Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 01:38 AM EDT

PDB ID	:	3F3G
Title	:	Crystal structure of the nucleoporin pair Nup85-Seh1, space group P212121
Authors	:	Debler, E.W.; Hseo, H.; Ma, Y.; Blobel, G.; Hoelz, A.
Deposited on	:	2008-10-30
Resolution	:	3.75 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

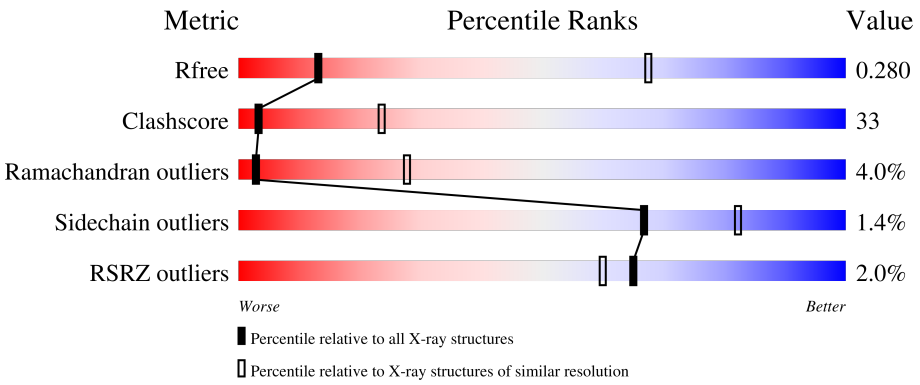
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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

Mol	Chain	Length	Quality of chain
1	A	351	.% 41% 43% • 15%
1	B	351	2% 38% 45% • 15%
1	E	351	3% 38% 45% • 15%
1	F	351	3% 40% 43% • 15%
2	C	570	2% 39% 43% • 14%

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Mol	Chain	Length	Quality of chain
2	D	570	% 39% 42% • 16%
2	G	570	% 40% 41% • 15%
2	H	570	% 39% 43% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25114 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 Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2379	1506	410	452	11	0	0	0
1	B	300	2379	1506	410	452	11	0	0	0
1	E	300	2379	1506	410	452	11	0	0	0
1	F	300	2379	1506	410	452	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	expression tag	UNP P53011
A	0	HIS	-	expression tag	UNP P53011
B	-1	PRO	-	expression tag	UNP P53011
B	0	HIS	-	expression tag	UNP P53011
E	-1	PRO	-	expression tag	UNP P53011
E	0	HIS	-	expression tag	UNP P53011
F	-1	PRO	-	expression tag	UNP P53011
F	0	HIS	-	expression tag	UNP P53011

- Molecule 2 is a protein called Nucleoporin NUP85.

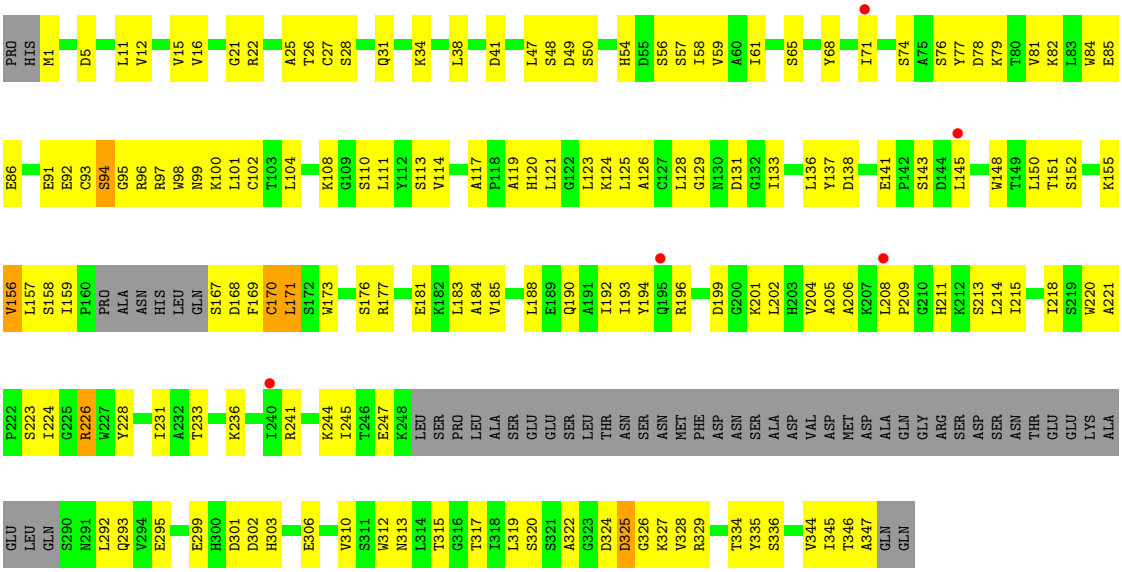
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	492	3938	2526	634	756	22	0	0	0
2	D	480	3850	2473	618	737	22	0	0	0
2	G	482	3863	2482	620	739	22	0	0	0
2	H	493	3947	2532	636	757	22	0	0	0

3 Residue-property plots (i)

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

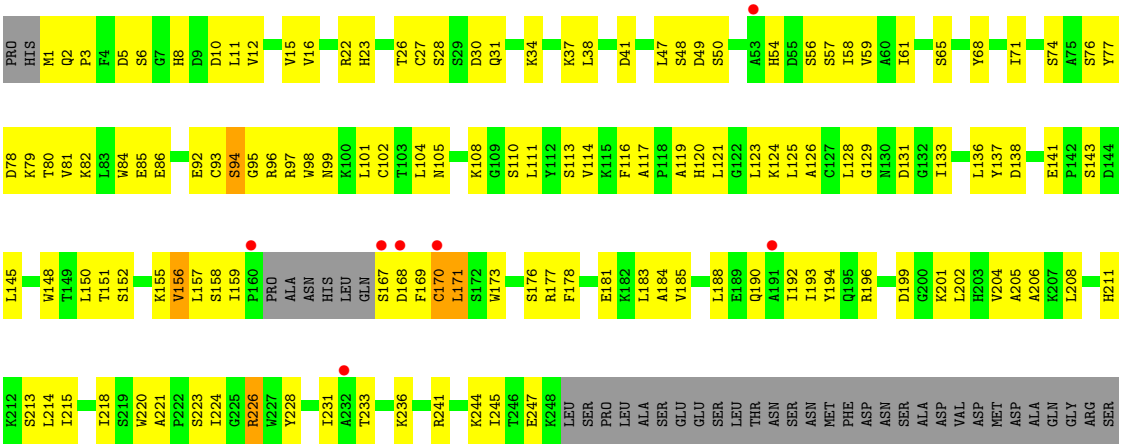
- Molecule 1: Nucleoporin SEH1

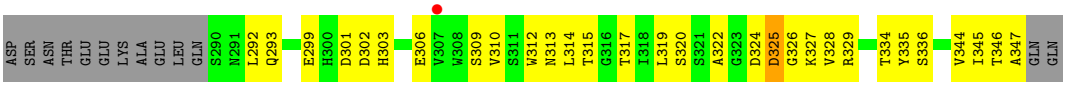
Chain A:



- Molecule 1: Nucleoporin SEH1

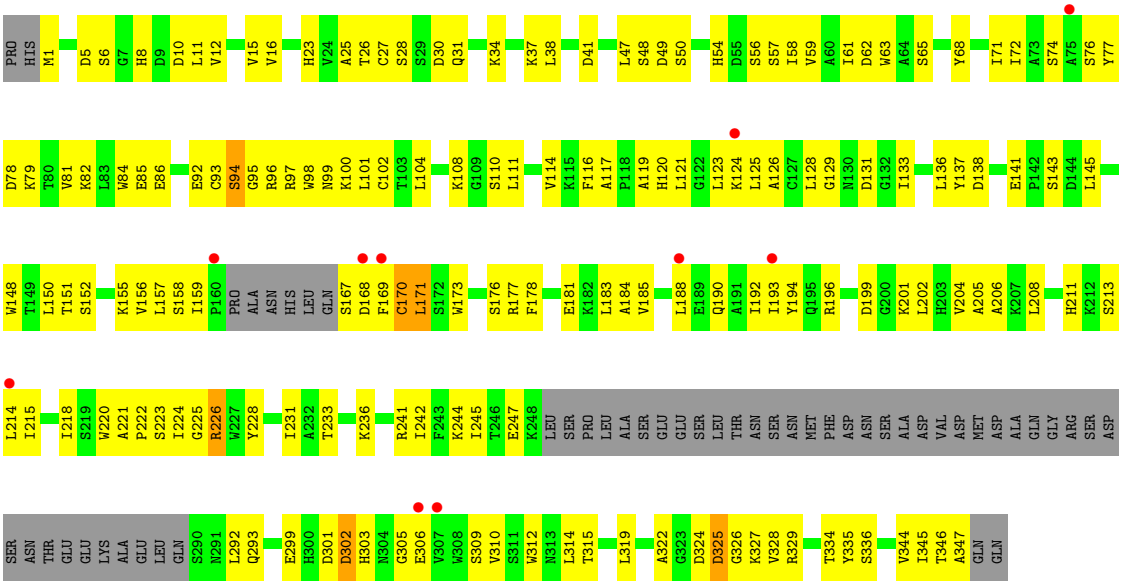
Chain B:





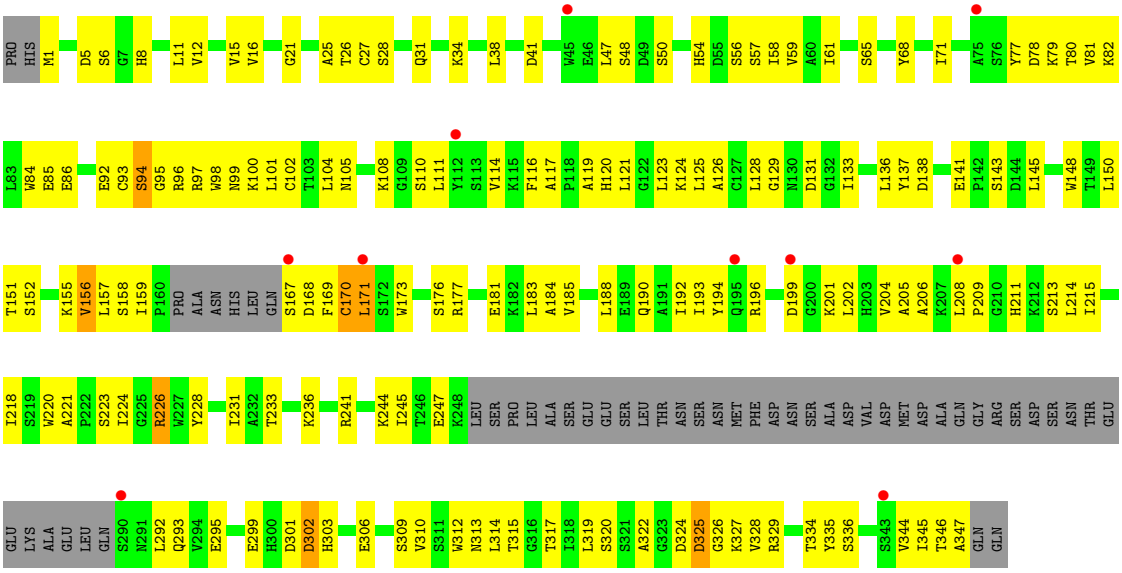
• Molecule 1: Nucleoporin SEH1

Chain E:



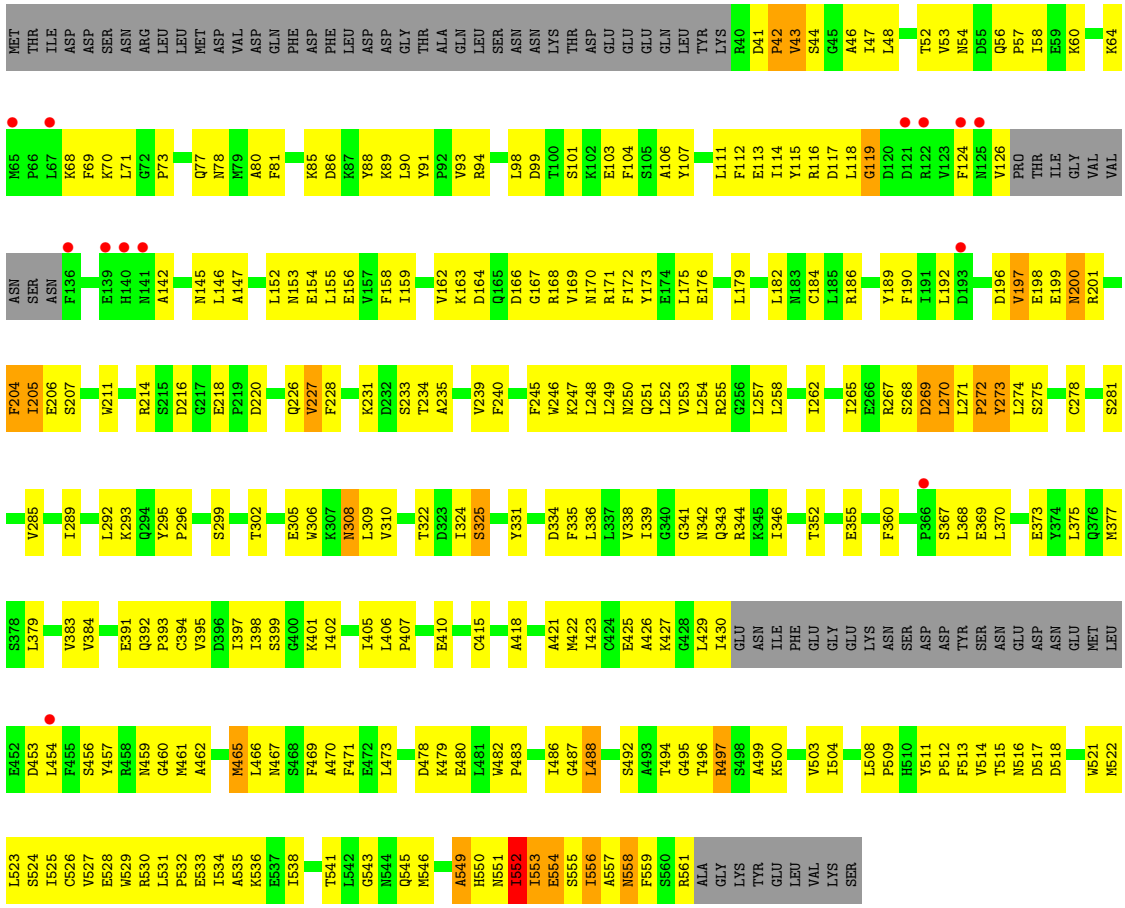
• Molecule 1: Nucleoporin SEH1

Chain F:



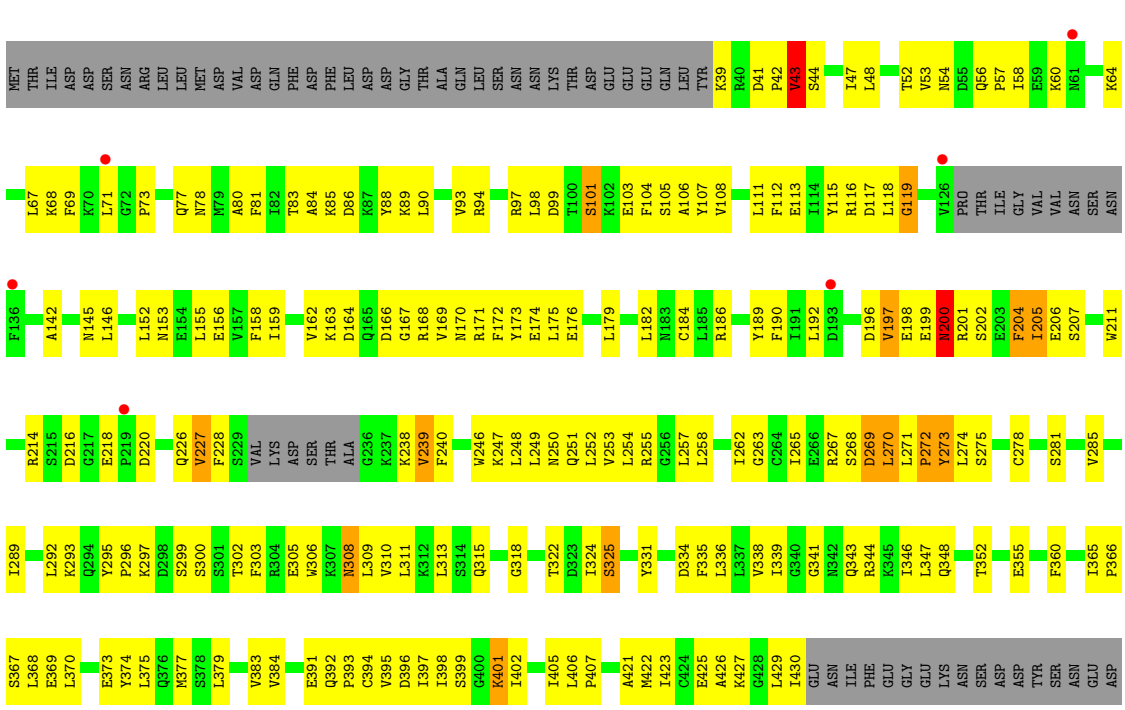
• Molecule 2: Nucleoporin NUP85

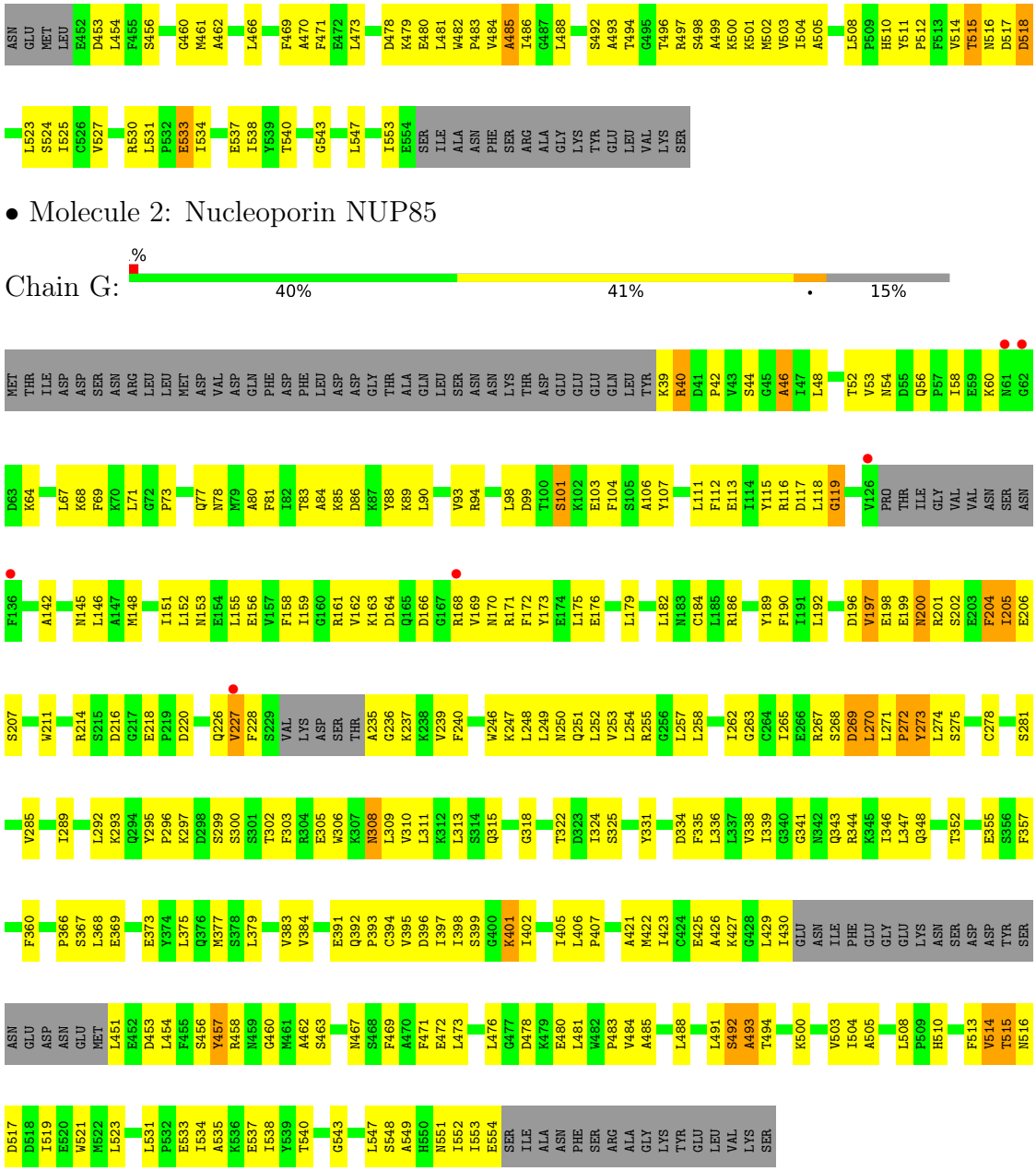
Chain C:



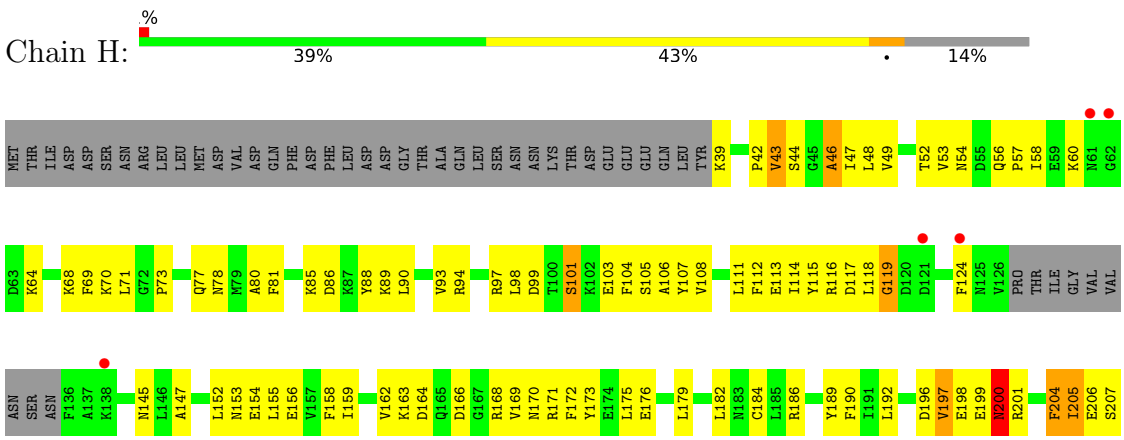
• Molecule 2: Nucleoporin NUP85

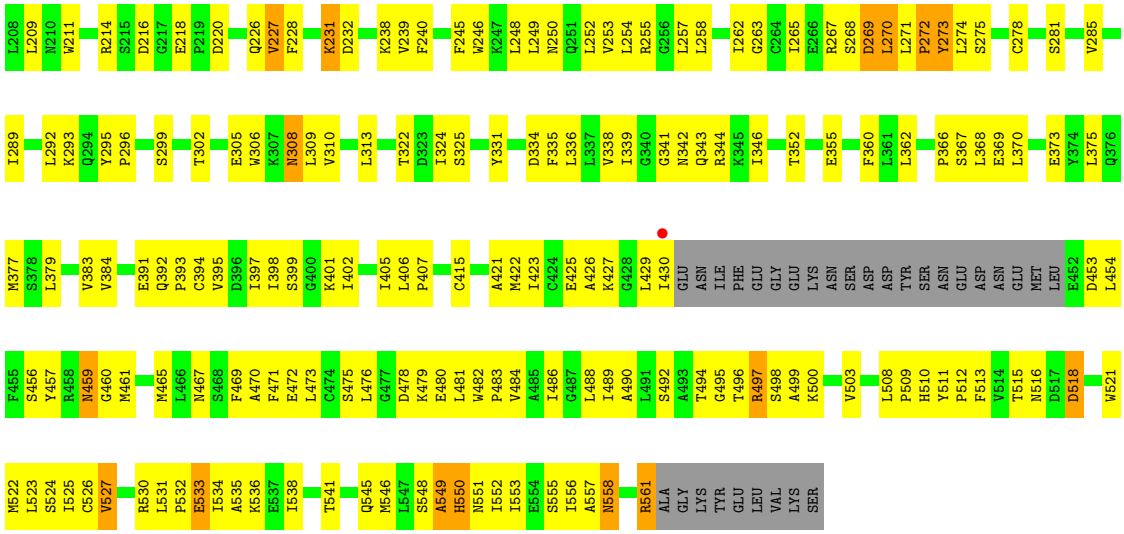
Chain D:





• Molecule 2: Nucleoporin NUP85




L208 L209 N210 W211 R214 S215 D216 G217 E218 P219 D220 Q226 V227 F228 K231 D232 K238 V239 F240 F245 W246 K247 L248 L249 N250 Q251 L252 V253 L254 R255 G256 L257 L258 I262 G263 C264 I265 E266 R267 S268 D269 L270 L271 P272 Y273 L274 S275 C278 S281 V285
I289 L292 K293 Q294 Y295 P296 S299 T302 E305 W306 K307 N308 L309 V310 L313 T322 D323 I324 S325 Y331 D334 F335 L336 L337 V338 I339 G340 G341 N342 Q343 R344 K345 I346 T352 E355 F360 L361 L362 P366 S367 L368 E369 L370 E373 Y374 L375 Q376
M377 S378 L379 V383 V384 E391 Q392 P393 C394 V395 D396 I397 I398 S399 G400 K401 I402 I405 L406 P407 C415 A421 M422 I423 G424 E425 A426 K427 G428 L429 I430 GLU ASN ILE PHE GLU GLY GLU LYS ASN SER ASP ASP TYR SER ASN GLU ASP ASN GLU MET LEU E452 D453 L454
F455 S456 Y457 R458 N459 G460 M461 M465 L466 N467 S468 F469 A470 F471 E472 L473 G474 S475 L476 G477 D478 K479 E480 L481 W482 P483 V484 A485 I486 G487 L488 I489 A490 L491 S492 A493 T494 G495 T496 R497 S498 A499 K500 V503 L508 P509 H510 Y511 P512 F513 V514 T515 N516 D517 D518 W521
M522 L523 S524 I525 C526 V527 R530 L531 P532 E533 I534 A535 K536 E537 I538 T541 Q545 M546 L547 S548 A549 H550 N551 I552 I553 E554 S555 I556 A557 N558 R561 ALA GLY LYS TYR GLU LEU VAL LYS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.38Å 106.49Å 358.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.75 47.52 – 3.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.75) 86.4 (47.52-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.243 , 0.272 0.254 , 0.280	Depositor DCC
R_{free} test set	2062 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å^2)	107.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 78.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.337 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	25114	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.40	0/2437	0.64	0/3301
1	B	0.39	0/2437	0.63	0/3301
1	E	0.39	0/2437	0.64	0/3301
1	F	0.40	0/2437	0.64	0/3301
2	C	0.58	2/4018 (0.0%)	0.67	1/5440 (0.0%)
2	D	0.53	1/3928 (0.0%)	0.67	2/5316 (0.0%)
2	G	0.50	1/3941 (0.0%)	0.66	1/5334 (0.0%)
2	H	0.59	3/4027 (0.1%)	0.67	1/5451 (0.0%)
All	All	0.50	7/25662 (0.0%)	0.66	5/34745 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	39	LYS	CD-CE	5.48	1.65	1.51
2	G	39	LYS	CD-CE	5.47	1.65	1.51
2	H	43	VAL	CB-CG2	5.46	1.64	1.52
2	D	39	LYS	CD-CE	5.43	1.64	1.51
2	C	552	ILE	CA-CB	5.22	1.66	1.54
2	C	554	GLU	CD-OE1	5.08	1.31	1.25
2	H	561	ARG	CZ-NH1	5.03	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	41	ASP	CB-CG-OD1	5.93	123.64	118.30
2	C	43	VAL	CB-CA-C	-5.84	100.30	111.40
2	D	43	VAL	N-CA-C	5.59	126.11	111.00
2	G	40	ARG	CB-CA-C	-5.31	99.77	110.40
2	H	39	LYS	CD-CE-NZ	5.21	123.68	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2379	0	2319	165	0
1	B	2379	0	2319	165	0
1	E	2379	0	2319	170	0
1	F	2379	0	2319	167	0
2	C	3938	0	3892	274	0
2	D	3850	0	3807	257	0
2	G	3863	0	3823	251	0
2	H	3947	0	3905	279	0
All	All	25114	0	24703	1642	0

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

All (1642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:VAL:HG13	2:C:48:LEU:HD22	1.27	1.10
2:D:42:PRO:HB3	2:D:48:LEU:HD22	1.37	1.04
2:H:42:PRO:HB3	2:H:48:LEU:HD22	1.42	0.99
2:H:42:PRO:HD3	2:H:48:LEU:HB2	1.40	0.99
2:D:42:PRO:CG	2:D:48:LEU:HB2	1.94	0.98
2:D:515:THR:HG22	2:D:517:ASP:H	1.24	0.98
1:A:211:HIS:NE2	1:A:233:THR:HG21	1.79	0.97
2:C:43:VAL:CG1	2:C:48:LEU:HD22	1.94	0.97
1:F:211:HIS:NE2	1:F:233:THR:HG21	1.81	0.95
1:B:211:HIS:NE2	1:B:233:THR:HG21	1.84	0.93
2:H:42:PRO:CD	2:H:48:LEU:HB2	1.99	0.92
1:B:81:VAL:HG23	1:B:111:LEU:HD13	1.49	0.92
1:E:81:VAL:HG23	1:E:111:LEU:HD13	1.49	0.91
1:F:81:VAL:HG23	1:F:111:LEU:HD13	1.52	0.91
1:E:211:HIS:NE2	1:E:233:THR:HG21	1.84	0.91
2:G:42:PRO:HD3	2:G:48:LEU:HB2	1.51	0.91
1:A:81:VAL:HG23	1:A:111:LEU:HD13	1.50	0.90
1:B:27:CYS:HB3	1:B:61:ILE:HD11	1.51	0.89
2:H:231:LYS:HE3	2:H:238:LYS:HG2	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:PRO:CB	2:D:48:LEU:HB2	2.03	0.88
1:F:220:TRP:HA	1:F:231:ILE:HG22	1.55	0.88
1:E:27:CYS:HB3	1:E:61:ILE:HD11	1.56	0.87
2:G:453:ASP:HB2	2:G:456:SER:HB2	1.54	0.87
1:A:220:TRP:HA	1:A:231:ILE:HG22	1.57	0.86
2:D:42:PRO:HB3	2:D:48:LEU:HB2	1.58	0.85
2:C:515:THR:HG22	2:C:517:ASP:H	1.41	0.85
1:A:27:CYS:HB3	1:A:61:ILE:HD11	1.59	0.84
2:C:553:ILE:O	2:C:556:ILE:HB	1.77	0.83
2:D:515:THR:HG22	2:D:517:ASP:N	1.94	0.83
1:E:220:TRP:HA	1:E:231:ILE:HG22	1.61	0.83
2:G:515:THR:HG22	2:G:517:ASP:H	1.43	0.82
1:F:27:CYS:HB3	1:F:61:ILE:HD11	1.60	0.82
1:A:213:SER:HB3	1:A:236:LYS:HB3	1.62	0.82
1:A:12:VAL:HA	1:A:28:SER:HB3	1.61	0.81
2:D:422:MET:HB2	2:D:466:LEU:HD11	1.62	0.81
2:H:42:PRO:HD3	2:H:48:LEU:CB	2.09	0.81
1:A:11:LEU:O	1:A:28:SER:HB2	1.80	0.81
1:F:104:LEU:HD13	1:F:137:TYR:CD2	2.16	0.81
1:B:104:LEU:HD13	1:B:137:TYR:CD2	2.16	0.80
2:H:499:ALA:O	2:H:503:VAL:HG23	1.80	0.80
1:E:104:LEU:HD13	1:E:137:TYR:CD2	2.15	0.80
2:D:249:LEU:O	2:D:253:VAL:HG23	1.80	0.80
1:B:220:TRP:HA	1:B:231:ILE:HG22	1.63	0.80
2:C:231:LYS:HE3	2:C:233:SER:HB3	1.64	0.80
1:B:213:SER:HB3	1:B:236:LYS:HB3	1.64	0.80
1:F:11:LEU:O	1:F:28:SER:HB2	1.82	0.80
1:F:12:VAL:HA	1:F:28:SER:HB3	1.62	0.80
1:E:11:LEU:O	1:E:28:SER:HB2	1.81	0.79
2:D:258:LEU:HD22	2:D:292:LEU:HD22	1.65	0.79
2:D:480:GLU:O	2:D:483:PRO:HD2	1.83	0.79
1:F:213:SER:HB3	1:F:236:LYS:HB3	1.65	0.79
1:A:104:LEU:HD13	1:A:137:TYR:CD2	2.17	0.79
1:B:27:CYS:CB	1:B:61:ILE:HD11	2.13	0.78
2:D:42:PRO:CD	2:D:48:LEU:HB2	2.13	0.78
1:E:213:SER:HB3	1:E:236:LYS:HB3	1.66	0.78
2:H:515:THR:HG22	2:H:516:ASN:H	1.47	0.78
2:H:521:TRP:CZ2	2:H:525:ILE:HD11	2.19	0.78
2:G:453:ASP:CB	2:G:456:SER:HB2	2.14	0.78
2:H:47:ILE:CD1	2:H:97:ARG:HE	1.96	0.78
2:D:42:PRO:HB3	2:D:48:LEU:CD2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:249:LEU:O	2:G:253:VAL:HG23	1.83	0.78
2:D:296:PRO:HG3	2:D:302:THR:HG22	1.66	0.77
2:G:296:PRO:HG3	2:G:302:THR:HG22	1.65	0.77
2:C:249:LEU:O	2:C:253:VAL:HG23	1.83	0.77
2:C:258:LEU:HD22	2:C:292:LEU:HD22	1.66	0.77
2:H:553:ILE:CA	2:H:556:ILE:HG22	2.15	0.76
1:A:211:HIS:CD2	1:A:233:THR:HG21	2.21	0.76
2:G:258:LEU:HD22	2:G:292:LEU:HD22	1.67	0.76
2:H:69:PHE:HE1	2:H:71:LEU:HD23	1.50	0.75
2:C:478:ASP:OD1	2:C:480:GLU:HB2	1.85	0.75
1:E:27:CYS:CB	1:E:61:ILE:HD11	2.16	0.75
2:H:258:LEU:HD22	2:H:292:LEU:HD22	1.68	0.75
2:H:296:PRO:HG3	2:H:302:THR:HG22	1.69	0.75
1:F:211:HIS:CD2	1:F:233:THR:HG21	2.20	0.75
1:B:211:HIS:CD2	1:B:233:THR:HG21	2.21	0.75
2:C:406:LEU:HB2	2:C:407:PRO:HD3	1.67	0.75
2:C:296:PRO:HG3	2:C:302:THR:HG22	1.69	0.75
1:E:12:VAL:HA	1:E:28:SER:HB3	1.67	0.75
1:F:54:HIS:HB3	1:F:78:ASP:OD2	1.86	0.75
2:G:42:PRO:CD	2:G:48:LEU:HB2	2.16	0.75
2:G:344:ARG:HH11	2:G:344:ARG:HG3	1.51	0.75
2:H:344:ARG:HH11	2:H:344:ARG:HG3	1.51	0.75
2:C:69:PHE:HE1	2:C:71:LEU:HD23	1.51	0.75
2:D:454:LEU:HD23	2:D:503:VAL:HG21	1.69	0.75
1:B:11:LEU:O	1:B:28:SER:HB2	1.87	0.75
2:H:515:THR:HG22	2:H:516:ASN:N	2.01	0.75
2:D:42:PRO:HD3	2:D:48:LEU:N	2.02	0.74
2:G:278:CYS:HB2	2:G:324:ILE:HG23	1.68	0.74
1:E:324:ASP:HB3	2:G:64:LYS:HG2	1.70	0.74
1:A:208:LEU:HD11	1:A:231:ILE:CD1	2.16	0.74
1:B:54:HIS:HB3	1:B:78:ASP:OD2	1.88	0.74
1:E:211:HIS:CD2	1:E:233:THR:HG21	2.22	0.74
2:H:533:GLU:HA	2:H:533:GLU:OE1	1.88	0.74
2:C:344:ARG:HH11	2:C:344:ARG:HG3	1.50	0.74
1:E:208:LEU:HD11	1:E:231:ILE:CD1	2.17	0.74
1:F:208:LEU:HD11	1:F:231:ILE:CD1	2.18	0.74
2:H:454:LEU:HD23	2:H:503:VAL:HG21	1.70	0.74
2:C:550:HIS:HA	2:C:553:ILE:CD1	2.17	0.73
2:C:499:ALA:O	2:C:503:VAL:HG23	1.87	0.73
2:H:406:LEU:HB2	2:H:407:PRO:HD3	1.69	0.73
2:C:555:SER:HA	2:C:558:ASN:OD1	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:CYS:CB	1:F:61:ILE:HD11	2.18	0.73
2:D:344:ARG:HH11	2:D:344:ARG:HG3	1.52	0.73
2:H:249:LEU:O	2:H:253:VAL:HG23	1.87	0.73
1:A:27:CYS:CB	1:A:61:ILE:HD11	2.19	0.73
1:F:324:ASP:HB3	2:H:64:LYS:HG2	1.71	0.73
2:D:406:LEU:HB2	2:D:407:PRO:HD3	1.71	0.72
2:D:69:PHE:HE1	2:D:71:LEU:HD23	1.52	0.72
1:A:54:HIS:HB3	1:A:78:ASP:OD2	1.89	0.72
2:G:480:GLU:O	2:G:483:PRO:HD2	1.89	0.72
1:B:12:VAL:HA	1:B:28:SER:HB3	1.69	0.72
1:E:54:HIS:HB3	1:E:78:ASP:OD2	1.88	0.72
1:B:81:VAL:HG23	1:B:111:LEU:CD1	2.19	0.72
2:H:42:PRO:CG	2:H:48:LEU:HB2	2.18	0.72
2:G:69:PHE:HE1	2:G:71:LEU:HD23	1.55	0.72
2:G:335:PHE:O	2:G:339:ILE:HG13	1.89	0.72
2:H:184:CYS:HB2	2:H:211:TRP:NE1	2.05	0.72
2:H:278:CYS:HB2	2:H:324:ILE:HG23	1.71	0.72
2:H:478:ASP:OD1	2:H:480:GLU:HB2	1.89	0.72
1:F:124:LYS:HG3	1:F:138:ASP:HB3	1.72	0.71
2:G:406:LEU:HB2	2:G:407:PRO:HD3	1.72	0.71
1:B:208:LEU:HD11	1:B:231:ILE:CD1	2.20	0.71
1:F:334:THR:HG22	1:F:335:TYR:N	2.05	0.71
2:H:335:PHE:O	2:H:339:ILE:HG13	1.90	0.71
2:H:552:ILE:O	2:H:556:ILE:N	2.23	0.71
2:D:184:CYS:HB2	2:D:211:TRP:NE1	2.05	0.71
2:H:511:TYR:HD2	2:H:522:MET:SD	2.13	0.71
2:D:278:CYS:HB2	2:D:324:ILE:HG23	1.71	0.71
2:G:402:ILE:HD12	2:G:429:LEU:HB3	1.71	0.71
2:C:278:CYS:HB2	2:C:324:ILE:HG23	1.72	0.71
2:C:402:ILE:HD12	2:C:429:LEU:HB3	1.71	0.71
2:D:43:VAL:HG23	2:D:44:SER:H	1.56	0.71
1:E:334:THR:HG22	1:E:335:TYR:N	2.05	0.71
2:C:454:LEU:HD23	2:C:503:VAL:HG21	1.73	0.71
2:H:484:VAL:O	2:H:488:LEU:HB2	1.91	0.70
1:B:324:ASP:HB3	2:D:64:LYS:HG2	1.73	0.70
2:D:402:ILE:HD12	2:D:429:LEU:HB3	1.73	0.70
1:B:334:THR:HG22	1:B:335:TYR:N	2.05	0.70
2:C:550:HIS:HA	2:C:553:ILE:HD12	1.72	0.70
2:G:523:LEU:HD21	2:G:538:ILE:HG21	1.73	0.70
1:A:124:LYS:HG3	1:A:138:ASP:HB3	1.74	0.70
2:C:335:PHE:O	2:C:339:ILE:HG13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLY:HA3	2:H:58:ILE:HD12	1.73	0.70
1:E:81:VAL:HG23	1:E:111:LEU:CD1	2.21	0.70
1:F:214:LEU:H	1:F:214:LEU:HD12	1.57	0.70
2:D:335:PHE:O	2:D:339:ILE:HG13	1.91	0.69
1:A:334:THR:HG22	1:A:335:TYR:N	2.06	0.69
1:F:345:ILE:HD13	2:H:93:VAL:HG11	1.74	0.69
2:G:515:THR:HG22	2:G:516:ASN:N	2.05	0.69
2:G:98:LEU:HD11	2:G:476:LEU:HD11	1.73	0.69
2:G:454:LEU:HD23	2:G:503:VAL:HG21	1.74	0.69
2:H:402:ILE:HD12	2:H:429:LEU:HB3	1.74	0.69
2:H:553:ILE:C	2:H:556:ILE:HG22	2.13	0.69
2:H:555:SER:HA	2:H:558:ASN:HB3	1.73	0.69
2:C:252:LEU:HD23	2:C:257:LEU:HD12	1.73	0.69
2:H:252:LEU:HD23	2:H:257:LEU:HD12	1.74	0.69
2:H:553:ILE:HA	2:H:556:ILE:CG2	2.22	0.69
1:F:27:CYS:SG	1:F:61:ILE:HD11	2.34	0.68
2:G:184:CYS:HB2	2:G:211:TRP:NE1	2.08	0.68
2:C:184:CYS:HB2	2:C:211:TRP:NE1	2.08	0.68
2:C:196:ASP:O	2:C:198:GLU:N	2.27	0.68
2:H:231:LYS:HG3	2:H:232:ASP:H	1.57	0.68
1:A:324:ASP:HB3	2:C:64:LYS:HG2	1.75	0.68
2:G:196:ASP:O	2:G:198:GLU:N	2.26	0.68
2:H:68:LYS:HB2	2:H:81:PHE:CE1	2.28	0.68
2:G:531:LEU:HD13	2:G:534:ILE:HD12	1.75	0.68
2:H:548:SER:O	2:H:552:ILE:HG13	1.94	0.68
2:C:265:ILE:HG21	2:C:289:ILE:HD11	1.76	0.68
2:C:515:THR:HG22	2:C:516:ASN:N	2.09	0.68
1:F:236:LYS:O	1:F:306:GLU:HG2	1.94	0.68
2:C:68:LYS:HB2	2:C:81:PHE:CE1	2.29	0.68
1:A:71:ILE:HD11	1:A:145:LEU:HD23	1.76	0.67
1:A:81:VAL:HG23	1:A:111:LEU:CD1	2.22	0.67
2:C:227:VAL:HG21	2:C:248:LEU:HD12	1.75	0.67
2:H:196:ASP:O	2:H:198:GLU:N	2.27	0.67
2:D:341:GLY:HA2	2:D:346:ILE:HD11	1.76	0.67
2:G:265:ILE:HG21	2:G:289:ILE:HD11	1.76	0.67
1:A:167:SER:HA	1:A:188:LEU:CD2	2.25	0.67
1:A:236:LYS:O	1:A:306:GLU:HG2	1.95	0.67
2:G:252:LEU:HD23	2:G:257:LEU:HD12	1.76	0.67
2:G:278:CYS:CB	2:G:324:ILE:HG23	2.24	0.67
1:F:11:LEU:O	1:F:11:LEU:HD12	1.94	0.67
1:A:177:ARG:HG2	1:A:177:ARG:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:ILE:HD11	1:F:145:LEU:HD23	1.77	0.67
1:B:85:GLU:HB3	1:B:101:LEU:HD21	1.77	0.67
2:C:89:LYS:N	2:C:89:LYS:HD2	2.09	0.67
1:F:167:SER:HA	1:F:188:LEU:CD2	2.24	0.67
2:H:47:ILE:HD13	2:H:97:ARG:HE	1.60	0.67
1:A:65:SER:OG	1:A:119:ALA:HB2	1.95	0.67
2:C:118:LEU:HD21	2:C:147:ALA:HB2	1.77	0.67
1:E:236:LYS:O	1:E:306:GLU:HG2	1.94	0.67
2:D:89:LYS:N	2:D:89:LYS:HD2	2.09	0.66
1:B:124:LYS:HG3	1:B:138:ASP:HB3	1.77	0.66
2:G:89:LYS:HD2	2:G:89:LYS:N	2.10	0.66
2:H:541:THR:O	2:H:545:GLN:HG3	1.95	0.66
1:A:214:LEU:HD12	1:A:214:LEU:H	1.60	0.66
2:C:511:TYR:HD2	2:C:522:MET:SD	2.19	0.66
2:C:533:GLU:OE1	2:C:536:LYS:HD2	1.96	0.66
1:F:85:GLU:HB3	1:F:101:LEU:HD21	1.78	0.66
2:G:169:VAL:HG12	2:G:170:ASN:H	1.59	0.66
1:A:209:PRO:HG3	2:D:315:GLN:HA	1.77	0.66
1:B:214:LEU:H	1:B:214:LEU:HD12	1.61	0.66
2:H:89:LYS:HD2	2:H:89:LYS:N	2.11	0.66
2:D:196:ASP:O	2:D:198:GLU:N	2.29	0.66
2:G:341:GLY:HA2	2:G:346:ILE:HD11	1.77	0.66
2:H:240:PHE:CE2	2:H:269:ASP:HB3	2.31	0.66
2:D:42:PRO:HD3	2:D:48:LEU:HB2	1.75	0.66
1:E:241:ARG:HG2	1:E:241:ARG:HH11	1.60	0.66
1:B:11:LEU:O	1:B:11:LEU:HD12	1.96	0.66
1:E:27:CYS:SG	1:E:61:ILE:HD11	2.35	0.66
1:E:214:LEU:H	1:E:214:LEU:HD12	1.60	0.66
2:H:105:SER:HB2	2:H:481:LEU:HD21	1.77	0.66
2:H:454:LEU:HB2	2:H:499:ALA:HB1	1.78	0.66
2:D:42:PRO:HB3	2:D:48:LEU:CB	2.26	0.66
1:E:167:SER:HA	1:E:188:LEU:CD2	2.26	0.66
1:B:236:LYS:O	1:B:306:GLU:HG2	1.96	0.65
1:B:329:ARG:HG2	1:B:344:VAL:HG22	1.77	0.65
2:C:41:ASP:O	2:C:48:LEU:N	2.27	0.65
1:B:177:ARG:O	1:B:177:ARG:HG2	1.96	0.65
2:D:201:ARG:CZ	2:D:205:ILE:HD11	2.26	0.65
1:E:329:ARG:HH12	2:G:44:SER:HB2	1.62	0.65
1:A:326:GLY:HA3	2:C:58:ILE:HD12	1.78	0.65
2:D:523:LEU:HD21	2:D:538:ILE:HG21	1.77	0.65
2:G:42:PRO:HB3	2:G:48:LEU:HD22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HG22	1:B:159:ILE:O	1.97	0.65
2:D:42:PRO:HG3	2:D:48:LEU:HB2	1.77	0.65
1:E:124:LYS:HG3	1:E:138:ASP:HB3	1.77	0.65
1:F:81:VAL:HG23	1:F:111:LEU:CD1	2.25	0.65
1:F:177:ARG:O	1:F:177:ARG:HG2	1.95	0.65
2:H:265:ILE:HG21	2:H:289:ILE:HD11	1.78	0.65
2:C:418:ALA:HB1	2:C:466:LEU:HD23	1.78	0.65
2:H:255:ARG:HB2	2:H:257:LEU:HG	1.77	0.65
2:C:124:PHE:HB2	2:C:426:ALA:O	1.97	0.65
2:H:533:GLU:OE1	2:H:536:LYS:HD2	1.96	0.65
1:A:345:ILE:HD13	2:C:93:VAL:HG11	1.79	0.65
1:E:159:ILE:HG22	1:E:159:ILE:O	1.97	0.65
1:E:177:ARG:O	1:E:177:ARG:HG2	1.97	0.65
1:B:27:CYS:SG	1:B:61:ILE:HD11	2.37	0.65
1:A:27:CYS:SG	1:A:61:ILE:HD11	2.37	0.64
2:D:278:CYS:CB	2:D:324:ILE:HG23	2.27	0.64
2:H:278:CYS:CB	2:H:324:ILE:HG23	2.27	0.64
2:H:335:PHE:CE2	2:H:339:ILE:HD11	2.32	0.64
2:H:546:MET:O	2:H:549:ALA:HB3	1.98	0.64
2:C:255:ARG:HB2	2:C:257:LEU:HG	1.78	0.64
1:B:241:ARG:HG2	1:B:241:ARG:HH11	1.62	0.64
2:C:201:ARG:CZ	2:C:205:ILE:HD11	2.27	0.64
2:C:278:CYS:HB3	2:C:281:SER:HB2	1.79	0.64
2:C:480:GLU:O	2:C:483:PRO:HD2	1.97	0.64
1:F:329:ARG:HG2	1:F:344:VAL:HG22	1.78	0.64
1:B:71:ILE:HD11	1:B:145:LEU:HD23	1.79	0.64
2:G:240:PHE:CE2	2:G:269:ASP:HB3	2.32	0.64
1:A:85:GLU:HB3	1:A:101:LEU:HD21	1.80	0.64
1:A:241:ARG:HG2	1:A:241:ARG:HH11	1.61	0.64
2:D:240:PHE:CE2	2:D:269:ASP:HB3	2.32	0.64
2:C:335:PHE:CE2	2:C:339:ILE:HD11	2.32	0.64
2:D:169:VAL:HG12	2:D:170:ASN:H	1.62	0.64
2:D:252:LEU:HD23	2:D:257:LEU:HD12	1.78	0.64
1:E:205:ALA:HB1	1:E:292:LEU:HD12	1.79	0.64
1:E:208:LEU:HD11	1:E:231:ILE:HD11	1.80	0.64
1:F:167:SER:HA	1:F:188:LEU:HD21	1.80	0.64
2:G:201:ARG:CZ	2:G:205:ILE:HD11	2.28	0.64
2:C:169:VAL:HG12	2:C:170:ASN:H	1.62	0.64
2:H:278:CYS:HB3	2:H:281:SER:HB2	1.80	0.64
2:C:240:PHE:CE2	2:C:269:ASP:HB3	2.33	0.63
2:H:201:ARG:CZ	2:H:205:ILE:HD11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:O	1:A:11:LEU:HD12	1.98	0.63
2:C:114:ILE:HD11	2:C:154:GLU:HG3	1.81	0.63
2:H:118:LEU:HD21	2:H:147:ALA:HB2	1.80	0.63
1:F:159:ILE:O	1:F:159:ILE:HG22	1.97	0.63
1:A:167:SER:HA	1:A:188:LEU:HD21	1.81	0.63
1:F:65:SER:OG	1:F:119:ALA:HB2	1.98	0.63
1:A:12:VAL:HA	1:A:28:SER:CB	2.29	0.63
1:A:159:ILE:O	1:A:159:ILE:HG22	1.99	0.63
2:C:278:CYS:CB	2:C:324:ILE:HG23	2.28	0.63
1:E:85:GLU:HB3	1:E:101:LEU:HD21	1.79	0.63
2:G:402:ILE:CD1	2:G:429:LEU:HD13	2.29	0.63
2:H:169:VAL:HG12	2:H:170:ASN:H	1.64	0.63
2:D:68:LYS:HB2	2:D:81:PHE:CE1	2.34	0.63
1:E:11:LEU:O	1:E:11:LEU:HD12	1.98	0.63
1:E:329:ARG:HG2	1:E:344:VAL:HG22	1.80	0.63
1:F:301:ASP:O	1:F:303:HIS:N	2.32	0.63
2:C:546:MET:O	2:C:549:ALA:HB3	1.99	0.63
2:D:265:ILE:HG21	2:D:289:ILE:HD11	1.80	0.63
1:F:335:TYR:HB3	2:G:373:GLU:HG3	1.80	0.63
2:H:192:LEU:HD11	2:H:204:PHE:CD2	2.33	0.63
2:C:43:VAL:HG13	2:C:48:LEU:CD2	2.18	0.63
1:F:241:ARG:HG2	1:F:241:ARG:HH11	1.63	0.63
1:F:334:THR:HG22	1:F:336:SER:H	1.63	0.63
2:G:278:CYS:HB3	2:G:281:SER:HB2	1.80	0.62
2:G:543:GLY:O	2:G:547:LEU:HG	1.99	0.62
2:H:114:ILE:HD11	2:H:154:GLU:HG3	1.81	0.62
2:H:453:ASP:HB3	2:H:456:SER:HB2	1.81	0.62
2:C:192:LEU:HD11	2:C:204:PHE:CD2	2.35	0.62
2:D:531:LEU:HD13	2:D:534:ILE:HD12	1.81	0.62
2:D:335:PHE:CE2	2:D:339:ILE:HD11	2.33	0.62
1:E:71:ILE:HD11	1:E:145:LEU:HD23	1.80	0.62
2:G:240:PHE:CD2	2:G:268:SER:HB2	2.34	0.62
2:G:197:VAL:HG12	2:G:197:VAL:O	1.99	0.62
2:H:531:LEU:HD13	2:H:534:ILE:HD12	1.80	0.62
2:C:496:THR:HG22	2:C:497:ARG:H	1.65	0.62
2:H:341:GLY:HA2	2:H:346:ILE:HD11	1.82	0.62
1:A:334:THR:HG22	1:A:336:SER:H	1.65	0.62
2:G:68:LYS:HB2	2:G:81:PHE:CE1	2.34	0.62
2:H:480:GLU:O	2:H:483:PRO:HD2	1.98	0.62
1:E:65:SER:OG	1:E:119:ALA:HB2	2.00	0.62
1:A:208:LEU:HD11	1:A:231:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLN:HG2	1:B:56:SER:O	2.00	0.62
2:C:541:THR:O	2:C:545:GLN:HG3	2.00	0.62
2:D:42:PRO:HD3	2:D:48:LEU:CB	2.29	0.62
1:A:329:ARG:HH12	2:C:44:SER:HB2	1.64	0.61
2:D:255:ARG:HB2	2:D:257:LEU:HG	1.81	0.61
2:C:197:VAL:O	2:C:197:VAL:HG12	1.99	0.61
2:D:278:CYS:HB3	2:D:281:SER:HB2	1.81	0.61
2:D:402:ILE:CD1	2:D:429:LEU:HD13	2.30	0.61
1:F:12:VAL:HA	1:F:28:SER:CB	2.30	0.61
2:H:197:VAL:O	2:H:197:VAL:HG12	1.99	0.61
1:B:167:SER:HA	1:B:188:LEU:CD2	2.30	0.61
1:B:345:ILE:HD13	2:D:93:VAL:HG11	1.83	0.61
2:D:197:VAL:O	2:D:197:VAL:HG12	2.00	0.61
2:D:240:PHE:CD2	2:D:269:ASP:HB3	2.35	0.61
2:G:255:ARG:HB2	2:G:257:LEU:HG	1.80	0.61
2:G:552:ILE:C	2:G:554:GLU:H	2.04	0.61
1:B:159:ILE:HD12	1:B:159:ILE:N	2.15	0.61
2:H:515:THR:HB	2:H:518:ASP:OD1	2.00	0.61
1:B:208:LEU:HD11	1:B:231:ILE:HD11	1.82	0.61
1:F:168:ASP:H	1:F:188:LEU:HD23	1.64	0.61
2:C:240:PHE:CD2	2:C:268:SER:HB2	2.35	0.61
1:E:168:ASP:H	1:E:188:LEU:HD23	1.65	0.61
2:H:456:SER:OG	2:H:457:TYR:N	2.33	0.61
1:B:131:ASP:OD2	1:B:133:ILE:HD12	2.01	0.61
1:B:205:ALA:HB1	1:B:292:LEU:HD12	1.83	0.61
2:G:478:ASP:OD1	2:G:480:GLU:HB2	2.01	0.61
2:H:240:PHE:CD2	2:H:268:SER:HB2	2.35	0.61
2:C:523:LEU:O	2:C:526:CYS:HB2	2.00	0.61
2:G:107:TYR:CZ	2:G:111:LEU:HD11	2.36	0.61
1:A:301:ASP:O	1:A:303:HIS:N	2.34	0.60
1:A:329:ARG:HG2	1:A:344:VAL:HG22	1.81	0.60
1:E:226:ARG:HH11	1:E:226:ARG:HG3	1.64	0.60
1:F:214:LEU:HD12	1:F:214:LEU:N	2.16	0.60
1:A:131:ASP:OD2	1:A:133:ILE:HD12	2.02	0.60
1:A:168:ASP:H	1:A:188:LEU:HD23	1.65	0.60
2:C:554:GLU:O	2:C:558:ASN:HB3	2.01	0.60
1:E:345:ILE:HD13	2:G:93:VAL:HG11	1.82	0.60
2:H:334:ASP:O	2:H:338:VAL:HG23	2.01	0.60
1:B:65:SER:OG	1:B:119:ALA:HB2	2.01	0.60
2:H:553:ILE:O	2:H:556:ILE:HG22	2.02	0.60
2:C:459:ASN:OD1	2:C:494:THR:HB	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:551:ASN:O	2:C:554:GLU:HB3	2.02	0.60
1:E:302:ASP:OD2	2:G:44:SER:HB3	2.01	0.60
1:A:312:TRP:CE2	1:A:319:LEU:HD13	2.36	0.60
2:C:515:THR:CG2	2:C:516:ASN:N	2.65	0.60
1:F:183:LEU:HD12	1:F:184:ALA:N	2.16	0.60
2:G:299:SER:HB3	2:G:302:THR:OG1	2.01	0.60
2:H:392:GLN:HB3	2:H:393:PRO:HD3	1.84	0.60
2:H:510:HIS:O	2:H:512:PRO:HD3	2.02	0.60
2:C:341:GLY:HA2	2:C:346:ILE:HD11	1.84	0.60
2:D:240:PHE:CD2	2:D:268:SER:HB2	2.36	0.60
1:E:334:THR:HG22	1:E:336:SER:H	1.67	0.60
2:H:240:PHE:CD2	2:H:269:ASP:HB3	2.37	0.60
2:H:553:ILE:HA	2:H:556:ILE:HG22	1.81	0.60
1:B:334:THR:HG22	1:B:336:SER:H	1.66	0.60
2:D:405:ILE:HG13	2:D:406:LEU:N	2.17	0.60
1:F:208:LEU:HD11	1:F:231:ILE:HD11	1.82	0.60
1:A:117:ALA:HB2	1:A:173:TRP:CZ2	2.37	0.59
1:B:145:LEU:H	1:B:145:LEU:HD12	1.67	0.59
2:D:299:SER:HB3	2:D:302:THR:OG1	2.01	0.59
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.66	0.59
1:E:131:ASP:OD2	1:E:133:ILE:HD12	2.02	0.59
1:E:231:ILE:CD1	1:E:245:ILE:HD11	2.32	0.59
2:G:240:PHE:CD2	2:G:269:ASP:HB3	2.37	0.59
1:E:159:ILE:HD12	1:E:159:ILE:N	2.17	0.59
1:F:312:TRP:CE2	1:F:319:LEU:HD13	2.36	0.59
1:E:12:VAL:HA	1:E:28:SER:CB	2.32	0.59
1:E:117:ALA:HB2	1:E:173:TRP:CZ2	2.37	0.59
1:E:225:GLY:HA2	2:G:503:VAL:HG22	1.85	0.59
2:G:335:PHE:CE2	2:G:339:ILE:HD11	2.38	0.59
2:G:383:VAL:HG12	2:G:384:VAL:N	2.17	0.59
2:H:108:VAL:HG22	2:H:469:PHE:HZ	1.67	0.59
2:C:107:TYR:CZ	2:C:111:LEU:HD11	2.38	0.59
1:A:31:GLN:HG2	1:A:56:SER:O	2.02	0.59
2:C:482:TRP:NE1	2:C:512:PRO:HD2	2.17	0.59
1:E:84:TRP:HA	1:E:99:ASN:O	2.03	0.59
2:C:392:GLN:HB3	2:C:393:PRO:HD3	1.85	0.59
1:E:10:ASP:C	2:G:88:TYR:HE2	2.06	0.59
2:G:515:THR:CG2	2:G:516:ASN:N	2.65	0.59
1:B:301:ASP:O	1:B:303:HIS:N	2.36	0.59
2:C:240:PHE:CD2	2:C:269:ASP:HB3	2.38	0.59
2:D:392:GLN:HB3	2:D:393:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:LEU:HA	1:F:129:GLY:HA2	1.85	0.59
1:F:159:ILE:HD12	1:F:159:ILE:N	2.18	0.59
1:F:226:ARG:HH11	1:F:226:ARG:HG3	1.68	0.59
2:G:192:LEU:HD11	2:G:204:PHE:CD2	2.37	0.59
1:B:117:ALA:HB2	1:B:173:TRP:CZ2	2.38	0.59
2:C:78:ASN:HB2	2:C:93:VAL:O	2.03	0.59
2:D:192:LEU:HD11	2:D:204:PHE:CD2	2.38	0.59
2:D:383:VAL:HG12	2:D:384:VAL:N	2.18	0.59
1:E:167:SER:HA	1:E:188:LEU:HD21	1.84	0.59
1:A:159:ILE:N	1:A:159:ILE:HD12	2.18	0.58
1:B:85:GLU:CB	1:B:101:LEU:HD21	2.32	0.58
2:C:231:LYS:CE	2:C:233:SER:HB3	2.30	0.58
1:E:77:TYR:HD1	1:E:110:SER:HB2	1.67	0.58
2:C:299:SER:HB3	2:C:302:THR:OG1	2.03	0.58
2:C:383:VAL:HG12	2:C:384:VAL:N	2.18	0.58
2:D:107:TYR:CZ	2:D:111:LEU:HD11	2.38	0.58
1:E:170:CYS:SG	1:E:218:ILE:HG22	2.42	0.58
2:G:274:LEU:HD22	2:G:281:SER:HB3	1.85	0.58
2:G:392:GLN:HB3	2:G:393:PRO:HD3	1.84	0.58
1:B:84:TRP:HA	1:B:99:ASN:O	2.03	0.58
2:D:306:TRP:O	2:D:310:VAL:HG23	2.03	0.58
1:F:85:GLU:CB	1:F:101:LEU:HD21	2.32	0.58
1:F:171:LEU:N	1:F:171:LEU:HD23	2.18	0.58
2:H:227:VAL:HG21	2:H:248:LEU:HD12	1.84	0.58
1:A:84:TRP:HA	1:A:99:ASN:O	2.04	0.58
2:C:295:TYR:HD1	2:C:296:PRO:HD2	1.68	0.58
2:C:334:ASP:O	2:C:338:VAL:HG23	2.03	0.58
1:E:171:LEU:HD23	1:E:171:LEU:N	2.18	0.58
1:E:194:TYR:CE1	1:E:204:VAL:HG22	2.39	0.58
1:F:325:ASP:O	1:F:327:LYS:HG3	2.03	0.58
1:B:168:ASP:H	1:B:188:LEU:HD23	1.68	0.58
1:E:325:ASP:O	1:E:327:LYS:HG3	2.03	0.58
2:G:113:GLU:O	2:G:116:ARG:HG2	2.04	0.58
2:G:451:LEU:CD2	2:G:458:ARG:HG3	2.33	0.58
1:A:171:LEU:N	1:A:171:LEU:HD23	2.17	0.58
2:C:274:LEU:HD22	2:C:281:SER:HB3	1.85	0.58
2:H:107:TYR:CZ	2:H:111:LEU:HD11	2.38	0.58
2:H:197:VAL:O	2:H:197:VAL:CG1	2.52	0.58
2:D:227:VAL:HG21	2:D:248:LEU:HD12	1.86	0.58
2:D:454:LEU:CD2	2:D:503:VAL:HG21	2.33	0.58
1:E:31:GLN:HG2	1:E:56:SER:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:394:CYS:O	2:G:398:ILE:HG22	2.04	0.58
2:H:274:LEU:HD22	2:H:281:SER:HB3	1.85	0.58
1:B:12:VAL:HA	1:B:28:SER:CB	2.34	0.58
1:B:171:LEU:HD23	1:B:171:LEU:N	2.18	0.58
2:C:521:TRP:CZ2	2:C:525:ILE:HD11	2.39	0.58
1:F:85:GLU:HB2	1:F:101:LEU:HD11	1.86	0.58
1:A:213:SER:CB	1:A:236:LYS:HB3	2.34	0.58
1:B:325:ASP:O	1:B:327:LYS:HG3	2.03	0.58
2:D:334:ASP:O	2:D:338:VAL:HG23	2.04	0.58
2:D:262:ILE:HG23	2:D:289:ILE:HG23	1.86	0.57
2:G:306:TRP:O	2:G:310:VAL:HG23	2.03	0.57
1:A:231:ILE:CD1	1:A:245:ILE:HD11	2.34	0.57
2:D:500:LYS:O	2:D:504:ILE:HG13	2.03	0.57
1:E:214:LEU:HD12	1:E:214:LEU:N	2.19	0.57
1:F:92:GLU:O	1:F:93:CYS:HB2	2.04	0.57
1:F:205:ALA:HB1	1:F:292:LEU:HD12	1.86	0.57
2:H:459:ASN:N	2:H:459:ASN:HD22	2.02	0.57
2:H:186:ARG:HG3	2:H:190:PHE:HB2	1.87	0.57
1:E:301:ASP:O	1:E:303:HIS:N	2.36	0.57
1:F:131:ASP:OD2	1:F:133:ILE:HD12	2.03	0.57
1:F:156:VAL:O	1:F:157:LEU:HG	2.03	0.57
2:G:42:PRO:HD3	2:G:48:LEU:CB	2.27	0.57
2:G:186:ARG:HG3	2:G:190:PHE:HB2	1.86	0.57
2:G:406:LEU:HD22	2:G:421:ALA:HB2	1.86	0.57
2:H:299:SER:HB3	2:H:302:THR:OG1	2.04	0.57
2:H:508:LEU:HD11	2:H:522:MET:HG3	1.85	0.57
1:A:183:LEU:HD12	1:A:184:ALA:N	2.20	0.57
1:B:156:VAL:O	1:B:157:LEU:HG	2.04	0.57
2:C:482:TRP:N	2:C:483:PRO:CD	2.67	0.57
2:D:524:SER:O	2:D:527:VAL:HB	2.03	0.57
2:H:166:ASP:HB3	2:H:169:VAL:CG2	2.35	0.57
2:C:478:ASP:O	2:C:480:GLU:N	2.37	0.57
1:E:176:SER:HB2	1:E:223:SER:OG	2.05	0.57
2:G:262:ILE:HG23	2:G:289:ILE:HG23	1.86	0.57
2:H:383:VAL:HG12	2:H:384:VAL:N	2.20	0.57
2:C:42:PRO:HB3	2:C:46:ALA:C	2.25	0.57
1:E:156:VAL:O	1:E:157:LEU:HG	2.04	0.57
1:E:183:LEU:HD12	1:E:184:ALA:N	2.20	0.57
1:F:77:TYR:HD1	1:F:110:SER:HB2	1.68	0.57
1:A:26:THR:HG22	1:A:27:CYS:H	1.68	0.57
1:A:85:GLU:CB	1:A:101:LEU:HD21	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HH11	1:A:226:ARG:HG3	1.70	0.57
2:D:113:GLU:O	2:D:116:ARG:HG2	2.05	0.57
2:D:425:GLU:HB2	2:D:430:ILE:HD11	1.86	0.57
2:D:515:THR:CG2	2:D:516:ASN:N	2.67	0.57
2:H:270:LEU:HG	2:H:271:LEU:N	2.20	0.57
1:A:205:ALA:HB1	1:A:292:LEU:HD12	1.87	0.57
1:B:176:SER:HB2	1:B:223:SER:OG	2.04	0.57
2:C:113:GLU:O	2:C:116:ARG:HG2	2.05	0.57
2:C:523:LEU:HD23	2:C:538:ILE:HD12	1.86	0.57
1:E:85:GLU:CB	1:E:101:LEU:HD21	2.35	0.57
1:F:84:TRP:HA	1:F:99:ASN:O	2.04	0.57
2:H:42:PRO:HG3	2:H:48:LEU:HB2	1.86	0.57
2:H:285:VAL:O	2:H:289:ILE:HG13	2.05	0.57
1:A:38:LEU:HD21	2:C:77:GLN:HG3	1.85	0.57
1:A:156:VAL:O	1:A:157:LEU:HG	2.05	0.57
1:B:231:ILE:CD1	1:B:245:ILE:HD11	2.35	0.57
1:F:117:ALA:HB2	1:F:173:TRP:CZ2	2.40	0.57
2:G:405:ILE:HG13	2:G:406:LEU:N	2.20	0.57
1:A:145:LEU:H	1:A:145:LEU:HD12	1.69	0.56
1:A:176:SER:HB2	1:A:223:SER:OG	2.05	0.56
2:C:197:VAL:O	2:C:197:VAL:CG1	2.53	0.56
2:C:394:CYS:O	2:C:398:ILE:HG22	2.05	0.56
2:C:496:THR:HG22	2:C:497:ARG:N	2.20	0.56
2:D:394:CYS:O	2:D:398:ILE:HG22	2.05	0.56
2:D:453:ASP:CB	2:D:456:SER:HB2	2.35	0.56
1:A:214:LEU:HD12	1:A:214:LEU:N	2.19	0.56
1:B:213:SER:CB	1:B:236:LYS:HB3	2.35	0.56
2:D:515:THR:HG22	2:D:516:ASN:N	2.20	0.56
1:E:158:SER:C	1:E:159:ILE:HD12	2.26	0.56
1:F:31:GLN:HG2	1:F:56:SER:O	2.05	0.56
2:G:425:GLU:HB2	2:G:430:ILE:HD11	1.87	0.56
2:C:163:LYS:HE3	2:C:168:ARG:HH21	1.70	0.56
2:C:550:HIS:O	2:C:553:ILE:HB	2.05	0.56
1:E:121:LEU:HD21	1:E:181:GLU:HB2	1.88	0.56
2:G:500:LYS:O	2:G:504:ILE:HG13	2.06	0.56
2:H:113:GLU:O	2:H:116:ARG:HG2	2.05	0.56
2:H:402:ILE:CD1	2:H:429:LEU:HD13	2.36	0.56
2:H:454:LEU:HD13	2:H:495:GLY:HA3	1.87	0.56
2:C:270:LEU:HG	2:C:271:LEU:N	2.19	0.56
2:C:534:ILE:O	2:C:538:ILE:HG13	2.06	0.56
2:D:42:PRO:CD	2:D:48:LEU:N	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:VAL:O	2:D:197:VAL:CG1	2.54	0.56
2:D:285:VAL:O	2:D:289:ILE:HG13	2.05	0.56
1:F:209:PRO:HG3	2:G:315:GLN:HA	1.88	0.56
1:B:194:TYR:CE1	1:B:204:VAL:HG22	2.40	0.56
1:B:322:ALA:HB2	1:B:328:VAL:HG22	1.87	0.56
2:C:554:GLU:O	2:C:558:ASN:N	2.35	0.56
2:D:199:GLU:HG2	2:D:199:GLU:O	2.06	0.56
2:H:231:LYS:HE3	2:H:238:LYS:CG	2.30	0.56
1:A:77:TYR:HD1	1:A:110:SER:HB2	1.69	0.56
2:C:393:PRO:O	2:C:397:ILE:HG13	2.05	0.56
1:A:228:TYR:HD2	1:A:244:LYS:HG3	1.71	0.56
1:B:26:THR:HG22	1:B:27:CYS:H	1.70	0.56
1:B:167:SER:HA	1:B:188:LEU:HD21	1.88	0.56
2:C:186:ARG:HG3	2:C:190:PHE:HB2	1.88	0.56
2:H:240:PHE:HD2	2:H:268:SER:HB2	1.71	0.56
1:A:57:SER:HB2	1:A:77:TYR:HD2	1.71	0.56
1:A:209:PRO:HB2	2:D:318:GLY:HA3	1.88	0.56
2:D:470:ALA:HA	2:D:473:LEU:HD12	1.86	0.56
1:F:228:TYR:HD2	1:F:244:LYS:HG3	1.70	0.56
2:G:285:VAL:O	2:G:289:ILE:HG13	2.06	0.56
2:G:296:PRO:CG	2:G:302:THR:HG22	2.36	0.56
1:B:158:SER:C	1:B:159:ILE:HD12	2.26	0.56
2:C:262:ILE:HG23	2:C:289:ILE:HG23	1.88	0.56
2:D:270:LEU:HG	2:D:271:LEU:N	2.20	0.56
2:D:393:PRO:O	2:D:397:ILE:HG13	2.06	0.56
2:D:274:LEU:HD22	2:D:281:SER:HB3	1.88	0.56
1:E:312:TRP:CE2	1:E:319:LEU:HD13	2.41	0.56
1:F:71:ILE:HD11	1:F:145:LEU:CD2	2.36	0.56
1:F:231:ILE:CD1	1:F:245:ILE:HD11	2.36	0.56
2:H:496:THR:HG22	2:H:498:SER:H	1.71	0.56
1:B:92:GLU:O	1:B:93:CYS:HB2	2.06	0.55
1:E:26:THR:HG22	1:E:27:CYS:H	1.70	0.55
2:G:197:VAL:O	2:G:197:VAL:CG1	2.52	0.55
2:H:391:GLU:O	2:H:395:VAL:HG23	2.05	0.55
1:B:214:LEU:HD12	1:B:214:LEU:N	2.20	0.55
2:G:240:PHE:HD2	2:G:268:SER:HB2	1.70	0.55
2:G:295:TYR:HD1	2:G:296:PRO:HD2	1.72	0.55
2:G:492:SER:O	2:G:494:THR:N	2.38	0.55
2:H:515:THR:CG2	2:H:516:ASN:H	2.16	0.55
1:A:111:LEU:HA	1:A:129:GLY:HA2	1.89	0.55
1:B:121:LEU:HD21	1:B:181:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:296:PRO:CG	2:D:302:THR:HG22	2.36	0.55
1:F:26:THR:HG22	1:F:27:CYS:H	1.70	0.55
1:F:121:LEU:HD21	1:F:181:GLU:HB2	1.87	0.55
1:F:209:PRO:HB2	2:G:318:GLY:HA3	1.88	0.55
2:G:484:VAL:O	2:G:488:LEU:HB2	2.05	0.55
1:F:145:LEU:HD12	1:F:145:LEU:H	1.71	0.55
1:A:335:TYR:HB3	2:D:373:GLU:HG3	1.88	0.55
1:B:77:TYR:HD1	1:B:110:SER:HB2	1.69	0.55
1:E:334:THR:CG2	1:E:335:TYR:N	2.70	0.55
2:G:42:PRO:HD2	2:G:46:ALA:O	2.07	0.55
2:H:406:LEU:HD22	2:H:421:ALA:HB2	1.88	0.55
1:A:325:ASP:O	1:A:327:LYS:HG3	2.06	0.55
1:B:57:SER:HB2	1:B:77:TYR:HD2	1.71	0.55
2:C:524:SER:O	2:C:527:VAL:HB	2.06	0.55
2:C:531:LEU:HD13	2:C:534:ILE:HD12	1.88	0.55
2:D:486:ILE:HD12	2:D:504:ILE:HG23	1.89	0.55
1:A:38:LEU:CD2	2:C:77:GLN:HG3	2.37	0.55
1:A:71:ILE:HD11	1:A:145:LEU:CD2	2.36	0.55
2:C:166:ASP:HB3	2:C:169:VAL:CG2	2.36	0.55
1:E:68:TYR:CG	1:E:123:LEU:HD13	2.42	0.55
1:F:38:LEU:HD21	2:H:77:GLN:HG3	1.88	0.55
2:H:553:ILE:HA	2:H:556:ILE:HG21	1.89	0.55
2:C:515:THR:HB	2:C:518:ASP:OD1	2.06	0.55
2:D:537:GLU:O	2:D:540:THR:HB	2.07	0.55
1:E:322:ALA:HB2	1:E:328:VAL:HG22	1.88	0.55
2:G:393:PRO:O	2:G:397:ILE:HG13	2.07	0.55
2:H:68:LYS:HD2	2:H:81:PHE:HE1	1.71	0.55
2:H:295:TYR:HD1	2:H:296:PRO:HD2	1.70	0.55
1:F:57:SER:HB2	1:F:77:TYR:HD2	1.71	0.55
2:G:199:GLU:O	2:G:199:GLU:HG2	2.06	0.55
1:A:92:GLU:O	1:A:93:CYS:HB2	2.07	0.55
2:D:484:VAL:O	2:D:488:LEU:HB2	2.07	0.55
1:F:334:THR:CG2	1:F:335:TYR:N	2.70	0.55
2:H:163:LYS:HE3	2:H:168:ARG:HH21	1.72	0.55
2:H:496:THR:HG22	2:H:497:ARG:N	2.22	0.55
1:B:96:ARG:HG2	1:B:96:ARG:HH11	1.71	0.54
1:B:241:ARG:NH1	1:B:299:GLU:OE2	2.40	0.54
2:D:197:VAL:HB	2:D:366:PRO:HB2	1.89	0.54
1:E:92:GLU:O	1:E:93:CYS:HB2	2.06	0.54
1:E:145:LEU:H	1:E:145:LEU:HD12	1.72	0.54
1:E:224:ILE:HD12	1:E:315:THR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:HIS:HB3	1:F:177:ARG:HG3	1.89	0.54
1:F:192:ILE:CG2	1:F:204:VAL:HG13	2.37	0.54
1:F:213:SER:CB	1:F:236:LYS:HB3	2.36	0.54
2:H:306:TRP:O	2:H:310:VAL:HG23	2.07	0.54
1:A:346:THR:OG1	1:A:347:ALA:N	2.39	0.54
1:B:312:TRP:CE2	1:B:319:LEU:HD13	2.41	0.54
1:B:324:ASP:C	1:B:326:GLY:H	2.09	0.54
1:B:326:GLY:HA3	2:D:58:ILE:HD12	1.88	0.54
2:C:240:PHE:HD2	2:C:268:SER:HB2	1.70	0.54
2:C:453:ASP:CB	2:C:456:SER:HB2	2.37	0.54
1:F:346:THR:OG1	1:F:347:ALA:N	2.38	0.54
1:B:71:ILE:HD11	1:B:145:LEU:CD2	2.37	0.54
2:C:425:GLU:HB2	2:C:430:ILE:HD11	1.89	0.54
2:D:186:ARG:HG3	2:D:190:PHE:HB2	1.88	0.54
2:D:379:LEU:HD22	2:D:384:VAL:HG22	1.90	0.54
1:E:336:SER:HA	2:H:370:LEU:HD22	1.89	0.54
2:H:394:CYS:O	2:H:398:ILE:HG22	2.07	0.54
2:H:534:ILE:O	2:H:538:ILE:HG13	2.08	0.54
1:A:26:THR:HG22	1:A:27:CYS:N	2.23	0.54
2:C:523:LEU:HD23	2:C:538:ILE:CD1	2.37	0.54
1:E:57:SER:HB2	1:E:77:TYR:HD2	1.72	0.54
1:A:85:GLU:HB2	1:A:101:LEU:HD11	1.88	0.54
1:B:336:SER:HA	2:C:370:LEU:HD22	1.88	0.54
1:F:104:LEU:HD13	1:F:137:TYR:CE2	2.42	0.54
1:F:181:GLU:OE1	1:F:196:ARG:HD3	2.07	0.54
2:G:52:THR:HG22	2:G:53:VAL:N	2.23	0.54
2:G:166:ASP:HB3	2:G:169:VAL:CG2	2.38	0.54
2:G:169:VAL:HG12	2:G:170:ASN:N	2.23	0.54
2:G:196:ASP:C	2:G:198:GLU:H	2.11	0.54
2:C:405:ILE:HG13	2:C:406:LEU:N	2.21	0.54
2:C:406:LEU:HD22	2:C:421:ALA:HB2	1.89	0.54
2:G:163:LYS:HE3	2:G:168:ARG:HH21	1.73	0.54
2:G:391:GLU:O	2:G:395:VAL:HG23	2.07	0.54
2:H:199:GLU:O	2:H:199:GLU:HG2	2.07	0.54
2:H:379:LEU:HD22	2:H:384:VAL:HG22	1.90	0.54
1:A:94:SER:OG	1:A:95:GLY:N	2.38	0.54
1:B:133:ILE:HG12	1:B:155:LYS:HG3	1.89	0.54
1:B:170:CYS:SG	1:B:218:ILE:HG22	2.48	0.54
1:E:85:GLU:HB2	1:E:101:LEU:HD11	1.88	0.54
1:E:104:LEU:HD13	1:E:137:TYR:CE2	2.42	0.54
1:F:194:TYR:CE1	1:F:204:VAL:HG22	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:ASP:HB3	2:H:64:LYS:CG	2.36	0.54
2:G:379:LEU:HD22	2:G:384:VAL:HG22	1.90	0.54
1:B:38:LEU:HD21	2:D:77:GLN:HG3	1.89	0.54
1:B:334:THR:CG2	1:B:335:TYR:N	2.70	0.54
2:C:52:THR:HG22	2:C:53:VAL:N	2.23	0.54
2:C:285:VAL:O	2:C:289:ILE:HG13	2.08	0.54
2:C:296:PRO:CG	2:C:302:THR:HG22	2.37	0.54
2:D:163:LYS:HE3	2:D:168:ARG:HH21	1.72	0.54
2:H:405:ILE:HG13	2:H:406:LEU:N	2.22	0.54
1:A:121:LEU:HD21	1:A:181:GLU:HB2	1.90	0.54
1:A:192:ILE:CG2	1:A:204:VAL:HG13	2.37	0.54
2:C:486:ILE:HD12	2:C:504:ILE:HG23	1.90	0.54
2:D:429:LEU:O	2:D:430:ILE:HG23	2.08	0.54
1:F:158:SER:C	1:F:159:ILE:HD12	2.28	0.54
2:G:344:ARG:HH11	2:G:344:ARG:CG	2.21	0.54
1:B:38:LEU:CD2	2:D:77:GLN:HG3	2.38	0.54
2:D:406:LEU:HD22	2:D:421:ALA:HB2	1.89	0.54
2:G:270:LEU:HG	2:G:271:LEU:N	2.23	0.54
2:H:393:PRO:O	2:H:397:ILE:HG13	2.07	0.54
2:H:515:THR:CG2	2:H:516:ASN:N	2.70	0.54
1:A:334:THR:CG2	1:A:335:TYR:N	2.71	0.53
1:B:85:GLU:HB2	1:B:101:LEU:HD11	1.88	0.53
1:B:96:ARG:HG2	1:B:96:ARG:NH1	2.23	0.53
2:C:43:VAL:HG23	2:C:44:SER:N	2.22	0.53
1:F:224:ILE:HD12	1:F:315:THR:HA	1.90	0.53
1:B:111:LEU:HA	1:B:129:GLY:HA2	1.91	0.53
2:C:199:GLU:HG2	2:C:199:GLU:O	2.08	0.53
2:C:556:ILE:HG22	2:C:557:ALA:N	2.23	0.53
1:A:194:TYR:CE1	1:A:204:VAL:HG22	2.43	0.53
1:B:181:GLU:OE1	1:B:196:ARG:HD3	2.08	0.53
2:D:152:LEU:O	2:D:156:GLU:HG3	2.09	0.53
2:D:240:PHE:HD2	2:D:268:SER:HB2	1.72	0.53
1:E:326:GLY:HA3	2:G:58:ILE:HD12	1.90	0.53
2:H:52:THR:HG22	2:H:53:VAL:N	2.22	0.53
2:D:52:THR:HG22	2:D:53:VAL:N	2.23	0.53
2:D:158:PHE:O	2:D:162:VAL:HG23	2.08	0.53
2:D:274:LEU:HD11	2:D:285:VAL:HG21	1.88	0.53
2:H:270:LEU:HD13	2:H:289:ILE:HD12	1.90	0.53
1:B:68:TYR:CG	1:B:123:LEU:HD13	2.44	0.53
1:E:133:ILE:HG12	1:E:155:LYS:HG3	1.91	0.53
2:H:262:ILE:HG23	2:H:289:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:521:TRP:CH2	2:H:525:ILE:HD11	2.44	0.53
1:A:128:LEU:HD22	1:A:185:VAL:CG1	2.38	0.53
1:A:158:SER:C	1:A:159:ILE:HD12	2.29	0.53
1:B:27:CYS:HB3	1:B:61:ILE:CD1	2.33	0.53
2:D:166:ASP:HB3	2:D:169:VAL:CG2	2.39	0.53
1:E:241:ARG:HG2	1:E:241:ARG:NH1	2.23	0.53
2:G:274:LEU:HD11	2:G:285:VAL:HG21	1.90	0.53
2:H:78:ASN:HB2	2:H:93:VAL:O	2.08	0.53
2:H:124:PHE:HB2	2:H:426:ALA:O	2.08	0.53
2:H:196:ASP:C	2:H:198:GLU:H	2.12	0.53
1:A:181:GLU:OE1	1:A:196:ARG:HD3	2.09	0.53
2:C:402:ILE:CD1	2:C:429:LEU:HD13	2.39	0.53
1:E:86:GLU:HB2	1:E:98:TRP:CH2	2.44	0.53
2:G:270:LEU:HD13	2:G:289:ILE:HD12	1.91	0.53
2:H:482:TRP:N	2:H:483:PRO:CD	2.72	0.53
2:C:306:TRP:O	2:C:310:VAL:HG23	2.09	0.53
1:E:38:LEU:HD21	2:G:77:GLN:HG3	1.89	0.53
1:E:71:ILE:HD11	1:E:145:LEU:CD2	2.39	0.53
1:F:26:THR:HG22	1:F:27:CYS:N	2.24	0.53
2:G:197:VAL:HB	2:G:366:PRO:HB2	1.91	0.53
1:A:241:ARG:HG2	1:A:241:ARG:NH1	2.24	0.53
2:C:68:LYS:HD2	2:C:81:PHE:HE1	1.74	0.53
2:D:270:LEU:HD13	2:D:289:ILE:HD12	1.91	0.53
2:D:391:GLU:O	2:D:395:VAL:HG23	2.09	0.53
2:D:422:MET:SD	2:D:423:ILE:N	2.82	0.53
1:E:96:ARG:HG2	1:E:96:ARG:HH11	1.72	0.53
1:E:324:ASP:C	1:E:326:GLY:H	2.12	0.53
2:G:86:ASP:HA	2:G:88:TYR:HE1	1.74	0.53
2:G:103:GLU:CD	2:G:103:GLU:H	2.11	0.53
1:A:104:LEU:HD13	1:A:137:TYR:CE2	2.43	0.53
1:A:133:ILE:HG12	1:A:155:LYS:HG3	1.90	0.53
2:C:270:LEU:HD13	2:C:289:ILE:HD12	1.91	0.53
2:C:521:TRP:CE2	2:C:525:ILE:HD11	2.44	0.53
1:E:111:LEU:HA	1:E:129:GLY:HA2	1.90	0.53
1:F:236:LYS:HG2	1:F:306:GLU:OE1	2.09	0.53
2:H:274:LEU:HD11	2:H:285:VAL:HG21	1.90	0.53
2:H:508:LEU:HB3	2:H:509:PRO:HD3	1.90	0.53
2:C:166:ASP:HB3	2:C:169:VAL:HG23	1.92	0.52
1:E:128:LEU:HD22	1:E:185:VAL:CG1	2.38	0.52
1:A:120:HIS:HB3	1:A:177:ARG:HG3	1.91	0.52
1:A:224:ILE:HD12	1:A:315:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NH1	1:A:299:GLU:OE2	2.42	0.52
1:E:194:TYR:HE1	1:E:204:VAL:HG22	1.74	0.52
1:F:326:GLY:CA	2:H:58:ILE:HD12	2.39	0.52
2:C:43:VAL:HG23	2:C:44:SER:H	1.74	0.52
2:C:274:LEU:HD11	2:C:285:VAL:HG21	1.90	0.52
2:C:379:LEU:HD22	2:C:384:VAL:HG22	1.91	0.52
2:C:470:ALA:O	2:C:473:LEU:HB2	2.09	0.52
1:E:15:VAL:HG21	2:G:90:LEU:HD21	1.91	0.52
1:E:213:SER:CB	1:E:236:LYS:HB3	2.37	0.52
1:F:120:HIS:CB	1:F:177:ARG:HG3	2.39	0.52
1:B:128:LEU:HD22	1:B:185:VAL:CG1	2.39	0.52
2:C:152:LEU:O	2:C:156:GLU:HG3	2.09	0.52
2:C:453:ASP:HB3	2:C:456:SER:HB2	1.90	0.52
1:E:26:THR:HG22	1:E:27:CYS:N	2.23	0.52
1:F:176:SER:HB2	1:F:223:SER:OG	2.09	0.52
2:H:379:LEU:CD2	2:H:384:VAL:HG22	2.39	0.52
2:H:453:ASP:CB	2:H:456:SER:HB2	2.39	0.52
2:C:391:GLU:O	2:C:395:VAL:HG23	2.09	0.52
1:E:141:GLU:HG2	1:E:143:SER:OG	2.08	0.52
1:F:190:GLN:O	1:F:215:ILE:HD12	2.10	0.52
1:F:241:ARG:NH1	1:F:299:GLU:OE2	2.43	0.52
2:H:166:ASP:HB3	2:H:169:VAL:HG23	1.92	0.52
2:H:308:ASN:C	2:H:308:ASN:HD22	2.13	0.52
2:H:425:GLU:HB2	2:H:430:ILE:HD11	1.91	0.52
1:E:346:THR:OG1	1:E:347:ALA:N	2.40	0.52
2:G:42:PRO:CG	2:G:48:LEU:HB2	2.39	0.52
1:A:324:ASP:C	1:A:326:GLY:H	2.13	0.52
1:B:104:LEU:HD13	1:B:137:TYR:CE2	2.43	0.52
1:B:192:ILE:CG2	1:B:204:VAL:HG13	2.39	0.52
2:C:196:ASP:C	2:C:198:GLU:H	2.12	0.52
1:E:96:ARG:HG2	1:E:96:ARG:NH1	2.24	0.52
1:E:192:ILE:CG2	1:E:204:VAL:HG13	2.40	0.52
1:F:324:ASP:C	1:F:326:GLY:H	2.13	0.52
1:B:183:LEU:HD12	1:B:184:ALA:N	2.24	0.52
1:B:190:GLN:O	1:B:215:ILE:HD12	2.09	0.52
2:D:68:LYS:HD2	2:D:81:PHE:HE1	1.74	0.52
1:F:141:GLU:HG2	1:F:143:SER:OG	2.10	0.52
2:G:204:PHE:HD1	2:G:205:ILE:N	2.07	0.52
2:H:508:LEU:HD11	2:H:522:MET:CG	2.40	0.52
1:A:190:GLN:O	1:A:215:ILE:HD12	2.10	0.52
1:B:120:HIS:HB3	1:B:177:ARG:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:492:SER:O	2:C:500:LYS:NZ	2.37	0.52
2:C:533:GLU:OE1	2:C:533:GLU:HA	2.10	0.52
1:F:128:LEU:HD22	1:F:185:VAL:CG1	2.40	0.52
1:F:322:ALA:HB2	1:F:328:VAL:HG22	1.91	0.52
1:A:322:ALA:HB2	1:A:328:VAL:HG22	1.91	0.52
1:A:334:THR:HG22	1:A:335:TYR:H	1.75	0.52
1:B:241:ARG:HG2	1:B:241:ARG:NH1	2.25	0.52
2:C:379:LEU:HD11	2:C:395:VAL:CG1	2.40	0.52
2:D:379:LEU:CD2	2:D:384:VAL:HG22	2.40	0.52
1:F:38:LEU:CD2	2:H:77:GLN:HG3	2.39	0.52
2:D:295:TYR:HD1	2:D:296:PRO:HD2	1.74	0.51
1:F:324:ASP:HB3	2:H:64:LYS:HB3	1.92	0.51
2:H:272:PRO:O	2:H:273:TYR:C	2.49	0.51
1:A:120:HIS:CB	1:A:177:ARG:HG3	2.40	0.51
2:D:204:PHE:HD1	2:D:205:ILE:N	2.08	0.51
1:B:224:ILE:HD12	1:B:315:THR:HA	1.91	0.51
2:D:196:ASP:C	2:D:198:GLU:H	2.13	0.51
1:E:329:ARG:NH1	2:G:44:SER:HB2	2.25	0.51
2:H:152:LEU:O	2:H:156:GLU:HG3	2.10	0.51
2:H:296:PRO:CG	2:H:302:THR:HG22	2.37	0.51
1:B:346:THR:OG1	1:B:347:ALA:N	2.41	0.51
2:G:379:LEU:CD2	2:G:384:VAL:HG22	2.40	0.51
2:H:103:GLU:H	2:H:103:GLU:CD	2.13	0.51
2:C:192:LEU:HD11	2:C:204:PHE:HD2	1.76	0.51
2:D:453:ASP:HB2	2:D:456:SER:HB2	1.91	0.51
1:F:214:LEU:H	1:F:214:LEU:CD1	2.22	0.51
2:G:537:GLU:O	2:G:540:THR:HB	2.10	0.51
2:H:335:PHE:CD2	2:H:339:ILE:HD11	2.46	0.51
1:B:26:THR:HG22	1:B:27:CYS:N	2.25	0.51
2:C:429:LEU:O	2:C:430:ILE:HG23	2.11	0.51
2:D:42:PRO:CD	2:D:47:ILE:C	2.79	0.51
2:D:78:ASN:HB2	2:D:93:VAL:O	2.11	0.51
2:D:86:ASP:HA	2:D:88:TYR:HE1	1.75	0.51
1:F:94:SER:OG	1:F:95:GLY:N	2.41	0.51
2:H:461:MET:O	2:H:465:MET:HG3	2.11	0.51
1:A:136:LEU:HD11	1:A:202:LEU:HD11	1.93	0.51
2:D:97:ARG:HD2	2:D:174:GLU:OE2	2.11	0.51
2:D:534:ILE:O	2:D:538:ILE:HG13	2.10	0.51
1:E:94:SER:OG	1:E:95:GLY:N	2.43	0.51
1:F:133:ILE:HG12	1:F:155:LYS:HG3	1.92	0.51
2:G:429:LEU:O	2:G:430:ILE:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ASP:C	2:D:88:TYR:HE2	2.14	0.51
1:B:86:GLU:HB2	1:B:98:TRP:CH2	2.46	0.51
1:B:94:SER:OG	1:B:95:GLY:N	2.44	0.51
1:B:334:THR:HG22	1:B:335:TYR:H	1.75	0.51
2:D:322:THR:HG23	2:D:324:ILE:HG12	1.92	0.51
1:E:190:GLN:O	1:E:215:ILE:HD12	2.11	0.51
1:F:241:ARG:HG2	1:F:241:ARG:NH1	2.26	0.51
2:G:369:GLU:HG2	2:H:457:TYR:O	2.11	0.51
1:A:108:LYS:HE2	1:A:133:ILE:CD1	2.40	0.51
1:B:228:TYR:HD2	1:B:244:LYS:HG3	1.76	0.51
2:C:56:GLN:HG3	2:C:56:GLN:O	2.11	0.51
2:D:42:PRO:CB	2:D:48:LEU:HD22	2.27	0.51
2:D:335:PHE:CD2	2:D:339:ILE:HD11	2.46	0.51
2:D:367:SER:C	2:D:369:GLU:H	2.14	0.51
1:E:34:LYS:HE2	1:E:50:SER:OG	2.11	0.51
1:E:221:ALA:HB2	1:E:312:TRP:CE2	2.46	0.51
2:C:103:GLU:H	2:C:103:GLU:CD	2.14	0.50
2:C:231:LYS:H	2:C:234:THR:HB	1.75	0.50
2:D:42:PRO:HB3	2:D:48:LEU:CG	2.40	0.50
1:E:241:ARG:NH1	1:E:299:GLU:OE2	2.43	0.50
1:E:245:ILE:HA	1:E:293:GLN:O	2.11	0.50
1:E:310:VAL:HG13	1:E:310:VAL:O	2.11	0.50
2:G:158:PHE:O	2:G:162:VAL:HG23	2.11	0.50
2:G:235:ALA:C	2:G:237:LYS:H	2.14	0.50
2:G:513:PHE:C	2:G:513:PHE:CD1	2.85	0.50
1:E:228:TYR:HD2	1:E:244:LYS:HG3	1.77	0.50
1:A:236:LYS:HG2	1:A:306:GLU:OE1	2.11	0.50
1:A:336:SER:HA	2:D:370:LEU:HD22	1.94	0.50
2:C:373:GLU:O	2:C:377:MET:HG3	2.12	0.50
2:C:508:LEU:HB3	2:C:509:PRO:HD3	1.94	0.50
2:G:481:LEU:O	2:G:484:VAL:HB	2.12	0.50
2:C:423:ILE:O	2:C:426:ALA:HB3	2.11	0.50
1:F:34:LYS:HE2	1:F:50:SER:OG	2.12	0.50
1:B:108:LYS:HE2	1:B:133:ILE:CD1	2.41	0.50
2:C:367:SER:C	2:C:369:GLU:H	2.15	0.50
2:D:246:TRP:CE2	2:D:331:TYR:HB3	2.47	0.50
1:E:231:ILE:HD11	1:E:245:ILE:HD11	1.93	0.50
1:F:295:GLU:HG2	2:G:311:LEU:HD21	1.94	0.50
2:G:422:MET:SD	2:G:423:ILE:N	2.85	0.50
2:C:375:LEU:HD11	2:C:395:VAL:HG13	1.94	0.50
2:C:557:ALA:O	2:C:561:ARG:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:246:TRP:CE2	2:G:331:TYR:HB3	2.47	0.50
2:H:492:SER:O	2:H:500:LYS:NZ	2.41	0.50
2:C:158:PHE:O	2:C:162:VAL:HG23	2.12	0.50
2:D:103:GLU:CD	2:D:103:GLU:H	2.15	0.50
2:G:514:VAL:HG12	2:G:515:THR:N	2.27	0.50
1:B:34:LYS:HE2	1:B:50:SER:OG	2.12	0.50
2:C:204:PHE:HD1	2:C:205:ILE:N	2.09	0.50
2:D:42:PRO:HD2	2:D:47:ILE:CA	2.42	0.50
2:G:152:LEU:O	2:G:156:GLU:HG3	2.12	0.50
2:C:169:VAL:HG12	2:C:170:ASN:N	2.27	0.50
2:C:379:LEU:CD2	2:C:384:VAL:HG22	2.42	0.50
2:D:271:LEU:N	2:D:272:PRO:CD	2.75	0.50
1:E:38:LEU:CD2	2:G:77:GLN:HG3	2.41	0.50
2:H:344:ARG:HH11	2:H:344:ARG:CG	2.21	0.50
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.27	0.49
2:D:169:VAL:HG12	2:D:170:ASN:N	2.25	0.49
2:D:190:PHE:CZ	2:D:427:LYS:HG3	2.47	0.49
1:F:221:ALA:HB2	1:F:312:TRP:CE2	2.47	0.49
2:G:214:ARG:O	2:G:214:ARG:HG3	2.12	0.49
2:G:451:LEU:CD1	2:G:458:ARG:HG3	2.42	0.49
2:H:379:LEU:HD11	2:H:395:VAL:CG1	2.42	0.49
1:B:194:TYR:HE1	1:B:204:VAL:HG22	1.77	0.49
2:D:214:ARG:O	2:D:214:ARG:HG3	2.11	0.49
1:E:120:HIS:HB3	1:E:177:ARG:HG3	1.94	0.49
2:G:68:LYS:HD2	2:G:81:PHE:HE1	1.77	0.49
2:G:166:ASP:HB3	2:G:169:VAL:HG23	1.94	0.49
2:G:322:THR:HG23	2:G:324:ILE:HG12	1.92	0.49
2:H:94:ARG:HH21	2:H:98:LEU:HB3	1.76	0.49
2:H:98:LEU:HD11	2:H:476:LEU:CD1	2.42	0.49
2:H:429:LEU:O	2:H:430:ILE:HG23	2.12	0.49
2:H:482:TRP:O	2:H:486:ILE:HG12	2.12	0.49
1:B:141:GLU:HG2	1:B:143:SER:OG	2.12	0.49
2:C:173:TYR:HA	2:C:176:GLU:HB2	1.93	0.49
2:D:56:GLN:O	2:D:56:GLN:HG3	2.11	0.49
1:F:194:TYR:HE1	1:F:204:VAL:HG22	1.77	0.49
1:A:86:GLU:HB2	1:A:98:TRP:CH2	2.47	0.49
1:A:221:ALA:HB2	1:A:312:TRP:CE2	2.47	0.49
1:E:128:LEU:HD22	1:E:185:VAL:HG11	1.94	0.49
2:G:334:ASP:O	2:G:338:VAL:HG23	2.10	0.49
2:G:367:SER:C	2:G:369:GLU:H	2.15	0.49
2:H:367:SER:C	2:H:369:GLU:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TYR:HE1	1:A:204:VAL:HG22	1.78	0.49
1:B:221:ALA:HB2	1:B:312:TRP:CE2	2.47	0.49
1:B:245:ILE:HA	1:B:293:GLN:O	2.11	0.49
2:C:69:PHE:HD2	2:C:80:ALA:HB2	1.76	0.49
2:C:69:PHE:CD2	2:C:80:ALA:HB2	2.47	0.49
1:E:27:CYS:HB3	1:E:61:ILE:CD1	2.37	0.49
2:G:192:LEU:HD11	2:G:204:PHE:HD2	1.77	0.49
2:G:227:VAL:HG21	2:G:248:LEU:HD12	1.93	0.49
1:A:141:GLU:HG2	1:A:143:SER:OG	2.12	0.49
2:C:42:PRO:HA	2:C:46:ALA:O	2.13	0.49
2:C:268:SER:O	2:C:272:PRO:HD2	2.12	0.49
2:C:482:TRP:N	2:C:483:PRO:HD3	2.25	0.49
1:F:136:LEU:HD11	1:F:202:LEU:HD11	1.94	0.49
2:C:86:ASP:HA	2:C:88:TYR:HE1	1.77	0.49
2:D:86:ASP:N	2:D:88:TYR:CE1	2.80	0.49
2:H:155:LEU:O	2:H:159:ILE:HG13	2.13	0.49
1:B:120:HIS:CB	1:B:177:ARG:HG3	2.43	0.49
2:C:335:PHE:CD2	2:C:339:ILE:HD11	2.48	0.49
1:F:334:THR:HG22	1:F:335:TYR:H	1.75	0.49
2:G:86:ASP:HA	2:G:88:TYR:CE1	2.48	0.49
2:D:166:ASP:HB3	2:D:169:VAL:HG23	1.95	0.49
2:D:272:PRO:O	2:D:273:TYR:C	2.50	0.49
2:G:69:PHE:HD2	2:G:80:ALA:HB2	1.76	0.49
2:H:231:LYS:HG3	2:H:232:ASP:N	2.27	0.49
2:H:398:ILE:HG23	2:H:399:SER:N	2.28	0.49
2:H:549:ALA:O	2:H:551:ASN:N	2.45	0.49
1:A:193:ILE:CD1	1:A:245:ILE:HD13	2.43	0.49
1:A:247:GLU:HB3	1:A:292:LEU:HD23	1.94	0.49
1:B:236:LYS:HG2	1:B:306:GLU:OE1	2.13	0.49
2:C:272:PRO:O	2:C:273:TYR:C	2.51	0.49
2:D:423:ILE:O	2:D:426:ALA:HB3	2.12	0.49
1:E:11:LEU:N	2:G:88:TYR:HE2	2.10	0.49
1:E:236:LYS:HG2	1:E:306:GLU:OE1	2.12	0.49
2:H:104:PHE:O	2:H:107:TYR:N	2.46	0.49
1:A:79:LYS:HG2	1:A:110:SER:N	2.28	0.48
1:A:128:LEU:HD22	1:A:185:VAL:HG11	1.95	0.48
2:C:535:ALA:HA	2:C:538:ILE:HD12	1.95	0.48
1:F:79:LYS:HG2	1:F:110:SER:N	2.27	0.48
1:F:231:ILE:HD11	1:F:245:ILE:HD11	1.95	0.48
2:H:231:LYS:NZ	2:H:238:LYS:HD3	2.28	0.48
1:F:168:ASP:H	1:F:188:LEU:CD2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:PHE:O	2:H:162:VAL:HG23	2.12	0.48
2:H:204:PHE:O	2:H:206:GLU:N	2.46	0.48
2:H:344:ARG:HG3	2:H:344:ARG:NH1	2.25	0.48
1:A:114:VAL:HG23	1:A:126:ALA:O	2.13	0.48
1:A:208:LEU:HD11	1:A:231:ILE:HD12	1.94	0.48
2:C:515:THR:HG22	2:C:517:ASP:N	2.20	0.48
2:H:173:TYR:HA	2:H:176:GLU:HB2	1.95	0.48
1:A:68:TYR:CG	1:A:123:LEU:HD13	2.49	0.48
1:B:247:GLU:HB3	1:B:292:LEU:HD23	1.95	0.48
2:G:515:THR:HG22	2:G:517:ASP:N	2.22	0.48
2:G:552:ILE:O	2:G:552:ILE:HG22	2.13	0.48
2:H:268:SER:O	2:H:272:PRO:HD2	2.13	0.48
1:A:138:ASP:HA	1:A:148:TRP:CE3	2.49	0.48
1:E:334:THR:HG22	1:E:335:TYR:H	1.74	0.48
2:G:56:GLN:HG3	2:G:56:GLN:O	2.13	0.48
2:G:69:PHE:CD2	2:G:80:ALA:HB2	2.49	0.48
2:C:322:THR:HG23	2:C:324:ILE:HG12	1.95	0.48
2:D:98:LEU:HD12	2:D:99:ASP:H	1.78	0.48
1:E:181:GLU:OE1	1:E:196:ARG:HD3	2.13	0.48
2:H:56:GLN:HG3	2:H:56:GLN:O	2.13	0.48
2:H:189:TYR:O	2:H:427:LYS:HE3	2.14	0.48
1:A:247:GLU:HB3	1:A:292:LEU:CD2	2.44	0.48
1:B:310:VAL:O	1:B:310:VAL:HG13	2.14	0.48
2:C:532:PRO:HG2	2:C:533:GLU:H	1.78	0.48
2:D:145:ASN:OD1	2:D:190:PHE:HA	2.14	0.48
2:D:308:ASN:HD22	2:D:308:ASN:C	2.16	0.48
1:E:214:LEU:H	1:E:214:LEU:CD1	2.25	0.48
1:E:324:ASP:HB3	2:G:64:LYS:CG	2.42	0.48
1:F:128:LEU:HD22	1:F:185:VAL:HG11	1.96	0.48
1:F:247:GLU:HB3	1:F:292:LEU:HD23	1.94	0.48
1:A:15:VAL:O	2:C:70:LYS:HD2	2.13	0.48
2:C:308:ASN:C	2:C:308:ASN:HD22	2.16	0.48
2:C:344:ARG:HH11	2:C:344:ARG:CG	2.20	0.48
2:D:344:ARG:HG3	2:D:344:ARG:NH1	2.26	0.48
2:D:478:ASP:O	2:D:480:GLU:N	2.47	0.48
2:G:398:ILE:HG23	2:G:399:SER:N	2.29	0.48
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.78	0.48
1:B:224:ILE:HG22	2:D:471:PHE:CZ	2.48	0.48
1:B:231:ILE:HD11	1:B:245:ILE:HD11	1.94	0.48
1:B:247:GLU:HB3	1:B:292:LEU:CD2	2.44	0.48
2:D:268:SER:O	2:D:272:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:GLU:HB2	1:F:98:TRP:CH2	2.48	0.48
2:G:523:LEU:HD23	2:G:538:ILE:CD1	2.43	0.48
2:H:169:VAL:HG12	2:H:170:ASN:N	2.27	0.48
2:C:155:LEU:O	2:C:159:ILE:HG13	2.13	0.48
2:C:271:LEU:N	2:C:272:PRO:CD	2.77	0.48
2:C:508:LEU:HD11	2:C:522:MET:HG3	1.96	0.48
2:D:204:PHE:O	2:D:206:GLU:N	2.47	0.48
2:D:398:ILE:HG23	2:D:399:SER:N	2.29	0.48
1:E:226:ARG:HG3	1:E:226:ARG:NH1	2.28	0.48
1:F:96:ARG:NH1	1:F:96:ARG:HG2	2.29	0.48
1:F:151:THR:HG22	1:F:152:SER:N	2.29	0.48
2:G:78:ASN:HB2	2:G:93:VAL:O	2.13	0.48
2:G:190:PHE:CZ	2:G:427:LYS:HG3	2.48	0.48
2:H:52:THR:HG22	2:H:54:ASN:H	1.79	0.48
2:H:422:MET:SD	2:H:423:ILE:N	2.87	0.48
2:H:459:ASN:HB3	2:H:494:THR:CB	2.44	0.48
2:H:471:PHE:O	2:H:473:LEU:N	2.47	0.48
1:B:214:LEU:H	1:B:214:LEU:CD1	2.25	0.47
2:C:86:ASP:HA	2:C:88:TYR:CE1	2.49	0.47
2:D:52:THR:HG22	2:D:54:ASN:H	1.79	0.47
2:D:313:LEU:HD23	2:D:313:LEU:C	2.35	0.47
1:E:54:HIS:HD2	1:E:58:ILE:HG12	1.78	0.47
1:E:193:ILE:CD1	1:E:245:ILE:HD13	2.44	0.47
2:G:173:TYR:HA	2:G:176:GLU:HB2	1.95	0.47
2:G:268:SER:O	2:G:272:PRO:HD2	2.13	0.47
2:H:192:LEU:HD11	2:H:204:PHE:HD2	1.75	0.47
1:E:247:GLU:HB3	1:E:292:LEU:HD23	1.96	0.47
1:F:54:HIS:CE1	1:F:82:LYS:HB2	2.49	0.47
1:F:108:LYS:HE2	1:F:133:ILE:CD1	2.44	0.47
2:G:86:ASP:N	2:G:88:TYR:CE1	2.82	0.47
2:G:117:ASP:C	2:G:119:GLY:H	2.18	0.47
2:G:469:PHE:O	2:G:472:GLU:N	2.47	0.47
2:H:69:PHE:HD2	2:H:80:ALA:HB2	1.79	0.47
2:C:52:THR:HG22	2:C:54:ASN:H	1.79	0.47
2:D:118:LEU:O	2:D:119:GLY:C	2.53	0.47
2:D:502:MET:O	2:D:505:ALA:HB3	2.15	0.47
1:E:108:LYS:HE2	1:E:133:ILE:CD1	2.43	0.47
1:E:120:HIS:CB	1:E:177:ARG:HG3	2.44	0.47
1:E:247:GLU:HB3	1:E:292:LEU:CD2	2.45	0.47
2:G:505:ALA:HB2	2:G:531:LEU:HD22	1.95	0.47
2:H:153:ASN:O	2:H:156:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HD22	1:B:185:VAL:HG11	1.97	0.47
1:F:247:GLU:HB3	1:F:292:LEU:CD2	2.44	0.47
2:G:250:ASN:O	2:G:254:LEU:HG	2.13	0.47
2:G:269:ASP:O	2:G:270:LEU:C	2.53	0.47
2:G:271:LEU:N	2:G:272:PRO:CD	2.77	0.47
2:H:204:PHE:HD1	2:H:205:ILE:N	2.12	0.47
2:H:470:ALA:O	2:H:473:LEU:HB2	2.15	0.47
2:C:204:PHE:O	2:C:206:GLU:N	2.48	0.47
2:D:86:ASP:HA	2:D:88:TYR:CE1	2.49	0.47
2:D:198:GLU:HA	2:D:300:SER:OG	2.14	0.47
1:F:96:ARG:HG2	1:F:96:ARG:HH11	1.80	0.47
1:F:310:VAL:HG13	1:F:310:VAL:O	2.15	0.47
2:G:118:LEU:O	2:G:119:GLY:C	2.52	0.47
2:G:204:PHE:O	2:G:206:GLU:N	2.48	0.47
2:G:240:PHE:HD2	2:G:268:SER:CB	2.28	0.47
2:H:532:PRO:O	2:H:535:ALA:HB3	2.15	0.47
1:A:310:VAL:O	1:A:310:VAL:HG13	2.15	0.47
2:C:42:PRO:HB3	2:C:46:ALA:O	2.14	0.47
2:D:228:PHE:CE2	2:D:267:ARG:HG3	2.49	0.47
2:G:112:PHE:O	2:G:115:TYR:HB3	2.14	0.47
1:A:97:ARG:HH11	1:A:97:ARG:HG3	1.80	0.47
1:A:214:LEU:H	1:A:214:LEU:CD1	2.26	0.47
1:A:324:ASP:HB3	2:C:64:LYS:CG	2.43	0.47
2:D:104:PHE:O	2:D:107:TYR:N	2.47	0.47
2:D:104:PHE:C	2:D:106:ALA:H	2.18	0.47
2:D:155:LEU:O	2:D:159:ILE:HG13	2.14	0.47
2:D:269:ASP:O	2:D:270:LEU:C	2.52	0.47
1:F:68:TYR:CG	1:F:123:LEU:HD13	2.49	0.47
2:G:155:LEU:O	2:G:159:ILE:HG13	2.14	0.47
2:G:505:ALA:HB2	2:G:531:LEU:CD2	2.45	0.47
2:H:98:LEU:HD12	2:H:99:ASP:H	1.79	0.47
2:H:184:CYS:HB2	2:H:211:TRP:CE2	2.49	0.47
2:H:322:THR:HG23	2:H:324:ILE:HG12	1.95	0.47
1:A:231:ILE:HD11	1:A:245:ILE:HD11	1.96	0.47
2:C:112:PHE:O	2:C:115:TYR:HB3	2.14	0.47
2:C:189:TYR:O	2:C:427:LYS:HE3	2.15	0.47
2:D:108:VAL:HG22	2:D:469:PHE:HZ	1.80	0.47
2:G:335:PHE:CD2	2:G:339:ILE:HD11	2.50	0.47
2:H:271:LEU:O	2:H:275:SER:HB3	2.15	0.47
2:H:375:LEU:HD11	2:H:395:VAL:HG13	1.96	0.47
1:A:168:ASP:H	1:A:188:LEU:CD2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:ILE:HG23	2:C:399:SER:N	2.29	0.47
2:D:112:PHE:O	2:D:115:TYR:HB3	2.15	0.47
2:D:173:TYR:HA	2:D:176:GLU:HB2	1.95	0.47
1:E:81:VAL:CG2	1:E:111:LEU:HD13	2.33	0.47
2:G:98:LEU:HD12	2:G:99:ASP:H	1.80	0.47
2:G:344:ARG:CG	2:G:344:ARG:NH1	2.78	0.47
2:G:451:LEU:HD21	2:G:458:ARG:HG3	1.97	0.47
2:H:373:GLU:O	2:H:377:MET:HG3	2.15	0.47
2:H:549:ALA:O	2:H:550:HIS:C	2.52	0.47
1:B:138:ASP:HA	1:B:148:TRP:CE3	2.50	0.47
2:C:269:ASP:O	2:C:270:LEU:O	2.32	0.47
2:C:454:LEU:HD13	2:C:495:GLY:HA3	1.97	0.47
2:D:99:ASP:OD2	2:D:171:ARG:NE	2.48	0.47
2:D:192:LEU:HD11	2:D:204:PHE:HD2	1.79	0.47
1:E:54:HIS:CE1	1:E:82:LYS:HB2	2.50	0.47
1:F:138:ASP:HA	1:F:148:TRP:CE3	2.50	0.47
1:F:193:ILE:CD1	1:F:245:ILE:HD13	2.44	0.47
2:G:457:TYR:C	2:G:457:TYR:CD1	2.89	0.47
2:G:508:LEU:O	2:G:510:HIS:N	2.48	0.47
1:A:324:ASP:HB3	2:C:64:LYS:HB3	1.96	0.46
2:D:201:ARG:NH2	2:D:303:PHE:CD1	2.83	0.46
2:D:344:ARG:HH11	2:D:344:ARG:CG	2.22	0.46
1:E:168:ASP:H	1:E:188:LEU:CD2	2.28	0.46
1:F:328:VAL:HG11	2:H:69:PHE:CG	2.50	0.46
2:G:52:THR:HG22	2:G:54:ASN:H	1.80	0.46
2:G:454:LEU:HD12	2:G:454:LEU:O	2.15	0.46
2:H:69:PHE:CD2	2:H:80:ALA:HB2	2.49	0.46
1:A:27:CYS:HB3	1:A:61:ILE:CD1	2.39	0.46
1:B:324:ASP:HB3	2:D:64:LYS:CG	2.45	0.46
2:C:94:ARG:HH21	2:C:98:LEU:HB3	1.80	0.46
2:G:548:SER:HA	2:G:551:ASN:ND2	2.30	0.46
2:H:112:PHE:O	2:H:115:TYR:HB3	2.15	0.46
2:H:216:ASP:OD2	2:H:218:GLU:HB2	2.15	0.46
1:B:151:THR:CG2	1:B:196:ARG:HH22	2.29	0.46
2:C:344:ARG:HG3	2:C:344:ARG:NH1	2.24	0.46
1:E:16:VAL:HG21	1:E:61:ILE:O	2.15	0.46
2:H:86:ASP:HA	2:H:88:TYR:HE1	1.79	0.46
2:H:271:LEU:N	2:H:272:PRO:CD	2.78	0.46
1:A:34:LYS:HE2	1:A:50:SER:OG	2.14	0.46
2:C:86:ASP:N	2:C:88:TYR:CE1	2.82	0.46
2:C:526:CYS:O	2:C:530:ARG:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLU:HB2	1:E:98:TRP:CZ3	2.50	0.46
1:F:97:ARG:HH11	1:F:97:ARG:HG3	1.80	0.46
1:F:169:PHE:O	1:F:170:CYS:HB3	2.16	0.46
2:G:272:PRO:O	2:G:273:TYR:C	2.53	0.46
2:H:423:ILE:O	2:H:426:ALA:HB3	2.14	0.46
1:B:226:ARG:HG3	1:B:226:ARG:NH1	2.30	0.46
2:C:460:GLY:C	2:C:462:ALA:N	2.69	0.46
2:C:478:ASP:C	2:C:480:GLU:N	2.69	0.46
2:C:552:ILE:O	2:C:556:ILE:HG13	2.16	0.46
1:F:295:GLU:HG2	2:G:311:LEU:CD2	2.46	0.46
1:F:302:ASP:OD2	2:H:44:SER:HB3	2.16	0.46
2:G:305:GLU:O	2:G:309:LEU:HG	2.15	0.46
2:C:457:TYR:CD1	2:C:457:TYR:C	2.89	0.46
2:C:478:ASP:C	2:C:480:GLU:H	2.19	0.46
2:D:153:ASN:O	2:D:156:GLU:N	2.46	0.46
2:D:240:PHE:HD2	2:D:268:SER:CB	2.29	0.46
2:D:496:THR:HB	2:D:499:ALA:H	1.81	0.46
1:B:76:SER:OG	1:B:77:TYR:N	2.48	0.46
2:C:271:LEU:O	2:C:275:SER:HB3	2.15	0.46
2:D:375:LEU:HD11	2:D:395:VAL:HG13	1.98	0.46
1:F:125:LEU:C	1:F:125:LEU:HD12	2.36	0.46
2:H:250:ASN:O	2:H:254:LEU:HG	2.16	0.46
1:B:125:LEU:HD12	1:B:125:LEU:C	2.36	0.46
2:C:269:ASP:O	2:C:270:LEU:C	2.53	0.46
2:D:184:CYS:HB2	2:D:211:TRP:CE2	2.50	0.46
1:E:125:LEU:C	1:E:125:LEU:HD12	2.36	0.46
2:G:216:ASP:OD2	2:G:218:GLU:HB2	2.16	0.46
2:G:289:ILE:O	2:G:293:LYS:HG3	2.15	0.46
2:G:423:ILE:O	2:G:426:ALA:HB3	2.16	0.46
1:A:169:PHE:O	1:A:170:CYS:HB3	2.16	0.46
1:B:48:SER:O	1:B:49:ASP:HB2	2.15	0.46
1:B:54:HIS:CE1	1:B:82:LYS:HB2	2.51	0.46
1:B:193:ILE:CD1	1:B:245:ILE:HD13	2.46	0.46
2:C:551:ASN:O	2:C:554:GLU:N	2.49	0.46
2:D:269:ASP:O	2:D:270:LEU:O	2.34	0.46
2:G:352:THR:OG1	2:G:355:GLU:HG3	2.15	0.46
2:H:86:ASP:N	2:H:88:TYR:CE1	2.82	0.46
1:A:54:HIS:CE1	1:A:82:LYS:HB2	2.51	0.46
2:C:43:VAL:CG1	2:C:48:LEU:CD2	2.79	0.46
2:D:343:GLN:HA	2:D:360:PHE:HE1	1.80	0.46
1:E:136:LEU:HD11	1:E:202:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ASP:HA	1:E:148:TRP:CE3	2.51	0.46
1:E:208:LEU:HD11	1:E:231:ILE:HD12	1.96	0.46
1:E:309:SER:HB3	2:G:68:LYS:HA	1.97	0.46
2:H:305:GLU:O	2:H:309:LEU:HG	2.16	0.46
2:H:344:ARG:CG	2:H:344:ARG:NH1	2.78	0.46
1:A:205:ALA:O	1:A:206:ALA:HB2	2.15	0.45
1:B:79:LYS:HG2	1:B:110:SER:N	2.31	0.45
2:C:480:GLU:O	2:C:483:PRO:CD	2.64	0.45
2:D:117:ASP:C	2:D:119:GLY:H	2.19	0.45
2:D:352:THR:OG1	2:D:355:GLU:HG3	2.16	0.45
2:G:171:ARG:O	2:G:175:LEU:HG	2.17	0.45
2:H:270:LEU:HD13	2:H:289:ILE:CD1	2.46	0.45
1:A:16:VAL:HG21	1:A:61:ILE:O	2.15	0.45
2:C:246:TRP:CE2	2:C:331:TYR:HB3	2.51	0.45
2:C:459:ASN:HD22	2:C:459:ASN:N	2.14	0.45
2:D:453:ASP:HB3	2:D:456:SER:HB2	1.97	0.45
2:D:482:TRP:O	2:D:485:ALA:HB3	2.16	0.45
2:D:523:LEU:HD23	2:D:538:ILE:CD1	2.47	0.45
1:E:101:LEU:O	1:E:102:CYS:HB2	2.16	0.45
1:F:208:LEU:HD11	1:F:231:ILE:HD12	1.96	0.45
2:G:104:PHE:O	2:G:107:TYR:N	2.49	0.45
2:G:308:ASN:HD22	2:G:308:ASN:C	2.19	0.45
2:G:313:LEU:HD23	2:G:313:LEU:C	2.36	0.45
2:G:379:LEU:HD11	2:G:395:VAL:CG1	2.47	0.45
2:G:515:THR:CG2	2:G:516:ASN:H	2.27	0.45
2:H:352:THR:OG1	2:H:355:GLU:HG3	2.16	0.45
1:A:326:GLY:CA	2:C:58:ILE:HD12	2.44	0.45
2:C:415:CYS:HB2	2:C:469:PHE:CE1	2.51	0.45
1:F:205:ALA:O	1:F:206:ALA:HB2	2.15	0.45
2:H:145:ASN:OD1	2:H:190:PHE:HA	2.15	0.45
1:A:151:THR:HG22	1:A:152:SER:N	2.30	0.45
1:B:136:LEU:HD11	1:B:202:LEU:HD11	1.98	0.45
2:C:41:ASP:HA	2:C:42:PRO:HD3	1.77	0.45
2:C:145:ASN:OD1	2:C:190:PHE:HA	2.16	0.45
2:C:184:CYS:HB2	2:C:211:TRP:CE2	2.51	0.45
2:H:245:PHE:O	2:H:248:LEU:HB3	2.17	0.45
2:C:69:PHE:CE1	2:C:71:LEU:HD23	2.41	0.45
2:D:263:GLY:O	2:D:267:ARG:HG2	2.17	0.45
2:D:289:ILE:O	2:D:293:LYS:HG3	2.17	0.45
1:F:114:VAL:HG23	1:F:126:ALA:O	2.16	0.45
2:G:153:ASN:O	2:G:156:GLU:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:531:LEU:HD13	2:H:534:ILE:CD1	2.46	0.45
1:A:86:GLU:HB2	1:A:98:TRP:CZ3	2.52	0.45
2:D:379:LEU:HD11	2:D:395:VAL:CG1	2.46	0.45
1:F:347:ALA:HB1	2:H:57:PRO:HG2	1.99	0.45
1:B:54:HIS:HD2	1:B:58:ILE:HG12	1.81	0.45
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.81	0.45
2:D:250:ASN:O	2:D:254:LEU:HG	2.17	0.45
1:E:74:SER:O	1:E:81:VAL:HG13	2.17	0.45
1:F:137:TYR:HE1	1:F:150:LEU:HG	1.80	0.45
2:H:81:PHE:HB3	2:H:90:LEU:HD23	1.99	0.45
2:H:190:PHE:CD1	2:H:190:PHE:N	2.85	0.45
2:H:523:LEU:O	2:H:526:CYS:HB2	2.17	0.45
1:A:1:MET:CE	2:C:94:ARG:HD2	2.46	0.45
1:B:81:VAL:CG2	1:B:111:LEU:HD13	2.32	0.45
1:B:168:ASP:H	1:B:188:LEU:CD2	2.29	0.45
2:C:163:LYS:CE	2:C:168:ARG:HH21	2.29	0.45
2:D:204:PHE:CD1	2:D:205:ILE:N	2.84	0.45
1:F:336:SER:HB2	2:G:343:GLN:OE1	2.17	0.45
2:H:240:PHE:HD2	2:H:268:SER:CB	2.29	0.45
2:H:289:ILE:O	2:H:293:LYS:HG3	2.17	0.45
1:B:114:VAL:O	1:B:114:VAL:HG13	2.17	0.45
2:C:204:PHE:CD1	2:C:204:PHE:C	2.90	0.45
2:C:216:ASP:OD2	2:C:218:GLU:HB2	2.16	0.45
2:C:552:ILE:O	2:C:556:ILE:N	2.36	0.45
2:D:99:ASP:OD1	2:D:101:SER:HB2	2.17	0.45
2:D:204:PHE:CD1	2:D:204:PHE:C	2.90	0.45
2:D:492:SER:O	2:D:494:THR:N	2.50	0.45
1:E:47:LEU:HD12	1:E:48:SER:N	2.32	0.45
1:E:151:THR:HG22	1:E:152:SER:N	2.31	0.45
2:G:336:LEU:HA	2:G:339:ILE:HD12	1.99	0.45
2:H:336:LEU:HA	2:H:339:ILE:HD12	1.99	0.45
2:C:98:LEU:HD12	2:C:99:ASP:H	1.81	0.45
2:C:153:ASN:O	2:C:156:GLU:N	2.48	0.45
1:F:15:VAL:O	2:H:70:LYS:HD2	2.17	0.45
2:G:269:ASP:O	2:G:270:LEU:O	2.35	0.45
1:B:334:THR:CG2	1:B:335:TYR:H	2.30	0.44
2:C:118:LEU:HD21	2:C:147:ALA:CB	2.46	0.44
2:C:190:PHE:CD1	2:C:190:PHE:N	2.85	0.44
2:C:422:MET:SD	2:C:423:ILE:N	2.90	0.44
2:D:247:LYS:O	2:D:251:GLN:HG3	2.18	0.44
2:D:498:SER:O	2:D:501:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:LEU:C	2:D:510:HIS:H	2.19	0.44
1:F:183:LEU:HD12	1:F:184:ALA:H	1.82	0.44
2:G:204:PHE:CD1	2:G:205:ILE:N	2.84	0.44
2:G:383:VAL:CG1	2:G:384:VAL:N	2.80	0.44
2:G:396:ASP:OD1	2:G:401:LYS:HE3	2.16	0.44
2:H:86:ASP:HA	2:H:88:TYR:CE1	2.52	0.44
2:H:118:LEU:O	2:H:119:GLY:C	2.56	0.44
2:H:482:TRP:N	2:H:483:PRO:HD3	2.32	0.44
1:A:334:THR:CG2	1:A:335:TYR:H	2.30	0.44
2:C:118:LEU:O	2:C:119:GLY:C	2.55	0.44
2:C:126:VAL:O	2:C:126:VAL:HG12	2.16	0.44
1:E:97:ARG:HH11	1:E:97:ARG:HG3	1.81	0.44
2:G:204:PHE:CD1	2:G:204:PHE:C	2.90	0.44
2:H:524:SER:O	2:H:527:VAL:N	2.50	0.44
2:C:104:PHE:C	2:C:106:ALA:H	2.20	0.44
2:C:179:LEU:O	2:C:182:LEU:N	2.50	0.44
2:C:240:PHE:HD2	2:C:268:SER:CB	2.29	0.44
2:C:523:LEU:CD2	2:C:538:ILE:CD1	2.95	0.44
2:D:305:GLU:O	2:D:309:LEU:HG	2.17	0.44
2:G:189:TYR:O	2:G:427:LYS:HE3	2.17	0.44
2:H:179:LEU:O	2:H:182:LEU:N	2.50	0.44
2:H:269:ASP:O	2:H:270:LEU:O	2.35	0.44
2:D:189:TYR:O	2:D:427:LYS:HE3	2.16	0.44
1:E:151:THR:CG2	1:E:196:ARG:HH22	2.31	0.44
1:E:334:THR:CG2	1:E:335:TYR:H	2.29	0.44
2:H:117:ASP:C	2:H:119:GLY:H	2.20	0.44
2:H:343:GLN:HA	2:H:360:PHE:HE1	1.82	0.44
2:H:471:PHE:C	2:H:473:LEU:N	2.71	0.44
2:H:531:LEU:CD1	2:H:534:ILE:HD12	2.48	0.44
1:B:309:SER:HB3	2:D:68:LYS:HA	1.99	0.44
2:C:352:THR:OG1	2:C:355:GLU:HG3	2.18	0.44
2:D:271:LEU:O	2:D:275:SER:HB3	2.18	0.44
2:D:373:GLU:O	2:D:377:MET:HG3	2.17	0.44
1:E:48:SER:O	1:E:49:ASP:HB2	2.17	0.44
1:E:76:SER:OG	1:E:77:TYR:N	2.50	0.44
1:E:224:ILE:HG22	2:G:503:VAL:HG13	1.99	0.44
1:F:171:LEU:HB3	1:F:185:VAL:HG13	1.99	0.44
2:G:235:ALA:O	2:G:237:LYS:N	2.48	0.44
1:B:16:VAL:HG21	1:B:61:ILE:O	2.18	0.44
2:C:42:PRO:CB	2:C:46:ALA:O	2.66	0.44
2:C:47:ILE:HG22	2:C:48:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:214:ARG:HG3	2:C:214:ARG:O	2.17	0.44
2:C:247:LYS:O	2:C:251:GLN:HG3	2.18	0.44
2:C:305:GLU:O	2:C:308:ASN:HB3	2.17	0.44
2:C:456:SER:OG	2:C:457:TYR:N	2.51	0.44
1:E:137:TYR:HE1	1:E:150:LEU:HG	1.81	0.44
2:G:145:ASN:OD1	2:G:190:PHE:HA	2.18	0.44
2:H:104:PHE:C	2:H:106:ALA:H	2.19	0.44
2:H:214:ARG:HG3	2:H:214:ARG:O	2.17	0.44
2:H:555:SER:CA	2:H:558:ASN:HB3	2.46	0.44
2:C:171:ARG:O	2:C:175:LEU:HG	2.18	0.44
2:C:344:ARG:CG	2:C:344:ARG:NH1	2.77	0.44
2:D:525:ILE:C	2:D:527:VAL:N	2.71	0.44
1:E:205:ALA:O	1:E:206:ALA:HB2	2.18	0.44
1:E:315:THR:HB	2:G:471:PHE:HD2	1.82	0.44
1:F:309:SER:HB3	2:H:68:LYS:HA	1.99	0.44
2:G:508:LEU:C	2:G:510:HIS:N	2.71	0.44
2:H:523:LEU:HD23	2:H:538:ILE:HD12	2.00	0.44
1:A:124:LYS:HA	1:A:138:ASP:HB3	1.99	0.44
1:A:125:LEU:C	1:A:125:LEU:HD12	2.38	0.44
1:B:86:GLU:HB2	1:B:98:TRP:CZ3	2.52	0.44
1:B:114:VAL:HG23	1:B:126:ALA:O	2.17	0.44
2:C:343:GLN:HA	2:C:360:PHE:HE1	1.82	0.44
2:C:551:ASN:O	2:C:554:GLU:CB	2.65	0.44
1:F:228:TYR:CD2	1:F:244:LYS:HG3	2.52	0.44
2:G:103:GLU:CD	2:G:103:GLU:N	2.71	0.44
2:G:163:LYS:CE	2:G:168:ARG:HH21	2.31	0.44
2:G:190:PHE:N	2:G:190:PHE:CD1	2.85	0.44
2:G:343:GLN:HA	2:G:360:PHE:HE1	1.82	0.44
2:H:163:LYS:CE	2:H:168:ARG:HH21	2.30	0.44
1:A:59:VAL:O	1:A:59:VAL:HG12	2.18	0.44
1:A:108:LYS:HE2	1:A:133:ILE:HD12	2.00	0.44
1:B:47:LEU:HD12	1:B:48:SER:N	2.32	0.44
2:C:81:PHE:HB3	2:C:90:LEU:HD23	2.00	0.44
2:D:171:ARG:O	2:D:175:LEU:HG	2.18	0.44
2:D:216:ASP:OD2	2:D:218:GLU:HB2	2.18	0.44
2:D:270:LEU:HD13	2:D:289:ILE:CD1	2.48	0.44
1:E:15:VAL:HB	2:G:81:PHE:CE2	2.53	0.44
1:F:334:THR:CG2	1:F:335:TYR:H	2.29	0.44
2:H:85:LYS:O	2:H:86:ASP:HB2	2.18	0.44
2:H:246:TRP:CE2	2:H:331:TYR:HB3	2.53	0.44
2:H:274:LEU:HD22	2:H:281:SER:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HE1	1:A:150:LEU:HG	1.82	0.43
1:B:1:MET:CE	2:D:94:ARG:HD2	2.47	0.43
1:B:15:VAL:HG21	2:D:90:LEU:HD21	2.00	0.43
1:B:137:TYR:HE1	1:B:150:LEU:HG	1.82	0.43
1:B:205:ALA:O	1:B:206:ALA:HB2	2.17	0.43
2:C:204:PHE:O	2:C:207:SER:N	2.51	0.43
2:C:289:ILE:O	2:C:293:LYS:HG3	2.17	0.43
2:D:104:PHE:C	2:D:106:ALA:N	2.72	0.43
2:D:336:LEU:HA	2:D:339:ILE:HD12	1.99	0.43
1:E:54:HIS:CD2	1:E:58:ILE:HG12	2.53	0.43
1:E:79:LYS:HG2	1:E:110:SER:N	2.33	0.43
1:F:310:VAL:HA	1:F:320:SER:O	2.17	0.43
1:F:345:ILE:HA	2:H:49:VAL:O	2.18	0.43
2:H:258:LEU:HD22	2:H:292:LEU:CD2	2.44	0.43
2:H:470:ALA:HB1	2:H:489:ILE:HG13	2.00	0.43
2:H:486:ILE:O	2:H:490:ALA:HB2	2.18	0.43
2:H:541:THR:HG22	2:H:545:GLN:NE2	2.33	0.43
1:B:74:SER:O	1:B:81:VAL:HG13	2.18	0.43
2:C:250:ASN:O	2:C:254:LEU:HG	2.17	0.43
2:D:69:PHE:CD2	2:D:80:ALA:HB2	2.53	0.43
2:D:197:VAL:CB	2:D:366:PRO:HB2	2.48	0.43
1:E:6:SER:HB2	1:E:8:HIS:HD2	1.84	0.43
1:E:10:ASP:C	2:G:88:TYR:CE2	2.90	0.43
1:F:170:CYS:SG	1:F:218:ILE:HG22	2.59	0.43
2:H:415:CYS:HB2	2:H:469:PHE:CE1	2.51	0.43
1:B:28:SER:OG	1:B:30:ASP:OD1	2.36	0.43
1:B:59:VAL:O	1:B:59:VAL:HG12	2.18	0.43
1:E:314:LEU:CD2	2:G:73:PRO:O	2.67	0.43
2:H:481:LEU:O	2:H:484:VAL:HB	2.19	0.43
1:A:25:ALA:O	1:A:61:ILE:HD12	2.18	0.43
1:B:145:LEU:HD12	1:B:145:LEU:N	2.33	0.43
1:B:169:PHE:O	1:B:170:CYS:HB3	2.19	0.43
2:C:515:THR:CG2	2:C:516:ASN:H	2.31	0.43
1:E:328:VAL:HG11	2:G:69:PHE:CG	2.53	0.43
2:H:526:CYS:O	2:H:530:ARG:N	2.47	0.43
1:A:170:CYS:SG	1:A:218:ILE:HG22	2.59	0.43
2:D:163:LYS:CE	2:D:168:ARG:HH21	2.29	0.43
2:D:344:ARG:NH1	2:D:344:ARG:CG	2.79	0.43
2:G:184:CYS:HB2	2:G:211:TRP:CE2	2.54	0.43
2:H:269:ASP:O	2:H:270:LEU:C	2.55	0.43
1:A:47:LEU:HD12	1:A:48:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:PHE:HB3	2:D:90:LEU:HD23	2.00	0.43
2:D:197:VAL:HB	2:D:366:PRO:O	2.19	0.43
2:D:492:SER:C	2:D:494:THR:H	2.22	0.43
1:E:199:ASP:OD2	1:E:201:LYS:HB2	2.18	0.43
1:F:101:LEU:O	1:F:102:CYS:HB2	2.17	0.43
2:G:104:PHE:C	2:G:106:ALA:H	2.21	0.43
2:G:151:ILE:O	2:G:152:LEU:C	2.57	0.43
2:G:198:GLU:HA	2:G:300:SER:OG	2.17	0.43
2:G:253:VAL:HG21	2:G:335:PHE:CE1	2.54	0.43
2:G:263:GLY:O	2:G:267:ARG:HG2	2.19	0.43
2:G:274:LEU:HD22	2:G:281:SER:CB	2.47	0.43
2:H:478:ASP:O	2:H:480:GLU:N	2.51	0.43
2:C:167:GLY:O	2:C:168:ARG:HG3	2.18	0.43
2:C:482:TRP:O	2:C:486:ILE:HG12	2.19	0.43
2:C:527:VAL:HG12	2:C:528:GLU:N	2.34	0.43
2:D:85:LYS:O	2:D:86:ASP:HB2	2.18	0.43
2:D:108:VAL:HG12	2:D:484:VAL:HG11	2.01	0.43
1:E:117:ALA:HB2	1:E:173:TRP:CE2	2.53	0.43
2:G:40:ARG:O	2:G:42:PRO:HD3	2.19	0.43
1:A:76:SER:OG	1:A:77:TYR:N	2.51	0.43
2:C:226:GLN:C	2:C:228:PHE:H	2.21	0.43
1:F:6:SER:HB2	1:F:8:HIS:HD2	1.84	0.43
2:H:555:SER:HA	2:H:558:ASN:OD1	2.19	0.43
2:C:117:ASP:C	2:C:119:GLY:H	2.22	0.43
2:C:258:LEU:HD22	2:C:292:LEU:CD2	2.42	0.43
2:D:253:VAL:HG21	2:D:335:PHE:CE1	2.53	0.43
1:E:169:PHE:O	1:E:170:CYS:HB3	2.19	0.43
2:G:81:PHE:HB3	2:G:90:LEU:HD23	2.00	0.43
2:G:99:ASP:OD1	2:G:101:SER:HB2	2.18	0.43
2:H:197:VAL:HB	2:H:366:PRO:HB2	2.01	0.43
2:H:459:ASN:OD1	2:H:494:THR:HB	2.18	0.43
1:A:328:VAL:HG11	2:C:69:PHE:CG	2.54	0.43
1:B:11:LEU:N	2:D:88:TYR:HE2	2.17	0.43
2:D:515:THR:HB	2:D:518:ASP:OD1	2.18	0.43
2:D:533:GLU:OE1	2:D:533:GLU:HA	2.19	0.43
2:G:67:LEU:HD12	2:G:81:PHE:O	2.19	0.43
2:G:247:LYS:O	2:G:251:GLN:HG3	2.19	0.43
2:G:460:GLY:O	2:G:463:SER:N	2.52	0.43
2:G:508:LEU:HB3	2:G:534:ILE:HD13	2.01	0.43
2:H:89:LYS:HD2	2:H:89:LYS:H	1.82	0.43
2:H:201:ARG:HG3	2:H:201:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:GLN:C	2:H:228:PHE:H	2.22	0.43
2:H:305:GLU:O	2:H:308:ASN:HB3	2.19	0.43
1:A:303:HIS:HD1	1:A:325:ASP:CG	2.22	0.42
2:C:104:PHE:O	2:C:107:TYR:N	2.51	0.42
2:C:270:LEU:HD13	2:C:289:ILE:CD1	2.49	0.42
2:C:406:LEU:HB2	2:C:407:PRO:CD	2.44	0.42
2:D:226:GLN:C	2:D:228:PHE:H	2.21	0.42
2:D:383:VAL:CG1	2:D:384:VAL:N	2.81	0.42
1:F:314:LEU:HD21	2:H:475:SER:OG	2.19	0.42
2:G:94:ARG:HH21	2:G:98:LEU:HB3	1.83	0.42
2:G:271:LEU:O	2:G:275:SER:HB3	2.19	0.42
2:G:519:ILE:O	2:G:523:LEU:HG	2.19	0.42
2:H:81:PHE:CD1	2:H:81:PHE:C	2.92	0.42
2:H:553:ILE:O	2:H:556:ILE:CG2	2.67	0.42
1:A:82:LYS:HE3	1:A:100:LYS:HD3	2.00	0.42
2:C:252:LEU:HD23	2:C:252:LEU:HA	1.89	0.42
2:C:529:TRP:O	2:C:530:ARG:HB2	2.18	0.42
1:F:86:GLU:HB2	1:F:98:TRP:CZ3	2.54	0.42
2:G:197:VAL:HB	2:G:366:PRO:O	2.19	0.42
2:G:460:GLY:C	2:G:462:ALA:N	2.72	0.42
2:H:204:PHE:O	2:H:207:SER:N	2.52	0.42
2:H:480:GLU:O	2:H:483:PRO:CD	2.66	0.42
2:C:89:LYS:HD2	2:C:89:LYS:H	1.80	0.42
1:E:114:VAL:O	1:E:114:VAL:HG13	2.19	0.42
1:B:314:LEU:CD2	2:D:73:PRO:O	2.67	0.42
2:C:204:PHE:CD1	2:C:205:ILE:N	2.87	0.42
2:D:324:ILE:O	2:D:325:SER:C	2.58	0.42
1:E:183:LEU:HD12	1:E:184:ALA:H	1.85	0.42
1:F:27:CYS:HB3	1:F:61:ILE:CD1	2.40	0.42
2:G:85:LYS:O	2:G:86:ASP:HB2	2.18	0.42
2:H:231:LYS:CG	2:H:232:ASP:H	2.29	0.42
1:A:199:ASP:OD2	1:A:201:LYS:HD2	2.19	0.42
1:B:22:ARG:HA	1:B:22:ARG:HD3	1.83	0.42
1:B:151:THR:HG22	1:B:152:SER:N	2.32	0.42
2:C:305:GLU:O	2:C:309:LEU:HG	2.20	0.42
2:D:86:ASP:CA	2:D:88:TYR:CE1	3.03	0.42
2:D:202:SER:HA	2:D:297:LYS:O	2.19	0.42
2:D:238:LYS:O	2:D:239:VAL:C	2.57	0.42
2:H:104:PHE:C	2:H:106:ALA:N	2.72	0.42
2:H:204:PHE:CD1	2:H:204:PHE:C	2.92	0.42
2:H:526:CYS:O	2:H:530:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:CYS:SG	1:B:27:CYS:O	2.78	0.42
2:D:69:PHE:HD2	2:D:80:ALA:HB2	1.83	0.42
2:D:179:LEU:O	2:D:182:LEU:N	2.52	0.42
2:D:498:SER:O	2:D:499:ALA:C	2.57	0.42
1:E:28:SER:OG	1:E:30:ASP:OD1	2.37	0.42
1:F:156:VAL:HG12	1:F:157:LEU:N	2.34	0.42
1:A:22:ARG:HD3	1:A:22:ARG:HA	1.85	0.42
1:A:199:ASP:OD2	1:A:201:LYS:HB2	2.20	0.42
1:B:101:LEU:O	1:B:102:CYS:HB2	2.18	0.42
2:C:103:GLU:CD	2:C:103:GLU:N	2.73	0.42
2:C:336:LEU:HA	2:C:339:ILE:HD12	2.00	0.42
2:C:487:GLY:O	2:C:488:LEU:C	2.57	0.42
2:D:89:LYS:HD2	2:D:89:LYS:H	1.82	0.42
2:D:94:ARG:HH21	2:D:98:LEU:HB3	1.83	0.42
2:D:112:PHE:CE1	2:D:488:LEU:HD13	2.54	0.42
1:E:59:VAL:O	1:E:59:VAL:HG12	2.19	0.42
1:F:80:THR:HG22	1:F:105:ASN:HA	2.01	0.42
1:F:199:ASP:OD2	1:F:201:LYS:HD2	2.19	0.42
2:G:145:ASN:O	2:G:148:MET:HB3	2.20	0.42
2:H:42:PRO:HD2	2:H:46:ALA:O	2.19	0.42
2:H:459:ASN:HB3	2:H:494:THR:HB	2.02	0.42
2:H:551:ASN:O	2:H:555:SER:HB2	2.20	0.42
1:B:117:ALA:HB2	1:B:173:TRP:CE2	2.55	0.42
1:B:178:PHE:CE2	2:D:502:MET:HG2	2.55	0.42
1:B:328:VAL:HG11	2:D:69:PHE:CG	2.55	0.42
2:D:396:ASP:OD1	2:D:401:LYS:HE3	2.19	0.42
1:F:116:PHE:HD1	1:F:124:LYS:O	2.03	0.42
2:H:103:GLU:CD	2:H:103:GLU:N	2.73	0.42
1:A:91:GLU:O	1:A:97:ARG:HD2	2.20	0.42
1:B:80:THR:HG22	1:B:105:ASN:HA	2.02	0.42
2:D:167:GLY:O	2:D:168:ARG:HG3	2.20	0.42
1:E:82:LYS:HE3	1:E:100:LYS:HD3	2.02	0.42
1:F:245:ILE:HA	1:F:293:GLN:O	2.20	0.42
2:G:204:PHE:O	2:G:207:SER:N	2.53	0.42
2:G:218:GLU:HA	2:G:220:ASP:N	2.35	0.42
2:G:270:LEU:HD13	2:G:289:ILE:CD1	2.49	0.42
2:H:342:ASN:O	2:H:343:GLN:C	2.58	0.42
1:A:114:VAL:HG13	1:A:114:VAL:O	2.20	0.42
1:A:310:VAL:HA	1:A:320:SER:O	2.20	0.42
1:A:313:ASN:HB3	1:A:317:THR:H	1.84	0.42
1:B:320:SER:HB3	2:D:71:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:ASP:C	2:C:198:GLU:N	2.73	0.42
2:C:274:LEU:HD22	2:C:281:SER:CB	2.49	0.42
2:D:365:ILE:HB	2:D:374:TYR:OH	2.20	0.42
2:D:492:SER:C	2:D:494:THR:N	2.74	0.42
1:E:114:VAL:HG23	1:E:126:ALA:O	2.19	0.42
2:G:69:PHE:CE1	2:G:71:LEU:HD23	2.45	0.42
2:G:373:GLU:O	2:G:377:MET:HG3	2.20	0.42
2:G:547:LEU:C	2:G:549:ALA:N	2.73	0.42
1:A:54:HIS:HD2	1:A:58:ILE:HG12	1.85	0.41
1:A:117:ALA:HB2	1:A:173:TRP:CE2	2.55	0.41
1:B:199:ASP:OD2	1:B:201:LYS:HB2	2.20	0.41
2:D:258:LEU:HD22	2:D:292:LEU:CD2	2.42	0.41
1:E:23:HIS:HD2	1:E:37:LYS:HA	1.84	0.41
1:E:61:ILE:HG22	1:E:62:ASP:N	2.35	0.41
1:E:124:LYS:HA	1:E:138:ASP:HB3	2.01	0.41
1:F:16:VAL:HG21	1:F:61:ILE:O	2.19	0.41
2:G:357:PHE:CE1	2:G:398:ILE:HD11	2.56	0.41
2:G:508:LEU:C	2:G:510:HIS:H	2.23	0.41
2:H:457:TYR:CD1	2:H:457:TYR:C	2.93	0.41
2:H:467:ASN:OD1	2:H:467:ASN:N	2.51	0.41
1:A:101:LEU:O	1:A:102:CYS:HB2	2.19	0.41
1:B:208:LEU:HD11	1:B:231:ILE:HD12	1.99	0.41
2:C:81:PHE:CD1	2:C:81:PHE:C	2.93	0.41
2:C:383:VAL:CG1	2:C:384:VAL:N	2.81	0.41
2:D:83:THR:O	2:D:84:ALA:HB2	2.20	0.41
2:D:103:GLU:CD	2:D:103:GLU:N	2.73	0.41
1:E:1:MET:CE	2:G:94:ARG:HD2	2.49	0.41
2:G:197:VAL:CB	2:G:366:PRO:HB2	2.50	0.41
2:G:226:GLN:C	2:G:228:PHE:H	2.23	0.41
2:G:473:LEU:HB2	2:G:485:ALA:HB2	2.02	0.41
2:H:469:PHE:O	2:H:470:ALA:C	2.58	0.41
1:A:48:SER:O	1:A:49:ASP:HB2	2.20	0.41
2:C:228:PHE:CE2	2:C:267:ARG:HG3	2.55	0.41
2:C:231:LYS:NZ	2:C:233:SER:HB3	2.35	0.41
2:D:142:ALA:O	2:D:146:LEU:HG	2.21	0.41
2:D:248:LEU:HD23	2:D:248:LEU:O	2.20	0.41
2:D:511:TYR:HA	2:D:512:PRO:HD3	1.81	0.41
1:F:47:LEU:HD12	1:F:48:SER:N	2.36	0.41
1:F:206:ALA:HB1	2:G:315:GLN:OE1	2.20	0.41
1:F:247:GLU:HG3	1:F:247:GLU:O	2.20	0.41
2:G:83:THR:O	2:G:84:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:201:ARG:NH2	2:G:303:PHE:CD1	2.88	0.41
2:G:491:LEU:O	2:G:493:ALA:N	2.54	0.41
2:H:171:ARG:O	2:H:175:LEU:HG	2.20	0.41
2:H:200:ASN:O	2:H:201:ARG:C	2.59	0.41
2:H:253:VAL:HG21	2:H:335:PHE:CE1	2.55	0.41
2:H:557:ALA:O	2:H:561:ARG:N	2.40	0.41
1:A:171:LEU:HB3	1:A:185:VAL:HG13	2.01	0.41
1:A:347:ALA:HB1	2:C:57:PRO:HG2	2.03	0.41
1:B:124:LYS:HA	1:B:138:ASP:HB3	2.02	0.41
2:C:167:GLY:O	2:C:168:ARG:CG	2.68	0.41
2:D:305:GLU:O	2:D:308:ASN:HB3	2.20	0.41
1:E:156:VAL:HG12	1:E:157:LEU:N	2.36	0.41
1:E:242:ILE:HD11	1:E:319:LEU:CD2	2.50	0.41
1:F:124:LYS:HA	1:F:138:ASP:HB3	2.01	0.41
2:H:201:ARG:HG3	2:H:201:ARG:HH11	1.85	0.41
1:A:21:GLY:HA3	2:C:73:PRO:HD2	2.02	0.41
1:A:226:ARG:HG3	1:A:226:ARG:NH1	2.34	0.41
1:B:303:HIS:HD1	1:B:325:ASP:CG	2.24	0.41
2:C:104:PHE:C	2:C:106:ALA:N	2.73	0.41
2:C:173:TYR:HD1	2:C:173:TYR:H	1.68	0.41
2:C:407:PRO:O	2:C:410:GLU:HB3	2.21	0.41
2:D:204:PHE:O	2:D:207:SER:N	2.53	0.41
1:E:199:ASP:OD2	1:E:201:LYS:HD2	2.20	0.41
1:F:199:ASP:OD2	1:F:201:LYS:HB2	2.20	0.41
2:G:228:PHE:CE2	2:G:267:ARG:HG3	2.56	0.41
2:H:263:GLY:O	2:H:267:ARG:HG2	2.19	0.41
1:A:81:VAL:CG2	1:A:111:LEU:HD13	2.36	0.41
1:B:23:HIS:HD2	1:B:37:LYS:HA	1.85	0.41
2:C:296:PRO:HD3	2:C:306:TRP:CD1	2.55	0.41
2:C:461:MET:O	2:C:465:MET:HG3	2.21	0.41
2:C:550:HIS:HA	2:C:553:ILE:CG1	2.50	0.41
2:D:57:PRO:HG2	2:D:58:ILE:H	1.86	0.41
2:D:190:PHE:CE2	2:D:427:LYS:HG3	2.56	0.41
1:E:54:HIS:HE1	1:E:82:LYS:HB2	1.85	0.41
1:F:54:HIS:HE1	1:F:82:LYS:HB2	1.85	0.41
2:G:375:LEU:HD11	2:G:395:VAL:HG13	2.01	0.41
2:H:383:VAL:CG1	2:H:384:VAL:N	2.83	0.41
2:H:532:PRO:O	2:H:536:LYS:HG3	2.21	0.41
2:C:245:PHE:O	2:C:248:LEU:HB3	2.20	0.41
2:D:190:PHE:N	2:D:190:PHE:CD1	2.87	0.41
2:D:313:LEU:HD23	2:D:313:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ALA:HA	1:E:173:TRP:CG	2.55	0.41
2:G:142:ALA:O	2:G:146:LEU:HG	2.21	0.41
2:H:478:ASP:C	2:H:480:GLU:N	2.74	0.41
1:B:54:HIS:HE1	1:B:82:LYS:HB2	1.86	0.41
1:B:156:VAL:HG12	1:B:157:LEU:N	2.35	0.41
2:C:205:ILE:O	2:C:205:ILE:HG22	2.20	0.41
2:C:511:TYR:CE2	2:C:513:PHE:HB3	2.56	0.41
2:D:466:LEU:HD23	2:D:466:LEU:HA	1.92	0.41
1:E:221:ALA:HA	1:E:222:PRO:HD3	1.87	0.41
2:G:104:PHE:C	2:G:106:ALA:N	2.74	0.41
2:G:253:VAL:HG21	2:G:335:PHE:HE1	1.85	0.41
2:G:347:LEU:O	2:G:348:GLN:C	2.57	0.41
2:G:456:SER:OG	2:G:457:TYR:N	2.54	0.41
2:G:516:ASN:HA	2:G:519:ILE:HD12	2.01	0.41
2:H:99:ASP:OD1	2:H:101:SER:HB2	2.20	0.41
2:H:173:TYR:HD1	2:H:173:TYR:H	1.69	0.41
2:H:313:LEU:C	2:H:313:LEU:HD23	2.41	0.41
1:A:145:LEU:HD12	1:A:145:LEU:N	2.36	0.41
1:A:151:THR:CG2	1:A:196:ARG:HH22	2.33	0.41
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.36	0.41
1:B:108:LYS:HE2	1:B:133:ILE:HD12	2.01	0.41
1:B:116:PHE:HD1	1:B:124:LYS:O	2.03	0.41
2:C:342:ASN:O	2:C:343:GLN:C	2.59	0.41
2:D:218:GLU:HA	2:D:220:ASP:N	2.35	0.41
2:D:347:LEU:O	2:D:348:GLN:C	2.59	0.41
1:F:25:ALA:O	1:F:61:ILE:HD12	2.20	0.41
1:F:54:HIS:HD2	1:F:58:ILE:HG12	1.86	0.41
1:F:226:ARG:HG3	1:F:226:ARG:NH1	2.33	0.41
1:F:303:HIS:HD1	1:F:325:ASP:CG	2.23	0.41
2:G:81:PHE:C	2:G:81:PHE:CD1	2.94	0.41
2:G:296:PRO:HD3	2:G:306:TRP:CD1	2.55	0.41
2:H:204:PHE:CD1	2:H:205:ILE:N	2.89	0.41
2:H:209:LEU:HD21	2:H:362:LEU:HD11	2.02	0.41
2:H:511:TYR:CE2	2:H:513:PHE:HB3	2.56	0.41
1:A:113:SER:HB3	1:A:170:CYS:HA	2.03	0.41
1:A:228:TYR:CD2	1:A:244:LYS:HG3	2.53	0.41
1:A:245:ILE:HA	1:A:293:GLN:O	2.20	0.41
1:B:6:SER:HB2	1:B:8:HIS:HD2	1.86	0.41
1:B:199:ASP:OD2	1:B:201:LYS:HD2	2.21	0.41
2:D:42:PRO:HD2	2:D:47:ILE:HA	2.01	0.41
2:D:105:SER:HB2	2:D:481:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:VAL:HG21	2:D:335:PHE:HE1	1.85	0.41
1:F:151:THR:CG2	1:F:196:ARG:HH22	2.34	0.41
1:F:313:ASN:HB3	1:F:317:THR:H	1.86	0.41
2:G:179:LEU:O	2:G:182:LEU:N	2.54	0.41
2:G:240:PHE:CE2	2:G:268:SER:HB2	2.56	0.41
2:G:305:GLU:O	2:G:308:ASN:HB3	2.21	0.41
2:G:523:LEU:HD23	2:G:538:ILE:HD12	2.02	0.41
2:H:406:LEU:O	2:H:407:PRO:C	2.59	0.41
2:H:467:ASN:HA	2:H:470:ALA:HB3	2.02	0.41
1:A:74:SER:O	1:A:81:VAL:HG13	2.21	0.40
1:B:15:VAL:HB	2:D:81:PHE:CE2	2.56	0.40
2:C:57:PRO:HG2	2:C:58:ILE:H	1.86	0.40
2:C:253:VAL:HG21	2:C:335:PHE:CE1	2.56	0.40
2:C:324:ILE:O	2:C:325:SER:C	2.60	0.40
2:D:543:GLY:O	2:D:547:LEU:HG	2.21	0.40
1:F:21:GLY:HA3	2:H:73:PRO:HD2	2.02	0.40
1:F:108:LYS:HE2	1:F:133:ILE:HD12	2.04	0.40
2:G:483:PRO:HA	2:G:521:TRP:HZ2	1.86	0.40
2:C:91:TYR:CD1	2:C:91:TYR:N	2.89	0.40
2:C:201:ARG:NH1	2:C:201:ARG:HG3	2.36	0.40
2:C:218:GLU:HA	2:C:220:ASP:N	2.35	0.40
2:D:367:SER:C	2:D:369:GLU:N	2.75	0.40
2:G:202:SER:HA	2:G:297:LYS:O	2.21	0.40
2:G:248:LEU:HD23	2:G:248:LEU:O	2.21	0.40
2:H:218:GLU:HA	2:H:220:ASP:N	2.36	0.40
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.35	0.40
1:B:2:GLN:HA	1:B:3:PRO:HD3	1.95	0.40
2:C:86:ASP:CA	2:C:88:TYR:CE1	3.05	0.40
2:C:142:ALA:O	2:C:146:LEU:HG	2.22	0.40
2:C:406:LEU:O	2:C:407:PRO:C	2.60	0.40
2:C:467:ASN:O	2:C:471:PHE:CD1	2.74	0.40
1:E:177:ARG:HD2	1:E:178:PHE:CE1	2.57	0.40
1:E:305:GLY:HA3	1:E:324:ASP:HB2	2.03	0.40
1:F:82:LYS:HE3	1:F:100:LYS:HD3	2.02	0.40
1:F:97:ARG:HG3	1:F:97:ARG:NH1	2.36	0.40
2:G:86:ASP:CA	2:G:88:TYR:CE1	3.03	0.40
2:G:535:ALA:O	2:G:538:ILE:HB	2.20	0.40
2:H:205:ILE:O	2:H:205:ILE:HG22	2.21	0.40
2:H:248:LEU:O	2:H:248:LEU:HD23	2.21	0.40
2:H:375:LEU:HB2	2:H:398:ILE:HD13	2.03	0.40
1:A:117:ALA:HA	1:A:173:TRP:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:HG2	2:D:311:LEU:HD21	2.04	0.40
2:C:85:LYS:O	2:C:86:ASP:HB2	2.21	0.40
2:D:200:ASN:O	2:D:201:ARG:C	2.60	0.40
2:D:274:LEU:HD22	2:D:281:SER:CB	2.50	0.40
2:D:296:PRO:HD3	2:D:306:TRP:CD1	2.55	0.40
1:E:25:ALA:O	1:E:61:ILE:HD12	2.21	0.40
1:F:1:MET:CE	2:H:94:ARG:HD2	2.51	0.40
1:F:59:VAL:O	1:F:59:VAL:HG12	2.20	0.40
1:F:117:ALA:HB2	1:F:173:TRP:CE2	2.56	0.40
1:A:1:MET:HE2	2:C:94:ARG:HD2	2.03	0.40
1:B:113:SER:HB3	1:B:170:CYS:HA	2.04	0.40
1:B:313:ASN:HB3	1:B:317:THR:H	1.86	0.40
2:C:558:ASN:CG	2:C:559:PHE:N	2.75	0.40
2:D:67:LEU:HD12	2:D:81:PHE:O	2.22	0.40
2:D:93:VAL:HG12	2:D:94:ARG:N	2.36	0.40
2:D:240:PHE:CE2	2:D:268:SER:HB2	2.57	0.40
2:D:460:GLY:O	2:D:462:ALA:N	2.54	0.40
2:D:508:LEU:C	2:D:510:HIS:N	2.75	0.40
1:E:63:TRP:CH2	1:E:72:ILE:HD11	2.56	0.40
1:E:116:PHE:HD1	1:E:124:LYS:O	2.03	0.40
1:F:345:ILE:CD1	2:H:93:VAL:HG11	2.48	0.40
2:G:467:ASN:O	2:G:471:PHE:HD1	2.05	0.40
2:H:166:ASP:HB3	2:H:169:VAL:HG21	2.04	0.40
2:H:367:SER:C	2:H:369:GLU:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/351 (84%)	240 (82%)	48 (16%)	6 (2%)	7 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	294/351 (84%)	243 (83%)	45 (15%)	6 (2%)	7	41
1	E	294/351 (84%)	242 (82%)	47 (16%)	5 (2%)	9	43
1	F	294/351 (84%)	242 (82%)	46 (16%)	6 (2%)	7	41
2	C	486/570 (85%)	378 (78%)	82 (17%)	26 (5%)	2	22
2	D	472/570 (83%)	371 (79%)	76 (16%)	25 (5%)	2	22
2	G	474/570 (83%)	370 (78%)	79 (17%)	25 (5%)	2	22
2	H	487/570 (85%)	384 (79%)	78 (16%)	25 (5%)	2	23
All	All	3095/3684 (84%)	2470 (80%)	501 (16%)	124 (4%)	3	28

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	B	302	ASP
2	C	197	VAL
2	C	200	ASN
2	C	270	LEU
2	C	273	TYR
2	D	43	VAL
2	D	197	VAL
2	D	200	ASN
2	D	270	LEU
2	D	273	TYR
2	D	515	THR
2	D	553	ILE
1	E	302	ASP
1	F	302	ASP
2	G	46	ALA
2	G	197	VAL
2	G	200	ASN
2	G	270	LEU
2	G	273	TYR
2	G	514	VAL
2	H	43	VAL
2	H	197	VAL
2	H	200	ASN
2	H	270	LEU
2	H	273	TYR
2	H	549	ALA
2	C	205	ILE

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Mol	Chain	Res	Type
2	C	235	ALA
2	C	239	VAL
2	C	272	PRO
2	C	479	LYS
2	C	549	ALA
2	C	552	ILE
2	C	556	ILE
2	D	205	ILE
2	D	239	VAL
2	D	272	PRO
2	D	479	LYS
2	D	514	VAL
2	G	205	ILE
2	G	239	VAL
2	G	272	PRO
2	G	493	ALA
2	H	46	ALA
2	H	239	VAL
2	H	272	PRO
2	H	550	HIS
1	A	94	SER
1	A	170	CYS
1	B	170	CYS
1	B	325	ASP
2	C	60	LYS
2	C	101	SER
2	C	543	GLY
2	D	60	LYS
2	D	101	SER
2	D	204	PHE
2	D	461	MET
2	D	493	ALA
1	E	94	SER
1	E	170	CYS
1	E	325	ASP
1	F	94	SER
1	F	170	CYS
1	F	325	ASP
2	G	60	LYS
2	G	101	SER
2	G	204	PHE
2	G	236	GLY

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Mol	Chain	Res	Type
2	G	492	SER
2	G	515	THR
2	H	60	LYS
2	H	101	SER
2	H	204	PHE
2	H	205	ILE
2	H	460	GLY
2	H	479	LYS
1	A	41	ASP
1	A	325	ASP
1	B	41	ASP
1	B	94	SER
2	C	42	PRO
2	C	164	ASP
2	C	172	PHE
2	C	204	PHE
2	C	325	SER
2	C	368	LEU
2	D	164	ASP
2	D	325	SER
2	D	401	LYS
1	E	41	ASP
1	F	41	ASP
2	G	164	ASP
2	G	325	SER
2	G	368	LEU
2	H	164	ASP
2	H	172	PHE
2	H	325	SER
2	H	472	GLU
2	C	119	GLY
2	C	401	LYS
2	D	119	GLY
2	D	172	PHE
2	D	368	LEU
2	D	485	ALA
2	G	119	GLY
2	G	161	ARG
2	G	172	PHE
2	H	368	LEU
2	H	401	LYS
2	C	227	VAL

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Mol	Chain	Res	Type
2	D	227	VAL
2	G	227	VAL
2	G	401	LYS
2	H	119	GLY
2	H	227	VAL
2	C	514	VAL
2	C	553	ILE
1	A	156	VAL
2	G	553	ILE
2	H	527	VAL
1	B	156	VAL
1	F	156	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/307 (85%)	259 (99%)	3 (1%)	73	85
1	B	262/307 (85%)	259 (99%)	3 (1%)	73	85
1	E	262/307 (85%)	259 (99%)	3 (1%)	73	85
1	F	262/307 (85%)	259 (99%)	3 (1%)	73	85
2	C	438/510 (86%)	431 (98%)	7 (2%)	62	80
2	D	428/510 (84%)	421 (98%)	7 (2%)	62	80
2	G	429/510 (84%)	424 (99%)	5 (1%)	71	84
2	H	439/510 (86%)	430 (98%)	9 (2%)	53	74
All	All	2782/3268 (85%)	2742 (99%)	40 (1%)	67	82

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	171	LEU
1	A	226	ARG

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Mol	Chain	Res	Type
1	B	5	ASP
1	B	171	LEU
1	B	226	ARG
2	C	200	ASN
2	C	269	ASP
2	C	308	ASN
2	C	465	MET
2	C	488	LEU
2	C	497	ARG
2	C	558	ASN
2	D	200	ASN
2	D	269	ASP
2	D	308	ASN
2	D	497	ARG
2	D	518	ASP
2	D	530	ARG
2	D	533	GLU
1	E	5	ASP
1	E	171	LEU
1	E	226	ARG
1	F	5	ASP
1	F	171	LEU
1	F	226	ARG
2	G	200	ASN
2	G	269	ASP
2	G	308	ASN
2	G	457	TYR
2	G	533	GLU
2	H	200	ASN
2	H	231	LYS
2	H	269	ASP
2	H	308	ASN
2	H	459	ASN
2	H	497	ARG
2	H	518	ASP
2	H	533	GLU
2	H	558	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	308	ASN

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Mol	Chain	Res	Type
2	C	545	GLN
2	D	308	ASN
2	G	551	ASN
2	H	308	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	300/351 (85%)	0.31	5 (1%)	70	65	97, 126, 151, 158	0
1	B	300/351 (85%)	0.30	8 (2%)	54	47	96, 125, 152, 160	0
1	E	300/351 (85%)	0.25	10 (3%)	46	40	97, 126, 152, 160	0
1	F	300/351 (85%)	0.33	10 (3%)	46	40	98, 126, 151, 158	0
2	C	492/570 (86%)	0.08	13 (2%)	56	49	90, 124, 170, 179	0
2	D	480/570 (84%)	0.02	6 (1%)	77	73	92, 122, 167, 180	0
2	G	482/570 (84%)	0.06	6 (1%)	79	75	92, 123, 167, 179	0
2	H	493/570 (86%)	0.16	6 (1%)	79	75	91, 125, 170, 183	0
All	All	3147/3684 (85%)	0.16	64 (2%)	65	60	90, 124, 162, 183	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	126	VAL	6.5
2	G	61	ASN	4.9
2	C	124	PHE	4.8
1	F	195	GLN	3.9
2	H	121	ASP	3.9
2	G	136	PHE	3.8
1	B	167	SER	3.8
1	B	168	ASP	3.8
2	C	122	ARG	3.3
2	C	121	ASP	3.1
2	H	430	ILE	3.0
1	B	307	VAL	2.9
2	H	124	PHE	2.9
1	E	306	GLU	2.9
2	C	136	PHE	2.9
1	B	160	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	75	ALA	2.8
1	E	160	PRO	2.8
2	C	141	ASN	2.7
2	C	67	LEU	2.7
2	G	227	VAL	2.7
2	H	61	ASN	2.7
1	E	169	PHE	2.6
1	A	195	GLN	2.6
1	F	112	TYR	2.6
1	F	45	TRP	2.5
2	C	454	LEU	2.5
2	C	139	GLU	2.5
1	A	145	LEU	2.4
1	E	188	LEU	2.4
2	C	366	PRO	2.4
1	F	199	ASP	2.3
2	D	71	LEU	2.3
1	F	208	LEU	2.3
1	A	71	ILE	2.3
1	F	167	SER	2.3
1	E	307	VAL	2.3
2	C	140	HIS	2.2
1	F	290	SER	2.2
2	D	136	PHE	2.2
1	E	168	ASP	2.2
2	D	219	PRO	2.2
1	B	191	ALA	2.2
2	C	193	ASP	2.2
1	F	171	LEU	2.2
2	H	138	LYS	2.2
2	G	168	ARG	2.1
1	E	124	LYS	2.1
1	E	214	LEU	2.1
2	G	126	VAL	2.1
2	C	125	ASN	2.1
1	E	75	ALA	2.1
1	B	170	CYS	2.1
1	A	208	LEU	2.1
2	H	62	GLY	2.1
2	C	65	MET	2.1
1	B	53	ALA	2.1
2	G	62	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	193	ILE	2.0
2	D	193	ASP	2.0
1	F	343	SER	2.0
2	D	61	ASN	2.0
1	A	240	ILE	2.0
1	B	232	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.