Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:14 pm BST

PDB ID	:	1IOK
Title	:	CRYSTAL STRUCTURE OF CHAPERONIN-60 FROM PARACOCCUS DENITRIFICANS
Authors	:	Fukami, T.A.; Yohda, M.; Taguchi, H.; Yoshida, M.; Miki, K.
Deposited on	:	2001-03-16
Resolution	:	3.20 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 ⓘ symbol.

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

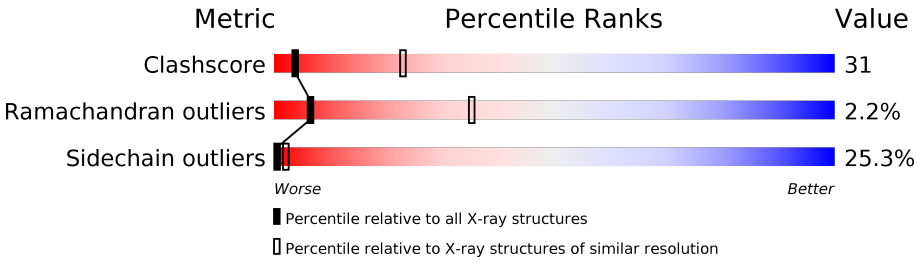
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	545	36% 42% 10% 12%
1	B	545	37% 42% 10% 12%
1	C	545	37% 41% 10% 12%
1	D	545	37% 42% 10% 12%
1	E	545	37% 41% 10% 12%
1	F	545	37% 41% 10% 12%
1	G	545	37% 41% 10% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25095 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 CHAPERONIN 60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	B	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	C	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	D	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	E	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	F	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	G	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			

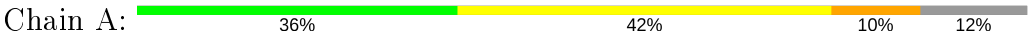
3 Residue-property plots (i)

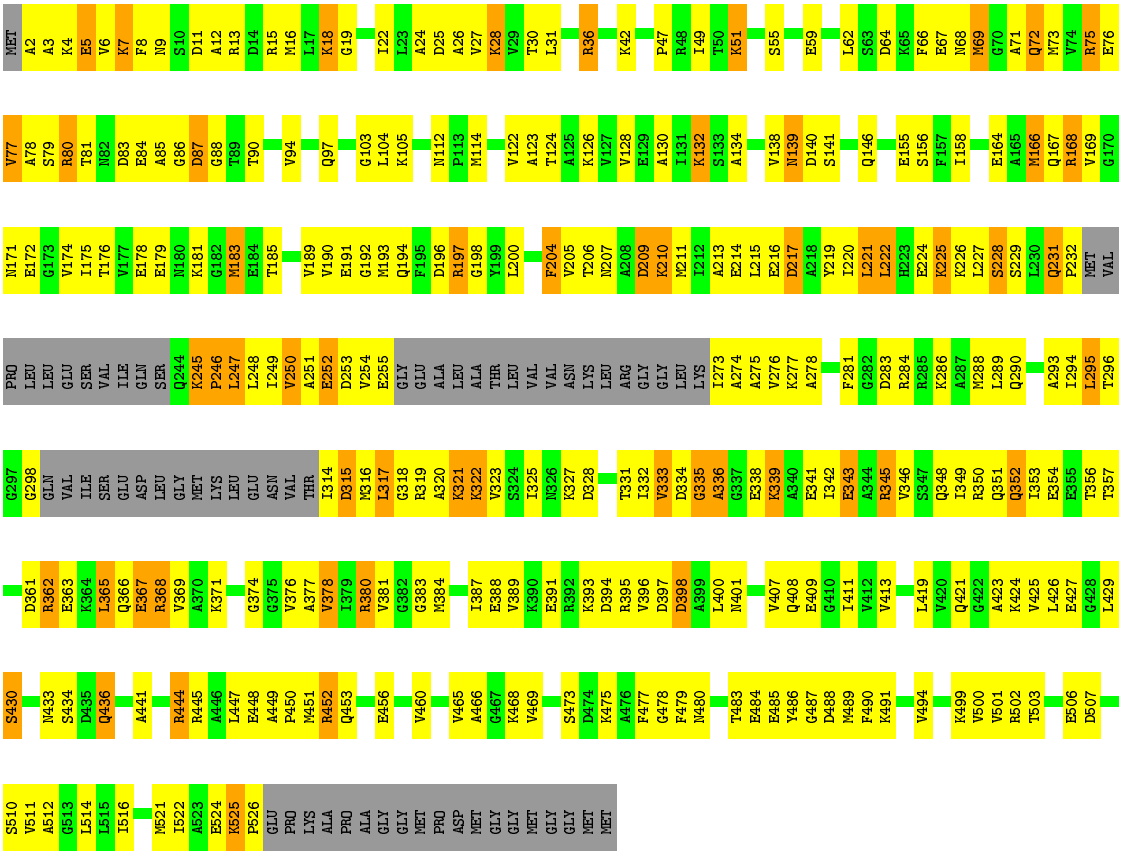
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: CHAPERONIN 60

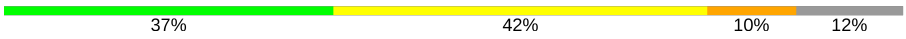
Chain A:

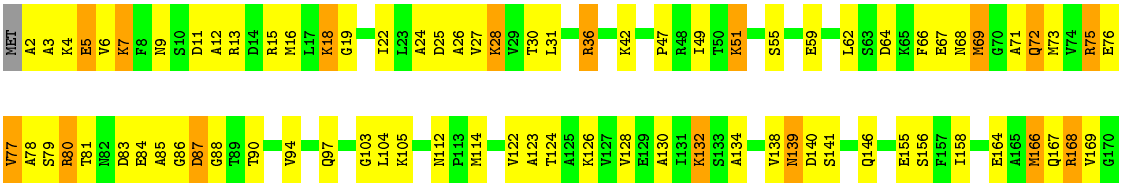


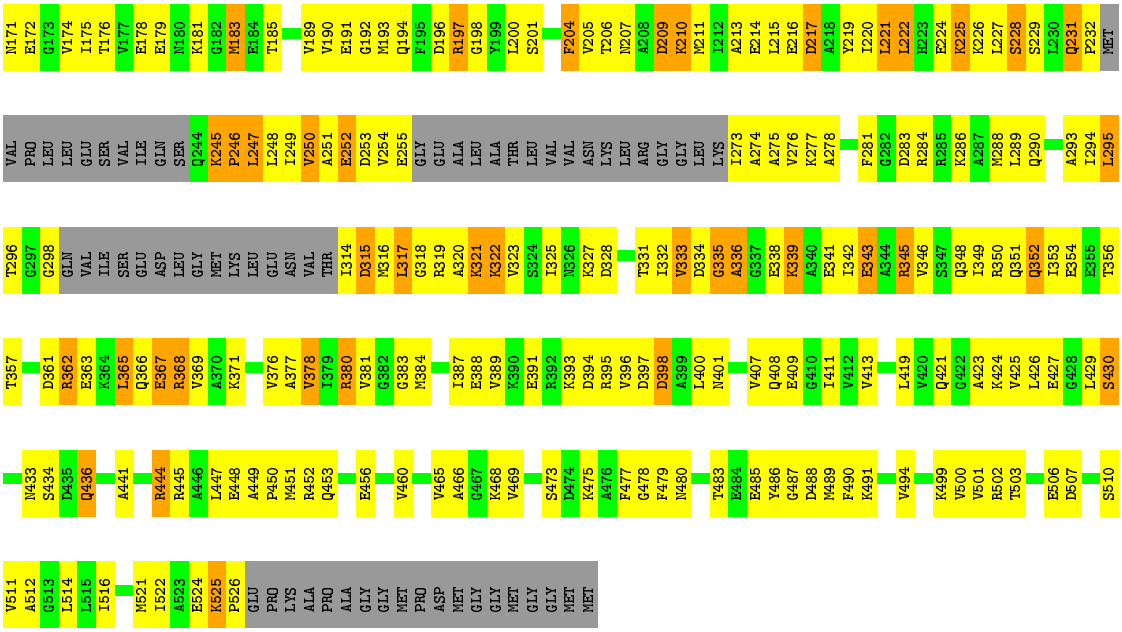


- Molecule 1: CHAPERONIN 60

Chain B:

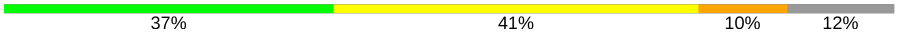


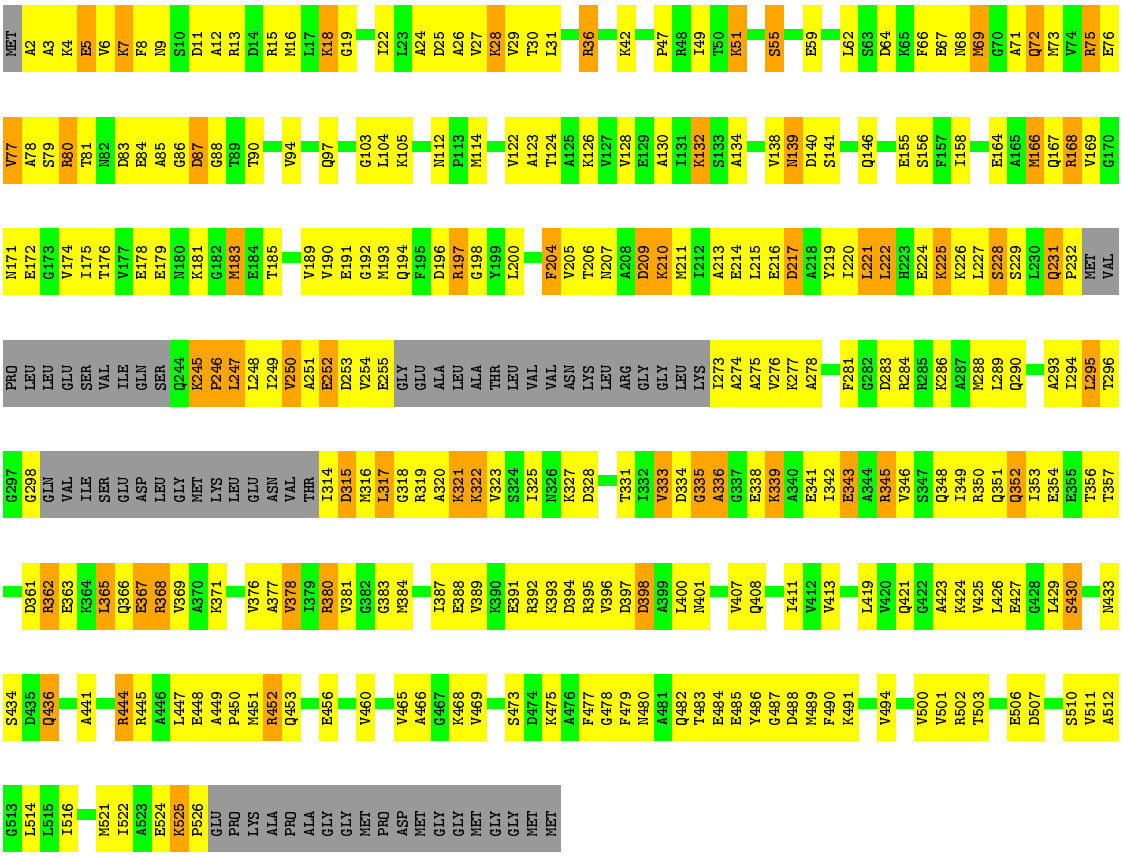




• Molecule 1: CHAPERONIN 60

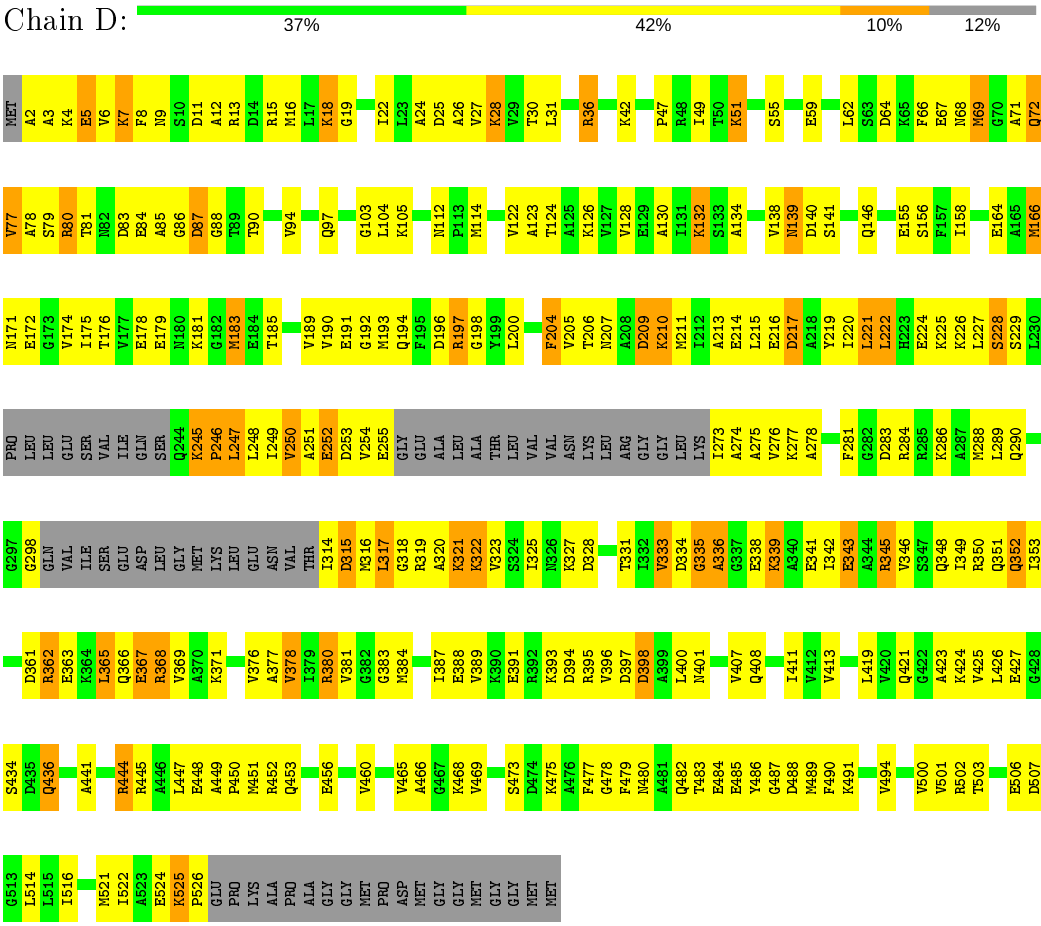
Chain C:





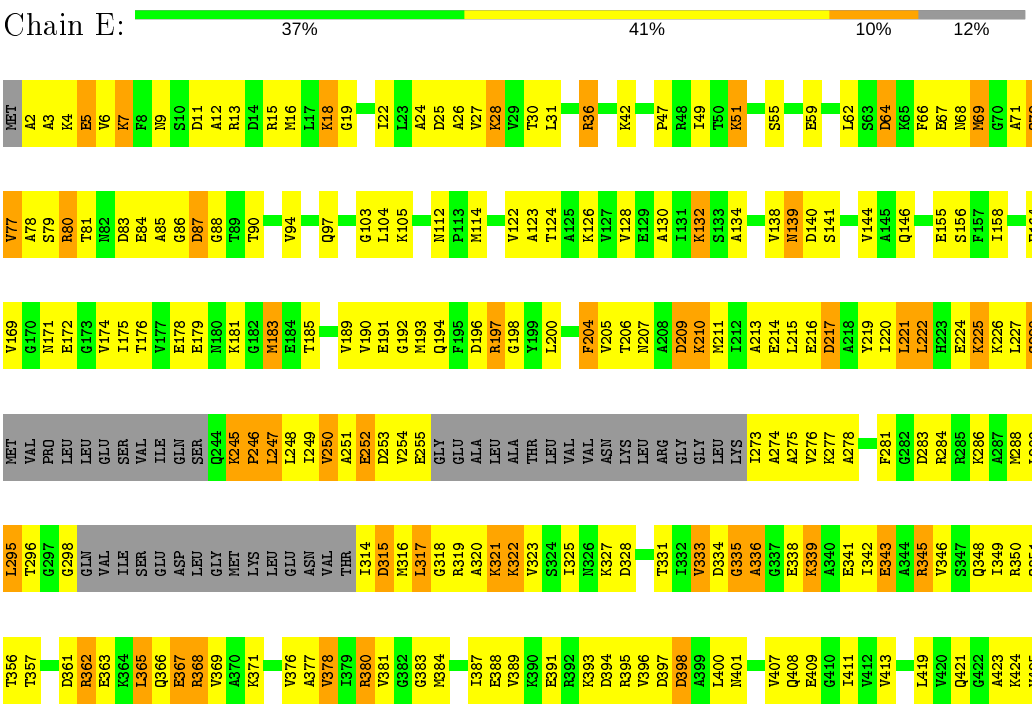
• Molecule 1: CHAPERONIN 60

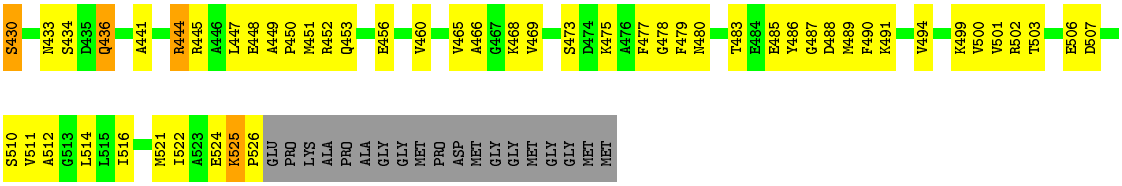
Chain D:



- Molecule 1: CHAPERONIN 60

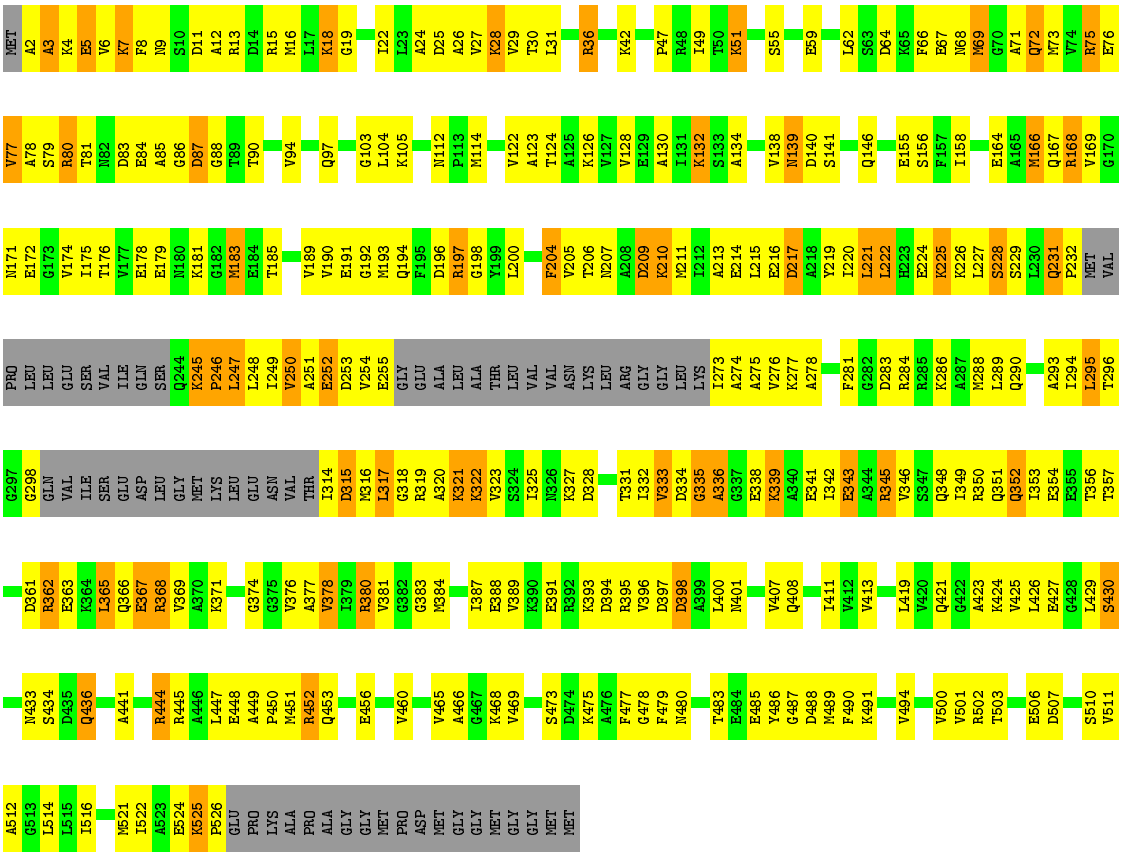
Chain E:





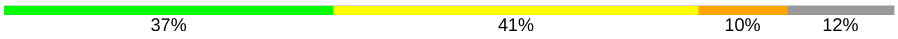
• Molecule 1: CHAPERONIN 60

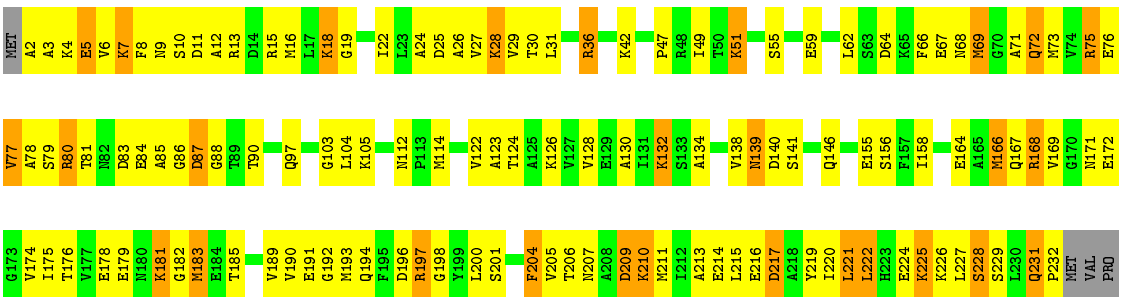
Chain F:

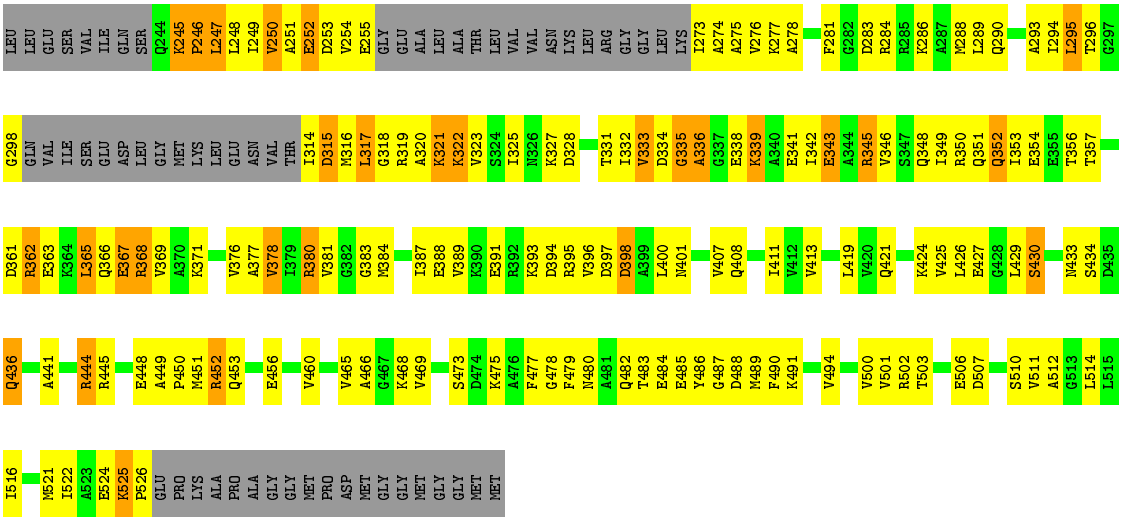


• Molecule 1: CHAPERONIN 60

Chain G:






LEU LEU GLU SER VAL ILE GLN SER Q244 K245 P246 L247 L248 I249 V250 A251 E252 D253 V254 E255 GLY GLU ALA LEU ALA THR LEU VAL VAL ASN LYS LEU ARG GLY GLY LEU LYS I273 A274 A275 V276 K277 A278 F281 G282 D283 R284 R285 K286 A287 M288 L289 Q290 A293 I294 L295 T296 G297
G298 GLN VAL ILE SER GLU ASP LEU GLY MET LYS LEU GLU ASN VAL THR I314 D315 M316 L317 G318 R319 A320 K321 K322 V323 S324 I325 N326 K327 D328 T331 I332 V333 D334 G335 A336 G337 E338 K339 A340 E341 I342 E343 A344 R345 V346 S347 Q348 I349 R350 Q351 Q352 I353 E354 E355 T356 T357
D361 R362 E363 R364 L365 Q366 E367 R368 V369 A370 K371 V376 A377 V378 I379 R380 V381 G382 G383 M384 I387 E388 V389 K390 E391 R392 K393 D394 R395 V396 D397 D398 A399 L400 N401 V407 Q408 I411 V412 V413 L419 V420 Q421 K424 V425 L426 E427 G428 L429 S430 N433 S434 D435
Q436 A441 R444 R445 E448 A449 P450 M451 R452 Q453 E456 V460 V465 A466 G467 K468 V469 S473 D474 K475 A476 F477 G478 F479 N480 A481 Q482 T483 E484 E485 Y486 G487 D488 M489 F490 K491 V494 V500 V501 R502 T503 E506 D507 S510 V511 A512 G513 L514 L515
I516 M521 I522 A523 E524 K525 P526 GLU PRO LYS ALA PRO ALA GLY GLY MET PRO ASP MET GLY GLY MET GLY GLY MET MET

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	286.36Å 286.36Å 153.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25095	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/3609	0.48	0/4855
1	B	0.33	0/3609	0.48	0/4855
1	C	0.32	0/3609	0.49	0/4855
1	D	0.34	0/3609	0.48	0/4855
1	E	0.33	0/3609	0.48	0/4855
1	F	0.32	0/3609	0.49	0/4855
1	G	0.33	0/3609	0.48	0/4855
All	All	0.33	0/25263	0.48	0/33985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3585	0	3657	233	0
1	B	3585	0	3657	231	0
1	C	3585	0	3657	229	0
1	D	3585	0	3657	228	0
1	E	3585	0	3657	231	0
1	F	3585	0	3657	235	0
1	G	3585	0	3657	231	0
All	All	25095	0	25599	1574	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 31.

All (1574) 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)
1:D:139:ASN:HD22	1:D:140:ASP:H	1.17	0.93
1:C:139:ASN:HD22	1:C:140:ASP:H	1.17	0.92
1:C:36:ARG:HG2	1:C:36:ARG:HH11	1.35	0.92
1:G:139:ASN:HD22	1:G:140:ASP:H	1.16	0.92
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.35	0.91
1:F:139:ASN:HD22	1:F:140:ASP:H	1.17	0.91
1:E:139:ASN:HD22	1:E:140:ASP:H	1.17	0.91
1:F:36:ARG:HH11	1:F:36:ARG:HG2	1.34	0.91
1:A:139:ASN:HD22	1:A:140:ASP:H	1.18	0.90
1:B:36:ARG:HH11	1:B:36:ARG:HG2	1.35	0.90
1:E:36:ARG:HG2	1:E:36:ARG:HH11	1.36	0.90
1:C:227:LEU:HB2	1:C:254:VAL:HA	1.54	0.89
1:F:227:LEU:HB2	1:F:254:VAL:HA	1.54	0.89
1:A:227:LEU:HB2	1:A:254:VAL:HA	1.55	0.89
1:G:227:LEU:HB2	1:G:254:VAL:HA	1.55	0.89
1:B:227:LEU:HB2	1:B:254:VAL:HA	1.55	0.89
1:B:139:ASN:HD22	1:B:140:ASP:H	1.18	0.88
1:D:227:LEU:HB2	1:D:254:VAL:HA	1.55	0.88
1:D:36:ARG:HH11	1:D:36:ARG:HG2	1.36	0.88
1:E:227:LEU:HB2	1:E:254:VAL:HA	1.55	0.88
1:G:36:ARG:HH11	1:G:36:ARG:HG2	1.40	0.86
1:A:228:SER:HA	1:A:255:GLU:HB2	1.58	0.85
1:G:228:SER:HA	1:G:255:GLU:HB2	1.59	0.85
1:B:228:SER:HA	1:B:255:GLU:HB2	1.59	0.84
1:C:228:SER:HA	1:C:255:GLU:HB2	1.59	0.83
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.60	0.83
1:E:228:SER:HA	1:E:255:GLU:HB2	1.59	0.83
1:F:514:LEU:HD13	1:G:49:ILE:HD12	1.61	0.82
1:D:228:SER:HA	1:D:255:GLU:HB2	1.59	0.82
1:F:228:SER:HA	1:F:255:GLU:HB2	1.59	0.82
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.62	0.82
1:B:514:LEU:HD13	1:C:49:ILE:HD12	1.63	0.81
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.62	0.81
1:A:322:LYS:HB3	1:A:333:VAL:HG23	1.63	0.81
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.62	0.81
1:D:322:LYS:HB3	1:D:333:VAL:HG23	1.63	0.81
1:F:322:LYS:HB3	1:F:333:VAL:HG23	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.61	0.80
1:E:322:LYS:HB3	1:E:333:VAL:HG23	1.63	0.80
1:A:49:ILE:HD12	1:G:514:LEU:HD13	1.63	0.80
1:G:322:LYS:HB3	1:G:333:VAL:HG23	1.64	0.80
1:C:514:LEU:HD13	1:D:49:ILE:HD12	1.63	0.80
1:B:322:LYS:HB3	1:B:333:VAL:HG23	1.64	0.80
1:C:322:LYS:HB3	1:C:333:VAL:HG23	1.64	0.80
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.61	0.79
1:F:250:VAL:HG13	1:F:276:VAL:HG23	1.65	0.78
1:A:197:ARG:HH11	1:A:277:LYS:HG2	1.49	0.78
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.64	0.78
1:G:250:VAL:HG13	1:G:276:VAL:HG23	1.66	0.78
1:D:197:ARG:HH11	1:D:277:LYS:HG2	1.49	0.77
1:A:250:VAL:HG13	1:A:276:VAL:HG23	1.66	0.77
1:E:197:ARG:HH11	1:E:277:LYS:HG2	1.50	0.77
1:B:380:ARG:HB2	1:B:380:ARG:HH11	1.50	0.77
1:B:197:ARG:HH11	1:B:277:LYS:HG2	1.50	0.77
1:D:250:VAL:HG13	1:D:276:VAL:HG23	1.66	0.77
1:F:197:ARG:HH11	1:F:277:LYS:HG2	1.50	0.77
1:G:197:ARG:HH11	1:G:277:LYS:HG2	1.50	0.77
1:E:250:VAL:HG13	1:E:276:VAL:HG23	1.67	0.77
1:E:380:ARG:HB2	1:E:380:ARG:HH11	1.50	0.77
1:C:250:VAL:HG13	1:C:276:VAL:HG23	1.66	0.77
1:A:380:ARG:HH11	1:A:380:ARG:HB2	1.50	0.76
1:G:380:ARG:HH11	1:G:380:ARG:HB2	1.50	0.76
1:C:197:ARG:HH11	1:C:277:LYS:HG2	1.50	0.76
1:C:380:ARG:HH11	1:C:380:ARG:HB2	1.50	0.76
1:F:380:ARG:HH11	1:F:380:ARG:HB2	1.50	0.76
1:C:413:VAL:HG12	1:C:489:MET:HB3	1.68	0.76
1:B:250:VAL:HG13	1:B:276:VAL:HG23	1.66	0.76
1:D:380:ARG:HH11	1:D:380:ARG:HB2	1.50	0.75
1:B:413:VAL:HG12	1:B:489:MET:HB3	1.69	0.75
1:G:413:VAL:HG12	1:G:489:MET:HB3	1.68	0.74
1:E:413:VAL:HG12	1:E:489:MET:HB3	1.68	0.74
1:A:413:VAL:HG12	1:A:489:MET:HB3	1.69	0.74
1:E:514:LEU:HD13	1:F:49:ILE:HD12	1.70	0.73
1:D:413:VAL:HG12	1:D:489:MET:HB3	1.70	0.73
1:F:413:VAL:HG12	1:F:489:MET:HB3	1.69	0.73
1:A:514:LEU:HD13	1:B:49:ILE:HD12	1.70	0.73
1:E:411:ILE:HD12	1:E:490:PHE:HE1	1.54	0.72
1:D:514:LEU:HD13	1:E:49:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ILE:HD12	1:C:490:PHE:HE1	1.54	0.72
1:B:128:VAL:HG13	1:B:502:ARG:HG3	1.70	0.72
1:F:411:ILE:HD12	1:F:490:PHE:HE1	1.53	0.72
1:E:226:LYS:HG2	1:E:252:GLU:HB2	1.72	0.71
1:D:128:VAL:HG13	1:D:502:ARG:HG3	1.72	0.71
1:B:411:ILE:HD12	1:B:490:PHE:HE1	1.56	0.71
1:A:411:ILE:HD12	1:A:490:PHE:HE1	1.55	0.71
1:D:411:ILE:HD12	1:D:490:PHE:HE1	1.55	0.71
1:C:7:LYS:HD2	1:C:66:PHE:CZ	2.25	0.71
1:D:226:LYS:HG2	1:D:252:GLU:HB2	1.72	0.71
1:E:128:VAL:HG13	1:E:502:ARG:HG3	1.73	0.71
1:F:346:VAL:HG12	1:F:350:ARG:HE	1.56	0.71
1:C:128:VAL:HG13	1:C:502:ARG:HG3	1.72	0.71
1:A:346:VAL:HG12	1:A:350:ARG:HE	1.56	0.70
1:C:226:LYS:HG2	1:C:252:GLU:HB2	1.73	0.70
1:G:128:VAL:HG13	1:G:502:ARG:HG3	1.72	0.70
1:D:139:ASN:HD22	1:D:140:ASP:N	1.90	0.70
1:G:346:VAL:HG12	1:G:350:ARG:HE	1.56	0.70
1:F:7:LYS:HD2	1:F:66:PHE:CZ	2.26	0.70
1:G:7:LYS:HD2	1:G:66:PHE:CZ	2.26	0.70
1:B:346:VAL:HG12	1:B:350:ARG:HE	1.56	0.70
1:B:36:ARG:NH1	1:B:36:ARG:HG2	2.07	0.70
1:F:128:VAL:HG13	1:F:502:ARG:HG3	1.73	0.70
1:G:226:LYS:HG2	1:G:252:GLU:HB2	1.72	0.70
1:D:36:ARG:NH1	1:D:36:ARG:HG2	2.07	0.70
1:A:448:GLU:O	1:A:452:ARG:HD2	1.91	0.70
1:C:346:VAL:HG12	1:C:350:ARG:HE	1.56	0.70
1:F:226:LYS:HG2	1:F:252:GLU:HB2	1.72	0.70
1:A:226:LYS:HG2	1:A:252:GLU:HB2	1.73	0.69
1:D:7:LYS:HD2	1:D:66:PHE:CZ	2.26	0.69
1:F:130:ALA:CB	1:F:425:VAL:HG21	2.22	0.69
1:G:411:ILE:HD12	1:G:490:PHE:HE1	1.57	0.69
1:B:226:LYS:HG2	1:B:252:GLU:HB2	1.72	0.69
1:E:7:LYS:HD2	1:E:66:PHE:CZ	2.26	0.69
1:E:130:ALA:CB	1:E:425:VAL:HG21	2.22	0.69
1:D:346:VAL:HG12	1:D:350:ARG:HE	1.56	0.69
1:A:130:ALA:CB	1:A:425:VAL:HG21	2.23	0.69
1:G:139:ASN:HD22	1:G:140:ASP:N	1.90	0.69
1:G:130:ALA:CB	1:G:425:VAL:HG21	2.23	0.69
1:C:130:ALA:CB	1:C:425:VAL:HG21	2.23	0.69
1:G:227:LEU:HD22	1:G:254:VAL:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:MET:HG2	1:G:171:ASN:HA	1.74	0.68
1:E:346:VAL:HG12	1:E:350:ARG:HE	1.57	0.68
1:A:73:MET:CE	1:B:49:ILE:HD11	2.23	0.68
1:C:448:GLU:O	1:C:452:ARG:HD2	1.92	0.68
1:A:128:VAL:HG13	1:A:502:ARG:HG3	1.74	0.68
1:A:366:GLN:O	1:A:369:VAL:HG12	1.94	0.68
1:B:139:ASN:HD22	1:B:140:ASP:N	1.91	0.68
1:B:7:LYS:HD2	1:B:66:PHE:CZ	2.29	0.68
1:F:166:MET:HG2	1:F:171:ASN:HA	1.76	0.68
1:B:130:ALA:CB	1:B:425:VAL:HG21	2.23	0.68
1:C:366:GLN:O	1:C:369:VAL:HG12	1.94	0.68
1:D:166:MET:HG2	1:D:171:ASN:HA	1.75	0.68
1:F:448:GLU:O	1:F:452:ARG:HD2	1.94	0.68
1:B:227:LEU:HD22	1:B:254:VAL:HG22	1.76	0.68
1:E:139:ASN:HD22	1:E:140:ASP:N	1.90	0.68
1:E:166:MET:HG2	1:E:171:ASN:HA	1.76	0.68
1:A:227:LEU:HD22	1:A:254:VAL:HG22	1.76	0.67
1:C:321:LYS:HB3	1:C:334:ASP:HB3	1.76	0.67
1:D:130:ALA:CB	1:D:425:VAL:HG21	2.23	0.67
1:C:227:LEU:HD22	1:C:254:VAL:HG22	1.77	0.67
1:C:139:ASN:HD22	1:C:140:ASP:N	1.91	0.67
1:F:227:LEU:HD22	1:F:254:VAL:HG22	1.76	0.67
1:G:448:GLU:O	1:G:452:ARG:HD2	1.93	0.67
1:E:227:LEU:HD22	1:E:254:VAL:HG22	1.76	0.67
1:D:321:LYS:HB3	1:D:334:ASP:HB3	1.77	0.67
1:D:366:GLN:O	1:D:369:VAL:HG12	1.94	0.67
1:F:366:GLN:O	1:F:369:VAL:HG12	1.93	0.67
1:A:132:LYS:HD3	1:A:502:ARG:HD3	1.76	0.67
1:D:227:LEU:HD22	1:D:254:VAL:HG22	1.77	0.67
1:E:130:ALA:HB2	1:E:425:VAL:HG21	1.77	0.67
1:G:366:GLN:O	1:G:369:VAL:HG12	1.93	0.66
1:A:7:LYS:HD2	1:A:66:PHE:CZ	2.29	0.66
1:B:166:MET:HG2	1:B:171:ASN:HA	1.76	0.66
1:G:132:LYS:HD3	1:G:502:ARG:HD3	1.77	0.66
1:A:166:MET:HG2	1:A:171:ASN:HA	1.76	0.66
1:C:166:MET:HG2	1:C:171:ASN:HA	1.75	0.66
1:C:183:MET:HG2	1:C:384:MET:SD	2.35	0.66
1:E:366:GLN:O	1:E:369:VAL:HG12	1.94	0.66
1:A:183:MET:HG2	1:A:384:MET:SD	2.36	0.66
1:B:366:GLN:O	1:B:369:VAL:HG12	1.95	0.66
1:F:231:GLN:NE2	1:F:231:GLN:H	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:LYS:HB3	1:G:334:ASP:HB3	1.76	0.66
1:B:321:LYS:HB3	1:B:334:ASP:HB3	1.78	0.66
1:F:130:ALA:HB2	1:F:425:VAL:HG21	1.77	0.66
1:B:448:GLU:O	1:B:452:ARG:HD2	1.96	0.66
1:D:183:MET:HG2	1:D:384:MET:SD	2.36	0.66
1:A:321:LYS:HB3	1:A:334:ASP:HB3	1.76	0.65
1:E:226:LYS:NZ	1:E:252:GLU:HB3	2.11	0.65
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.77	0.65
1:F:321:LYS:HB3	1:F:334:ASP:HB3	1.77	0.65
1:B:183:MET:HG2	1:B:384:MET:SD	2.37	0.65
1:D:226:LYS:NZ	1:D:252:GLU:HB3	2.12	0.65
1:F:219:TYR:HB2	1:F:247:LEU:HA	1.79	0.65
1:A:219:TYR:HB2	1:A:247:LEU:HA	1.78	0.65
1:D:130:ALA:HB2	1:D:425:VAL:HG21	1.79	0.65
1:D:231:GLN:H	1:D:231:GLN:NE2	1.94	0.65
1:B:130:ALA:HB2	1:B:425:VAL:HG21	1.78	0.65
1:B:231:GLN:NE2	1:B:231:GLN:H	1.95	0.65
1:G:231:GLN:H	1:G:231:GLN:NE2	1.94	0.65
1:C:226:LYS:NZ	1:C:252:GLU:HB3	2.12	0.65
1:E:448:GLU:O	1:E:452:ARG:HD2	1.97	0.65
1:C:130:ALA:HB2	1:C:425:VAL:HG21	1.78	0.65
1:E:231:GLN:H	1:E:231:GLN:NE2	1.95	0.65
1:F:132:LYS:HD3	1:F:502:ARG:HD3	1.78	0.65
1:C:231:GLN:H	1:C:231:GLN:NE2	1.95	0.65
1:G:36:ARG:HG2	1:G:36:ARG:NH1	2.10	0.65
1:A:231:GLN:H	1:A:231:GLN:NE2	1.95	0.64
1:B:128:VAL:HG13	1:B:502:ARG:CG	2.27	0.64
1:E:209:ASP:HB3	1:E:210:LYS:NZ	2.12	0.64
1:B:72:GLN:HE22	1:B:75:ARG:NH1	1.95	0.64
1:A:226:LYS:NZ	1:A:252:GLU:HB3	2.12	0.64
1:C:209:ASP:HB3	1:C:210:LYS:NZ	2.12	0.64
1:C:36:ARG:HG2	1:C:36:ARG:NH1	2.07	0.64
1:D:448:GLU:O	1:D:452:ARG:HD2	1.97	0.64
1:D:73:MET:CE	1:E:49:ILE:HD11	2.27	0.64
1:F:429:LEU:HD12	1:F:430:SER:H	1.62	0.64
1:G:77:VAL:HA	1:G:80:ARG:HD3	1.79	0.64
1:D:429:LEU:HD12	1:D:430:SER:H	1.63	0.64
1:E:183:MET:HG2	1:E:384:MET:SD	2.37	0.64
1:F:226:LYS:NZ	1:F:252:GLU:HB3	2.12	0.64
1:G:183:MET:HG2	1:G:384:MET:SD	2.36	0.64
1:A:77:VAL:HA	1:A:80:ARG:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASP:HB3	1:B:210:LYS:NZ	2.13	0.64
1:A:130:ALA:HB2	1:A:425:VAL:HG21	1.78	0.64
1:E:219:TYR:HB2	1:E:247:LEU:HA	1.78	0.64
1:B:226:LYS:NZ	1:B:252:GLU:HB3	2.12	0.64
1:D:132:LYS:HD3	1:D:502:ARG:HD3	1.78	0.64
1:G:130:ALA:HB2	1:G:425:VAL:HG21	1.79	0.64
1:G:209:ASP:HB3	1:G:210:LYS:NZ	2.13	0.64
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.05	0.64
1:B:219:TYR:HB2	1:B:247:LEU:HA	1.78	0.64
1:D:209:ASP:HB3	1:D:210:LYS:NZ	2.13	0.64
1:F:183:MET:HG2	1:F:384:MET:SD	2.38	0.64
1:G:250:VAL:HA	1:G:276:VAL:O	1.98	0.64
1:C:132:LYS:HD3	1:C:502:ARG:HD3	1.79	0.64
1:D:190:VAL:HG12	1:D:191:GLU:H	1.62	0.64
1:D:77:VAL:HA	1:D:80:ARG:HD3	1.78	0.64
1:G:219:TYR:HB2	1:G:247:LEU:HA	1.78	0.64
1:G:226:LYS:NZ	1:G:252:GLU:HB3	2.13	0.64
1:A:429:LEU:HD12	1:A:430:SER:H	1.64	0.63
1:D:219:TYR:HB2	1:D:247:LEU:HA	1.79	0.63
1:F:250:VAL:HA	1:F:276:VAL:O	1.98	0.63
1:F:77:VAL:HA	1:F:80:ARG:HD3	1.80	0.63
1:A:209:ASP:HB3	1:A:210:LYS:NZ	2.13	0.63
1:F:209:ASP:HB3	1:F:210:LYS:NZ	2.13	0.63
1:F:72:GLN:HE22	1:F:75:ARG:NH1	1.96	0.63
1:C:219:TYR:HB2	1:C:247:LEU:HA	1.79	0.63
1:E:77:VAL:HA	1:E:80:ARG:HD3	1.80	0.63
1:F:139:ASN:HD22	1:F:140:ASP:N	1.91	0.63
1:E:84:GLU:HG3	1:E:500:VAL:HG22	1.81	0.63
1:E:72:GLN:HE22	1:E:75:ARG:NH1	1.96	0.63
1:G:72:GLN:HE22	1:G:75:ARG:NH1	1.97	0.63
1:C:250:VAL:HA	1:C:276:VAL:O	1.98	0.63
1:G:128:VAL:HG13	1:G:502:ARG:CG	2.28	0.63
1:E:248:LEU:HA	1:E:274:ALA:HB3	1.81	0.63
1:A:250:VAL:HA	1:A:276:VAL:O	1.99	0.62
1:B:250:VAL:HA	1:B:276:VAL:O	1.98	0.62
1:D:250:VAL:HA	1:D:276:VAL:O	1.99	0.62
1:B:77:VAL:HA	1:B:80:ARG:HD3	1.79	0.62
1:C:429:LEU:HD12	1:C:430:SER:H	1.63	0.62
1:E:250:VAL:HA	1:E:276:VAL:O	1.98	0.62
1:F:138:VAL:HG12	1:F:407:VAL:HG12	1.81	0.62
1:C:72:GLN:HE22	1:C:75:ARG:NH1	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:VAL:HG13	1:E:502:ARG:CG	2.29	0.62
1:E:73:MET:CE	1:F:49:ILE:HD11	2.30	0.62
1:A:176:THR:O	1:A:378:VAL:HG23	2.00	0.62
1:A:138:VAL:HG12	1:A:407:VAL:HG12	1.82	0.62
1:B:174:VAL:HG22	1:B:376:VAL:HG13	1.81	0.62
1:B:429:LEU:HD12	1:B:430:SER:H	1.64	0.62
1:B:176:THR:O	1:B:378:VAL:HG23	1.99	0.62
1:C:190:VAL:HG12	1:C:191:GLU:H	1.63	0.62
1:E:429:LEU:HD12	1:E:430:SER:H	1.65	0.62
1:F:248:LEU:HA	1:F:274:ALA:HB3	1.82	0.62
1:B:84:GLU:HG3	1:B:500:VAL:HG22	1.81	0.62
1:C:128:VAL:HG13	1:C:502:ARG:CG	2.28	0.62
1:C:176:THR:O	1:C:378:VAL:HG23	1.99	0.62
1:C:193:MET:HB2	1:C:295:LEU:HD22	1.82	0.62
1:E:174:VAL:HG22	1:E:376:VAL:HG13	1.82	0.62
1:F:36:ARG:NH1	1:F:36:ARG:HG2	2.07	0.62
1:D:174:VAL:HG22	1:D:376:VAL:HG13	1.82	0.62
1:E:132:LYS:HD3	1:E:502:ARG:HD3	1.79	0.62
1:C:73:MET:CE	1:D:49:ILE:HD11	2.30	0.62
1:F:84:GLU:HG3	1:F:500:VAL:HG22	1.82	0.62
1:F:176:THR:O	1:F:378:VAL:HG23	2.00	0.62
1:G:429:LEU:HD12	1:G:430:SER:H	1.63	0.62
1:A:525:LYS:HD2	1:A:526:PRO:HD2	1.82	0.61
1:D:248:LEU:HA	1:D:274:ALA:HB3	1.82	0.61
1:G:190:VAL:HG12	1:G:191:GLU:H	1.65	0.61
1:A:128:VAL:HG13	1:A:502:ARG:CG	2.29	0.61
1:B:477:PHE:HA	1:B:487:GLY:O	1.99	0.61
1:D:128:VAL:HG13	1:D:502:ARG:CG	2.29	0.61
1:A:174:VAL:HG22	1:A:376:VAL:HG13	1.82	0.61
1:B:138:VAL:HG12	1:B:407:VAL:HG12	1.83	0.61
1:B:248:LEU:HA	1:B:274:ALA:HB3	1.82	0.61
1:B:132:LYS:HD3	1:B:502:ARG:HD3	1.80	0.61
1:C:174:VAL:HG22	1:C:376:VAL:HG13	1.83	0.61
1:A:139:ASN:HD22	1:A:140:ASP:N	1.92	0.61
1:A:49:ILE:HD11	1:G:73:MET:CE	2.31	0.61
1:C:221:LEU:HD11	1:C:249:ILE:HG23	1.82	0.61
1:C:248:LEU:HA	1:C:274:ALA:HB3	1.82	0.61
1:C:77:VAL:HA	1:C:80:ARG:HD3	1.81	0.61
1:E:409:GLU:OE2	1:E:499:LYS:HG3	1.99	0.61
1:A:193:MET:HB2	1:A:295:LEU:HD22	1.82	0.61
1:B:221:LEU:HD11	1:B:249:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:LYS:HD2	1:F:526:PRO:HD2	1.82	0.61
1:F:73:MET:CE	1:G:49:ILE:HD11	2.30	0.61
1:G:248:LEU:HA	1:G:274:ALA:HB3	1.82	0.61
1:A:248:LEU:HA	1:A:274:ALA:HB3	1.82	0.61
1:E:367:GLU:HG3	1:E:368:ARG:N	2.16	0.61
1:G:221:LEU:HD11	1:G:249:ILE:HG23	1.82	0.61
1:B:193:MET:HB2	1:B:295:LEU:HD22	1.82	0.61
1:E:525:LYS:HD2	1:E:526:PRO:HD2	1.82	0.61
1:F:73:MET:HE3	1:G:49:ILE:HD11	1.82	0.61
1:F:75:ARG:HG2	1:F:75:ARG:NH1	2.16	0.61
1:A:72:GLN:HE22	1:A:75:ARG:NH1	1.99	0.61
1:B:73:MET:HE3	1:C:49:ILE:HD11	1.82	0.61
1:D:525:LYS:HD2	1:D:526:PRO:HD2	1.82	0.61
1:A:49:ILE:HD11	1:G:73:MET:HE3	1.82	0.61
1:G:193:MET:HB2	1:G:295:LEU:HD22	1.82	0.61
1:F:174:VAL:HG22	1:F:376:VAL:HG13	1.84	0.60
1:G:525:LYS:HD2	1:G:526:PRO:HD2	1.83	0.60
1:D:176:THR:O	1:D:378:VAL:HG23	2.01	0.60
1:D:193:MET:HB2	1:D:295:LEU:HD22	1.83	0.60
1:F:221:LEU:HD11	1:F:249:ILE:HG23	1.82	0.60
1:D:84:GLU:HG3	1:D:500:VAL:HG22	1.83	0.60
1:G:174:VAL:HG22	1:G:376:VAL:HG13	1.84	0.60
1:G:477:PHE:HA	1:G:487:GLY:O	2.01	0.60
1:E:221:LEU:HD11	1:E:249:ILE:HG23	1.82	0.60
1:E:75:ARG:HG2	1:E:75:ARG:NH1	2.17	0.60
1:B:367:GLU:HG3	1:B:368:ARG:N	2.16	0.60
1:B:525:LYS:HD2	1:B:526:PRO:HD2	1.83	0.60
1:C:73:MET:HE3	1:D:49:ILE:HD11	1.81	0.60
1:F:128:VAL:HG13	1:F:502:ARG:CG	2.30	0.60
1:F:367:GLU:HG3	1:F:368:ARG:N	2.16	0.60
1:C:22:ILE:HG21	1:C:62:LEU:HD21	1.84	0.60
1:C:296:THR:O	1:C:336:ALA:HB3	2.02	0.60
1:G:367:GLU:HG3	1:G:368:ARG:N	2.16	0.60
1:C:367:GLU:HG3	1:C:368:ARG:N	2.16	0.60
1:C:138:VAL:HG12	1:C:407:VAL:HG12	1.83	0.60
1:E:176:THR:O	1:E:378:VAL:HG23	2.01	0.60
1:A:221:LEU:HD11	1:A:249:ILE:HG23	1.84	0.60
1:C:477:PHE:HA	1:C:487:GLY:O	2.02	0.60
1:C:525:LYS:HD2	1:C:526:PRO:HD2	1.83	0.60
1:C:84:GLU:HG3	1:C:500:VAL:HG22	1.83	0.60
1:D:73:MET:HE3	1:E:49:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:HE22	1:D:75:ARG:NH1	2.00	0.60
1:E:193:MET:HB2	1:E:295:LEU:HD22	1.82	0.60
1:F:477:PHE:HA	1:F:487:GLY:O	2.02	0.60
1:G:84:GLU:HG3	1:G:500:VAL:HG22	1.83	0.59
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.32	0.59
1:B:73:MET:CE	1:C:49:ILE:HD11	2.32	0.59
1:F:296:THR:O	1:F:336:ALA:HB3	2.02	0.59
1:G:219:TYR:H	1:G:247:LEU:HA	1.66	0.59
1:A:477:PHE:HA	1:A:487:GLY:O	2.02	0.59
1:C:352:GLN:O	1:C:356:THR:HG23	2.02	0.59
1:D:352:GLN:O	1:D:356:THR:HG23	2.02	0.59
1:F:193:MET:HB2	1:F:295:LEU:HD22	1.82	0.59
1:A:84:GLU:HG3	1:A:500:VAL:HG22	1.82	0.59
1:D:296:THR:O	1:D:336:ALA:HB3	2.02	0.59
1:D:367:GLU:HG3	1:D:368:ARG:N	2.16	0.59
1:A:73:MET:HE3	1:B:49:ILE:HD11	1.83	0.59
1:C:219:TYR:H	1:C:247:LEU:HA	1.66	0.59
1:D:219:TYR:H	1:D:247:LEU:HA	1.67	0.59
1:E:73:MET:HE3	1:F:49:ILE:HD11	1.84	0.59
1:G:138:VAL:HG12	1:G:407:VAL:HG12	1.85	0.59
1:A:296:THR:O	1:A:336:ALA:HB3	2.02	0.59
1:A:367:GLU:HG3	1:A:368:ARG:N	2.16	0.59
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.33	0.59
1:F:219:TYR:H	1:F:247:LEU:HA	1.67	0.59
1:A:219:TYR:H	1:A:247:LEU:HA	1.67	0.59
1:B:71:ALA:O	1:B:75:ARG:HB3	2.02	0.59
1:C:158:ILE:HG23	1:C:396:VAL:HG22	1.84	0.59
1:F:352:GLN:O	1:F:356:THR:HG23	2.03	0.59
1:G:296:THR:O	1:G:336:ALA:HB3	2.03	0.59
1:B:77:VAL:HG12	1:B:78:ALA:N	2.18	0.59
1:E:352:GLN:O	1:E:356:THR:HG23	2.03	0.59
1:A:394:ASP:O	1:A:398:ASP:HB2	2.03	0.59
1:B:296:THR:O	1:B:336:ALA:HB3	2.03	0.59
1:D:221:LEU:HD11	1:D:249:ILE:HG23	1.83	0.59
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.33	0.59
1:F:483:THR:OG1	1:F:485:GLU:HG2	2.03	0.59
1:E:219:TYR:H	1:E:247:LEU:HA	1.66	0.59
1:E:477:PHE:HA	1:E:487:GLY:O	2.03	0.59
1:D:158:ILE:HG23	1:D:396:VAL:HG22	1.85	0.58
1:F:411:ILE:CD1	1:F:490:PHE:HE1	2.16	0.58
1:B:219:TYR:H	1:B:247:LEU:HA	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:VAL:HG12	1:E:191:GLU:H	1.67	0.58
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.85	0.58
1:A:168:ARG:HG2	1:A:189:VAL:HG21	1.86	0.58
1:D:77:VAL:HG12	1:D:78:ALA:N	2.17	0.58
1:G:394:ASP:O	1:G:398:ASP:HB2	2.03	0.58
1:D:394:ASP:O	1:D:398:ASP:HB2	2.03	0.58
1:G:352:GLN:O	1:G:356:THR:HG23	2.03	0.58
1:C:483:THR:OG1	1:C:485:GLU:HG2	2.03	0.58
1:C:394:ASP:O	1:C:398:ASP:HB2	2.03	0.58
1:E:296:THR:O	1:E:336:ALA:HB3	2.03	0.58
1:G:483:THR:OG1	1:G:485:GLU:HG2	2.04	0.58
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.86	0.58
1:F:168:ARG:HG2	1:F:189:VAL:HG21	1.86	0.58
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.85	0.58
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.32	0.58
1:B:25:ASP:HA	1:B:28:LYS:HD2	1.86	0.58
1:D:22:ILE:HG21	1:D:62:LEU:HD21	1.86	0.58
1:G:71:ALA:O	1:G:75:ARG:HB3	2.04	0.58
1:D:477:PHE:HA	1:D:487:GLY:O	2.04	0.58
1:A:483:THR:OG1	1:A:485:GLU:HG2	2.04	0.58
1:A:19:GLY:HA3	1:A:67:GLU:O	2.04	0.58
1:C:77:VAL:HG12	1:C:78:ALA:N	2.18	0.58
1:E:138:VAL:HG12	1:E:407:VAL:HG12	1.85	0.58
1:G:365:LEU:O	1:G:368:ARG:HG3	2.04	0.58
1:G:176:THR:O	1:G:378:VAL:HG23	2.04	0.58
1:A:488:ASP:OD1	1:A:490:PHE:HB2	2.04	0.57
1:B:158:ILE:HG23	1:B:396:VAL:HG22	1.84	0.57
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.33	0.57
1:A:352:GLN:O	1:A:356:THR:HG23	2.03	0.57
1:B:394:ASP:O	1:B:398:ASP:HB2	2.04	0.57
1:B:468:LYS:HD3	1:B:486:TYR:CZ	2.39	0.57
1:B:168:ARG:HG2	1:B:189:VAL:HG21	1.87	0.57
1:B:352:GLN:O	1:B:356:THR:HG23	2.03	0.57
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.85	0.57
1:B:75:ARG:HG2	1:B:75:ARG:NH1	2.19	0.57
1:D:138:VAL:HG12	1:D:407:VAL:HG12	1.86	0.57
1:F:77:VAL:HG12	1:F:78:ALA:N	2.19	0.57
1:G:158:ILE:HG23	1:G:396:VAL:HG22	1.85	0.57
1:G:25:ASP:HA	1:G:28:LYS:HD2	1.86	0.57
1:E:36:ARG:HG2	1:E:36:ARG:NH1	2.08	0.57
1:F:158:ILE:HG23	1:F:396:VAL:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:ASP:OD1	1:F:490:PHE:HB2	2.04	0.57
1:G:75:ARG:NH1	1:G:75:ARG:HG2	2.18	0.57
1:C:168:ARG:HG2	1:C:189:VAL:HG21	1.86	0.57
1:C:411:ILE:CD1	1:C:490:PHE:HE1	2.16	0.57
1:D:502:ARG:O	1:D:506:GLU:HG3	2.04	0.57
1:F:75:ARG:HH11	1:F:75:ARG:HG2	1.68	0.57
1:A:365:LEU:O	1:A:368:ARG:HG3	2.05	0.57
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.86	0.57
1:F:468:LYS:HD3	1:F:486:TYR:CZ	2.40	0.57
1:B:409:GLU:OE2	1:B:499:LYS:HG3	2.05	0.57
1:C:226:LYS:HZ1	1:C:252:GLU:HB3	1.69	0.57
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.20	0.57
1:B:483:THR:OG1	1:B:485:GLU:HG2	2.05	0.57
1:F:71:ALA:O	1:F:75:ARG:HB3	2.05	0.57
1:A:59:GLU:O	1:G:4:LYS:HD2	2.05	0.57
1:C:245:LYS:NZ	1:C:319:ARG:HH21	2.03	0.57
1:E:168:ARG:HG2	1:E:189:VAL:HG21	1.87	0.57
1:E:365:LEU:O	1:E:368:ARG:HG3	2.05	0.57
1:E:75:ARG:HG2	1:E:75:ARG:HH11	1.67	0.57
1:G:168:ARG:HG2	1:G:189:VAL:HG21	1.87	0.57
1:B:190:VAL:HG12	1:B:191:GLU:H	1.68	0.57
1:B:451:MET:HE1	1:B:466:ALA:HA	1.87	0.57
1:G:77:VAL:HG12	1:G:78:ALA:N	2.18	0.57
1:A:31:LEU:HD13	1:A:90:THR:CG2	2.35	0.56
1:F:365:LEU:O	1:F:368:ARG:HG3	2.05	0.56
1:F:394:ASP:O	1:F:398:ASP:HB2	2.05	0.56
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.35	0.56
1:A:71:ALA:O	1:A:75:ARG:HB3	2.05	0.56
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.85	0.56
1:D:168:ARG:HG2	1:D:189:VAL:HG21	1.87	0.56
1:D:483:THR:OG1	1:D:485:GLU:HG2	2.04	0.56
1:E:22:ILE:HG21	1:E:62:LEU:HD21	1.87	0.56
1:E:394:ASP:O	1:E:398:ASP:HB2	2.05	0.56
1:E:71:ALA:O	1:E:75:ARG:HB3	2.05	0.56
1:G:468:LYS:HD3	1:G:486:TYR:CZ	2.41	0.56
1:G:502:ARG:O	1:G:506:GLU:HG3	2.05	0.56
1:A:158:ILE:HG23	1:A:396:VAL:HG22	1.85	0.56
1:B:365:LEU:O	1:B:368:ARG:HG3	2.05	0.56
1:B:479:PHE:N	1:B:489:MET:HE1	2.20	0.56
1:B:81:THR:HG23	1:B:503:THR:HG22	1.87	0.56
1:C:468:LYS:HD3	1:C:486:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.85	0.56
1:E:245:LYS:NZ	1:E:319:ARG:HH21	2.04	0.56
1:A:22:ILE:HG21	1:A:62:LEU:HD21	1.87	0.56
1:C:31:LEU:HD13	1:C:90:THR:CG2	2.36	0.56
1:D:468:LYS:HD3	1:D:486:TYR:CZ	2.40	0.56
1:F:245:LYS:NZ	1:F:319:ARG:HH21	2.03	0.56
1:G:19:GLY:HA3	1:G:67:GLU:O	2.06	0.56
1:A:77:VAL:HG12	1:A:78:ALA:N	2.19	0.56
1:C:75:ARG:HG2	1:C:75:ARG:NH1	2.20	0.56
1:D:81:THR:HG23	1:D:503:THR:HG22	1.88	0.56
1:E:411:ILE:CD1	1:E:490:PHE:HE1	2.19	0.56
1:G:13:ARG:HD3	1:G:104:LEU:HD22	1.88	0.56
1:A:209:ASP:HB3	1:A:210:LYS:HZ1	1.71	0.56
1:B:226:LYS:HZ1	1:B:252:GLU:HB3	1.69	0.56
1:B:393:LYS:O	1:B:397:ASP:HB2	2.05	0.56
1:D:411:ILE:CD1	1:D:490:PHE:HE1	2.19	0.56
1:D:4:LYS:HD2	1:E:59:GLU:O	2.06	0.56
1:F:25:ASP:HA	1:F:28:LYS:HD2	1.88	0.56
1:A:245:LYS:NZ	1:A:319:ARG:HH21	2.04	0.56
1:A:411:ILE:CD1	1:A:490:PHE:HE1	2.19	0.56
1:D:488:ASP:OD1	1:D:490:PHE:HB2	2.06	0.56
1:F:28:LYS:HG3	1:F:453:GLN:OE1	2.06	0.56
1:G:400:LEU:HG	1:G:400:LEU:O	2.06	0.56
1:A:393:LYS:O	1:A:397:ASP:HB2	2.06	0.56
1:A:81:THR:HG23	1:A:503:THR:HG22	1.88	0.56
1:D:25:ASP:HA	1:D:28:LYS:HD2	1.88	0.56
1:E:483:THR:OG1	1:E:485:GLU:HG2	2.05	0.56
1:G:245:LYS:NZ	1:G:319:ARG:HH21	2.04	0.56
1:A:468:LYS:HD3	1:A:486:TYR:CZ	2.40	0.56
1:B:245:LYS:NZ	1:B:319:ARG:HH21	2.04	0.56
1:C:200:LEU:HD23	1:C:275:ALA:O	2.06	0.56
1:C:71:ALA:O	1:C:75:ARG:HB3	2.06	0.56
1:E:209:ASP:HB3	1:E:210:LYS:HZ1	1.70	0.56
1:G:75:ARG:HH11	1:G:75:ARG:HG2	1.69	0.56
1:B:488:ASP:OD1	1:B:490:PHE:HB2	2.05	0.56
1:C:393:LYS:O	1:C:397:ASP:HB2	2.06	0.56
1:D:71:ALA:O	1:D:75:ARG:HB3	2.06	0.56
1:E:158:ILE:HG23	1:E:396:VAL:HG22	1.87	0.56
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.35	0.56
1:D:13:ARG:HD3	1:D:104:LEU:HD22	1.88	0.55
1:E:13:ARG:HD3	1:E:104:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:GLY:HA3	1:F:67:GLU:O	2.06	0.55
1:B:75:ARG:HG2	1:B:75:ARG:HH11	1.71	0.55
1:C:25:ASP:HA	1:C:28:LYS:HD2	1.88	0.55
1:C:19:GLY:HA3	1:C:67:GLU:O	2.06	0.55
1:E:25:ASP:HA	1:E:28:LYS:HD2	1.89	0.55
1:A:25:ASP:HA	1:A:28:LYS:HD2	1.88	0.55
1:A:69:MET:HG2	1:B:47:PRO:HB3	1.88	0.55
1:D:365:LEU:O	1:D:368:ARG:HG3	2.05	0.55
1:E:488:ASP:OD1	1:E:490:PHE:HB2	2.05	0.55
1:E:77:VAL:HG12	1:E:78:ALA:N	2.19	0.55
1:F:393:LYS:O	1:F:397:ASP:HB2	2.06	0.55
1:F:31:LEU:HD13	1:F:90:THR:CG2	2.36	0.55
1:G:393:LYS:O	1:G:397:ASP:HB2	2.06	0.55
1:B:19:GLY:HA3	1:B:67:GLU:O	2.06	0.55
1:C:488:ASP:OD1	1:C:490:PHE:HB2	2.05	0.55
1:D:245:LYS:NZ	1:D:319:ARG:HH21	2.04	0.55
1:D:393:LYS:O	1:D:397:ASP:HB2	2.07	0.55
1:F:502:ARG:O	1:F:506:GLU:HG3	2.06	0.55
1:G:488:ASP:OD1	1:G:490:PHE:HB2	2.07	0.55
1:A:200:LEU:HD23	1:A:275:ALA:O	2.07	0.55
1:B:342:ILE:O	1:B:346:VAL:HG23	2.06	0.55
1:B:22:ILE:HG21	1:B:62:LEU:HD21	1.89	0.55
1:C:349:ILE:HG21	1:C:369:VAL:HB	1.89	0.55
1:E:226:LYS:HG2	1:E:252:GLU:CB	2.37	0.55
1:E:342:ILE:O	1:E:346:VAL:HG23	2.07	0.55
1:F:227:LEU:HB3	1:F:254:VAL:HG13	1.89	0.55
1:F:400:LEU:HG	1:F:400:LEU:O	2.07	0.55
1:G:200:LEU:HD23	1:G:275:ALA:O	2.07	0.55
1:G:411:ILE:CD1	1:G:490:PHE:HE1	2.20	0.55
1:B:200:LEU:HD23	1:B:275:ALA:O	2.07	0.55
1:B:502:ARG:O	1:B:506:GLU:HG3	2.06	0.55
1:E:393:LYS:O	1:E:397:ASP:HB2	2.06	0.55
1:A:227:LEU:HB3	1:A:254:VAL:HG13	1.88	0.55
1:B:411:ILE:CD1	1:B:490:PHE:HE1	2.20	0.55
1:F:342:ILE:O	1:F:346:VAL:HG23	2.07	0.55
1:A:13:ARG:HD3	1:A:104:LEU:HD22	1.89	0.55
1:C:5:GLU:HG3	1:C:525:LYS:HD3	1.88	0.55
1:C:75:ARG:HG2	1:C:75:ARG:HH11	1.72	0.55
1:E:468:LYS:HD3	1:E:486:TYR:CZ	2.42	0.55
1:F:30:THR:HB	1:F:51:LYS:O	2.06	0.55
1:G:2:ALA:O	1:G:4:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HG3	1:A:453:GLN:OE1	2.06	0.55
1:A:342:ILE:O	1:A:346:VAL:HG23	2.06	0.55
1:D:342:ILE:O	1:D:346:VAL:HG23	2.07	0.55
1:F:413:VAL:CG1	1:F:489:MET:HB3	2.37	0.55
1:G:227:LEU:HB3	1:G:254:VAL:HG13	1.89	0.55
1:A:502:ARG:O	1:A:506:GLU:HG3	2.06	0.54
1:A:31:LEU:HD13	1:A:90:THR:HG21	1.88	0.54
1:B:31:LEU:HD13	1:B:90:THR:CG2	2.37	0.54
1:B:441:ALA:O	1:B:445:ARG:HD3	2.07	0.54
1:D:349:ILE:HG21	1:D:369:VAL:HB	1.89	0.54
1:E:413:VAL:CG1	1:E:489:MET:HB3	2.37	0.54
1:E:81:THR:HG23	1:E:503:THR:HG22	1.90	0.54
1:E:4:LYS:HD2	1:F:59:GLU:O	2.07	0.54
1:G:31:LEU:HD13	1:G:90:THR:HG21	1.89	0.54
1:G:460:VAL:HG21	1:G:479:PHE:HZ	1.73	0.54
1:A:5:GLU:HG3	1:A:525:LYS:HD3	1.88	0.54
1:A:24:ALA:HB3	1:A:97:GLN:NE2	2.23	0.54
1:C:365:LEU:O	1:C:368:ARG:HG3	2.06	0.54
1:C:179:GLU:HA	1:C:381:VAL:HG23	1.90	0.54
1:G:342:ILE:O	1:G:346:VAL:HG23	2.07	0.54
1:E:200:LEU:HD23	1:E:275:ALA:O	2.07	0.54
1:F:22:ILE:HG21	1:F:62:LEU:HD21	1.89	0.54
1:G:31:LEU:HD13	1:G:90:THR:CG2	2.37	0.54
1:D:179:GLU:HA	1:D:381:VAL:HG23	1.90	0.54
1:F:31:LEU:HD13	1:F:90:THR:HG21	1.89	0.54
1:G:192:GLY:HA2	1:G:295:LEU:HD21	1.90	0.54
1:A:226:LYS:HG2	1:A:252:GLU:CB	2.38	0.54
1:B:349:ILE:HG21	1:B:369:VAL:HB	1.90	0.54
1:C:502:ARG:O	1:C:506:GLU:HG3	2.06	0.54
1:D:200:LEU:HD23	1:D:275:ALA:O	2.08	0.54
1:B:5:GLU:HG3	1:B:525:LYS:HD3	1.88	0.54
1:C:226:LYS:HG2	1:C:252:GLU:CB	2.38	0.54
1:C:451:MET:HE1	1:C:466:ALA:HA	1.90	0.54
1:C:460:VAL:HG21	1:C:479:PHE:HZ	1.72	0.54
1:C:31:LEU:HD13	1:C:90:THR:HG21	1.89	0.54
1:D:5:GLU:HG3	1:D:525:LYS:HD3	1.89	0.54
1:E:5:GLU:HG3	1:E:525:LYS:HD3	1.88	0.54
1:F:179:GLU:HA	1:F:381:VAL:HG23	1.90	0.54
1:F:452:ARG:O	1:F:456:GLU:HG2	2.08	0.54
1:G:413:VAL:CG1	1:G:489:MET:HB3	2.38	0.54
1:B:383:GLY:N	1:B:389:VAL:HG22	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LYS:HG3	1:C:453:GLN:OE1	2.07	0.54
1:E:227:LEU:HB3	1:E:254:VAL:HG13	1.89	0.54
1:F:226:LYS:HG2	1:F:252:GLU:CB	2.38	0.54
1:F:2:ALA:O	1:F:4:LYS:HG2	2.08	0.54
1:A:383:GLY:N	1:A:389:VAL:HG22	2.23	0.54
1:C:342:ILE:O	1:C:346:VAL:HG23	2.07	0.54
1:E:349:ILE:HG21	1:E:369:VAL:HB	1.90	0.54
1:F:200:LEU:HD23	1:F:275:ALA:O	2.08	0.54
1:G:349:ILE:HG21	1:G:369:VAL:HB	1.90	0.54
1:E:2:ALA:O	1:E:4:LYS:HG2	2.07	0.54
1:E:400:LEU:O	1:E:400:LEU:HG	2.07	0.54
1:F:383:GLY:N	1:F:389:VAL:HG22	2.23	0.54
1:F:81:THR:HG23	1:F:503:THR:HG22	1.90	0.54
1:G:5:GLU:HG3	1:G:525:LYS:HD3	1.89	0.54
1:D:31:LEU:HD13	1:D:90:THR:CG2	2.38	0.54
1:B:13:ARG:HD3	1:B:104:LEU:HD22	1.90	0.53
1:B:179:GLU:HA	1:B:381:VAL:HG23	1.90	0.53
1:C:250:VAL:HG12	1:C:278:ALA:HA	1.90	0.53
1:D:75:ARG:HG2	1:D:75:ARG:NH1	2.23	0.53
1:E:460:VAL:HG21	1:E:479:PHE:HZ	1.73	0.53
1:G:179:GLU:HA	1:G:381:VAL:HG23	1.90	0.53
1:G:441:ALA:O	1:G:445:ARG:HD3	2.07	0.53
1:G:479:PHE:N	1:G:489:MET:HE1	2.23	0.53
1:D:250:VAL:HG12	1:D:278:ALA:HA	1.90	0.53
1:F:349:ILE:HG21	1:F:369:VAL:HB	1.90	0.53
1:F:5:GLU:HG3	1:F:525:LYS:HD3	1.89	0.53
1:C:178:GLU:O	1:C:381:VAL:HG22	2.08	0.53
1:C:383:GLY:N	1:C:389:VAL:HG22	2.23	0.53
1:C:400:LEU:HG	1:C:400:LEU:O	2.07	0.53
1:C:81:THR:HG23	1:C:503:THR:HG22	1.90	0.53
1:E:179:GLU:HA	1:E:381:VAL:HG23	1.90	0.53
1:F:190:VAL:HG12	1:F:191:GLU:H	1.72	0.53
1:A:349:ILE:HG21	1:A:369:VAL:HB	1.89	0.53
1:A:413:VAL:CG1	1:A:489:MET:HB3	2.38	0.53
1:B:250:VAL:HG12	1:B:278:ALA:HA	1.90	0.53
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.73	0.53
1:B:226:LYS:HG2	1:B:252:GLU:CB	2.38	0.53
1:G:183:MET:HB3	1:G:384:MET:HE1	1.90	0.53
1:A:192:GLY:HA2	1:A:295:LEU:HD21	1.91	0.53
1:B:227:LEU:HB3	1:B:254:VAL:HG13	1.89	0.53
1:C:192:GLY:HA2	1:C:295:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HB2	1:C:289:LEU:HD22	1.91	0.53
1:C:66:PHE:HA	1:C:69:MET:HE2	1.91	0.53
1:D:226:LYS:HG2	1:D:252:GLU:CB	2.38	0.53
1:E:24:ALA:HB3	1:E:97:GLN:NE2	2.23	0.53
1:E:451:MET:HE1	1:E:466:ALA:HA	1.90	0.53
1:G:81:THR:HG23	1:G:503:THR:HG22	1.91	0.53
1:A:197:ARG:NH1	1:A:277:LYS:HG2	2.23	0.53
1:B:222:LEU:HB2	1:B:289:LEU:HD22	1.91	0.53
1:C:413:VAL:CG1	1:C:489:MET:HB3	2.37	0.53
1:F:192:GLY:HA2	1:F:295:LEU:HD21	1.90	0.53
1:A:2:ALA:O	1:A:4:LYS:HG2	2.09	0.53
1:B:139:ASN:ND2	1:B:139:ASN:H	2.07	0.53
1:B:400:LEU:O	1:B:400:LEU:HG	2.07	0.53
1:C:227:LEU:HB3	1:C:254:VAL:HG13	1.89	0.53
1:D:400:LEU:O	1:D:400:LEU:HG	2.07	0.53
1:F:209:ASP:HB3	1:F:210:LYS:HZ1	1.73	0.53
1:A:66:PHE:HA	1:A:69:MET:HE2	1.91	0.53
1:D:178:GLU:O	1:D:381:VAL:HG22	2.09	0.53
1:D:227:LEU:HB3	1:D:254:VAL:HG13	1.89	0.53
1:E:502:ARG:O	1:E:506:GLU:HG3	2.09	0.53
1:F:24:ALA:HB3	1:F:97:GLN:NE2	2.24	0.53
1:F:103:GLY:HA3	1:F:516:ILE:HD11	1.91	0.53
1:G:178:GLU:O	1:G:381:VAL:HG22	2.09	0.53
1:G:24:ALA:HB3	1:G:97:GLN:NE2	2.24	0.53
1:A:179:GLU:HA	1:A:381:VAL:HG23	1.91	0.53
1:B:178:GLU:O	1:B:381:VAL:HG22	2.09	0.53
1:B:460:VAL:HG21	1:B:479:PHE:HZ	1.74	0.53
1:D:441:ALA:O	1:D:445:ARG:HD3	2.09	0.53
1:D:452:ARG:O	1:D:456:GLU:HG2	2.09	0.53
1:F:178:GLU:O	1:F:381:VAL:HG22	2.09	0.53
1:G:30:THR:HB	1:G:51:LYS:O	2.09	0.53
1:A:190:VAL:HG12	1:A:191:GLU:H	1.73	0.52
1:A:479:PHE:N	1:A:489:MET:HE1	2.24	0.52
1:C:139:ASN:H	1:C:139:ASN:ND2	2.08	0.52
1:C:452:ARG:O	1:C:456:GLU:HG2	2.09	0.52
1:E:479:PHE:N	1:E:489:MET:HE1	2.24	0.52
1:A:250:VAL:HG12	1:A:278:ALA:HA	1.90	0.52
1:B:192:GLY:HA2	1:B:295:LEU:HD21	1.91	0.52
1:C:460:VAL:HG21	1:C:479:PHE:CZ	2.45	0.52
1:D:2:ALA:O	1:D:4:LYS:HG2	2.08	0.52
1:E:383:GLY:N	1:E:389:VAL:HG22	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:LEU:HG	1:F:318:GLY:N	2.24	0.52
1:G:139:ASN:ND2	1:G:139:ASN:H	2.06	0.52
1:G:383:GLY:N	1:G:389:VAL:HG22	2.25	0.52
1:E:250:VAL:HG12	1:E:278:ALA:HA	1.89	0.52
1:A:421:GLN:O	1:A:424:LYS:HB2	2.09	0.52
1:A:460:VAL:HG21	1:A:479:PHE:HZ	1.73	0.52
1:B:66:PHE:HA	1:B:69:MET:HE2	1.92	0.52
1:E:19:GLY:HA3	1:E:67:GLU:O	2.09	0.52
1:F:13:ARG:HD3	1:F:104:LEU:HD22	1.91	0.52
1:F:426:LEU:HB2	1:F:444:ARG:HD2	1.91	0.52
1:A:18:LYS:HB3	1:A:67:GLU:HG2	1.92	0.52
1:C:426:LEU:HB2	1:C:444:ARG:HD2	1.91	0.52
1:D:31:LEU:HD13	1:D:90:THR:HG21	1.91	0.52
1:D:413:VAL:CG1	1:D:489:MET:HB3	2.38	0.52
1:D:30:THR:HB	1:D:51:LYS:O	2.09	0.52
1:D:86:GLY:C	1:D:88:GLY:H	2.13	0.52
1:E:139:ASN:H	1:E:139:ASN:ND2	2.07	0.52
1:E:317:LEU:HG	1:E:318:GLY:N	2.25	0.52
1:F:460:VAL:HG21	1:F:479:PHE:HZ	1.73	0.52
1:A:47:PRO:HB3	1:G:69:MET:HG2	1.91	0.52
1:A:222:LEU:HB2	1:A:289:LEU:HD22	1.91	0.52
1:A:441:ALA:O	1:A:445:ARG:HD3	2.09	0.52
1:A:30:THR:HB	1:A:51:LYS:O	2.10	0.52
1:B:317:LEU:HG	1:B:318:GLY:N	2.25	0.52
1:B:413:VAL:CG1	1:B:489:MET:HB3	2.38	0.52
1:D:139:ASN:H	1:D:139:ASN:ND2	2.08	0.52
1:C:4:LYS:HD2	1:D:59:GLU:O	2.08	0.52
1:D:7:LYS:HD2	1:D:66:PHE:CE1	2.45	0.52
1:E:197:ARG:NH1	1:E:277:LYS:HG2	2.24	0.52
1:E:365:LEU:HD11	1:E:368:ARG:HH21	1.75	0.52
1:F:222:LEU:HB2	1:F:289:LEU:HD22	1.91	0.52
1:G:365:LEU:HD11	1:G:368:ARG:HH21	1.75	0.52
1:G:66:PHE:HA	1:G:69:MET:CE	2.40	0.52
1:B:2:ALA:O	1:B:4:LYS:HG2	2.09	0.52
1:D:185:THR:HA	1:D:380:ARG:O	2.10	0.52
1:D:192:GLY:HA2	1:D:295:LEU:HD21	1.91	0.52
1:D:383:GLY:N	1:D:389:VAL:HG22	2.24	0.52
1:E:433:ASN:N	1:E:433:ASN:OD1	2.42	0.52
1:E:31:LEU:HD13	1:E:90:THR:CG2	2.40	0.52
1:G:250:VAL:HG12	1:G:278:ALA:HA	1.90	0.52
1:B:30:THR:HB	1:B:51:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ALA:O	1:C:445:ARG:HD3	2.10	0.52
1:D:460:VAL:HG21	1:D:479:PHE:HZ	1.74	0.52
1:D:69:MET:HG2	1:E:47:PRO:HB3	1.91	0.52
1:E:192:GLY:HA2	1:E:295:LEU:HD21	1.91	0.52
1:E:421:GLN:O	1:E:424:LYS:HB2	2.10	0.52
1:F:477:PHE:CE1	1:F:486:TYR:HB3	2.45	0.52
1:G:86:GLY:C	1:G:88:GLY:H	2.14	0.52
1:A:66:PHE:HA	1:A:69:MET:CE	2.40	0.52
1:B:86:GLY:C	1:B:88:GLY:H	2.13	0.52
1:D:66:PHE:HA	1:D:69:MET:HE2	1.92	0.52
1:E:452:ARG:O	1:E:456:GLU:HG2	2.10	0.52
1:G:7:LYS:HD2	1:G:66:PHE:CE1	2.44	0.52
1:B:365:LEU:HD11	1:B:368:ARG:HH21	1.75	0.52
1:D:222:LEU:HB2	1:D:289:LEU:HD22	1.91	0.52
1:E:185:THR:HA	1:E:380:ARG:O	2.10	0.52
1:E:365:LEU:HG	1:E:368:ARG:HE	1.75	0.52
1:E:31:LEU:HD13	1:E:90:THR:HG21	1.91	0.52
1:B:103:GLY:HA3	1:B:516:ILE:HD11	1.91	0.51
1:B:31:LEU:HD13	1:B:90:THR:HG21	1.90	0.51
1:C:30:THR:HB	1:C:51:LYS:O	2.09	0.51
1:E:138:VAL:O	1:E:138:VAL:HG12	2.09	0.51
1:E:169:VAL:CG2	1:E:377:ALA:HB2	2.41	0.51
1:F:185:THR:HA	1:F:380:ARG:O	2.10	0.51
1:F:365:LEU:HG	1:F:368:ARG:HE	1.76	0.51
1:G:452:ARG:O	1:G:456:GLU:HG2	2.10	0.51
1:F:4:LYS:HD2	1:G:59:GLU:O	2.10	0.51
1:G:22:ILE:HG21	1:G:62:LEU:HD21	1.91	0.51
1:A:365:LEU:HG	1:A:368:ARG:HE	1.76	0.51
1:C:13:ARG:HD3	1:C:104:LEU:HD22	1.93	0.51
1:C:421:GLN:O	1:C:424:LYS:HB2	2.10	0.51
1:E:460:VAL:HG21	1:E:479:PHE:CZ	2.45	0.51
1:G:220:ILE:HG23	1:G:248:LEU:HD22	1.92	0.51
1:G:197:ARG:NH1	1:G:277:LYS:HG2	2.24	0.51
1:G:322:LYS:HB3	1:G:333:VAL:CG2	2.39	0.51
1:A:185:THR:HA	1:A:380:ARG:O	2.10	0.51
1:A:460:VAL:HG21	1:A:479:PHE:CZ	2.45	0.51
1:C:317:LEU:HG	1:C:318:GLY:N	2.25	0.51
1:C:7:LYS:HD2	1:C:66:PHE:CE1	2.45	0.51
1:D:220:ILE:HG23	1:D:248:LEU:HD22	1.93	0.51
1:E:220:ILE:HG23	1:E:248:LEU:HD22	1.93	0.51
1:E:222:LEU:HB2	1:E:289:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LYS:HG3	1:E:453:GLN:OE1	2.11	0.51
1:E:66:PHE:HA	1:E:69:MET:CE	2.41	0.51
1:F:197:ARG:NH1	1:F:277:LYS:HG2	2.24	0.51
1:G:226:LYS:HG2	1:G:252:GLU:CB	2.38	0.51
1:G:222:LEU:HB2	1:G:289:LEU:HD22	1.91	0.51
1:G:317:LEU:HG	1:G:318:GLY:N	2.25	0.51
1:B:24:ALA:HB3	1:B:97:GLN:NE2	2.26	0.51
1:C:86:GLY:C	1:C:88:GLY:H	2.14	0.51
1:D:28:LYS:HG3	1:D:453:GLN:OE1	2.11	0.51
1:F:322:LYS:HB3	1:F:333:VAL:CG2	2.38	0.51
1:F:479:PHE:N	1:F:489:MET:HE1	2.25	0.51
1:B:452:ARG:O	1:B:456:GLU:HG2	2.11	0.51
1:B:468:LYS:HD3	1:B:486:TYR:CE1	2.46	0.51
1:C:6:VAL:HG22	1:C:522:ILE:HG12	1.92	0.51
1:D:451:MET:HE1	1:D:466:ALA:HA	1.92	0.51
1:D:468:LYS:HD3	1:D:486:TYR:CE1	2.45	0.51
1:D:479:PHE:N	1:D:489:MET:HE1	2.26	0.51
1:F:460:VAL:HG21	1:F:479:PHE:CZ	2.45	0.51
1:F:7:LYS:HD2	1:F:66:PHE:CE1	2.44	0.51
1:A:26:ALA:HA	1:G:8:PHE:HE1	1.76	0.51
1:C:185:THR:HA	1:C:380:ARG:O	2.10	0.51
1:A:317:LEU:HG	1:A:318:GLY:N	2.25	0.51
1:A:400:LEU:HG	1:A:400:LEU:O	2.10	0.51
1:D:365:LEU:HD11	1:D:368:ARG:HH21	1.76	0.51
1:E:178:GLU:O	1:E:381:VAL:HG22	2.10	0.51
1:F:284:ARG:HA	1:F:284:ARG:HH11	1.76	0.51
1:G:365:LEU:HG	1:G:368:ARG:HE	1.76	0.51
1:G:421:GLN:O	1:G:424:LYS:HB2	2.11	0.51
1:G:426:LEU:HB2	1:G:444:ARG:HD2	1.92	0.51
1:A:139:ASN:H	1:A:139:ASN:ND2	2.07	0.51
1:A:452:ARG:O	1:A:456:GLU:HG2	2.11	0.51
1:C:66:PHE:HA	1:C:69:MET:CE	2.41	0.51
1:D:433:ASN:OD1	1:D:433:ASN:N	2.44	0.51
1:F:220:ILE:HG23	1:F:248:LEU:HD22	1.93	0.51
1:F:250:VAL:HG12	1:F:278:ALA:HA	1.91	0.51
1:G:185:THR:HA	1:G:380:ARG:O	2.10	0.51
1:G:460:VAL:HG21	1:G:479:PHE:CZ	2.45	0.51
1:A:284:ARG:HA	1:A:284:ARG:HH11	1.76	0.51
1:A:489:MET:HG3	1:A:494:VAL:HB	1.93	0.51
1:B:185:THR:HA	1:B:380:ARG:O	2.10	0.51
1:B:64:ASP:OD1	1:B:64:ASP:C	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ALA:HB3	1:C:97:GLN:NE2	2.26	0.51
1:E:7:LYS:HD2	1:E:66:PHE:CE1	2.45	0.51
1:F:421:GLN:O	1:F:424:LYS:HB2	2.10	0.51
1:A:178:GLU:O	1:A:381:VAL:HG22	2.11	0.51
1:C:103:GLY:HA3	1:C:516:ILE:HD11	1.92	0.51
1:D:421:GLN:O	1:D:424:LYS:HB2	2.11	0.51
1:D:19:GLY:HA3	1:D:67:GLU:O	2.10	0.51
1:E:24:ALA:O	1:E:28:LYS:HD2	2.11	0.51
1:E:441:ALA:O	1:E:445:ARG:HD3	2.11	0.51
1:G:103:GLY:HA3	1:G:516:ILE:HD11	1.93	0.51
1:G:18:LYS:HB3	1:G:67:GLU:HG2	1.93	0.51
1:B:314:ILE:HD12	1:B:315:ASP:N	2.26	0.50
1:C:314:ILE:HD12	1:C:315:ASP:N	2.26	0.50
1:D:460:VAL:HG21	1:D:479:PHE:CZ	2.46	0.50
1:E:226:LYS:HZ1	1:E:252:GLU:HB3	1.76	0.50
1:F:139:ASN:H	1:F:139:ASN:ND2	2.07	0.50
1:A:314:ILE:HD12	1:A:315:ASP:N	2.26	0.50
1:A:86:GLY:C	1:A:88:GLY:H	2.14	0.50
1:B:433:ASN:OD1	1:B:433:ASN:N	2.42	0.50
1:C:365:LEU:HG	1:C:368:ARG:HE	1.76	0.50
1:C:479:PHE:N	1:C:489:MET:HE1	2.26	0.50
1:D:66:PHE:HA	1:D:69:MET:CE	2.41	0.50
1:E:426:LEU:HB2	1:E:444:ARG:HD2	1.93	0.50
1:E:6:VAL:HG22	1:E:522:ILE:HG12	1.94	0.50
1:F:433:ASN:OD1	1:F:433:ASN:N	2.43	0.50
1:F:86:GLY:C	1:F:88:GLY:H	2.14	0.50
1:G:433:ASN:OD1	1:G:436:GLN:HB2	2.12	0.50
1:G:477:PHE:CE1	1:G:486:TYR:HB3	2.46	0.50
1:B:362:ARG:HE	1:B:363:GLU:N	2.09	0.50
1:B:460:VAL:HG21	1:B:479:PHE:CZ	2.47	0.50
1:A:4:LYS:HD2	1:B:59:GLU:O	2.10	0.50
1:C:18:LYS:HB3	1:C:67:GLU:HG2	1.93	0.50
1:C:220:ILE:HG23	1:C:248:LEU:HD22	1.93	0.50
1:D:231:GLN:N	1:D:232:PRO:HD2	2.27	0.50
1:D:365:LEU:HG	1:D:368:ARG:HE	1.76	0.50
1:E:231:GLN:N	1:E:232:PRO:HD2	2.26	0.50
1:G:433:ASN:OD1	1:G:433:ASN:N	2.44	0.50
1:G:28:LYS:HG3	1:G:453:GLN:OE1	2.12	0.50
1:A:220:ILE:HG23	1:A:248:LEU:HD22	1.93	0.50
1:B:66:PHE:HA	1:B:69:MET:CE	2.42	0.50
1:C:231:GLN:N	1:C:232:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LEU:HG	1:D:318:GLY:N	2.25	0.50
1:D:169:VAL:CG2	1:D:377:ALA:HB2	2.42	0.50
1:D:426:LEU:HB2	1:D:444:ARG:HD2	1.92	0.50
1:F:362:ARG:HE	1:F:363:GLU:N	2.09	0.50
1:G:362:ARG:HE	1:G:363:GLU:N	2.09	0.50
1:A:169:VAL:CG2	1:A:377:ALA:HB2	2.41	0.50
1:B:231:GLN:N	1:B:232:PRO:HD2	2.27	0.50
1:C:365:LEU:HD11	1:C:368:ARG:HH21	1.76	0.50
1:D:477:PHE:CE1	1:D:486:TYR:HB3	2.46	0.50
1:E:103:GLY:HA3	1:E:516:ILE:HD11	1.93	0.50
1:E:18:LYS:HB3	1:E:67:GLU:HG2	1.93	0.50
1:E:284:ARG:HA	1:E:284:ARG:HH11	1.76	0.50
1:G:451:MET:HE1	1:G:466:ALA:HA	1.94	0.50
1:A:426:LEU:HB2	1:A:444:ARG:HD2	1.92	0.50
1:A:409:GLU:OE2	1:A:499:LYS:HG3	2.11	0.50
1:C:362:ARG:HE	1:C:363:GLU:N	2.10	0.50
1:C:433:ASN:OD1	1:C:433:ASN:N	2.45	0.50
1:C:433:ASN:OD1	1:C:436:GLN:HB2	2.12	0.50
1:D:284:ARG:HA	1:D:284:ARG:HH11	1.76	0.50
1:D:64:ASP:OD1	1:D:64:ASP:C	2.50	0.50
1:E:30:THR:HB	1:E:51:LYS:O	2.11	0.50
1:F:169:VAL:CG2	1:F:377:ALA:HB2	2.42	0.50
1:F:441:ALA:O	1:F:445:ARG:HD3	2.11	0.50
1:F:66:PHE:HA	1:F:69:MET:CE	2.41	0.50
1:B:284:ARG:HA	1:B:284:ARG:HH11	1.76	0.50
1:B:224:GLU:HG3	1:B:286:LYS:NZ	2.27	0.50
1:B:4:LYS:HD2	1:C:59:GLU:O	2.11	0.50
1:C:24:ALA:O	1:C:28:LYS:HD2	2.12	0.50
1:D:221:LEU:HD21	1:D:249:ILE:HG12	1.94	0.50
1:D:222:LEU:HD13	1:D:289:LEU:HB3	1.94	0.50
1:F:138:VAL:HG12	1:F:138:VAL:O	2.11	0.50
1:G:314:ILE:HD12	1:G:315:ASP:N	2.26	0.50
1:G:339:LYS:HB3	1:G:343:GLU:OE2	2.12	0.50
1:A:433:ASN:OD1	1:A:433:ASN:N	2.43	0.50
1:B:365:LEU:HG	1:B:368:ARG:HE	1.76	0.50
1:B:28:LYS:HG3	1:B:453:GLN:OE1	2.12	0.50
1:C:138:VAL:O	1:C:138:VAL:HG12	2.10	0.50
1:C:468:LYS:HD3	1:C:486:TYR:CE1	2.47	0.50
1:D:226:LYS:HZ3	1:D:252:GLU:HB3	1.77	0.50
1:D:314:ILE:HD12	1:D:315:ASP:N	2.26	0.50
1:A:477:PHE:CE1	1:A:486:TYR:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLY:C	1:E:88:GLY:H	2.14	0.50
1:F:314:ILE:HD12	1:F:315:ASP:N	2.26	0.50
1:G:169:VAL:CG2	1:G:377:ALA:HB2	2.42	0.50
1:A:138:VAL:O	1:A:138:VAL:HG12	2.11	0.49
1:B:169:VAL:CG2	1:B:377:ALA:HB2	2.41	0.49
1:D:224:GLU:HG3	1:D:286:LYS:NZ	2.27	0.49
1:D:322:LYS:HB3	1:D:333:VAL:CG2	2.39	0.49
1:D:75:ARG:HH11	1:D:75:ARG:HG2	1.76	0.49
1:E:224:GLU:HG3	1:E:286:LYS:NZ	2.27	0.49
1:F:365:LEU:HD11	1:F:368:ARG:HH21	1.76	0.49
1:A:362:ARG:HE	1:A:363:GLU:N	2.10	0.49
1:B:220:ILE:HG23	1:B:248:LEU:HD22	1.93	0.49
1:B:222:LEU:HD13	1:B:289:LEU:HB3	1.94	0.49
1:B:322:LYS:HB3	1:B:333:VAL:CG2	2.39	0.49
1:C:222:LEU:HD13	1:C:289:LEU:HB3	1.94	0.49
1:F:224:GLU:HG3	1:F:286:LYS:NZ	2.27	0.49
1:A:248:LEU:HD13	1:A:323:VAL:HG11	1.95	0.49
1:A:365:LEU:HD11	1:A:368:ARG:HH21	1.76	0.49
1:C:2:ALA:O	1:C:4:LYS:HG2	2.11	0.49
1:C:169:VAL:CG2	1:C:377:ALA:HB2	2.42	0.49
1:A:231:GLN:N	1:A:232:PRO:HD2	2.27	0.49
1:A:322:LYS:HB3	1:A:333:VAL:CG2	2.38	0.49
1:A:361:ASP:OD1	1:A:365:LEU:HD13	2.13	0.49
1:B:248:LEU:HD13	1:B:323:VAL:HG11	1.95	0.49
1:B:339:LYS:HB3	1:B:343:GLU:OE2	2.13	0.49
1:C:224:GLU:HG3	1:C:286:LYS:NZ	2.28	0.49
1:C:361:ASP:OD1	1:C:365:LEU:HD13	2.13	0.49
1:E:314:ILE:HD12	1:E:315:ASP:N	2.26	0.49
1:F:11:ASP:CG	1:F:15:ARG:HH12	2.16	0.49
1:F:451:MET:CE	1:F:465:VAL:HG12	2.42	0.49
1:F:451:MET:HE1	1:F:466:ALA:HA	1.94	0.49
1:A:339:LYS:HB3	1:A:343:GLU:OE2	2.13	0.49
1:B:433:ASN:OD1	1:B:436:GLN:HB2	2.13	0.49
1:C:227:LEU:HD13	1:C:254:VAL:HG22	1.95	0.49
1:A:224:GLU:HG3	1:A:286:LYS:NZ	2.27	0.49
1:A:221:LEU:HD21	1:A:249:ILE:HG12	1.94	0.49
1:B:138:VAL:HG12	1:B:138:VAL:O	2.11	0.49
1:B:361:ASP:OD1	1:B:365:LEU:HD13	2.13	0.49
1:D:362:ARG:HE	1:D:363:GLU:N	2.09	0.49
1:E:248:LEU:HD13	1:E:323:VAL:HG11	1.95	0.49
1:E:169:VAL:HG21	1:E:377:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:GLN:N	1:F:232:PRO:HD2	2.27	0.49
1:F:64:ASP:C	1:F:64:ASP:OD1	2.51	0.49
1:G:284:ARG:HA	1:G:284:ARG:HH11	1.76	0.49
1:G:66:PHE:HA	1:G:69:MET:HE2	1.94	0.49
1:D:248:LEU:HD13	1:D:323:VAL:HG11	1.95	0.49
1:G:248:LEU:HD13	1:G:323:VAL:HG11	1.95	0.49
1:B:122:VAL:HG12	1:B:123:ALA:N	2.28	0.49
1:C:284:ARG:HA	1:C:284:ARG:HH11	1.76	0.49
1:D:18:LYS:HB3	1:D:67:GLU:HG2	1.93	0.49
1:D:227:LEU:HD13	1:D:254:VAL:HG22	1.95	0.49
1:E:339:LYS:HB3	1:E:343:GLU:OE2	2.12	0.49
1:E:477:PHE:CE1	1:E:486:TYR:HB3	2.47	0.49
1:G:231:GLN:N	1:G:232:PRO:HD2	2.27	0.49
1:G:227:LEU:HD13	1:G:254:VAL:HG22	1.94	0.49
1:G:469:VAL:HG22	1:G:478:GLY:HA2	1.94	0.49
1:G:501:VAL:HG12	1:G:501:VAL:O	2.13	0.49
1:A:222:LEU:HD13	1:A:289:LEU:HB3	1.94	0.49
1:A:69:MET:HG2	1:B:47:PRO:HG3	1.95	0.49
1:C:339:LYS:HB3	1:C:343:GLU:OE2	2.13	0.49
1:E:213:ALA:HB3	1:E:325:ILE:HB	1.95	0.49
1:F:489:MET:HG3	1:F:494:VAL:HB	1.95	0.49
1:F:6:VAL:HG22	1:F:522:ILE:HG12	1.95	0.49
1:G:138:VAL:HG12	1:G:138:VAL:O	2.13	0.49
1:B:227:LEU:HD13	1:B:254:VAL:HG22	1.95	0.49
1:B:469:VAL:HG22	1:B:478:GLY:HA2	1.95	0.49
1:C:477:PHE:CE1	1:C:486:TYR:HB3	2.47	0.49
1:E:362:ARG:HE	1:E:363:GLU:N	2.09	0.49
1:G:222:LEU:HD13	1:G:289:LEU:HB3	1.94	0.49
1:G:468:LYS:HD3	1:G:486:TYR:CE1	2.47	0.49
1:G:64:ASP:OD1	1:G:64:ASP:C	2.51	0.49
1:A:64:ASP:OD1	1:A:64:ASP:C	2.51	0.48
1:B:421:GLN:O	1:B:424:LYS:HB2	2.12	0.48
1:B:477:PHE:CE1	1:B:486:TYR:HB3	2.47	0.48
1:D:339:LYS:HB3	1:D:343:GLU:OE2	2.13	0.48
1:D:469:VAL:HG22	1:D:478:GLY:HA2	1.95	0.48
1:E:221:LEU:HD21	1:E:249:ILE:HG12	1.95	0.48
1:E:361:ASP:OD1	1:E:365:LEU:HD13	2.13	0.48
1:E:433:ASN:OD1	1:E:436:GLN:HB2	2.13	0.48
1:F:122:VAL:HG12	1:F:123:ALA:N	2.27	0.48
1:A:341:GLU:O	1:A:345:ARG:HG2	2.13	0.48
1:D:24:ALA:HB3	1:D:97:GLN:NE2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:LEU:HD13	1:E:289:LEU:HB3	1.94	0.48
1:E:468:LYS:HD3	1:E:486:TYR:CE1	2.48	0.48
1:F:248:LEU:HD13	1:F:323:VAL:HG11	1.95	0.48
1:G:221:LEU:HD21	1:G:249:ILE:HG12	1.94	0.48
1:G:341:GLU:O	1:G:345:ARG:HG2	2.14	0.48
1:A:451:MET:HE1	1:A:466:ALA:HA	1.95	0.48
1:B:18:LYS:HB3	1:B:67:GLU:HG2	1.95	0.48
1:C:248:LEU:HD13	1:C:323:VAL:HG11	1.95	0.48
1:C:322:LYS:HB3	1:C:333:VAL:CG2	2.39	0.48
1:E:227:LEU:HD13	1:E:254:VAL:HG22	1.95	0.48
1:C:341:GLU:O	1:C:345:ARG:HG2	2.13	0.48
1:F:222:LEU:HD13	1:F:289:LEU:HB3	1.94	0.48
1:F:213:ALA:HB3	1:F:325:ILE:HB	1.96	0.48
1:F:361:ASP:OD1	1:F:365:LEU:HD13	2.13	0.48
1:F:468:LYS:HD3	1:F:486:TYR:CE1	2.47	0.48
1:F:69:MET:HG2	1:G:47:PRO:HB3	1.95	0.48
1:G:451:MET:CE	1:G:465:VAL:HG12	2.44	0.48
1:B:7:LYS:HD2	1:B:66:PHE:CE1	2.48	0.48
1:D:501:VAL:O	1:D:501:VAL:HG12	2.13	0.48
1:F:24:ALA:O	1:F:28:LYS:HD2	2.14	0.48
1:F:433:ASN:OD1	1:F:436:GLN:HB2	2.14	0.48
1:G:213:ALA:HB3	1:G:325:ILE:HB	1.95	0.48
1:G:224:GLU:HG3	1:G:286:LYS:NZ	2.28	0.48
1:B:426:LEU:HB2	1:B:444:ARG:HD2	1.94	0.48
1:B:501:VAL:O	1:B:501:VAL:HG12	2.14	0.48
1:C:221:LEU:HD21	1:C:249:ILE:HG12	1.95	0.48
1:A:433:ASN:OD1	1:A:436:GLN:HB2	2.14	0.48
1:A:469:VAL:HG22	1:A:478:GLY:HA2	1.95	0.48
1:C:122:VAL:HG12	1:C:123:ALA:N	2.29	0.48
1:C:469:VAL:HG22	1:C:478:GLY:HA2	1.94	0.48
1:D:433:ASN:OD1	1:D:436:GLN:HB2	2.14	0.48
1:F:501:VAL:HG12	1:F:501:VAL:O	2.13	0.48
1:A:468:LYS:HD3	1:A:486:TYR:CE1	2.48	0.48
1:C:64:ASP:C	1:C:64:ASP:OD1	2.52	0.48
1:D:11:ASP:CG	1:D:15:ARG:HH12	2.17	0.48
1:D:8:PHE:HE1	1:E:26:ALA:HA	1.78	0.48
1:E:12:ALA:HB1	1:E:521:MET:HG3	1.96	0.48
1:G:122:VAL:HG12	1:G:123:ALA:N	2.27	0.48
1:G:190:VAL:HG11	1:G:334:ASP:CG	2.34	0.48
1:C:489:MET:HG3	1:C:494:VAL:HB	1.95	0.48
1:D:361:ASP:OD1	1:D:365:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:VAL:HG11	1:F:334:ASP:CB	2.43	0.48
1:F:339:LYS:HB3	1:F:343:GLU:OE2	2.13	0.48
1:F:183:MET:HB3	1:F:384:MET:HE1	1.95	0.48
1:B:169:VAL:HG21	1:B:377:ALA:HB2	1.95	0.48
1:D:122:VAL:HG12	1:D:123:ALA:N	2.29	0.48
1:F:341:GLU:O	1:F:345:ARG:HG2	2.14	0.48
1:G:6:VAL:HG22	1:G:522:ILE:HG12	1.95	0.48
1:B:227:LEU:CB	1:B:254:VAL:HG13	2.44	0.47
1:B:341:GLU:O	1:B:345:ARG:HG2	2.14	0.47
1:D:220:ILE:HD12	1:D:248:LEU:HD22	1.96	0.47
1:E:322:LYS:HB3	1:E:333:VAL:CG2	2.39	0.47
1:E:469:VAL:HG22	1:E:478:GLY:HA2	1.96	0.47
1:G:124:THR:O	1:G:128:VAL:HG23	2.14	0.47
1:A:501:VAL:HG12	1:A:501:VAL:O	2.14	0.47
1:B:205:VAL:HG12	1:B:207:ASN:H	1.79	0.47
1:C:227:LEU:CB	1:C:254:VAL:HG13	2.44	0.47
1:C:501:VAL:O	1:C:501:VAL:HG12	2.13	0.47
1:D:138:VAL:HG12	1:D:138:VAL:O	2.12	0.47
1:E:341:GLU:O	1:E:345:ARG:HG2	2.14	0.47
1:F:221:LEU:HD21	1:F:249:ILE:HG12	1.94	0.47
1:A:213:ALA:HB3	1:A:325:ILE:HB	1.96	0.47
1:B:205:VAL:HG12	1:B:207:ASN:N	2.30	0.47
1:B:221:LEU:HD21	1:B:249:ILE:HG12	1.95	0.47
1:C:183:MET:HB3	1:C:384:MET:HE1	1.96	0.47
1:D:489:MET:HG3	1:D:494:VAL:HB	1.96	0.47
1:E:64:ASP:C	1:E:64:ASP:OD1	2.52	0.47
1:F:227:LEU:HD13	1:F:254:VAL:HG22	1.95	0.47
1:A:227:LEU:HD13	1:A:254:VAL:HG22	1.96	0.47
1:D:169:VAL:HG21	1:D:377:ALA:HB2	1.96	0.47
1:F:226:LYS:HZ3	1:F:252:GLU:HB3	1.79	0.47
1:F:469:VAL:HG22	1:F:478:GLY:HA2	1.95	0.47
1:A:362:ARG:HE	1:A:363:GLU:HB2	1.79	0.47
1:A:7:LYS:HD2	1:A:66:PHE:CE1	2.49	0.47
1:D:219:TYR:CD1	1:D:247:LEU:HD12	2.50	0.47
1:D:341:GLU:O	1:D:345:ARG:HG2	2.14	0.47
1:F:220:ILE:HD12	1:F:248:LEU:HD22	1.95	0.47
1:B:220:ILE:HD12	1:B:248:LEU:HD22	1.96	0.47
1:C:220:ILE:HD12	1:C:248:LEU:HD22	1.96	0.47
1:A:220:ILE:HD12	1:A:248:LEU:HD22	1.95	0.47
1:F:169:VAL:HG21	1:F:377:ALA:HB2	1.96	0.47
1:G:362:ARG:HE	1:G:363:GLU:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:361:ASP:OD1	1:G:365:LEU:HD13	2.13	0.47
1:A:221:LEU:HD21	1:A:249:ILE:CG1	2.45	0.47
1:B:174:VAL:O	1:B:174:VAL:HG22	2.14	0.47
1:D:227:LEU:CB	1:D:254:VAL:HG13	2.44	0.47
1:D:197:ARG:NH1	1:D:277:LYS:HG2	2.23	0.47
1:D:321:LYS:CB	1:D:334:ASP:HB3	2.45	0.47
1:F:77:VAL:HG21	1:F:511:VAL:HG13	1.97	0.47
1:G:227:LEU:CB	1:G:254:VAL:HG13	2.44	0.47
1:A:226:LYS:HZ1	1:A:252:GLU:HB3	1.78	0.47
1:A:289:LEU:O	1:A:293:ALA:HB2	2.15	0.47
1:B:219:TYR:CD1	1:B:247:LEU:HD12	2.50	0.47
1:B:183:MET:HB3	1:B:384:MET:HE1	1.97	0.47
1:E:227:LEU:CB	1:E:254:VAL:HG13	2.45	0.47
1:F:18:LYS:HB3	1:F:67:GLU:HG2	1.96	0.47
1:G:220:ILE:HD12	1:G:248:LEU:HD22	1.96	0.47
1:G:429:LEU:HD12	1:G:430:SER:N	2.30	0.47
1:B:362:ARG:HE	1:B:363:GLU:HB2	1.79	0.47
1:B:158:ILE:CG2	1:B:396:VAL:HG22	2.45	0.47
1:C:11:ASP:CG	1:C:15:ARG:HH12	2.18	0.47
1:C:213:ALA:HB3	1:C:325:ILE:HB	1.96	0.47
1:C:362:ARG:HE	1:C:363:GLU:HB2	1.80	0.47
1:C:511:VAL:HG23	1:C:512:ALA:N	2.29	0.47
1:D:124:THR:O	1:D:128:VAL:HG23	2.15	0.47
1:E:220:ILE:HD12	1:E:248:LEU:HD22	1.96	0.47
1:A:169:VAL:HG21	1:A:377:ALA:HB2	1.96	0.47
1:A:174:VAL:O	1:A:174:VAL:HG22	2.14	0.47
1:A:227:LEU:CB	1:A:254:VAL:HG13	2.44	0.47
1:B:213:ALA:HB3	1:B:325:ILE:HB	1.96	0.47
1:C:197:ARG:NH1	1:C:277:LYS:HG2	2.24	0.47
1:C:158:ILE:CG2	1:C:396:VAL:HG22	2.45	0.47
1:C:451:MET:CE	1:C:465:VAL:HG12	2.45	0.47
1:D:174:VAL:O	1:D:174:VAL:HG22	2.14	0.47
1:D:213:ALA:HB3	1:D:325:ILE:HB	1.96	0.47
1:F:227:LEU:CB	1:F:254:VAL:HG13	2.44	0.47
1:G:11:ASP:CG	1:G:15:ARG:HH12	2.18	0.47
1:G:219:TYR:CD1	1:G:247:LEU:HD12	2.50	0.47
1:A:69:MET:HG2	1:B:47:PRO:CB	2.45	0.46
1:C:112:ASN:OD1	1:C:114:MET:N	2.49	0.46
1:C:321:LYS:CB	1:C:334:ASP:HB3	2.45	0.46
1:F:221:LEU:HD21	1:F:249:ILE:CG1	2.45	0.46
1:G:24:ALA:O	1:G:28:LYS:HD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.45	0.46
1:A:205:VAL:HG12	1:A:207:ASN:N	2.30	0.46
1:A:24:ALA:O	1:A:28:LYS:HD2	2.15	0.46
1:C:429:LEU:HD12	1:C:430:SER:N	2.30	0.46
1:D:198:GLY:O	1:D:276:VAL:HG12	2.15	0.46
1:D:362:ARG:HE	1:D:363:GLU:HB2	1.79	0.46
1:E:205:VAL:HG12	1:E:207:ASN:H	1.79	0.46
1:E:489:MET:HG3	1:E:494:VAL:HB	1.97	0.46
1:G:221:LEU:HD21	1:G:249:ILE:CG1	2.46	0.46
1:G:226:LYS:HZ1	1:G:252:GLU:HB3	1.79	0.46
1:G:169:VAL:HG21	1:G:377:ALA:HB2	1.97	0.46
1:A:205:VAL:HG12	1:A:207:ASN:H	1.80	0.46
1:A:219:TYR:CD1	1:A:247:LEU:HD12	2.50	0.46
1:B:36:ARG:NH1	1:B:36:ARG:CG	2.76	0.46
1:B:489:MET:HG3	1:B:494:VAL:HB	1.97	0.46
1:D:158:ILE:CG2	1:D:396:VAL:HG22	2.46	0.46
1:E:511:VAL:HG23	1:E:512:ALA:N	2.30	0.46
1:F:219:TYR:CD1	1:F:247:LEU:HD12	2.50	0.46
1:G:209:ASP:HB3	1:G:210:LYS:HZ2	1.80	0.46
1:A:11:ASP:CG	1:A:15:ARG:HH12	2.19	0.46
1:B:24:ALA:O	1:B:28:LYS:HD2	2.16	0.46
1:C:205:VAL:HG12	1:C:207:ASN:N	2.31	0.46
1:C:77:VAL:HG21	1:C:511:VAL:HG13	1.98	0.46
1:E:221:LEU:O	1:E:250:VAL:HG23	2.16	0.46
1:F:383:GLY:H	1:F:389:VAL:HG22	1.81	0.46
1:F:158:ILE:CG2	1:F:396:VAL:HG22	2.46	0.46
1:C:205:VAL:HG12	1:C:207:ASN:H	1.80	0.46
1:D:289:LEU:O	1:D:293:ALA:HB2	2.16	0.46
1:E:66:PHE:HA	1:E:69:MET:HE2	1.96	0.46
1:G:489:MET:HG3	1:G:494:VAL:HB	1.98	0.46
1:A:122:VAL:HG12	1:A:123:ALA:N	2.31	0.46
1:A:158:ILE:CG2	1:A:396:VAL:HG22	2.46	0.46
1:B:429:LEU:HD12	1:B:430:SER:N	2.31	0.46
1:C:219:TYR:CD1	1:C:247:LEU:HD12	2.51	0.46
1:C:169:VAL:HG21	1:C:377:ALA:HB2	1.96	0.46
1:D:429:LEU:HD12	1:D:430:SER:N	2.29	0.46
1:E:11:ASP:CG	1:E:15:ARG:HH12	2.18	0.46
1:E:219:TYR:CD1	1:E:247:LEU:HD12	2.51	0.46
1:F:227:LEU:HB2	1:F:254:VAL:CA	2.37	0.46
1:D:103:GLY:HA3	1:D:516:ILE:HD11	1.96	0.46
1:D:205:VAL:HG12	1:D:207:ASN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:VAL:HG12	1:E:123:ALA:N	2.29	0.46
1:E:205:VAL:HG12	1:E:207:ASN:N	2.30	0.46
1:G:205:VAL:HG12	1:G:207:ASN:H	1.80	0.46
1:G:351:GLN:HA	1:G:354:GLU:HB2	1.98	0.46
1:B:197:ARG:NH1	1:B:277:LYS:HG2	2.23	0.46
1:D:205:VAL:HG12	1:D:207:ASN:N	2.31	0.46
1:D:351:GLN:HA	1:D:354:GLU:HB2	1.98	0.46
1:C:69:MET:HG2	1:D:47:PRO:HB3	1.98	0.46
1:E:174:VAL:HG22	1:E:174:VAL:O	2.15	0.46
1:E:198:GLY:O	1:E:276:VAL:HG12	2.16	0.46
1:E:383:GLY:H	1:E:389:VAL:HG22	1.81	0.46
1:F:351:GLN:HA	1:F:354:GLU:HB2	1.98	0.46
1:F:362:ARG:HE	1:F:363:GLU:HB2	1.79	0.46
1:F:80:ARG:HB2	1:F:80:ARG:HH11	1.81	0.46
1:G:69:MET:HB2	1:G:69:MET:HE3	1.53	0.46
1:A:217:ASP:O	1:A:246:PRO:HD2	2.16	0.46
1:A:90:THR:O	1:A:94:VAL:HG23	2.16	0.46
1:B:221:LEU:HD21	1:B:249:ILE:CG1	2.46	0.46
1:C:289:LEU:O	1:C:293:ALA:HB2	2.16	0.46
1:D:221:LEU:HD21	1:D:249:ILE:CG1	2.45	0.46
1:D:62:LEU:H	1:D:68:ASN:HD22	1.64	0.46
1:E:289:LEU:O	1:E:293:ALA:HB2	2.15	0.46
1:E:77:VAL:HG21	1:E:511:VAL:HG13	1.98	0.46
1:A:128:VAL:HG11	1:A:506:GLU:OE2	2.16	0.46
1:A:6:VAL:HG22	1:A:522:ILE:HG12	1.98	0.46
1:B:451:MET:CE	1:B:465:VAL:HG12	2.46	0.46
1:C:294:ILE:HD11	1:C:345:ARG:NH1	2.31	0.46
1:D:217:ASP:O	1:D:246:PRO:HD2	2.16	0.46
1:E:194:GLN:HG3	1:E:331:THR:OG1	2.16	0.46
1:G:62:LEU:H	1:G:68:ASN:HD22	1.63	0.46
1:C:217:ASP:O	1:C:246:PRO:HD2	2.16	0.45
1:G:80:ARG:HB2	1:G:80:ARG:HH11	1.81	0.45
1:A:175:ILE:HG22	1:A:176:THR:N	2.31	0.45
1:A:451:MET:CE	1:A:465:VAL:HG12	2.47	0.45
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.46	0.45
1:D:36:ARG:NH1	1:D:36:ARG:CG	2.75	0.45
1:D:69:MET:HE3	1:D:69:MET:HB2	1.53	0.45
1:E:221:LEU:HD21	1:E:249:ILE:CG1	2.46	0.45
1:E:351:GLN:HA	1:E:354:GLU:HB2	1.99	0.45
1:F:217:ASP:O	1:F:246:PRO:HD2	2.17	0.45
1:F:194:GLN:HG3	1:F:331:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:GLY:O	1:G:276:VAL:HG12	2.16	0.45
1:G:217:ASP:O	1:G:246:PRO:HD2	2.16	0.45
1:A:351:GLN:HA	1:A:354:GLU:HB2	1.99	0.45
1:A:103:GLY:HA3	1:A:516:ILE:HD11	1.97	0.45
1:B:12:ALA:HB1	1:B:521:MET:SD	2.57	0.45
1:B:11:ASP:CG	1:B:15:ARG:HH12	2.19	0.45
1:B:289:LEU:O	1:B:293:ALA:HB2	2.15	0.45
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.46	0.45
1:C:351:GLN:HA	1:C:354:GLU:HB2	1.98	0.45
1:C:478:GLY:HA3	1:C:489:MET:HE3	1.97	0.45
1:D:112:ASN:OD1	1:D:114:MET:N	2.49	0.45
1:E:225:LYS:HB2	1:E:226:LYS:H	1.62	0.45
1:E:362:ARG:HE	1:E:363:GLU:HB2	1.80	0.45
1:G:112:ASN:OD1	1:G:114:MET:N	2.49	0.45
1:G:378:VAL:HG22	1:G:378:VAL:O	2.16	0.45
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.47	0.45
1:B:321:LYS:CB	1:B:334:ASP:HB3	2.46	0.45
1:D:320:ALA:HA	1:D:335:GLY:O	2.17	0.45
1:D:348:GLN:O	1:D:352:GLN:HB2	2.17	0.45
1:D:378:VAL:O	1:D:378:VAL:HG22	2.17	0.45
1:F:112:ASN:OD1	1:F:114:MET:N	2.49	0.45
1:F:507:ASP:O	1:F:510:SER:HB3	2.17	0.45
1:B:348:GLN:O	1:B:352:GLN:HB2	2.17	0.45
1:B:80:ARG:HB2	1:B:80:ARG:HH11	1.82	0.45
1:C:383:GLY:H	1:C:389:VAL:HG22	1.82	0.45
1:E:112:ASN:OD1	1:E:114:MET:N	2.50	0.45
1:F:221:LEU:O	1:F:250:VAL:HG23	2.16	0.45
1:F:289:LEU:O	1:F:293:ALA:HB2	2.15	0.45
1:G:289:LEU:O	1:G:293:ALA:HB2	2.16	0.45
1:A:247:LEU:HB3	1:A:273:ILE:HD12	1.99	0.45
1:A:69:MET:HB2	1:A:69:MET:HE3	1.55	0.45
1:A:77:VAL:HG21	1:A:511:VAL:HG13	1.99	0.45
1:B:351:GLN:HA	1:B:354:GLU:HB2	1.98	0.45
1:C:221:LEU:O	1:C:250:VAL:HG23	2.16	0.45
1:F:128:VAL:HG11	1:F:506:GLU:OE2	2.17	0.45
1:F:66:PHE:HA	1:F:69:MET:HE2	1.97	0.45
1:G:194:GLN:HG3	1:G:331:THR:OG1	2.17	0.45
1:G:221:LEU:O	1:G:250:VAL:HG23	2.16	0.45
1:B:247:LEU:HB3	1:B:273:ILE:HD12	1.99	0.45
1:C:124:THR:O	1:C:128:VAL:HG23	2.16	0.45
1:C:198:GLY:O	1:C:276:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ALA:HA	1:C:335:GLY:O	2.17	0.45
1:E:501:VAL:O	1:E:501:VAL:HG12	2.16	0.45
1:E:69:MET:HG2	1:F:47:PRO:HB3	1.99	0.45
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.46	0.45
1:F:478:GLY:HA3	1:F:489:MET:HE3	1.99	0.45
1:G:204:PHE:CE1	1:G:273:ILE:HG23	2.52	0.45
1:G:205:VAL:HG12	1:G:207:ASN:N	2.30	0.45
1:A:12:ALA:HB1	1:A:521:MET:HG3	1.99	0.45
1:A:221:LEU:O	1:A:250:VAL:HG23	2.16	0.45
1:C:348:GLN:O	1:C:352:GLN:HB2	2.17	0.45
1:E:348:GLN:O	1:E:352:GLN:HB2	2.17	0.45
1:E:69:MET:HE3	1:E:69:MET:HB2	1.50	0.45
1:E:80:ARG:HB2	1:E:80:ARG:HH11	1.82	0.45
1:B:217:ASP:O	1:B:246:PRO:HD2	2.17	0.45
1:D:221:LEU:O	1:D:250:VAL:HG23	2.16	0.45
1:E:217:ASP:O	1:E:246:PRO:HD2	2.17	0.45
1:F:204:PHE:CE1	1:F:273:ILE:HG23	2.52	0.45
1:F:511:VAL:HG23	1:F:512:ALA:N	2.32	0.45
1:A:124:THR:O	1:A:128:VAL:HG23	2.17	0.45
1:A:383:GLY:H	1:A:389:VAL:HG22	1.81	0.45
1:A:429:LEU:HD12	1:A:430:SER:N	2.29	0.45
1:B:112:ASN:OD1	1:B:114:MET:N	2.50	0.45
1:B:194:GLN:HG3	1:B:331:THR:OG1	2.17	0.45
1:C:480:ASN:O	1:C:484:GLU:N	2.45	0.45
1:C:62:LEU:H	1:C:68:ASN:HD22	1.64	0.45
1:C:72:GLN:HE22	1:C:75:ARG:CZ	2.30	0.45
1:D:175:ILE:HG22	1:D:176:THR:N	2.32	0.45
1:G:478:GLY:HA3	1:G:489:MET:HE3	1.99	0.45
1:B:225:LYS:HB2	1:B:226:LYS:H	1.62	0.44
1:B:383:GLY:H	1:B:389:VAL:HG22	1.81	0.44
1:C:174:VAL:O	1:C:174:VAL:HG22	2.16	0.44
1:C:221:LEU:HD21	1:C:249:ILE:CG1	2.47	0.44
1:C:80:ARG:HH11	1:C:80:ARG:HB2	1.82	0.44
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.47	0.44
1:D:383:GLY:H	1:D:389:VAL:HG22	1.82	0.44
1:D:511:VAL:HG23	1:D:512:ALA:N	2.33	0.44
1:D:6:VAL:HG22	1:D:522:ILE:HG12	1.98	0.44
1:G:158:ILE:CG2	1:G:396:VAL:HG22	2.46	0.44
1:A:194:GLN:HG3	1:A:331:THR:OG1	2.17	0.44
1:B:198:GLY:O	1:B:276:VAL:HG12	2.18	0.44
1:C:204:PHE:CE1	1:C:273:ILE:HG23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:THR:O	1:D:94:VAL:HG23	2.17	0.44
1:E:320:ALA:HA	1:E:335:GLY:O	2.18	0.44
1:E:294:ILE:HD11	1:E:345:ARG:NH1	2.32	0.44
1:E:423:ALA:HB2	1:E:447:LEU:HD13	1.98	0.44
1:F:294:ILE:HD11	1:F:345:ARG:NH1	2.33	0.44
1:A:198:GLY:O	1:A:276:VAL:HG12	2.17	0.44
1:B:12:ALA:HB1	1:B:521:MET:HG3	1.98	0.44
1:B:221:LEU:O	1:B:250:VAL:HG23	2.16	0.44
1:B:6:VAL:HG22	1:B:522:ILE:HG12	1.99	0.44
1:C:247:LEU:HB3	1:C:273:ILE:HD12	1.99	0.44
1:D:507:ASP:O	1:D:510:SER:HB3	2.17	0.44
1:E:451:MET:CE	1:E:466:ALA:HA	2.48	0.44
1:F:247:LEU:HB3	1:F:273:ILE:HD12	1.99	0.44
1:G:174:VAL:HG22	1:G:174:VAL:O	2.16	0.44
1:G:294:ILE:HD11	1:G:345:ARG:NH1	2.32	0.44
1:G:348:GLN:O	1:G:352:GLN:HB2	2.17	0.44
1:B:69:MET:HB2	1:B:69:MET:HE3	1.55	0.44
1:C:128:VAL:HG11	1:C:506:GLU:OE2	2.18	0.44
1:E:158:ILE:CG2	1:E:396:VAL:HG22	2.48	0.44
1:F:320:ALA:HA	1:F:335:GLY:O	2.18	0.44
1:G:320:ALA:HA	1:G:335:GLY:O	2.17	0.44
1:A:80:ARG:HB2	1:A:80:ARG:HH11	1.82	0.44
1:C:90:THR:O	1:C:94:VAL:HG23	2.17	0.44
1:D:13:ARG:CD	1:D:104:LEU:HD22	2.47	0.44
1:D:423:ALA:HB2	1:D:447:LEU:HD13	1.99	0.44
1:E:204:PHE:CE1	1:E:273:ILE:HG23	2.53	0.44
1:F:245:LYS:HZ1	1:F:319:ARG:HH21	1.64	0.44
1:F:429:LEU:HD12	1:F:430:SER:N	2.29	0.44
1:G:219:TYR:N	1:G:246:PRO:O	2.51	0.44
1:A:183:MET:HB3	1:A:384:MET:HE1	1.99	0.44
1:A:480:ASN:HD21	1:A:483:THR:HG23	1.83	0.44
1:C:245:LYS:HZ1	1:C:319:ARG:HH21	1.65	0.44
1:D:183:MET:HB3	1:D:384:MET:HE1	2.00	0.44
1:D:231:GLN:N	1:D:231:GLN:NE2	2.65	0.44
1:D:80:ARG:HH11	1:D:80:ARG:HB2	1.82	0.44
1:E:429:LEU:HD12	1:E:430:SER:N	2.31	0.44
1:E:62:LEU:H	1:E:68:ASN:HD22	1.66	0.44
1:F:205:VAL:HG12	1:F:207:ASN:N	2.31	0.44
1:F:205:VAL:HG12	1:F:207:ASN:H	1.81	0.44
1:F:231:GLN:NE2	1:F:231:GLN:N	2.65	0.44
1:F:219:TYR:N	1:F:246:PRO:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:ARG:CD	1:G:104:LEU:HD22	2.48	0.44
1:G:488:ASP:HB3	1:G:491:LYS:HG3	1.99	0.44
1:G:511:VAL:HG23	1:G:512:ALA:N	2.33	0.44
1:A:511:VAL:HG23	1:A:512:ALA:N	2.32	0.44
1:B:72:GLN:HE22	1:B:75:ARG:CZ	2.31	0.44
1:C:126:LYS:HG3	1:C:429:LEU:CD2	2.48	0.44
1:D:194:GLN:HG3	1:D:331:THR:OG1	2.18	0.44
1:E:75:ARG:HH11	1:E:75:ARG:CG	2.30	0.44
1:F:175:ILE:HG22	1:F:176:THR:N	2.32	0.44
1:F:348:GLN:O	1:F:352:GLN:HB2	2.17	0.44
1:G:72:GLN:HE22	1:G:75:ARG:CZ	2.31	0.44
1:B:77:VAL:HG21	1:B:511:VAL:HG13	2.00	0.44
1:C:190:VAL:HG12	1:C:191:GLU:N	2.32	0.44
1:C:225:LYS:HG3	1:C:225:LYS:H	1.61	0.44
1:C:69:MET:HE3	1:C:69:MET:HB2	1.59	0.44
1:D:423:ALA:HB2	1:D:447:LEU:CD1	2.47	0.44
1:E:175:ILE:HG22	1:E:176:THR:N	2.33	0.44
1:F:174:VAL:HG22	1:F:174:VAL:O	2.17	0.44
1:G:507:ASP:O	1:G:510:SER:HB3	2.18	0.44
1:G:77:VAL:HG21	1:G:511:VAL:HG13	2.00	0.44
1:A:13:ARG:CD	1:A:104:LEU:HD22	2.48	0.44
1:A:320:ALA:HA	1:A:335:GLY:O	2.17	0.44
1:A:348:GLN:O	1:A:352:GLN:HB2	2.18	0.44
1:B:320:ALA:HA	1:B:335:GLY:O	2.17	0.44
1:D:24:ALA:O	1:D:28:LYS:HD2	2.17	0.44
1:E:219:TYR:N	1:E:246:PRO:O	2.51	0.44
1:E:247:LEU:HB3	1:E:273:ILE:HD12	1.99	0.44
1:F:198:GLY:O	1:F:276:VAL:HG12	2.17	0.44
1:A:219:TYR:N	1:A:246:PRO:O	2.51	0.43
1:B:451:MET:CE	1:B:466:ALA:HA	2.48	0.43
1:C:175:ILE:HG22	1:C:176:THR:N	2.33	0.43
1:C:349:ILE:HG22	1:C:353:ILE:HD11	2.00	0.43
1:E:72:GLN:HE22	1:E:75:ARG:CZ	2.30	0.43
1:F:126:LYS:HG3	1:F:429:LEU:CD2	2.48	0.43
1:A:204:PHE:CE1	1:A:273:ILE:HG23	2.54	0.43
1:A:8:PHE:HE1	1:B:26:ALA:HA	1.83	0.43
1:B:294:ILE:HD11	1:B:345:ARG:NH1	2.33	0.43
1:C:227:LEU:CD1	1:C:251:ALA:HB3	2.48	0.43
1:C:12:ALA:HB1	1:C:521:MET:HG3	1.99	0.43
1:D:139:ASN:N	1:D:139:ASN:ND2	2.66	0.43
1:D:349:ILE:HG22	1:D:353:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:HE22	1:D:75:ARG:CZ	2.31	0.43
1:E:365:LEU:HA	1:E:368:ARG:HG2	2.00	0.43
1:F:480:ASN:HD21	1:F:483:THR:HG23	1.84	0.43
1:A:112:ASN:OD1	1:A:114:MET:N	2.51	0.43
1:A:488:ASP:HB3	1:A:491:LYS:HG3	2.00	0.43
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.48	0.43
1:G:128:VAL:HG11	1:G:506:GLU:OE2	2.19	0.43
1:G:225:LYS:HG3	1:G:225:LYS:H	1.62	0.43
1:G:174:VAL:HG13	1:G:376:VAL:HA	2.00	0.43
1:B:488:ASP:HB3	1:B:491:LYS:HG3	1.99	0.43
1:D:247:LEU:HB3	1:D:273:ILE:HD12	1.99	0.43
1:E:423:ALA:HB2	1:E:447:LEU:CD1	2.48	0.43
1:F:488:ASP:HB3	1:F:491:LYS:HG3	1.99	0.43
1:F:62:LEU:H	1:F:68:ASN:HD22	1.66	0.43
1:B:103:GLY:HA3	1:B:516:ILE:CD1	2.49	0.43
1:C:139:ASN:N	1:C:139:ASN:ND2	2.67	0.43
1:D:227:LEU:CD1	1:D:251:ALA:HB3	2.48	0.43
1:C:8:PHE:HE1	1:D:26:ALA:HA	1.84	0.43
1:D:294:ILE:HD11	1:D:345:ARG:NH1	2.32	0.43
1:E:13:ARG:CD	1:E:104:LEU:HD22	2.48	0.43
1:F:225:LYS:HB2	1:F:226:LYS:H	1.62	0.43
1:F:227:LEU:CD1	1:F:251:ALA:HB3	2.48	0.43
1:G:12:ALA:HB1	1:G:521:MET:SD	2.58	0.43
1:G:175:ILE:HG22	1:G:176:THR:N	2.33	0.43
1:G:247:LEU:HB3	1:G:273:ILE:HD12	2.00	0.43
1:B:204:PHE:CE1	1:B:273:ILE:HG23	2.53	0.43
1:B:511:VAL:HG23	1:B:512:ALA:N	2.34	0.43
1:B:69:MET:HG2	1:C:47:PRO:HB3	2.01	0.43
1:D:204:PHE:CE1	1:D:273:ILE:HG23	2.53	0.43
1:D:480:ASN:HD21	1:D:483:THR:HG23	1.84	0.43
1:E:12:ALA:HB1	1:E:521:MET:SD	2.59	0.43
1:E:451:MET:CE	1:E:465:VAL:HG12	2.49	0.43
1:F:365:LEU:HA	1:F:368:ARG:HG2	2.00	0.43
1:G:75:ARG:HH11	1:G:75:ARG:CG	2.31	0.43
1:A:478:GLY:HA3	1:A:489:MET:HE3	1.99	0.43
1:B:349:ILE:HG22	1:B:353:ILE:HD11	2.00	0.43
1:D:365:LEU:HA	1:D:368:ARG:HG2	2.00	0.43
1:D:451:MET:CE	1:D:465:VAL:HG12	2.49	0.43
1:E:224:GLU:HG3	1:E:286:LYS:CE	2.49	0.43
1:F:103:GLY:HA3	1:F:516:ILE:CD1	2.49	0.43
1:F:124:THR:O	1:F:128:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:HD11	1:A:345:ARG:NH1	2.33	0.43
1:A:480:ASN:O	1:A:484:GLU:N	2.47	0.43
1:B:227:LEU:CD1	1:B:251:ALA:HB3	2.49	0.43
1:B:365:LEU:HA	1:B:368:ARG:HG2	2.00	0.43
1:C:488:ASP:HB3	1:C:491:LYS:HG3	1.99	0.43
1:C:103:GLY:HA3	1:C:516:ILE:CD1	2.49	0.43
1:D:224:GLU:HG3	1:D:286:LYS:CE	2.49	0.43
1:D:478:GLY:HA3	1:D:489:MET:HE3	2.00	0.43
1:F:349:ILE:HG22	1:F:353:ILE:HD11	2.00	0.43
1:F:451:MET:CE	1:F:466:ALA:HA	2.49	0.43
1:A:321:LYS:CB	1:A:334:ASP:HB3	2.45	0.43
1:B:175:ILE:HG22	1:B:176:THR:N	2.33	0.43
1:B:224:GLU:HG3	1:B:286:LYS:CE	2.49	0.43
1:B:507:ASP:O	1:B:510:SER:HB3	2.18	0.43
1:C:224:GLU:HG3	1:C:286:LYS:CE	2.49	0.43
1:C:194:GLN:HG3	1:C:331:THR:OG1	2.17	0.43
1:C:365:LEU:HA	1:C:368:ARG:HG2	2.01	0.43
1:C:507:ASP:O	1:C:510:SER:HB3	2.19	0.43
1:D:12:ALA:HB1	1:D:521:MET:HG3	2.00	0.43
1:E:128:VAL:HG11	1:E:506:GLU:OE2	2.18	0.43
1:G:227:LEU:CD1	1:G:251:ALA:HB3	2.49	0.43
1:G:365:LEU:HA	1:G:368:ARG:HG2	2.00	0.43
1:A:225:LYS:HB2	1:A:226:LYS:H	1.62	0.43
1:A:227:LEU:CD1	1:A:251:ALA:HB3	2.48	0.43
1:B:126:LYS:HG3	1:B:429:LEU:CD2	2.49	0.43
1:B:62:LEU:H	1:B:68:ASN:HD22	1.65	0.43
1:D:488:ASP:HB3	1:D:491:LYS:HG3	2.00	0.43
1:E:124:THR:O	1:E:128:VAL:HG23	2.19	0.43
1:E:478:GLY:HA3	1:E:489:MET:HE3	2.01	0.43
1:G:383:GLY:H	1:G:389:VAL:HG22	1.83	0.43
1:A:24:ALA:O	1:A:28:LYS:HB3	2.18	0.42
1:A:451:MET:HE1	1:A:465:VAL:HG12	2.01	0.42
1:D:480:ASN:O	1:D:484:GLU:N	2.48	0.42
1:E:227:LEU:CD1	1:E:251:ALA:HB3	2.48	0.42
1:E:248:LEU:CA	1:E:274:ALA:HB3	2.49	0.42
1:D:69:MET:HG2	1:E:47:PRO:HG3	2.00	0.42
1:F:13:ARG:CD	1:F:104:LEU:HD22	2.49	0.42
1:F:75:ARG:HH11	1:F:75:ARG:CG	2.30	0.42
1:A:365:LEU:HA	1:A:368:ARG:HG2	2.00	0.42
1:B:231:GLN:N	1:B:231:GLN:NE2	2.65	0.42
1:B:449:ALA:CB	1:B:450:PRO:HD3	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ASP:HA	1:C:320:ALA:O	2.19	0.42
1:D:128:VAL:O	1:D:128:VAL:HG12	2.18	0.42
1:F:226:LYS:HZ1	1:F:252:GLU:HB3	1.84	0.42
1:F:26:ALA:O	1:F:29:VAL:HG22	2.18	0.42
1:F:321:LYS:CB	1:F:334:ASP:HB3	2.45	0.42
1:A:507:ASP:O	1:A:510:SER:HB3	2.19	0.42
1:B:378:VAL:HG22	1:B:378:VAL:O	2.19	0.42
1:A:126:LYS:HG3	1:A:429:LEU:CD2	2.49	0.42
1:A:62:LEU:H	1:A:68:ASN:HD22	1.65	0.42
1:C:227:LEU:HD11	1:C:251:ALA:HB3	2.02	0.42
1:C:451:MET:CE	1:C:466:ALA:HA	2.48	0.42
1:D:219:TYR:N	1:D:246:PRO:O	2.52	0.42
1:E:378:VAL:O	1:E:378:VAL:HG22	2.19	0.42
1:D:69:MET:HG2	1:E:47:PRO:CB	2.49	0.42
1:E:488:ASP:HB3	1:E:491:LYS:HG3	2.00	0.42
1:F:220:ILE:CD1	1:F:248:LEU:HD22	2.49	0.42
1:G:248:LEU:CA	1:G:274:ALA:HB3	2.49	0.42
1:A:224:GLU:HG3	1:A:286:LYS:CE	2.49	0.42
1:A:349:ILE:HG22	1:A:353:ILE:HD11	2.01	0.42
1:A:423:ALA:HB2	1:A:447:LEU:HD13	2.01	0.42
1:B:124:THR:O	1:B:128:VAL:HG23	2.19	0.42
1:B:174:VAL:HG13	1:B:376:VAL:HA	2.02	0.42
1:B:90:THR:O	1:B:94:VAL:HG23	2.20	0.42
1:C:174:VAL:HG13	1:C:376:VAL:HA	2.01	0.42
1:C:19:GLY:O	1:C:71:ALA:HB2	2.20	0.42
1:F:126:LYS:HG3	1:F:429:LEU:HD22	2.00	0.42
1:G:321:LYS:CB	1:G:334:ASP:HB3	2.45	0.42
1:G:480:ASN:HD21	1:G:483:THR:HG23	1.84	0.42
1:A:174:VAL:HG13	1:A:376:VAL:HA	2.02	0.42
1:A:220:ILE:CD1	1:A:248:LEU:HD22	2.50	0.42
1:E:126:LYS:HG3	1:E:429:LEU:CD2	2.49	0.42
1:F:12:ALA:HB1	1:F:521:MET:HG3	2.01	0.42
1:F:36:ARG:CG	1:F:36:ARG:NH1	2.75	0.42
1:G:380:ARG:HH11	1:G:380:ARG:CB	2.28	0.42
1:C:112:ASN:OD1	1:C:112:ASN:C	2.58	0.42
1:D:112:ASN:C	1:D:112:ASN:OD1	2.58	0.42
1:E:221:LEU:HG	1:E:249:ILE:HA	2.02	0.42
1:F:72:GLN:HE22	1:F:75:ARG:CZ	2.31	0.42
1:A:112:ASN:OD1	1:A:112:ASN:C	2.58	0.42
1:A:2:ALA:O	1:A:3:ALA:C	2.57	0.42
1:C:220:ILE:CD1	1:C:248:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LYS:HG3	1:D:429:LEU:CD2	2.49	0.42
1:D:227:LEU:HD11	1:D:251:ALA:HB3	2.02	0.42
1:D:298:GLY:HA2	1:D:317:LEU:C	2.40	0.42
1:D:174:VAL:HG13	1:D:376:VAL:HA	2.01	0.42
1:E:139:ASN:ND2	1:E:139:ASN:N	2.66	0.42
1:E:321:LYS:CB	1:E:334:ASP:HB3	2.45	0.42
1:E:507:ASP:O	1:E:510:SER:HB3	2.20	0.42
1:F:2:ALA:O	1:F:3:ALA:C	2.57	0.42
1:B:13:ARG:CD	1:B:104:LEU:HD22	2.49	0.42
1:B:112:ASN:C	1:B:112:ASN:OD1	2.59	0.42
1:B:128:VAL:HG11	1:B:506:GLU:OE2	2.20	0.42
1:B:227:LEU:HD11	1:B:251:ALA:HB3	2.02	0.42
1:B:423:ALA:HB2	1:B:447:LEU:HD13	2.01	0.42
1:D:128:VAL:HG11	1:D:506:GLU:OE2	2.19	0.42
1:D:451:MET:CE	1:D:466:ALA:HA	2.49	0.42
1:E:220:ILE:CD1	1:E:248:LEU:HD22	2.50	0.42
1:F:123:ALA:HB1	1:F:426:LEU:HD22	2.02	0.42
1:G:224:GLU:HG3	1:G:286:LYS:CE	2.50	0.42
1:A:139:ASN:ND2	1:A:139:ASN:N	2.66	0.42
1:A:217:ASP:HA	1:A:320:ALA:O	2.20	0.42
1:B:219:TYR:N	1:B:246:PRO:O	2.52	0.42
1:B:221:LEU:HG	1:B:249:ILE:HA	2.02	0.42
1:D:215:LEU:HD22	1:D:274:ALA:HB2	2.02	0.42
1:D:220:ILE:CD1	1:D:248:LEU:HD22	2.50	0.42
1:D:77:VAL:HG21	1:D:511:VAL:HG13	2.02	0.42
1:F:215:LEU:HD22	1:F:274:ALA:HB2	2.02	0.42
1:G:225:LYS:HB2	1:G:226:LYS:H	1.62	0.42
1:G:215:LEU:HD22	1:G:274:ALA:HB2	2.02	0.42
1:G:349:ILE:HG22	1:G:353:ILE:HD11	2.01	0.42
1:G:126:LYS:HG3	1:G:429:LEU:CD2	2.50	0.42
1:A:378:VAL:O	1:A:378:VAL:HG22	2.20	0.41
1:C:219:TYR:N	1:C:246:PRO:O	2.52	0.41
1:C:298:GLY:HA2	1:C:317:LEU:C	2.40	0.41
1:E:90:THR:O	1:E:94:VAL:HG23	2.20	0.41
1:F:224:GLU:HG3	1:F:286:LYS:CE	2.49	0.41
1:A:215:LEU:HD22	1:A:274:ALA:HB2	2.02	0.41
1:A:423:ALA:HB2	1:A:447:LEU:CD1	2.50	0.41
1:B:139:ASN:N	1:B:139:ASN:ND2	2.66	0.41
1:E:7:LYS:HB3	1:E:12:ALA:HB2	2.03	0.41
1:E:298:GLY:HA2	1:E:317:LEU:C	2.41	0.41
1:F:323:VAL:HG13	1:F:332:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HB3	1:A:12:ALA:HB2	2.03	0.41
1:B:75:ARG:HH11	1:B:75:ARG:CG	2.32	0.41
1:C:221:LEU:HG	1:C:249:ILE:HA	2.03	0.41
1:C:480:ASN:HD21	1:C:483:THR:HG23	1.85	0.41
1:D:220:ILE:HG23	1:D:248:LEU:CD2	2.50	0.41
1:F:423:ALA:HB2	1:F:447:LEU:HD13	2.01	0.41
1:F:69:MET:HE3	1:F:69:MET:HB2	1.53	0.41
1:G:112:ASN:C	1:G:112:ASN:OD1	2.58	0.41
1:A:227:LEU:HD11	1:A:251:ALA:HB3	2.02	0.41
1:C:126:LYS:HG3	1:C:429:LEU:HD22	2.02	0.41
1:C:220:ILE:HG23	1:C:248:LEU:CD2	2.51	0.41
1:C:423:ALA:HB2	1:C:447:LEU:CD1	2.50	0.41
1:E:227:LEU:HB2	1:E:254:VAL:CA	2.38	0.41
1:E:217:ASP:HA	1:E:320:ALA:O	2.21	0.41
1:F:217:ASP:HA	1:F:320:ALA:O	2.21	0.41
1:F:221:LEU:HG	1:F:249:ILE:HA	2.03	0.41
1:G:220:ILE:CD1	1:G:248:LEU:HD22	2.50	0.41
1:G:12:ALA:HB1	1:G:521:MET:HG3	2.03	0.41
1:A:451:MET:CE	1:A:466:ALA:HA	2.50	0.41
1:A:12:ALA:HB1	1:A:521:MET:SD	2.60	0.41
1:B:215:LEU:HD22	1:B:274:ALA:HB2	2.02	0.41
1:B:220:ILE:CD1	1:B:248:LEU:HD22	2.50	0.41
1:B:80:ARG:HB2	1:B:80:ARG:NH1	2.36	0.41
1:E:349:ILE:HG22	1:E:353:ILE:HD11	2.01	0.41
1:E:36:ARG:CG	1:E:36:ARG:NH1	2.76	0.41
1:E:2:ALA:O	1:E:3:ALA:C	2.58	0.41
1:B:2:ALA:O	1:B:3:ALA:C	2.59	0.41
1:B:423:ALA:HB2	1:B:447:LEU:CD1	2.51	0.41
1:C:215:LEU:HD22	1:C:274:ALA:HB2	2.03	0.41
1:D:221:LEU:HG	1:D:249:ILE:HA	2.03	0.41
1:E:174:VAL:HG13	1:E:376:VAL:HA	2.01	0.41
1:F:220:ILE:HG23	1:F:248:LEU:CD2	2.50	0.41
1:F:298:GLY:HA2	1:F:317:LEU:C	2.41	0.41
1:F:174:VAL:HG13	1:F:376:VAL:HA	2.02	0.41
1:F:8:PHE:HE1	1:G:26:ALA:HA	1.86	0.41
1:G:24:ALA:O	1:G:28:LYS:HB3	2.20	0.41
1:G:298:GLY:HA2	1:G:317:LEU:C	2.41	0.41
1:C:24:ALA:O	1:C:28:LYS:HB3	2.21	0.41
1:E:245:LYS:HZ1	1:E:319:ARG:HH21	1.66	0.41
1:E:480:ASN:HD21	1:E:483:THR:HG23	1.85	0.41
1:E:103:GLY:HA3	1:E:516:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:LEU:HD11	1:F:251:ALA:HB3	2.02	0.41
1:G:231:GLN:N	1:G:231:GLN:NE2	2.65	0.41
1:A:248:LEU:CB	1:A:274:ALA:HB3	2.51	0.41
1:B:220:ILE:HG23	1:B:248:LEU:CD2	2.51	0.41
1:B:248:LEU:CB	1:B:274:ALA:HB3	2.51	0.41
1:C:26:ALA:O	1:C:29:VAL:HG22	2.21	0.41
1:C:378:VAL:HG22	1:C:378:VAL:O	2.21	0.41
1:D:227:LEU:HB2	1:D:254:VAL:CA	2.38	0.41
1:D:248:LEU:CA	1:D:274:ALA:HB3	2.49	0.41
1:D:2:ALA:O	1:D:3:ALA:C	2.59	0.41
1:D:126:LYS:HG3	1:D:429:LEU:HD22	2.02	0.41
1:D:482:GLN:HA	1:D:482:GLN:NE2	2.36	0.41
1:G:181:LYS:HB2	1:G:182:GLY:H	1.78	0.41
1:A:298:GLY:HA2	1:A:317:LEU:C	2.41	0.41
1:C:482:GLN:HA	1:C:482:GLN:NE2	2.36	0.41
1:F:423:ALA:HB2	1:F:447:LEU:CD1	2.51	0.41
1:G:2:ALA:O	1:G:3:ALA:C	2.58	0.41
1:G:36:ARG:CG	1:G:36:ARG:NH1	2.79	0.41
1:A:220:ILE:HG23	1:A:248:LEU:CD2	2.51	0.41
1:A:231:GLN:N	1:A:231:GLN:NE2	2.65	0.41
1:A:190:VAL:HG11	1:A:334:ASP:CB	2.51	0.41
1:C:13:ARG:CD	1:C:104:LEU:HD22	2.50	0.41
1:C:423:ALA:HB2	1:C:447:LEU:HD13	2.02	0.41
1:E:220:ILE:HG23	1:E:248:LEU:CD2	2.50	0.41
1:E:227:LEU:HD11	1:E:251:ALA:HB3	2.02	0.41
1:E:215:LEU:HD22	1:E:274:ALA:HB2	2.03	0.41
1:F:451:MET:HE1	1:F:465:VAL:HG12	2.02	0.41
1:F:90:THR:O	1:F:94:VAL:HG23	2.21	0.41
1:A:221:LEU:HG	1:A:249:ILE:HA	2.03	0.41
1:A:72:GLN:HE22	1:A:75:ARG:CZ	2.34	0.41
1:B:298:GLY:HA2	1:B:317:LEU:C	2.41	0.41
1:C:55:SER:O	1:C:59:GLU:HG2	2.20	0.41
1:F:380:ARG:HH11	1:F:380:ARG:CB	2.29	0.41
1:F:7:LYS:HB3	1:F:12:ALA:HB2	2.03	0.40
1:F:489:MET:HG3	1:F:494:VAL:O	2.21	0.40
1:G:220:ILE:HG23	1:G:248:LEU:CD2	2.50	0.40
1:G:248:LEU:CB	1:G:274:ALA:HB3	2.51	0.40
1:G:26:ALA:O	1:G:29:VAL:HG22	2.21	0.40
1:G:323:VAL:HG13	1:G:332:ILE:HG12	2.03	0.40
1:B:201:SER:O	1:B:204:PHE:HB2	2.21	0.40
1:B:480:ASN:HD21	1:B:483:THR:HG23	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ARG:HB2	1:C:80:ARG:NH1	2.36	0.40
1:D:19:GLY:HA2	1:D:62:LEU:HD11	2.03	0.40
1:E:112:ASN:C	1:E:112:ASN:OD1	2.58	0.40
1:G:103:GLY:HA3	1:G:516:ILE:CD1	2.50	0.40
1:G:227:LEU:HD11	1:G:251:ALA:HB3	2.03	0.40
1:A:323:VAL:HG13	1:A:332:ILE:HG12	2.03	0.40
1:B:7:LYS:HB3	1:B:12:ALA:HB2	2.04	0.40
1:E:126:LYS:HG3	1:E:429:LEU:HD22	2.02	0.40
1:F:190:VAL:HG12	1:F:191:GLU:N	2.36	0.40
1:F:80:ARG:HB2	1:F:80:ARG:NH1	2.35	0.40
1:G:217:ASP:HA	1:G:320:ALA:O	2.22	0.40
1:G:480:ASN:O	1:G:484:GLU:N	2.48	0.40
1:B:217:ASP:HA	1:B:320:ALA:O	2.22	0.40
1:B:323:VAL:HG13	1:B:332:ILE:HG12	2.03	0.40
1:F:378:VAL:HG22	1:F:378:VAL:O	2.21	0.40
1:A:80:ARG:NH1	1:A:80:ARG:HB2	2.36	0.40
1:C:2:ALA:O	1:C:3:ALA:C	2.60	0.40
1:E:144:VAL:O	1:E:144:VAL:CG1	2.70	0.40
1:G:201:SER:O	1:G:204:PHE:HB2	2.21	0.40
1:G:482:GLN:NE2	1:G:482:GLN:HA	2.37	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	474/545 (87%)	404 (85%)	59 (12%)	11 (2%)	6 34
1	B	474/545 (87%)	405 (85%)	59 (12%)	10 (2%)	7 37
1	C	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	7 37
1	D	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	7 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	7 37
1	F	474/545 (87%)	404 (85%)	58 (12%)	12 (2%)	5 32
1	G	474/545 (87%)	405 (85%)	59 (12%)	10 (2%)	7 37
All	All	3318/3815 (87%)	2830 (85%)	415 (12%)	73 (2%)	6 35

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	85	ALA
1	A	228	SER
1	A	378	VAL
1	B	9	ASN
1	B	85	ALA
1	B	134	ALA
1	B	228	SER
1	B	378	VAL
1	C	9	ASN
1	C	85	ALA
1	C	134	ALA
1	C	228	SER
1	C	378	VAL
1	D	9	ASN
1	D	85	ALA
1	D	228	SER
1	D	378	VAL
1	E	9	ASN
1	E	85	ALA
1	E	134	ALA
1	E	228	SER
1	E	378	VAL
1	F	9	ASN
1	F	85	ALA
1	F	228	SER
1	F	378	VAL
1	G	9	ASN
1	G	85	ALA
1	G	228	SER
1	G	378	VAL
1	A	134	ALA
1	A	335	GLY

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Mol	Chain	Res	Type
1	B	335	GLY
1	C	335	GLY
1	D	134	ALA
1	D	335	GLY
1	E	335	GLY
1	F	134	ALA
1	F	335	GLY
1	G	134	ALA
1	G	335	GLY
1	A	87	ASP
1	A	336	ALA
1	A	475	LYS
1	B	87	ASP
1	B	336	ALA
1	B	475	LYS
1	C	87	ASP
1	C	336	ALA
1	C	475	LYS
1	D	87	ASP
1	D	336	ALA
1	D	475	LYS
1	E	87	ASP
1	E	336	ALA
1	E	475	LYS
1	F	87	ASP
1	F	336	ALA
1	F	475	LYS
1	G	87	ASP
1	G	336	ALA
1	G	475	LYS
1	F	3	ALA
1	A	246	PRO
1	B	246	PRO
1	C	246	PRO
1	D	246	PRO
1	F	246	PRO
1	E	246	PRO
1	G	246	PRO
1	F	374	GLY
1	A	374	GLY

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	372/421 (88%)	278 (75%)	94 (25%)	0 2
1	B	372/421 (88%)	279 (75%)	93 (25%)	0 2
1	C	372/421 (88%)	277 (74%)	95 (26%)	0 2
1	D	372/421 (88%)	279 (75%)	93 (25%)	0 2
1	E	372/421 (88%)	278 (75%)	94 (25%)	0 2
1	F	372/421 (88%)	278 (75%)	94 (25%)	0 2
1	G	372/421 (88%)	277 (74%)	95 (26%)	0 2
All	All	2604/2947 (88%)	1946 (75%)	658 (25%)	0 2

All (658) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	LYS
1	A	16	MET
1	A	18	LYS
1	A	28	LYS
1	A	36	ARG
1	A	42	LYS
1	A	51	LYS
1	A	55	SER
1	A	69	MET
1	A	72	GLN
1	A	75	ARG
1	A	76	GLU
1	A	77	VAL
1	A	79	SER
1	A	80	ARG
1	A	83	ASP
1	A	87	ASP
1	A	105	LYS
1	A	132	LYS

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Mol	Chain	Res	Type
1	A	139	ASN
1	A	141	SER
1	A	146	GLN
1	A	155	GLU
1	A	156	SER
1	A	164	GLU
1	A	166	MET
1	A	167	GLN
1	A	168	ARG
1	A	172	GLU
1	A	181	LYS
1	A	183	MET
1	A	196	ASP
1	A	197	ARG
1	A	204	PHE
1	A	206	THR
1	A	209	ASP
1	A	210	LYS
1	A	211	MET
1	A	214	GLU
1	A	216	GLU
1	A	217	ASP
1	A	221	LEU
1	A	222	LEU
1	A	225	LYS
1	A	229	SER
1	A	231	GLN
1	A	245	LYS
1	A	247	LEU
1	A	250	VAL
1	A	252	GLU
1	A	253	ASP
1	A	281	PHE
1	A	283	ASP
1	A	288	MET
1	A	290	GLN
1	A	295	LEU
1	A	315	ASP
1	A	316	MET
1	A	317	LEU
1	A	321	LYS
1	A	322	LYS

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Mol	Chain	Res	Type
1	A	327	LYS
1	A	328	ASP
1	A	333	VAL
1	A	338	GLU
1	A	339	LYS
1	A	343	GLU
1	A	345	ARG
1	A	352	GLN
1	A	357	THR
1	A	362	ARG
1	A	365	LEU
1	A	367	GLU
1	A	368	ARG
1	A	371	LYS
1	A	380	ARG
1	A	387	ILE
1	A	388	GLU
1	A	391	GLU
1	A	395	ARG
1	A	398	ASP
1	A	401	ASN
1	A	408	GLN
1	A	419	LEU
1	A	427	GLU
1	A	430	SER
1	A	434	SER
1	A	436	GLN
1	A	444	ARG
1	A	452	ARG
1	A	473	SER
1	A	524	GLU
1	A	525	LYS
1	B	5	GLU
1	B	7	LYS
1	B	16	MET
1	B	18	LYS
1	B	28	LYS
1	B	36	ARG
1	B	42	LYS
1	B	51	LYS
1	B	55	SER
1	B	69	MET

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Mol	Chain	Res	Type
1	B	72	GLN
1	B	75	ARG
1	B	76	GLU
1	B	77	VAL
1	B	79	SER
1	B	80	ARG
1	B	83	ASP
1	B	87	ASP
1	B	105	LYS
1	B	132	LYS
1	B	139	ASN
1	B	141	SER
1	B	146	GLN
1	B	155	GLU
1	B	156	SER
1	B	164	GLU
1	B	166	MET
1	B	167	GLN
1	B	168	ARG
1	B	172	GLU
1	B	181	LYS
1	B	183	MET
1	B	196	ASP
1	B	197	ARG
1	B	204	PHE
1	B	206	THR
1	B	209	ASP
1	B	210	LYS
1	B	211	MET
1	B	214	GLU
1	B	216	GLU
1	B	217	ASP
1	B	221	LEU
1	B	222	LEU
1	B	225	LYS
1	B	229	SER
1	B	231	GLN
1	B	245	LYS
1	B	247	LEU
1	B	250	VAL
1	B	252	GLU
1	B	253	ASP

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Mol	Chain	Res	Type
1	B	281	PHE
1	B	283	ASP
1	B	288	MET
1	B	290	GLN
1	B	295	LEU
1	B	315	ASP
1	B	316	MET
1	B	317	LEU
1	B	321	LYS
1	B	322	LYS
1	B	327	LYS
1	B	328	ASP
1	B	333	VAL
1	B	338	GLU
1	B	339	LYS
1	B	343	GLU
1	B	345	ARG
1	B	352	GLN
1	B	357	THR
1	B	362	ARG
1	B	365	LEU
1	B	367	GLU
1	B	368	ARG
1	B	371	LYS
1	B	380	ARG
1	B	387	ILE
1	B	388	GLU
1	B	391	GLU
1	B	395	ARG
1	B	398	ASP
1	B	401	ASN
1	B	408	GLN
1	B	419	LEU
1	B	427	GLU
1	B	430	SER
1	B	434	SER
1	B	436	GLN
1	B	444	ARG
1	B	473	SER
1	B	524	GLU
1	B	525	LYS
1	C	5	GLU

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Mol	Chain	Res	Type
1	C	7	LYS
1	C	16	MET
1	C	18	LYS
1	C	28	LYS
1	C	36	ARG
1	C	42	LYS
1	C	51	LYS
1	C	55	SER
1	C	69	MET
1	C	72	GLN
1	C	75	ARG
1	C	76	GLU
1	C	77	VAL
1	C	79	SER
1	C	80	ARG
1	C	83	ASP
1	C	87	ASP
1	C	105	LYS
1	C	132	LYS
1	C	139	ASN
1	C	141	SER
1	C	146	GLN
1	C	155	GLU
1	C	156	SER
1	C	164	GLU
1	C	166	MET
1	C	167	GLN
1	C	168	ARG
1	C	172	GLU
1	C	181	LYS
1	C	183	MET
1	C	196	ASP
1	C	197	ARG
1	C	204	PHE
1	C	206	THR
1	C	209	ASP
1	C	210	LYS
1	C	211	MET
1	C	214	GLU
1	C	216	GLU
1	C	217	ASP
1	C	221	LEU

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Mol	Chain	Res	Type
1	C	222	LEU
1	C	225	LYS
1	C	229	SER
1	C	231	GLN
1	C	245	LYS
1	C	247	LEU
1	C	250	VAL
1	C	252	GLU
1	C	253	ASP
1	C	281	PHE
1	C	283	ASP
1	C	288	MET
1	C	290	GLN
1	C	295	LEU
1	C	315	ASP
1	C	316	MET
1	C	317	LEU
1	C	321	LYS
1	C	322	LYS
1	C	327	LYS
1	C	328	ASP
1	C	333	VAL
1	C	338	GLU
1	C	339	LYS
1	C	343	GLU
1	C	345	ARG
1	C	352	GLN
1	C	357	THR
1	C	362	ARG
1	C	365	LEU
1	C	367	GLU
1	C	368	ARG
1	C	371	LYS
1	C	380	ARG
1	C	387	ILE
1	C	388	GLU
1	C	391	GLU
1	C	392	ARG
1	C	395	ARG
1	C	398	ASP
1	C	401	ASN
1	C	408	GLN

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Mol	Chain	Res	Type
1	C	419	LEU
1	C	427	GLU
1	C	430	SER
1	C	434	SER
1	C	436	GLN
1	C	444	ARG
1	C	452	ARG
1	C	473	SER
1	C	524	GLU
1	C	525	LYS
1	D	5	GLU
1	D	7	LYS
1	D	16	MET
1	D	18	LYS
1	D	28	LYS
1	D	36	ARG
1	D	42	LYS
1	D	51	LYS
1	D	55	SER
1	D	69	MET
1	D	72	GLN
1	D	75	ARG
1	D	76	GLU
1	D	77	VAL
1	D	79	SER
1	D	80	ARG
1	D	83	ASP
1	D	87	ASP
1	D	105	LYS
1	D	132	LYS
1	D	139	ASN
1	D	141	SER
1	D	146	GLN
1	D	155	GLU
1	D	156	SER
1	D	164	GLU
1	D	166	MET
1	D	167	GLN
1	D	168	ARG
1	D	172	GLU
1	D	181	LYS
1	D	183	MET

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Mol	Chain	Res	Type
1	D	196	ASP
1	D	197	ARG
1	D	204	PHE
1	D	206	THR
1	D	209	ASP
1	D	210	LYS
1	D	211	MET
1	D	214	GLU
1	D	216	GLU
1	D	217	ASP
1	D	221	LEU
1	D	222	LEU
1	D	225	LYS
1	D	229	SER
1	D	231	GLN
1	D	245	LYS
1	D	247	LEU
1	D	250	VAL
1	D	252	GLU
1	D	253	ASP
1	D	281	PHE
1	D	283	ASP
1	D	288	MET
1	D	290	GLN
1	D	295	LEU
1	D	315	ASP
1	D	316	MET
1	D	317	LEU
1	D	321	LYS
1	D	322	LYS
1	D	327	LYS
1	D	328	ASP
1	D	333	VAL
1	D	338	GLU
1	D	339	LYS
1	D	343	GLU
1	D	345	ARG
1	D	352	GLN
1	D	357	THR
1	D	362	ARG
1	D	365	LEU
1	D	367	GLU

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Mol	Chain	Res	Type
1	D	368	ARG
1	D	371	LYS
1	D	380	ARG
1	D	387	ILE
1	D	388	GLU
1	D	391	GLU
1	D	395	ARG
1	D	398	ASP
1	D	401	ASN
1	D	408	GLN
1	D	419	LEU
1	D	427	GLU
1	D	430	SER
1	D	434	SER
1	D	436	GLN
1	D	444	ARG
1	D	473	SER
1	D	524	GLU
1	D	525	LYS
1	E	5	GLU
1	E	7	LYS
1	E	16	MET
1	E	18	LYS
1	E	28	LYS
1	E	36	ARG
1	E	42	LYS
1	E	51	LYS
1	E	55	SER
1	E	64	ASP
1	E	69	MET
1	E	72	GLN
1	E	75	ARG
1	E	76	GLU
1	E	77	VAL
1	E	79	SER
1	E	80	ARG
1	E	83	ASP
1	E	87	ASP
1	E	105	LYS
1	E	132	LYS
1	E	139	ASN
1	E	141	SER

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Mol	Chain	Res	Type
1	E	146	GLN
1	E	155	GLU
1	E	156	SER
1	E	164	GLU
1	E	166	MET
1	E	167	GLN
1	E	168	ARG
1	E	172	GLU
1	E	181	LYS
1	E	183	MET
1	E	196	ASP
1	E	197	ARG
1	E	204	PHE
1	E	206	THR
1	E	209	ASP
1	E	210	LYS
1	E	211	MET
1	E	214	GLU
1	E	216	GLU
1	E	217	ASP
1	E	221	LEU
1	E	222	LEU
1	E	225	LYS
1	E	229	SER
1	E	231	GLN
1	E	245	LYS
1	E	247	LEU
1	E	250	VAL
1	E	252	GLU
1	E	253	ASP
1	E	281	PHE
1	E	283	ASP
1	E	288	MET
1	E	290	GLN
1	E	295	LEU
1	E	315	ASP
1	E	316	MET
1	E	317	LEU
1	E	321	LYS
1	E	322	LYS
1	E	327	LYS
1	E	328	ASP

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Mol	Chain	Res	Type
1	E	333	VAL
1	E	338	GLU
1	E	339	LYS
1	E	343	GLU
1	E	345	ARG
1	E	352	GLN
1	E	357	THR
1	E	362	ARG
1	E	365	LEU
1	E	367	GLU
1	E	368	ARG
1	E	371	LYS
1	E	380	ARG
1	E	387	ILE
1	E	388	GLU
1	E	391	GLU
1	E	395	ARG
1	E	398	ASP
1	E	401	ASN
1	E	408	GLN
1	E	419	LEU
1	E	427	GLU
1	E	430	SER
1	E	434	SER
1	E	436	GLN
1	E	444	ARG
1	E	473	SER
1	E	524	GLU
1	E	525	LYS
1	F	5	GLU
1	F	7	LYS
1	F	16	MET
1	F	18	LYS
1	F	28	LYS
1	F	36	ARG
1	F	42	LYS
1	F	51	LYS
1	F	55	SER
1	F	69	MET
1	F	72	GLN
1	F	75	ARG
1	F	76	GLU

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Mol	Chain	Res	Type
1	F	77	VAL
1	F	79	SER
1	F	80	ARG
1	F	83	ASP
1	F	87	ASP
1	F	105	LYS
1	F	132	LYS
1	F	139	ASN
1	F	141	SER
1	F	146	GLN
1	F	155	GLU
1	F	156	SER
1	F	164	GLU
1	F	166	MET
1	F	167	GLN
1	F	168	ARG
1	F	172	GLU
1	F	181	LYS
1	F	183	MET
1	F	196	ASP
1	F	197	ARG
1	F	204	PHE
1	F	206	THR
1	F	209	ASP
1	F	210	LYS
1	F	211	MET
1	F	214	GLU
1	F	216	GLU
1	F	217	ASP
1	F	221	LEU
1	F	222	LEU
1	F	225	LYS
1	F	229	SER
1	F	231	GLN
1	F	245	LYS
1	F	247	LEU
1	F	250	VAL
1	F	252	GLU
1	F	253	ASP
1	F	281	PHE
1	F	283	ASP
1	F	288	MET

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Mol	Chain	Res	Type
1	F	290	GLN
1	F	295	LEU
1	F	315	ASP
1	F	316	MET
1	F	317	LEU
1	F	321	LYS
1	F	322	LYS
1	F	327	LYS
1	F	328	ASP
1	F	333	VAL
1	F	338	GLU
1	F	339	LYS
1	F	343	GLU
1	F	345	ARG
1	F	352	GLN
1	F	357	THR
1	F	362	ARG
1	F	365	LEU
1	F	367	GLU
1	F	368	ARG
1	F	371	LYS
1	F	380	ARG
1	F	387	ILE
1	F	388	GLU
1	F	391	GLU
1	F	395	ARG
1	F	398	ASP
1	F	401	ASN
1	F	408	GLN
1	F	419	LEU
1	F	427	GLU
1	F	430	SER
1	F	434	SER
1	F	436	GLN
1	F	444	ARG
1	F	452	ARG
1	F	473	SER
1	F	524	GLU
1	F	525	LYS
1	G	5	GLU
1	G	7	LYS
1	G	10	SER

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Mol	Chain	Res	Type
1	G	16	MET
1	G	18	LYS
1	G	28	LYS
1	G	36	ARG
1	G	42	LYS
1	G	51	LYS
1	G	55	SER
1	G	69	MET
1	G	72	GLN
1	G	75	ARG
1	G	76	GLU
1	G	77	VAL
1	G	79	SER
1	G	80	ARG
1	G	83	ASP
1	G	87	ASP
1	G	105	LYS
1	G	132	LYS
1	G	139	ASN
1	G	141	SER
1	G	146	GLN
1	G	155	GLU
1	G	156	SER
1	G	164	GLU
1	G	166	MET
1	G	167	GLN
1	G	168	ARG
1	G	172	GLU
1	G	181	LYS
1	G	183	MET
1	G	196	ASP
1	G	197	ARG
1	G	204	PHE
1	G	206	THR
1	G	209	ASP
1	G	210	LYS
1	G	211	MET
1	G	214	GLU
1	G	216	GLU
1	G	217	ASP
1	G	221	LEU
1	G	222	LEU

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Mol	Chain	Res	Type
1	G	225	LYS
1	G	229	SER
1	G	231	GLN
1	G	245	LYS
1	G	247	LEU
1	G	250	VAL
1	G	252	GLU
1	G	253	ASP
1	G	281	PHE
1	G	283	ASP
1	G	288	MET
1	G	290	GLN
1	G	295	LEU
1	G	315	ASP
1	G	316	MET
1	G	317	LEU
1	G	321	LYS
1	G	322	LYS
1	G	327	LYS
1	G	328	ASP
1	G	333	VAL
1	G	338	GLU
1	G	339	LYS
1	G	343	GLU
1	G	345	ARG
1	G	352	GLN
1	G	357	THR
1	G	362	ARG
1	G	365	LEU
1	G	367	GLU
1	G	368	ARG
1	G	371	LYS
1	G	380	ARG
1	G	387	ILE
1	G	388	GLU
1	G	391	GLU
1	G	395	ARG
1	G	398	ASP
1	G	401	ASN
1	G	408	GLN
1	G	419	LEU
1	G	427	GLU

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Mol	Chain	Res	Type
1	G	430	SER
1	G	434	SER
1	G	436	GLN
1	G	444	ARG
1	G	452	ARG
1	G	473	SER
1	G	524	GLU
1	G	525	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	72	GLN
1	A	97	GLN
1	A	139	ASN
1	A	153	ASN
1	A	194	GLN
1	A	231	GLN
1	A	348	GLN
1	A	352	GLN
1	A	480	ASN
1	B	68	ASN
1	B	72	GLN
1	B	97	GLN
1	B	139	ASN
1	B	153	ASN
1	B	194	GLN
1	B	231	GLN
1	B	348	GLN
1	B	352	GLN
1	B	480	ASN
1	C	37	ASN
1	C	68	ASN
1	C	72	GLN
1	C	97	GLN
1	C	139	ASN
1	C	153	ASN
1	C	194	GLN
1	C	231	GLN
1	C	348	GLN
1	C	352	GLN

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Mol	Chain	Res	Type
1	C	480	ASN
1	D	68	ASN
1	D	72	GLN
1	D	139	ASN
1	D	153	ASN
1	D	194	GLN
1	D	231	GLN
1	D	348	GLN
1	D	352	GLN
1	D	480	ASN
1	E	68	ASN
1	E	72	GLN
1	E	97	GLN
1	E	139	ASN
1	E	153	ASN
1	E	231	GLN
1	E	348	GLN
1	E	352	GLN
1	E	480	ASN
1	F	68	ASN
1	F	72	GLN
1	F	97	GLN
1	F	139	ASN
1	F	153	ASN
1	F	194	GLN
1	F	231	GLN
1	F	348	GLN
1	F	352	GLN
1	F	480	ASN
1	G	68	ASN
1	G	72	GLN
1	G	97	GLN
1	G	139	ASN
1	G	153	ASN
1	G	194	GLN
1	G	231	GLN
1	G	348	GLN
1	G	352	GLN
1	G	480	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.