0.43
1:A:361:ILE:HD12	1:A:425:THR:CG2	2.46	0.43
1:B:200:TYR:CD2	1:B:257:PHE:CE2	3.06	0.43
1:B:270:ASP:H	1:B:326:VAL:CB	2.23	0.43
1:B:54:GLU:CD	1:B:60:LYS:NZ	2.72	0.43
1:C:338:ILE:O	1:C:339:PRO:C	2.56	0.43
2:D:32:ILE:HG22	2:D:33:LEU:HG	2.01	0.43
2:D:456:ALA:HB1	2:D:470:ALA:HB2	2.01	0.43
2:E:282:GLN:HG2	2:E:285:LEU:N	2.33	0.43
2:E:253:LEU:HB3	2:E:306:SER:HB2	2.00	0.43
1:B:180:ILE:HD11	1:B:216:LEU:CD1	2.48	0.43
1:B:439:GLU:HA	1:B:442:VAL:CG1	2.49	0.43
1:B:427:LEU:HD22	1:B:444:VAL:CG2	2.49	0.43
1:C:199:LEU:HD12	1:C:263:HIS:O	2.18	0.43
1:C:337:TYR:O	1:C:338:ILE:C	2.55	0.43
2:F:200:MET:HB3	2:F:205:VAL:CG2	2.46	0.43
2:F:223:ASN:N	2:F:223:ASN:HD22	2.16	0.43
2:F:388:ILE:CD1	2:F:396:LEU:HD11	2.48	0.43
3:G:251:ASN:O	3:G:255:GLN:HB2	2.18	0.43
1:A:400:VAL:O	1:A:401:ALA:C	2.56	0.43
1:B:338:ILE:HA	1:B:341:ASN:ND2	2.25	0.43
1:C:210:ARG:HG2	1:C:235:THR:HG21	2.00	0.43
1:C:268:TYR:CZ	1:C:305:LEU:HD21	2.53	0.43
2:D:321:ALA:HB3	2:D:322:PRO:HD3	2.00	0.43
2:D:440:GLY:HA2	2:D:463:ILE:HB	2.00	0.43
2:E:367:HIS:O	2:E:367:HIS:HD2	2.01	0.43
1:A:35:GLY:C	1:A:36:ASP:OD1	2.57	0.43
1:B:291:ARG:HB3	1:B:337:TYR:CE1	2.53	0.43
1:B:32:LEU:CG	1:B:42:HIS:HB2	2.49	0.43
1:B:87:ILE:H	1:B:87:ILE:CD1	2.24	0.43
1:C:300:TYR:HB2	2:E:229:ARG:HH22	1.83	0.43
1:C:353:GLU:HB2	1:C:356:LEU:CD1	2.49	0.43
1:C:446:TYR:HE1	1:C:450:ARG:NH1	2.16	0.43
1:C:471:HIS:CE1	1:C:475:GLN:OE1	2.72	0.43
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.35	0.43
2:F:229:ARG:O	2:F:232:VAL:HG23	2.18	0.43
2:F:258:ILE:HD11	2:F:292:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLY:HA2	5:A:1511:ANP:PA	2.59	0.43
1:A:217:VAL:HG23	1:A:218:LYS:N	2.34	0.43
1:A:24:ASP:OD1	1:A:26:GLU:HB3	2.18	0.43
1:A:289:PRO:HG3	2:D:275:ILE:HG21	1.99	0.43
1:A:28:THR:HG22	1:A:89:LYS:HG2	1.99	0.43
1:C:436:MET:CE	1:C:441:GLN:HA	2.48	0.43
2:D:197:TYR:CZ	2:D:201:ILE:HD11	2.53	0.43
1:A:283:LEU:HD22	2:D:275:ILE:HB	2.01	0.43
2:D:443:GLN:O	2:D:446:ALA:HB3	2.19	0.43
2:E:94:ILE:HG12	2:E:217:LEU:HD12	2.00	0.43
2:F:143:LEU:HD22	2:F:375:GLN:CG	2.48	0.43
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.99	0.43
1:A:410:LEU:O	1:A:411:ASP:HB3	2.18	0.43
1:B:38:ILE:HG13	1:B:284:LEU:HB3	2.00	0.43
1:B:347:ASP:HA	1:B:373:ARG:HH12	1.81	0.43
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.53	0.43
1:C:446:TYR:CE1	1:C:450:ARG:NH1	2.87	0.43
2:E:231:ARG:O	2:E:232:VAL:C	2.57	0.43
2:E:345:TYR:HA	2:E:346:PRO:C	2.39	0.43
2:E:472:LYS:O	2:E:472:LYS:HG2	2.19	0.43
2:E:48:GLU:OE2	2:E:117:HIS:NE2	2.39	0.43
1:A:286:ARG:NH2	2:F:273:GLY:O	2.52	0.43
2:F:396:LEU:O	2:F:401:LYS:HG3	2.18	0.43
2:F:422:GLU:HG2	2:F:427:HIS:O	2.18	0.43
1:A:359:LYS:CG	2:D:379:GLN:HG2	2.49	0.43
1:B:141:SER:O	1:B:142:VAL:C	2.56	0.43
1:C:387:ALA:O	1:C:388:GLY:C	2.56	0.43
1:C:52:MET:HG3	1:C:53:VAL:N	2.33	0.43
2:E:256:ASP:O	2:E:257:ASN:HB2	2.18	0.43
2:E:253:LEU:O	2:E:306:SER:HA	2.18	0.43
2:F:140:VAL:CG1	2:F:146:TYR:CE2	3.01	0.43
2:F:391:LEU:O	2:F:395:GLU:HG2	2.17	0.43
1:A:104:LEU:HD11	1:A:200:TYR:HD2	1.82	0.43
1:A:194:ASP:OD2	1:A:196:LYS:HB2	2.18	0.43
1:A:489:ILE:HG22	1:A:494:ASP:HB2	2.00	0.43
1:B:156:LEU:HD13	1:B:367:VAL:HG13	2.01	0.43
1:B:34:ILE:HD13	1:B:82:ILE:CG2	2.49	0.43
2:D:181:SER:OG	2:D:252:LEU:HB2	2.19	0.43
2:E:230:ALA:HB2	2:E:264:ALA:HB1	2.01	0.43
2:E:243:PHE:C	2:E:251:VAL:HG21	2.39	0.43
2:E:281:TYR:HB3	2:E:285:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:168:GLU:HA	2:F:168:GLU:OE1	2.18	0.43
4:H:12:ALA:O	4:H:15:VAL:HB	2.19	0.43
4:H:29:GLU:O	4:H:33:TYR:CD1	2.72	0.43
1:A:105:GLY:HA2	1:A:226:MET:O	2.18	0.43
1:A:313:ASN:OD1	1:A:316:PHE:HD1	2.02	0.43
1:B:150:ILE:HA	1:B:430:GLN:HE22	1.83	0.43
1:B:97:VAL:HG11	1:B:249:SER:OG	2.19	0.43
1:B:357:PHE:CZ	1:B:362:ARG:NH1	2.87	0.43
1:B:458:PRO:O	1:B:460:LYS:N	2.51	0.43
1:C:468:PHE:O	1:C:471:HIS:N	2.42	0.43
2:D:139:VAL:HG22	2:D:414:LEU:CB	2.47	0.43
2:D:89:GLU:H	2:D:89:GLU:CD	2.21	0.43
2:E:152:ILE:HA	2:E:331:ALA:O	2.18	0.43
2:E:430:LYS:HE3	2:E:465:GLU:OE1	2.19	0.43
2:F:370:VAL:HG22	2:F:442:GLN:HG2	2.01	0.43
1:B:309:ALA:O	1:B:310:ALA:HB2	2.19	0.43
1:B:76:PHE:CD1	1:B:76:PHE:N	2.87	0.43
1:B:99:VAL:HG13	1:B:256:TYR:CG	2.54	0.43
1:C:398:ARG:HH11	1:C:398:ARG:HG2	1.84	0.43
2:D:285:LEU:HD23	2:D:285:LEU:O	2.19	0.43
1:A:369:LEU:CD2	2:D:341:GLU:HG2	2.49	0.43
2:D:96:ASN:ND2	2:D:98:ILE:N	2.66	0.43
2:E:23:VAL:O	2:E:58:VAL:HG22	2.19	0.43
2:E:98:ILE:HD11	2:E:100:GLU:CD	2.39	0.43
2:F:203:SER:OG	2:F:205:VAL:HG22	2.19	0.43
1:A:224:ASP:OD2	1:A:227:LYS:NZ	2.44	0.43
1:A:156:LEU:HD13	1:A:367:VAL:HG11	2.01	0.43
1:A:489:ILE:N	1:A:489:ILE:HD12	2.33	0.43
1:B:137:ILE:CB	1:B:138:PRO:HD3	2.47	0.43
1:B:270:ASP:OD1	1:B:270:ASP:C	2.56	0.43
1:C:52:MET:HE3	1:C:76:PHE:HE1	1.84	0.43
2:D:269:SER:O	2:D:272:LEU:HB2	2.19	0.43
2:D:333:THR:CG2	2:D:348:VAL:HG22	2.49	0.43
2:E:284:THR:O	2:E:285:LEU:C	2.57	0.43
2:E:396:LEU:O	2:E:401:LYS:HG3	2.19	0.43
2:F:203:SER:OG	2:F:205:VAL:HG13	2.18	0.43
2:F:221:GLN:HB2	2:F:223:ASN:HD21	1.84	0.43
4:H:19:GLY:O	4:H:22:PHE:HB3	2.19	0.43
1:B:337:TYR:HB3	1:B:338:ILE:HD12	2.01	0.42
1:B:386:VAL:HG23	1:B:387:ALA:N	2.34	0.42
1:B:55:PHE:O	1:B:56:SER:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:ILE:HG22	2:D:102:ILE:CG1	2.49	0.42
2:E:292:MET:CE	2:E:296:ILE:HD12	2.49	0.42
2:E:66:THR:HB	2:E:69:LEU:HD12	2.01	0.42
2:F:167:MET:CE	2:F:420:VAL:HG11	2.49	0.42
2:F:220:GLY:CA	2:F:232:VAL:HG11	2.49	0.42
2:F:454:GLU:O	2:F:456:ALA:N	2.52	0.42
2:F:464:GLU:CD	2:F:464:GLU:H	2.22	0.42
2:F:279:VAL:HG22	3:G:255:GLN:HG2	1.97	0.42
1:A:76:PHE:N	1:A:76:PHE:CD1	2.86	0.42
1:B:166:LEU:HD11	1:B:327:ILE:HB	2.01	0.42
1:B:472:VAL:CG2	1:B:473:ILE:N	2.81	0.42
1:B:28:THR:HG23	1:B:88:VAL:O	2.19	0.42
1:C:509:GLU:O	1:C:510:ALA:C	2.58	0.42
2:D:277:SER:OG	2:D:278:ALA:N	2.52	0.42
2:D:395:GLU:OE1	2:D:395:GLU:HA	2.19	0.42
2:E:346:PRO:HB2	2:E:348:VAL:HG23	2.01	0.42
1:A:132:LYS:NZ	2:E:64:ASP:OD2	2.52	0.42
2:F:357:ILE:HG22	2:F:357:ILE:O	2.18	0.42
2:F:391:LEU:HD13	2:F:395:GLU:HG3	2.01	0.42
3:G:15:ASN:ND2	4:H:7:ASN:HD22	2.17	0.42
3:G:77:LEU:HD12	3:G:77:LEU:O	2.19	0.42
1:A:99:VAL:CG1	1:A:256:TYR:HB2	2.48	0.42
1:A:280:GLN:NE2	2:F:284:THR:HG22	2.33	0.42
1:A:28:THR:CG2	1:A:29:GLY:H	2.32	0.42
1:A:502:THR:C	1:A:504:PHE:H	2.21	0.42
1:B:172:GLN:NE2	5:B:1511:ANP:O3G	2.52	0.42
1:B:163:GLN:O	1:B:322:THR:HG23	2.19	0.42
1:C:30:ARG:HH11	1:C:30:ARG:HG2	1.82	0.42
1:C:376:SER:O	1:C:378:ALA:N	2.49	0.42
1:C:462:THR:C	1:C:464:PHE:N	2.71	0.42
2:F:243:PHE:HB2	2:F:251:VAL:HG21	2.01	0.42
1:A:286:ARG:NH1	2:F:275:ILE:HD11	2.35	0.42
2:F:412:ARG:HH12	2:F:455:GLN:NE2	2.17	0.42
3:G:15:ASN:O	3:G:18:LYS:N	2.51	0.42
1:A:165:GLU:O	1:A:325:PRO:HD2	2.18	0.42
1:A:152:ALA:HA	1:A:428:LEU:HD22	2.00	0.42
1:B:144:GLU:O	1:B:161:ARG:HG3	2.19	0.42
1:B:64:LEU:C	1:B:65:ASN:HD22	2.23	0.42
2:D:183:PHE:HD1	2:D:254:PHE:HB2	1.84	0.42
2:D:292:MET:HE2	2:D:293:GLN:HA	2.00	0.42
2:E:251:VAL:CG1	2:E:252:LEU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:412:ARG:NH1	2:E:455:GLN:NE2	2.67	0.42
2:E:458:TYR:O	2:E:460:VAL:HG13	2.19	0.42
1:C:280:GLN:HE22	2:F:287:THR:HG21	1.84	0.42
4:H:29:GLU:O	4:H:32:ARG:CB	2.52	0.42
1:B:180:ILE:HD11	1:B:216:LEU:HD21	2.00	0.42
1:B:209:LYS:HE3	1:B:211:SER:OG	2.18	0.42
1:B:94:ILE:CG1	1:B:95:VAL:H	2.26	0.42
1:C:329:THR:HG21	1:C:334:VAL:CG1	2.49	0.42
1:C:188:ARG:NH2	1:C:437:ALA:HB2	2.30	0.42
2:D:138:LYS:NZ	2:D:413:PHE:CE1	2.84	0.42
2:D:419:GLN:C	2:D:421:ALA:H	2.23	0.42
2:E:226:PRO:O	2:E:227:GLY:C	2.58	0.42
2:E:87:GLY:HA2	2:E:242:TYR:CD2	2.53	0.42
2:E:314:ALA:O	2:E:315:ASP:HB2	2.18	0.42
2:E:346:PRO:O	2:E:348:VAL:N	2.52	0.42
2:E:377:ILE:CG2	2:E:378:LEU:N	2.82	0.42
2:F:346:PRO:C	2:F:348:VAL:H	2.21	0.42
1:A:55:PHE:O	1:A:56:SER:C	2.58	0.42
1:B:151:LYS:HB2	1:B:151:LYS:NZ	2.34	0.42
1:B:286:ARG:NH1	2:E:275:ILE:HG13	2.34	0.42
1:B:463:LYS:NZ	1:B:509:GLU:O	2.51	0.42
1:C:36:ASP:HB2	1:C:284:LEU:HD22	2.00	0.42
1:C:386:VAL:O	1:C:449:VAL:HG11	2.19	0.42
1:B:136:ILE:HG23	2:F:194:ASN:HA	2.02	0.42
1:A:49:ALA:O	1:A:50:GLU:HB2	2.19	0.42
1:B:140:ILE:HG13	1:B:141:SER:H	1.84	0.42
2:D:252:LEU:HD23	2:D:252:LEU:HA	1.86	0.42
2:E:148:LYS:HB2	2:E:148:LYS:HE3	1.84	0.42
2:E:151:LYS:HD2	2:E:296:ILE:O	2.20	0.42
1:B:83:LYS:NZ	2:E:29:LEU:O	2.40	0.42
2:E:41:ARG:HG2	2:E:41:ARG:NH1	2.34	0.42
2:F:181:SER:CB	2:F:215:VAL:HG13	2.50	0.42
2:F:241:GLU:HA	2:F:304:ILE:HD11	2.01	0.42
1:A:181:ASP:O	1:A:184:ILE:N	2.52	0.42
1:A:407:GLY:HA3	1:A:410:LEU:CD1	2.49	0.42
1:B:441:GLN:HA	1:B:444:VAL:HG22	2.00	0.42
1:C:109:ASP:OD2	1:C:111:LEU:N	2.51	0.42
2:D:382:LYS:HB3	4:H:6:ASP:HB3	2.02	0.42
2:D:452:LEU:HD11	2:D:467:VAL:HG22	2.01	0.42
2:E:132:ILE:CD1	2:E:145:PRO:HB3	2.49	0.42
2:E:336:SER:HG	2:E:339:ILE:HG12	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PHE:CE2	3:G:23:MET:HA	2.54	0.42
1:A:240:ALA:HB3	1:A:241:PRO:HD3	2.02	0.42
1:A:442:VAL:HG23	1:A:443:ALA:N	2.34	0.42
2:D:192:GLU:O	2:D:195:ASP:HB2	2.19	0.42
2:D:220:GLY:N	2:D:232:VAL:HG11	2.34	0.42
2:E:189:ARG:HB2	2:E:192:GLU:OE1	2.20	0.42
2:E:185:GLY:HA3	2:E:219:TYR:CD2	2.54	0.42
2:E:93:ARG:HH11	2:E:93:ARG:HG3	1.85	0.42
1:B:307:GLU:HG3	2:F:222:MET:HB2	2.00	0.42
2:F:275:ILE:O	2:F:283:PRO:HG3	2.19	0.42
2:F:419:GLN:HA	2:F:429:GLY:HA3	2.01	0.42
2:F:455:GLN:HA	2:F:455:GLN:OE1	2.19	0.42
2:F:457:PHE:N	2:F:457:PHE:CD1	2.87	0.42
2:F:458:TYR:CE1	2:F:459:MET:HG2	2.54	0.42
1:B:383:MET:O	1:B:385:GLN:N	2.53	0.42
2:D:196:LEU:O	2:D:196:LEU:HG	2.20	0.42
2:D:230:ALA:HB2	2:D:264:ALA:HB1	2.01	0.42
2:D:281:TYR:CB	2:D:285:LEU:HD12	2.48	0.42
2:D:333:THR:HG22	2:D:348:VAL:HG22	2.02	0.42
2:E:360:PRO:HG3	2:E:368:TYR:CD2	2.54	0.42
2:E:463:ILE:O	2:E:466:ALA:HB3	2.19	0.42
2:F:146:TYR:HB3	2:F:152:ILE:HD11	2.00	0.42
1:A:188:ARG:HG2	1:A:189:PHE:CE1	2.55	0.42
1:A:356:LEU:O	1:A:361:ILE:HB	2.20	0.42
1:A:55:PHE:CE2	1:A:82:ILE:HD13	2.55	0.42
1:C:423:ARG:HG2	1:C:423:ARG:HH11	1.85	0.42
2:D:142:LEU:O	2:D:358:MET:HE3	2.20	0.42
2:D:455:GLN:OE1	2:D:455:GLN:N	2.40	0.42
2:F:226:PRO:N	2:F:229:ARG:NH1	2.67	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD2	1.87	0.42
1:A:432:GLN:NE2	1:A:433:TYR:CZ	2.87	0.42
1:A:457:GLU:HB3	1:A:460:LYS:HD3	2.00	0.42
1:B:54:GLU:CG	1:B:60:LYS:NZ	2.81	0.42
1:C:34:ILE:HD12	1:C:38:ILE:O	2.18	0.42
1:A:218:LYS:CE	1:A:222:ASP:OD2	2.68	0.42
1:A:381:ARG:NE	1:A:488:LYS:HZ3	2.17	0.42
1:A:99:VAL:HG22	1:A:253:MET:HA	2.02	0.42
1:B:94:ILE:HG21	1:B:128:ARG:NE	2.34	0.42
1:C:188:ARG:HH21	1:C:437:ALA:CB	2.30	0.42
1:C:362:ARG:NH2	2:D:372:ARG:CD	2.79	0.42
2:D:376:LYS:O	2:D:380:ASP:OD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:ILE:H	2:E:137:ILE:HG12	1.70	0.42
2:F:134:VAL:HA	2:F:141:ASP:OD1	2.20	0.42
2:F:432:VAL:HA	2:F:433:PRO:HD3	1.90	0.42
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.47	0.42
1:A:251:CYS:SG	1:A:321:LEU:HD21	2.60	0.42
1:B:102:GLU:HG3	1:B:123:SER:N	2.34	0.42
1:B:434:SER:N	1:B:435:PRO:HD3	2.35	0.42
1:B:444:VAL:HG23	1:B:445:ILE:N	2.33	0.42
1:C:35:GLY:O	1:C:36:ASP:C	2.57	0.42
2:D:112:GLN:NE2	2:D:242:TYR:OH	2.52	0.42
2:F:212:THR:O	2:F:214:LYS:HD2	2.20	0.42
3:G:250:PHE:O	3:G:254:ARG:N	2.51	0.42
4:H:4:SER:CA	4:H:7:ASN:HD21	2.32	0.42
1:A:153:VAL:C	1:A:155:SER:N	2.72	0.42
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.01	0.42
2:D:168:GLU:OE2	2:D:172:ASN:ND2	2.52	0.42
2:D:292:MET:HE1	2:D:293:GLN:HG2	2.02	0.42
2:F:257:ASN:ND2	2:F:260:ARG:HG3	2.34	0.42
2:E:389:ALA:CA	4:H:18:ALA:HB2	2.50	0.42
1:A:313:ASN:OD1	1:A:313:ASN:O	2.38	0.42
1:A:438:ILE:O	1:A:441:GLN:HB2	2.20	0.42
1:B:268:TYR:O	1:B:270:ASP:N	2.53	0.42
1:C:129:VAL:HA	1:C:252:SER:OG	2.20	0.42
1:C:486:ASP:C	1:C:488:LYS:N	2.72	0.42
2:D:242:TYR:CD1	2:D:246:GLN:HG3	2.54	0.42
2:D:237:LEU:HD21	2:D:295:ARG:HB2	2.01	0.42
2:D:93:ARG:HH11	2:D:93:ARG:HG3	1.84	0.42
2:F:168:GLU:HG2	2:F:418:PHE:CG	2.55	0.42
2:E:280:GLY:HA2	3:G:262:LEU:HD21	2.01	0.42
1:A:140:ILE:HG23	1:A:311:LYS:HG3	2.01	0.42
1:A:44:LEU:HB3	1:A:47:VAL:HG11	2.01	0.42
1:C:178:ILE:HD11	1:C:363:PRO:HB2	2.02	0.42
1:C:30:ARG:HG2	1:C:30:ARG:NH1	2.35	0.42
1:C:327:ILE:HD13	1:C:327:ILE:HA	1.86	0.42
1:C:397:TYR:CD1	1:C:418:LEU:HD23	2.54	0.42
1:C:382:ALA:HB2	1:C:488:LYS:HA	2.00	0.42
1:C:136:ILE:O	2:E:194:ASN:OD1	2.38	0.42
2:E:381:TYR:CE1	4:H:22:PHE:HZ	2.37	0.42
2:E:139:VAL:HG22	2:E:414:LEU:HD22	2.01	0.42
2:E:63:MET:O	2:E:64:ASP:HB2	2.20	0.42
2:F:275:ILE:HG23	3:G:266:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:TYR:HB3	1:B:271:LEU:HD21	2.02	0.42
1:B:28:THR:O	1:B:44:LEU:N	2.46	0.42
1:C:211:SER:O	1:C:214:ALA:HB3	2.20	0.42
2:E:162:LYS:HE2	2:E:256:ASP:OD2	2.19	0.42
1:A:139:ARG:CZ	2:E:190:THR:HG21	2.50	0.42
2:E:242:TYR:CD1	2:E:246:GLN:HG3	2.55	0.42
2:E:421:ALA:HB1	2:E:425:THR:HG21	2.02	0.42
1:A:151:LYS:HB2	1:A:151:LYS:NZ	2.35	0.42
1:A:149:GLY:N	1:A:154:ASP:OD2	2.49	0.42
1:A:354:THR:CG2	1:A:358:TYR:CE2	3.03	0.42
1:A:36:ASP:O	1:A:284:LEU:HB3	2.20	0.42
1:B:444:VAL:HG22	1:B:445:ILE:N	2.34	0.42
1:C:108:VAL:HA	1:C:113:ASN:O	2.20	0.42
1:C:40:ARG:HA	1:C:40:ARG:HD3	1.93	0.42
2:D:351:LEU:HD12	2:D:382:LYS:HD2	2.01	0.42
1:A:215:GLN:NE2	2:D:128:VAL:HA	2.35	0.42
1:A:210:ARG:CG	1:A:235:THR:HG21	2.50	0.42
1:A:161:ARG:HH11	1:A:263:HIS:HB2	1.84	0.42
1:A:391:LYS:O	1:A:393:GLU:N	2.52	0.42
1:A:472:VAL:CG2	1:A:473:ILE:N	2.81	0.42
1:A:468:PHE:HA	1:A:504:PHE:CZ	2.55	0.42
1:B:270:ASP:OD1	1:B:270:ASP:O	2.38	0.42
1:C:168:ILE:HA	1:C:327:ILE:O	2.18	0.42
1:C:351:PHE:CZ	1:C:353:GLU:HG2	2.55	0.42
1:C:188:ARG:NH2	1:C:436:MET:C	2.72	0.42
2:D:370:VAL:O	2:D:374:VAL:HG23	2.19	0.42
2:D:33:LEU:O	2:D:81:PRO:HA	2.20	0.42
2:E:135:THR:OG1	2:E:141:ASP:OD2	2.31	0.42
1:A:66:LEU:HB2	2:E:16:VAL:HB	2.02	0.42
2:F:200:MET:HB3	2:F:205:VAL:HG22	2.01	0.42
2:F:396:LEU:HB3	2:F:400:ASP:HB2	2.02	0.42
1:A:180:ILE:HD13	1:A:180:ILE:HA	1.89	0.41
1:A:38:ILE:CG1	1:A:285:LEU:HD21	2.32	0.41
1:A:432:GLN:CD	1:A:433:TYR:CZ	2.93	0.41
1:B:381:ARG:CD	1:B:488:LYS:HB3	2.48	0.41
1:C:144:GLU:HA	1:C:145:PRO:HD3	1.88	0.41
2:D:17:ILE:HG22	2:D:271:LEU:HD22	2.02	0.41
2:E:188:GLU:HB2	2:E:221:GLN:OE1	2.19	0.41
2:E:24:GLN:HA	2:E:57:THR:HA	2.02	0.41
2:F:289:MET:HG3	2:F:293:GLN:CG	2.50	0.41
2:F:464:GLU:N	2:F:464:GLU:CD	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG22	1:A:350:ILE:HD13	2.02	0.41
1:A:76:PHE:HD1	1:A:76:PHE:N	2.19	0.41
1:B:166:LEU:HD11	1:B:327:ILE:CG1	2.50	0.41
1:C:156:LEU:CB	1:C:391:LYS:HE2	2.39	0.41
1:C:420:ARG:HG3	1:C:420:ARG:HH11	1.85	0.41
2:E:390:ILE:C	2:E:392:GLY:H	2.23	0.41
3:G:12:SER:HA	4:H:7:ASN:HB2	2.01	0.41
1:A:171:ARG:HB2	1:A:171:ARG:HH11	1.84	0.41
1:A:295:PRO:O	1:A:298:VAL:HG22	2.19	0.41
1:B:292:GLU:HB3	1:B:294:TYR:CE1	2.55	0.41
1:B:331:ALA:C	1:B:333:ASP:N	2.74	0.41
1:B:76:PHE:N	1:B:76:PHE:HD1	2.18	0.41
1:C:457:GLU:HA	1:C:458:PRO:HD3	1.78	0.41
2:D:234:LEU:HD23	2:D:292:MET:HG3	2.02	0.41
1:C:340:THR:HG21	2:E:314:ALA:HB2	2.02	0.41
2:F:67:GLU:H	2:F:67:GLU:CD	2.23	0.41
3:G:11:LYS:HB3	3:G:11:LYS:HE2	1.80	0.41
1:A:28:THR:HG22	1:A:89:LYS:HA	2.02	0.41
1:B:283:LEU:CD2	1:B:289:PRO:HG3	2.50	0.41
1:B:140:ILE:CG2	1:B:311:LYS:HG3	2.51	0.41
1:B:35:GLY:O	1:B:36:ASP:CB	2.69	0.41
1:C:300:TYR:CZ	1:C:304:ARG:HD3	2.55	0.41
1:C:164:ARG:O	1:C:346:THR:HB	2.19	0.41
1:C:482:LYS:HB2	1:C:482:LYS:HE3	1.86	0.41
2:D:188:GLU:HB3	2:D:189:ARG:H	1.73	0.41
2:E:210:ASP:O	2:E:212:THR:N	2.54	0.41
2:E:15:ALA:O	2:E:21:VAL:HA	2.20	0.41
2:E:345:TYR:HA	2:E:346:PRO:C	2.41	0.41
1:A:109:ASP:OD2	1:A:113:ASN:HB2	2.19	0.41
1:A:41:VAL:HG22	1:A:88:VAL:HG21	2.03	0.41
1:C:209:LYS:HB3	1:C:209:LYS:HE2	1.76	0.41
2:D:207:ASN:HB3	2:D:210:ASP:O	2.20	0.41
2:E:139:VAL:HG22	2:E:414:LEU:CD2	2.50	0.41
2:E:257:ASN:N	2:E:309:ALA:HB3	2.34	0.41
4:H:6:ASP:O	4:H:6:ASP:CG	2.58	0.41
1:A:464:PHE:HE1	1:A:505:LEU:HD12	1.85	0.41
2:E:221:GLN:O	2:E:224:GLU:HB2	2.20	0.41
2:E:237:LEU:HD21	2:E:295:ARG:HB2	2.02	0.41
2:E:412:ARG:NH1	2:E:455:GLN:HE21	2.18	0.41
2:E:95:MET:SD	2:E:99:GLY:HA2	2.60	0.41
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:430:LYS:HA	2:F:430:LYS:HD3	1.94	0.41
1:A:141:SER:O	1:A:143:ARG:HD2	2.20	0.41
1:A:286:ARG:HA	2:F:275:ILE:CD1	2.50	0.41
1:A:156:LEU:HD11	1:A:428:LEU:CD2	2.51	0.41
1:B:456:LEU:HD23	1:B:461:ILE:HD13	2.02	0.41
1:C:505:LEU:HD22	1:C:505:LEU:C	2.41	0.41
2:E:325:THR:O	2:E:328:HIS:HB2	2.20	0.41
2:E:464:GLU:C	2:E:466:ALA:N	2.74	0.41
2:F:101:PRO:HB3	2:F:108:ILE:CD1	2.50	0.41
1:A:102:GLU:HG3	1:A:122:GLY:O	2.20	0.41
1:A:403:PHE:CZ	3:G:25:MET:CE	3.03	0.41
1:B:432:GLN:OE1	5:B:1511:ANP:H2'	2.19	0.41
1:C:111:LEU:HA	1:C:111:LEU:HD23	1.81	0.41
1:C:291:ARG:HB3	1:C:337:TYR:CZ	2.53	0.41
1:C:416:GLN:O	1:C:419:SER:HB2	2.20	0.41
1:C:439:GLU:HG2	1:C:440:GLU:N	2.36	0.41
2:E:441:PHE:O	2:E:445:LEU:HG	2.20	0.41
2:F:157:GLY:HA3	2:F:315:ASP:OD1	2.20	0.41
3:G:251:ASN:O	3:G:252:ARG:C	2.57	0.41
1:A:48:GLN:HB2	1:A:51:GLU:HB2	2.02	0.41
1:A:96:ASP:OD2	1:A:126:ARG:NH2	2.53	0.41
1:C:257:PHE:H	1:C:257:PHE:HD1	1.69	0.41
1:C:37:GLY:HA2	1:C:79:ASP:OD1	2.20	0.41
2:D:425:THR:HG23	5:D:1478:ANP:H2	2.03	0.41
2:D:440:GLY:O	2:D:444:ILE:HG13	2.20	0.41
2:E:138:LYS:HG2	2:E:437:THR:HG23	2.01	0.41
2:F:33:LEU:HD13	2:F:117:HIS:CG	2.55	0.41
2:F:146:TYR:CZ	2:F:152:ILE:HG21	2.55	0.41
2:F:275:ILE:HA	2:F:276:PRO:HD3	1.93	0.41
4:H:30:GLU:O	4:H:34:PHE:N	2.53	0.41
1:A:265:LEU:HG	1:A:267:ILE:CD1	2.50	0.41
1:A:370:SER:O	1:A:371:VAL:HG13	2.20	0.41
1:B:107:VAL:HG12	1:B:115:ILE:HG13	2.03	0.41
1:C:164:ARG:HH11	1:C:164:ARG:HG2	1.85	0.41
1:C:219:ARG:CZ	1:C:433:TYR:CZ	3.04	0.41
1:C:264:ALA:O	1:C:321:LEU:HA	2.21	0.41
1:C:372:SER:C	1:C:374:VAL:H	2.23	0.41
2:F:412:ARG:CG	2:F:412:ARG:NH1	2.81	0.41
1:A:505:LEU:O	1:A:508:PHE:HB3	2.21	0.41
1:C:145:PRO:O	1:C:161:ARG:HG3	2.20	0.41
1:C:202:ILE:HA	1:C:230:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:467:VAL:O	2:E:470:ALA:HB3	2.21	0.41
2:F:93:ARG:HG3	2:F:93:ARG:HH11	1.85	0.41
4:H:15:VAL:O	4:H:16:ARG:C	2.59	0.41
1:B:168:ILE:HD11	1:B:329:THR:CG2	2.51	0.41
1:B:352:LEU:HA	1:B:364:ALA:O	2.20	0.41
1:B:359:LYS:HG2	1:B:359:LYS:O	2.20	0.41
1:C:390:MET:HG3	1:C:424:LEU:HD13	2.02	0.41
1:C:219:ARG:CD	1:C:433:TYR:CE2	3.01	0.41
1:C:458:PRO:O	1:C:460:LYS:N	2.53	0.41
2:D:310:ILE:HD13	2:D:325:THR:CG2	2.51	0.41
2:D:339:ILE:HG23	2:D:344:ILE:HB	2.02	0.41
2:E:384:LEU:O	2:E:388:ILE:HG12	2.20	0.41
2:F:153:GLY:HA3	2:F:329:LEU:CD1	2.49	0.41
3:G:14:LYS:HA	3:G:243:ILE:CD1	2.48	0.41
1:A:460:LYS:O	1:A:461:ILE:C	2.58	0.41
1:C:210:ARG:O	1:C:214:ALA:N	2.51	0.41
1:C:392:LEU:O	1:C:396:GLN:HB2	2.20	0.41
2:D:132:ILE:HG13	2:D:145:PRO:HB2	2.01	0.41
2:E:473:LEU:HB3	4:H:34:PHE:HZ	1.71	0.41
2:F:454:GLU:C	2:F:456:ALA:H	2.23	0.41
1:A:34:ILE:CG2	2:F:52:HIS:HB2	2.51	0.41
1:A:33:SER:HB2	2:F:52:HIS:O	2.21	0.41
3:G:3:LEU:O	3:G:4:LYS:C	2.57	0.41
4:H:25:ARG:HD3	4:H:29:GLU:HG2	2.02	0.41
1:A:91:THR:C	1:A:93:ALA:N	2.74	0.41
1:A:94:ILE:HG12	1:A:95:VAL:N	2.35	0.41
1:B:116:ASP:C	1:B:118:LYS:H	2.23	0.41
1:B:131:LEU:HA	1:B:131:LEU:HD23	1.87	0.41
1:B:319:GLY:O	1:B:320:SER:HB3	2.21	0.41
1:C:202:ILE:CD1	1:C:254:GLY:HA2	2.50	0.41
1:C:255:GLU:CD	1:C:308:ARG:HH21	2.21	0.41
1:C:337:TYR:O	1:C:338:ILE:C	2.58	0.41
1:C:297:ASP:HA	2:D:267:GLU:HG2	2.02	0.41
2:F:220:GLY:HA3	2:F:232:VAL:HG21	2.02	0.41
2:F:346:PRO:O	2:F:348:VAL:N	2.49	0.41
1:A:271:LEU:HB3	1:A:302:HIS:NE2	2.36	0.41
1:A:271:LEU:HB2	1:A:327:ILE:HD11	2.02	0.41
1:A:383:MET:CE	1:A:442:VAL:HG12	2.51	0.41
1:B:336:ALA:O	1:B:339:PRO:HD2	2.21	0.41
1:B:97:VAL:O	1:B:97:VAL:HG23	2.21	0.41
2:D:24:GLN:HA	2:D:57:THR:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:329:LEU:HD12	2:E:332:THR:HG22	2.02	0.41
2:E:412:ARG:HG3	2:E:412:ARG:NH1	2.34	0.41
2:F:144:ALA:N	2:F:145:PRO:HD3	2.35	0.41
1:A:135:GLY:O	1:A:139:ARG:NE	2.51	0.41
1:A:338:ILE:O	1:A:341:ASN:HB2	2.19	0.41
1:C:268:TYR:CZ	1:C:305:LEU:HD11	2.55	0.41
2:D:188:GLU:O	2:D:221:GLN:HB3	2.21	0.41
2:D:470:ALA:O	2:D:473:LEU:HB2	2.20	0.41
2:E:359:ASP:OD1	2:E:360:PRO:HD2	2.21	0.41
2:E:94:ILE:HD11	2:E:197:TYR:CG	2.55	0.41
2:F:200:MET:HB3	2:F:205:VAL:CG2	2.51	0.41
1:B:427:LEU:HD11	1:B:453:LEU:HD12	2.03	0.41
1:C:420:ARG:O	1:C:424:LEU:HG	2.21	0.41
1:C:65:ASN:HB2	1:C:72:GLY:HA3	2.02	0.41
2:E:293:GLN:NE2	2:E:308:GLN:OE1	2.48	0.41
2:F:203:SER:HB2	2:F:420:VAL:CG1	2.34	0.41
2:F:144:ALA:HB1	2:F:354:THR:O	2.21	0.41
1:A:390:MET:CE	1:A:445:ILE:HD12	2.50	0.41
1:C:360:GLY:O	1:C:362:ARG:N	2.54	0.41
1:C:437:ALA:HB3	1:C:440:GLU:OE2	2.21	0.41
2:D:82:ILE:HB	2:D:116:ILE:HG12	2.03	0.41
2:D:88:PRO:O	2:D:91:LEU:HB2	2.20	0.41
2:E:234:LEU:O	2:E:238:THR:N	2.48	0.41
2:F:25:PHE:HZ	2:F:36:LEU:HD13	1.86	0.41
1:A:100:GLY:HA2	1:A:256:TYR:CD2	2.56	0.41
1:A:151:LYS:HE2	1:A:427:LEU:O	2.21	0.41
1:B:349:GLN:HB2	1:B:351:PHE:CE1	2.55	0.41
1:B:439:GLU:OE2	1:B:484:ARG:NE	2.53	0.41
1:C:423:ARG:HA	1:C:461:ILE:HD11	2.01	0.41
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.51	0.41
2:F:172:ASN:ND2	2:F:431:LEU:CD1	2.83	0.41
2:F:445:LEU:C	2:F:447:GLY:N	2.73	0.41
2:F:36:LEU:HA	2:F:76:LEU:O	2.19	0.41
3:G:246:LEU:O	3:G:250:PHE:N	2.52	0.41
2:F:386:ASP:OD2	4:H:13:GLY:HA3	2.21	0.41
1:A:45:ARG:NH1	1:A:45:ARG:HG2	2.34	0.41
1:B:432:GLN:HG2	1:B:433:TYR:CG	2.56	0.41
1:C:270:ASP:OD1	1:C:272:SER:HB2	2.20	0.41
1:C:349:GLN:O	1:C:349:GLN:HG2	2.20	0.41
1:C:486:ASP:O	1:C:488:LYS:HB2	2.21	0.41
1:A:330:GLN:HB3	2:D:318:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:96:ASN:HB2	2:E:102:ILE:HG23	2.02	0.41
2:E:163:THR:HG22	2:E:196:LEU:HD13	2.03	0.41
2:F:245:ASP:C	2:F:247:GLU:H	2.24	0.41
4:H:12:ALA:HB1	4:H:16:ARG:CZ	2.51	0.41
1:A:98:PRO:HG3	1:A:126:ARG:HH12	1.86	0.41
1:A:164:ARG:HH11	1:A:164:ARG:HG2	1.86	0.41
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.96	0.41
1:B:278:TYR:HA	1:B:281:MET:HE3	2.02	0.41
1:C:432:GLN:NE2	2:D:359:ASP:OD2	2.53	0.41
2:E:237:LEU:HD21	2:E:295:ARG:CB	2.51	0.41
4:H:4:SER:HA	4:H:7:ASN:CG	2.41	0.41
1:A:148:THR:O	1:A:182:THR:HA	2.21	0.41
1:A:236:ALA:O	2:D:290:GLY:HA3	2.21	0.41
1:A:247:PRO:O	1:A:268:TYR:HE2	2.04	0.41
1:A:34:ILE:HG22	2:D:52:HIS:HB2	2.03	0.41
1:A:48:GLN:HB3	2:E:68:GLY:CA	2.50	0.41
1:B:137:ILE:HD13	1:B:137:ILE:HA	1.88	0.41
1:B:83:LYS:HB2	1:B:83:LYS:HE3	1.88	0.41
1:C:303:SER:HA	1:C:345:ILE:HD13	2.03	0.41
1:C:398:ARG:O	1:C:401:ALA:HB3	2.21	0.41
2:E:132:ILE:HD12	2:E:145:PRO:HB3	2.03	0.41
2:E:341:GLU:C	2:E:343:GLY:N	2.74	0.41
1:A:213:VAL:O	1:A:217:VAL:HG13	2.20	0.40
1:A:460:LYS:C	1:A:462:THR:N	2.73	0.40
1:B:238:ASP:O	1:B:243:GLN:NE2	2.50	0.40
1:B:199:LEU:HD12	1:B:263:HIS:O	2.20	0.40
1:B:457:GLU:HB3	1:B:460:LYS:HD3	2.03	0.40
1:B:489:ILE:HD12	1:B:489:ILE:N	2.36	0.40
1:C:168:ILE:O	1:C:351:PHE:HA	2.21	0.40
2:D:339:ILE:O	2:D:342:LEU:HB2	2.20	0.40
2:F:167:MET:HE3	2:F:420:VAL:CG1	2.51	0.40
1:A:246:ALA:HB3	1:A:247:PRO:HD3	2.02	0.40
1:A:300:TYR:O	1:A:304:ARG:NH1	2.54	0.40
1:B:216:LEU:O	1:B:220:LEU:HG	2.20	0.40
1:B:357:PHE:CE1	1:B:362:ARG:CZ	3.04	0.40
1:B:96:ASP:HA	1:B:128:ARG:HA	2.03	0.40
1:C:205:ALA:C	1:C:206:ILE:HD12	2.41	0.40
1:C:349:GLN:HB3	1:C:349:GLN:HE21	1.73	0.40
2:D:94:ILE:HG12	2:D:217:LEU:HD12	2.02	0.40
2:E:66:THR:HB	2:E:69:LEU:HD12	2.03	0.40
2:E:94:ILE:HG22	2:E:102:ILE:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:29:GLU:O	4:H:33:TYR:HD1	2.04	0.40
1:B:76:PHE:CE2	1:B:111:LEU:HD11	2.56	0.40
1:B:102:GLU:OE2	1:B:124:LYS:HG3	2.22	0.40
1:B:71:VAL:O	1:B:71:VAL:HG12	2.21	0.40
1:C:279:ARG:O	1:C:283:LEU:HG	2.21	0.40
1:C:451:GLY:HA2	1:C:454:ASP:OD1	2.22	0.40
1:C:49:ALA:O	1:C:50:GLU:CB	2.69	0.40
2:D:259:PHE:CE2	2:D:263:GLN:HB2	2.55	0.40
1:A:106:ARG:NH2	1:A:119:GLY:O	2.46	0.40
1:A:379:GLN:CG	1:A:383:MET:HG3	2.50	0.40
1:B:442:VAL:O	1:B:446:TYR:CB	2.64	0.40
1:C:68:PRO:HD3	2:D:15:ALA:HB2	2.01	0.40
2:D:152:ILE:HB	2:D:306:SER:O	2.21	0.40
2:D:298:THR:HG23	2:D:302:GLY:O	2.21	0.40
2:D:430:LYS:NZ	2:D:465:GLU:OE1	2.51	0.40
2:F:193:GLY:HA2	2:F:219:TYR:OH	2.21	0.40
1:A:226:MET:HA	1:A:229:THR:HB	2.03	0.40
1:A:345:ILE:O	2:D:189:ARG:NE	2.55	0.40
1:C:245:LEU:O	1:C:248:TYR:N	2.53	0.40
1:C:280:GLN:HG2	1:C:284:LEU:CD1	2.52	0.40
1:C:423:ARG:HA	1:C:461:ILE:HD13	2.03	0.40
1:C:490:SER:O	1:C:493:SER:N	2.54	0.40
2:D:15:ALA:HB3	2:D:22:ASP:HB2	2.03	0.40
2:D:269:SER:CB	2:D:282:GLN:HB3	2.52	0.40
2:D:293:GLN:CD	2:D:308:GLN:HE22	2.25	0.40
2:D:329:LEU:CD1	2:D:332:THR:HG22	2.51	0.40
2:E:64:ASP:OD1	2:E:65:GLY:N	2.53	0.40
2:F:276:PRO:HD2	3:G:266:ILE:CD1	2.51	0.40
2:F:297:THR:HB	2:F:298:THR:H	1.68	0.40
1:A:36:ASP:CB	1:A:284:LEU:HD22	2.51	0.40
1:A:348:GLY:C	1:A:349:GLN:NE2	2.75	0.40
1:A:357:PHE:C	1:A:357:PHE:CD2	2.95	0.40
1:A:156:LEU:HD13	1:A:367:VAL:HG13	2.03	0.40
1:B:167:ILE:O	1:B:326:VAL:HA	2.21	0.40
1:B:424:LEU:O	1:B:427:LEU:HB2	2.21	0.40
1:B:450:ARG:HB3	1:B:452:TYR:HE1	1.87	0.40
1:B:99:VAL:HG21	1:B:127:ARG:HB3	2.03	0.40
1:C:106:ARG:HB3	1:C:106:ARG:HE	1.74	0.40
1:C:156:LEU:CD1	1:C:391:LYS:HG3	2.49	0.40
2:D:139:VAL:HG22	2:D:414:LEU:CD2	2.51	0.40
2:E:181:SER:O	2:E:215:VAL:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:ILE:HD11	2:E:445:LEU:HD23	2.03	0.40
2:E:93:ARG:HG3	2:E:93:ARG:HH11	1.86	0.40
4:H:29:GLU:O	4:H:33:TYR:N	2.54	0.40
1:A:154:ASP:CB	1:A:441:GLN:HE22	2.30	0.40
1:C:224:ASP:CG	1:C:224:ASP:O	2.60	0.40
1:C:362:ARG:O	1:C:429:LYS:HA	2.22	0.40
1:C:32:LEU:CD2	1:C:42:HIS:HB2	2.50	0.40
1:C:439:GLU:HG2	1:C:440:GLU:HG3	2.02	0.40
1:C:501:VAL:O	1:C:502:THR:C	2.60	0.40
2:E:464:GLU:O	2:E:466:ALA:N	2.54	0.40
2:F:12:ARG:HH11	2:F:12:ARG:HG3	1.85	0.40
1:A:140:ILE:CG1	1:A:143:ARG:NH2	2.79	0.40
1:A:170:ASP:O	1:A:173:THR:OG1	2.30	0.40
1:A:312:MET:HB2	1:A:319:GLY:O	2.21	0.40
1:A:67:GLU:HB2	1:A:70:ASN:O	2.22	0.40
1:B:217:VAL:CG2	1:B:218:LYS:N	2.84	0.40
2:E:93:ARG:NE	2:E:103:ASP:OD2	2.45	0.40
2:F:85:PRO:HD2	2:F:95:MET:CE	2.51	0.40
3:G:242:MET:HB2	3:G:242:MET:HE3	1.95	0.40
2:D:275:ILE:HG23	3:G:269:ALA:HB2	2.02	0.40
4:H:12:ALA:HB1	4:H:16:ARG:NH2	2.36	0.40
1:A:270:ASP:HA	1:A:326:VAL:C	2.39	0.40
1:A:349:GLN:HB2	1:A:351:PHE:CE1	2.57	0.40
1:A:426:GLU:HB2	1:A:461:ILE:HG21	2.04	0.40
1:C:300:TYR:CE1	2:E:224:GLU:O	2.75	0.40
1:C:175:LYS:NZ	1:C:328:GLU:HA	2.36	0.40
1:C:497:LEU:HD23	1:C:500:ILE:HD12	2.03	0.40
2:D:221:GLN:N	2:D:221:GLN:HE21	2.19	0.40
2:D:404:VAL:O	2:D:408:ARG:HG3	2.21	0.40
2:E:10:THR:CG2	2:E:11:GLY:N	2.84	0.40
1:B:406:PHE:CE1	2:E:395:GLU:HB3	2.49	0.40
1:A:352:LEU:O	1:A:353:GLU:HG3	2.21	0.40
1:A:422:VAL:CG2	1:A:423:ARG:NH1	2.83	0.40
1:A:427:LEU:HD21	1:A:453:LEU:CD1	2.51	0.40
1:B:165:GLU:OE2	1:B:371:VAL:O	2.40	0.40
1:C:446:TYR:CD2	1:C:497:LEU:HB3	2.55	0.40
1:C:53:VAL:HG22	1:C:61:GLY:O	2.22	0.40
2:D:180:TYR:CD2	2:D:180:TYR:N	2.87	0.40
2:D:227:GLY:O	2:D:230:ALA:HB3	2.22	0.40
2:E:139:VAL:HG23	2:E:140:VAL:H	1.87	0.40
2:E:279:VAL:O	2:E:279:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:289:MET:HG3	2:E:328:HIS:CD2	2.57	0.40
2:E:444:ILE:HD13	2:E:449:TYR:CD1	2.57	0.40
2:F:12:ARG:HE	2:F:74:LYS:CE	2.35	0.40
3:G:20:THR:HG21	3:G:235:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	485/510 (95%)	398 (82%)	63 (13%)	24 (5%)	2	7
1	1-B	475/510 (93%)	408 (86%)	56 (12%)	11 (2%)	6	21
1	1-C	484/510 (95%)	411 (85%)	58 (12%)	15 (3%)	4	14
1	2-A	475/510 (93%)	416 (88%)	48 (10%)	11 (2%)	6	21
1	2-B	485/510 (95%)	413 (85%)	59 (12%)	13 (3%)	5	17
1	2-C	476/510 (93%)	390 (82%)	64 (13%)	22 (5%)	2	7
2	1-D	467/482 (97%)	411 (88%)	50 (11%)	6 (1%)	12	36
2	1-E	464/482 (96%)	396 (85%)	59 (13%)	9 (2%)	8	26
2	1-F	464/482 (96%)	400 (86%)	54 (12%)	10 (2%)	6	22
2	2-D	464/482 (96%)	408 (88%)	46 (10%)	10 (2%)	6	22
2	2-E	465/482 (96%)	400 (86%)	52 (11%)	13 (3%)	5	17
2	2-F	464/482 (96%)	400 (86%)	53 (11%)	11 (2%)	6	20
3	1-G	88/272 (32%)	78 (89%)	9 (10%)	1 (1%)	14	41
3	2-G	88/272 (32%)	76 (86%)	11 (12%)	1 (1%)	14	41
4	1-H	35/84 (42%)	20 (57%)	10 (29%)	5 (14%)	0	0
4	2-H	42/84 (50%)	30 (71%)	10 (24%)	2 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5921/6664 (89%)	5055 (85%)	702 (12%)	164 (3%)	5	17

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	123	SER
1	1-A	141	SER
1	1-A	270	ASP
1	1-A	387	ALA
1	1-A	404	ALA
1	1-A	409	ASP
1	1-C	25	LEU
1	1-C	123	SER
1	1-C	337	TYR
1	1-C	483	ILE
2	1-D	27	GLU
2	1-D	109	LYS
2	1-E	65	GLY
2	1-E	109	LYS
1	2-A	270	ASP
1	2-B	332	GLY
1	2-B	337	TYR
1	2-C	337	TYR
1	2-C	364	ALA
2	2-D	347	ALA
2	2-E	109	LYS
2	2-E	246	GLN
2	2-F	391	LEU
4	2-H	13	GLY
1	1-A	341	ASN
1	1-A	357	PHE
1	1-B	57	SER
1	1-B	118	LYS
1	1-B	270	ASP
1	1-B	337	TYR
1	1-B	459	SER
1	1-C	45	ARG
1	1-C	270	ASP
1	1-C	364	ALA
1	1-C	388	GLY
2	1-D	246	GLN
2	1-E	157	GLY

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Mol	Chain	Res	Type
2	1-E	211	ALA
2	1-F	28	GLY
2	1-F	455	GLN
4	1-H	13	GLY
1	2-A	57	SER
1	2-A	337	TYR
1	2-A	379	GLN
1	2-A	452	TYR
1	2-B	45	ARG
1	2-B	192	GLY
1	2-B	270	ASP
1	2-B	409	ASP
1	2-C	20	ASP
1	2-C	236	ALA
1	2-C	361	ILE
1	2-C	373	ARG
1	2-C	388	GLY
1	2-C	431	GLY
2	2-D	211	ALA
2	2-D	247	GLU
2	2-D	420	VAL
2	2-E	27	GLU
2	2-F	19	ALA
2	2-F	109	LYS
2	2-F	211	ALA
2	2-F	347	ALA
2	2-F	390	ILE
3	2-G	81	ILE
1	1-A	50	GLU
1	1-A	110	ALA
1	1-A	188	ARG
1	1-A	358	TYR
1	1-A	388	GLY
1	1-A	391	LYS
1	1-A	392	LEU
1	1-B	384	LYS
1	1-C	175	LYS
1	1-C	269	ASP
1	1-C	459	SER
1	1-C	487	GLY
2	1-F	246	GLN
2	1-F	247	GLU

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Mol	Chain	Res	Type
4	1-H	22	PHE
1	2-A	154	ASP
1	2-A	175	LYS
1	2-A	195	GLU
1	2-A	385	GLN
1	2-B	123	SER
1	2-B	397	TYR
1	2-B	411	ASP
1	2-C	45	ARG
1	2-C	141	SER
1	2-C	246	ALA
1	2-C	288	PRO
1	2-C	377	ALA
2	2-D	257	ASN
2	2-D	455	GLN
2	2-E	33	LEU
2	2-E	96	ASN
2	2-E	122	GLU
2	2-E	347	ALA
2	2-F	257	ASN
2	2-F	392	GLY
2	2-F	455	GLN
4	2-H	21	ALA
1	1-A	25	LEU
1	1-A	376	SER
1	1-A	385	GLN
2	1-D	327	ALA
2	1-E	391	LEU
2	1-F	397	SER
2	1-F	446	ALA
4	1-H	25	ARG
1	2-B	118	LYS
1	2-B	364	ALA
1	2-C	79	ASP
1	2-C	270	ASP
1	2-C	295	PRO
1	2-C	458	PRO
1	2-C	491	GLU
2	2-D	142	LEU
1	1-A	287	ARG
1	1-A	375	GLY
1	1-A	486	ASP

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Mol	Chain	Res	Type
1	1-B	236	ALA
1	1-C	188	ARG
1	1-C	468	PHE
2	1-D	347	ALA
2	1-E	257	ASN
2	1-E	390	ILE
2	1-F	81	PRO
1	2-A	411	ASP
1	2-C	95	VAL
2	2-D	109	LYS
2	2-E	197	TYR
2	2-E	257	ASN
2	2-E	465	GLU
1	1-A	86	ASP
1	1-A	93	ALA
2	1-F	132	ILE
2	1-F	161	GLY
4	1-H	20	GLY
1	2-B	385	GLN
2	2-D	416	GLN
1	1-B	178	ILE
2	2-F	97	VAL
1	1-B	246	ALA
1	1-C	458	PRO
4	1-H	8	VAL
1	2-A	421	GLY
1	2-C	438	ILE
1	2-C	461	ILE
2	2-D	322	PRO
1	1-B	117	GLY
2	1-D	279	VAL
2	1-F	98	ILE
1	2-C	180	ILE
2	2-E	279	VAL
2	2-F	65	GLY
1	1-A	461	ILE
1	1-B	458	PRO
2	1-E	31	PRO
2	1-E	321	ALA
3	1-G	81	ILE
1	2-B	449	VAL
2	2-E	232	VAL

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Mol	Chain	Res	Type
2	2-E	362	ILE

### 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	1-A	393/412 (95%)	379 (96%)	14 (4%)	35	69
1	1-B	388/412 (94%)	374 (96%)	14 (4%)	35	69
1	1-C	394/412 (96%)	375 (95%)	19 (5%)	25	58
1	2-A	388/412 (94%)	368 (95%)	20 (5%)	23	55
1	2-B	393/412 (95%)	373 (95%)	20 (5%)	24	55
1	2-C	389/412 (94%)	371 (95%)	18 (5%)	27	60
2	1-D	379/386 (98%)	369 (97%)	10 (3%)	46	79
2	1-E	376/386 (97%)	366 (97%)	10 (3%)	44	78
2	1-F	376/386 (97%)	363 (96%)	13 (4%)	36	70
2	2-D	376/386 (97%)	362 (96%)	14 (4%)	34	68
2	2-E	377/386 (98%)	368 (98%)	9 (2%)	49	81
2	2-F	376/386 (97%)	364 (97%)	12 (3%)	39	73
3	1-G	78/230 (34%)	75 (96%)	3 (4%)	33	67
3	2-G	79/230 (34%)	73 (92%)	6 (8%)	13	36
4	1-H	25/68 (37%)	23 (92%)	2 (8%)	12	34
4	2-H	30/68 (44%)	28 (93%)	2 (7%)	16	43
All	All	4817/5384 (90%)	4631 (96%)	186 (4%)	32	66

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	45	ARG
1	1-A	47	VAL
1	1-A	62	MET

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Mol	Chain	Res	Type
1	1-A	86	ASP
1	1-A	102	GLU
1	1-A	121	ILE
1	1-A	140	ILE
1	1-A	164	ARG
1	1-A	211	SER
1	1-A	357	PHE
1	1-A	403	PHE
1	1-A	462	THR
1	1-A	479	LEU
1	1-A	499	GLU
1	1-B	38	ILE
1	1-B	86	ASP
1	1-B	140	ILE
1	1-B	143	ARG
1	1-B	163	GLN
1	1-B	164	ARG
1	1-B	171	ARG
1	1-B	217	VAL
1	1-B	218	LYS
1	1-B	270	ASP
1	1-B	276	VAL
1	1-B	298	VAL
1	1-B	371	VAL
1	1-B	389	THR
1	1-C	47	VAL
1	1-C	52	MET
1	1-C	63	SER
1	1-C	164	ARG
1	1-C	166	LEU
1	1-C	189	PHE
1	1-C	208	GLN
1	1-C	211	SER
1	1-C	216	LEU
1	1-C	244	TYR
1	1-C	272	SER
1	1-C	337	TYR
1	1-C	349	GLN
1	1-C	354	THR
1	1-C	397	TYR
1	1-C	415	GLN
1	1-C	423	ARG

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Mol	Chain	Res	Type
1	1-C	444	VAL
1	1-C	479	LEU
2	1-D	43	THR
2	1-D	112	GLN
2	1-D	232	VAL
2	1-D	250	ASP
2	1-D	257	ASN
2	1-D	282	GLN
2	1-D	292	MET
2	1-D	315	ASP
2	1-D	358	MET
2	1-D	383	SER
2	1-E	67	GLU
2	1-E	215	VAL
2	1-E	223	ASN
2	1-E	232	VAL
2	1-E	246	GLN
2	1-E	257	ASN
2	1-E	282	GLN
2	1-E	308	GLN
2	1-E	336	SER
2	1-E	395	GLU
2	1-F	34	ASN
2	1-F	67	GLU
2	1-F	95	MET
2	1-F	96	ASN
2	1-F	97	VAL
2	1-F	139	VAL
2	1-F	166	ILE
2	1-F	213	SER
2	1-F	221	GLN
2	1-F	223	ASN
2	1-F	282	GLN
2	1-F	303	SER
2	1-F	393	MET
3	1-G	77	LEU
3	1-G	230	THR
3	1-G	262	LEU
4	1-H	29	GLU
4	1-H	34	PHE
1	2-A	56	SER
1	2-A	86	ASP

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Mol	Chain	Res	Type
1	2-A	99	VAL
1	2-A	143	ARG
1	2-A	164	ARG
1	2-A	171	ARG
1	2-A	181	ASP
1	2-A	217	VAL
1	2-A	218	LYS
1	2-A	270	ASP
1	2-A	276	VAL
1	2-A	298	VAL
1	2-A	349	GLN
1	2-A	371	VAL
1	2-A	380	THR
1	2-A	383	MET
1	2-A	389	THR
1	2-A	486	ASP
1	2-A	499	GLU
1	2-A	505	LEU
1	2-B	34	ILE
1	2-B	45	ARG
1	2-B	50	GLU
1	2-B	99	VAL
1	2-B	121	ILE
1	2-B	136	ILE
1	2-B	140	ILE
1	2-B	164	ARG
1	2-B	193	THR
1	2-B	216	LEU
1	2-B	269	ASP
1	2-B	272	SER
1	2-B	335	SER
1	2-B	337	TYR
1	2-B	340	THR
1	2-B	354	THR
1	2-B	403	PHE
1	2-B	442	VAL
1	2-B	449	VAL
1	2-B	499	GLU
1	2-C	45	ARG
1	2-C	52	MET
1	2-C	79	ASP
1	2-C	181	ASP

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Mol	Chain	Res	Type
1	2-C	208	GLN
1	2-C	216	LEU
1	2-C	217	VAL
1	2-C	229	THR
1	2-C	235	THR
1	2-C	272	SER
1	2-C	338	ILE
1	2-C	349	GLN
1	2-C	381	ARG
1	2-C	397	TYR
1	2-C	432	GLN
1	2-C	479	LEU
1	2-C	486	ASP
1	2-C	505	LEU
2	2-D	67	GLU
2	2-D	95	MET
2	2-D	96	ASN
2	2-D	128	VAL
2	2-D	166	ILE
2	2-D	221	GLN
2	2-D	223	ASN
2	2-D	232	VAL
2	2-D	237	LEU
2	2-D	259	PHE
2	2-D	274	ARG
2	2-D	282	GLN
2	2-D	303	SER
2	2-D	393	MET
2	2-E	112	GLN
2	2-E	181	SER
2	2-E	232	VAL
2	2-E	257	ASN
2	2-E	282	GLN
2	2-E	292	MET
2	2-E	315	ASP
2	2-E	358	MET
2	2-E	394	ASP
2	2-F	43	THR
2	2-F	67	GLU
2	2-F	78	SER
2	2-F	223	ASN
2	2-F	232	VAL

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Mol	Chain	Res	Type
2	2-F	246	GLN
2	2-F	252	LEU
2	2-F	282	GLN
2	2-F	308	GLN
2	2-F	358	MET
2	2-F	380	ASP
2	2-F	395	GLU
3	2-G	10	LEU
3	2-G	77	LEU
3	2-G	249	THR
3	2-G	255	GLN
3	2-G	262	LEU
3	2-G	267	SER
4	2-H	22	PHE
4	2-H	34	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	190	ASN
1	1-A	208	GLN
1	1-A	263	HIS
1	1-A	349	GLN
1	1-A	396	GLN
1	1-A	405	GLN
1	1-A	415	GLN
1	1-B	46	ASN
1	1-B	65	ASN
1	1-B	215	GLN
1	1-B	341	ASN
1	1-B	503	ASN
1	1-C	65	ASN
1	1-C	208	GLN
1	1-C	215	GLN
1	1-C	263	HIS
1	1-C	349	GLN
1	1-C	415	GLN
1	1-C	432	GLN
1	1-C	441	GLN
1	1-C	471	HIS
1	1-C	476	HIS
2	1-D	39	GLN

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Mol	Chain	Res	Type
2	1-D	177	HIS
2	1-D	249	GLN
2	1-D	282	GLN
2	1-D	442	GLN
2	1-E	194	ASN
2	1-E	223	ASN
2	1-E	246	GLN
2	1-E	257	ASN
2	1-E	263	GLN
2	1-E	282	GLN
2	1-E	293	GLN
2	1-E	308	GLN
2	1-E	328	HIS
2	1-E	367	HIS
2	1-E	411	GLN
2	1-E	455	GLN
2	1-F	96	ASN
2	1-F	221	GLN
2	1-F	223	ASN
2	1-F	249	GLN
2	1-F	282	GLN
2	1-F	308	GLN
2	1-F	328	HIS
2	1-F	385	GLN
2	1-F	443	GLN
3	1-G	82	HIS
3	1-G	238	ASN
4	1-H	7	ASN
1	2-A	46	ASN
1	2-A	48	GLN
1	2-A	65	ASN
1	2-A	113	ASN
1	2-A	208	GLN
1	2-A	379	GLN
1	2-A	466	ASN
1	2-A	503	ASN
1	2-B	113	ASN
1	2-B	405	GLN
1	2-B	415	GLN
1	2-B	432	GLN
1	2-B	471	HIS
1	2-B	503	ASN

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Mol	Chain	Res	Type
1	2-C	78	ASN
1	2-C	208	GLN
1	2-C	260	ASN
1	2-C	263	HIS
1	2-C	349	GLN
1	2-C	379	GLN
1	2-C	396	GLN
1	2-C	415	GLN
1	2-C	430	GLN
1	2-C	476	HIS
2	2-D	96	ASN
2	2-D	221	GLN
2	2-D	223	ASN
2	2-D	249	GLN
2	2-D	282	GLN
2	2-D	308	GLN
2	2-D	385	GLN
2	2-E	39	GLN
2	2-E	130	GLN
2	2-E	194	ASN
2	2-E	198	HIS
2	2-E	221	GLN
2	2-E	223	ASN
2	2-E	282	GLN
2	2-E	328	HIS
2	2-E	442	GLN
2	2-F	96	ASN
2	2-F	194	ASN
2	2-F	221	GLN
2	2-F	223	ASN
2	2-F	246	GLN
2	2-F	257	ASN
2	2-F	282	GLN
2	2-F	293	GLN
2	2-F	367	HIS
2	2-F	411	GLN
3	2-G	234	ASN
4	2-H	41	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ANP	2-D	1478	6	29,33,33	1.54	6 (20%)	31,52,52	1.90	6 (19%)
5	ANP	1-A	1511	6	29,33,33	1.43	4 (13%)	31,52,52	1.38	4 (12%)
5	ANP	1-B	1511	6	29,33,33	1.48	5 (17%)	31,52,52	1.55	5 (16%)
5	ANP	2-F	1478	6	29,33,33	1.74	8 (27%)	31,52,52	1.73	6 (19%)
5	ANP	1-C	1511	6	29,33,33	1.35	3 (10%)	31,52,52	1.45	2 (6%)
5	ANP	2-B	1511	6	29,33,33	1.35	4 (13%)	31,52,52	1.19	3 (9%)
5	ANP	1-F	1478	6	29,33,33	1.59	6 (20%)	31,52,52	1.76	5 (16%)
5	ANP	1-D	1478	6	29,33,33	1.75	7 (24%)	31,52,52	1.80	8 (25%)
5	ANP	2-A	1511	6	29,33,33	1.57	5 (17%)	31,52,52	1.68	4 (12%)
5	ANP	2-C	1511	6	29,33,33	1.52	6 (20%)	31,52,52	1.66	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	2-D	1478	6	-	8/14/38/38	0/3/3/3
5	ANP	1-A	1511	6	-	7/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	1-B	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	2-F	1478	6	-	9/14/38/38	0/3/3/3
5	ANP	1-C	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	2-B	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	1-F	1478	6	-	9/14/38/38	0/3/3/3
5	ANP	1-D	1478	6	-	9/14/38/38	0/3/3/3
5	ANP	2-A	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	2-C	1511	6	-	7/14/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-F	1478	ANP	PG-O2G	-5.33	1.42	1.56
5	1-D	1478	ANP	PG-O2G	-5.05	1.43	1.56
5	2-A	1511	ANP	PG-O2G	-4.48	1.44	1.56
5	1-C	1511	ANP	PG-O2G	-4.26	1.45	1.56
5	2-C	1511	ANP	PG-O1G	4.24	1.52	1.46
5	1-F	1478	ANP	PG-O2G	-4.16	1.45	1.56
5	2-B	1511	ANP	PG-O2G	-4.04	1.45	1.56
5	2-D	1478	ANP	PG-O2G	-3.82	1.46	1.56
5	2-A	1511	ANP	PB-O2B	-3.79	1.46	1.56
5	1-B	1511	ANP	PG-O2G	-3.76	1.46	1.56
5	1-A	1511	ANP	PB-O2B	-3.73	1.46	1.56
5	2-C	1511	ANP	PG-O2G	-3.61	1.47	1.56
5	1-A	1511	ANP	PG-O2G	-3.61	1.47	1.56
5	1-D	1478	ANP	PB-O3A	-3.35	1.54	1.59
5	1-D	1478	ANP	PG-O1G	3.22	1.51	1.46
5	1-B	1511	ANP	C4-N3	3.22	1.40	1.35
5	1-F	1478	ANP	PG-O1G	3.11	1.51	1.46
5	1-A	1511	ANP	PG-O1G	3.06	1.51	1.46
5	2-A	1511	ANP	PG-O1G	2.99	1.50	1.46
5	2-F	1478	ANP	PG-O1G	2.96	1.50	1.46
5	1-D	1478	ANP	PG-N3B	-2.91	1.55	1.63
5	2-C	1511	ANP	PB-O2B	-2.84	1.49	1.56
5	1-B	1511	ANP	PG-O1G	2.79	1.50	1.46
5	2-D	1478	ANP	C2-N1	2.73	1.39	1.33
5	1-F	1478	ANP	PB-O2B	-2.70	1.49	1.56
5	2-F	1478	ANP	PG-O3G	-2.64	1.49	1.56
5	1-B	1511	ANP	PB-O2B	-2.62	1.49	1.56
5	2-B	1511	ANP	C4-N3	2.56	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-D	1478	ANP	C4-N3	2.52	1.39	1.35
5	2-D	1478	ANP	PG-O3G	-2.51	1.50	1.56
5	1-C	1511	ANP	PB-O2B	-2.51	1.50	1.56
5	2-F	1478	ANP	PB-O2B	-2.50	1.50	1.56
5	2-D	1478	ANP	PG-O1G	2.49	1.50	1.46
5	2-F	1478	ANP	C2-N1	2.48	1.38	1.33
5	2-F	1478	ANP	PG-N3B	-2.46	1.56	1.63
5	2-C	1511	ANP	C2-N1	2.42	1.38	1.33
5	2-D	1478	ANP	PB-O2B	-2.39	1.50	1.56
5	2-A	1511	ANP	C4-N3	2.38	1.38	1.35
5	2-B	1511	ANP	C2-N1	2.38	1.38	1.33
5	2-F	1478	ANP	C4-N3	2.26	1.38	1.35
5	2-F	1478	ANP	PB-O3A	-2.22	1.56	1.59
5	2-C	1511	ANP	PG-O3G	-2.22	1.50	1.56
5	1-F	1478	ANP	PG-N3B	-2.20	1.57	1.63
5	1-B	1511	ANP	C2-N1	2.16	1.37	1.33
5	1-F	1478	ANP	C2-N1	2.12	1.37	1.33
5	2-B	1511	ANP	PG-O3G	-2.09	1.51	1.56
5	2-A	1511	ANP	C5'-C4'	-2.07	1.45	1.51
5	1-D	1478	ANP	C3'-C4'	-2.07	1.47	1.53
5	1-D	1478	ANP	C4-N3	2.06	1.38	1.35
5	1-F	1478	ANP	C2'-C3'	-2.06	1.47	1.53
5	2-C	1511	ANP	C4-N3	2.05	1.38	1.35
5	1-C	1511	ANP	PG-O3G	-2.04	1.51	1.56
5	1-A	1511	ANP	C2-N1	2.02	1.37	1.33
5	1-D	1478	ANP	PG-O3G	-2.02	1.51	1.56

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2-D	1478	ANP	O1G-PG-N3B	-6.80	101.76	111.77
5	2-F	1478	ANP	O1G-PG-N3B	-6.45	102.27	111.77
5	1-F	1478	ANP	O1G-PG-N3B	-5.65	103.45	111.77
5	2-C	1511	ANP	O1G-PG-N3B	-5.49	103.68	111.77
5	2-A	1511	ANP	O1G-PG-N3B	-5.34	103.91	111.77
5	1-B	1511	ANP	O1G-PG-N3B	-5.23	104.07	111.77
5	1-C	1511	ANP	O1G-PG-N3B	-5.02	104.38	111.77
5	1-D	1478	ANP	O1G-PG-N3B	-4.96	104.47	111.77
5	1-A	1511	ANP	O1G-PG-N3B	-4.67	104.90	111.77
5	2-D	1478	ANP	O1B-PB-N3B	-4.28	105.47	111.77
5	1-D	1478	ANP	O1B-PB-N3B	-3.41	106.75	111.77
5	2-F	1478	ANP	O1B-PB-N3B	-3.30	106.91	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1-F	1478	ANP	O1B-PB-N3B	-3.29	106.92	111.77
5	2-C	1511	ANP	O1B-PB-N3B	-3.14	107.14	111.77
5	1-D	1478	ANP	O4'-C4'-C5'	3.03	119.35	109.37
5	1-D	1478	ANP	O2B-PB-O3A	3.03	114.74	104.64
5	2-D	1478	ANP	O4'-C4'-C5'	2.89	118.88	109.37
5	2-B	1511	ANP	O1G-PG-N3B	-2.88	107.53	111.77
5	2-A	1511	ANP	C5-C6-N6	2.81	124.63	120.35
5	1-F	1478	ANP	O4'-C4'-C5'	2.79	118.57	109.37
5	1-A	1511	ANP	O5'-C5'-C4'	2.68	118.21	108.99
5	1-B	1511	ANP	O4'-C4'-C5'	2.59	117.89	109.37
5	1-B	1511	ANP	C3'-C2'-C1'	2.58	104.87	100.98
5	1-D	1478	ANP	O3G-PG-O2G	2.55	114.44	107.64
5	2-D	1478	ANP	O2B-PB-O3A	2.49	112.94	104.64
5	1-F	1478	ANP	O2B-PB-O3A	2.39	112.63	104.64
5	2-A	1511	ANP	C3'-C2'-C1'	2.35	104.51	100.98
5	1-F	1478	ANP	C4-C5-N7	2.31	111.81	109.40
5	1-A	1511	ANP	C4-C5-N7	2.22	111.71	109.40
5	2-F	1478	ANP	C3'-C2'-C1'	2.21	104.30	100.98
5	2-D	1478	ANP	O3G-PG-O1G	-2.19	107.94	113.45
5	2-F	1478	ANP	O2B-PB-O3A	2.16	111.84	104.64
5	1-A	1511	ANP	C5-C6-N6	2.15	123.61	120.35
5	1-D	1478	ANP	C4-C5-N7	2.13	111.62	109.40
5	1-D	1478	ANP	C1'-N9-C4	-2.13	122.89	126.64
5	2-B	1511	ANP	C5-C6-N6	2.13	123.59	120.35
5	1-C	1511	ANP	O2G-PG-O1G	-2.11	108.14	113.45
5	2-F	1478	ANP	C4-C5-N7	2.10	111.58	109.40
5	2-B	1511	ANP	O2B-PB-O3A	2.09	111.62	104.64
5	2-D	1478	ANP	C4-C5-N7	2.09	111.58	109.40
5	1-B	1511	ANP	C2'-C3'-C4'	2.07	106.66	102.64
5	2-A	1511	ANP	C2'-C3'-C4'	2.07	106.66	102.64
5	1-B	1511	ANP	C4-C5-N7	2.06	111.54	109.40
5	2-F	1478	ANP	O4'-C4'-C5'	2.03	116.04	109.37
5	1-D	1478	ANP	O2G-PG-O1G	-2.02	108.39	113.45
5	2-C	1511	ANP	C4-C5-N7	2.01	111.49	109.40

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	2-D	1478	ANP	PB-N3B-PG-O1G
5	2-D	1478	ANP	PG-N3B-PB-O1B
5	2-D	1478	ANP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	2-D	1478	ANP	C5'-O5'-PA-O1A
5	2-D	1478	ANP	C5'-O5'-PA-O2A
5	1-A	1511	ANP	PB-N3B-PG-O1G
5	1-A	1511	ANP	PG-N3B-PB-O1B
5	1-A	1511	ANP	C5'-O5'-PA-O1A
5	1-A	1511	ANP	C5'-O5'-PA-O2A
5	1-B	1511	ANP	PB-N3B-PG-O1G
5	1-B	1511	ANP	PG-N3B-PB-O1B
5	1-B	1511	ANP	C5'-O5'-PA-O1A
5	1-B	1511	ANP	C5'-O5'-PA-O2A
5	2-F	1478	ANP	PB-N3B-PG-O1G
5	2-F	1478	ANP	PG-N3B-PB-O1B
5	2-F	1478	ANP	PA-O3A-PB-O1B
5	2-F	1478	ANP	PA-O3A-PB-O2B
5	2-F	1478	ANP	C5'-O5'-PA-O1A
5	2-F	1478	ANP	C5'-O5'-PA-O2A
5	2-F	1478	ANP	O4'-C4'-C5'-O5'
5	2-F	1478	ANP	C3'-C4'-C5'-O5'
5	1-C	1511	ANP	PB-N3B-PG-O1G
5	1-C	1511	ANP	PG-N3B-PB-O1B
5	1-C	1511	ANP	C5'-O5'-PA-O1A
5	1-C	1511	ANP	C5'-O5'-PA-O2A
5	1-C	1511	ANP	O4'-C4'-C5'-O5'
5	2-B	1511	ANP	PB-N3B-PG-O1G
5	2-B	1511	ANP	PG-N3B-PB-O1B
5	2-B	1511	ANP	C5'-O5'-PA-O1A
5	2-B	1511	ANP	C5'-O5'-PA-O2A
5	2-B	1511	ANP	O4'-C4'-C5'-O5'
5	1-F	1478	ANP	PB-N3B-PG-O1G
5	1-F	1478	ANP	PG-N3B-PB-O1B
5	1-F	1478	ANP	PA-O3A-PB-O1B
5	1-F	1478	ANP	PA-O3A-PB-O2B
5	1-F	1478	ANP	C5'-O5'-PA-O1A
5	1-F	1478	ANP	C5'-O5'-PA-O2A
5	1-D	1478	ANP	PB-N3B-PG-O1G
5	1-D	1478	ANP	PG-N3B-PB-O1B
5	1-D	1478	ANP	PA-O3A-PB-O1B
5	1-D	1478	ANP	PA-O3A-PB-O2B
5	1-D	1478	ANP	C5'-O5'-PA-O1A
5	1-D	1478	ANP	C5'-O5'-PA-O2A
5	1-D	1478	ANP	O4'-C4'-C5'-O5'
5	2-A	1511	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
5	2-A	1511	ANP	PG-N3B-PB-O1B
5	2-A	1511	ANP	C5'-O5'-PA-O1A
5	2-A	1511	ANP	C5'-O5'-PA-O2A
5	2-C	1511	ANP	PB-N3B-PG-O1G
5	2-C	1511	ANP	PG-N3B-PB-O1B
5	2-C	1511	ANP	C5'-O5'-PA-O1A
5	2-C	1511	ANP	C5'-O5'-PA-O2A
5	2-C	1511	ANP	O4'-C4'-C5'-O5'
5	2-D	1478	ANP	C3'-C4'-C5'-O5'
5	1-B	1511	ANP	O4'-C4'-C5'-O5'
5	1-B	1511	ANP	C3'-C4'-C5'-O5'
5	1-C	1511	ANP	C3'-C4'-C5'-O5'
5	2-B	1511	ANP	C3'-C4'-C5'-O5'
5	1-F	1478	ANP	O4'-C4'-C5'-O5'
5	1-F	1478	ANP	C3'-C4'-C5'-O5'
5	1-D	1478	ANP	C3'-C4'-C5'-O5'
5	2-A	1511	ANP	O4'-C4'-C5'-O5'
5	2-A	1511	ANP	C3'-C4'-C5'-O5'
5	2-C	1511	ANP	C3'-C4'-C5'-O5'
5	2-D	1478	ANP	O4'-C4'-C5'-O5'
5	2-D	1478	ANP	C5'-O5'-PA-O3A
5	1-A	1511	ANP	C5'-O5'-PA-O3A
5	2-A	1511	ANP	C5'-O5'-PA-O3A
5	2-C	1511	ANP	C5'-O5'-PA-O3A
5	1-A	1511	ANP	C3'-C4'-C5'-O5'
5	1-A	1511	ANP	O4'-C4'-C5'-O5'
5	1-B	1511	ANP	C5'-O5'-PA-O3A
5	2-F	1478	ANP	C5'-O5'-PA-O3A
5	1-C	1511	ANP	C5'-O5'-PA-O3A
5	2-B	1511	ANP	C5'-O5'-PA-O3A
5	1-F	1478	ANP	C5'-O5'-PA-O3A
5	1-D	1478	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

10 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2-D	1478	ANP	4	0
5	1-A	1511	ANP	4	0
5	1-B	1511	ANP	4	0
5	2-F	1478	ANP	4	0
5	1-C	1511	ANP	3	0

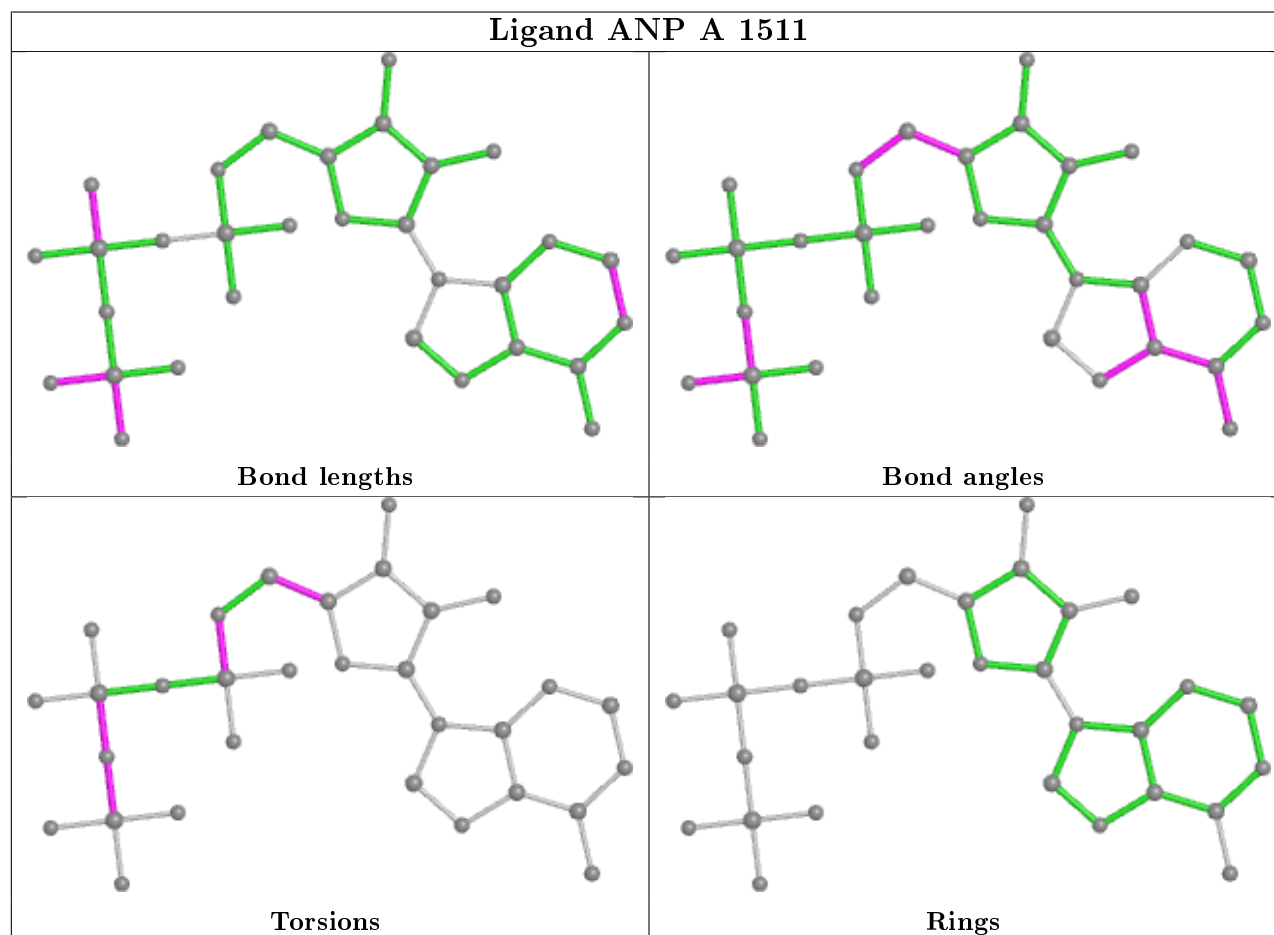
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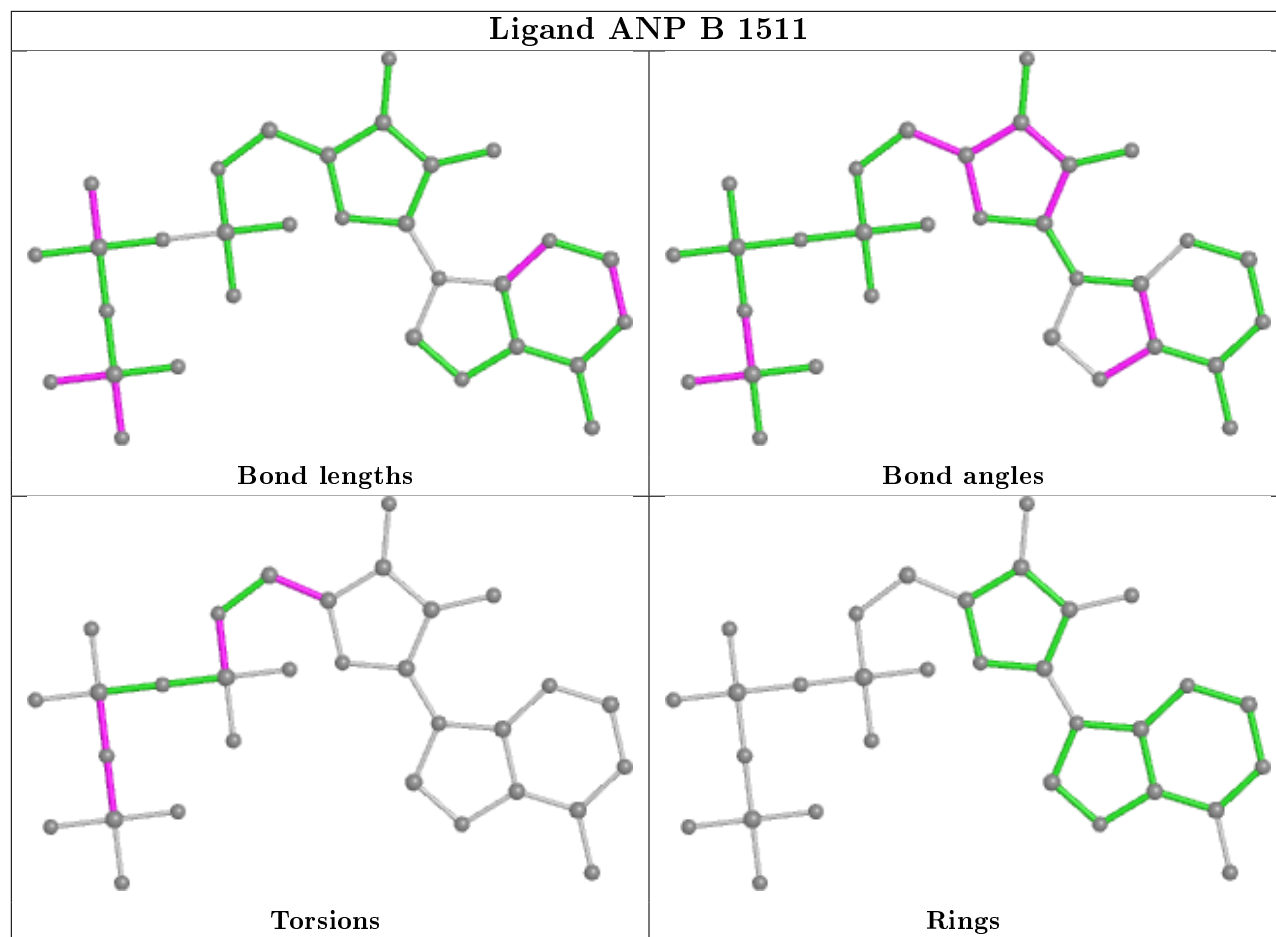


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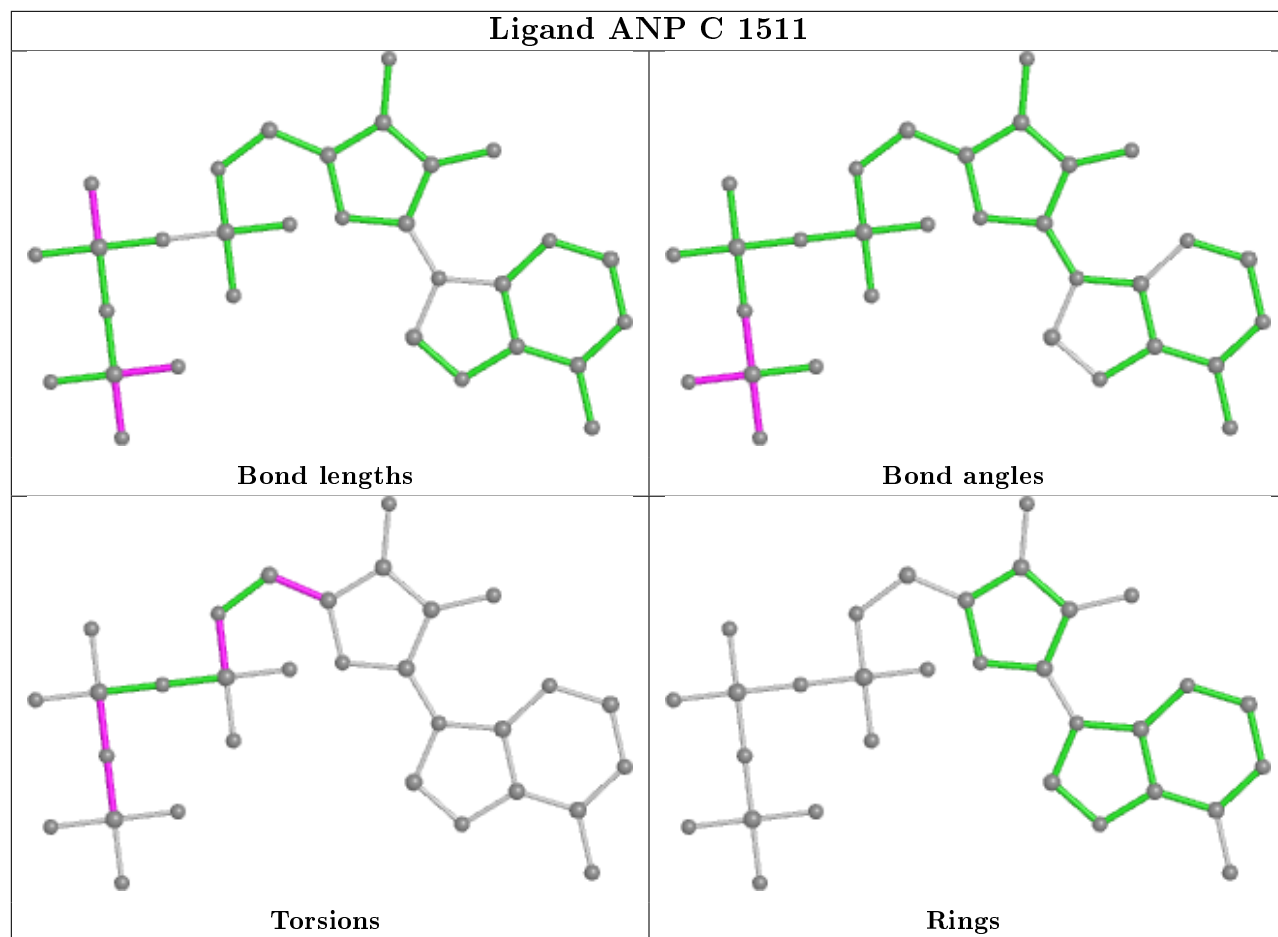
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2-B	1511	ANP	4	0
5	1-F	1478	ANP	3	0
5	1-D	1478	ANP	5	0
5	2-A	1511	ANP	6	0
5	2-C	1511	ANP	5	0

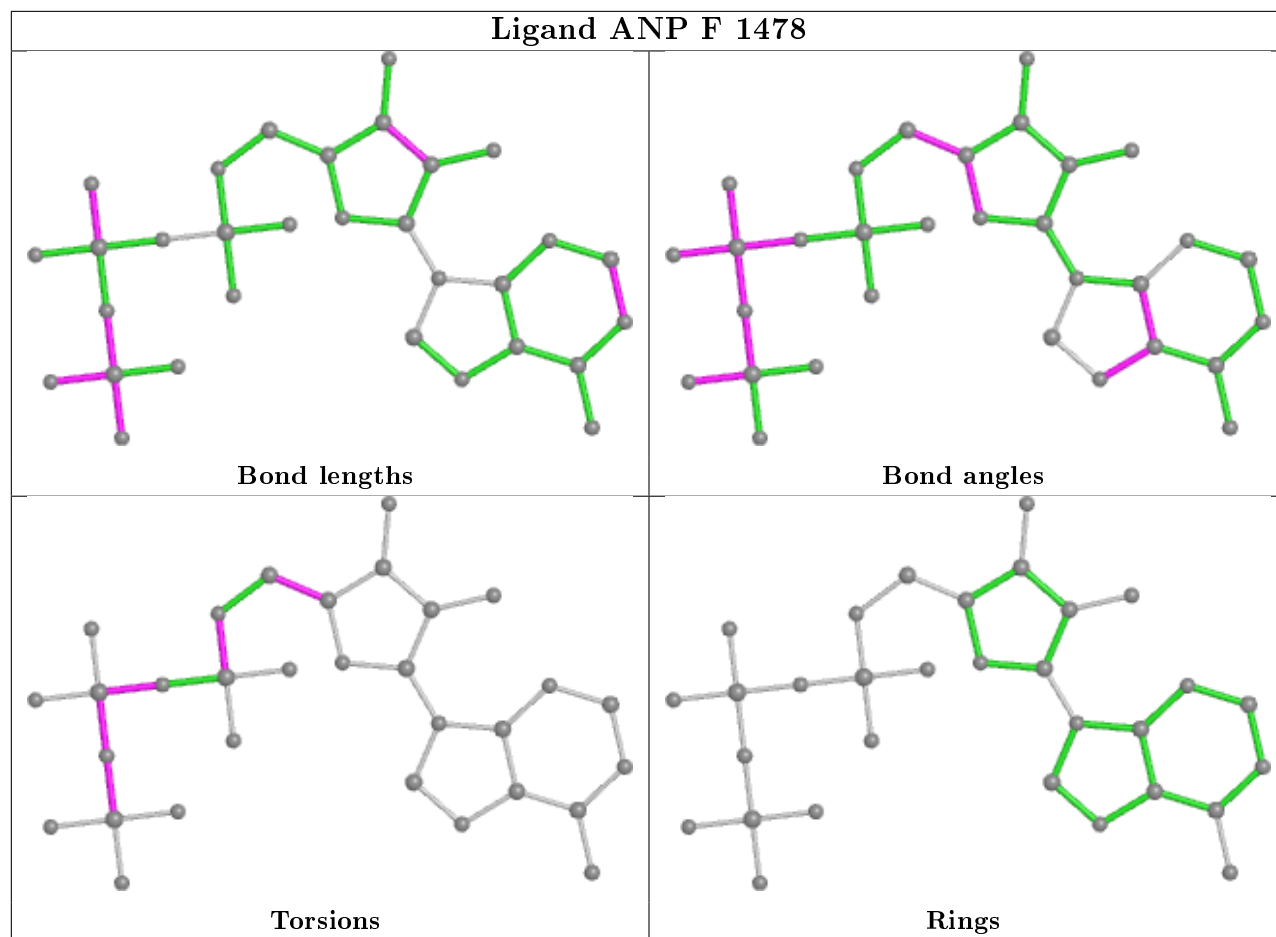
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

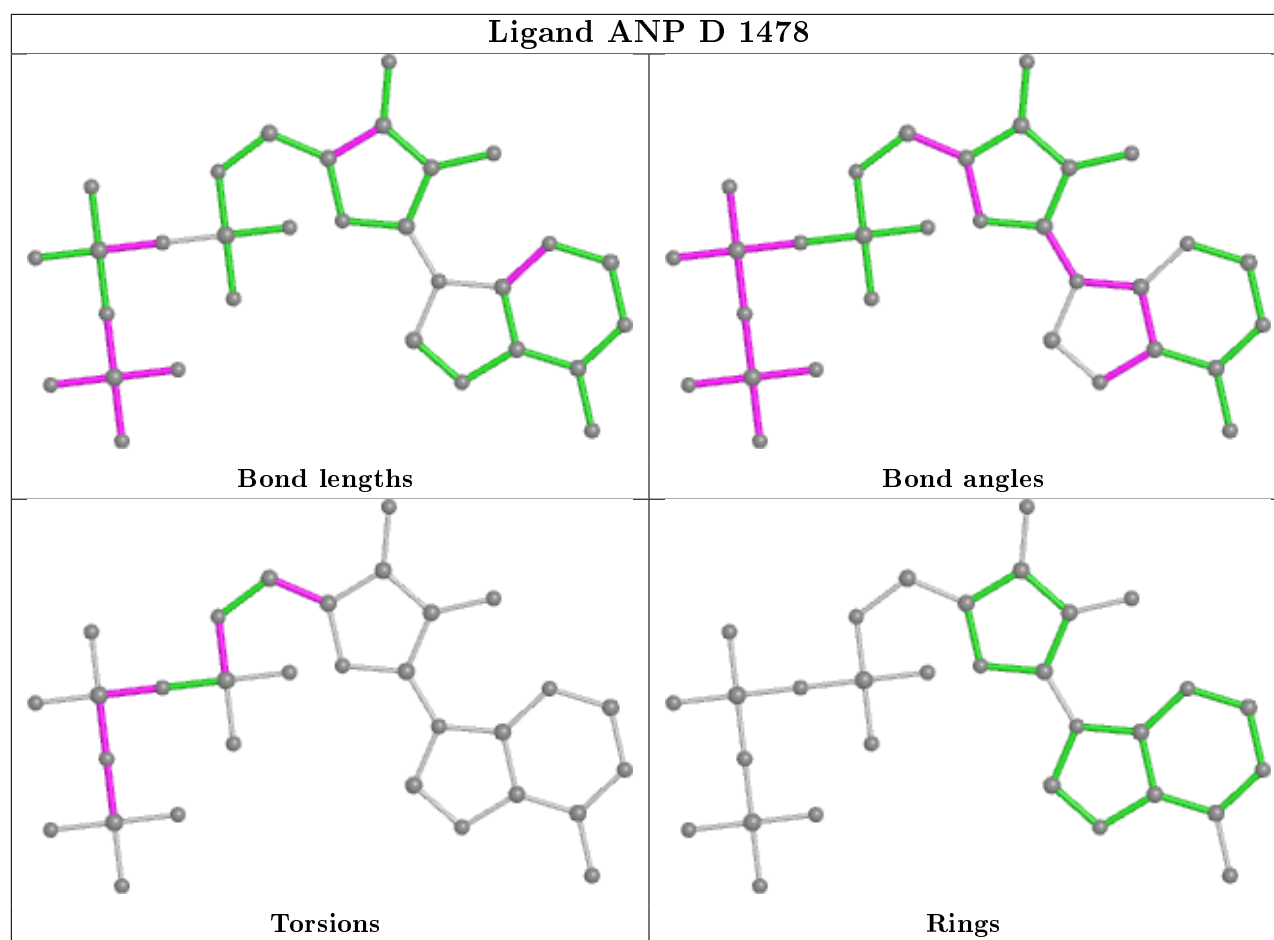




## Ligand ANP C 1511







## 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	1-A	487/510 (95%)	-0.05	19 (3%) 39 29	33, 55, 103, 139	487 (100%)
1	1-B	479/510 (93%)	0.11	33 (6%) 16 10	38, 59, 88, 127	479 (100%)
1	1-C	488/510 (95%)	0.24	35 (7%) 15 8	37, 65, 99, 147	488 (100%)
1	2-A	479/510 (93%)	-0.14	12 (2%) 57 47	33, 55, 102, 139	479 (100%)
1	2-B	487/510 (95%)	0.15	39 (8%) 12 6	38, 59, 96, 128	487 (100%)
1	2-C	480/510 (94%)	0.19	31 (6%) 18 11	37, 65, 97, 130	480 (100%)
2	1-D	469/482 (97%)	0.41	43 (9%) 9 5	36, 56, 91, 117	469 (100%)
2	1-E	466/482 (96%)	0.83	88 (18%) 1 1	41, 65, 98, 111	466 (100%)
2	1-F	466/482 (96%)	0.43	46 (9%) 7 4	28, 60, 106, 135	466 (100%)
2	2-D	466/482 (96%)	0.40	42 (9%) 9 5	36, 56, 89, 112	466 (100%)
2	2-E	467/482 (96%)	0.84	89 (19%) 1 1	41, 65, 99, 111	467 (100%)
2	2-F	466/482 (96%)	0.43	46 (9%) 7 4	28, 60, 106, 135	466 (100%)
3	1-G	94/272 (34%)	1.83	32 (34%) 0 0	33, 71, 120, 123	94 (100%)
3	2-G	94/272 (34%)	1.78	30 (31%) 0 0	33, 71, 117, 123	94 (100%)
4	1-H	37/84 (44%)	2.39	18 (48%) 0 0	70, 90, 110, 115	37 (100%)
4	2-H	44/84 (52%)	2.53	23 (52%) 0 0	70, 93, 112, 118	44 (100%)
All	All	5969/6664 (89%)	0.39	626 (10%) 9 3	28, 61, 102, 147	5969 (100%)

All (626) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	414	THR	14.5
1	2-C	414	THR	14.5
2	1-F	394	ASP	14.1
2	2-F	394	ASP	14.1
2	1-F	391	LEU	13.2

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Mol	Chain	Res	Type	RSRZ
2	2-F	391	LEU	13.2
1	1-A	408	SER	11.2
1	1-A	406	PHE	9.7
1	1-C	413	ALA	9.7
1	2-C	413	ALA	9.7
1	1-B	510	ALA	8.9
1	2-B	510	ALA	8.9
1	1-C	20	ASP	8.7
1	2-C	20	ASP	8.7
2	1-F	395	GLU	8.6
2	2-F	395	GLU	8.6
2	1-D	387	ILE	8.5
2	2-D	387	ILE	8.5
4	1-H	35	ARG	8.3
4	2-H	35	ARG	8.3
2	1-F	387	ILE	8.1
2	2-F	387	ILE	8.1
4	1-H	12	ALA	8.0
4	2-H	12	ALA	8.0
2	1-E	201	ILE	8.0
2	2-E	201	ILE	8.0
3	1-G	227	ALA	8.0
3	2-G	227	ALA	8.0
1	1-A	407	GLY	7.9
1	1-C	19	ALA	7.6
1	2-C	19	ALA	7.6
1	1-C	22	SER	7.3
1	2-C	22	SER	7.3
1	1-C	21	THR	7.3
1	2-C	21	THR	7.3
2	1-E	336	SER	7.3
2	2-E	336	SER	7.3
3	1-G	226	SER	7.0
3	2-G	226	SER	7.0
2	1-D	469	LYS	6.8
2	2-D	469	LYS	6.8
2	1-F	399	GLU	6.8
2	2-F	399	GLU	6.8
2	1-E	302	GLY	6.7
2	2-E	302	GLY	6.7
3	1-G	82	HIS	6.6
3	2-G	82	HIS	6.6

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Mol	Chain	Res	Type	RSRZ
2	1-D	400	ASP	6.5
2	2-D	400	ASP	6.5
2	1-E	288	ASP	6.4
2	2-E	288	ASP	6.4
3	1-G	223	SER	6.3
3	2-G	223	SER	6.3
2	1-F	364	GLY	6.3
2	2-F	364	GLY	6.3
1	1-C	404	ALA	6.2
2	1-F	362	ILE	6.2
2	2-F	362	ILE	6.2
2	1-D	391	LEU	6.1
2	2-D	391	LEU	6.1
2	1-E	352	ASP	6.0
2	2-E	352	ASP	6.0
2	1-D	467	VAL	6.0
2	2-D	467	VAL	6.0
2	1-F	455	GLN	5.9
2	2-F	455	GLN	5.9
3	1-G	233	ASP	5.8
3	2-G	233	ASP	5.8
2	2-E	475	GLU	5.8
1	2-B	408	SER	5.8
1	1-C	417	LEU	5.7
1	2-C	417	LEU	5.7
2	1-E	394	ASP	5.6
2	2-E	394	ASP	5.6
4	1-H	15	VAL	5.6
4	2-H	15	VAL	5.6
2	1-F	458	TYR	5.5
2	2-F	458	TYR	5.5
2	1-E	180	TYR	5.5
2	2-E	180	TYR	5.5
4	2-H	46	LYS	5.4
2	1-D	395	GLU	5.2
2	2-D	395	GLU	5.2
1	1-C	510	ALA	5.2
1	2-C	510	ALA	5.2
3	1-G	83	SER	5.2
3	1-G	234	ASN	5.1
3	2-G	234	ASN	5.1
2	1-E	464	GLU	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	2-E	464	GLU	5.1
2	1-F	453	PRO	5.1
2	2-F	453	PRO	5.1
2	1-D	462	PRO	5.0
2	2-D	462	PRO	5.0
2	1-E	159	GLY	5.0
2	2-E	159	GLY	5.0
1	1-A	409	ASP	4.9
1	1-A	412	ALA	4.9
1	2-A	412	ALA	4.9
1	1-C	409	ASP	4.9
2	1-E	211	ALA	4.9
2	2-E	211	ALA	4.9
4	1-H	24	LYS	4.8
4	2-H	24	LYS	4.8
1	1-B	489	ILE	4.8
1	2-B	489	ILE	4.8
4	2-H	41	GLN	4.8
2	1-D	394	ASP	4.7
2	2-D	394	ASP	4.7
1	1-B	61	GLY	4.7
1	2-B	61	GLY	4.7
2	1-D	28	GLY	4.7
2	2-D	28	GLY	4.7
2	1-E	76	LEU	4.6
2	2-E	76	LEU	4.6
2	1-F	473	LEU	4.6
2	2-F	473	LEU	4.6
2	1-E	139	VAL	4.5
2	2-E	139	VAL	4.5
1	1-C	410	LEU	4.4
2	1-E	175	LYS	4.4
2	2-E	175	LYS	4.4
2	1-F	338	ALA	4.4
2	2-F	338	ALA	4.4
3	1-G	251	ASN	4.4
3	2-G	251	ASN	4.4
1	1-B	56	SER	4.4
1	2-B	56	SER	4.4
2	1-E	340	ALA	4.4
2	2-E	340	ALA	4.4
3	2-G	216	SER	4.3

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Mol	Chain	Res	Type	RSRZ
2	1-F	278	ALA	4.3
2	2-F	278	ALA	4.3
1	1-C	392	LEU	4.3
1	2-C	392	LEU	4.3
3	1-G	86	ALA	4.3
2	1-D	388	ILE	4.3
2	2-D	388	ILE	4.3
2	1-E	451	HIS	4.3
2	2-E	451	HIS	4.3
2	1-E	386	ASP	4.3
2	1-F	315	ASP	4.3
2	2-E	386	ASP	4.3
2	2-F	315	ASP	4.3
2	1-E	392	GLY	4.3
2	2-E	392	GLY	4.3
4	1-H	31	GLU	4.3
4	2-H	31	GLU	4.3
1	1-C	399	GLU	4.2
1	2-C	399	GLU	4.2
2	1-E	273	GLY	4.2
2	2-E	273	GLY	4.2
2	1-F	402	LEU	4.2
2	2-F	402	LEU	4.2
2	1-E	261	PHE	4.2
2	2-E	261	PHE	4.2
2	1-E	339	ILE	4.2
2	2-E	339	ILE	4.2
2	1-D	176	ALA	4.1
2	2-D	176	ALA	4.1
4	1-H	39	LYS	4.2
4	2-H	39	LYS	4.2
2	1-E	351	LEU	4.1
2	2-E	351	LEU	4.1
3	1-G	5	ASP	4.1
3	2-G	5	ASP	4.1
4	1-H	37	ARG	4.1
4	2-H	37	ARG	4.1
2	1-E	438	ILE	4.1
2	2-E	438	ILE	4.1
2	1-F	279	VAL	4.0
2	2-F	279	VAL	4.0
1	2-B	406	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
3	2-G	220	SER	4.0
3	1-G	265	ILE	4.0
3	2-G	265	ILE	4.0
4	2-H	45	LEU	4.0
2	1-D	475	GLU	4.0
2	1-D	390	ILE	4.0
2	2-D	390	ILE	4.0
2	1-F	393	MET	3.9
2	2-F	393	MET	3.9
2	1-D	474	ALA	3.9
2	2-D	474	ALA	3.9
3	1-G	224	GLU	3.9
3	2-G	224	GLU	3.9
2	1-D	389	ALA	3.9
2	2-D	389	ALA	3.9
2	1-D	458	TYR	3.9
2	2-D	458	TYR	3.9
2	1-E	441	PHE	3.9
2	2-E	441	PHE	3.9
2	1-E	436	GLU	3.8
2	2-E	436	GLU	3.8
2	1-E	354	THR	3.8
2	2-E	354	THR	3.8
2	1-E	424	PHE	3.8
2	2-E	424	PHE	3.8
3	1-G	247	THR	3.8
3	2-G	247	THR	3.8
1	1-B	401	ALA	3.8
1	2-B	401	ALA	3.8
3	1-G	244	ASP	3.8
3	2-G	244	ASP	3.8
4	2-H	42	LEU	3.8
1	1-A	510	ALA	3.8
1	2-A	510	ALA	3.8
2	1-E	90	THR	3.8
2	2-E	90	THR	3.8
1	1-C	34	ILE	3.8
1	2-C	34	ILE	3.8
2	1-D	473	LEU	3.8
2	2-D	473	LEU	3.8
2	1-F	161	GLY	3.8
2	2-F	161	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	1-E	338	ALA	3.7
2	2-E	338	ALA	3.7
2	1-F	351	LEU	3.7
2	2-F	351	LEU	3.7
1	1-B	493	SER	3.7
1	2-B	493	SER	3.7
2	1-F	386	ASP	3.7
2	2-F	386	ASP	3.7
3	1-G	6	ILE	3.7
3	2-G	6	ILE	3.7
2	1-E	412	ARG	3.7
2	2-E	412	ARG	3.7
2	1-E	428	LEU	3.6
2	2-E	428	LEU	3.6
2	1-F	385	GLN	3.6
2	2-F	385	GLN	3.6
2	1-F	388	ILE	3.6
2	2-F	388	ILE	3.6
2	1-E	118	ALA	3.6
2	2-E	118	ALA	3.6
2	1-D	338	ALA	3.6
2	1-D	421	ALA	3.6
2	2-D	338	ALA	3.6
2	2-D	421	ALA	3.6
2	1-D	108	ILE	3.6
2	1-E	341	GLU	3.6
2	2-D	108	ILE	3.6
2	2-E	341	GLU	3.6
2	1-E	77	ASP	3.6
2	2-E	77	ASP	3.6
1	1-A	415	GLN	3.6
1	2-A	415	GLN	3.6
2	1-D	139	VAL	3.5
2	2-D	139	VAL	3.5
3	2-G	215	TYR	3.5
3	1-G	252	ARG	3.5
3	2-G	252	ARG	3.5
1	1-C	194	ASP	3.5
1	2-C	194	ASP	3.5
2	1-F	401	LYS	3.5
2	2-F	401	LYS	3.5
1	1-C	412	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	2-C	412	ALA	3.5
2	1-E	104	GLU	3.5
2	2-E	104	GLU	3.5
1	1-A	509	GLU	3.5
1	2-A	509	GLU	3.5
2	1-E	210	ASP	3.4
2	2-E	210	ASP	3.4
4	1-H	17	ASP	3.4
4	2-H	17	ASP	3.4
2	1-E	262	THR	3.4
2	2-E	262	THR	3.4
4	2-H	47	LYS	3.4
2	1-D	436	GLU	3.4
2	2-D	436	GLU	3.4
4	1-H	7	ASN	3.4
4	2-H	7	ASN	3.4
1	1-C	489	ILE	3.4
1	2-C	489	ILE	3.4
2	1-D	9	THR	3.4
2	1-D	437	THR	3.4
2	2-D	9	THR	3.4
2	2-D	437	THR	3.4
2	1-F	449	TYR	3.4
2	2-F	449	TYR	3.4
1	1-B	447	ALA	3.3
1	2-B	447	ALA	3.3
4	1-H	23	GLY	3.3
4	2-H	23	GLY	3.3
1	1-B	508	PHE	3.3
1	2-B	508	PHE	3.3
1	1-B	509	GLU	3.3
1	2-B	509	GLU	3.3
3	1-G	250	PHE	3.3
3	2-G	250	PHE	3.3
2	1-E	68	GLY	3.3
2	2-E	68	GLY	3.3
2	1-F	448	GLU	3.3
2	2-F	448	GLU	3.3
2	1-E	246	GLN	3.3
2	2-E	246	GLN	3.3
4	1-H	33	TYR	3.3
4	2-H	33	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
2	1-E	418	PHE	3.2
2	2-E	418	PHE	3.2
4	1-H	22	PHE	3.2
4	2-H	22	PHE	3.2
2	1-D	471	ASP	3.2
2	2-D	471	ASP	3.2
1	1-B	387	ALA	3.2
1	2-B	387	ALA	3.2
2	1-F	445	LEU	3.2
2	2-F	445	LEU	3.2
2	1-F	467	VAL	3.2
2	2-F	467	VAL	3.2
2	1-E	36	LEU	3.2
2	2-E	36	LEU	3.2
2	1-F	343	GLY	3.2
2	2-F	343	GLY	3.2
2	1-D	203	SER	3.2
2	2-D	203	SER	3.2
2	1-E	378	LEU	3.2
2	2-E	378	LEU	3.2
4	1-H	18	ALA	3.1
4	2-H	18	ALA	3.1
4	1-H	40	GLU	3.1
4	2-H	40	GLU	3.1
2	1-D	109	LYS	3.1
2	2-D	109	LYS	3.1
1	2-B	405	GLN	3.1
4	1-H	5	GLY	3.1
4	2-H	5	GLY	3.1
1	1-A	487	GLY	3.1
1	2-A	487	GLY	3.1
1	1-A	402	ALA	3.0
1	1-B	89	LYS	3.0
1	2-B	89	LYS	3.0
1	1-C	24	ASP	3.0
1	2-C	24	ASP	3.0
2	1-D	110	THR	3.0
2	2-D	110	THR	3.0
1	1-C	23	VAL	3.0
1	2-C	23	VAL	3.0
2	1-D	177	HIS	3.0
2	1-E	359	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	1-E	471	ASP	3.0
2	2-D	177	HIS	3.0
2	2-E	359	ASP	3.0
2	2-E	471	ASP	3.0
2	1-D	440	GLY	3.0
2	2-D	440	GLY	3.0
3	1-G	87	LYS	3.0
1	1-C	334	VAL	3.0
1	2-C	334	VAL	3.0
2	1-F	389	ALA	3.0
2	2-F	389	ALA	3.0
2	1-F	405	SER	3.0
2	2-F	405	SER	3.0
2	1-F	400	ASP	3.0
2	2-F	400	ASP	3.0
3	2-G	219	GLU	3.0
4	1-H	11	SER	3.0
4	2-H	11	SER	3.0
2	1-E	197	TYR	3.0
2	2-E	197	TYR	3.0
1	1-B	224	ASP	3.0
1	2-B	224	ASP	3.0
2	1-D	132	ILE	3.0
2	2-D	132	ILE	3.0
2	1-F	446	ALA	2.9
2	2-F	446	ALA	2.9
2	1-F	409	LYS	2.9
2	2-F	409	LYS	2.9
1	1-B	414	THR	2.9
1	2-B	414	THR	2.9
2	1-D	250	ASP	2.9
2	2-D	250	ASP	2.9
2	1-E	357	ILE	2.9
2	2-E	357	ILE	2.9
2	1-F	384	LEU	2.9
2	2-F	384	LEU	2.9
3	1-G	230	THR	2.9
3	2-G	230	THR	2.9
1	1-B	87	ILE	2.9
1	2-B	87	ILE	2.9
1	1-B	412	ALA	2.9
1	2-B	412	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-C	454	ASP	2.8
1	2-C	454	ASP	2.8
1	1-B	386	VAL	2.8
1	2-B	386	VAL	2.8
2	1-F	426	GLY	2.8
2	2-F	426	GLY	2.8
3	1-G	85	VAL	2.8
2	1-F	390	ILE	2.8
2	2-F	390	ILE	2.8
2	1-E	245	ASP	2.8
2	2-E	245	ASP	2.8
1	1-C	124	LYS	2.8
1	2-C	124	LYS	2.8
2	1-F	26	ASP	2.8
2	2-F	26	ASP	2.8
2	1-E	402	LEU	2.8
2	2-E	402	LEU	2.8
1	1-C	403	PHE	2.7
2	1-E	29	LEU	2.7
2	2-E	29	LEU	2.7
3	1-G	271	ALA	2.7
3	2-G	271	ALA	2.7
2	1-E	179	GLY	2.7
2	2-E	179	GLY	2.7
1	1-C	509	GLU	2.7
1	2-C	509	GLU	2.7
3	1-G	14	LYS	2.7
3	2-G	14	LYS	2.7
1	1-C	381	ARG	2.7
1	2-C	381	ARG	2.7
2	1-E	242	TYR	2.7
2	2-E	242	TYR	2.7
3	1-G	88	GLN	2.7
2	1-E	106	GLY	2.7
2	2-E	106	GLY	2.7
2	1-E	368	TYR	2.7
2	2-E	368	TYR	2.7
1	1-B	59	LEU	2.7
1	2-B	59	LEU	2.7
2	1-E	466	ALA	2.7
2	2-E	466	ALA	2.7
2	1-E	383	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	2-E	383	SER	2.7
2	1-E	425	THR	2.7
2	2-E	425	THR	2.7
2	1-E	455	GLN	2.7
2	2-E	455	GLN	2.7
2	1-E	200	MET	2.7
2	2-E	200	MET	2.7
2	1-E	400	ASP	2.6
2	2-E	400	ASP	2.6
3	1-G	222	THR	2.6
3	2-G	222	THR	2.6
3	1-G	248	LEU	2.6
3	2-G	248	LEU	2.6
2	1-F	142	LEU	2.6
2	2-F	142	LEU	2.6
2	1-E	437	THR	2.6
2	2-E	437	THR	2.6
2	1-E	376	LYS	2.6
2	1-F	111	LYS	2.6
2	2-E	376	LYS	2.6
2	2-F	111	LYS	2.6
2	1-E	387	ILE	2.6
2	2-E	387	ILE	2.6
1	1-A	296	GLY	2.6
1	1-C	130	GLY	2.6
1	2-A	296	GLY	2.6
1	2-C	130	GLY	2.6
2	1-D	92	GLY	2.6
2	2-D	92	GLY	2.6
1	1-C	123	SER	2.6
1	2-C	123	SER	2.6
2	1-E	198	HIS	2.6
2	2-E	198	HIS	2.6
3	1-G	84	SER	2.6
1	2-B	409	ASP	2.6
2	1-D	10	THR	2.5
2	2-D	10	THR	2.5
1	1-C	103	LEU	2.5
1	2-C	103	LEU	2.5
2	1-E	380	ASP	2.5
2	2-E	380	ASP	2.5
2	1-D	470	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	2-D	470	ALA	2.5
2	1-D	384	LEU	2.5
2	2-D	384	LEU	2.5
2	1-E	393	MET	2.5
2	2-E	393	MET	2.5
2	1-E	395	GLU	2.5
2	2-E	395	GLU	2.5
2	1-F	427	HIS	2.5
2	2-F	427	HIS	2.5
1	1-C	395	ALA	2.5
1	2-C	395	ALA	2.5
2	1-E	422	GLU	2.5
2	2-E	422	GLU	2.5
2	1-E	442	GLN	2.5
2	2-E	442	GLN	2.5
2	1-E	349	ASP	2.4
2	2-E	349	ASP	2.4
1	1-A	403	PHE	2.4
1	1-B	448	GLY	2.4
1	2-B	448	GLY	2.4
1	1-A	442	VAL	2.4
1	1-C	47	VAL	2.4
1	2-A	442	VAL	2.4
1	2-C	47	VAL	2.4
2	1-E	26	ASP	2.4
2	2-E	26	ASP	2.4
2	1-D	88	PRO	2.4
2	2-D	88	PRO	2.4
2	1-E	382	LYS	2.4
2	2-E	382	LYS	2.4
2	1-E	375	GLN	2.4
2	2-E	375	GLN	2.4
3	1-G	4	LYS	2.4
3	2-G	4	LYS	2.4
2	1-E	379	GLN	2.3
2	2-E	379	GLN	2.3
2	1-D	438	ILE	2.3
2	2-D	438	ILE	2.3
1	1-B	53	VAL	2.3
1	2-B	53	VAL	2.3
1	1-B	486	ASP	2.3
1	2-B	486	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	1-E	337	ARG	2.3
2	2-E	337	ARG	2.3
2	1-D	403	THR	2.3
2	2-D	403	THR	2.3
2	1-E	301	LYS	2.3
2	2-E	301	LYS	2.3
2	1-E	391	LEU	2.3
2	2-E	391	LEU	2.3
1	1-B	25	LEU	2.3
1	2-B	25	LEU	2.3
1	1-A	46	ASN	2.3
1	2-A	46	ASN	2.3
1	1-A	47	VAL	2.3
1	2-A	47	VAL	2.3
1	1-B	479	LEU	2.3
1	2-B	479	LEU	2.3
2	1-E	381	TYR	2.3
2	2-E	381	TYR	2.3
4	1-H	21	ALA	2.3
4	2-H	21	ALA	2.3
1	1-C	416	GLN	2.3
1	2-C	416	GLN	2.3
2	1-E	56	SER	2.3
2	2-E	56	SER	2.3
1	1-B	85	GLY	2.3
1	2-B	85	GLY	2.3
2	1-E	10	THR	2.3
2	2-E	10	THR	2.3
1	1-A	410	LEU	2.3
1	1-C	418	LEU	2.3
1	2-A	410	LEU	2.3
1	2-C	418	LEU	2.3
1	1-B	354	THR	2.2
1	2-B	354	THR	2.2
2	1-D	454	GLU	2.2
2	2-D	454	GLU	2.2
3	1-G	24	LYS	2.2
3	2-G	24	LYS	2.2
1	2-B	403	PHE	2.2
1	1-B	30	ARG	2.2
1	2-B	30	ARG	2.2
2	1-F	398	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	2-F	398	GLU	2.2
2	1-E	208	LEU	2.2
2	2-E	208	LEU	2.2
2	1-E	321	ALA	2.2
2	2-E	321	ALA	2.2
2	1-F	403	THR	2.2
2	2-F	403	THR	2.2
1	1-B	227	LYS	2.2
1	2-B	227	LYS	2.2
2	1-E	396	LEU	2.2
2	2-E	396	LEU	2.2
2	1-E	309	ALA	2.2
2	2-E	309	ALA	2.2
2	1-E	401	LYS	2.1
2	2-E	401	LYS	2.1
3	1-G	253	THR	2.1
3	2-G	253	THR	2.1
1	1-B	456	LEU	2.1
1	2-B	456	LEU	2.1
1	1-A	405	GLN	2.1
1	1-C	137	ILE	2.1
1	2-C	137	ILE	2.1
1	1-B	60	LYS	2.1
1	2-B	60	LYS	2.1
2	1-F	25	PHE	2.1
2	2-F	25	PHE	2.1
4	1-H	4	SER	2.1
4	2-H	4	SER	2.1
2	1-D	327	ALA	2.1
2	1-E	474	ALA	2.1
2	2-D	327	ALA	2.1
2	2-E	474	ALA	2.1
1	1-B	287	ARG	2.1
1	2-B	287	ARG	2.1
2	1-F	361	ASN	2.1
2	2-F	361	ASN	2.1
1	1-A	418	LEU	2.1
1	2-A	418	LEU	2.1
2	1-E	371	ALA	2.1
2	2-E	371	ALA	2.1
2	1-E	257	ASN	2.1
2	2-E	257	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-C	502	THR	2.1
1	2-C	502	THR	2.1
2	1-E	411	GLN	2.1
2	1-F	352	ASP	2.1
2	2-E	411	GLN	2.1
2	2-F	352	ASP	2.1
3	1-G	25	MET	2.1
3	2-G	25	MET	2.1
2	1-D	396	LEU	2.1
2	1-F	457	PHE	2.1
2	2-D	396	LEU	2.1
2	2-F	457	PHE	2.1
2	1-E	291	THR	2.1
2	2-E	291	THR	2.1
1	1-A	263	HIS	2.0
1	2-A	263	HIS	2.0
1	1-B	382	ALA	2.0
1	2-B	382	ALA	2.0
1	2-B	407	GLY	2.0
1	1-C	318	GLY	2.0
1	2-C	318	GLY	2.0
3	1-G	23	MET	2.0
3	2-G	23	MET	2.0
1	1-B	376	SER	2.0
1	1-B	483	ILE	2.0
1	2-B	376	SER	2.0
1	2-B	483	ILE	2.0
1	1-B	55	PHE	2.0
1	2-B	55	PHE	2.0
3	1-G	221	THR	2.0
3	2-G	221	THR	2.0
2	1-D	25	PHE	2.0
2	2-D	25	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

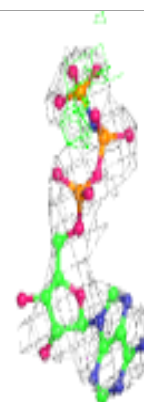
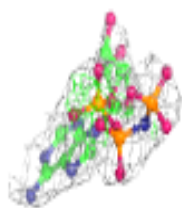
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	2-F	1479	1/1	0.76	0.35	62,62,62,62	1
6	MG	1-F	1479	1/1	0.76	0.35	44,44,44,44	1
5	ANP	2-F	1478	31/31	0.89	0.24	49,69,75,79	31
5	ANP	1-F	1478	31/31	0.89	0.24	33,52,59,61	31
6	MG	1-B	1512	1/1	0.90	0.55	57,57,57,57	1
6	MG	2-B	1512	1/1	0.90	0.55	45,45,45,45	1
6	MG	1-A	1512	1/1	0.92	0.47	39,39,39,39	1
6	MG	2-A	1512	1/1	0.92	0.47	41,41,41,41	1
6	MG	1-C	1512	1/1	0.94	0.42	46,46,46,46	1
6	MG	2-C	1512	1/1	0.94	0.42	44,44,44,44	1
5	ANP	1-C	1511	31/31	0.95	0.20	29,44,58,62	31
5	ANP	2-A	1511	31/31	0.95	0.19	40,59,70,76	31
5	ANP	2-C	1511	31/31	0.95	0.20	36,64,75,78	31
5	ANP	1-A	1511	31/31	0.95	0.19	39,57,65,70	31
6	MG	1-D	1479	1/1	0.96	0.39	60,60,60,60	1
6	MG	2-D	1479	1/1	0.96	0.39	47,47,47,47	1
5	ANP	1-D	1478	31/31	0.97	0.18	40,54,62,62	31
5	ANP	2-B	1511	31/31	0.97	0.16	40,54,61,67	31
5	ANP	2-D	1478	31/31	0.97	0.18	39,48,56,58	31
5	ANP	1-B	1511	31/31	0.97	0.16	41,68,80,81	31

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ANP F 1478:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP C 1511:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

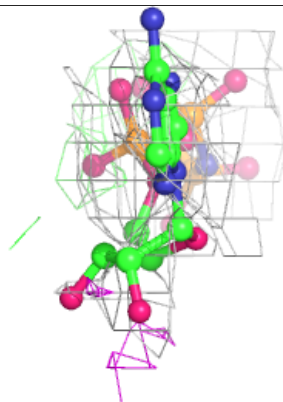
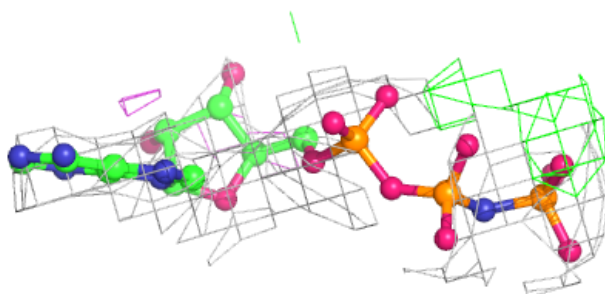
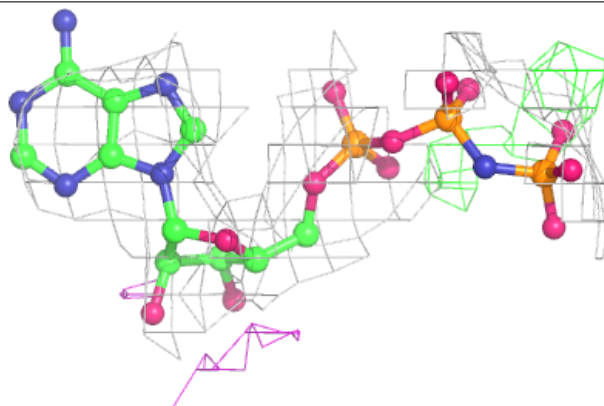


**Electron density around ANP A 1511:**

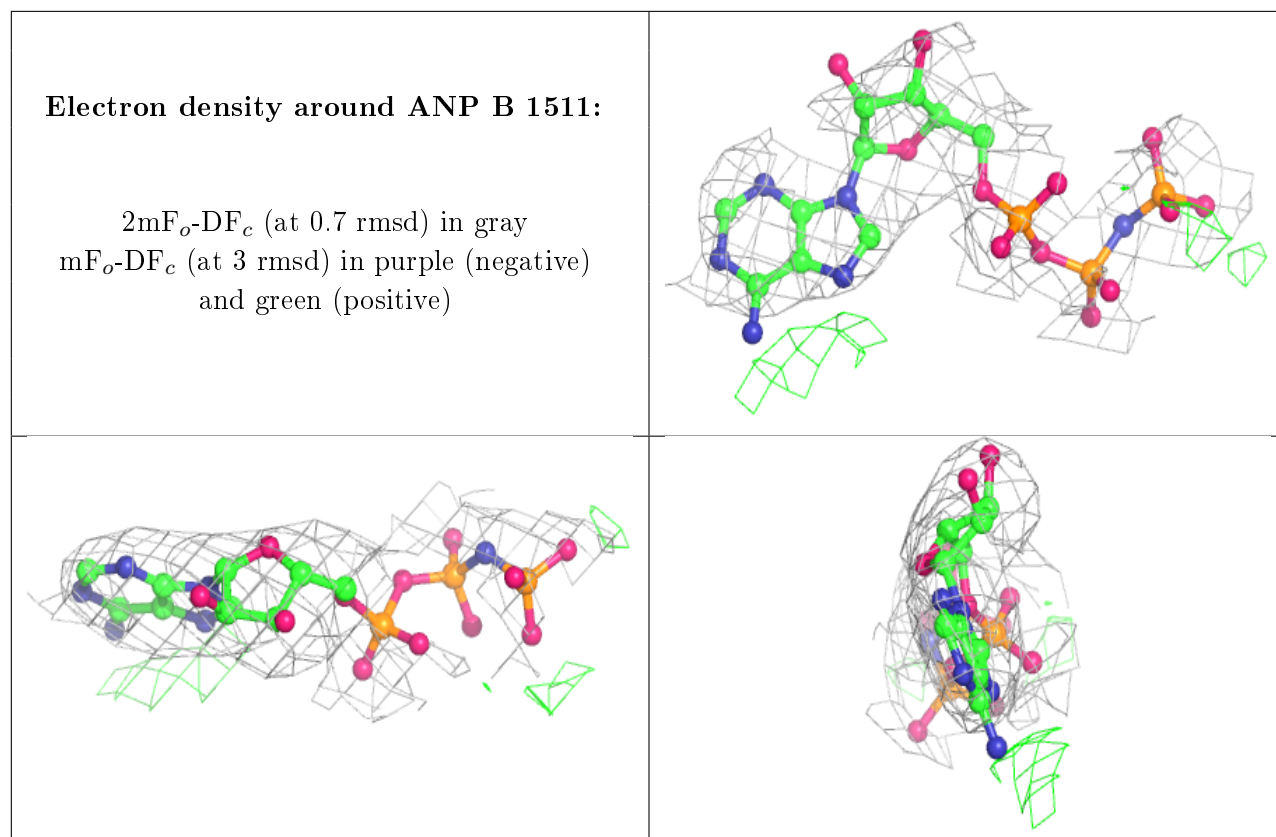
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP D 1478:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.