Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:37 AM EDT

PDB ID	:	1M3I
Title	:	Perfringolysin O, new crystal form
Authors	:	Rossjohn, J.; Parker, M.; Polekhina, G.; Feil, S.; Tweten, R.
Deposited on	:	2002-06-28
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

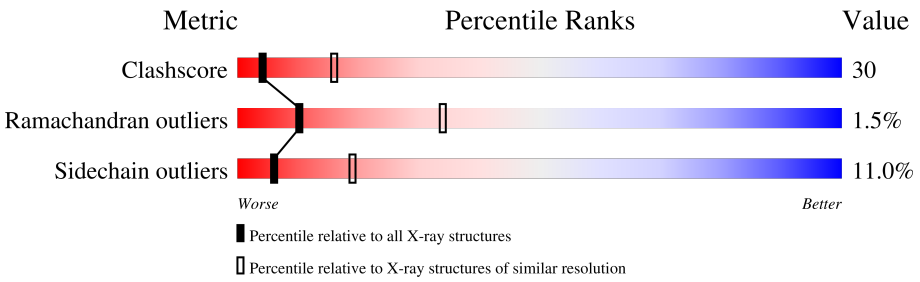
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	49% 44% 6% •
1	B	471	54% 39% 6% •
1	C	471	41% 49% 8% •
1	D	471	45% 47% 6% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14920 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 perfringolysin O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3657	2304	614	734	5	0	0	0
1	B	465	3657	2304	614	734	5	0	0	0
1	C	465	3657	2304	614	734	5	0	0	0
1	D	465	3657	2304	614	734	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	LEU	PHE	see remark 999	UNP P19995
B	114	LEU	PHE	see remark 999	UNP P19995
C	114	LEU	PHE	see remark 999	UNP P19995
D	114	LEU	PHE	see remark 999	UNP P19995

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	70	70	70	0	0
2	B	88	88	88	0	0
2	C	58	58	58	0	0
2	D	76	76	76	0	0

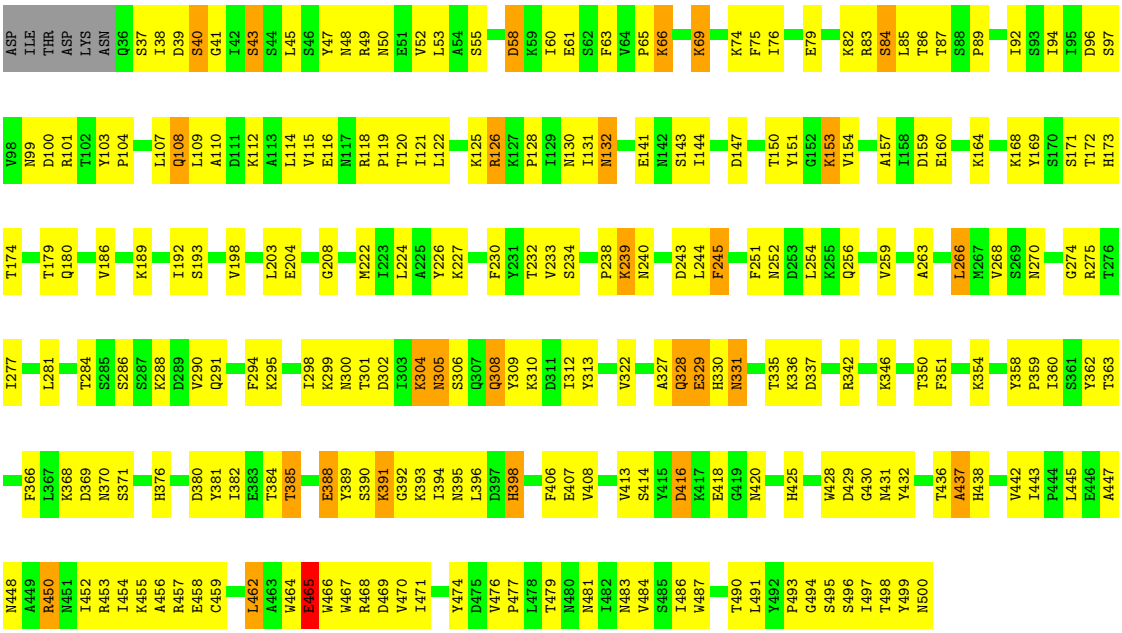
3 Residue-property plots (i)

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

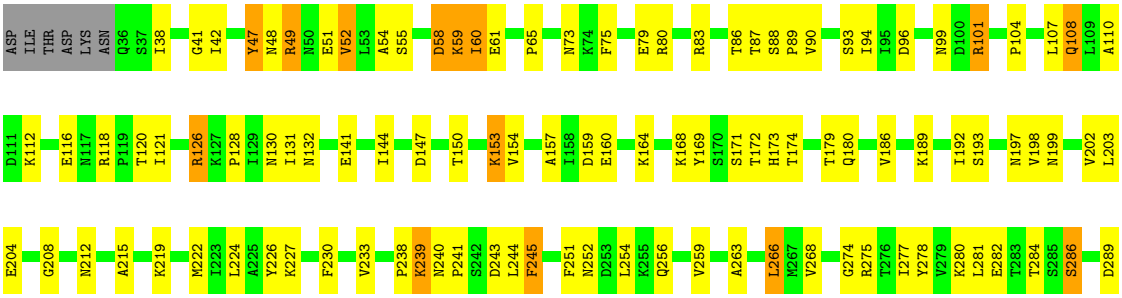
• Molecule 1: perfringolysin O

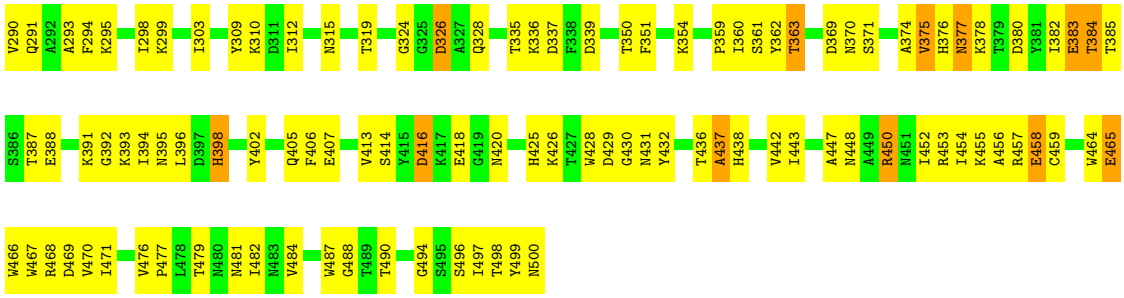
Chain A: 49% 44% 6% •



• Molecule 1: perfringolysin O

Chain B: 54% 39% 6% •



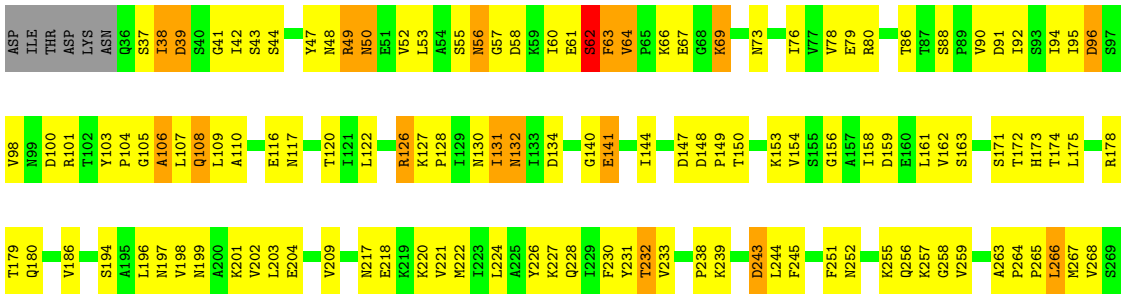


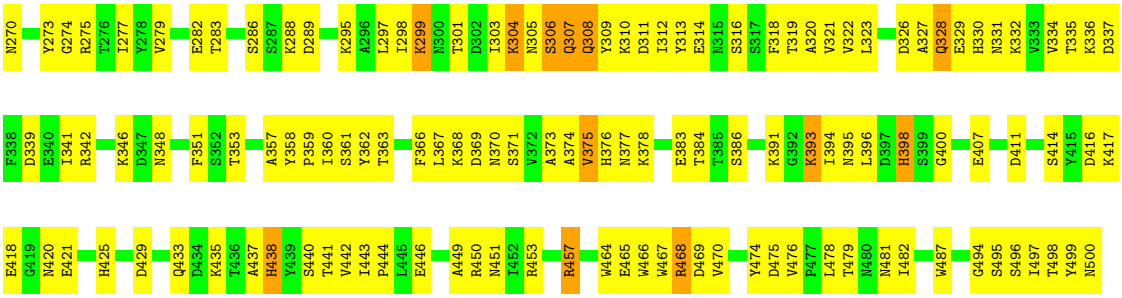
- Molecule 1: perfringolysin O

Chain C:

- Molecule 1: perfringolysin O

Chain D:




N270 Y273 G274 R275 T276 I277 Y278 V279 E282 T283 S286 S287 K288 D289 K295 A296 L297 I298 K299 N300 T301 D302 I303 K304 N305 S306 Q307 Q308 Y309 K310 D311 I312 Y313 E314 N315 S316 S317 F318 T319 A320 V321 V322 L323 D326 A327 Q328 E329 H330 N331 K332 V333 V334 T335 K336 D337
F338 D339 E340 I341 R342 K346 D347 N348 F351 S352 T353 A357 Y358 P359 I360 S361 Y362 T363 F366 L367 K368 D369 N370 S371 V372 A373 A374 V375 H376 N377 K378 E383 T384 T385 S386 K391 G392 K393 I394 N395 L396 D397 H398 S399 G400 E407 D411 S414 Y415 D416 K417
E418 G419 N420 E421 H425 D429 Q433 D434 K435 T436 A437 H438 Y439 S440 T441 V442 I443 P444 L445 E446 A449 R450 N451 I452 R453 R457 W464 E465 W466 W467 R468 D469 V470 Y474 D475 V476 P477 L478 T479 N480 N481 I482 W487 G494 S495 S496 I497 T498 Y499 N500

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	130.41Å 130.41Å 129.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	95.2 (20.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14920	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.35	0/3728	0.57	0/5062
1	B	0.36	0/3728	0.56	0/5062
1	C	0.37	0/3728	0.57	1/5062 (0.0%)
1	D	0.35	0/3728	0.56	0/5062
All	All	0.36	0/14912	0.57	1/20248 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	300	ASN	N-CA-C	6.46	128.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3657	0	3611	211	0
1	B	3657	0	3611	174	0
1	C	3657	0	3611	275	0
1	D	3657	0	3611	214	0
2	A	70	0	0	14	0
2	B	88	0	0	6	0
2	C	58	0	0	4	0
2	D	76	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14920	0	14444	860	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 30.

All (860) 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:A:335:THR:HG22	1:A:337:ASP:H	1.27	0.99
1:B:335:THR:HG22	1:B:337:ASP:H	1.28	0.98
1:A:87:THR:HG22	1:A:89:PRO:HD3	1.45	0.97
1:C:289:ASP:HB3	1:C:309:TYR:HE1	1.25	0.94
1:A:301:THR:O	1:A:304:LYS:HG3	1.68	0.94
1:C:296:ALA:HB2	1:C:303:ILE:HD13	1.52	0.91
1:C:82:LYS:HA	1:C:382:ILE:HA	1.50	0.91
1:D:457:ARG:HD2	1:D:469:ASP:OD2	1.71	0.90
1:A:109:LEU:HD21	1:A:122:LEU:HD21	1.53	0.89
1:A:104:PRO:HG2	1:A:131:ILE:HD11	1.54	0.88
1:C:481:ASN:HB2	1:C:500:ASN:HB2	1.56	0.88
1:D:481:ASN:HB2	1:D:500:ASN:HB2	1.56	0.87
1:C:457:ARG:HD2	1:C:469:ASP:OD2	1.75	0.87
1:C:90:VAL:HG12	1:C:374:ALA:HB2	1.58	0.86
1:A:481:ASN:HB2	1:A:500:ASN:HB2	1.58	0.85
1:C:66:LYS:HG3	1:C:79:GLU:HG3	1.59	0.85
1:D:457:ARG:HG3	1:D:468:ARG:O	1.78	0.84
1:A:222:MET:HE1	1:A:298:ILE:HD11	1.60	0.84
1:A:75:PHE:HB2	1:A:447:ALA:HB3	1.60	0.83
1:A:131:ILE:HG22	1:A:144:ILE:HG22	1.59	0.83
1:B:481:ASN:HB2	1:B:500:ASN:HB2	1.61	0.82
1:A:464:TRP:HA	1:A:467:TRP:CE3	2.14	0.82
1:B:456:ALA:HB3	1:B:471:ILE:HG22	1.61	0.82
1:B:465:GLU:OE2	1:D:91:ASP:HB2	1.79	0.82
1:C:259:VAL:HG13	1:C:265:PRO:HD3	1.61	0.82
1:D:259:VAL:HG13	1:D:265:PRO:HD3	1.62	0.82
1:B:131:ILE:HG22	1:B:144:ILE:HG22	1.59	0.81
1:A:456:ALA:HB3	1:A:471:ILE:HG22	1.60	0.81
1:D:110:ALA:HB2	1:D:266:LEU:HD21	1.63	0.81
1:A:37:SER:HB3	1:A:40:SER:OG	1.80	0.80
1:A:288:LYS:HB2	2:A:542:HOH:O	1.81	0.80
1:D:429:ASP:HB3	2:D:553:HOH:O	1.81	0.80
1:C:457:ARG:HG3	1:C:468:ARG:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ALA:HB2	1:C:266:LEU:HD21	1.65	0.79
1:B:73:ASN:HA	1:B:391:LYS:HE2	1.64	0.78
1:B:457:ARG:HD2	1:B:469:ASP:OD2	1.84	0.78
1:D:69:LYS:HG3	1:D:76:ILE:HB	1.65	0.77
1:A:458:GLU:OE2	1:A:490:THR:HG23	1.85	0.77
1:A:75:PHE:CE1	1:A:448:ASN:HB3	2.20	0.77
1:C:289:ASP:HB2	1:C:308:GLN:NE2	2.00	0.76
1:C:275:ARG:HB3	1:C:325:GLY:H	1.50	0.76
1:B:458:GLU:OE2	1:B:490:THR:HG23	1.86	0.76
1:D:335:THR:HG22	1:D:337:ASP:H	1.49	0.76
1:D:61:GLU:HG3	1:D:62:SER:H	1.50	0.75
1:C:39:ASP:OD1	1:C:240:ASN:HB3	1.86	0.75
1:C:44:SER:HA	1:C:368:LYS:HZ2	1.50	0.75
1:C:37:SER:O	1:C:251:PHE:HB2	1.86	0.75
1:D:80:ARG:HG2	1:D:384:THR:HG22	1.69	0.74
1:A:126:ARG:HB2	1:A:244:LEU:O	1.87	0.74
1:D:37:SER:O	1:D:251:PHE:HB2	1.86	0.74
1:C:335:THR:HG22	1:C:337:ASP:H	1.51	0.74
1:C:108:GLN:HG2	1:C:121:ILE:HD13	1.69	0.73
1:D:61:GLU:CG	1:D:62:SER:H	2.01	0.73
1:B:86:THR:OG1	1:B:378:LYS:HG3	1.88	0.73
1:D:88:SER:HA	1:D:375:VAL:O	1.88	0.73
1:A:55:SER:HB3	1:A:115:VAL:HG13	1.69	0.73
1:B:126:ARG:HB2	1:B:244:LEU:O	1.88	0.73
1:C:105:GLY:O	1:C:267:MET:HG3	1.89	0.73
1:C:64:VAL:HB	1:C:80:ARG:NH1	2.03	0.72
1:A:469:ASP:OD2	1:C:180:GLN:HA	1.89	0.72
1:C:36:GLN:O	1:C:251:PHE:HB3	1.89	0.72
1:D:295:LYS:HD2	2:D:539:HOH:O	1.90	0.72
1:D:312:ILE:H	1:D:312:ILE:HD12	1.55	0.71
1:A:252:ASN:O	1:A:256:GLN:HB2	1.90	0.71
1:A:457:ARG:HB2	1:A:464:TRP:CZ3	2.25	0.71
1:C:107:LEU:HD11	1:C:126:ARG:HH21	1.55	0.71
1:C:44:SER:HA	1:C:368:LYS:NZ	2.04	0.71
1:B:464:TRP:HA	1:B:467:TRP:CE3	2.25	0.71
1:A:384:THR:HG22	1:A:385:THR:N	2.06	0.71
1:A:39:ASP:O	1:A:43:SER:HB2	1.90	0.71
1:C:109:LEU:HD21	1:C:122:LEU:HD11	1.72	0.70
1:A:66:LYS:HB2	1:A:66:LYS:NZ	2.05	0.70
1:B:252:ASN:O	1:B:256:GLN:HB2	1.90	0.70
1:D:37:SER:C	1:D:251:PHE:HB2	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:LYS:HE2	1:D:446:GLU:OE1	1.92	0.70
1:C:87:THR:HG22	1:C:89:PRO:HD3	1.73	0.70
1:D:127:LYS:HG3	1:D:245:PHE:O	1.92	0.70
1:B:222:MET:HE3	1:B:298:ILE:HD11	1.72	0.70
1:C:105:GLY:H	1:C:268:VAL:HB	1.56	0.70
1:B:286:SER:HB2	1:B:388:GLU:HB3	1.73	0.69
1:D:322:VAL:HG21	1:D:327:ALA:HB1	1.73	0.69
1:D:94:ILE:HD13	1:D:359:PRO:HB2	1.74	0.69
1:A:342:ARG:HD3	2:A:503:HOH:O	1.92	0.69
1:C:89:PRO:C	1:C:91:ASP:H	1.95	0.69
1:C:98:VAL:HG21	1:C:329:GLU:OE2	1.92	0.69
1:D:322:VAL:CG2	1:D:331:ASN:HB3	2.23	0.69
1:A:84:SER:HB2	1:A:380:ASP:OD2	1.93	0.68
1:C:49:ARG:HD3	2:C:505:HOH:O	1.93	0.68
1:A:131:ILE:CG2	1:A:144:ILE:HG22	2.23	0.68
1:D:60:ILE:HG22	1:D:61:GLU:N	2.08	0.68
1:A:310:LYS:HA	1:A:310:LYS:HE2	1.75	0.68
1:B:131:ILE:CG2	1:B:144:ILE:HG22	2.24	0.68
1:A:48:ASN:O	1:A:52:VAL:HG13	1.94	0.68
1:C:127:LYS:HG3	1:C:245:PHE:O	1.93	0.68
1:C:104:PRO:HD2	1:C:154:VAL:HG11	1.75	0.68
1:C:289:ASP:HB3	1:C:309:TYR:CE1	2.18	0.68
1:A:131:ILE:HG12	1:A:233:VAL:HG12	1.76	0.67
1:C:418:GLU:HB2	1:C:420:ASN:ND2	2.08	0.67
1:A:222:MET:HE1	1:A:298:ILE:CD1	2.23	0.67
1:C:83:ARG:HB2	1:C:381:TYR:CE1	2.29	0.67
1:D:418:GLU:HB2	1:D:420:ASN:ND2	2.09	0.67
1:C:134:ASP:OD1	1:C:232:THR:HG23	1.95	0.67
1:B:90:VAL:O	1:B:363:THR:HG22	1.94	0.67
1:A:96:ASP:OD2	1:A:99:ASN:HB2	1.95	0.67
1:A:462:LEU:HD11	1:C:232:THR:OG1	1.95	0.67
1:C:53:LEU:HD13	1:C:115:VAL:HG22	1.75	0.67
1:B:198:VAL:HG21	1:B:203:LEU:HD21	1.77	0.66
1:D:134:ASP:OD1	1:D:232:THR:HG23	1.96	0.66
1:D:398:HIS:O	1:D:438:HIS:HA	1.96	0.66
1:D:319:THR:HG23	1:D:334:VAL:HG22	1.75	0.66
1:A:55:SER:HB3	1:A:115:VAL:CG1	2.25	0.66
1:A:109:LEU:HD12	2:A:554:HOH:O	1.95	0.66
1:B:90:VAL:HG12	1:B:374:ALA:HB2	1.77	0.66
1:B:295:LYS:HE2	1:B:299:LYS:NZ	2.11	0.66
1:C:335:THR:HG22	1:C:336:LYS:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:HG2	1:B:61:GLU:O	1.96	0.66
1:D:52:VAL:HB	2:D:568:HOH:O	1.95	0.65
1:C:278:TYR:HE1	1:C:323:LEU:HD22	1.61	0.65
1:D:94:ILE:HG13	1:D:361:SER:HA	1.77	0.65
1:B:131:ILE:HG12	1:B:233:VAL:HG12	1.79	0.65
1:D:335:THR:HG22	1:D:336:LYS:H	1.60	0.65
1:C:80:ARG:HH11	1:C:80:ARG:HG3	1.61	0.65
1:D:61:GLU:HG3	1:D:62:SER:N	2.12	0.65
1:A:346:LYS:HG3	2:A:527:HOH:O	1.97	0.65
1:B:369:ASP:OD2	1:B:371:SER:HB3	1.96	0.65
1:C:398:HIS:O	1:C:438:HIS:HA	1.96	0.65
1:B:222:MET:HE1	1:B:294:PHE:HB3	1.79	0.64
1:D:396:LEU:HB2	1:D:441:THR:HG22	1.80	0.64
1:A:66:LYS:HB2	1:A:66:LYS:HZ3	1.62	0.64
1:B:107:LEU:HD11	1:B:126:ARG:HH21	1.61	0.64
1:C:103:TYR:CD1	1:C:154:VAL:HG21	2.32	0.64
1:D:94:ILE:CD1	1:D:359:PRO:HB2	2.26	0.64
1:A:75:PHE:CD1	1:A:448:ASN:HB3	2.32	0.64
1:B:426:LYS:HD2	2:B:548:HOH:O	1.98	0.64
1:C:199:ASN:HB3	1:C:202:VAL:HG23	1.80	0.64
1:A:198:VAL:HG21	1:A:203:LEU:HD21	1.79	0.64
1:A:398:HIS:O	1:A:438:HIS:HA	1.97	0.64
1:C:308:GLN:NE2	1:C:312:ILE:HD11	2.12	0.64
1:A:395:ASN:HD22	1:A:442:VAL:HG22	1.61	0.64
1:D:148:ASP:HB3	1:D:153:LYS:HE2	1.80	0.64
1:D:335:THR:HG22	1:D:336:LYS:N	2.12	0.64
1:C:64:VAL:HB	1:C:80:ARG:HH12	1.63	0.64
1:A:491:LEU:HD22	1:C:176:PRO:HG2	1.80	0.64
1:C:191:GLN:HA	1:C:379:THR:HG21	1.80	0.64
1:C:61:GLU:HA	1:C:61:GLU:OE1	1.97	0.64
1:A:395:ASN:ND2	1:A:442:VAL:HG22	2.13	0.63
1:B:476:VAL:HG13	1:B:499:TYR:OH	1.98	0.63
1:D:322:VAL:O	1:D:323:LEU:HD23	1.98	0.63
1:B:395:ASN:HD22	1:B:442:VAL:HG22	1.62	0.63
1:C:293:ALA:HB2	1:C:309:TYR:CD1	2.34	0.63
1:D:199:ASN:HB3	1:D:202:VAL:HG23	1.80	0.63
1:B:80:ARG:HD3	1:B:382:ILE:HG21	1.79	0.63
1:A:396:LEU:HD23	1:A:484:VAL:HB	1.81	0.62
1:C:217:ASN:ND2	1:C:384:THR:HB	2.14	0.62
1:C:289:ASP:HB2	1:C:308:GLN:CD	2.19	0.62
1:B:398:HIS:O	1:B:438:HIS:HA	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:OG1	1:A:153:LYS:HB2	1.99	0.62
1:A:369:ASP:OD2	1:A:371:SER:HB3	1.99	0.62
1:A:302:ASP:HA	1:A:304:LYS:HE3	1.80	0.62
1:C:335:THR:HG22	1:C:336:LYS:N	2.14	0.62
1:D:63:PHE:N	1:D:63:PHE:CD2	2.68	0.62
1:C:97:SER:O	1:C:358:TYR:HB3	2.00	0.62
1:A:295:LYS:HE2	1:A:299:LYS:NZ	2.14	0.61
1:A:304:LYS:HD2	1:A:304:LYS:N	2.15	0.61
1:B:395:ASN:ND2	1:B:442:VAL:HG22	2.14	0.61
1:B:173:HIS:HB2	1:B:354:LYS:HG3	1.82	0.61
1:C:191:GLN:HG3	1:C:381:TYR:CD2	2.35	0.61
1:C:227:LYS:HE3	1:C:360:ILE:HG22	1.81	0.61
1:C:296:ALA:HB2	1:C:303:ILE:CD1	2.27	0.61
1:D:116:GLU:O	1:D:117:ASN:HB2	2.00	0.61
1:D:196:LEU:O	1:D:198:VAL:HG13	2.01	0.61
1:B:315:ASN:HB2	2:B:561:HOH:O	2.01	0.61
1:B:326:ASP:OD1	1:B:326:ASP:N	2.33	0.61
1:B:396:LEU:HD23	1:B:484:VAL:HB	1.82	0.61
1:A:335:THR:HG22	1:A:336:LYS:N	2.15	0.61
1:B:222:MET:CE	1:B:298:ILE:HD11	2.31	0.61
1:A:157:ALA:O	1:A:160:GLU:HB2	2.00	0.61
1:A:470:VAL:HG12	1:A:495:SER:HB3	1.83	0.61
1:C:75:PHE:O	1:C:389:TYR:HB2	2.01	0.61
1:A:125:LYS:HE3	2:A:504:HOH:O	1.99	0.60
1:A:335:THR:HG22	1:A:336:LYS:H	1.66	0.60
1:A:254:LEU:HB3	1:A:259:VAL:HG21	1.84	0.60
1:C:148:ASP:HB3	1:C:153:LYS:HE2	1.83	0.60
1:A:173:HIS:HB2	1:A:354:LYS:HG3	1.83	0.60
1:B:324:GLY:HA3	2:B:501:HOH:O	2.01	0.60
1:C:172:THR:HG22	1:C:174:THR:H	1.66	0.60
1:C:196:LEU:O	1:C:198:VAL:HG13	2.01	0.60
1:C:308:GLN:HG3	1:C:309:TYR:N	2.15	0.60
1:C:222:MET:HE1	1:C:298:ILE:HD11	1.83	0.60
1:B:131:ILE:HG22	1:B:144:ILE:CG2	2.30	0.60
1:C:37:SER:C	1:C:251:PHE:HB2	2.23	0.60
1:C:53:LEU:HD22	1:C:115:VAL:HG23	1.84	0.60
1:D:98:VAL:HG21	1:D:329:GLU:HG2	1.83	0.60
1:A:37:SER:C	1:A:251:PHE:HB2	2.23	0.59
1:A:476:VAL:HG13	1:A:499:TYR:OH	2.01	0.59
1:D:172:THR:HG22	1:D:174:THR:H	1.66	0.59
1:C:80:ARG:HD3	1:C:384:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ILE:HG13	1:C:96:ASP:H	1.66	0.59
1:C:351:PHE:HE2	2:C:535:HOH:O	1.83	0.59
1:D:78:VAL:HG11	1:D:217:ASN:HD21	1.67	0.59
1:A:119:PRO:HD3	2:A:502:HOH:O	2.03	0.59
1:A:131:ILE:HG22	1:A:144:ILE:CG2	2.31	0.59
1:B:457:ARG:HB2	1:B:464:TRP:CZ3	2.36	0.59
1:A:222:MET:CE	1:A:298:ILE:HD11	2.30	0.59
1:A:328:GLN:CG	1:A:329:GLU:H	2.16	0.59
1:B:150:THR:OG1	1:B:153:LYS:HB2	2.03	0.59
1:B:487:TRP:CH2	1:B:496:SER:HB3	2.36	0.59
1:C:81:GLN:C	1:C:382:ILE:HG13	2.23	0.59
1:A:487:TRP:CH2	1:A:496:SER:HB3	2.38	0.59
1:A:45:LEU:O	1:A:368:LYS:NZ	2.32	0.59
1:A:418:GLU:HB2	1:A:420:ASN:ND2	2.17	0.59
1:A:128:PRO:HB3	1:A:147:ASP:HA	1.85	0.58
1:A:384:THR:CG2	1:A:385:THR:N	2.66	0.58
1:B:335:THR:HG22	1:B:336:LYS:N	2.18	0.58
1:C:47:TYR:CD1	1:C:52:VAL:HG11	2.38	0.58
1:C:82:LYS:HD2	1:C:380:ASP:HB3	1.84	0.58
1:D:337:ASP:OD1	1:D:339:ASP:HB2	2.04	0.58
1:C:45:LEU:H	1:C:368:LYS:HZ2	1.50	0.58
1:D:140:GLY:O	1:D:141:GLU:HG3	2.03	0.58
1:A:101:ARG:HG2	2:A:546:HOH:O	2.03	0.58
1:A:391:LYS:HB3	1:A:445:LEU:O	2.04	0.58
1:B:157:ALA:O	1:B:160:GLU:HB2	2.04	0.58
1:C:186:VAL:HG23	1:C:221:VAL:O	2.04	0.58
1:A:75:PHE:HB2	1:A:447:ALA:CB	2.33	0.58
1:B:108:GLN:HE21	1:B:121:ILE:CD1	2.16	0.58
1:C:116:GLU:O	1:C:117:ASN:HB2	2.03	0.58
1:D:416:ASP:OD2	1:D:420:ASN:HB2	2.04	0.58
1:D:453:ARG:NH2	2:D:515:HOH:O	2.35	0.58
1:B:477:PRO:O	1:B:479:THR:HG23	2.04	0.58
1:C:286:SER:OG	1:C:386:SER:HB3	2.04	0.58
1:D:275:ARG:HA	1:D:360:ILE:HD11	1.85	0.58
1:A:41:GLY:HA3	1:A:251:PHE:CD1	2.39	0.57
1:B:254:LEU:HB3	1:B:259:VAL:HG21	1.86	0.57
1:C:158:ILE:O	1:C:162:VAL:HG23	2.03	0.57
1:D:61:GLU:CG	1:D:62:SER:N	2.66	0.57
1:D:109:LEU:HD22	1:D:263:ALA:O	2.03	0.57
1:D:147:ASP:O	1:D:149:PRO:HD3	2.04	0.57
1:A:464:TRP:HA	1:A:467:TRP:CZ3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:MET:HE3	1:B:298:ILE:CD1	2.34	0.57
1:C:140:GLY:O	1:C:141:GLU:HG3	2.04	0.57
1:D:275:ARG:NH1	1:D:326:ASP:HB2	2.19	0.57
1:A:60:ILE:HG13	1:A:61:GLU:N	2.20	0.57
1:B:418:GLU:HB2	1:B:420:ASN:ND2	2.19	0.57
1:C:279:VAL:HA	1:C:319:THR:O	2.03	0.57
1:C:337:ASP:OD1	1:C:339:ASP:HB2	2.04	0.57
1:C:498:THR:HG22	1:C:499:TYR:N	2.19	0.57
1:B:295:LYS:HE2	1:B:299:LYS:HZ1	1.68	0.57
1:A:498:THR:HG22	1:A:499:TYR:N	2.19	0.57
1:C:252:ASN:O	1:C:256:GLN:HB2	2.04	0.57
1:C:416:ASP:OD2	1:C:420:ASN:HB2	2.04	0.57
1:A:222:MET:HE2	1:A:294:PHE:HB3	1.87	0.57
1:C:89:PRO:HD2	1:C:375:VAL:HG13	1.87	0.57
1:C:91:ASP:O	1:C:92:ILE:HG13	2.05	0.57
1:C:128:PRO:HB3	1:C:147:ASP:HA	1.87	0.57
1:C:175:LEU:HB2	1:C:351:PHE:CZ	2.40	0.57
1:B:458:GLU:CD	1:B:490:THR:HG23	2.25	0.57
1:D:128:PRO:HB3	1:D:147:ASP:HA	1.87	0.57
1:A:172:THR:HG22	1:A:174:THR:H	1.70	0.57
1:C:45:LEU:HD23	1:C:261:ASN:OD1	2.05	0.57
1:C:147:ASP:O	1:C:149:PRO:HD3	2.04	0.57
1:D:222:MET:HE1	1:D:298:ILE:HD11	1.86	0.57
1:D:230:PHE:HB3	1:D:351:PHE:CE1	2.40	0.57
1:B:454:ILE:HG21	1:B:484:VAL:HG21	1.86	0.56
1:D:127:LYS:N	1:D:244:LEU:O	2.36	0.56
1:C:323:LEU:HD23	1:C:323:LEU:O	2.05	0.56
1:D:158:ILE:O	1:D:162:VAL:HG23	2.05	0.56
1:D:230:PHE:CE2	1:D:274:GLY:HA2	2.40	0.56
1:A:103:TYR:CD1	1:A:154:VAL:HG21	2.40	0.56
1:A:335:THR:HG22	1:A:337:ASP:N	2.10	0.56
1:B:128:PRO:HB3	1:B:147:ASP:HA	1.88	0.56
1:B:487:TRP:HH2	1:B:496:SER:HB3	1.68	0.56
1:C:396:LEU:HB2	1:C:441:THR:HG22	1.86	0.56
1:D:107:LEU:HD11	1:D:126:ARG:HH21	1.70	0.56
1:D:498:THR:HG22	1:D:499:TYR:N	2.19	0.56
1:A:477:PRO:O	1:A:479:THR:HG23	2.05	0.56
1:C:90:VAL:HA	1:C:374:ALA:HA	1.88	0.56
1:D:175:LEU:HB2	1:D:351:PHE:CE2	2.40	0.56
1:B:454:ILE:HD13	1:B:484:VAL:HG21	1.88	0.56
1:C:382:ILE:O	1:C:382:ILE:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ARG:NH1	1:C:80:ARG:HG3	2.20	0.56
1:D:175:LEU:HB2	1:D:351:PHE:CZ	2.40	0.56
1:B:335:THR:HG22	1:B:336:LYS:H	1.70	0.56
1:C:230:PHE:HB3	1:C:351:PHE:CE1	2.41	0.56
1:D:252:ASN:O	1:D:256:GLN:HB2	2.06	0.56
1:A:454:ILE:HG21	1:A:484:VAL:HG21	1.88	0.56
1:C:230:PHE:CE2	1:C:274:GLY:HA2	2.41	0.56
1:A:52:VAL:HG23	1:A:53:LEU:N	2.20	0.55
1:A:416:ASP:OD2	1:A:420:ASN:HB2	2.06	0.55
1:B:263:ALA:HB2	2:B:563:HOH:O	2.06	0.55
1:C:320:ALA:HB3	1:C:333:VAL:HB	1.89	0.55
1:A:92:ILE:HD12	1:A:362:TYR:O	2.06	0.55
1:C:98:VAL:HG12	1:C:358:TYR:CD1	2.41	0.55
1:D:60:ILE:CG2	1:D:61:GLU:N	2.69	0.55
1:B:416:ASP:OD2	1:B:420:ASN:HB2	2.06	0.55
1:C:479:THR:HB	1:C:500:ASN:O	2.07	0.55
1:A:108:GLN:HA	1:A:120:THR:O	2.06	0.55
1:A:322:VAL:H	1:A:331:ASN:ND2	2.03	0.55
1:A:487:TRP:HH2	1:A:496:SER:HB3	1.70	0.55
1:D:321:VAL:HG12	1:D:332:LYS:HA	1.89	0.55
1:C:86:THR:HG23	1:C:378:LYS:HG2	1.88	0.55
1:A:49:ARG:NH2	2:A:517:HOH:O	2.40	0.55
1:B:498:THR:HG22	1:B:499:TYR:N	2.21	0.55
1:C:198:VAL:HG21	1:C:203:LEU:HD21	1.88	0.55
1:A:87:THR:CG2	1:A:89:PRO:HD3	2.29	0.55
1:C:127:LYS:N	1:C:244:LEU:O	2.35	0.55
1:C:39:ASP:OD2	1:C:242:SER:N	2.39	0.55
1:D:186:VAL:HG23	1:D:221:VAL:O	2.06	0.55
1:D:303:ILE:O	1:D:306:SER:HB3	2.07	0.55
1:A:306:SER:HB3	1:A:308:GLN:HG3	1.88	0.54
1:B:204:GLU:O	1:B:208:GLY:HA2	2.07	0.54
1:C:97:SER:O	1:C:359:PRO:HD2	2.06	0.54
1:D:49:ARG:HB3	1:D:366:PHE:CE1	2.43	0.54
1:D:64:VAL:HG12	1:D:417:LYS:O	2.06	0.54
1:D:95:ILE:HG13	1:D:117:ASN:HD22	1.72	0.54
1:A:335:THR:CG2	1:A:337:ASP:H	2.11	0.54
1:C:175:LEU:HB2	1:C:351:PHE:CE2	2.41	0.54
1:D:179:THR:HB	2:D:562:HOH:O	2.06	0.54
1:A:428:TRP:HA	2:A:544:HOH:O	2.07	0.54
1:D:69:LYS:O	1:D:76:ILE:N	2.39	0.54
1:D:103:TYR:HB2	1:D:104:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:GLN:O	1:D:435:LYS:HG2	2.07	0.54
1:A:304:LYS:HD2	1:A:304:LYS:H	1.72	0.54
1:C:73:ASN:HA	1:C:391:LYS:HD2	1.88	0.54
1:C:308:GLN:HE21	1:C:312:ILE:HD11	1.71	0.54
1:D:57:GLY:HA3	1:D:378:LYS:O	2.07	0.54
1:D:309:TYR:HA	1:D:312:ILE:HD13	1.89	0.54
1:B:94:ILE:HD13	1:B:359:PRO:HB2	1.88	0.54
1:C:53:LEU:HG	1:C:114:LEU:HD23	1.88	0.54
1:D:39:ASP:OD2	1:D:39:ASP:N	2.41	0.54
1:D:198:VAL:HG21	1:D:203:LEU:HD21	1.88	0.54
1:A:47:TYR:CD1	1:A:52:VAL:HG11	2.42	0.54
1:C:98:VAL:HG12	1:C:358:TYR:CE1	2.43	0.54
1:A:470:VAL:HG11	1:A:486:ILE:HB	1.89	0.54
1:C:131:ILE:HG22	1:C:144:ILE:HG22	1.90	0.54
1:A:458:GLU:CD	1:A:490:THR:HG23	2.27	0.54
1:B:172:THR:HG22	1:B:174:THR:H	1.73	0.54
1:B:289:ASP:HB3	1:B:309:TYR:HE1	1.72	0.54
1:C:227:LYS:HZ1	1:C:361:SER:CB	2.21	0.54
1:D:105:GLY:N	1:D:268:VAL:O	2.36	0.54
1:D:328:GLN:O	1:D:331:ASN:HB2	2.08	0.54
1:D:109:LEU:HD22	1:D:263:ALA:HB1	1.90	0.54
1:A:110:ALA:HB2	1:A:266:LEU:HD21	1.91	0.53
1:C:89:PRO:C	1:C:91:ASP:N	2.62	0.53
1:A:328:GLN:HG2	1:A:329:GLU:HG2	1.90	0.53
1:D:90:VAL:HG12	1:D:374:ALA:HB2	1.89	0.53
1:A:310:LYS:HE2	1:A:313:TYR:HD1	1.72	0.53
1:D:78:VAL:HG11	1:D:217:ASN:ND2	2.24	0.53
1:C:47:TYR:HB2	1:C:52:VAL:CG1	2.38	0.53
1:C:53:LEU:CD2	1:C:115:VAL:HG23	2.39	0.53
1:C:191:GLN:CA	1:C:379:THR:HG21	2.38	0.53
1:D:86:THR:HA	1:D:377:ASN:O	2.07	0.53
1:D:109:LEU:HD12	1:D:120:THR:HG21	1.89	0.53
1:C:85:LEU:C	1:C:85:LEU:HD23	2.29	0.53
1:C:100:ASP:C	1:C:102:THR:H	2.12	0.53
1:A:396:LEU:HD11	1:A:443:ILE:HD11	1.90	0.53
2:A:541:HOH:O	1:C:462:LEU:HD22	2.08	0.53
1:D:479:THR:HB	1:D:500:ASN:O	2.08	0.53
1:C:83:ARG:N	1:C:381:TYR:O	2.40	0.53
1:A:63:PHE:O	1:A:65:PRO:HD3	2.08	0.53
1:C:110:ALA:HB2	1:C:266:LEU:CD2	2.38	0.53
1:C:217:ASN:HD21	1:C:384:THR:HB	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:TYR:O	1:C:295:LYS:NZ	2.42	0.52
1:D:67:GLU:HG2	1:D:69:LYS:HD3	1.90	0.52
1:B:141:GLU:HB3	1:B:164:LYS:HE2	1.92	0.52
1:D:369:ASP:OD2	1:D:371:SER:HB3	2.09	0.52
1:C:79:GLU:HB2	1:C:385:THR:OG1	2.10	0.52
1:D:304:LYS:O	1:D:313:TYR:HE1	1.91	0.52
1:B:131:ILE:HD12	1:B:154:VAL:HG13	1.92	0.52
1:C:38:ILE:HD12	1:C:242:SER:HB3	1.91	0.52
1:C:148:ASP:H	1:C:153:LYS:HE2	1.75	0.52
1:C:265:PRO:HB2	1:C:367:LEU:HD12	1.91	0.52
1:C:465:GLU:CD	1:C:465:GLU:H	2.12	0.52
1:A:484:VAL:HG22	1:A:497:ILE:HD12	1.92	0.52
1:C:433:GLN:O	1:C:435:LYS:HG2	2.10	0.52
1:B:59:LYS:HD2	1:B:59:LYS:N	2.24	0.52
1:B:89:PRO:HD2	1:B:375:VAL:O	2.10	0.52
1:B:396:LEU:HD11	1:B:443:ILE:HD11	1.91	0.52
1:C:53:LEU:HD22	1:C:115:VAL:CG2	2.40	0.52
1:C:280:LYS:O	1:C:318:PHE:HA	2.10	0.52
1:A:392:GLY:HA3	1:A:479:THR:O	2.10	0.52
1:B:60:ILE:HG23	1:B:60:ILE:O	2.09	0.52
1:B:335:THR:HG22	1:B:337:ASP:N	2.11	0.52
1:B:459:CYS:HA	1:B:467:TRP:CE2	2.45	0.52
1:B:179:THR:HA	1:B:227:LYS:O	2.10	0.52
1:A:350:THR:CG2	1:A:351:PHE:N	2.72	0.52
1:B:392:GLY:HA3	1:B:479:THR:O	2.10	0.52
1:C:53:LEU:HD21	1:C:111:ASP:O	2.10	0.52
1:A:38:ILE:HG12	1:A:254:LEU:HD11	1.90	0.51
1:C:95:ILE:HG23	1:C:117:ASN:HD22	1.75	0.51
1:C:369:ASP:OD2	1:C:371:SER:HB3	2.09	0.51
1:D:131:ILE:HG22	1:D:144:ILE:HG22	1.92	0.51
1:A:457:ARG:HD2	1:A:469:ASP:OD1	2.11	0.51
1:C:61:GLU:HG3	1:C:62:SER:N	2.26	0.51
1:C:310:LYS:NZ	1:C:314:GLU:HG3	2.25	0.51
1:B:107:LEU:CD1	1:B:126:ARG:HH21	2.22	0.51
1:B:464:TRP:HA	1:B:467:TRP:CZ3	2.45	0.51
1:C:302:ASP:OD1	1:C:302:ASP:N	2.42	0.51
1:D:110:ALA:HB2	1:D:266:LEU:CD2	2.36	0.51
1:D:148:ASP:H	1:D:153:LYS:HE2	1.74	0.51
1:D:265:PRO:HB2	1:D:367:LEU:HD12	1.92	0.51
1:D:308:GLN:CA	1:D:308:GLN:HE21	2.24	0.51
1:C:265:PRO:HG2	1:C:367:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:HD13	1:A:484:VAL:HG21	1.93	0.51
1:B:350:THR:CG2	1:B:351:PHE:N	2.73	0.51
1:D:63:PHE:N	1:D:63:PHE:HD2	2.09	0.51
1:D:358:TYR:HB3	1:D:359:PRO:HD2	1.91	0.51
1:A:452:ILE:HD12	1:A:476:VAL:O	2.11	0.51
1:B:293:ALA:HB2	1:B:309:TYR:CD1	2.46	0.51
1:C:100:ASP:HB3	1:C:102:THR:OG1	2.10	0.51
1:A:222:MET:HE3	1:A:281:LEU:HD13	1.93	0.51
1:A:239:LYS:HG3	1:A:240:ASN:ND2	2.26	0.51
1:A:458:GLU:HG2	1:A:459:CYS:H	1.75	0.51
1:D:148:ASP:CB	1:D:153:LYS:HE2	2.40	0.51
1:B:239:LYS:HG3	1:B:240:ASN:ND2	2.26	0.51
1:B:484:VAL:HG22	1:B:497:ILE:HD12	1.91	0.51
1:D:55:SER:OG	1:D:377:ASN:HA	2.10	0.51
1:A:491:LEU:HD22	1:C:176:PRO:CG	2.40	0.51
1:C:104:PRO:HD2	1:C:154:VAL:CG1	2.40	0.51
1:D:238:PRO:HG3	1:D:244:LEU:HG	1.93	0.51
1:B:458:GLU:O	1:B:467:TRP:HB3	2.11	0.51
1:C:36:GLN:C	1:C:251:PHE:HB3	2.31	0.51
1:C:80:ARG:HD3	1:C:384:THR:HG21	1.93	0.51
1:C:89:PRO:O	1:C:91:ASP:N	2.44	0.51
1:D:144:ILE:HB	1:D:161:LEU:HD21	1.93	0.51
1:A:141:GLU:HB3	1:A:164:LYS:HE2	1.92	0.50
1:A:407:GLU:HG3	1:A:432:TYR:CZ	2.46	0.50
1:A:470:VAL:HG22	1:A:493:PRO:CB	2.41	0.50
1:B:107:LEU:CG	1:B:126:ARG:HH21	2.24	0.50
1:C:80:ARG:HG2	1:C:384:THR:HG22	1.93	0.50
1:C:275:ARG:HA	1:C:360:ILE:HD11	1.93	0.50
1:A:368:LYS:NZ	2:A:551:HOH:O	2.44	0.50
1:B:55:SER:OG	1:B:377:ASN:HB2	2.11	0.50
1:C:41:GLY:O	1:C:45:LEU:HD12	2.11	0.50
1:C:108:GLN:HB2	1:C:266:LEU:HD12	1.93	0.50
1:A:350:THR:HG22	1:A:351:PHE:N	2.25	0.50
1:B:498:THR:HG22	1:B:499:TYR:H	1.76	0.50
1:B:110:ALA:HB2	1:B:266:LEU:HD21	1.94	0.50
1:C:47:TYR:HB2	1:C:52:VAL:HG11	1.94	0.50
1:C:321:VAL:HG23	1:C:321:VAL:O	2.11	0.50
1:D:398:HIS:CE1	1:D:400:GLY:H	2.30	0.50
1:D:230:PHE:HZ	1:D:275:ARG:NH1	2.10	0.50
1:D:270:ASN:O	1:D:362:TYR:HB2	2.12	0.50
1:A:37:SER:O	1:A:251:PHE:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:HG22	1:B:351:PHE:N	2.26	0.50
1:B:452:ILE:HD12	1:B:476:VAL:O	2.12	0.50
1:C:95:ILE:HG23	1:C:117:ASN:HB3	1.94	0.50
1:C:227:LYS:NZ	1:C:361:SER:CB	2.75	0.50
1:D:150:THR:O	1:D:154:VAL:HG23	2.11	0.50
1:D:465:GLU:H	1:D:465:GLU:CD	2.13	0.50
1:A:498:THR:HG22	1:A:499:TYR:H	1.76	0.50
1:B:222:MET:HE2	1:B:281:LEU:HD13	1.94	0.50
1:D:222:MET:HE3	1:D:224:LEU:HD21	1.94	0.50
1:A:85:LEU:HD23	1:A:86:THR:N	2.27	0.50
1:A:131:ILE:HD12	1:A:154:VAL:HG13	1.94	0.50
1:C:238:PRO:HG3	1:C:244:LEU:HG	1.93	0.50
1:C:295:LYS:HE2	1:C:299:LYS:NZ	2.27	0.50
1:D:50:ASN:HA	1:D:376:HIS:NE2	2.26	0.50
1:A:204:GLU:O	1:A:208:GLY:HA2	2.11	0.49
1:D:53:LEU:CD1	1:D:373:ALA:HB1	2.42	0.49
1:D:425:HIS:HE1	1:D:453:ARG:NH2	2.10	0.49
1:A:322:VAL:H	1:A:331:ASN:HD21	1.60	0.49
1:A:394:ILE:HD13	1:A:454:ILE:HD11	1.94	0.49
1:B:309:TYR:O	1:B:312:ILE:N	2.45	0.49
1:D:98:VAL:HG11	1:D:329:GLU:CG	2.41	0.49
1:D:107:LEU:CD2	1:D:267:MET:HB2	2.42	0.49
1:A:66:LYS:NZ	1:A:79:GLU:HG3	2.26	0.49
1:B:407:GLU:HG3	1:B:432:TYR:CZ	2.48	0.49
1:B:464:TRP:O	1:B:466:TRP:N	2.46	0.49
1:C:109:LEU:CD2	1:C:122:LEU:HD11	2.40	0.49
1:C:126:ARG:HG3	1:C:149:PRO:HD2	1.93	0.49
1:A:132:ASN:ND2	1:A:143:SER:OG	2.35	0.49
1:A:291:GLN:O	1:A:295:LYS:HG3	2.13	0.49
1:C:78:VAL:HG12	1:C:386:SER:OG	2.13	0.49
1:D:395:ASN:HD22	1:D:442:VAL:HG22	1.77	0.49
1:A:245:PHE:N	1:A:245:PHE:CD1	2.80	0.49
1:A:328:GLN:CG	1:A:329:GLU:HG2	2.42	0.49
1:A:407:GLU:HG3	1:A:432:TYR:OH	2.12	0.49
1:B:104:PRO:HG2	1:B:131:ILE:HD11	1.94	0.49
1:B:245:PHE:CD1	1:B:245:PHE:N	2.80	0.49
1:D:58:ASP:HB3	2:D:524:HOH:O	2.12	0.49
1:C:377:ASN:ND2	1:C:378:LYS:H	2.10	0.49
1:C:497:ILE:HG23	1:C:497:ILE:O	2.12	0.49
1:D:66:LYS:HG3	1:D:79:GLU:HG2	1.94	0.49
1:A:131:ILE:HG12	1:A:233:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ILE:HG13	1:C:39:ASP:H	1.77	0.49
1:D:47:TYR:CE2	1:D:264:PRO:HB3	2.46	0.49
1:B:96:ASP:OD2	1:B:99:ASN:HB2	2.13	0.49
1:C:270:ASN:O	1:C:362:TYR:HB2	2.13	0.49
1:C:300:ASN:O	1:C:300:ASN:ND2	2.39	0.49
1:A:464:TRP:C	1:A:466:TRP:H	2.16	0.49
1:B:468:ARG:HB3	1:D:178:ARG:HA	1.94	0.49
1:C:255:LYS:HA	1:C:259:VAL:O	2.12	0.49
1:D:96:ASP:OD2	1:D:100:ASP:HB2	2.13	0.49
2:B:528:HOH:O	1:C:440:SER:HB3	2.12	0.48
1:C:91:ASP:HA	1:C:363:THR:HG22	1.95	0.48
1:C:144:ILE:HB	1:C:161:LEU:HD21	1.95	0.48
1:D:303:ILE:HG22	1:D:309:TYR:CE2	2.48	0.48
1:D:446:GLU:OE1	1:D:446:GLU:HA	2.12	0.48
1:D:41:GLY:HA3	1:D:251:PHE:CZ	2.49	0.48
1:A:76:ILE:HD13	1:A:76:ILE:N	2.27	0.48
1:A:384:THR:CG2	1:A:385:THR:H	2.26	0.48
1:A:470:VAL:HG22	1:A:493:PRO:HB3	1.96	0.48
1:B:402:TYR:CD1	1:B:458:GLU:HG3	2.48	0.48
1:B:405:GLN:HG3	1:B:459:CYS:SG	2.54	0.48
1:C:288:LYS:HG3	1:C:289:ASP:OD2	2.14	0.48
1:D:265:PRO:HG2	1:D:367:LEU:HD12	1.95	0.48
1:A:82:LYS:HA	1:A:382:ILE:HG12	1.95	0.48
1:C:451:ASN:O	1:C:453:ARG:NH1	2.47	0.48
1:C:105:GLY:N	1:C:268:VAL:O	2.46	0.48
1:C:150:THR:O	1:C:154:VAL:HG23	2.13	0.48
1:D:295:LYS:HE2	1:D:299:LYS:NZ	2.29	0.48
1:A:413:VAL:HG12	1:A:448:ASN:HB2	1.95	0.48
1:B:226:TYR:HB2	1:B:277:ILE:HB	1.96	0.48
1:D:308:GLN:HG3	1:D:309:TYR:N	2.29	0.48
1:D:201:LYS:N	1:D:201:LYS:HE2	2.28	0.48
1:A:226:TYR:HB2	1:A:277:ILE:HB	1.95	0.47
1:B:275:ARG:HA	1:B:360:ILE:HD11	1.96	0.47
1:D:498:THR:CG2	1:D:499:TYR:N	2.77	0.47
1:A:418:GLU:HB2	1:A:420:ASN:HD21	1.79	0.47
1:B:108:GLN:HE21	1:B:121:ILE:HD13	1.79	0.47
1:B:335:THR:CG2	1:B:337:ASP:H	2.12	0.47
1:C:61:GLU:HG3	1:C:62:SER:H	1.80	0.47
1:C:148:ASP:CB	1:C:153:LYS:HE2	2.44	0.47
1:C:217:ASN:ND2	1:C:384:THR:CB	2.77	0.47
1:D:465:GLU:HG2	1:D:466:TRP:CZ3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HA	1:A:360:ILE:HD11	1.97	0.47
1:D:476:VAL:HG11	1:D:482:ILE:HD13	1.95	0.47
1:C:60:ILE:O	1:C:82:LYS:NZ	2.36	0.47
1:C:76:ILE:CD1	1:C:388:GLU:HG3	2.45	0.47
1:A:222:MET:CE	1:A:224:LEU:HD21	2.45	0.47
1:C:394:ILE:HB	1:C:443:ILE:HB	1.97	0.47
1:A:179:THR:HA	1:A:227:LYS:O	2.15	0.47
1:A:491:LEU:CD2	1:C:176:PRO:HG2	2.44	0.47
1:B:54:ALA:HA	1:B:376:HIS:O	2.15	0.47
1:B:88:SER:N	1:B:89:PRO:HD3	2.30	0.47
1:B:116:GLU:O	1:B:118:ARG:HG2	2.15	0.47
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.80	0.47
1:C:98:VAL:HG13	1:C:324:GLY:O	2.15	0.47
1:C:222:MET:HE3	1:C:224:LEU:HD21	1.97	0.47
1:D:106:ALA:O	1:D:267:MET:HG3	2.15	0.47
1:D:283:THR:HB	1:D:316:SER:OG	2.14	0.47
1:D:487:TRP:NE1	1:D:494:GLY:HA3	2.29	0.47
1:C:267:MET:HG2	1:C:268:VAL:N	2.30	0.47
1:C:358:TYR:HB3	1:C:359:PRO:HD2	1.96	0.47
1:A:268:VAL:HG13	1:A:362:TYR:CD1	2.50	0.47
1:C:285:SER:HB3	1:C:312:ILE:HG23	1.96	0.47
1:C:375:VAL:HG22	1:C:376:HIS:N	2.30	0.47
1:D:451:ASN:O	1:D:453:ARG:NH1	2.48	0.47
1:B:295:LYS:NZ	1:D:474:TYR:O	2.48	0.47
1:C:86:THR:HG23	1:C:378:LYS:CG	2.45	0.47
1:C:498:THR:CG2	1:C:499:TYR:N	2.78	0.47
1:A:126:ARG:HG3	1:A:126:ARG:HH11	1.80	0.46
1:B:407:GLU:HG3	1:B:432:TYR:OH	2.13	0.46
1:D:48:ASN:O	1:D:52:VAL:HG22	2.15	0.46
1:D:224:LEU:HB2	1:D:279:VAL:HB	1.97	0.46
1:A:109:LEU:HB3	1:A:263:ALA:HB1	1.97	0.46
1:B:94:ILE:HD12	1:B:361:SER:HA	1.97	0.46
1:D:126:ARG:HG3	1:D:149:PRO:HD2	1.96	0.46
1:B:413:VAL:HG12	1:B:448:ASN:HB2	1.98	0.46
1:C:95:ILE:CG2	1:C:117:ASN:HB3	2.45	0.46
1:C:227:LYS:NZ	1:C:361:SER:HB3	2.30	0.46
1:C:425:HIS:HE1	1:C:453:ARG:NH2	2.13	0.46
1:A:116:GLU:O	1:A:118:ARG:HG2	2.16	0.46
1:B:75:PHE:HB2	1:B:447:ALA:HB3	1.96	0.46
1:C:60:ILE:HG13	1:C:61:GLU:N	2.31	0.46
1:B:222:MET:HE3	1:B:224:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:TRP:N	1:B:494:GLY:O	2.48	0.46
1:C:48:ASN:O	1:C:52:VAL:HG22	2.16	0.46
1:C:108:GLN:HE21	1:C:121:ILE:HD11	1.80	0.46
1:C:446:GLU:OE1	1:C:446:GLU:HA	2.14	0.46
1:A:101:ARG:HB3	1:A:151:TYR:CG	2.50	0.46
1:C:39:ASP:CG	1:C:242:SER:H	2.18	0.46
1:D:92:ILE:O	1:D:361:SER:HA	2.16	0.46
1:D:339:ASP:O	1:D:342:ARG:HB2	2.16	0.46
1:A:186:VAL:HG13	1:A:192:ILE:HB	1.98	0.46
1:C:94:ILE:HG22	1:C:360:ILE:O	2.15	0.46
1:C:187:TYR:CE2	1:C:383:GLU:HG2	2.50	0.46
1:C:321:VAL:HA	1:C:331:ASN:O	2.16	0.46
1:C:476:VAL:HG11	1:C:482:ILE:HD13	1.96	0.46
1:B:83:ARG:HH22	1:D:421:GLU:CD	2.19	0.46
1:B:418:GLU:HB2	1:B:420:ASN:HD21	1.80	0.46
1:C:201:LYS:HE2	1:C:201:LYS:N	2.31	0.46
1:D:64:VAL:O	1:D:80:ARG:HD2	2.16	0.46
1:D:270:ASN:HB2	1:D:363:THR:OG1	2.15	0.46
1:D:301:THR:O	1:D:304:LYS:HG3	2.16	0.46
1:B:101:ARG:NH1	1:B:101:ARG:HG2	2.31	0.45
1:B:168:LYS:HE2	1:B:169:TYR:OH	2.16	0.45
1:B:222:MET:CE	1:B:224:LEU:HD21	2.46	0.45
1:C:76:ILE:HD13	1:C:388:GLU:HA	1.97	0.45
1:C:290:VAL:HG22	1:C:312:ILE:HD13	1.98	0.45
1:A:306:SER:O	1:A:309:TYR:N	2.49	0.45
1:C:220:LYS:O	1:C:282:GLU:HA	2.16	0.45
1:C:224:LEU:HB2	1:C:279:VAL:HB	1.97	0.45
1:D:60:ILE:CG2	1:D:61:GLU:H	2.29	0.45
1:D:288:LYS:HG3	1:D:289:ASP:OD2	2.16	0.45
1:B:41:GLY:HA3	1:B:251:PHE:CD1	2.52	0.45
1:C:42:ILE:HD12	1:C:241:PRO:CB	2.46	0.45
1:C:78:VAL:HA	1:C:385:THR:O	2.16	0.45
1:C:398:HIS:CE1	1:C:400:GLY:H	2.34	0.45
1:D:38:ILE:O	1:D:42:ILE:HG13	2.17	0.45
1:D:320:ALA:HB2	1:D:341:ILE:HD12	1.98	0.45
1:A:96:ASP:O	1:A:100:ASP:N	2.48	0.45
1:A:168:LYS:HE2	1:A:169:TYR:OH	2.17	0.45
1:C:465:GLU:HG2	1:C:466:TRP:CZ3	2.52	0.45
1:D:148:ASP:H	1:D:153:LYS:CE	2.30	0.45
1:B:458:GLU:OE1	1:B:490:THR:HG23	2.17	0.45
1:C:96:ASP:O	1:C:100:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASN:HB2	1:C:363:THR:OG1	2.17	0.45
1:A:38:ILE:HG22	1:A:39:ASP:N	2.32	0.45
1:A:60:ILE:CG1	1:A:61:GLU:N	2.80	0.45
1:A:295:LYS:HE2	1:A:299:LYS:HZ1	1.78	0.45
1:B:42:ILE:CD1	1:B:241:PRO:HB3	2.47	0.45
1:B:94:ILE:HD12	1:B:361:SER:CA	2.46	0.45
1:C:395:ASN:HD22	1:C:442:VAL:HG22	1.80	0.45
1:A:85:LEU:HD21	1:A:87:THR:OG1	2.16	0.45
1:A:406:PHE:HB2	1:A:428:TRP:HZ3	1.80	0.45
1:D:320:ALA:HB2	1:D:341:ILE:HG23	1.99	0.45
1:A:85:LEU:HD23	1:A:85:LEU:C	2.37	0.45
1:A:108:GLN:O	1:A:266:LEU:HD12	2.17	0.45
1:B:47:TYR:O	1:B:47:TYR:CD1	2.69	0.45
1:B:186:VAL:HG13	1:B:192:ILE:HB	1.98	0.45
1:B:280:LYS:HB3	1:B:319:THR:HB	1.98	0.45
1:C:47:TYR:HD1	1:C:52:VAL:HG11	1.81	0.45
1:C:227:LYS:HE3	1:C:360:ILE:CG2	2.47	0.45
1:A:110:ALA:HB2	1:A:266:LEU:CD2	2.47	0.45
1:B:384:THR:O	1:B:384:THR:HG22	2.17	0.45
1:C:312:ILE:O	1:C:316:SER:HB2	2.17	0.45
1:D:47:TYR:HB2	1:D:52:VAL:HG11	1.99	0.45
1:D:231:TYR:OH	1:D:357:ALA:HB3	2.17	0.45
1:B:309:TYR:O	1:B:310:LYS:C	2.55	0.44
1:D:91:ASP:OD2	1:D:361:SER:HB2	2.17	0.44
1:A:222:MET:HE3	1:A:224:LEU:HD21	1.99	0.44
1:C:180:GLN:HB2	1:C:227:LYS:HB3	1.97	0.44
1:A:47:TYR:HD1	1:A:52:VAL:HG11	1.82	0.44
1:A:94:ILE:CD1	1:A:359:PRO:HB2	2.48	0.44
1:A:97:SER:HB3	1:A:358:TYR:HB3	1.99	0.44
1:A:109:LEU:CD2	1:A:122:LEU:HD21	2.37	0.44
1:A:416:ASP:OD1	1:A:418:GLU:N	2.51	0.44
1:D:156:GLY:O	1:D:159:ASP:HB2	2.16	0.44
1:D:255:LYS:HA	1:D:259:VAL:O	2.17	0.44
1:A:114:LEU:HD12	2:A:502:HOH:O	2.17	0.44
1:B:73:ASN:ND2	1:B:391:LYS:HE3	2.32	0.44
1:B:335:THR:HG21	1:B:337:ASP:HB3	2.00	0.44
1:B:394:ILE:HD13	1:B:454:ILE:HD11	1.99	0.44
1:C:49:ARG:NH2	1:C:369:ASP:OD2	2.50	0.44
1:C:278:TYR:CE1	1:C:323:LEU:HD22	2.47	0.44
1:C:457:ARG:HG2	1:C:467:TRP:HB2	2.00	0.44
1:A:69:LYS:HE3	1:A:69:LYS:HB3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:HE2	1:A:299:LYS:HZ2	1.80	0.44
1:A:329:GLU:H	1:A:329:GLU:HG2	1.45	0.44
1:A:487:TRP:N	1:A:494:GLY:O	2.47	0.44
1:B:75:PHE:CB	1:B:447:ALA:HB3	2.48	0.44
1:B:406:PHE:HB2	1:B:428:TRP:HZ3	1.83	0.44
1:C:339:ASP:O	1:C:342:ARG:HB2	2.17	0.44
1:D:222:MET:CE	1:D:298:ILE:HD11	2.48	0.44
1:D:393:LYS:HD2	2:D:512:HOH:O	2.18	0.44
1:B:83:ARG:NH2	1:D:421:GLU:OE1	2.48	0.44
1:B:268:VAL:HG13	1:B:362:TYR:CD1	2.53	0.44
1:D:425:HIS:CE1	1:D:453:ARG:NH2	2.85	0.44
1:A:58:ASP:OD2	1:A:58:ASP:N	2.50	0.44
1:A:232:THR:HG21	1:C:466:TRP:CD1	2.53	0.44
1:A:234:SER:HB3	1:A:270:ASN:OD1	2.18	0.44
1:A:327:ALA:HA	2:A:543:HOH:O	2.18	0.44
1:A:406:PHE:O	1:A:431:ASN:HA	2.17	0.44
1:A:465:GLU:HG3	1:A:466:TRP:CZ3	2.53	0.44
1:B:73:ASN:ND2	1:B:391:LYS:CE	2.80	0.44
1:B:416:ASP:OD1	1:B:418:GLU:N	2.50	0.44
1:C:303:ILE:CG1	1:C:304:LYS:N	2.80	0.44
1:D:267:MET:HG2	1:D:268:VAL:N	2.32	0.44
1:C:98:VAL:HG21	1:C:329:GLU:CD	2.36	0.44
1:C:156:GLY:O	1:C:159:ASP:HB2	2.17	0.44
1:C:275:ARG:NH1	1:C:326:ASP:HB2	2.33	0.44
1:D:37:SER:O	1:D:38:ILE:C	2.56	0.44
1:D:407:GLU:HB2	1:D:464:TRP:CH2	2.53	0.44
1:A:66:LYS:HZ1	1:A:79:GLU:HG3	1.83	0.44
1:A:244:LEU:HA	2:A:550:HOH:O	2.18	0.44
1:C:36:GLN:N	2:C:518:HOH:O	2.50	0.44
1:C:58:ASP:O	1:C:380:ASP:HB2	2.18	0.44
1:C:231:TYR:OH	1:C:357:ALA:HB3	2.18	0.44
1:D:126:ARG:HB2	1:D:244:LEU:O	2.18	0.44
1:B:303:ILE:HD13	1:B:303:ILE:N	2.33	0.43
1:B:457:ARG:HG3	1:B:468:ARG:O	2.18	0.43
1:A:101:ARG:O	1:A:151:TYR:CD1	2.71	0.43
1:A:425:HIS:CE1	1:A:453:ARG:NH2	2.86	0.43
1:B:49:ARG:O	1:B:52:VAL:HG22	2.17	0.43
1:C:41:GLY:HA3	1:C:251:PHE:CD1	2.54	0.43
1:D:96:ASP:HB2	1:D:100:ASP:HB3	2.00	0.43
1:D:180:GLN:HB2	1:D:227:LYS:HB3	1.99	0.43
1:D:310:LYS:O	1:D:314:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:THR:CG2	1:D:336:LYS:H	2.30	0.43
1:A:192:ILE:HG23	1:A:193:SER:N	2.34	0.43
1:C:91:ASP:C	1:C:92:ILE:HG13	2.39	0.43
1:D:98:VAL:HG11	1:D:329:GLU:HG3	2.00	0.43
1:D:226:TYR:HB2	1:D:277:ILE:HB	1.99	0.43
1:D:497:ILE:HG23	1:D:497:ILE:O	2.18	0.43
1:A:172:THR:CG2	1:A:174:THR:H	2.31	0.43
1:B:189:LYS:O	1:B:193:SER:HB3	2.19	0.43
1:C:90:VAL:HA	1:C:374:ALA:CB	2.48	0.43
1:D:96:ASP:CB	1:D:100:ASP:CB	2.97	0.43
1:A:238:PRO:HB2	1:A:243:ASP:HB2	2.01	0.43
1:B:101:ARG:HG2	1:B:101:ARG:HH11	1.83	0.43
1:B:131:ILE:HG12	1:B:233:VAL:CG1	2.46	0.43
1:C:66:LYS:HG3	1:C:79:GLU:CG	2.38	0.43
1:C:90:VAL:HA	1:C:374:ALA:CA	2.48	0.43
1:C:148:ASP:H	1:C:153:LYS:CE	2.32	0.43
1:C:187:TYR:CZ	1:C:383:GLU:HG2	2.53	0.43
1:D:263:ALA:N	1:D:264:PRO:HD3	2.34	0.43
1:A:180:GLN:HB2	1:A:227:LYS:HB3	1.99	0.43
1:B:94:ILE:HD12	1:B:361:SER:N	2.33	0.43
1:B:172:THR:CG2	1:B:174:THR:H	2.32	0.43
1:C:108:GLN:HE21	1:C:121:ILE:CD1	2.32	0.43
1:C:265:PRO:HB2	1:C:367:LEU:CD1	2.48	0.43
1:B:275:ARG:NH2	1:B:350:THR:O	2.52	0.43
1:B:457:ARG:CZ	1:D:180:GLN:NE2	2.82	0.43
1:C:122:LEU:HD22	1:C:257:LYS:CB	2.49	0.43
1:C:275:ARG:HH11	1:C:326:ASP:HB2	1.84	0.43
1:C:407:GLU:HB2	1:C:464:TRP:CH2	2.54	0.43
1:B:48:ASN:CG	1:B:51:GLU:HG2	2.39	0.43
1:B:407:GLU:HB3	1:B:455:LYS:HB3	2.01	0.43
1:B:456:ALA:O	1:B:470:VAL:N	2.47	0.43
1:C:263:ALA:N	1:C:264:PRO:HD3	2.34	0.43
1:D:95:ILE:HG13	1:D:117:ASN:ND2	2.33	0.43
1:D:220:LYS:O	1:D:282:GLU:HA	2.19	0.43
1:D:312:ILE:HD12	1:D:312:ILE:N	2.28	0.43
1:A:75:PHE:O	1:A:389:TYR:HB2	2.19	0.43
1:B:406:PHE:O	1:B:431:ASN:HA	2.19	0.43
1:D:109:LEU:HD12	1:D:120:THR:CG2	2.49	0.43
1:B:199:ASN:HB3	1:B:202:VAL:HG23	2.01	0.42
1:B:425:HIS:CE1	1:B:453:ARG:NH2	2.87	0.42
1:B:488:GLY:N	2:B:525:HOH:O	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:HIS:CE1	1:C:453:ARG:NH2	2.87	0.42
1:C:487:TRP:NE1	1:C:494:GLY:HA3	2.34	0.42
1:A:305:ASN:O	1:A:306:SER:C	2.58	0.42
1:A:408:VAL:N	1:A:431:ASN:HD21	2.17	0.42
1:B:83:ARG:NH1	1:D:421:GLU:OE1	2.51	0.42
1:B:108:GLN:HA	1:B:120:THR:O	2.19	0.42
1:C:122:LEU:HD22	1:C:257:LYS:HB2	2.00	0.42
1:C:300:ASN:ND2	1:C:300:ASN:C	2.73	0.42
1:C:300:ASN:C	1:C:300:ASN:HD22	2.20	0.42
1:D:487:TRP:HH2	1:D:496:SER:HB3	1.83	0.42
1:D:56:ASN:HD22	1:D:57:GLY:N	2.18	0.42
1:A:483:ASN:O	1:A:497:ILE:HA	2.19	0.42
1:B:360:ILE:HD13	1:B:360:ILE:HA	1.80	0.42
1:D:172:THR:HG22	1:D:173:HIS:N	2.34	0.42
1:A:407:GLU:HB3	1:A:455:LYS:HB3	2.01	0.42
1:C:107:LEU:CD1	1:C:126:ARG:HH21	2.25	0.42
1:C:204:GLU:HA	1:C:209:VAL:H	1.85	0.42
1:D:273:TYR:HA	1:D:358:TYR:O	2.19	0.42
1:B:180:GLN:HB2	1:B:227:LYS:HB3	2.01	0.42
1:A:144:ILE:HG21	1:A:157:ALA:HB1	2.02	0.42
1:B:230:PHE:CE2	1:B:274:GLY:HA2	2.54	0.42
1:B:291:GLN:O	1:B:295:LYS:HG3	2.20	0.42
1:C:303:ILE:CG1	1:C:304:LYS:H	2.33	0.42
1:D:53:LEU:HD11	1:D:373:ALA:HB1	2.01	0.42
1:D:107:LEU:HD23	1:D:267:MET:HB2	2.01	0.42
1:D:478:LEU:HD22	2:D:534:HOH:O	2.20	0.42
1:A:107:LEU:O	1:A:121:ILE:HA	2.19	0.42
1:A:230:PHE:CE2	1:A:274:GLY:HA2	2.55	0.42
1:A:464:TRP:O	1:A:466:TRP:N	2.47	0.42
1:C:41:GLY:HA3	1:C:251:PHE:CE1	2.55	0.42
1:C:273:TYR:HA	1:C:358:TYR:O	2.19	0.42
1:D:173:HIS:HB2	1:D:353:THR:OG1	2.20	0.42
1:D:199:ASN:OD1	1:D:201:LYS:HG2	2.20	0.42
1:A:407:GLU:HA	1:A:431:ASN:ND2	2.35	0.42
1:B:238:PRO:HB2	1:B:243:ASP:HB2	2.01	0.42
1:C:126:ARG:HB2	1:C:244:LEU:O	2.20	0.42
1:C:407:GLU:HG3	1:C:432:TYR:OH	2.20	0.42
1:D:295:LYS:HA	1:D:298:ILE:HD12	2.02	0.42
1:A:52:VAL:HG21	1:A:366:PHE:CZ	2.54	0.41
1:A:52:VAL:CG2	1:A:53:LEU:N	2.83	0.41
1:A:436:THR:O	1:A:437:ALA:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:HE2	1:B:282:GLU:OE2	2.19	0.41
1:C:226:TYR:HB2	1:C:277:ILE:HB	2.02	0.41
1:C:259:VAL:HG13	1:C:265:PRO:CD	2.41	0.41
1:C:265:PRO:CG	1:C:367:LEU:HD12	2.50	0.41
1:D:394:ILE:HB	1:D:443:ILE:HB	2.01	0.41
1:A:429:ASP:C	1:A:431:ASN:H	2.24	0.41
1:B:61:GLU:O	1:B:61:GLU:CG	2.68	0.41
1:C:500:ASN:ND2	2:C:525:HOH:O	2.54	0.41
1:D:258:GLY:O	1:D:263:ALA:HB3	2.20	0.41
1:D:457:ARG:HG2	1:D:467:TRP:HB2	2.01	0.41
1:B:110:ALA:HB2	1:B:266:LEU:CD2	2.50	0.41
1:B:192:ILE:HG23	1:B:193:SER:N	2.34	0.41
1:D:122:LEU:HD22	1:D:257:LYS:CB	2.50	0.41
1:D:310:LYS:HE2	1:D:310:LYS:HA	2.02	0.41
1:A:308:GLN:O	1:A:312:ILE:HG13	2.20	0.41
1:A:453:ARG:HH11	1:A:453:ARG:HG2	1.85	0.41
1:C:172:THR:HG22	1:C:173:HIS:N	2.36	0.41
1:C:274:GLY:O	1:C:360:ILE:HD11	2.21	0.41
1:C:295:LYS:HA	1:C:298:ILE:HD12	2.01	0.41
1:D:122:LEU:HD22	1:D:257:LYS:HB2	2.02	0.41
1:D:339:ASP:O	1:D:342:ARG:N	2.54	0.41
1:A:74:LYS:NZ	1:A:388:GLU:HG2	2.36	0.41
1:A:83:ARG:HB3	1:A:381:TYR:CZ	2.55	0.41
1:A:94:ILE:HD12	1:A:359:PRO:HB2	2.03	0.41
1:A:103:TYR:HB2	1:A:104:PRO:HD2	2.01	0.41
1:B:108:GLN:HE21	1:B:121:ILE:HD11	1.86	0.41
1:C:52:VAL:HG21	1:C:366:PHE:CZ	2.55	0.41
1:C:92:ILE:HG21	1:C:362:TYR:CZ	2.56	0.41
1:D:306:SER:O	1:D:307:GLN:C	2.58	0.41
1:A:413:VAL:HB	1:A:450:ARG:HD3	2.02	0.41
1:B:413:VAL:HB	1:B:450:ARG:HD3	2.02	0.41
1:D:476:VAL:CG1	1:D:482:ILE:HD13	2.50	0.41
1:B:38:ILE:HA	1:B:251:PHE:HB2	2.01	0.41
1:C:61:GLU:OE1	1:C:61:GLU:CA	2.66	0.41
1:C:108:GLN:HB2	1:C:266:LEU:CD1	2.50	0.41
1:C:325:GLY:HA2	1:C:358:TYR:HD1	1.86	0.41
1:D:50:ASN:HA	1:D:376:HIS:CE1	2.56	0.41
1:D:108:GLN:HA	1:D:120:THR:O	2.21	0.41
1:D:204:GLU:HA	1:D:209:VAL:H	1.85	0.41
1:A:50:ASN:HA	1:A:376:HIS:NE2	2.35	0.41
1:A:189:LYS:O	1:A:193:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:HG21	1:A:337:ASP:HB3	2.02	0.41
1:B:198:VAL:HG11	1:B:278:TYR:CE2	2.56	0.41
1:C:407:GLU:HG3	1:C:432:TYR:CE2	2.56	0.41
1:D:78:VAL:HG22	1:D:386:SER:HB2	2.02	0.41
1:D:265:PRO:HB2	1:D:367:LEU:CD1	2.51	0.41
1:D:444:PRO:HD2	2:D:503:HOH:O	2.21	0.41
1:A:309:TYR:HA	1:A:312:ILE:HD12	2.02	0.41
1:A:491:LEU:C	1:A:493:PRO:HD3	2.41	0.41
1:C:105:GLY:HA2	1:C:267:MET:CG	2.51	0.41
1:C:222:MET:CE	1:C:281:LEU:HD13	2.51	0.41
1:D:96:ASP:CB	1:D:100:ASP:HB3	2.51	0.41
1:D:132:ASN:O	1:D:233:VAL:HA	2.21	0.41
1:D:274:GLY:O	1:D:360:ILE:HD11	2.21	0.41
1:B:337:ASP:OD1	1:B:339:ASP:HB2	2.20	0.41
1:C:64:VAL:CB	1:C:80:ARG:NH1	2.80	0.41
1:D:307:GLN:O	1:D:310:LYS:HB2	2.21	0.41
1:D:335:THR:CG2	1:D:336:LYS:N	2.80	0.41
1:B:144:ILE:HG21	1:B:157:ALA:HB1	2.03	0.40
1:B:212:ASN:O	1:B:215:ALA:N	2.54	0.40
1:C:254:LEU:C	1:C:256:GLN:H	2.25	0.40
1:C:310:LYS:HE2	1:C:313:TYR:HB2	2.03	0.40
1:B:436:THR:O	1:B:437:ALA:C	2.59	0.40
1:C:154:VAL:O	1:C:158:ILE:HG13	2.21	0.40
1:C:191:GLN:N	1:C:379:THR:HG21	2.35	0.40
1:D:238:PRO:CB	1:D:243:ASP:HB2	2.52	0.40
1:D:417:LYS:HB2	1:D:417:LYS:NZ	2.36	0.40
1:B:42:ILE:HD12	1:B:241:PRO:CB	2.51	0.40
1:B:83:ARG:HG3	1:B:383:GLU:HB2	2.03	0.40
1:C:228:GLN:OE1	1:C:348:ASN:O	2.39	0.40
1:C:350:THR:HG22	1:C:351:PHE:N	2.37	0.40
1:D:53:LEU:HD23	1:D:53:LEU:HA	1.95	0.40
1:D:109:LEU:CD2	1:D:263:ALA:O	2.69	0.40
1:D:465:GLU:HG2	1:D:466:TRP:CE3	2.56	0.40
1:D:470:VAL:HG12	1:D:495:SER:HB3	2.04	0.40
1:B:497:ILE:HG23	1:B:497:ILE:O	2.21	0.40
1:C:132:ASN:O	1:C:233:VAL:HA	2.21	0.40
1:C:189:LYS:HA	1:C:211:PHE:CE2	2.57	0.40
1:C:199:ASN:OD1	1:C:201:LYS:HG2	2.21	0.40
1:C:338:PHE:O	1:C:341:ILE:HB	2.22	0.40
1:A:335:THR:CG2	1:A:336:LYS:N	2.83	0.40
1:B:429:ASP:C	1:B:431:ASN:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:PRO:HG2	1:B:499:TYR:CE2	2.57	0.40
1:B:482:ILE:HG23	1:B:497:ILE:HD11	2.04	0.40
1:C:335:THR:CG2	1:C:336:LYS:N	2.82	0.40
1:C:476:VAL:CG1	1:C:482:ILE:HD13	2.51	0.40
1:D:228:GLN:OE1	1:D:348:ASN:O	2.40	0.40
1:D:297:LEU:HD21	1:D:318:PHE:CZ	2.56	0.40
1:D:411:ASP:O	1:D:449:ALA:HA	2.22	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	463/471 (98%)	421 (91%)	35 (8%)	7 (2%)	10 34
1	B	463/471 (98%)	417 (90%)	39 (8%)	7 (2%)	10 34
1	C	463/471 (98%)	416 (90%)	41 (9%)	6 (1%)	12 37
1	D	463/471 (98%)	424 (92%)	31 (7%)	8 (2%)	9 31
All	All	1852/1884 (98%)	1678 (91%)	146 (8%)	28 (2%)	10 34

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	B	58	ASP
1	D	38	ILE
1	D	62	SER
1	A	465	GLU
1	B	465	GLU
1	D	438	HIS
1	A	416	ASP

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Mol	Chain	Res	Type
1	B	416	ASP
1	C	90	VAL
1	C	368	LYS
1	C	437	ALA
1	C	438	HIS
1	D	368	LYS
1	D	437	ALA
1	A	437	ALA
1	B	437	ALA
1	D	307	GLN
1	A	330	HIS
1	B	65	PRO
1	C	141	GLU
1	D	106	ALA
1	D	141	GLU
1	A	430	GLY
1	C	38	ILE
1	A	290	VAL
1	B	290	VAL
1	B	430	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	412/418 (99%)	374 (91%)	38 (9%)	9 27
1	B	412/418 (99%)	372 (90%)	40 (10%)	8 25
1	C	412/418 (99%)	357 (87%)	55 (13%)	4 11
1	D	412/418 (99%)	364 (88%)	48 (12%)	5 16
All	All	1648/1672 (99%)	1467 (89%)	181 (11%)	6 19

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER

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Mol	Chain	Res	Type
1	A	43	SER
1	A	58	ASP
1	A	66	LYS
1	A	69	LYS
1	A	84	SER
1	A	108	GLN
1	A	112	LYS
1	A	126	ARG
1	A	130	ASN
1	A	132	ASN
1	A	153	LYS
1	A	159	ASP
1	A	171	SER
1	A	239	LYS
1	A	245	PHE
1	A	266	LEU
1	A	284	THR
1	A	286	SER
1	A	300	ASN
1	A	304	LYS
1	A	305	ASN
1	A	308	GLN
1	A	328	GLN
1	A	329	GLU
1	A	331	ASN
1	A	363	THR
1	A	370	ASN
1	A	385	THR
1	A	388	GLU
1	A	390	SER
1	A	391	LYS
1	A	393	LYS
1	A	398	HIS
1	A	414	SER
1	A	450	ARG
1	A	465	GLU
1	A	468	ARG
1	B	47	TYR
1	B	49	ARG
1	B	52	VAL
1	B	58	ASP
1	B	59	LYS

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Mol	Chain	Res	Type
1	B	60	ILE
1	B	79	GLU
1	B	87	THR
1	B	93	SER
1	B	101	ARG
1	B	108	GLN
1	B	112	LYS
1	B	126	ARG
1	B	130	ASN
1	B	132	ASN
1	B	153	LYS
1	B	159	ASP
1	B	171	SER
1	B	197	ASN
1	B	239	LYS
1	B	245	PHE
1	B	266	LEU
1	B	284	THR
1	B	286	SER
1	B	326	ASP
1	B	328	GLN
1	B	363	THR
1	B	370	ASN
1	B	375	VAL
1	B	377	ASN
1	B	380	ASP
1	B	383	GLU
1	B	384	THR
1	B	385	THR
1	B	387	THR
1	B	393	LYS
1	B	398	HIS
1	B	414	SER
1	B	450	ARG
1	B	458	GLU
1	C	45	LEU
1	C	49	ARG
1	C	52	VAL
1	C	53	LEU
1	C	58	ASP
1	C	64	VAL
1	C	69	LYS

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Mol	Chain	Res	Type
1	C	74	LYS
1	C	80	ARG
1	C	84	SER
1	C	85	LEU
1	C	86	THR
1	C	93	SER
1	C	100	ASP
1	C	126	ARG
1	C	130	ASN
1	C	131	ILE
1	C	132	ASN
1	C	163	SER
1	C	171	SER
1	C	194	SER
1	C	197	ASN
1	C	218	GLU
1	C	232	THR
1	C	239	LYS
1	C	243	ASP
1	C	266	LEU
1	C	286	SER
1	C	299	LYS
1	C	300	ASN
1	C	302	ASP
1	C	304	LYS
1	C	306	SER
1	C	308	GLN
1	C	310	LYS
1	C	311	ASP
1	C	317	SER
1	C	326	ASP
1	C	331	ASN
1	C	346	LYS
1	C	370	ASN
1	C	378	LYS
1	C	379	THR
1	C	384	THR
1	C	386	SER
1	C	387	THR
1	C	390	SER
1	C	393	LYS
1	C	398	HIS

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Mol	Chain	Res	Type
1	C	414	SER
1	C	440	SER
1	C	450	ARG
1	C	457	ARG
1	C	468	ARG
1	C	475	ASP
1	D	39	ASP
1	D	43	SER
1	D	44	SER
1	D	49	ARG
1	D	50	ASN
1	D	56	ASN
1	D	62	SER
1	D	63	PHE
1	D	64	VAL
1	D	69	LYS
1	D	73	ASN
1	D	96	ASP
1	D	101	ARG
1	D	108	GLN
1	D	126	ARG
1	D	130	ASN
1	D	131	ILE
1	D	132	ASN
1	D	163	SER
1	D	171	SER
1	D	194	SER
1	D	197	ASN
1	D	218	GLU
1	D	232	THR
1	D	239	LYS
1	D	243	ASP
1	D	266	LEU
1	D	286	SER
1	D	299	LYS
1	D	304	LYS
1	D	305	ASN
1	D	306	SER
1	D	308	GLN
1	D	311	ASP
1	D	328	GLN
1	D	330	HIS

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Mol	Chain	Res	Type
1	D	346	LYS
1	D	370	ASN
1	D	375	VAL
1	D	383	GLU
1	D	393	LYS
1	D	398	HIS
1	D	414	SER
1	D	440	SER
1	D	450	ARG
1	D	457	ARG
1	D	468	ARG
1	D	475	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	108	GLN
1	A	132	ASN
1	A	197	ASN
1	A	217	ASN
1	A	240	ASN
1	A	307	GLN
1	A	328	GLN
1	A	331	ASN
1	A	395	ASN
1	A	420	ASN
1	A	483	ASN
1	A	500	ASN
1	B	73	ASN
1	B	108	GLN
1	B	132	ASN
1	B	197	ASN
1	B	217	ASN
1	B	240	ASN
1	B	308	GLN
1	B	395	ASN
1	B	420	ASN
1	B	483	ASN
1	B	500	ASN
1	C	48	ASN
1	C	99	ASN

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Mol	Chain	Res	Type
1	C	108	GLN
1	C	117	ASN
1	C	197	ASN
1	C	205	ASN
1	C	217	ASN
1	C	308	GLN
1	C	315	ASN
1	C	331	ASN
1	C	370	ASN
1	C	377	ASN
1	C	395	ASN
1	C	420	ASN
1	C	483	ASN
1	C	500	ASN
1	D	56	ASN
1	D	73	ASN
1	D	99	ASN
1	D	108	GLN
1	D	117	ASN
1	D	180	GLN
1	D	197	ASN
1	D	205	ASN
1	D	217	ASN
1	D	308	GLN
1	D	330	HIS
1	D	395	ASN
1	D	420	ASN
1	D	451	ASN
1	D	483	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.