



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 01:32 AM EDT

PDB ID : 2NYM
Title : Crystal Structure of Protein Phosphatase 2A (PP2A) with C-terminus truncated catalytic subunit
Authors : Chen, Y.; Xing, Y.; Xu, Y.; Chao, Y.; Lin, Z.; Jeffrey, P.D.; Shi, Y.
Deposited on : unknown
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

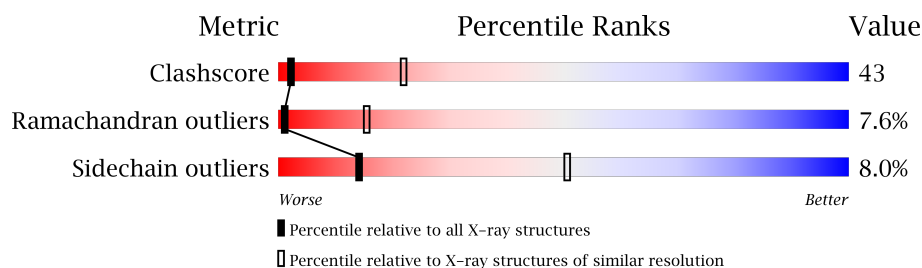
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)


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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	<div> <div></div> <div>37% 54% 7% .</div> </div>
1	D	582	<div> <div></div> <div>42% 49% 8% .</div> </div>
2	B	388	<div> <div></div> <div>32% 54% 12% .</div> </div>
2	E	388	<div> <div></div> <div>29% 57% 13% .</div> </div>
3	C	293	<div> <div></div> <div>39% 53% 8%</div> </div>
3	F	293	<div> <div></div> <div>42% 50% 8%</div> </div>
4	G	7	<div> <div></div> <div>86% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	H	7	 57% 43%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20212 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 Protein phosphatase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	Se	0	0	0
			4535	2881	764	863	14	13			
1	D	582	Total	C	N	O	S	Se	0	0	0
			4535	2881	764	863	14	13			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	Se	0	0	0
			3131	2043	513	561	3	11			
2	E	388	Total	C	N	O	S	Se	0	0	0
			3131	2043	513	561	3	11			

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	293	Total	C	N	O	S	0	0	0
			2367	1497	405	450	15			
3	F	293	Total	C	N	O	S	0	0	0
			2367	1497	405	450	15			

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	0	0	0
			71	49	10	12			
4	H	7	Total	C	N	O	0	0	0
			71	49	10	12			

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

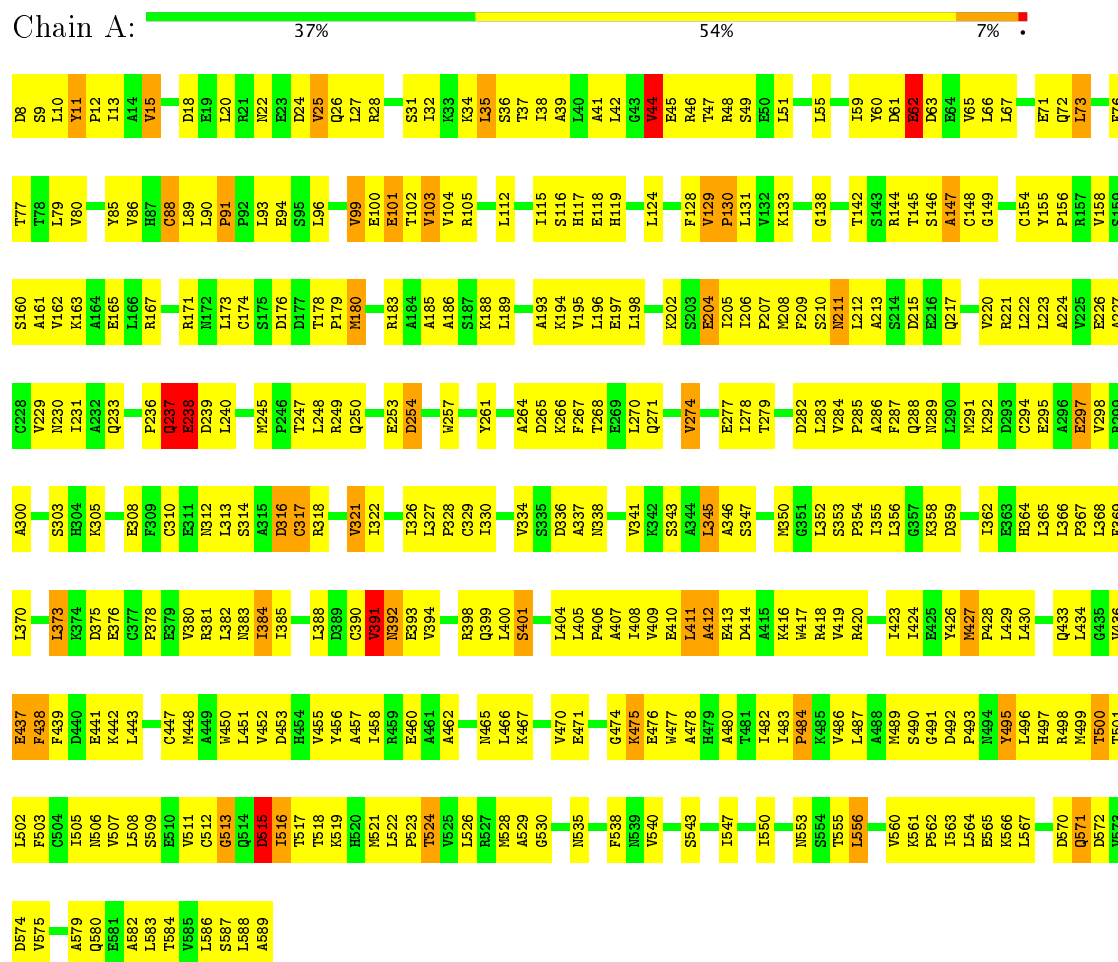
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total 2	Mn 2	0	0
5	F	2	Total 2	Mn 2	0	0

3 Residue-property plots

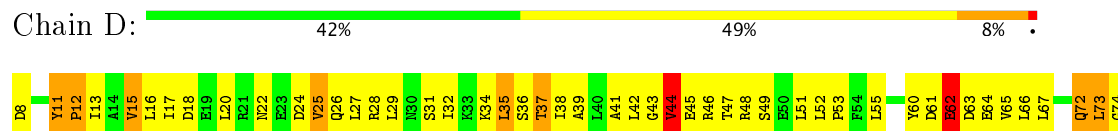
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

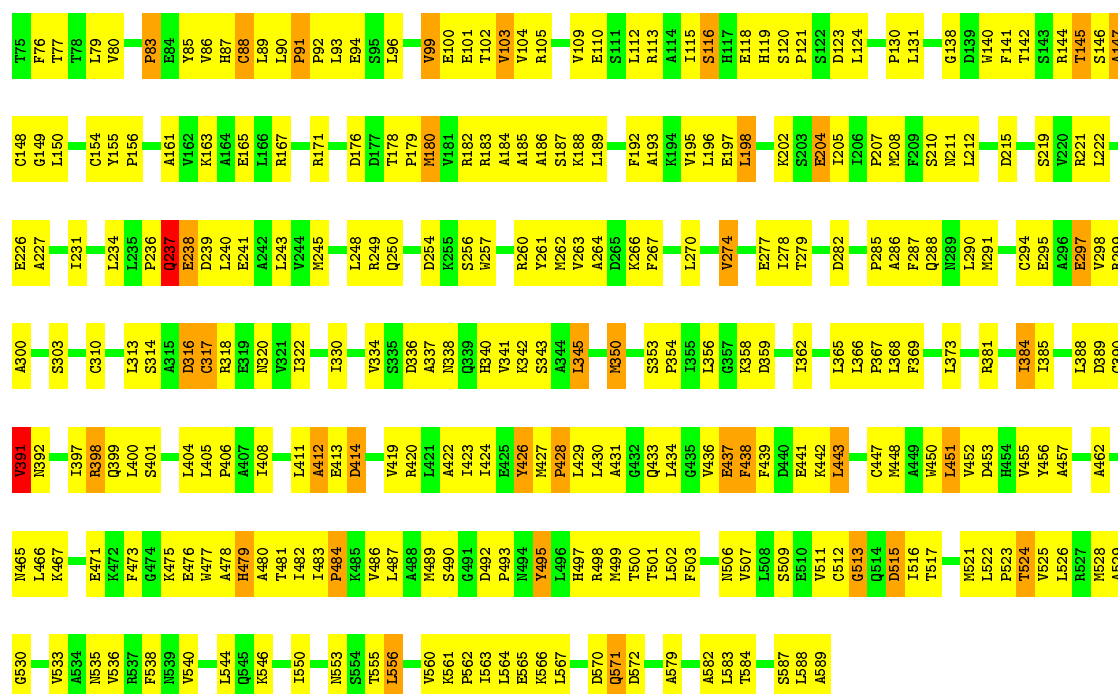
Note EDS was not executed.

• Molecule 1: Protein phosphatase 2



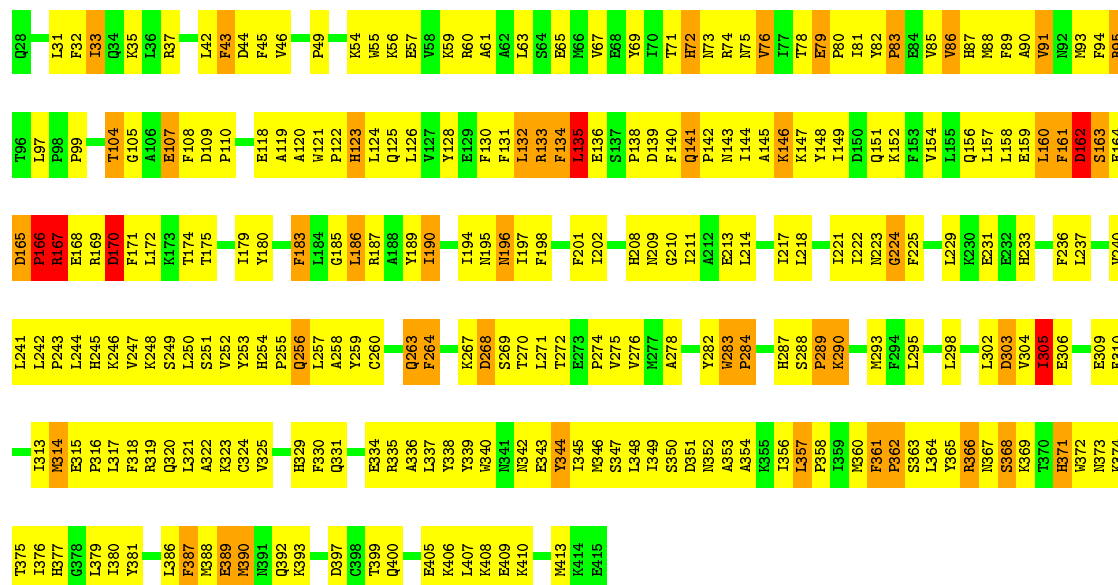
• Molecule 1: Protein phosphatase 2





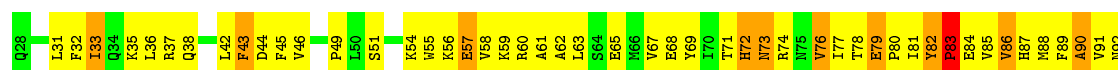
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

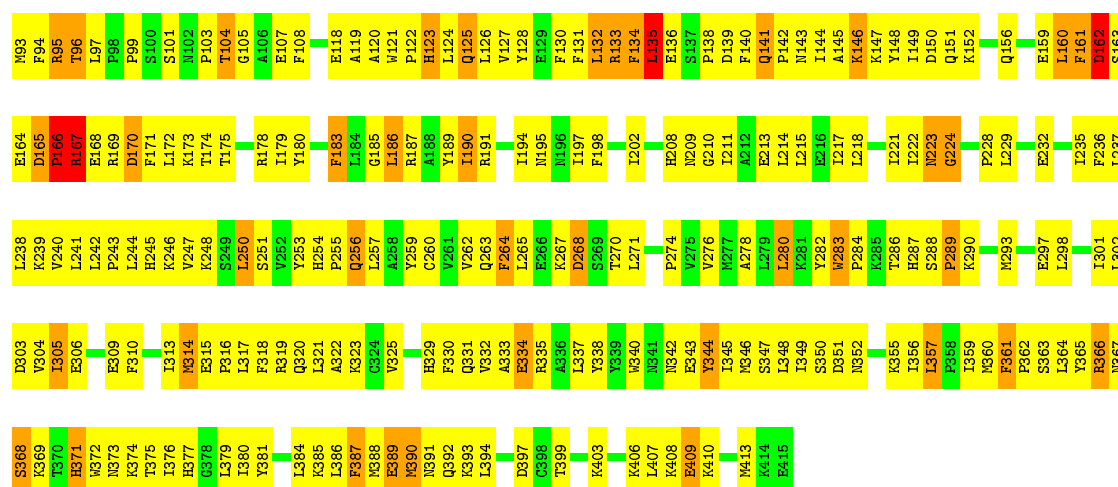
Chain B: 32% 54% 12%



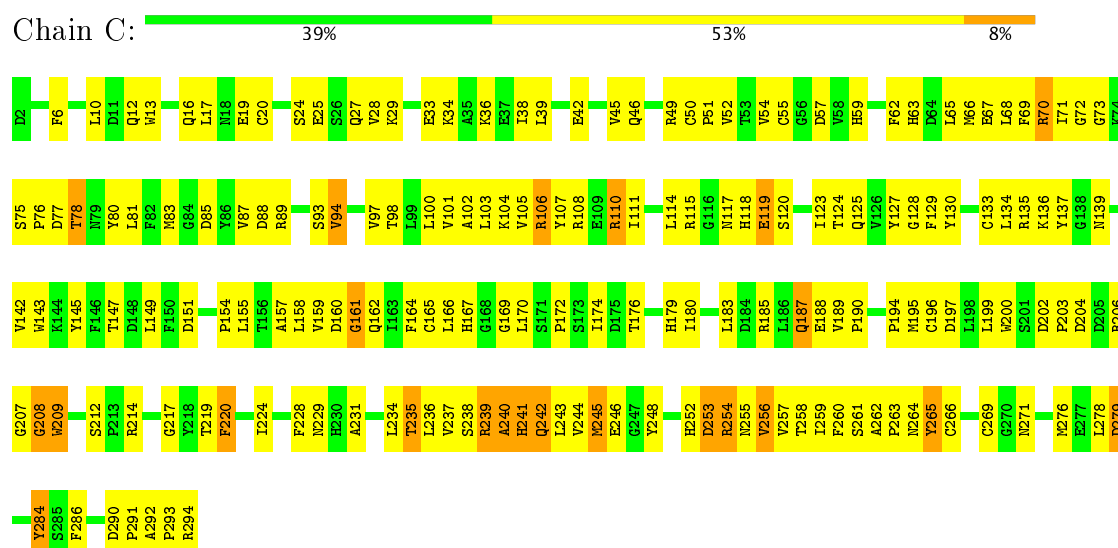
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

Chain E: 29% 57% 13%

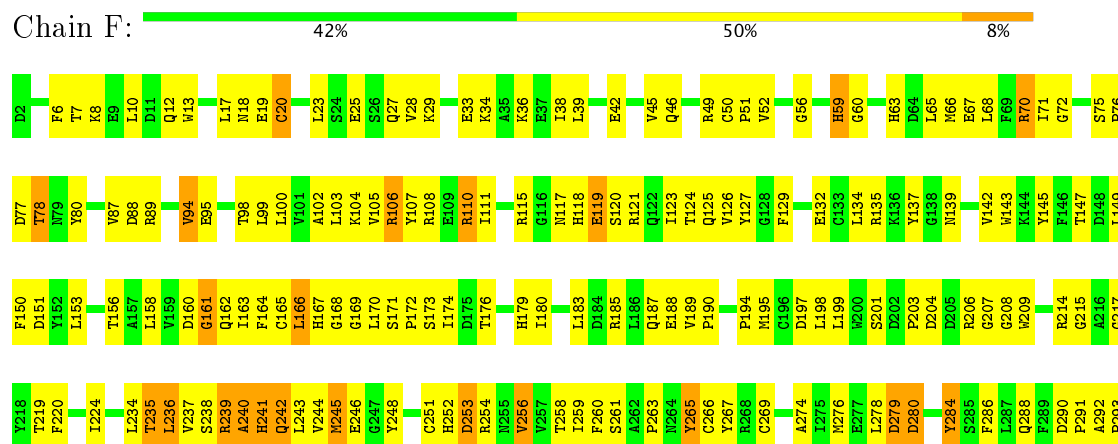




• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform




• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



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- Molecule 4: microcystin LR

Chain G:  86% 14%



41 75 76 77

- Molecule 4: microcystin LR

Chain H:  57% 43%



41 42 75 76 77

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.17Å 158.86Å 270.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.60	Depositor
% Data completeness (in resolution range)	97.4 (100.00-3.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20212	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACB, DAL, DAM, MN, 1ZN, FGA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/4596	0.69	0/6218
1	D	0.58	1/4596 (0.0%)	0.75	0/6218
2	B	0.47	0/3202	0.70	3/4326 (0.1%)
2	E	0.53	0/3202	0.74	5/4326 (0.1%)
3	C	0.45	0/2424	0.71	1/3285 (0.0%)
3	F	0.50	0/2424	0.72	1/3285 (0.0%)
4	G	0.34	0/17	0.88	0/19
4	H	0.42	0/17	0.88	0/19
All	All	0.51	1/20478 (0.0%)	0.72	10/27696 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	154	CYS	CB-SG	-5.13	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	ASP	N-CA-C	7.87	132.25	111.00
2	E	162	ASP	N-CA-C	7.41	131.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	163	SER	N-CA-C	6.42	128.34	111.00
2	E	162	ASP	C-N-CA	-5.82	107.16	121.70
3	C	128	GLY	N-CA-C	5.52	126.90	113.10
2	B	49	PRO	N-CA-CB	5.52	109.92	103.30
2	E	280	LEU	CA-CB-CG	-5.37	102.95	115.30
2	E	49	PRO	N-CA-CB	5.35	109.72	103.30
3	F	168	GLY	N-CA-C	5.12	125.90	113.10
2	B	163	SER	N-CA-C	5.07	124.69	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	426	TYR	Sidechain
2	E	82	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4535	0	4637	389	0
1	D	4535	0	4637	351	0
2	B	3131	0	3050	305	0
2	E	3131	0	3050	311	0
3	C	2367	0	2268	196	0
3	F	2367	0	2268	198	0
4	G	71	0	68	2	0
4	H	71	0	68	2	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20212	0	20046	1722	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 43.

All (1722) 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)
3:F:237:VAL:HB	3:F:256:VAL:HG23	1.30	1.14
1:D:350:MSE:HE1	1:D:391:VAL:HG13	1.32	1.12
2:E:325:VAL:HG13	2:E:337:LEU:HD11	1.32	1.09
2:B:325:VAL:HG13	2:B:337:LEU:HD11	1.35	1.03
1:A:278:ILE:HD12	1:A:278:ILE:H	1.22	1.03
1:D:278:ILE:HD12	1:D:278:ILE:H	1.23	0.99
2:B:388:MSE:HE2	2:B:392:GLN:HE22	1.27	0.96
3:C:237:VAL:HB	3:C:256:VAL:HG23	1.48	0.96
2:B:190:ILE:O	2:B:194:ILE:HG13	1.64	0.96
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.01	0.95
1:A:526:LEU:HD22	1:A:563:ILE:HG21	1.49	0.94
3:C:209:TRP:H	3:C:224:ILE:HD11	1.31	0.94
3:F:209:TRP:H	3:F:224:ILE:HD11	1.34	0.92
1:A:180:MSE:HE2	1:A:183:ARG:HH22	1.32	0.92
2:E:165:ASP:O	2:E:167:ARG:N	2.03	0.92
3:C:70:ARG:HG3	3:C:70:ARG:HH11	1.34	0.91
2:E:43:PHE:O	2:E:45:PHE:N	2.04	0.91
1:A:428:PRO:HD3	1:A:465:ASN:HD21	1.36	0.90
2:B:118:GLU:H	2:B:164:GLU:HG2	1.34	0.90
1:D:22:ASN:ND2	1:D:27:LEU:HD12	1.89	0.88
1:D:350:MSE:HE1	1:D:391:VAL:CG1	2.02	0.88
2:E:164:GLU:O	2:E:165:ASP:O	1.91	0.88
2:B:93:MSE:HA	2:B:93:MSE:HE3	1.54	0.88
2:B:288:SER:HB2	2:B:289:PRO:HD3	1.55	0.87
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.05	0.87
1:D:490:SER:HB2	1:D:528:MSE:HE3	1.56	0.87
1:A:571:GLN:HE22	3:C:49:ARG:HH22	1.23	0.86
1:A:102:THR:HG22	1:A:105:ARG:NH2	1.89	0.86
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.57	0.86
1:A:388:LEU:HD13	1:A:408:ILE:HD11	1.57	0.86
1:D:20:LEU:HD23	1:D:31:SER:HB3	1.58	0.86
1:D:427:MSE:HA	1:D:427:MSE:HE3	1.58	0.86
1:A:300:ALA:HB2	1:A:341:VAL:HG22	1.57	0.86
1:D:20:LEU:HD23	1:D:31:SER:CB	2.05	0.85
3:F:28:VAL:HG11	3:F:142:VAL:HG13	1.55	0.85
2:B:80:PRO:HG2	2:B:82:TYR:CE2	2.12	0.85
3:C:209:TRP:N	3:C:224:ILE:HD11	1.89	0.85
2:E:313:ILE:O	2:E:316:PRO:HD2	1.76	0.85
1:A:227:ALA:O	1:A:231:ILE:HG13	1.76	0.85
3:C:13:TRP:HE1	3:C:27:GLN:HE21	1.23	0.85
1:D:35:LEU:HD21	1:D:55:LEU:HD11	1.58	0.85
1:D:25:VAL:HG22	1:D:28:ARG:NH2	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.12	0.84
1:A:385:ILE:HD11	1:A:411:LEU:HG	1.56	0.84
2:E:167:ARG:HH11	2:E:167:ARG:CB	1.90	0.84
1:A:564:LEU:HD22	1:A:583:LEU:HD21	1.57	0.83
1:A:38:ILE:O	1:A:42:LEU:HB2	1.78	0.83
1:D:350:MSE:CE	1:D:391:VAL:HG13	2.08	0.83
1:D:526:LEU:HD22	1:D:563:ILE:HG21	1.61	0.83
1:A:427:MSE:HA	1:A:427:MSE:HE3	1.58	0.83
2:B:340:TRP:HA	2:B:346:MSE:HE3	1.59	0.82
3:F:209:TRP:N	3:F:224:ILE:HD11	1.94	0.82
1:D:452:VAL:O	1:D:452:VAL:HG12	1.79	0.82
3:F:244:VAL:HG23	3:F:244:VAL:O	1.80	0.82
3:C:170:LEU:H	3:C:220:PHE:HE2	1.23	0.82
2:B:165:ASP:O	2:B:167:ARG:N	2.13	0.81
2:B:43:PHE:O	2:B:45:PHE:N	2.12	0.81
3:F:251:CYS:SG	3:F:256:VAL:HG12	2.20	0.81
1:A:35:LEU:HB3	1:A:72:GLN:HG2	1.63	0.81
2:E:202:ILE:HD11	2:E:244:LEU:HG	1.63	0.81
1:A:492:ASP:OD2	1:A:493:PRO:HD2	1.79	0.81
3:C:162:GLN:HB3	3:C:235:THR:CG2	2.11	0.81
3:C:203:PRO:HA	3:C:220:PHE:CE1	2.16	0.80
3:F:197:ASP:OD1	3:F:217:GLY:HA2	1.80	0.80
3:C:123:ILE:HG23	3:C:127:TYR:HD2	1.46	0.80
1:A:564:LEU:HD22	1:A:583:LEU:CD2	2.10	0.80
2:E:288:SER:HB2	2:E:289:PRO:HD3	1.64	0.80
2:E:388:MSE:HE2	2:E:392:GLN:HE22	1.46	0.80
1:A:270:LEU:O	1:A:274:VAL:HG23	1.81	0.80
2:E:80:PRO:HG2	2:E:82:TYR:CD2	2.16	0.80
3:C:13:TRP:HE1	3:C:27:GLN:NE2	1.80	0.80
1:D:77:THR:HG21	1:D:118:GLU:HG3	1.65	0.80
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.65	0.79
1:A:385:ILE:HD12	1:A:423:ILE:HD11	1.64	0.79
1:D:171:ARG:HH21	1:D:204:GLU:CG	1.96	0.79
1:A:364:HIS:O	1:A:367:PRO:HD2	1.83	0.79
3:C:166:LEU:HD23	3:C:239:ARG:HB3	1.64	0.79
1:D:149:GLY:HA2	1:D:188:LYS:HD2	1.63	0.78
1:D:278:ILE:CD1	1:D:278:ILE:H	1.95	0.78
3:F:214:ARG:HH11	3:F:214:ARG:HG2	1.48	0.78
1:D:270:LEU:O	1:D:274:VAL:HG23	1.84	0.78
1:D:390:CYS:O	1:D:392:ASN:N	2.16	0.78
1:A:310:CYS:HA	1:A:313:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:340:TRP:HA	2:E:346:MSE:HE3	1.65	0.78
3:F:276:MET:HB2	3:F:286:PHE:CE1	2.19	0.78
1:D:429:LEU:O	1:D:433:GLN:HG3	1.83	0.78
1:D:561:LYS:HB3	1:D:562:PRO:HD3	1.66	0.77
2:E:186:LEU:HB3	2:E:190:ILE:HD13	1.64	0.77
2:E:164:GLU:O	2:E:165:ASP:C	2.22	0.77
2:E:149:ILE:HG22	2:E:149:ILE:O	1.82	0.77
2:E:128:TYR:HB3	2:E:171:PHE:CD2	2.20	0.77
2:B:160:LEU:O	2:B:162:ASP:N	2.18	0.77
2:B:157:LEU:HA	2:B:160:LEU:HD12	1.67	0.76
3:F:165:CYS:HA	3:F:238:SER:O	1.84	0.76
2:B:80:PRO:HG2	2:B:82:TYR:CD2	2.21	0.76
3:C:68:LEU:HD23	3:C:68:LEU:C	2.06	0.76
1:A:25:VAL:HG22	1:A:28:ARG:NH2	2.00	0.76
3:F:162:GLN:HB3	3:F:235:THR:CG2	2.15	0.76
3:F:6:PHE:HE2	3:F:34:LYS:HG3	1.49	0.76
2:E:218:LEU:HD23	2:E:221:ILE:HD12	1.67	0.76
1:A:205:ILE:HA	1:A:208:MSE:HE3	1.66	0.76
1:D:145:THR:HG22	1:D:146:SER:N	2.01	0.76
1:A:490:SER:HB2	1:A:528:MSE:HE3	1.69	0.75
1:A:48:ARG:HD3	1:A:80:VAL:O	1.86	0.75
1:A:347:SER:HB3	1:A:383:ASN:HD22	1.51	0.75
3:C:120:SER:O	3:C:124:THR:HG23	1.87	0.75
1:D:278:ILE:N	1:D:278:ILE:HD12	2.00	0.75
1:D:561:LYS:O	1:D:565:GLU:HG2	1.85	0.75
2:B:388:MSE:HE2	2:B:392:GLN:NE2	2.00	0.75
2:B:121:TRP:N	2:B:122:PRO:HD2	2.02	0.75
1:A:358:LYS:O	1:A:362:ILE:HG13	1.86	0.74
1:D:90:LEU:HB2	1:D:91:PRO:HD3	1.67	0.74
2:B:164:GLU:O	2:B:165:ASP:O	2.04	0.74
2:E:167:ARG:HB3	2:E:167:ARG:HH11	1.51	0.74
1:A:382:LEU:HD13	1:A:419:VAL:HG22	1.69	0.74
2:E:373:ASN:O	2:E:375:THR:N	2.20	0.74
2:E:128:TYR:HB3	2:E:171:PHE:HD2	1.53	0.74
1:D:38:ILE:O	1:D:42:LEU:HB2	1.88	0.74
1:A:467:LYS:O	1:A:471:GLU:HG3	1.88	0.74
2:E:318:PHE:HD2	2:E:360:MSE:HE2	1.52	0.74
2:B:305:ILE:HD13	2:B:306:GLU:H	1.52	0.74
1:A:564:LEU:O	1:A:564:LEU:HD23	1.87	0.73
3:F:204:ASP:OD2	3:F:206:ARG:HG2	1.86	0.73
2:B:186:LEU:HB3	2:B:190:ILE:HD13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:THR:C	2:B:80:PRO:HD2	2.07	0.73
1:D:492:ASP:OD2	1:D:493:PRO:HD2	1.88	0.73
3:F:239:ARG:HH12	3:F:242:GLN:CG	1.99	0.73
3:C:197:ASP:OD1	3:C:217:GLY:HA2	1.88	0.73
2:E:325:VAL:HG22	2:E:337:LEU:HD12	1.68	0.73
3:C:70:ARG:NH1	3:C:70:ARG:HG3	1.99	0.73
1:A:288:GLN:HA	1:A:291:MSE:HE3	1.71	0.73
3:F:89:ARG:HD2	3:F:266:CYS:SG	2.28	0.73
3:F:203:PRO:HA	3:F:220:PHE:CE1	2.23	0.73
3:F:137:TYR:CD2	3:F:142:VAL:HG21	2.24	0.72
1:A:163:LYS:O	1:A:167:ARG:HG3	1.90	0.72
2:E:349:ILE:HG23	2:E:356:ILE:HG21	1.71	0.72
1:A:237:GLN:O	1:A:240:LEU:HB2	1.89	0.72
3:C:203:PRO:HD2	3:C:242:GLN:OE1	1.89	0.72
3:C:6:PHE:HE2	3:C:34:LYS:HG3	1.53	0.72
1:A:22:ASN:ND2	1:A:27:LEU:HD12	2.05	0.72
1:A:452:VAL:O	1:A:452:VAL:HG12	1.90	0.72
2:E:286:THR:HG22	3:F:134:LEU:HB3	1.72	0.72
1:A:35:LEU:HD11	1:A:51:LEU:HD11	1.72	0.72
2:B:313:ILE:O	2:B:316:PRO:HD2	1.88	0.72
1:D:197:GLU:CD	1:D:197:GLU:H	1.93	0.72
1:A:401:SER:HB3	1:A:434:LEU:HD21	1.72	0.71
2:E:169:ARG:HB3	2:E:213:GLU:HG2	1.72	0.71
3:F:237:VAL:HB	3:F:256:VAL:CG2	2.14	0.71
1:A:274:VAL:HG12	1:A:278:ILE:HB	1.72	0.71
3:C:239:ARG:HH12	3:C:242:GLN:CG	2.02	0.71
1:A:428:PRO:HD3	1:A:465:ASN:ND2	2.06	0.71
3:C:240:ALA:HA	3:C:258:THR:HG23	1.72	0.71
1:A:35:LEU:HD21	1:A:55:LEU:HD11	1.72	0.71
3:C:54:VAL:HG22	3:C:81:LEU:HD22	1.71	0.71
3:F:80:TYR:HB2	3:F:111:ILE:HG22	1.71	0.71
1:A:100:GLU:O	1:A:105:ARG:NH1	2.23	0.71
1:D:310:CYS:HA	1:D:313:LEU:HD12	1.73	0.71
2:E:88:MSE:HE2	2:E:92:ASN:ND2	2.06	0.71
3:F:124:THR:HB	3:F:129:PHE:HB3	1.72	0.71
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.73	0.71
2:B:157:LEU:O	2:B:160:LEU:HB2	1.91	0.70
2:E:237:LEU:HD13	2:E:264:PHE:CD2	2.26	0.70
3:F:174:ILE:HD13	3:F:180:ILE:HG12	1.73	0.70
3:F:194:PRO:HG2	3:F:195:MET:H	1.55	0.70
2:B:325:VAL:CG1	2:B:337:LEU:HD11	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:THR:HG22	1:D:105:ARG:NH2	2.06	0.70
1:A:278:ILE:HD12	1:A:278:ILE:N	2.04	0.70
1:A:76:PHE:HB2	1:A:89:LEU:HD21	1.74	0.70
2:E:318:PHE:CD2	2:E:360:MSE:HE2	2.27	0.70
1:A:261:TYR:HA	1:A:298:VAL:HG22	1.72	0.70
1:A:278:ILE:CD1	1:A:278:ILE:H	2.01	0.70
1:A:381:ARG:HH12	1:A:414:ASP:CG	1.94	0.70
2:B:318:PHE:CD2	2:B:360:MSE:HE2	2.27	0.70
2:E:373:ASN:ND2	2:E:376:ILE:HG23	2.05	0.70
3:F:183:LEU:HD21	3:F:194:PRO:HG3	1.74	0.70
3:C:244:VAL:O	3:C:244:VAL:HG23	1.91	0.70
1:A:452:VAL:HG13	1:A:497:HIS:CD2	2.27	0.70
3:C:166:LEU:CD2	3:C:239:ARG:HB3	2.22	0.70
2:E:93:MSE:HE3	2:E:93:MSE:HA	1.71	0.70
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.74	0.69
1:D:401:SER:HB3	1:D:434:LEU:HD21	1.74	0.69
2:E:118:GLU:H	2:E:164:GLU:HG2	1.57	0.69
1:D:453:ASP:OD1	1:D:455:VAL:HG12	1.92	0.69
2:E:165:ASP:O	2:E:166:PRO:C	2.31	0.69
2:E:237:LEU:HD13	2:E:264:PHE:CG	2.27	0.69
3:C:204:ASP:HB2	3:C:219:THR:HB	1.75	0.69
1:D:115:ILE:O	1:D:119:HIS:CD2	2.46	0.69
2:B:132:LEU:C	2:B:134:PHE:H	1.96	0.69
3:C:42:GLU:HB3	3:C:46:GLN:OE1	1.92	0.69
1:D:205:ILE:HA	1:D:208:MSE:HE3	1.73	0.69
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.23	0.69
3:C:89:ARG:HD2	3:C:266:CYS:SG	2.32	0.69
1:D:227:ALA:O	1:D:231:ILE:HG13	1.93	0.69
2:E:406:LYS:O	2:E:406:LYS:HD3	1.93	0.69
1:A:44:VAL:HG22	1:A:45:GLU:N	2.06	0.69
1:A:571:GLN:HE22	3:C:49:ARG:NH2	1.88	0.69
1:D:100:GLU:O	1:D:105:ARG:NH1	2.26	0.69
1:D:366:LEU:HB3	1:D:367:PRO:HD3	1.75	0.69
1:D:44:VAL:HG22	1:D:45:GLU:N	2.08	0.69
1:D:452:VAL:HG13	1:D:497:HIS:CD2	2.27	0.68
3:F:115:ARG:NH1	3:F:151:ASP:HA	2.08	0.68
1:A:180:MSE:HE2	1:A:183:ARG:NH2	2.08	0.68
2:E:121:TRP:N	2:E:122:PRO:HD2	2.08	0.68
1:A:390:CYS:O	1:A:392:ASN:N	2.25	0.68
2:B:164:GLU:O	2:B:165:ASP:C	2.30	0.68
2:E:72:HIS:O	2:E:74:ARG:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ARG:HH11	2:B:167:ARG:CB	2.07	0.68
1:D:455:VAL:HG23	3:F:71:ILE:HG13	1.74	0.68
1:D:274:VAL:HG12	1:D:278:ILE:HB	1.76	0.68
1:D:385:ILE:HD12	1:D:423:ILE:HD11	1.76	0.68
1:A:179:PRO:HB2	1:A:180:MSE:HE3	1.76	0.68
1:A:25:VAL:HG22	1:A:28:ARG:HH21	1.58	0.68
2:E:78:THR:C	2:E:80:PRO:HD2	2.14	0.68
1:A:112:LEU:O	1:A:116:SER:HB3	1.94	0.68
1:D:113:ARG:O	1:D:116:SER:HB3	1.94	0.68
1:A:178:THR:HB	1:A:180:MSE:HG2	1.75	0.67
3:C:204:ASP:OD2	3:C:206:ARG:HG2	1.94	0.67
2:E:43:PHE:C	2:E:45:PHE:H	1.98	0.67
2:B:218:LEU:O	2:B:222:ILE:HG13	1.95	0.67
2:E:80:PRO:HG2	2:E:82:TYR:HD2	1.57	0.67
2:B:118:GLU:H	2:B:164:GLU:CG	2.06	0.67
2:B:121:TRP:H	2:B:122:PRO:HD2	1.57	0.67
1:D:161:ALA:O	1:D:165:GLU:HG3	1.95	0.67
2:E:325:VAL:HG22	2:E:337:LEU:CD1	2.24	0.67
3:F:240:ALA:HA	3:F:258:THR:HG23	1.76	0.67
3:C:10:LEU:HD11	3:C:105:VAL:HG12	1.77	0.67
1:D:20:LEU:HD23	1:D:31:SER:HB2	1.76	0.67
2:E:132:LEU:C	2:E:134:PHE:H	1.97	0.67
2:B:251:SER:HA	2:B:293:MSE:HE1	1.77	0.67
1:D:144:ARG:HH21	1:D:176:ASP:CG	1.98	0.67
2:B:276:VAL:HG11	2:B:313:ILE:HG21	1.77	0.67
2:B:284:PRO:HG2	2:B:290:LYS:HB3	1.77	0.67
3:C:104:LYS:N	3:C:111:ILE:HD11	2.09	0.67
2:E:166:PRO:O	2:E:169:ARG:N	2.28	0.67
1:D:506:ASN:HB3	1:D:546:LYS:HG2	1.77	0.66
2:E:325:VAL:CG1	2:E:337:LEU:HD11	2.18	0.66
2:E:340:TRP:HH2	2:E:360:MSE:HE3	1.59	0.66
3:F:204:ASP:HB2	3:F:219:THR:HB	1.77	0.66
2:B:164:GLU:HB3	2:B:168:GLU:HB3	1.76	0.66
1:D:171:ARG:HH21	1:D:204:GLU:HG3	1.58	0.66
1:D:287:PHE:CD2	1:D:291:MSE:HE2	2.30	0.66
3:F:239:ARG:HH12	3:F:242:GLN:HG2	1.59	0.66
1:A:466:LEU:HD22	1:A:482:ILE:HD13	1.76	0.66
2:B:118:GLU:N	2:B:164:GLU:HG2	2.10	0.66
2:B:237:LEU:HD13	2:B:264:PHE:CG	2.30	0.66
2:B:85:VAL:HG13	2:B:130:PHE:CE2	2.30	0.66
2:E:166:PRO:O	2:E:167:ARG:C	2.32	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:GLN:HB3	3:C:235:THR:HG22	1.78	0.66
2:B:242:LEU:HD13	2:B:278:ALA:CB	2.26	0.66
2:E:83:PRO:HB3	2:E:148:TYR:CD1	2.31	0.66
3:C:236:LEU:HD11	3:C:257:VAL:HG12	1.78	0.66
3:F:162:GLN:HB3	3:F:235:THR:HG21	1.77	0.66
1:A:73:LEU:O	1:A:89:LEU:HD23	1.96	0.66
2:B:218:LEU:HA	2:B:221:ILE:HD12	1.78	0.66
2:B:80:PRO:HG2	2:B:82:TYR:HE2	1.61	0.66
2:E:79:GLU:N	2:E:80:PRO:CD	2.58	0.66
3:F:10:LEU:HD11	3:F:105:VAL:HG12	1.75	0.66
3:F:170:LEU:H	3:F:220:PHE:HE2	1.40	0.66
3:C:117:ASN:ND2	3:C:241:HIS:HE1	1.93	0.66
2:E:242:LEU:N	2:E:243:PRO:HD2	2.11	0.66
2:B:133:ARG:HA	2:B:136:GLU:OE2	1.96	0.65
3:F:143:TRP:CE2	3:F:147:THR:HG21	2.30	0.65
2:B:133:ARG:HA	2:B:136:GLU:HG2	1.78	0.65
2:B:372:TRP:HZ2	3:C:125:GLN:HE22	1.44	0.65
2:B:87:HIS:O	2:B:91:VAL:HG23	1.96	0.65
1:D:189:LEU:HD11	1:D:205:ILE:HG23	1.77	0.65
2:B:310:PHE:CD1	2:B:348:LEU:HD13	2.31	0.65
3:C:276:MET:HB2	3:C:286:PHE:CE1	2.31	0.65
1:D:94:GLU:HG3	1:D:131:LEU:HG	1.76	0.65
2:B:318:PHE:HD2	2:B:360:MSE:HE2	1.61	0.65
2:B:79:GLU:N	2:B:80:PRO:CD	2.59	0.65
2:E:391:ASN:OD1	2:E:394:LEU:HB2	1.96	0.65
2:B:166:PRO:O	2:B:169:ARG:N	2.30	0.65
3:C:13:TRP:NE1	3:C:27:GLN:NE2	2.45	0.65
1:A:211:ASN:HD22	1:A:211:ASN:N	1.94	0.65
1:D:20:LEU:CD2	1:D:31:SER:HB3	2.26	0.65
3:F:166:LEU:HD23	3:F:239:ARG:HB3	1.77	0.65
3:C:194:PRO:HG2	3:C:195:MET:H	1.61	0.65
2:E:208:HIS:CD2	2:E:210:GLY:H	2.15	0.65
1:A:343:SER:HA	1:A:380:VAL:HG22	1.79	0.64
1:D:358:LYS:O	1:D:362:ILE:HG13	1.96	0.64
1:D:564:LEU:HD22	1:D:583:LEU:HD21	1.78	0.64
1:D:66:LEU:HD22	1:D:96:LEU:HD21	1.79	0.64
1:D:448:MSE:HE1	1:D:466:LEU:HD21	1.79	0.64
1:D:79:LEU:H	1:D:79:LEU:HD12	1.62	0.64
2:E:131:PHE:O	2:E:134:PHE:HB3	1.96	0.64
3:F:17:LEU:HD13	3:F:99:LEU:HA	1.79	0.64
1:D:261:TYR:HA	1:D:298:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:CD1	1:A:408:ILE:HD11	2.26	0.64
1:A:452:VAL:HG22	1:A:497:HIS:HD2	1.63	0.64
3:F:244:VAL:O	3:F:246:GLU:N	2.30	0.64
1:A:237:GLN:CD	1:A:278:ILE:HD11	2.18	0.64
1:A:439:PHE:HD1	1:A:443:LEU:HD23	1.63	0.64
2:B:349:ILE:HG23	2:B:356:ILE:HG21	1.78	0.64
2:E:222:ILE:HD13	2:E:264:PHE:HD1	1.61	0.64
2:E:223:ASN:HD22	2:E:263:GLN:HE21	1.44	0.64
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.79	0.64
2:B:373:ASN:O	2:B:375:THR:N	2.31	0.64
2:E:255:PRO:HG2	2:E:256:GLN:NE2	2.12	0.64
2:E:54:LYS:O	2:E:56:LYS:N	2.25	0.64
1:A:179:PRO:HB2	1:A:183:ARG:HH12	1.62	0.64
3:C:55:CYS:SG	3:C:68:LEU:HD11	2.37	0.64
1:D:286:ALA:O	1:D:290:LEU:HD12	1.98	0.64
2:E:208:HIS:HD2	2:E:210:GLY:H	1.44	0.64
1:D:381:ARG:O	1:D:385:ILE:HG12	1.97	0.64
1:A:427:MSE:HB3	1:A:428:PRO:CD	2.28	0.63
1:D:282:ASP:O	1:D:285:PRO:HD2	1.98	0.63
2:B:313:ILE:HD12	2:B:313:ILE:N	2.13	0.63
2:B:302:LEU:HD11	2:B:317:LEU:HD21	1.80	0.63
3:C:34:LYS:O	3:C:38:ILE:HG13	1.96	0.63
2:E:186:LEU:HB3	2:E:190:ILE:CD1	2.27	0.63
1:A:405:LEU:N	1:A:406:PRO:CD	2.62	0.63
2:E:71:THR:HG21	2:E:133:ARG:HH11	1.63	0.63
1:A:347:SER:HB3	1:A:383:ASN:ND2	2.12	0.63
1:A:526:LEU:CD2	1:A:563:ILE:HG21	2.23	0.63
3:F:29:LYS:HB2	3:F:145:TYR:CE1	2.33	0.63
3:C:176:THR:H	3:C:179:HIS:HD2	1.44	0.63
1:D:564:LEU:HD22	1:D:583:LEU:CD2	2.29	0.63
3:F:104:LYS:N	3:F:111:ILE:HD11	2.13	0.63
2:B:43:PHE:C	2:B:45:PHE:H	2.01	0.63
2:E:164:GLU:OE2	2:E:167:ARG:HB2	1.98	0.63
2:B:149:ILE:O	2:B:149:ILE:HG22	1.98	0.63
1:D:424:ILE:HG12	1:D:450:TRP:CE3	2.34	0.63
1:A:261:TYR:CA	1:A:298:VAL:HG22	2.29	0.63
2:B:166:PRO:O	2:B:167:ARG:C	2.36	0.63
2:B:335:ARG:HG3	2:B:335:ARG:HH11	1.64	0.63
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.81	0.62
3:C:162:GLN:HB3	3:C:235:THR:HG21	1.80	0.62
2:E:189:TYR:O	2:E:190:ILE:C	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:PHE:O	2:B:134:PHE:HB3	1.99	0.62
3:C:209:TRP:CZ3	3:C:220:PHE:HB3	2.35	0.62
3:C:220:PHE:HA	3:C:224:ILE:HD12	1.80	0.62
1:D:587:SER:O	1:D:588:LEU:HD23	1.99	0.62
1:A:20:LEU:HD23	1:A:31:SER:CB	2.29	0.62
1:D:564:LEU:HD23	1:D:564:LEU:O	1.99	0.62
2:E:190:ILE:O	2:E:194:ILE:HG13	1.99	0.62
2:E:276:VAL:HG11	2:E:313:ILE:CG2	2.30	0.62
3:F:164:PHE:HB2	3:F:234:LEU:HD13	1.81	0.62
2:B:63:LEU:O	2:B:67:VAL:HG23	1.99	0.62
1:D:571:GLN:HE22	3:F:49:ARG:HH22	1.44	0.62
3:F:65:LEU:O	3:F:68:LEU:HB3	1.99	0.62
2:B:289:PRO:O	2:B:293:MSE:HG3	2.00	0.62
3:C:276:MET:CE	3:C:278:LEU:HD21	2.29	0.62
1:A:388:LEU:C	1:A:390:CYS:N	2.53	0.62
2:B:144:ILE:O	2:B:144:ILE:HG22	2.00	0.62
2:B:268:ASP:OD1	2:B:270:THR:HB	2.00	0.62
3:F:50:CYS:HB2	3:F:51:PRO:HA	1.80	0.62
1:A:20:LEU:HD23	1:A:31:SER:HB3	1.82	0.62
1:D:397:ILE:HG13	1:D:397:ILE:O	1.99	0.62
2:E:223:ASN:ND2	2:E:263:GLN:HE21	1.96	0.62
2:E:409:GLU:O	2:E:413:MSE:HB2	2.00	0.62
2:E:88:MSE:HE2	2:E:92:ASN:HD21	1.63	0.62
2:B:325:VAL:HG22	2:B:337:LEU:CD1	2.30	0.62
2:E:145:ALA:O	2:E:147:LYS:N	2.33	0.62
1:D:345:LEU:O	1:D:345:LEU:HG	2.00	0.62
3:F:243:LEU:HD12	3:F:260:PHE:CE2	2.35	0.62
3:F:45:VAL:HG12	3:F:45:VAL:O	1.98	0.62
1:A:124:LEU:HD23	1:A:128:PHE:HB3	1.81	0.62
1:D:487:LEU:C	1:D:489:MSE:H	2.02	0.62
3:F:162:GLN:HB3	3:F:235:THR:HG22	1.81	0.62
1:A:452:VAL:HG13	1:A:497:HIS:NE2	2.15	0.61
2:B:222:ILE:O	2:B:224:GLY:N	2.33	0.61
1:D:35:LEU:HD21	1:D:55:LEU:CD1	2.29	0.61
2:E:284:PRO:HG3	2:E:290:LYS:HE2	1.81	0.61
2:E:222:ILE:O	2:E:224:GLY:N	2.32	0.61
1:A:571:GLN:NE2	3:C:49:ARG:HH22	1.95	0.61
2:E:302:LEU:HA	2:E:305:ILE:HB	1.82	0.61
2:E:63:LEU:O	2:E:67:VAL:HG23	2.00	0.61
1:A:204:GLU:O	1:A:207:PRO:HD2	2.00	0.61
1:A:336:ASP:OD1	1:A:337:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:373:ASN:C	2:E:375:THR:H	2.03	0.61
1:A:13:ILE:HG21	1:A:41:ALA:HB3	1.83	0.61
1:A:495:TYR:CE1	1:A:496:LEU:HG	2.35	0.61
2:B:208:HIS:CD2	2:B:210:GLY:H	2.18	0.61
3:C:284:TYR:N	3:C:284:TYR:CD2	2.66	0.61
1:D:93:LEU:HD13	1:D:112:LEU:HD23	1.82	0.61
1:A:490:SER:CB	1:A:528:MSE:HE3	2.29	0.61
2:B:133:ARG:HG2	2:B:136:GLU:OE2	1.99	0.61
1:D:72:GLN:O	1:D:74:GLY:N	2.34	0.61
2:B:313:ILE:HG22	2:B:317:LEU:HB2	1.83	0.61
2:B:85:VAL:HG11	2:B:134:PHE:CD1	2.36	0.61
3:C:214:ARG:HH11	3:C:214:ARG:HG2	1.66	0.61
1:D:35:LEU:HB3	1:D:72:GLN:HG2	1.83	0.61
2:E:56:LYS:O	2:E:58:VAL:HG23	2.01	0.61
2:B:169:ARG:HA	2:B:172:LEU:HD12	1.83	0.61
2:B:313:ILE:HD12	2:B:313:ILE:H	1.66	0.61
1:D:52:LEU:HB2	1:D:53:PRO:HD3	1.81	0.61
2:E:342:ASN:HB3	2:E:345:ILE:HB	1.83	0.61
1:D:467:LYS:O	1:D:471:GLU:HG3	2.01	0.60
3:F:290:ASP:HB3	3:F:291:PRO:HD2	1.82	0.60
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.31	0.60
1:A:316:ASP:O	1:A:317:CYS:HB3	2.00	0.60
1:A:356:LEU:HD12	1:A:365:LEU:HD11	1.83	0.60
1:A:343:SER:CA	1:A:380:VAL:HG22	2.30	0.60
2:B:287:HIS:ND1	2:B:290:LYS:HB2	2.16	0.60
2:E:144:ILE:O	2:E:144:ILE:HG22	2.00	0.60
3:F:13:TRP:HE1	3:F:27:GLN:HE21	1.47	0.60
2:B:154:VAL:HG11	2:B:190:ILE:HD12	1.83	0.60
2:B:325:VAL:HG22	2:B:337:LEU:HD12	1.83	0.60
3:F:169:GLY:HA3	3:F:220:PHE:HE2	1.65	0.60
1:A:257:TRP:CH2	2:B:99:PRO:HB3	2.36	0.60
1:A:60:TYR:HB2	1:A:66:LEU:HD21	1.84	0.60
3:F:45:VAL:HG22	3:F:156:THR:OG1	2.01	0.60
1:A:101:GLU:HG2	2:B:246:LYS:NZ	2.16	0.60
1:A:388:LEU:C	1:A:390:CYS:H	2.03	0.60
2:E:284:PRO:HG2	2:E:290:LYS:HB3	1.83	0.60
2:E:305:ILE:HD13	2:E:306:GLU:H	1.66	0.60
3:F:123:ILE:HG23	3:F:127:TYR:HD2	1.65	0.60
2:B:164:GLU:OE2	2:B:167:ARG:HB2	2.01	0.60
2:B:305:ILE:HD13	2:B:306:GLU:N	2.16	0.60
1:D:490:SER:CB	1:D:528:MSE:HE3	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:245:HIS:CE1	2:E:257:LEU:HD21	2.37	0.60
2:E:267:LYS:O	2:E:268:ASP:HB2	2.01	0.60
2:B:321:LEU:HB3	2:B:360:MSE:HE1	1.84	0.60
1:D:260:ARG:HH11	1:D:260:ARG:HG3	1.67	0.60
1:A:76:PHE:O	1:A:80:VAL:HG12	2.01	0.60
3:C:39:LEU:HD12	3:C:149:LEU:HD11	1.84	0.60
3:F:214:ARG:NH1	3:F:214:ARG:HG2	2.15	0.60
2:B:165:ASP:O	2:B:166:PRO:C	2.38	0.59
2:E:160:LEU:O	2:E:162:ASP:N	2.33	0.59
3:F:203:PRO:HD2	3:F:242:GLN:OE1	2.01	0.59
1:A:310:CYS:HB3	1:A:322:ILE:HD11	1.84	0.59
1:A:401:SER:HA	1:A:405:LEU:HB2	1.83	0.59
3:C:65:LEU:O	3:C:68:LEU:HB3	2.03	0.59
1:A:35:LEU:HD21	1:A:55:LEU:CD1	2.32	0.59
1:D:506:ASN:N	1:D:506:ASN:HD22	2.00	0.59
1:D:66:LEU:HD22	1:D:96:LEU:CD2	2.32	0.59
1:D:52:LEU:HD11	1:D:89:LEU:HD12	1.85	0.59
2:E:133:ARG:HA	2:E:136:GLU:HG2	1.84	0.59
2:E:136:GLU:OE1	2:E:178:ARG:NH1	2.35	0.59
2:E:159:GLU:O	2:E:161:PHE:N	2.36	0.59
2:E:85:VAL:HG11	2:E:134:PHE:CD1	2.38	0.59
1:A:292:LYS:HE2	1:A:329:CYS:SG	2.42	0.59
1:A:526:LEU:HD22	1:A:563:ILE:HD13	1.83	0.59
2:B:288:SER:HB2	2:B:289:PRO:CD	2.31	0.59
2:B:79:GLU:N	2:B:80:PRO:HD2	2.17	0.59
1:D:556:LEU:O	1:D:560:VAL:HB	2.02	0.59
2:E:124:LEU:O	2:E:126:LEU:N	2.35	0.59
2:E:375:THR:HG22	2:E:379:LEU:HD12	1.85	0.59
1:A:495:TYR:O	1:A:499:MSE:HG3	2.02	0.59
1:A:556:LEU:O	1:A:560:VAL:HB	2.02	0.59
2:B:373:ASN:C	2:B:375:THR:H	2.06	0.59
1:D:12:PRO:O	1:D:15:VAL:HG12	2.03	0.59
1:D:500:THR:O	1:D:503:PHE:HB2	2.03	0.59
2:E:389:GLU:O	2:E:390:MSE:HB2	2.03	0.59
2:E:67:VAL:C	2:E:69:TYR:H	2.06	0.59
2:B:208:HIS:HD2	2:B:210:GLY:H	1.49	0.58
1:D:226:GLU:OE2	1:D:266:LYS:HE3	2.02	0.58
2:E:340:TRP:CH2	2:E:360:MSE:HE3	2.37	0.58
2:E:340:TRP:NE1	2:E:387:PHE:CE1	2.70	0.58
2:E:79:GLU:N	2:E:80:PRO:HD2	2.16	0.58
2:B:31:LEU:C	2:B:33:ILE:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:ILE:O	2:B:349:ILE:HG13	2.02	0.58
1:D:452:VAL:O	1:D:452:VAL:CG1	2.51	0.58
3:F:162:GLN:O	3:F:235:THR:HG22	2.02	0.58
2:B:237:LEU:HD12	2:B:241:LEU:HD12	1.86	0.58
2:E:121:TRP:H	2:E:122:PRO:HD2	1.68	0.58
2:E:361:PHE:O	2:E:363:SER:N	2.36	0.58
2:E:372:TRP:HZ2	3:F:125:GLN:HE22	1.50	0.58
2:B:342:ASN:HB3	2:B:345:ILE:HB	1.84	0.58
1:D:48:ARG:HD3	1:D:80:VAL:O	2.03	0.58
1:D:498:ARG:HH11	1:D:498:ARG:HB2	1.69	0.58
1:D:500:THR:HA	1:D:503:PHE:HD1	1.67	0.58
3:F:199:LEU:N	3:F:199:LEU:HD12	2.18	0.58
2:B:128:TYR:HB3	2:B:171:PHE:CD2	2.38	0.58
2:E:104:THR:OG1	2:E:105:GLY:N	2.37	0.58
1:A:426:TYR:CZ	1:A:430:LEU:HG	2.38	0.58
1:A:495:TYR:HA	1:A:498:ARG:HB3	1.85	0.58
2:B:240:VAL:O	2:B:243:PRO:HG2	2.03	0.58
2:E:164:GLU:C	2:E:165:ASP:O	2.42	0.58
2:B:208:HIS:HB3	2:B:211:ILE:HD13	1.85	0.58
3:C:239:ARG:HH12	3:C:242:GLN:HG2	1.69	0.58
3:C:17:LEU:CD1	3:C:98:THR:HG22	2.34	0.58
2:E:373:ASN:HD22	2:E:376:ILE:HG23	1.67	0.58
2:B:166:PRO:HB3	2:B:170:ASP:OD1	2.04	0.58
2:B:72:HIS:O	2:B:74:ARG:N	2.37	0.58
3:C:185:ARG:HA	3:C:195:MET:SD	2.44	0.58
1:D:571:GLN:NE2	3:F:49:ARG:HH22	2.02	0.58
2:E:186:LEU:O	2:E:190:ILE:HD13	2.03	0.58
1:A:427:MSE:HA	1:A:427:MSE:CE	2.32	0.57
3:F:239:ARG:HD3	3:F:240:ALA:N	2.19	0.57
3:F:87:VAL:O	3:F:88:ASP:HB2	2.04	0.57
1:A:467:LYS:HB2	1:A:507:VAL:HG12	1.83	0.57
2:B:67:VAL:C	2:B:69:TYR:H	2.07	0.57
1:A:318:ARG:HD3	1:A:355:ILE:HG23	1.87	0.57
1:A:405:LEU:O	1:A:409:VAL:HG23	2.05	0.57
3:F:13:TRP:HE1	3:F:27:GLN:NE2	2.01	0.57
3:C:100:LEU:HA	3:C:103:LEU:HD12	1.85	0.57
1:D:405:LEU:HD13	1:D:405:LEU:C	2.24	0.57
2:E:218:LEU:O	2:E:222:ILE:HG13	2.05	0.57
1:A:572:ASP:OD2	3:C:110:ARG:NH2	2.38	0.57
2:E:175:THR:O	2:E:179:ILE:HG13	2.04	0.57
2:B:393:LYS:HG2	2:B:397:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:LEU:N	3:C:220:PHE:HE2	1.98	0.57
3:F:6:PHE:CE2	3:F:34:LYS:HG3	2.36	0.57
2:B:236:PHE:O	2:B:240:VAL:HB	2.04	0.57
1:D:330:ILE:HG23	1:D:345:LEU:HD11	1.86	0.57
1:A:287:PHE:CD2	1:A:291:MSE:HE2	2.40	0.57
1:A:498:ARG:HB2	1:A:498:ARG:HH11	1.69	0.57
2:B:195:ASN:O	2:B:198:PHE:N	2.38	0.57
2:B:267:LYS:O	2:B:268:ASP:HB2	2.04	0.57
2:B:186:LEU:O	2:B:190:ILE:HD13	2.05	0.57
2:B:210:GLY:O	2:B:214:LEU:HD12	2.05	0.57
3:C:6:PHE:CE2	3:C:34:LYS:HG3	2.37	0.57
1:D:34:LYS:O	1:D:37:THR:HG23	2.05	0.57
1:D:565:GLU:C	1:D:567:LEU:H	2.06	0.57
2:E:276:VAL:HG11	2:E:313:ILE:HG21	1.87	0.57
2:E:297:GLU:O	2:E:301:ILE:HG13	2.04	0.57
2:B:63:LEU:C	2:B:65:GLU:H	2.07	0.57
1:D:189:LEU:CD1	1:D:205:ILE:HD12	2.34	0.57
1:D:462:ALA:O	1:D:465:ASN:HB3	2.04	0.57
1:D:475:LYS:HB2	1:D:516:ILE:CD1	2.35	0.57
1:D:572:ASP:OD2	3:F:110:ARG:NH2	2.37	0.57
1:A:158:VAL:HG21	1:A:162:VAL:HG12	1.87	0.56
3:C:165:CYS:HA	3:C:238:SER:O	2.04	0.56
3:C:240:ALA:HB1	3:C:259:ILE:O	2.04	0.56
2:E:251:SER:HA	2:E:293:MSE:HE1	1.86	0.56
3:F:176:THR:H	3:F:179:HIS:HD2	1.52	0.56
1:A:102:THR:HG22	1:A:105:ARG:CZ	2.35	0.56
1:A:226:GLU:OE2	1:A:266:LYS:HE3	2.04	0.56
3:C:158:LEU:CD2	3:C:161:GLY:HA2	2.35	0.56
1:D:336:ASP:O	1:D:342:LYS:HE2	2.05	0.56
2:E:71:THR:HG21	2:E:133:ARG:NH1	2.20	0.56
2:E:313:ILE:HD12	2:E:313:ILE:N	2.20	0.56
3:F:34:LYS:O	3:F:38:ILE:HG13	2.05	0.56
1:A:63:ASP:OD2	1:A:101:GLU:HG3	2.05	0.56
3:C:252:HIS:O	3:C:255:ASN:HB2	2.04	0.56
1:D:426:TYR:O	1:D:426:TYR:CD1	2.58	0.56
2:E:134:PHE:CD2	2:E:135:LEU:N	2.73	0.56
2:E:237:LEU:HD23	2:E:238:LEU:CD2	2.35	0.56
2:B:357:LEU:HD22	2:B:387:PHE:CE2	2.40	0.56
1:D:392:ASN:HD21	1:D:433:GLN:HE22	1.51	0.56
2:E:151:GLN:HB3	2:E:189:TYR:CE2	2.40	0.56
1:A:237:GLN:HA	1:A:240:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:O	1:A:26:GLN:N	2.38	0.56
1:D:60:TYR:CD2	1:D:65:VAL:HG11	2.40	0.56
2:E:31:LEU:C	2:E:33:ILE:H	2.08	0.56
1:A:197:GLU:CD	1:A:197:GLU:H	2.08	0.56
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.88	0.56
1:D:22:ASN:HD21	1:D:27:LEU:HD12	1.68	0.56
2:E:80:PRO:HG2	2:E:82:TYR:CE2	2.41	0.56
3:F:274:ALA:HB2	3:F:288:GLN:HA	1.88	0.56
1:A:129:VAL:HG12	1:A:130:PRO:HD3	1.88	0.56
1:A:196:LEU:HD12	1:A:205:ILE:HG12	1.87	0.56
1:A:215:ASP:O	1:A:221:ARG:NH1	2.37	0.56
2:B:54:LYS:O	2:B:56:LYS:N	2.29	0.56
1:D:587:SER:C	1:D:588:LEU:HD23	2.25	0.56
2:E:134:PHE:C	2:E:134:PHE:CD2	2.76	0.56
1:A:411:LEU:O	1:A:413:GLU:N	2.39	0.56
1:A:48:ARG:CB	1:A:48:ARG:HH11	2.19	0.56
1:D:142:THR:O	1:D:145:THR:HB	2.06	0.56
2:E:93:MSE:HE2	2:E:128:TYR:OH	2.05	0.56
2:E:329:HIS:CD2	2:E:331:GLN:HB2	2.40	0.56
1:A:144:ARG:HH21	1:A:176:ASP:CG	2.09	0.56
1:A:322:ILE:CD1	1:A:355:ILE:HG21	2.35	0.56
1:A:189:LEU:HD22	1:A:212:LEU:HD12	1.87	0.56
1:A:229:VAL:O	1:A:233:GLN:HG3	2.06	0.56
1:A:94:GLU:HG3	1:A:131:LEU:HG	1.87	0.56
3:C:80:TYR:HB2	3:C:111:ILE:HG22	1.87	0.56
3:C:51:PRO:O	3:C:52:VAL:HG13	2.06	0.56
1:D:115:ILE:O	1:D:119:HIS:HD2	1.85	0.56
1:D:356:LEU:HD12	1:D:365:LEU:HD11	1.88	0.56
2:E:223:ASN:HD22	2:E:263:GLN:NE2	2.03	0.56
2:E:287:HIS:CE1	2:E:289:PRO:HB2	2.41	0.55
3:F:7:THR:O	3:F:7:THR:HG22	2.06	0.55
1:A:417:TRP:CZ2	1:A:418:ARG:NH1	2.74	0.55
2:E:271:LEU:O	2:E:274:PRO:HG2	2.06	0.55
1:A:362:ILE:HG23	1:A:366:LEU:CD2	2.37	0.55
1:A:561:LYS:O	1:A:565:GLU:HG2	2.06	0.55
1:A:73:LEU:HB2	1:A:93:LEU:HD21	1.88	0.55
2:B:83:PRO:HB3	2:B:148:TYR:CD1	2.42	0.55
2:B:85:VAL:HG13	2:B:130:PHE:CZ	2.41	0.55
1:D:237:GLN:O	1:D:240:LEU:HB2	2.07	0.55
1:A:24:ASP:OD2	1:A:24:ASP:O	2.24	0.55
1:A:448:MSE:HE1	1:A:466:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.71	0.55
2:E:247:VAL:HG12	2:E:248:LYS:N	2.22	0.55
2:E:240:VAL:O	2:E:243:PRO:HG2	2.07	0.55
2:E:313:ILE:H	2:E:313:ILE:HD12	1.72	0.55
3:C:10:LEU:HD13	3:C:106:ARG:HB2	1.89	0.55
3:C:174:ILE:HD13	3:C:180:ILE:HG12	1.87	0.55
3:C:50:CYS:HB2	3:C:51:PRO:HA	1.87	0.55
1:D:571:GLN:HE22	3:F:49:ARG:NH2	2.05	0.55
1:A:565:GLU:C	1:A:567:LEU:H	2.10	0.55
2:B:71:THR:HG21	2:B:133:ARG:HH11	1.72	0.55
2:B:260:CYS:O	2:B:264:PHE:HB2	2.07	0.55
2:E:375:THR:HG22	2:E:379:LEU:CD1	2.36	0.55
3:F:244:VAL:CG2	3:F:244:VAL:O	2.51	0.55
1:A:353:SER:HB2	1:A:354:PRO:CD	2.37	0.55
1:A:429:LEU:O	1:A:433:GLN:HG3	2.07	0.55
2:E:35:LYS:O	2:E:38:GLN:N	2.40	0.55
1:A:400:LEU:HD12	1:A:404:LEU:HD23	1.88	0.55
2:E:388:MSE:HE2	2:E:392:GLN:NE2	2.19	0.55
1:A:570:ASP:OD2	1:A:571:GLN:N	2.40	0.55
2:B:255:PRO:HG2	2:B:256:GLN:NE2	2.22	0.55
2:B:257:LEU:O	2:B:260:CYS:N	2.40	0.55
1:D:477:TRP:CH2	1:D:482:ILE:HD11	2.42	0.55
1:D:499:MSE:HE1	3:F:77:ASP:O	2.06	0.55
3:C:166:LEU:O	3:C:166:LEU:HD23	2.07	0.54
3:C:209:TRP:CD2	3:C:224:ILE:HD13	2.42	0.54
1:D:67:LEU:HA	1:D:104:VAL:HG22	1.88	0.54
1:D:179:PRO:HD2	1:D:180:MSE:HE3	1.89	0.54
1:D:300:ALA:HB2	1:D:341:VAL:HG22	1.88	0.54
1:D:427:MSE:HA	1:D:427:MSE:CE	2.35	0.54
1:D:438:PHE:O	1:D:438:PHE:HD1	1.90	0.54
1:A:237:GLN:O	1:A:238:GLU:C	2.45	0.54
1:A:392:ASN:HB3	1:A:400:LEU:HD22	1.89	0.54
1:A:85:TYR:O	1:A:88:CYS:HB2	2.07	0.54
2:B:249:SER:O	2:B:252:VAL:HG23	2.06	0.54
2:E:138:PRO:O	2:E:140:PHE:CD1	2.60	0.54
3:F:106:ARG:HG3	3:F:107:TYR:N	2.22	0.54
1:A:455:VAL:HG23	3:C:71:ILE:HG13	1.90	0.54
2:B:124:LEU:O	2:B:126:LEU:N	2.41	0.54
3:F:115:ARG:HH12	3:F:151:ASP:HA	1.71	0.54
3:C:76:PRO:HD3	3:C:107:TYR:CE2	2.42	0.54
1:D:441:GLU:HG2	1:D:442:LYS:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLU:HG2	2:B:246:LYS:HZ2	1.71	0.54
1:A:154:CYS:O	1:A:158:VAL:HG13	2.07	0.54
2:B:169:ARG:O	2:B:172:LEU:N	2.40	0.54
2:B:183:PHE:CD1	2:B:183:PHE:N	2.76	0.54
3:C:183:LEU:HD21	3:C:194:PRO:HG3	1.88	0.54
2:E:183:PHE:N	2:E:183:PHE:CD1	2.75	0.54
3:F:137:TYR:CG	3:F:142:VAL:HG21	2.42	0.54
1:A:439:PHE:CD1	1:A:443:LEU:HD23	2.42	0.54
1:A:517:THR:HA	1:A:521:MSE:HE2	1.88	0.54
1:D:163:LYS:O	1:D:167:ARG:HG3	2.08	0.54
1:D:411:LEU:O	1:D:413:GLU:N	2.41	0.54
2:E:141:GLN:HB2	2:E:144:ILE:HG13	1.89	0.54
2:E:350:SER:O	2:E:352:ASN:N	2.39	0.54
3:F:158:LEU:CD2	3:F:161:GLY:HA2	2.37	0.54
1:A:283:LEU:O	1:A:287:PHE:N	2.33	0.54
2:B:169:ARG:HB3	2:B:213:GLU:HG2	1.90	0.54
1:D:77:THR:CG2	1:D:118:GLU:HG3	2.37	0.54
1:D:517:THR:HG23	1:D:521:MSE:HE3	1.88	0.54
1:D:77:THR:HG21	1:D:118:GLU:CG	2.36	0.54
1:A:155:TYR:CE2	1:A:196:LEU:HD23	2.43	0.54
1:A:90:LEU:HD22	1:A:131:LEU:HD13	1.89	0.54
2:B:302:LEU:HA	2:B:305:ILE:HB	1.88	0.54
2:B:371:HIS:CG	2:B:376:ILE:HD11	2.43	0.54
3:C:203:PRO:CA	3:C:220:PHE:CE1	2.89	0.54
3:C:170:LEU:HD12	3:C:220:PHE:CD2	2.43	0.54
3:C:59:HIS:CD2	3:C:265:TYR:CE2	2.96	0.54
1:D:104:VAL:HG12	1:D:105:ARG:N	2.22	0.54
1:D:500:THR:HA	1:D:503:PHE:CD1	2.43	0.54
2:E:107:GLU:HG3	2:E:108:PHE:CE1	2.41	0.54
1:A:382:LEU:CD1	1:A:419:VAL:HG22	2.37	0.54
2:B:409:GLU:O	2:B:413:MSE:HB2	2.08	0.54
2:B:65:GLU:C	2:B:67:VAL:H	2.09	0.54
1:D:178:THR:HB	1:D:180:MSE:HG2	1.89	0.54
1:D:526:LEU:HD22	1:D:563:ILE:HD13	1.90	0.54
3:F:160:ASP:O	3:F:162:GLN:N	2.41	0.54
1:A:102:THR:HG22	1:A:105:ARG:HH22	1.72	0.53
1:A:25:VAL:CG1	1:A:62:GLU:HG2	2.38	0.53
2:B:244:LEU:HD22	2:B:253:TYR:CE1	2.44	0.53
2:E:152:LYS:O	2:E:156:GLN:HG3	2.08	0.53
2:E:65:GLU:C	2:E:67:VAL:H	2.11	0.53
3:F:190:PRO:HD3	3:F:195:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:TYR:O	2:B:190:ILE:C	2.45	0.53
2:B:373:ASN:HD21	2:B:375:THR:HB	1.73	0.53
1:D:385:ILE:HD11	1:D:411:LEU:HG	1.90	0.53
1:D:536:VAL:O	1:D:540:VAL:HG23	2.08	0.53
1:A:178:THR:HB	1:A:180:MSE:CG	2.38	0.53
1:D:419:VAL:O	1:D:422:ALA:HB3	2.08	0.53
2:E:381:TYR:CE2	2:E:385:LYS:HE3	2.43	0.53
3:F:183:LEU:HD21	3:F:194:PRO:CG	2.38	0.53
1:A:452:VAL:HG22	1:A:497:HIS:CD2	2.44	0.53
2:B:283:TRP:HH2	2:B:295:LEU:HD23	1.74	0.53
2:B:335:ARG:HG3	2:B:335:ARG:NH1	2.21	0.53
1:D:316:ASP:O	1:D:317:CYS:HB3	2.07	0.53
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.43	0.53
1:A:450:TRP:O	1:A:452:VAL:N	2.42	0.53
1:D:522:LEU:N	1:D:523:PRO:CD	2.72	0.53
2:B:284:PRO:CG	2:B:290:LYS:HB3	2.38	0.53
2:B:76:VAL:HG12	2:B:76:VAL:O	2.08	0.53
1:A:373:LEU:HD12	1:A:411:LEU:HD21	1.91	0.53
1:A:400:LEU:CD1	1:A:404:LEU:HD23	2.39	0.53
1:A:382:LEU:HD13	1:A:419:VAL:CG2	2.38	0.53
1:A:124:LEU:HD23	1:A:128:PHE:CB	2.39	0.53
2:B:372:TRP:HZ2	3:C:125:GLN:NE2	2.07	0.53
2:E:132:LEU:O	2:E:134:PHE:N	2.42	0.53
1:A:245:MSE:O	1:A:249:ARG:HG3	2.09	0.53
1:A:48:ARG:HB3	1:A:48:ARG:HH11	1.74	0.53
3:C:73:GLY:HA3	3:C:78:THR:HG21	1.90	0.53
2:E:257:LEU:O	2:E:260:CYS:N	2.42	0.53
1:A:487:LEU:C	1:A:489:MSE:H	2.11	0.53
3:C:244:VAL:O	3:C:246:GLU:N	2.42	0.53
2:E:134:PHE:CG	2:E:135:LEU:N	2.76	0.53
3:F:170:LEU:N	3:F:220:PHE:HE2	2.07	0.53
3:F:284:TYR:CD2	3:F:284:TYR:N	2.76	0.53
1:A:142:THR:O	1:A:145:THR:HB	2.09	0.52
1:A:179:PRO:HB2	1:A:183:ARG:NH1	2.24	0.52
1:A:528:MSE:C	1:A:530:GLY:H	2.13	0.52
2:B:371:HIS:CD2	2:B:376:ILE:HD11	2.44	0.52
2:B:85:VAL:O	2:B:88:MSE:HB3	2.09	0.52
3:C:123:ILE:HG23	3:C:127:TYR:CD2	2.36	0.52
1:A:486:VAL:O	1:A:486:VAL:HG12	2.10	0.52
3:F:171:SER:HB2	3:F:197:ASP:CB	2.38	0.52
3:F:25:GLU:OE1	3:F:139:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:C	1:A:484:PRO:HD2	2.29	0.52
2:B:222:ILE:HD13	2:B:264:PHE:HD1	1.74	0.52
2:B:329:HIS:CD2	2:B:331:GLN:HB2	2.44	0.52
2:E:371:HIS:CG	2:E:376:ILE:HD11	2.44	0.52
1:A:579:ALA:O	1:A:582:ALA:HB3	2.09	0.52
2:B:166:PRO:O	2:B:170:ASP:N	2.42	0.52
2:B:186:LEU:HB3	2:B:190:ILE:CD1	2.38	0.52
2:E:217:ILE:O	2:E:221:ILE:HG13	2.09	0.52
2:E:71:THR:O	2:E:73:ASN:N	2.41	0.52
3:F:17:LEU:HD11	3:F:98:THR:HG22	1.91	0.52
2:B:154:VAL:O	2:B:157:LEU:HB3	2.09	0.52
2:B:259:TYR:O	2:B:263:GLN:HB2	2.10	0.52
3:C:137:TYR:CD2	3:C:142:VAL:HG21	2.44	0.52
1:D:35:LEU:HD11	1:D:51:LEU:HD11	1.92	0.52
1:D:452:VAL:HG13	1:D:497:HIS:HD2	1.71	0.52
2:E:124:LEU:O	2:E:127:VAL:N	2.42	0.52
2:E:356:ILE:HG22	2:E:357:LEU:N	2.25	0.52
3:C:143:TRP:CE2	3:C:147:THR:HG21	2.44	0.52
1:D:63:ASP:O	1:D:64:GLU:C	2.48	0.52
3:F:203:PRO:CA	3:F:220:PHE:CE1	2.93	0.52
2:B:175:THR:O	2:B:179:ILE:HG13	2.10	0.52
1:D:438:PHE:C	1:D:438:PHE:CD1	2.83	0.52
2:E:236:PHE:O	2:E:240:VAL:HB	2.09	0.52
2:E:376:ILE:HA	2:E:379:LEU:HB2	1.92	0.52
3:F:171:SER:HB2	3:F:197:ASP:HB3	1.91	0.52
2:B:344:TYR:O	2:B:347:SER:HB3	2.10	0.52
1:A:462:ALA:O	1:A:465:ASN:HB3	2.10	0.52
2:B:134:PHE:C	2:B:136:GLU:H	2.14	0.52
2:B:242:LEU:N	2:B:243:PRO:HD2	2.25	0.52
2:B:202:ILE:HD11	2:B:244:LEU:HG	1.91	0.52
3:C:24:SER:OG	3:C:27:GLN:HG3	2.09	0.52
1:D:184:ALA:O	1:D:185:ALA:C	2.48	0.52
2:E:180:TYR:CE1	2:E:187:ARG:HG2	2.45	0.52
1:A:174:CYS:SG	1:A:185:ALA:HB1	2.50	0.52
1:A:229:VAL:HG22	1:A:270:LEU:CD2	2.40	0.52
1:D:447:CYS:O	1:D:448:MSE:HE2	2.10	0.52
1:D:478:ALA:C	1:D:480:ALA:H	2.13	0.52
2:E:169:ARG:O	2:E:170:ASP:C	2.48	0.52
1:A:76:PHE:CB	1:A:89:LEU:HD21	2.41	0.51
2:B:104:THR:OG1	2:B:105:GLY:N	2.43	0.51
1:D:353:SER:HB2	1:D:354:PRO:CD	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:163:ILE:HG23	3:F:236:LEU:HG	1.92	0.51
3:F:237:VAL:O	3:F:256:VAL:HA	2.10	0.51
1:A:343:SER:N	1:A:380:VAL:HG22	2.24	0.51
1:D:525:VAL:O	1:D:540:VAL:HG13	2.10	0.51
2:E:350:SER:C	2:E:352:ASN:H	2.14	0.51
1:A:338:ASN:HD22	1:A:341:VAL:HG23	1.76	0.51
2:B:198:PHE:CE2	2:B:211:ILE:HG13	2.45	0.51
3:C:117:ASN:CG	3:C:241:HIS:CE1	2.84	0.51
1:D:61:ASP:O	1:D:62:GLU:C	2.49	0.51
2:E:330:PHE:O	2:E:334:GLU:HB2	2.11	0.51
1:A:138:GLY:O	1:A:144:ARG:HD2	2.10	0.51
2:B:198:PHE:HE2	2:B:211:ILE:HG13	1.75	0.51
2:B:388:MSE:O	2:B:390:MSE:N	2.44	0.51
2:B:95:ARG:NH2	2:B:168:GLU:OE2	2.44	0.51
1:A:240:LEU:O	1:A:245:MSE:HG2	2.09	0.51
2:B:376:ILE:HA	2:B:379:LEU:HB2	1.91	0.51
1:D:260:ARG:NH1	1:D:260:ARG:HG3	2.25	0.51
1:D:424:ILE:HG12	1:D:450:TRP:CD2	2.46	0.51
3:F:103:LEU:C	3:F:111:ILE:HD11	2.30	0.51
3:F:194:PRO:O	3:F:195:MET:C	2.49	0.51
3:F:172:PRO:HG3	3:F:209:TRP:CE2	2.46	0.51
3:F:209:TRP:CD2	3:F:224:ILE:HD13	2.46	0.51
1:A:515:ASP:OD1	1:A:519:LYS:HE2	2.10	0.51
2:B:356:ILE:HG22	2:B:357:LEU:N	2.24	0.51
2:B:248:LYS:HD3	2:B:290:LYS:HZ3	1.76	0.51
1:D:528:MSE:O	1:D:530:GLY:N	2.44	0.51
3:F:120:SER:O	3:F:124:THR:HG23	2.11	0.51
1:A:317:CYS:O	1:A:321:VAL:HG13	2.11	0.51
1:D:179:PRO:HB2	1:D:183:ARG:HH12	1.76	0.51
1:D:211:ASN:HD22	1:D:211:ASN:N	2.07	0.51
3:F:209:TRP:N	3:F:224:ILE:CD1	2.71	0.51
3:F:239:ARG:HH11	3:F:258:THR:HG23	1.74	0.51
1:A:522:LEU:N	1:A:523:PRO:CD	2.73	0.51
3:C:164:PHE:HB2	3:C:234:LEU:HD13	1.93	0.51
3:C:208:GLY:O	3:C:209:TRP:C	2.49	0.51
3:C:240:ALA:O	3:C:241:HIS:HB2	2.10	0.51
3:C:243:LEU:HD12	3:C:260:PHE:CE2	2.45	0.51
3:C:17:LEU:HD11	3:C:98:THR:HG22	1.93	0.51
1:D:141:PHE:CD1	1:D:142:THR:N	2.78	0.51
1:D:438:PHE:O	1:D:438:PHE:CD1	2.64	0.51
2:B:134:PHE:CD2	2:B:135:LEU:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:GLN:O	2:B:323:LYS:N	2.43	0.51
2:E:310:PHE:CD1	2:E:348:LEU:HD13	2.46	0.51
1:A:373:LEU:HD11	1:A:385:ILE:HD13	1.91	0.50
1:A:448:MSE:HA	1:A:448:MSE:HE2	1.93	0.50
1:A:475:LYS:HB2	1:A:516:ILE:CD1	2.41	0.50
2:B:121:TRP:N	2:B:122:PRO:CD	2.72	0.50
2:B:310:PHE:O	2:B:314:MSE:HB2	2.11	0.50
1:A:388:LEU:O	1:A:390:CYS:N	2.44	0.50
1:A:401:SER:HB3	1:A:434:LEU:CD2	2.39	0.50
2:B:93:MSE:O	2:B:95:ARG:HG3	2.12	0.50
3:C:12:GLN:HE22	3:C:16:GLN:HB2	1.76	0.50
3:C:260:PHE:CE2	3:C:262:ALA:HB3	2.47	0.50
3:C:45:VAL:HG12	3:C:45:VAL:O	2.11	0.50
1:D:495:TYR:HA	1:D:498:ARG:HB3	1.93	0.50
2:E:132:LEU:C	2:E:134:PHE:N	2.64	0.50
2:E:31:LEU:O	2:E:33:ILE:N	2.40	0.50
3:F:158:LEU:HD12	3:F:163:ILE:O	2.11	0.50
1:A:424:ILE:HG12	1:A:450:TRP:CD2	2.47	0.50
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.32	0.50
3:C:62:PHE:O	3:C:65:LEU:HB3	2.12	0.50
2:E:89:PHE:CE2	2:E:93:MSE:HG3	2.46	0.50
1:A:447:CYS:O	1:A:448:MSE:HE2	2.11	0.50
2:B:132:LEU:C	2:B:134:PHE:N	2.64	0.50
3:C:25:GLU:OE1	3:C:139:ASN:ND2	2.45	0.50
1:D:479:HIS:ND1	1:D:479:HIS:O	2.44	0.50
1:D:506:ASN:N	1:D:506:ASN:ND2	2.58	0.50
2:E:169:ARG:O	2:E:172:LEU:N	2.44	0.50
2:E:320:GLN:O	2:E:323:LYS:N	2.43	0.50
1:D:257:TRP:CE2	2:E:99:PRO:HD3	2.46	0.50
3:C:261:SER:O	3:C:263:PRO:HD3	2.12	0.50
3:F:293:PRO:HG2	3:F:293:PRO:O	2.11	0.50
1:A:196:LEU:HD12	1:A:205:ILE:CG1	2.42	0.50
1:A:420:ARG:O	1:A:424:ILE:HG13	2.11	0.50
1:A:498:ARG:NH1	1:A:498:ARG:HB2	2.27	0.50
2:B:118:GLU:HB3	2:B:164:GLU:HG3	1.93	0.50
2:B:141:GLN:HB2	2:B:144:ILE:HG13	1.93	0.50
2:B:151:GLN:HB3	2:B:189:TYR:CE2	2.46	0.50
2:E:183:PHE:C	2:E:185:GLY:N	2.65	0.50
2:E:222:ILE:HD13	2:E:264:PHE:CD1	2.45	0.50
1:A:482:ILE:C	1:A:484:PRO:CD	2.80	0.50
1:D:481:THR:HG22	1:D:481:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:GLU:O	2:E:319:ARG:HB2	2.10	0.50
3:F:121:ARG:NH1	3:F:188:GLU:OE1	2.45	0.50
1:A:67:LEU:HD13	1:A:103:VAL:HG12	1.93	0.50
2:B:134:PHE:C	2:B:134:PHE:CD2	2.85	0.50
2:E:42:LEU:O	2:E:59:LYS:HE3	2.12	0.50
2:E:87:HIS:O	2:E:91:VAL:HG23	2.12	0.50
3:F:119:GLU:CA	3:F:119:GLU:OE1	2.60	0.50
2:B:373:ASN:ND2	2:B:375:THR:HB	2.27	0.49
1:D:120:SER:O	1:D:121:PRO:C	2.49	0.49
1:D:186:ALA:HA	1:D:212:LEU:HD13	1.92	0.49
1:D:381:ARG:HH12	1:D:414:ASP:CG	2.16	0.49
1:D:89:LEU:O	1:D:92:PRO:HD2	2.11	0.49
2:E:242:LEU:HD13	2:E:278:ALA:HB3	1.94	0.49
1:A:303:SER:HB3	1:A:345:LEU:HB2	1.95	0.49
1:A:438:PHE:CD1	1:A:438:PHE:C	2.85	0.49
3:C:68:LEU:HD23	3:C:69:PHE:N	2.27	0.49
1:D:257:TRP:CZ2	2:E:99:PRO:HD3	2.46	0.49
2:E:85:VAL:HG13	2:E:130:PHE:CE2	2.46	0.49
2:E:59:LYS:C	2:E:61:ALA:N	2.65	0.49
2:E:65:GLU:C	2:E:67:VAL:N	2.65	0.49
1:A:148:CYS:SG	1:A:173:LEU:HD13	2.52	0.49
1:A:253:GLU:O	1:A:254:ASP:O	2.30	0.49
1:A:526:LEU:CD2	1:A:563:ILE:HD13	2.42	0.49
1:D:241:GLU:O	1:D:241:GLU:HG3	2.12	0.49
1:D:79:LEU:N	1:D:79:LEU:HD12	2.27	0.49
2:E:93:MSE:HE2	2:E:128:TYR:CZ	2.48	0.49
2:E:180:TYR:CE1	2:E:187:ARG:HA	2.47	0.49
3:F:88:ASP:O	3:F:89:ARG:HB2	2.12	0.49
1:A:456:TYR:CE1	1:A:460:GLU:HB2	2.47	0.49
1:A:493:PRO:C	1:A:498:ARG:HH12	2.15	0.49
2:B:353:ALA:O	2:B:354:ALA:C	2.50	0.49
3:C:71:ILE:HG22	3:C:72:GLY:N	2.27	0.49
2:E:93:MSE:O	2:E:95:ARG:HG3	2.12	0.49
2:B:75:ASN:O	2:B:76:VAL:HG23	2.12	0.49
1:D:138:GLY:O	1:D:144:ARG:HD2	2.12	0.49
1:D:146:SER:O	1:D:148:CYS:N	2.46	0.49
3:F:166:LEU:HD23	3:F:166:LEU:O	2.12	0.49
1:A:36:SER:HB3	1:A:72:GLN:NE2	2.28	0.49
2:B:357:LEU:HD12	2:B:361:PHE:CD1	2.48	0.49
3:C:242:GLN:O	3:C:244:VAL:HG13	2.13	0.49
1:D:362:ILE:HD13	1:D:399:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:ASP:O	1:D:498:ARG:NH1	2.46	0.49
3:F:236:LEU:HD12	3:F:237:VAL:N	2.27	0.49
3:F:242:GLN:O	3:F:244:VAL:HG13	2.12	0.49
1:A:364:HIS:C	1:A:367:PRO:HD2	2.33	0.49
2:B:319:ARG:O	2:B:322:ALA:HB3	2.13	0.49
3:C:252:HIS:O	3:C:253:ASP:C	2.51	0.49
3:F:70:ARG:HG3	3:F:70:ARG:HH11	1.77	0.49
1:A:509:SER:OG	1:A:547:ILE:HG22	2.13	0.49
2:B:132:LEU:O	2:B:134:PHE:N	2.43	0.49
2:B:242:LEU:HD13	2:B:278:ALA:HB3	1.95	0.49
2:B:357:LEU:HD22	2:B:387:PHE:CD2	2.48	0.49
3:C:239:ARG:HD3	3:C:240:ALA:N	2.27	0.49
1:D:11:TYR:N	1:D:12:PRO:HD2	2.27	0.49
2:E:268:ASP:OD1	2:E:270:THR:HB	2.12	0.49
2:E:304:VAL:HG12	2:E:304:VAL:O	2.11	0.49
2:E:59:LYS:C	2:E:61:ALA:H	2.15	0.49
1:A:326:ILE:N	1:A:326:ILE:HD12	2.27	0.49
1:A:512:CYS:O	1:A:513:GLY:O	2.31	0.49
2:B:283:TRP:HH2	2:B:295:LEU:CD2	2.26	0.49
2:B:380:ILE:O	2:B:381:TYR:C	2.51	0.49
2:B:65:GLU:C	2:B:67:VAL:N	2.66	0.49
3:C:276:MET:HE2	3:C:278:LEU:HD21	1.95	0.49
3:F:119:GLU:HG3	3:F:150:PHE:CD1	2.47	0.49
1:A:492:ASP:OD2	1:A:493:PRO:CD	2.56	0.49
1:A:61:ASP:O	1:A:62:GLU:C	2.51	0.49
2:B:201:PHE:HD2	2:B:244:LEU:HD21	1.78	0.49
2:B:63:LEU:C	2:B:65:GLU:N	2.66	0.49
3:C:12:GLN:NE2	3:C:16:GLN:HB2	2.27	0.49
3:C:188:GLU:HG3	3:C:189:VAL:N	2.28	0.49
1:D:336:ASP:OD1	1:D:337:ALA:N	2.46	0.49
1:D:437:GLU:CD	1:D:437:GLU:H	2.16	0.49
1:D:486:VAL:O	1:D:486:VAL:HG12	2.13	0.49
3:F:160:ASP:C	3:F:162:GLN:H	2.17	0.49
3:F:166:LEU:CD2	3:F:239:ARG:HB3	2.43	0.49
1:A:265:ASP:O	1:A:305:LYS:HE3	2.13	0.48
1:A:34:LYS:O	1:A:36:SER:N	2.47	0.48
2:B:134:PHE:O	2:B:136:GLU:N	2.46	0.48
2:B:164:GLU:C	2:B:165:ASP:O	2.52	0.48
2:B:164:GLU:HB3	2:B:168:GLU:CB	2.43	0.48
1:D:250:GLN:O	1:D:250:GLN:NE2	2.45	0.48
1:D:310:CYS:HB3	1:D:322:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:LEU:HD12	1:D:404:LEU:HD23	1.95	0.48
2:E:242:LEU:HD13	2:E:278:ALA:CB	2.43	0.48
2:E:278:ALA:C	2:E:280:LEU:N	2.65	0.48
2:E:408:LYS:C	2:E:410:LYS:H	2.17	0.48
2:B:361:PHE:O	2:B:363:SER:N	2.46	0.48
1:D:317:CYS:O	1:D:318:ARG:C	2.52	0.48
2:E:121:TRP:C	2:E:123:HIS:H	2.17	0.48
2:E:121:TRP:C	2:E:123:HIS:N	2.66	0.48
2:E:80:PRO:O	2:E:82:TYR:N	2.46	0.48
3:F:176:THR:O	3:F:179:HIS:HB2	2.14	0.48
1:A:77:THR:HG21	1:A:118:GLU:CD	2.33	0.48
2:B:169:ARG:O	2:B:170:ASP:C	2.52	0.48
1:D:102:THR:O	1:D:103:VAL:C	2.49	0.48
1:D:261:TYR:O	1:D:264:ALA:HB3	2.14	0.48
1:D:427:MSE:HB3	1:D:428:PRO:CD	2.43	0.48
3:F:13:TRP:NE1	3:F:27:GLN:NE2	2.60	0.48
1:A:36:SER:HB3	1:A:72:GLN:HE21	1.78	0.48
1:A:438:PHE:O	1:A:438:PHE:CD1	2.66	0.48
2:B:35:LYS:C	2:B:37:ARG:H	2.16	0.48
2:B:94:PHE:CD2	2:B:94:PHE:N	2.77	0.48
3:C:57:ASP:O	3:C:261:SER:HB2	2.14	0.48
1:A:155:TYR:HE1	1:A:163:LYS:O	1.97	0.48
2:B:313:ILE:CG2	2:B:317:LEU:HB2	2.43	0.48
2:B:357:LEU:HD12	2:B:361:PHE:HD1	1.78	0.48
2:E:180:TYR:HE1	2:E:187:ARG:HA	1.79	0.48
2:E:306:GLU:O	2:E:309:GLU:HB2	2.14	0.48
3:F:94:VAL:HG23	3:F:132:GLU:OE2	2.13	0.48
3:F:276:MET:HB2	3:F:286:PHE:HE1	1.77	0.48
1:A:450:TRP:C	1:A:452:VAL:N	2.66	0.48
2:B:237:LEU:HD13	2:B:264:PHE:CD2	2.48	0.48
2:B:367:ASN:O	2:B:369:LYS:N	2.47	0.48
3:C:63:HIS:O	3:C:66:MET:HB2	2.13	0.48
1:D:262:MSE:O	1:D:263:VAL:C	2.49	0.48
1:D:570:ASP:OD2	1:D:571:GLN:N	2.45	0.48
2:E:288:SER:HB2	2:E:289:PRO:CD	2.41	0.48
2:E:376:ILE:HG13	2:E:377:HIS:N	2.28	0.48
2:E:86:VAL:O	2:E:87:HIS:C	2.51	0.48
3:F:121:ARG:HH11	3:F:121:ARG:HG3	1.78	0.48
1:D:180:MSE:HE2	1:D:183:ARG:HH22	1.78	0.48
1:D:448:MSE:HE2	1:D:448:MSE:HA	1.95	0.48
1:D:90:LEU:CB	1:D:91:PRO:HD3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:LEU:C	2:E:162:ASP:H	2.15	0.48
3:F:123:ILE:O	3:F:126:VAL:N	2.46	0.48
2:B:158:LEU:O	2:B:159:GLU:C	2.52	0.48
2:B:305:ILE:HD12	2:B:310:PHE:N	2.29	0.48
3:C:119:GLU:OE1	3:C:119:GLU:CA	2.62	0.48
1:D:392:ASN:ND2	1:D:433:GLN:HE22	2.11	0.48
1:A:261:TYR:O	1:A:264:ALA:HB3	2.14	0.48
1:A:426:TYR:O	1:A:426:TYR:CD1	2.67	0.48
2:B:367:ASN:C	2:B:369:LYS:H	2.17	0.48
3:C:172:PRO:HG3	3:C:209:TRP:CE2	2.49	0.48
3:C:243:LEU:HD12	3:C:260:PHE:CD2	2.49	0.48
1:D:334:VAL:HG21	1:D:368:LEU:HD13	1.95	0.48
3:F:251:CYS:SG	3:F:256:VAL:CG1	2.98	0.48
1:A:441:GLU:HG2	1:A:442:LYS:HE2	1.95	0.48
1:A:46:ARG:O	1:A:49:SER:N	2.46	0.48
2:B:208:HIS:HD2	2:B:210:GLY:N	2.10	0.48
1:D:390:CYS:O	1:D:391:VAL:C	2.53	0.48
1:D:412:ALA:O	1:D:413:GLU:CG	2.61	0.48
2:E:121:TRP:N	2:E:122:PRO:CD	2.77	0.48
3:F:118:HIS:ND1	3:F:123:ILE:HG21	2.28	0.48
3:F:51:PRO:HB3	3:F:279:ASP:C	2.34	0.48
1:A:179:PRO:O	1:A:183:ARG:HG3	2.13	0.47
1:A:73:LEU:CB	1:A:93:LEU:HD21	2.44	0.47
2:B:132:LEU:HD21	2:B:174:THR:HG22	1.96	0.47
3:C:115:ARG:NH1	3:C:151:ASP:HA	2.29	0.47
3:C:244:VAL:CG2	3:C:244:VAL:O	2.61	0.47
1:D:189:LEU:HD12	1:D:205:ILE:HD12	1.95	0.47
1:D:384:ILE:CG2	1:D:385:ILE:N	2.77	0.47
1:D:588:LEU:O	1:D:589:ALA:HB2	2.14	0.47
2:E:346:MSE:HE2	2:E:349:ILE:HD12	1.96	0.47
2:E:399:THR:CG2	2:E:403:LYS:HE3	2.44	0.47
1:A:13:ILE:HG21	1:A:41:ALA:CB	2.44	0.47
1:A:391:VAL:O	1:A:394:VAL:N	2.40	0.47
1:A:407:ALA:O	1:A:410:GLU:N	2.46	0.47
3:C:276:MET:HE3	3:C:278:LEU:HD21	1.96	0.47
1:D:439:PHE:CD1	1:D:443:LEU:HD23	2.49	0.47
1:A:456:TYR:C	1:A:456:TYR:CD1	2.87	0.47
2:B:71:THR:HG21	2:B:133:ARG:NH1	2.28	0.47
3:C:253:ASP:O	3:C:254:ARG:C	2.52	0.47
3:C:265:TYR:HB3	3:C:269:CYS:HB2	1.96	0.47
1:D:241:GLU:CG	1:D:241:GLU:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:GLU:C	1:D:567:LEU:N	2.67	0.47
2:E:35:LYS:C	2:E:37:ARG:H	2.17	0.47
3:F:117:ASN:H	3:F:167:HIS:CD2	2.33	0.47
3:F:56:GLY:HA3	3:F:259:ILE:O	2.14	0.47
1:A:282:ASP:O	1:A:285:PRO:HD2	2.14	0.47
1:A:411:LEU:C	1:A:413:GLU:H	2.18	0.47
2:B:254:HIS:N	2:B:255:PRO:HD2	2.29	0.47
2:B:89:PHE:CE2	2:B:93:MSE:HG3	2.50	0.47
3:C:170:LEU:HB2	3:C:220:PHE:CD2	2.49	0.47
1:D:525:VAL:HG12	1:D:525:VAL:O	2.15	0.47
1:D:560:VAL:HG12	1:D:561:LYS:N	2.30	0.47
2:E:262:VAL:O	2:E:265:LEU:N	2.48	0.47
3:F:198:LEU:C	3:F:199:LEU:HD12	2.35	0.47
3:F:239:ARG:C	3:F:239:ARG:HD3	2.34	0.47
1:A:283:LEU:HA	1:A:286:ALA:HB3	1.95	0.47
3:C:176:THR:O	3:C:179:HIS:HB2	2.15	0.47
2:E:119:ALA:O	2:E:120:ALA:HB3	2.14	0.47
1:A:144:ARG:NH2	1:A:176:ASP:OD1	2.46	0.47
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.96	0.47
2:B:121:TRP:O	2:B:123:HIS:N	2.47	0.47
1:D:146:SER:O	1:D:147:ALA:C	2.53	0.47
1:D:241:GLU:OE1	1:D:249:ARG:NH2	2.48	0.47
1:D:25:VAL:CG2	1:D:28:ARG:NH2	2.69	0.47
2:E:350:SER:C	2:E:352:ASN:N	2.68	0.47
1:A:287:PHE:O	1:A:291:MSE:HG3	2.15	0.47
1:A:20:LEU:HD23	1:A:31:SER:HB2	1.96	0.47
1:A:438:PHE:HD1	1:A:438:PHE:O	1.98	0.47
1:A:489:MSE:C	1:A:491:GLY:H	2.16	0.47
2:B:121:TRP:C	2:B:123:HIS:N	2.66	0.47
2:B:276:VAL:HG11	2:B:313:ILE:CG2	2.43	0.47
2:B:407:LEU:HD23	2:B:407:LEU:C	2.35	0.47
3:C:93:SER:O	3:C:94:VAL:C	2.53	0.47
1:D:237:GLN:O	1:D:238:GLU:C	2.53	0.47
1:D:438:PHE:C	1:D:438:PHE:HD1	2.17	0.47
1:D:487:LEU:C	1:D:489:MSE:N	2.68	0.47
1:D:61:ASP:N	1:D:62:GLU:OE2	2.48	0.47
2:E:121:TRP:O	2:E:123:HIS:N	2.48	0.47
2:E:169:ARG:HD2	2:E:213:GLU:OE1	2.15	0.47
3:F:203:PRO:HB3	3:F:220:PHE:HE1	1.80	0.47
3:F:204:ASP:CB	3:F:219:THR:HB	2.43	0.47
3:F:276:MET:CE	3:F:278:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ALA:O	1:A:303:SER:HB2	2.15	0.47
1:A:366:LEU:HD12	1:A:369:PHE:HD1	1.79	0.47
2:B:320:GLN:O	2:B:321:LEU:C	2.51	0.47
3:C:204:ASP:CB	3:C:219:THR:HB	2.42	0.47
1:D:261:TYR:CD2	1:D:261:TYR:C	2.88	0.47
2:E:367:ASN:C	2:E:369:LYS:H	2.18	0.47
2:E:76:VAL:O	2:E:76:VAL:HG12	2.15	0.47
2:B:389:GLU:O	2:B:390:MSE:HB2	2.15	0.47
2:E:132:LEU:HD21	2:E:174:THR:HG22	1.97	0.47
2:E:302:LEU:HD11	2:E:317:LEU:HD21	1.97	0.47
2:E:376:ILE:O	2:E:377:HIS:C	2.51	0.47
3:F:169:GLY:CA	3:F:220:PHE:HE2	2.27	0.47
2:B:119:ALA:O	2:B:120:ALA:HB3	2.14	0.47
2:B:321:LEU:CB	2:B:360:MSE:HE1	2.45	0.47
1:D:267:PHE:CE2	1:D:287:PHE:HB2	2.50	0.47
1:D:428:PRO:HD3	1:D:465:ASN:ND2	2.30	0.47
2:E:310:PHE:O	2:E:314:MSE:HB2	2.15	0.47
2:B:350:SER:C	2:B:352:ASN:H	2.17	0.47
1:A:499:MSE:HE1	3:C:77:ASP:O	2.15	0.47
2:E:94:PHE:CD2	2:E:94:PHE:N	2.80	0.47
3:F:240:ALA:HB1	3:F:259:ILE:O	2.15	0.47
3:F:76:PRO:HD3	3:F:107:TYR:CE2	2.50	0.47
1:A:268:THR:HG21	1:A:308:GLU:HG2	1.97	0.46
1:A:322:ILE:CG2	1:A:356:LEU:HD21	2.45	0.46
1:A:528:MSE:C	1:A:530:GLY:N	2.68	0.46
1:A:587:SER:O	1:A:588:LEU:HD23	2.15	0.46
3:C:214:ARG:NH1	3:C:214:ARG:HG2	2.28	0.46
1:D:155:TYR:HB3	1:D:156:PRO:HD3	1.97	0.46
1:D:144:ARG:NH2	1:D:176:ASP:OD1	2.47	0.46
1:D:483:ILE:N	1:D:484:PRO:CD	2.78	0.46
1:A:12:PRO:O	1:A:15:VAL:HG12	2.15	0.46
1:A:236:PRO:HG2	1:A:239:ASP:OD2	2.15	0.46
1:A:366:LEU:HA	1:A:369:PHE:CD1	2.50	0.46
1:A:560:VAL:O	1:A:563:ILE:HG22	2.16	0.46
1:A:80:VAL:HG22	1:A:80:VAL:O	2.15	0.46
1:A:86:VAL:C	1:A:88:CYS:H	2.18	0.46
2:B:342:ASN:O	2:B:343:GLU:C	2.53	0.46
1:D:489:MSE:HB3	1:D:501:THR:OG1	2.15	0.46
2:E:107:GLU:HG2	2:E:107:GLU:H	1.34	0.46
2:E:143:ASN:C	2:E:145:ALA:H	2.15	0.46
2:E:254:HIS:N	2:E:255:PRO:HD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG12	1:A:130:PRO:CD	2.45	0.46
1:A:24:ASP:OD2	1:A:24:ASP:C	2.54	0.46
1:A:353:SER:HB2	1:A:354:PRO:HD3	1.97	0.46
3:C:51:PRO:O	3:C:52:VAL:CG1	2.63	0.46
1:D:120:SER:O	1:D:123:ASP:N	2.48	0.46
1:D:155:TYR:CE2	1:D:196:LEU:HD23	2.50	0.46
1:D:401:SER:HA	1:D:405:LEU:HB2	1.98	0.46
1:D:451:LEU:HD12	1:D:451:LEU:HA	1.78	0.46
3:F:190:PRO:HD3	3:F:195:MET:HE1	1.96	0.46
1:A:362:ILE:HG23	1:A:366:LEU:HD23	1.97	0.46
1:A:500:THR:O	1:A:503:PHE:HB2	2.16	0.46
2:B:121:TRP:C	2:B:123:HIS:H	2.18	0.46
2:B:134:PHE:CG	2:B:135:LEU:N	2.83	0.46
2:B:241:LEU:O	2:B:244:LEU:HB2	2.16	0.46
2:B:399:THR:O	2:B:400:GLN:C	2.54	0.46
2:B:71:THR:CG2	2:B:133:ARG:HH11	2.27	0.46
3:C:103:LEU:C	3:C:111:ILE:HD11	2.35	0.46
3:C:87:VAL:O	3:C:88:ASP:HB2	2.15	0.46
1:D:205:ILE:HD13	1:D:208:MSE:HE3	1.97	0.46
1:D:497:HIS:O	1:D:500:THR:HB	2.15	0.46
1:D:528:MSE:C	1:D:530:GLY:H	2.18	0.46
2:E:289:PRO:O	2:E:293:MSE:HG3	2.15	0.46
3:F:123:ILE:HG22	3:F:124:THR:N	2.30	0.46
1:A:189:LEU:HD21	1:A:209:PHE:HA	1.97	0.46
1:A:327:LEU:N	1:A:328:PRO:CD	2.79	0.46
1:A:560:VAL:HG12	1:A:561:LYS:N	2.31	0.46
1:D:43:GLY:O	1:D:44:VAL:C	2.54	0.46
1:D:90:LEU:HB2	1:D:91:PRO:CD	2.42	0.46
1:D:140:TRP:CH2	2:E:239:LYS:HB3	2.51	0.46
2:E:305:ILE:HD13	2:E:306:GLU:N	2.31	0.46
2:E:345:ILE:O	2:E:349:ILE:HG13	2.15	0.46
3:F:143:TRP:O	3:F:147:THR:HG23	2.16	0.46
1:D:388:LEU:C	1:D:390:CYS:H	2.18	0.46
1:D:427:MSE:O	1:D:428:PRO:C	2.54	0.46
2:E:243:PRO:O	2:E:246:LYS:HB2	2.15	0.46
2:E:320:GLN:O	2:E:321:LEU:C	2.54	0.46
2:E:310:PHE:CG	2:E:348:LEU:HD13	2.51	0.46
1:A:222:LEU:HD23	1:A:223:LEU:H	1.81	0.46
1:A:253:GLU:O	1:A:254:ASP:C	2.53	0.46
1:A:385:ILE:CD1	1:A:411:LEU:HG	2.38	0.46
1:A:489:MSE:C	1:A:491:GLY:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:MSE:O	1:A:501:THR:N	2.49	0.46
1:A:506:ASN:HD21	1:A:543:SER:HB3	1.80	0.46
1:D:350:MSE:HE2	1:D:369:PHE:CE1	2.50	0.46
1:D:405:LEU:N	1:D:406:PRO:CD	2.79	0.46
1:D:512:CYS:O	1:D:513:GLY:O	2.34	0.46
2:E:95:ARG:NH2	2:E:168:GLU:OE2	2.48	0.46
3:F:169:GLY:CA	3:F:201:SER:HB2	2.46	0.46
2:B:138:PRO:O	2:B:140:PHE:CD1	2.68	0.46
1:D:189:LEU:HD11	1:D:205:ILE:HD12	1.97	0.46
2:E:250:LEU:HD23	2:E:290:LYS:HG2	1.97	0.46
2:E:349:ILE:HA	2:E:356:ILE:HD12	1.97	0.46
1:A:456:TYR:CD2	3:C:73:GLY:HA2	2.50	0.46
2:B:310:PHE:CG	2:B:348:LEU:HD13	2.51	0.46
3:C:239:ARG:O	3:C:240:ALA:HB2	2.16	0.46
1:D:131:LEU:C	1:D:131:LEU:HD23	2.36	0.46
1:D:330:ILE:O	1:D:334:VAL:HG23	2.16	0.46
2:E:247:VAL:HG12	2:E:248:LYS:H	1.81	0.46
2:E:388:MSE:O	2:E:390:MSE:N	2.49	0.46
1:A:221:ARG:O	1:A:224:ALA:HB3	2.15	0.46
1:A:310:CYS:C	1:A:312:ASN:N	2.70	0.46
1:A:378:PRO:O	1:A:382:LEU:HB2	2.16	0.46
2:B:180:TYR:CE1	2:B:187:ARG:HG2	2.50	0.46
2:B:242:LEU:HD11	2:B:275:VAL:HA	1.97	0.46
2:B:304:VAL:O	2:B:305:ILE:C	2.54	0.46
2:B:376:ILE:O	2:B:377:HIS:C	2.54	0.46
3:C:118:HIS:ND1	3:C:123:ILE:HG21	2.31	0.46
3:C:190:PRO:O	3:C:196:CYS:HB2	2.16	0.46
1:D:109:VAL:HG13	1:D:150:LEU:HD21	1.97	0.46
3:F:117:ASN:CG	3:F:241:HIS:CE1	2.89	0.46
3:F:252:HIS:O	3:F:253:ASP:C	2.55	0.46
1:A:116:SER:HA	1:A:119:HIS:CD2	2.51	0.45
3:C:154:PRO:HA	3:C:185:ARG:CD	2.46	0.45
1:D:46:ARG:O	1:D:49:SER:N	2.45	0.45
1:D:479:HIS:O	1:D:479:HIS:CG	2.69	0.45
1:D:528:MSE:C	1:D:530:GLY:N	2.69	0.45
2:E:246:LYS:HE2	2:E:246:LYS:HB3	1.76	0.45
2:E:78:THR:HG22	2:E:78:THR:O	2.15	0.45
3:F:100:LEU:HA	3:F:103:LEU:HD12	1.97	0.45
3:F:76:PRO:HG3	3:F:107:TYR:CE1	2.50	0.45
1:A:204:GLU:C	1:A:207:PRO:HD2	2.37	0.45
2:B:143:ASN:HA	2:B:146:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:PHE:HD2	2:B:360:MSE:CE	2.29	0.45
3:C:248:TYR:HA	3:C:258:THR:O	2.16	0.45
3:C:76:PRO:CB	3:C:110:ARG:HG3	2.46	0.45
1:D:115:ILE:O	1:D:115:ILE:HG13	2.14	0.45
1:D:511:VAL:HG23	1:D:511:VAL:O	2.17	0.45
1:D:560:VAL:O	1:D:563:ILE:HG22	2.16	0.45
2:E:172:LEU:O	2:E:173:LYS:C	2.55	0.45
3:F:176:THR:H	3:F:179:HIS:CD2	2.34	0.45
1:A:161:ALA:O	1:A:165:GLU:HG3	2.15	0.45
1:A:483:ILE:N	1:A:484:PRO:CD	2.79	0.45
2:B:248:LYS:NZ	2:B:290:LYS:HZ3	2.14	0.45
3:C:120:SER:OG	3:C:123:ILE:HD13	2.15	0.45
3:C:176:THR:H	3:C:179:HIS:CD2	2.29	0.45
3:C:240:ALA:CB	3:C:259:ILE:O	2.65	0.45
1:D:63:ASP:OD2	1:D:101:GLU:HG3	2.16	0.45
1:D:179:PRO:HB2	1:D:183:ARG:NH1	2.31	0.45
2:E:161:PHE:CD2	2:E:214:LEU:HG	2.52	0.45
2:E:276:VAL:HG11	2:E:313:ILE:HG23	1.96	0.45
1:A:452:VAL:CG1	1:A:452:VAL:O	2.61	0.45
1:A:582:ALA:O	1:A:586:LEU:HD12	2.17	0.45
2:B:154:VAL:HG11	2:B:190:ILE:CD1	2.47	0.45
2:B:217:ILE:O	2:B:221:ILE:HG13	2.16	0.45
2:B:305:ILE:CD1	2:B:310:PHE:N	2.79	0.45
2:B:361:PHE:N	2:B:362:PRO:HD2	2.30	0.45
3:C:124:THR:HB	3:C:129:PHE:HB3	1.98	0.45
3:C:59:HIS:CD2	3:C:265:TYR:HE2	2.34	0.45
1:D:180:MSE:HE3	1:D:180:MSE:H	1.82	0.45
1:D:408:ILE:HD13	1:D:426:TYR:HE2	1.82	0.45
1:D:441:GLU:HG2	1:D:442:LYS:HG2	1.97	0.45
1:D:579:ALA:O	1:D:582:ALA:HB3	2.16	0.45
1:D:96:LEU:O	1:D:99:VAL:HG23	2.16	0.45
2:E:132:LEU:HD21	2:E:174:THR:CG2	2.46	0.45
3:F:18:ASN:C	3:F:20:CYS:N	2.70	0.45
3:F:244:VAL:O	3:F:245:MET:C	2.54	0.45
1:A:11:TYR:O	1:A:12:PRO:C	2.53	0.45
1:A:517:THR:HG23	1:A:521:MSE:HE3	1.97	0.45
2:B:180:TYR:CE1	2:B:187:ARG:HA	2.52	0.45
2:B:42:LEU:O	2:B:59:LYS:HE3	2.16	0.45
3:C:62:PHE:HD2	3:C:63:HIS:CD2	2.35	0.45
1:D:123:ASP:O	1:D:124:LEU:C	2.53	0.45
1:D:401:SER:HB3	1:D:434:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:VAL:HB	1:D:473:PHE:CD1	2.51	0.45
1:D:521:MSE:C	1:D:523:PRO:HD2	2.36	0.45
1:A:474:GLY:HA3	1:A:476:GLU:OE2	2.16	0.45
1:A:517:THR:HG23	1:A:521:MSE:CE	2.45	0.45
2:B:320:GLN:C	2:B:322:ALA:N	2.69	0.45
1:D:179:PRO:CB	1:D:183:ARG:NH1	2.80	0.45
1:D:24:ASP:O	1:D:26:GLN:N	2.49	0.45
1:D:29:LEU:CD1	1:D:64:GLU:HG2	2.47	0.45
2:E:145:ALA:O	2:E:146:LYS:C	2.55	0.45
2:E:346:MSE:CE	2:E:349:ILE:HD12	2.47	0.45
1:A:131:LEU:HD23	1:A:131:LEU:C	2.37	0.45
1:A:146:SER:O	1:A:147:ALA:C	2.55	0.45
1:A:179:PRO:CD	2:B:196:ASN:ND2	2.79	0.45
1:A:362:ILE:HD13	1:A:399:GLN:HG3	1.99	0.45
2:B:107:GLU:HG3	2:B:108:PHE:CE1	2.52	0.45
2:B:194:ILE:HG23	2:B:214:LEU:HD22	1.98	0.45
2:B:313:ILE:O	2:B:316:PRO:CD	2.62	0.45
2:B:406:LYS:O	2:B:406:LYS:HD3	2.17	0.45
3:C:46:GLN:O	3:C:157:ALA:HA	2.16	0.45
3:C:97:VAL:HG13	3:C:98:THR:N	2.32	0.45
2:E:208:HIS:HB3	2:E:211:ILE:HD13	1.99	0.45
3:F:17:LEU:HD23	3:F:17:LEU:HA	1.72	0.45
1:A:322:ILE:HD12	1:A:355:ILE:HG21	1.97	0.45
1:A:492:ASP:O	1:A:498:ARG:NH1	2.49	0.45
1:A:495:TYR:CD1	1:A:496:LEU:N	2.85	0.45
2:B:350:SER:O	2:B:352:ASN:N	2.50	0.45
3:C:117:ASN:ND2	3:C:241:HIS:CE1	2.80	0.45
3:C:155:LEU:HD22	3:C:199:LEU:HD11	1.98	0.45
3:C:33:GLU:O	3:C:36:LYS:N	2.50	0.45
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.99	0.45
1:A:384:ILE:CG2	1:A:385:ILE:N	2.79	0.45
1:A:400:LEU:HD12	1:A:404:LEU:CD2	2.47	0.45
1:A:411:LEU:C	1:A:413:GLU:N	2.71	0.45
1:A:96:LEU:O	1:A:99:VAL:HG23	2.17	0.45
2:B:356:ILE:C	2:B:358:PRO:HD2	2.37	0.45
2:B:80:PRO:O	2:B:82:TYR:HD2	2.00	0.45
3:C:229:ASN:OD1	3:C:237:VAL:HG23	2.17	0.45
2:E:166:PRO:HA	2:E:169:ARG:HB2	1.98	0.45
2:E:93:MSE:HE3	2:E:93:MSE:CA	2.41	0.45
3:F:189:VAL:HA	3:F:195:MET:HE2	1.99	0.45
1:A:350:MSE:C	1:A:352:LEU:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:LEU:HD22	1:D:588:LEU:HD11	1.99	0.45
2:E:313:ILE:HG22	2:E:317:LEU:HB2	1.98	0.45
1:A:277:GLU:C	1:A:279:THR:N	2.69	0.44
1:A:314:SER:HB3	1:A:317:CYS:SG	2.57	0.44
1:A:452:VAL:CG2	1:A:497:HIS:HD2	2.30	0.44
1:A:509:SER:O	1:A:550:ILE:HD13	2.17	0.44
2:B:298:LEU:HD21	2:B:317:LEU:HD13	1.98	0.44
2:B:329:HIS:NE2	2:B:331:GLN:HB2	2.31	0.44
3:C:24:SER:O	3:C:27:GLN:N	2.49	0.44
1:D:179:PRO:CB	1:D:183:ARG:HH12	2.30	0.44
1:D:48:ARG:HG2	1:D:80:VAL:HG22	1.98	0.44
2:E:166:PRO:O	2:E:170:ASP:N	2.50	0.44
3:F:199:LEU:N	3:F:199:LEU:CD1	2.79	0.44
3:F:240:ALA:HA	3:F:258:THR:CG2	2.45	0.44
3:F:6:PHE:C	3:F:8:LYS:H	2.21	0.44
1:A:162:VAL:HA	1:A:165:GLU:HG3	2.00	0.44
1:A:535:ASN:HA	1:A:538:PHE:CD2	2.47	0.44
2:B:330:PHE:O	2:B:334:GLU:HB2	2.18	0.44
2:B:93:MSE:CE	2:B:93:MSE:HA	2.36	0.44
3:C:162:GLN:O	3:C:235:THR:HG22	2.17	0.44
1:D:155:TYR:CZ	1:D:163:LYS:HB3	2.53	0.44
1:D:300:ALA:O	1:D:303:SER:HB2	2.16	0.44
1:D:427:MSE:O	1:D:429:LEU:N	2.50	0.44
1:D:439:PHE:HD1	1:D:443:LEU:HD23	1.80	0.44
2:E:183:PHE:O	2:E:185:GLY:N	2.50	0.44
2:E:384:LEU:HA	2:E:384:LEU:HD23	1.70	0.44
3:F:123:ILE:O	3:F:124:THR:C	2.56	0.44
3:F:276:MET:HE3	3:F:278:LEU:HD21	1.99	0.44
3:F:51:PRO:O	3:F:52:VAL:HG13	2.17	0.44
1:A:450:TRP:C	1:A:452:VAL:H	2.21	0.44
2:B:133:ARG:HA	2:B:136:GLU:CG	2.46	0.44
1:D:85:TYR:O	1:D:88:CYS:HB2	2.17	0.44
2:E:195:ASN:O	2:E:198:PHE:N	2.51	0.44
2:E:282:TYR:O	2:E:283:TRP:C	2.55	0.44
2:E:366:ARG:O	2:E:368:SER:N	2.44	0.44
3:F:99:LEU:O	3:F:102:ALA:HB3	2.17	0.44
1:A:286:ALA:O	1:A:289:ASN:HB2	2.17	0.44
1:A:405:LEU:N	1:A:406:PRO:HD3	2.33	0.44
2:B:315:GLU:HB2	2:B:316:PRO:CD	2.48	0.44
3:C:212:SER:C	3:C:214:ARG:H	2.19	0.44
1:D:566:LYS:HG2	1:D:566:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:VAL:O	2:E:88:MSE:HB3	2.17	0.44
3:F:164:PHE:CB	3:F:234:LEU:HD13	2.47	0.44
3:F:42:GLU:HB3	3:F:46:GLN:OE1	2.17	0.44
1:A:25:VAL:CG2	1:A:28:ARG:HH21	2.28	0.44
2:B:69:TYR:CZ	2:B:75:ASN:ND2	2.86	0.44
3:C:189:VAL:O	4:G:5:1ZN:H9	2.18	0.44
2:E:284:PRO:CG	2:E:290:LYS:HB3	2.48	0.44
3:F:119:GLU:N	3:F:119:GLU:OE1	2.51	0.44
3:F:7:THR:O	3:F:7:THR:CG2	2.64	0.44
1:A:345:LEU:HD23	1:A:346:ALA:N	2.33	0.44
1:A:401:SER:HA	1:A:405:LEU:CB	2.46	0.44
3:C:70:ARG:HH11	3:C:70:ARG:CG	2.14	0.44
1:D:155:TYR:CE1	1:D:163:LYS:HB3	2.53	0.44
1:D:411:LEU:C	1:D:413:GLU:N	2.70	0.44
2:E:165:ASP:OD2	2:E:166:PRO:HD2	2.17	0.44
2:E:63:LEU:C	2:E:65:GLU:H	2.20	0.44
2:E:63:LEU:C	2:E:65:GLU:N	2.71	0.44
3:F:29:LYS:HD2	3:F:145:TYR:CZ	2.53	0.44
1:A:183:ARG:O	1:A:186:ALA:HB3	2.17	0.44
1:A:350:MSE:C	1:A:352:LEU:H	2.19	0.44
1:A:405:LEU:O	1:A:405:LEU:HD22	2.17	0.44
1:A:453:ASP:OD2	1:A:458:ILE:HG21	2.18	0.44
1:A:580:GLN:C	1:A:582:ALA:H	2.19	0.44
3:C:117:ASN:H	3:C:167:HIS:CD2	2.35	0.44
1:D:16:LEU:HD23	1:D:16:LEU:N	2.32	0.44
1:D:202:LYS:HG2	1:D:243:LEU:CD1	2.47	0.44
1:D:262:MSE:C	1:D:264:ALA:N	2.69	0.44
2:E:399:THR:HG22	2:E:403:LYS:HE3	1.99	0.44
1:A:115:ILE:O	1:A:119:HIS:HD2	2.01	0.44
1:A:171:ARG:HG3	1:A:208:MSE:HG2	2.00	0.44
2:B:283:TRP:HA	2:B:284:PRO:HD3	1.87	0.44
2:B:80:PRO:O	2:B:82:TYR:N	2.51	0.44
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.80	0.44
1:D:277:GLU:C	1:D:279:THR:N	2.71	0.44
1:D:412:ALA:O	1:D:413:GLU:HG3	2.18	0.44
1:D:73:LEU:HA	1:D:73:LEU:HD23	1.79	0.44
2:E:118:GLU:N	2:E:164:GLU:HG2	2.28	0.44
3:F:103:LEU:HB3	3:F:111:ILE:HD13	1.99	0.44
3:F:274:ALA:CB	3:F:288:GLN:HA	2.46	0.44
3:F:39:LEU:HD12	3:F:149:LEU:HD11	1.98	0.44
1:A:210:SER:O	1:A:213:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:NH1	1:A:48:ARG:CB	2.81	0.44
2:B:109:ASP:HA	2:B:110:PRO:HD2	1.81	0.44
2:B:167:ARG:HH11	2:B:167:ARG:HB3	1.79	0.44
3:C:143:TRP:O	3:C:147:THR:HG23	2.18	0.44
3:C:159:VAL:HG11	3:C:278:LEU:HD12	2.00	0.44
1:D:245:MSE:O	1:D:249:ARG:HG3	2.18	0.44
1:D:317:CYS:O	1:D:320:ASN:N	2.51	0.44
2:E:159:GLU:C	2:E:161:PHE:N	2.72	0.44
2:E:367:ASN:O	2:E:369:LYS:N	2.51	0.44
2:E:373:ASN:C	2:E:375:THR:N	2.69	0.44
1:A:46:ARG:O	1:A:47:THR:C	2.55	0.43
1:A:39:ALA:HB2	1:A:51:LEU:HD23	1.99	0.43
2:B:80:PRO:HG2	2:B:82:TYR:HD2	1.79	0.43
1:A:257:TRP:CZ2	2:B:99:PRO:HB3	2.52	0.43
1:D:486:VAL:O	1:D:501:THR:HG23	2.17	0.43
2:E:223:ASN:ND2	2:E:263:GLN:NE2	2.63	0.43
2:E:357:LEU:HD12	2:E:361:PHE:CD1	2.53	0.43
1:A:318:ARG:CD	1:A:355:ILE:HG23	2.48	0.43
1:A:528:MSE:O	1:A:530:GLY:N	2.51	0.43
2:B:67:VAL:C	2:B:69:TYR:N	2.71	0.43
3:C:166:LEU:HD11	3:C:169:GLY:O	2.17	0.43
1:D:236:PRO:HG2	1:D:239:ASP:OD2	2.18	0.43
2:E:208:HIS:HD2	2:E:209:ASN:N	2.16	0.43
2:E:79:GLU:O	2:E:80:PRO:C	2.56	0.43
3:F:158:LEU:HA	3:F:158:LEU:HD12	1.79	0.43
1:A:369:PHE:O	1:A:373:LEU:HB2	2.19	0.43
1:A:587:SER:C	1:A:588:LEU:HD23	2.37	0.43
1:A:71:GLU:HG2	1:A:71:GLU:O	2.16	0.43
3:C:134:LEU:O	3:C:136:LYS:N	2.51	0.43
3:C:185:ARG:O	3:C:187:GLN:N	2.50	0.43
1:D:42:LEU:HD23	1:D:47:THR:N	2.33	0.43
1:D:564:LEU:HD21	1:D:582:ALA:HB3	1.99	0.43
1:D:91:PRO:HB2	1:D:92:PRO:HD3	2.00	0.43
2:E:183:PHE:C	2:E:185:GLY:H	2.21	0.43
2:E:259:TYR:O	2:E:263:GLN:HB2	2.18	0.43
3:F:244:VAL:HG21	3:F:248:TYR:HA	1.99	0.43
2:B:282:TYR:O	2:B:283:TRP:C	2.57	0.43
2:B:313:ILE:HG22	2:B:317:LEU:CB	2.47	0.43
2:B:363:SER:HA	2:B:366:ARG:HB2	2.00	0.43
2:B:89:PHE:C	2:B:91:VAL:H	2.21	0.43
3:C:244:VAL:O	3:C:245:MET:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ASP:O	3:C:89:ARG:HB2	2.18	0.43
1:D:178:THR:HB	1:D:180:MSE:CG	2.48	0.43
1:D:556:LEU:CD2	1:D:588:LEU:HD11	2.48	0.43
2:E:393:LYS:HG2	2:E:397:ASP:OD2	2.19	0.43
3:F:68:LEU:C	3:F:68:LEU:HD23	2.38	0.43
1:A:102:THR:O	1:A:103:VAL:C	2.57	0.43
1:A:60:TYR:CD2	1:A:65:VAL:HG11	2.54	0.43
2:B:247:VAL:HG12	2:B:248:LYS:N	2.34	0.43
2:B:357:LEU:CD1	2:B:361:PHE:CD1	3.01	0.43
2:B:80:PRO:O	2:B:82:TYR:CD2	2.71	0.43
1:D:11:TYR:O	1:D:12:PRO:C	2.56	0.43
1:D:420:ARG:NH2	1:D:453:ASP:OD1	2.50	0.43
2:E:208:HIS:HD2	2:E:210:GLY:N	2.13	0.43
1:A:412:ALA:HB1	1:A:450:TRP:HZ2	1.83	0.43
2:B:305:ILE:CD1	2:B:309:GLU:HB2	2.48	0.43
3:C:237:VAL:O	3:C:256:VAL:HA	2.19	0.43
3:C:68:LEU:HD21	3:C:80:TYR:CE1	2.54	0.43
1:D:22:ASN:ND2	1:D:24:ASP:HB3	2.34	0.43
1:D:34:LYS:O	1:D:36:SER:N	2.51	0.43
1:D:17:ILE:HG12	1:D:38:ILE:HG23	2.01	0.43
1:D:411:LEU:C	1:D:413:GLU:H	2.21	0.43
1:D:478:ALA:O	1:D:480:ALA:N	2.52	0.43
2:E:267:LYS:O	2:E:268:ASP:CB	2.66	0.43
2:E:313:ILE:O	2:E:316:PRO:CD	2.56	0.43
2:E:67:VAL:C	2:E:69:TYR:N	2.70	0.43
3:F:108:ARG:HB2	3:F:108:ARG:HE	1.52	0.43
1:A:248:LEU:HD11	1:A:270:LEU:HD13	2.01	0.43
1:A:334:VAL:HG21	1:A:368:LEU:HD22	1.99	0.43
1:A:565:GLU:C	1:A:567:LEU:N	2.72	0.43
3:C:117:ASN:HB2	3:C:200:TRP:CZ2	2.54	0.43
3:C:6:PHE:CE2	3:C:34:LYS:HE3	2.53	0.43
3:C:73:GLY:CA	3:C:78:THR:HG21	2.48	0.43
1:D:179:PRO:O	1:D:182:ARG:N	2.52	0.43
1:D:398:ARG:O	1:D:400:LEU:N	2.52	0.43
2:E:89:PHE:CZ	2:E:93:MSE:HG3	2.54	0.43
3:F:239:ARG:HH11	3:F:258:THR:CG2	2.32	0.43
1:A:438:PHE:HD1	1:A:438:PHE:C	2.22	0.43
2:B:31:LEU:C	2:B:33:ILE:N	2.72	0.43
3:C:20:CYS:SG	3:C:20:CYS:O	2.77	0.43
1:D:338:ASN:HD22	1:D:341:VAL:HG23	1.84	0.43
1:D:492:ASP:OD2	1:D:493:PRO:CD	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:SER:O	1:D:550:ILE:HD13	2.19	0.43
1:D:79:LEU:H	1:D:79:LEU:CD1	2.29	0.43
1:D:48:ARG:HG2	1:D:80:VAL:CG2	2.49	0.43
2:E:145:ALA:O	2:E:148:TYR:N	2.25	0.43
2:E:407:LEU:C	2:E:407:LEU:HD23	2.38	0.43
2:E:408:LYS:O	2:E:410:LYS:N	2.52	0.43
1:A:367:PRO:O	1:A:370:LEU:HB2	2.18	0.43
2:B:340:TRP:NE1	2:B:387:PHE:CE1	2.78	0.43
3:C:29:LYS:HB2	3:C:145:TYR:CE1	2.54	0.43
3:C:172:PRO:HG3	3:C:209:TRP:CD2	2.53	0.43
1:D:262:MSE:O	1:D:264:ALA:N	2.52	0.43
1:D:76:PHE:O	1:D:80:VAL:HG12	2.19	0.43
2:E:103:PRO:HG3	2:E:108:PHE:CD2	2.54	0.43
2:E:391:ASN:ND2	2:E:394:LEU:HD12	2.34	0.43
3:F:170:LEU:HD12	3:F:220:PHE:CD2	2.54	0.43
3:F:209:TRP:CZ3	3:F:220:PHE:HB3	2.54	0.43
3:F:203:PRO:HD2	3:F:239:ARG:NH2	2.33	0.43
1:A:124:LEU:CD2	1:A:128:PHE:HB3	2.47	0.43
1:A:502:LEU:HD11	1:A:540:VAL:HG23	2.01	0.43
1:A:560:VAL:O	1:A:561:LYS:C	2.57	0.43
2:B:233:HIS:O	2:B:236:PHE:HB3	2.19	0.43
2:B:245:HIS:CE1	2:B:257:LEU:HD21	2.54	0.43
2:B:86:VAL:O	2:B:87:HIS:C	2.58	0.43
3:C:83:MET:HA	3:C:114:LEU:HB2	2.00	0.43
1:D:180:MSE:CE	1:D:180:MSE:H	2.32	0.43
1:D:356:LEU:HD12	1:D:365:LEU:CD1	2.49	0.43
2:E:124:LEU:O	2:E:125:GLN:C	2.57	0.43
2:E:31:LEU:C	2:E:33:ILE:N	2.73	0.43
2:E:321:LEU:CB	2:E:360:MSE:HE1	2.49	0.43
3:F:265:TYR:HB3	3:F:269:CYS:HB2	2.00	0.43
1:A:179:PRO:CB	1:A:183:ARG:HH12	2.31	0.42
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.85	0.42
2:B:161:PHE:CD2	2:B:214:LEU:HG	2.53	0.42
1:D:67:LEU:CA	1:D:104:VAL:HG22	2.48	0.42
1:D:204:GLU:C	1:D:207:PRO:HD2	2.40	0.42
1:D:535:ASN:HA	1:D:538:PHE:CD2	2.52	0.42
2:E:57:GLU:HB2	2:E:58:VAL:H	1.63	0.42
1:D:256:SER:OG	2:E:96:THR:HG21	2.19	0.42
1:A:202:LYS:O	1:A:206:ILE:HB	2.20	0.42
1:A:51:LEU:HD12	1:A:51:LEU:O	2.20	0.42
1:A:487:LEU:HD22	1:A:524:THR:OG1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:SER:C	2:B:352:ASN:N	2.71	0.42
1:D:94:GLU:HG3	1:D:131:LEU:CD1	2.49	0.42
1:D:498:ARG:NH1	1:D:498:ARG:HB2	2.32	0.42
1:D:39:ALA:HB2	1:D:51:LEU:HD23	2.01	0.42
2:E:332:VAL:HG12	2:E:333:ALA:N	2.34	0.42
2:E:337:LEU:HD12	2:E:337:LEU:N	2.34	0.42
2:E:344:TYR:O	2:E:347:SER:HB3	2.19	0.42
3:F:117:ASN:OD1	3:F:167:HIS:CD2	2.55	0.42
1:A:420:ARG:NE	1:A:453:ASP:OD2	2.49	0.42
1:A:79:LEU:HD12	1:A:79:LEU:H	1.83	0.42
3:C:85:ASP:CG	3:C:167:HIS:CE1	2.92	0.42
1:D:388:LEU:HD13	1:D:408:ILE:HD11	2.02	0.42
1:D:456:TYR:O	1:D:457:ALA:C	2.57	0.42
1:D:44:VAL:HG13	1:D:45:GLU:H	1.84	0.42
2:E:313:ILE:HG22	2:E:317:LEU:CB	2.50	0.42
2:E:342:ASN:O	2:E:343:GLU:C	2.58	0.42
2:E:408:LYS:C	2:E:410:LYS:N	2.73	0.42
1:A:456:TYR:O	1:A:457:ALA:C	2.58	0.42
1:A:477:TRP:CH2	1:A:482:ILE:HD11	2.54	0.42
2:B:272:THR:O	2:B:276:VAL:HG23	2.19	0.42
2:B:321:LEU:O	2:B:325:VAL:HG23	2.19	0.42
3:C:104:LYS:CA	3:C:111:ILE:HD11	2.48	0.42
3:C:188:GLU:O	3:C:190:PRO:HD3	2.20	0.42
1:D:192:PHE:CZ	1:D:196:LEU:HD21	2.55	0.42
1:D:434:LEU:HD23	1:D:434:LEU:HA	1.66	0.42
2:E:118:GLU:H	2:E:164:GLU:CG	2.28	0.42
2:E:241:LEU:HA	2:E:241:LEU:HD23	1.88	0.42
2:E:320:GLN:C	2:E:322:ALA:N	2.72	0.42
2:E:35:LYS:O	2:E:37:ARG:N	2.52	0.42
2:E:61:ALA:O	2:E:63:LEU:N	2.52	0.42
1:A:588:LEU:O	1:A:589:ALA:HB2	2.19	0.42
2:B:318:PHE:CD2	2:B:360:MSE:CE	2.99	0.42
1:D:171:ARG:HG3	1:D:208:MSE:HG2	2.02	0.42
1:D:274:VAL:CG1	1:D:278:ILE:HB	2.46	0.42
1:D:353:SER:CB	1:D:354:PRO:CD	2.97	0.42
1:A:412:ALA:O	1:A:413:GLU:CG	2.68	0.42
1:A:470:VAL:HG21	1:A:508:LEU:HD12	2.01	0.42
3:C:33:GLU:O	3:C:34:LYS:C	2.58	0.42
1:D:219:SER:HA	1:D:222:LEU:HD22	2.00	0.42
1:D:248:LEU:HD11	1:D:270:LEU:HD13	2.02	0.42
1:D:366:LEU:HA	1:D:369:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:VAL:O	1:D:455:VAL:HG13	2.19	0.42
2:E:124:LEU:C	2:E:126:LEU:N	2.72	0.42
2:E:344:TYR:HE1	2:E:348:LEU:HD11	1.84	0.42
3:F:121:ARG:HG3	3:F:121:ARG:NH1	2.34	0.42
3:F:169:GLY:HA3	3:F:220:PHE:CE2	2.51	0.42
4:H:2:LEU:H	4:H:7:DAM:C	2.33	0.42
1:A:261:TYR:C	1:A:261:TYR:CD2	2.93	0.42
1:A:310:CYS:C	1:A:312:ASN:H	2.22	0.42
2:B:248:LYS:NZ	2:B:290:LYS:NZ	2.67	0.42
2:B:376:ILE:HG13	2:B:377:HIS:N	2.34	0.42
3:C:101:VAL:O	3:C:102:ALA:C	2.58	0.42
3:C:119:GLU:N	3:C:119:GLU:OE1	2.53	0.42
3:C:183:LEU:HD21	3:C:194:PRO:CG	2.49	0.42
2:E:167:ARG:CG	2:E:167:ARG:HH11	2.31	0.42
2:E:356:ILE:O	2:E:359:ILE:N	2.42	0.42
2:E:80:PRO:O	2:E:82:TYR:HD2	2.02	0.42
2:E:89:PHE:O	2:E:91:VAL:N	2.51	0.42
2:E:90:ALA:HB1	2:E:94:PHE:CD1	2.54	0.42
3:F:237:VAL:CB	3:F:256:VAL:HG23	2.22	0.42
3:F:280:ASP:N	3:F:280:ASP:OD2	2.53	0.42
1:A:236:PRO:O	1:A:237:GLN:C	2.58	0.42
1:A:310:CYS:HB3	1:A:322:ILE:CD1	2.49	0.42
2:B:107:GLU:H	2:B:107:GLU:HG2	1.46	0.42
2:B:250:LEU:HA	2:B:253:TYR:CE2	2.55	0.42
2:B:357:LEU:CD1	2:B:361:PHE:HD1	2.33	0.42
2:B:373:ASN:C	2:B:375:THR:N	2.71	0.42
1:D:389:ASP:N	1:D:389:ASP:OD2	2.52	0.42
1:D:414:ASP:OD1	1:D:419:VAL:HG11	2.19	0.42
2:E:253:TYR:CD2	2:E:253:TYR:N	2.86	0.42
3:F:10:LEU:HD23	3:F:13:TRP:CE3	2.54	0.42
1:A:521:MSE:C	1:A:523:PRO:HD2	2.40	0.42
2:B:160:LEU:C	2:B:162:ASP:N	2.73	0.42
2:B:324:CYS:HB3	2:B:336:ALA:HB2	2.01	0.42
2:B:397:ASP:O	2:B:400:GLN:HB3	2.19	0.42
3:C:170:LEU:CD2	3:C:228:PHE:CD2	3.03	0.42
3:C:68:LEU:HD21	3:C:80:TYR:HE1	1.85	0.42
3:C:81:LEU:HD23	3:C:81:LEU:O	2.20	0.42
1:D:93:LEU:HB3	1:D:112:LEU:HD21	2.01	0.42
1:D:94:GLU:HB2	1:D:131:LEU:HD12	2.01	0.42
1:D:525:VAL:CG1	1:D:525:VAL:O	2.68	0.42
1:D:498:ARG:HG3	1:D:528:MSE:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:304:VAL:CG1	2:E:304:VAL:O	2.67	0.42
3:F:12:GLN:O	3:F:13:TRP:C	2.57	0.42
3:F:172:PRO:O	3:F:174:ILE:N	2.52	0.42
1:A:13:ILE:HD13	1:A:41:ALA:HB2	2.02	0.42
1:A:477:TRP:CH2	1:A:482:ILE:CD1	3.02	0.42
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.77	0.42
2:B:183:PHE:C	2:B:185:GLY:H	2.22	0.42
2:B:246:LYS:HB3	2:B:246:LYS:HE2	1.82	0.42
2:B:375:THR:HG22	2:B:379:LEU:CD1	2.50	0.42
3:C:110:ARG:HD3	3:C:110:ARG:HA	1.86	0.42
1:D:93:LEU:CB	1:D:112:LEU:HD21	2.50	0.42
1:D:198:LEU:HD13	1:D:198:LEU:C	2.41	0.42
1:D:398:ARG:O	1:D:399:GLN:C	2.58	0.42
1:D:560:VAL:O	1:D:561:LYS:C	2.59	0.42
2:E:373:ASN:ND2	2:E:376:ILE:H	2.18	0.42
2:E:67:VAL:O	2:E:69:TYR:N	2.53	0.42
3:F:190:PRO:HD3	3:F:195:MET:HE2	2.02	0.42
3:F:266:CYS:O	3:F:267:TYR:HB2	2.20	0.42
3:F:70:ARG:HG3	3:F:70:ARG:NH1	2.35	0.42
1:A:229:VAL:HG22	1:A:270:LEU:HD23	2.02	0.41
1:A:574:ASP:O	1:A:575:VAL:C	2.58	0.41
2:B:271:LEU:O	2:B:274:PRO:HG2	2.20	0.41
3:C:166:LEU:HD11	3:C:169:GLY:C	2.39	0.41
3:C:242:GLN:O	3:C:243:LEU:C	2.57	0.41
1:D:366:LEU:O	1:D:369:PHE:HB2	2.19	0.41
2:E:160:LEU:C	2:E:162:ASP:N	2.72	0.41
2:E:215:LEU:HD13	2:E:257:LEU:HA	2.02	0.41
2:E:321:LEU:HB3	2:E:360:MSE:HE1	2.01	0.41
1:A:193:ALA:O	1:A:195:VAL:N	2.53	0.41
1:A:412:ALA:O	1:A:413:GLU:HG3	2.20	0.41
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.55	0.41
1:A:470:VAL:HG11	1:A:511:VAL:HG23	2.02	0.41
1:A:515:ASP:O	1:A:518:THR:N	2.52	0.41
2:B:208:HIS:CD2	2:B:209:ASN:N	2.89	0.41
2:E:329:HIS:HE1	3:F:125:GLN:O	2.02	0.41
3:F:59:HIS:CD2	3:F:265:TYR:CE2	3.08	0.41
1:A:217:GLN:O	1:A:220:VAL:HB	2.20	0.41
1:A:489:MSE:O	1:A:491:GLY:N	2.53	0.41
2:B:159:GLU:O	2:B:161:PHE:N	2.54	0.41
2:B:218:LEU:HD23	2:B:221:ILE:HD12	2.02	0.41
2:B:254:HIS:O	2:B:257:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:TYR:HE1	2:B:348:LEU:HD21	1.85	0.41
2:E:161:PHE:CE2	2:E:214:LEU:HG	2.54	0.41
2:E:355:LYS:O	2:E:359:ILE:HG13	2.20	0.41
3:F:6:PHE:C	3:F:8:LYS:N	2.74	0.41
1:A:102:THR:HA	1:A:105:ARG:HG2	2.01	0.41
1:A:104:VAL:HG12	1:A:105:ARG:N	2.35	0.41
1:A:391:VAL:O	1:A:393:GLU:N	2.54	0.41
1:A:499:MSE:O	1:A:500:THR:C	2.58	0.41
2:B:152:LYS:O	2:B:156:GLN:HG3	2.20	0.41
2:B:166:PRO:HA	2:B:169:ARG:HB2	2.01	0.41
3:C:203:PRO:HA	3:C:220:PHE:CD1	2.54	0.41
1:D:234:LEU:HD23	1:D:234:LEU:N	2.35	0.41
1:D:340:HIS:HA	1:D:343:SER:HB3	2.03	0.41
1:D:86:VAL:C	1:D:88:CYS:H	2.24	0.41
1:D:73:LEU:CB	1:D:93:LEU:HD21	2.50	0.41
2:E:348:LEU:O	2:E:349:ILE:C	2.58	0.41
2:E:365:TYR:O	2:E:366:ARG:C	2.59	0.41
2:E:380:ILE:O	2:E:381:TYR:C	2.56	0.41
3:F:119:GLU:HG3	3:F:150:PHE:CE1	2.55	0.41
3:F:261:SER:O	3:F:263:PRO:HD3	2.20	0.41
1:A:179:PRO:CB	1:A:183:ARG:NH1	2.83	0.41
1:A:247:THR:O	1:A:250:GLN:HB3	2.19	0.41
1:A:366:LEU:N	1:A:367:PRO:CD	2.84	0.41
2:B:257:LEU:O	2:B:258:ALA:C	2.59	0.41
2:B:31:LEU:O	2:B:33:ILE:N	2.47	0.41
3:C:108:ARG:HE	3:C:108:ARG:HB2	1.62	0.41
3:C:264:ASN:O	3:C:265:TYR:O	2.39	0.41
1:D:533:VAL:HG12	1:D:535:ASN:HB2	2.02	0.41
1:D:67:LEU:O	1:D:67:LEU:HD12	2.19	0.41
1:D:48:ARG:CD	1:D:80:VAL:O	2.67	0.41
2:E:164:GLU:HB3	2:E:168:GLU:HB3	2.02	0.41
2:E:344:TYR:CD1	2:E:344:TYR:C	2.94	0.41
3:F:19:GLU:O	3:F:20:CYS:HB3	2.19	0.41
3:F:27:GLN:O	3:F:28:VAL:C	2.57	0.41
1:A:149:GLY:HA2	1:A:188:LYS:HD2	2.01	0.41
1:A:420:ARG:HH21	1:A:455:VAL:HG12	1.86	0.41
2:B:141:GLN:HB3	2:B:142:PRO:HD2	2.02	0.41
2:B:346:MSE:CE	2:B:349:ILE:HD12	2.50	0.41
3:C:130:TYR:O	3:C:133:CYS:HB2	2.20	0.41
3:C:162:GLN:CB	3:C:235:THR:HG22	2.49	0.41
3:C:293:PRO:O	3:C:293:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:PRO:O	1:D:15:VAL:N	2.39	0.41
1:D:215:ASP:O	1:D:221:ARG:NH1	2.54	0.41
2:E:134:PHE:C	2:E:136:GLU:H	2.24	0.41
2:E:169:ARG:HD2	2:E:213:GLU:CD	2.41	0.41
3:F:170:LEU:N	3:F:220:PHE:CE2	2.70	0.41
1:A:206:ILE:O	1:A:209:PHE:HB3	2.20	0.41
1:A:350:MSE:HE2	1:A:391:VAL:HG13	2.02	0.41
1:A:375:ASP:OD2	1:A:376:GLU:N	2.53	0.41
2:B:183:PHE:C	2:B:185:GLY:N	2.74	0.41
2:B:313:ILE:N	2:B:313:ILE:CD1	2.83	0.41
2:B:360:MSE:O	2:B:364:LEU:HG	2.21	0.41
2:B:408:LYS:C	2:B:410:LYS:H	2.23	0.41
2:B:59:LYS:C	2:B:61:ALA:N	2.74	0.41
3:C:97:VAL:HG13	3:C:98:THR:H	1.85	0.41
3:C:17:LEU:HD13	3:C:98:THR:HG22	2.01	0.41
1:D:299:ARG:O	1:D:300:ALA:C	2.58	0.41
2:E:248:LYS:C	2:E:250:LEU:H	2.23	0.41
1:A:366:LEU:HB3	1:A:367:PRO:HD3	2.02	0.41
1:A:437:GLU:CD	1:A:437:GLU:H	2.24	0.41
2:B:295:LEU:HD23	2:B:295:LEU:HA	1.77	0.41
2:B:94:PHE:N	2:B:94:PHE:HD2	2.18	0.41
1:D:184:ALA:O	1:D:187:SER:N	2.54	0.41
1:D:388:LEU:C	1:D:390:CYS:N	2.73	0.41
2:E:276:VAL:HG12	2:E:280:LEU:HD12	2.02	0.41
2:E:42:LEU:CB	2:E:63:LEU:HD21	2.51	0.41
3:F:153:LEU:O	3:F:185:ARG:HD2	2.20	0.41
3:F:220:PHE:HA	3:F:224:ILE:HD12	2.03	0.41
1:A:211:ASN:ND2	1:A:211:ASN:N	2.64	0.41
1:A:222:LEU:HD23	1:A:223:LEU:N	2.36	0.41
1:A:25:VAL:HG11	1:A:62:GLU:HG2	2.02	0.41
1:A:478:ALA:C	1:A:480:ALA:H	2.23	0.41
2:B:253:TYR:CD2	2:B:253:TYR:N	2.88	0.41
2:B:405:GLU:O	2:B:406:LYS:C	2.59	0.41
3:C:127:TYR:OH	4:G:5:1ZN:H21	2.21	0.41
1:D:313:LEU:O	1:D:314:SER:C	2.59	0.41
1:D:502:LEU:HD11	1:D:540:VAL:HG23	2.02	0.41
2:E:134:PHE:O	2:E:136:GLU:N	2.53	0.41
2:E:164:GLU:OE2	2:E:164:GLU:C	2.59	0.41
2:E:191:ARG:NH1	2:E:232:GLU:OE1	2.54	0.41
2:E:242:LEU:O	2:E:245:HIS:ND1	2.49	0.41
2:E:335:ARG:HG3	2:E:335:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:407:LEU:O	2:E:407:LEU:HD23	2.21	0.41
3:F:71:ILE:HG22	3:F:72:GLY:N	2.36	0.41
1:A:288:GLN:O	1:A:291:MSE:N	2.54	0.41
1:A:411:LEU:HD13	1:A:411:LEU:HA	1.92	0.41
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.86	0.41
2:B:267:LYS:O	2:B:268:ASP:CB	2.69	0.41
3:C:160:ASP:O	3:C:162:GLN:N	2.54	0.41
3:C:194:PRO:O	3:C:195:MET:C	2.59	0.41
3:C:252:HIS:O	3:C:253:ASP:O	2.38	0.41
1:D:32:ILE:O	1:D:35:LEU:HB2	2.20	0.41
2:E:313:ILE:CG2	2:E:317:LEU:HB2	2.51	0.41
3:F:171:SER:HB2	3:F:197:ASP:HB2	2.03	0.41
3:F:248:TYR:CE2	3:F:286:PHE:CD2	3.09	0.41
3:F:63:HIS:O	3:F:66:MET:HB2	2.21	0.41
1:A:455:VAL:HG23	3:C:71:ILE:HA	2.03	0.41
2:B:145:ALA:O	2:B:147:LYS:N	2.54	0.41
2:B:357:LEU:CD2	2:B:387:PHE:CD2	3.04	0.41
1:D:24:ASP:OD2	1:D:24:ASP:C	2.59	0.41
1:D:73:LEU:HB3	1:D:93:LEU:HD21	2.03	0.41
2:E:250:LEU:HD23	2:E:290:LYS:CG	2.51	0.41
2:E:360:MSE:O	2:E:364:LEU:HG	2.20	0.41
3:F:244:VAL:HG21	3:F:248:TYR:CA	2.50	0.41
3:F:33:GLU:O	3:F:36:LYS:N	2.54	0.41
1:A:155:TYR:OH	1:A:167:ARG:HD3	2.21	0.40
1:A:330:ILE:O	1:A:334:VAL:HG23	2.20	0.40
1:A:353:SER:N	1:A:354:PRO:HD2	2.35	0.40
1:A:99:VAL:HG12	1:A:100:GLU:N	2.36	0.40
1:A:9:SER:OG	1:A:10:LEU:N	2.54	0.40
2:B:221:ILE:HG22	2:B:225:PHE:CE2	2.56	0.40
2:B:365:TYR:O	2:B:366:ARG:C	2.59	0.40
2:B:407:LEU:C	2:B:407:LEU:CD2	2.90	0.40
3:C:68:LEU:C	3:C:68:LEU:CD2	2.78	0.40
1:D:13:ILE:HG21	1:D:41:ALA:HB3	2.03	0.40
3:F:118:HIS:C	3:F:120:SER:H	2.25	0.40
3:F:256:VAL:O	3:F:256:VAL:HG12	2.22	0.40
1:A:115:ILE:O	1:A:119:HIS:CD2	2.74	0.40
1:A:22:ASN:ND2	1:A:24:ASP:HB3	2.36	0.40
1:A:277:GLU:O	1:A:279:THR:N	2.55	0.40
2:B:217:ILE:HG22	2:B:221:ILE:HD11	2.03	0.40
2:B:89:PHE:CZ	2:B:93:MSE:HG3	2.56	0.40
3:C:76:PRO:HB2	3:C:110:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ILE:HG22	1:D:322:ILE:O	2.21	0.40
2:E:150:ASP:CG	2:E:151:GLN:N	2.74	0.40
3:F:76:PRO:O	3:F:78:THR:N	2.55	0.40
3:F:23:LEU:HG	3:F:98:THR:HG21	2.02	0.40
1:A:129:VAL:CG1	1:A:133:LYS:HE3	2.52	0.40
1:A:300:ALA:HB2	1:A:341:VAL:CG2	2.39	0.40
2:B:121:TRP:HB3	2:B:122:PRO:CD	2.51	0.40
2:B:248:LYS:HZ2	2:B:290:LYS:HZ3	1.70	0.40
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.90	0.40
3:C:169:GLY:HA3	3:C:220:PHE:HE2	1.85	0.40
1:D:109:VAL:O	1:D:110:GLU:C	2.59	0.40
1:D:193:ALA:O	1:D:195:VAL:N	2.55	0.40
1:D:411:LEU:HD13	1:D:411:LEU:HA	1.95	0.40
1:D:29:LEU:HD13	1:D:64:GLU:HG2	2.03	0.40
2:E:141:GLN:HB3	2:E:142:PRO:HD2	2.03	0.40
2:E:357:LEU:HD12	2:E:361:PHE:HD1	1.86	0.40
3:F:147:THR:HA	3:F:150:PHE:CD2	2.57	0.40
1:A:267:PHE:CE2	1:A:287:PHE:HB2	2.57	0.40
1:A:32:ILE:O	1:A:35:LEU:HB2	2.21	0.40
3:C:19:GLU:O	3:C:20:CYS:HB3	2.22	0.40
1:D:211:ASN:N	1:D:211:ASN:ND2	2.70	0.40
1:D:288:GLN:HA	1:D:291:MSE:HE3	2.04	0.40
1:D:46:ARG:O	1:D:47:THR:C	2.59	0.40
1:D:524:THR:O	1:D:528:MSE:HG3	2.21	0.40
1:D:94:GLU:HG3	1:D:131:LEU:CG	2.45	0.40
2:E:84:GLU:O	2:E:88:MSE:HB2	2.21	0.40
3:F:28:VAL:HG21	3:F:142:VAL:HG13	2.02	0.40
3:F:147:THR:O	3:F:150:PHE:HB2	2.22	0.40
3:F:215:GLY:HA3	4:H:5:1ZN:H14	2.03	0.40
3:F:240:ALA:CB	3:F:259:ILE:O	2.70	0.40
1:A:501:THR:O	1:A:505:ILE:HG13	2.21	0.40
1:A:79:LEU:HD12	1:A:79:LEU:N	2.36	0.40
2:B:302:LEU:HD12	2:B:339:TYR:HE2	1.87	0.40
2:B:366:ARG:O	2:B:368:SER:N	2.50	0.40
3:C:100:LEU:HA	3:C:100:LEU:HD23	1.77	0.40
3:C:202:ASP:HA	3:C:239:ARG:NH2	2.37	0.40
1:D:525:VAL:HG12	1:D:544:LEU:HD21	2.03	0.40
2:E:372:TRP:CZ2	3:F:125:GLN:NE2	2.88	0.40
2:E:86:VAL:O	2:E:89:PHE:N	2.54	0.40
3:F:94:VAL:HB	3:F:95:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/582 (100%)	419 (72%)	127 (22%)	34 (6%)	2	23
1	D	580/582 (100%)	434 (75%)	116 (20%)	30 (5%)	2	25
2	B	386/388 (100%)	248 (64%)	90 (23%)	48 (12%)	0	7
2	E	386/388 (100%)	248 (64%)	90 (23%)	48 (12%)	0	7
3	C	291/293 (99%)	219 (75%)	57 (20%)	15 (5%)	2	25
3	F	291/293 (99%)	229 (79%)	45 (16%)	17 (6%)	2	23
4	G	1/7 (14%)	1 (100%)	0	0	100	100
4	H	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2516/2540 (99%)	1799 (72%)	525 (21%)	192 (8%)	1	15

All (192) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	44	VAL
1	A	254	ASP
1	A	317	CYS
1	A	391	VAL
2	B	44	ASP
2	B	55	TRP
2	B	73	ASN
2	B	76	VAL
2	B	81	ILE
2	B	104	THR
2	B	125	GLN
2	B	146	LYS
2	B	161	PHE
2	B	166	PRO
2	B	223	ASN
2	B	229	LEU

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Mol	Chain	Res	Type
2	B	268	ASP
2	B	314	MSE
2	B	368	SER
2	B	374	LYS
3	C	94	VAL
3	C	241	HIS
3	C	265	TYR
1	D	25	VAL
1	D	44	VAL
1	D	73	LEU
1	D	254	ASP
1	D	317	CYS
1	D	391	VAL
2	E	43	PHE
2	E	44	ASP
2	E	55	TRP
2	E	57	GLU
2	E	72	HIS
2	E	73	ASN
2	E	104	THR
2	E	146	LYS
2	E	165	ASP
2	E	166	PRO
2	E	229	LEU
2	E	268	ASP
2	E	314	MSE
2	E	368	SER
2	E	374	LYS
3	F	245	MET
3	F	265	TYR
1	A	35	LEU
1	A	147	ALA
1	A	237	GLN
1	A	238	GLU
1	A	274	VAL
1	A	412	ALA
1	A	513	GLY
2	B	33	ILE
2	B	43	PHE
2	B	57	GLU
2	B	72	HIS
2	B	135	LEU

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Mol	Chain	Res	Type
2	B	165	ASP
2	B	167	ARG
2	B	283	TRP
2	B	389	GLU
2	B	390	MSE
3	C	161	GLY
3	C	207	GLY
3	C	208	GLY
3	C	245	MET
3	C	253	ASP
3	C	279	ASP
1	D	35	LEU
1	D	103	VAL
1	D	147	ALA
1	D	479	HIS
1	D	513	GLY
1	D	515	ASP
2	E	33	ILE
2	E	76	VAL
2	E	81	ILE
2	E	86	VAL
2	E	125	GLN
2	E	160	LEU
2	E	161	PHE
2	E	223	ASN
2	E	283	TRP
2	E	351	ASP
2	E	389	GLU
2	E	390	MSE
3	F	60	GLY
3	F	161	GLY
3	F	241	HIS
1	A	62	GLU
1	A	73	LEU
1	A	194	LYS
1	A	359	ASP
1	A	392	ASN
1	A	451	LEU
1	A	571	GLN
2	B	90	ALA
2	B	133	ARG
2	B	160	LEU

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Mol	Chain	Res	Type
2	B	351	ASP
3	C	135	ARG
3	C	231	ALA
3	C	240	ALA
3	C	254	ARG
1	D	62	GLU
1	D	237	GLN
1	D	412	ALA
1	D	431	ALA
1	D	553	ASN
1	D	571	GLN
2	E	32	PHE
2	E	36	LEU
2	E	62	ALA
2	E	68	GLU
2	E	83	PRO
2	E	90	ALA
2	E	133	ARG
2	E	135	LEU
2	E	167	ARG
2	E	224	GLY
3	F	20	CYS
3	F	59	HIS
3	F	106	ARG
3	F	135	ARG
3	F	207	GLY
3	F	279	ASP
1	A	99	VAL
1	A	401	SER
1	A	515	ASP
2	B	32	PHE
2	B	170	ASP
2	B	224	GLY
2	B	303	ASP
2	B	366	ARG
3	C	106	ARG
3	C	209	TRP
1	D	359	ASP
1	D	529	ALA
2	E	51	SER
2	E	190	ILE
2	E	250	LEU

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Mol	Chain	Res	Type
2	E	409	GLU
3	F	173	SER
3	F	253	ASP
3	F	254	ARG
1	A	297	GLU
1	A	416	LYS
1	A	500	THR
1	A	529	ALA
1	A	566	LYS
1	A	584	THR
2	B	163	SER
2	B	196	ASN
2	B	305	ILE
1	D	72	GLN
1	D	83	PRO
1	D	238	GLU
1	D	297	GLU
3	F	94	VAL
3	F	240	ALA
1	A	271	GLN
1	A	484	PRO
1	A	553	ASN
2	B	141	GLN
2	B	269	SER
1	D	484	PRO
1	D	584	THR
2	E	362	PRO
2	E	366	ARG
1	A	103	VAL
2	B	46	VAL
2	B	190	ILE
1	D	274	VAL
2	E	46	VAL
2	B	362	PRO
1	D	12	PRO
1	D	428	PRO
1	A	516	ILE
2	B	79	GLU
2	B	91	VAL
2	B	284	PRO
3	F	208	GLY
1	A	91	PRO

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Mol	Chain	Res	Type
2	B	86	VAL
1	D	99	VAL
2	E	79	GLU
2	E	141	GLN
2	B	83	PRO
2	E	77	ILE
2	E	228	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/496 (103%)	467 (92%)	42 (8%)	13	49
1	D	509/496 (103%)	468 (92%)	41 (8%)	14	50
2	B	331/351 (94%)	300 (91%)	31 (9%)	10	44
2	E	331/351 (94%)	298 (90%)	33 (10%)	9	41
3	C	259/259 (100%)	245 (95%)	14 (5%)	26	65
3	F	259/259 (100%)	244 (94%)	15 (6%)	23	62
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	2202/2216 (99%)	2026 (92%)	176 (8%)	14	50

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	11	TYR
1	A	15	VAL
1	A	18	ASP
1	A	37	THR
1	A	44	VAL
1	A	59	ILE
1	A	62	GLU

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Mol	Chain	Res	Type
1	A	88	CYS
1	A	101	GLU
1	A	117	HIS
1	A	129	VAL
1	A	130	PRO
1	A	160	SER
1	A	180	MSE
1	A	198	LEU
1	A	204	GLU
1	A	211	ASN
1	A	230	ASN
1	A	237	GLN
1	A	238	GLU
1	A	294	CYS
1	A	295	GLU
1	A	297	GLU
1	A	316	ASP
1	A	321	VAL
1	A	345	LEU
1	A	373	LEU
1	A	384	ILE
1	A	391	VAL
1	A	398	ARG
1	A	411	LEU
1	A	427	MSE
1	A	436	VAL
1	A	437	GLU
1	A	438	PHE
1	A	475	LYS
1	A	495	TYR
1	A	515	ASP
1	A	524	THR
1	A	555	THR
1	A	556	LEU
2	B	60	ARG
2	B	95	ARG
2	B	97	LEU
2	B	107	GLU
2	B	123	HIS
2	B	132	LEU
2	B	134	PHE
2	B	135	LEU

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Mol	Chain	Res	Type
2	B	139	ASP
2	B	162	ASP
2	B	166	PRO
2	B	167	ARG
2	B	170	ASP
2	B	183	PHE
2	B	186	LEU
2	B	197	ILE
2	B	231	GLU
2	B	256	GLN
2	B	263	GLN
2	B	264	PHE
2	B	289	PRO
2	B	290	LYS
2	B	303	ASP
2	B	305	ILE
2	B	338	TYR
2	B	344	TYR
2	B	357	LEU
2	B	361	PHE
2	B	371	HIS
2	B	386	LEU
2	B	387	PHE
3	C	70	ARG
3	C	75	SER
3	C	78	THR
3	C	110	ARG
3	C	119	GLU
3	C	187	GLN
3	C	220	PHE
3	C	235	THR
3	C	239	ARG
3	C	242	GLN
3	C	256	VAL
3	C	279	ASP
3	C	284	TYR
3	C	294	ARG
1	D	8	ASP
1	D	11	TYR
1	D	15	VAL
1	D	18	ASP
1	D	37	THR

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Mol	Chain	Res	Type
1	D	44	VAL
1	D	62	GLU
1	D	83	PRO
1	D	87	HIS
1	D	88	CYS
1	D	91	PRO
1	D	116	SER
1	D	130	PRO
1	D	145	THR
1	D	180	MSE
1	D	198	LEU
1	D	204	GLU
1	D	210	SER
1	D	237	GLN
1	D	294	CYS
1	D	295	GLU
1	D	297	GLU
1	D	316	ASP
1	D	345	LEU
1	D	350	MSE
1	D	373	LEU
1	D	384	ILE
1	D	391	VAL
1	D	398	ARG
1	D	414	ASP
1	D	430	LEU
1	D	437	GLU
1	D	438	PHE
1	D	443	LEU
1	D	451	LEU
1	D	476	GLU
1	D	495	TYR
1	D	515	ASP
1	D	524	THR
1	D	555	THR
1	D	556	LEU
2	E	60	ARG
2	E	83	PRO
2	E	95	ARG
2	E	96	THR
2	E	97	LEU
2	E	101	SER

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Mol	Chain	Res	Type
2	E	123	HIS
2	E	132	LEU
2	E	134	PHE
2	E	135	LEU
2	E	139	ASP
2	E	162	ASP
2	E	166	PRO
2	E	167	ARG
2	E	170	ASP
2	E	183	PHE
2	E	186	LEU
2	E	197	ILE
2	E	235	ILE
2	E	256	GLN
2	E	264	PHE
2	E	289	PRO
2	E	298	LEU
2	E	303	ASP
2	E	305	ILE
2	E	334	GLU
2	E	338	TYR
2	E	344	TYR
2	E	357	LEU
2	E	361	PHE
2	E	371	HIS
2	E	386	LEU
2	E	387	PHE
3	F	70	ARG
3	F	75	SER
3	F	78	THR
3	F	110	ARG
3	F	119	GLU
3	F	166	LEU
3	F	187	GLN
3	F	235	THR
3	F	236	LEU
3	F	239	ARG
3	F	242	GLN
3	F	256	VAL
3	F	280	ASP
3	F	284	TYR
3	F	294	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	72	GLN
1	A	119	HIS
1	A	172	ASN
1	A	200	ASN
1	A	211	ASN
1	A	230	ASN
1	A	250	GLN
1	A	271	GLN
1	A	338	ASN
1	A	383	ASN
1	A	399	GLN
1	A	465	ASN
1	A	497	HIS
1	A	506	ASN
1	A	514	GLN
1	A	571	GLN
1	A	580	GLN
2	B	208	HIS
2	B	209	ASN
2	B	223	ASN
2	B	254	HIS
2	B	329	HIS
2	B	373	ASN
2	B	392	GLN
3	C	12	GLN
3	C	63	HIS
3	C	141	ASN
3	C	179	HIS
3	C	187	GLN
3	C	288	GLN
1	D	22	ASN
1	D	26	GLN
1	D	72	GLN
1	D	119	HIS
1	D	200	ASN
1	D	211	ASN
1	D	230	ASN
1	D	250	GLN
1	D	271	GLN
1	D	338	ASN

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Mol	Chain	Res	Type
1	D	392	ASN
1	D	399	GLN
1	D	433	GLN
1	D	465	ASN
1	D	497	HIS
1	D	506	ASN
1	D	571	GLN
1	D	580	GLN
2	E	208	HIS
2	E	223	ASN
2	E	254	HIS
2	E	329	HIS
2	E	331	GLN
2	E	373	ASN
2	E	392	GLN
3	F	12	GLN
3	F	44	ASN
3	F	63	HIS
3	F	141	ASN
3	F	179	HIS
3	F	187	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
4	DAL	G	1	4	4,4,5	3.27	1 (25%)	1,4,6	0.37	0
4	ACB	G	3	4	4,8,9	1.64	1 (25%)	3,10,12	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	1ZN	G	5	4	22,23,24	1.18	2 (9%)	24,29,31	0.94	1 (4%)
4	FGA	G	6	4	3,8,9	1.47	0	2,9,11	0.98	0
4	DAM	G	7	3,4	5,5,6	2.39	2 (40%)	3,5,7	3.07	1 (33%)
4	DAL	H	1	4	4,4,5	3.01	1 (25%)	1,4,6	0.30	0
4	ACB	H	3	4	4,8,9	1.60	1 (25%)	3,10,12	0.73	0
4	1ZN	H	5	4	22,23,24	0.95	0	24,29,31	0.83	0
4	FGA	H	6	4	3,8,9	1.29	0	2,9,11	1.12	0
4	DAM	H	7	3,4	5,5,6	2.56	2 (40%)	3,5,7	3.13	2 (66%)

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
4	DAL	G	1	4	-	0/0/2/4	0/0/0/0
4	ACB	G	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	G	5	4	-	0/22/25/27	0/1/1/1
4	FGA	G	6	4	-	0/3/8/9	0/0/0/0
4	DAM	G	7	3,4	-	0/0/4/6	0/0/0/0
4	DAL	H	1	4	-	0/0/2/4	0/0/0/0
4	ACB	H	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	H	5	4	-	0/22/25/27	0/1/1/1
4	FGA	H	6	4	-	0/3/8/9	0/0/0/0
4	DAM	H	7	3,4	-	0/0/4/6	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	1ZN	C18-C17	-2.63	1.52	1.55
4	G	5	1ZN	C5-C4	2.09	1.43	1.38
4	H	3	ACB	CB-CA	2.39	1.57	1.55
4	G	3	ACB	CB-CA	2.74	1.57	1.55
4	G	7	DAM	C-CA	3.00	1.50	1.45
4	H	7	DAM	C-CA	3.36	1.50	1.45
4	G	7	DAM	CA-N	3.96	1.44	1.34
4	H	7	DAM	CA-N	4.18	1.45	1.34
4	H	1	DAL	CA-C	5.93	1.58	1.50
4	G	1	DAL	CA-C	6.44	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	7	DAM	O-C-CA	-5.00	118.90	125.07
4	G	7	DAM	O-C-CA	-4.93	118.98	125.07
4	G	5	1ZN	C17-C16-C15	-2.36	119.91	123.70
4	H	7	DAM	CB-CA-N	-2.08	120.57	125.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	5	1ZN	2	0
4	H	5	1ZN	1	0
4	H	7	DAM	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.