Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 11:29 PM EDT

PDB ID	:	1EWV
Title	:	CRYSTAL STRUCTURE OF METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1 LIGAND FREE FORM II
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Deposited on	:	2000-04-27
Resolution	:	4.00 Å(reported)

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

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

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

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

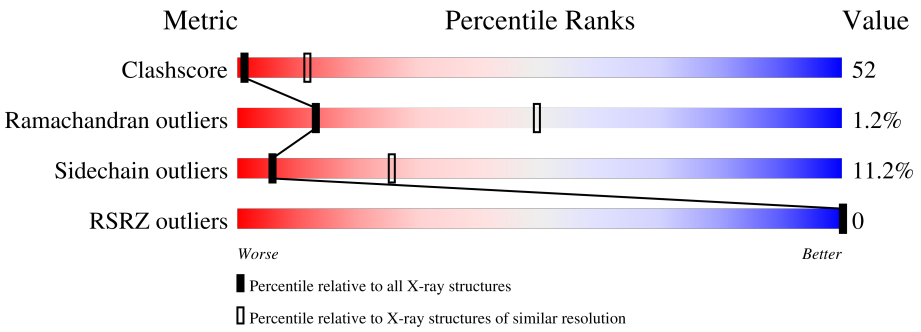
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 4.00 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	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	490	30% 53% 8% 9%
1	B	490	34% 50% 8% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7120 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 METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1.

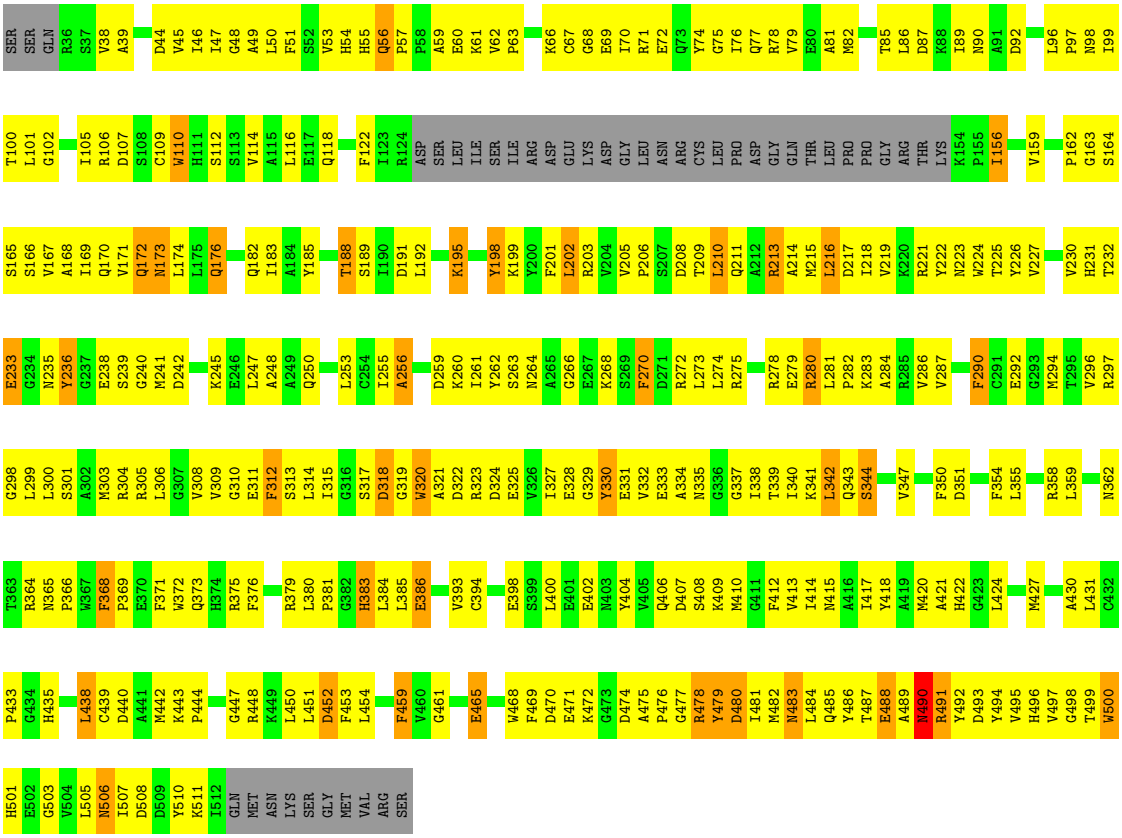
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	3560	2258	620	662	20	0	0	0
			Total	C	N	O	S			
1	B	448	3560	2258	620	662	20	0	0	0

3 Residue-property plots (i)

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

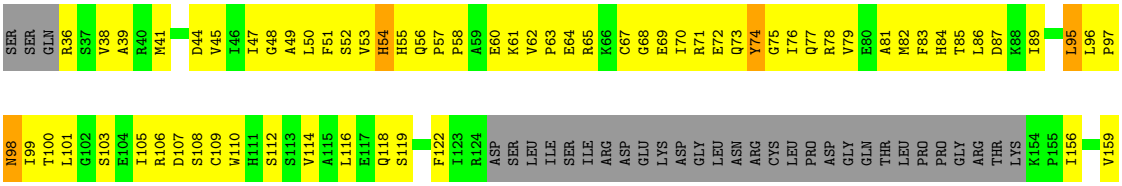
• Molecule 1: METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1

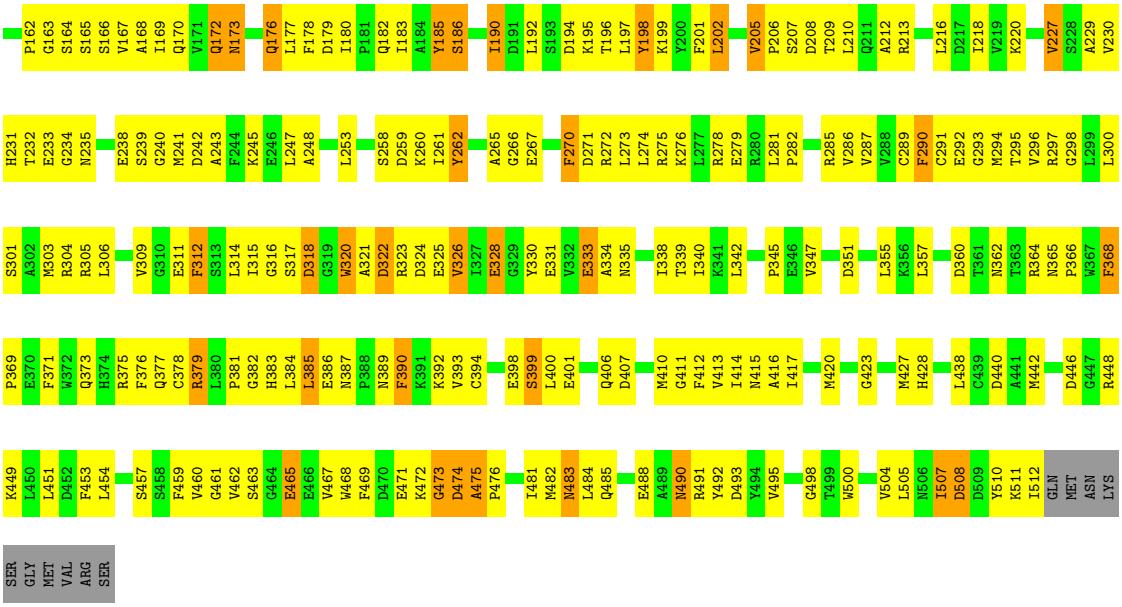
Chain A: 30% 53% 8% 9%



• Molecule 1: METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1

Chain B: 34% 50% 8% 9%




P162 G163 S164 S165 S166 V167 A168 I169 Q170 V171 Q172 N173 Q176 L177 F178 D179 I180 P181 Q182 I183 A184 Y185 S186 I190 D191 L192 S193 D194 K195 T196 L197 Y198 K199 Y200 F201 L202 V205 P206 S207 D208 T209 L210 Q211 A212 R213 L216 D217 I218 V219 K220 V227 S228 A229 V230
H231 T232 E233 G234 N235 E238 S239 G240 M241 D242 A243 F244 K245 E246 L247 A248 L253 S258 D259 K260 I261 Y262 A265 G266 E267 F270 D271 R272 L273 L274 R275 K276 L277 R278 E279 R280 L281 P282 R285 V286 V287 V288 C289 F290 C291 E292 G293 M294 T295 V296 R297 G298 L299 L300
S301 A302 M303 R304 R305 L306 V309 G310 E311 F312 S313 L314 I315 G316 S317 D318 G319 W320 A321 D322 R323 D324 E325 V326 I327 E328 G329 Y330 E331 V332 E333 A334 N335 I338 T339 I340 K341 L342 P345 E346 V347 D351 L355 K356 L357 D360 T361 N362 T363 R364 N365 P366 W367 F368
P369 E370 F371 W372 Q373 H374 R375 F376 Q377 C378 R379 L380 P381 G382 H383 L384 L385 E386 N387 P388 N389 F390 K391 K392 V393 C394 E398 S399 L400 E401 Q406 D407 M410 G411 F412 V413 I414 N415 A416 I417 M420 G423 M427 H428 L438 C439 D440 A441 M442 D446 G447 R448
K449 L450 L451 D452 F453 L454 S457 S458 F459 V460 G461 V462 S463 G464 E465 E466 V467 W468 F469 D470 E471 K472 G473 D474 A475 P476 I481 M482 N483 L484 Q485 E488 A489 N490 R491 Y492 D493 Y494 V495 G498 T499 W500 V504 L505 N506 I507 D508 D509 Y510 K511 I512 GLN MET ASN LYS
SER GLY MET VAL ARG SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.79Å 94.53Å 95.45Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 19.92 – 3.99	Depositor EDS
% Data completeness (in resolution range)	89.1 (20.00-4.00) 89.0 (19.92-3.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.328 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 24.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.73	6/3640 (0.2%)	0.95	0/4923
1	B	0.66	2/3640 (0.1%)	0.94	0/4923
All	All	0.70	8/7280 (0.1%)	0.95	0/9846

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TRP	NE1-CE2	8.80	1.49	1.37
1	A	500	TRP	NE1-CE2	8.73	1.49	1.37
1	A	372	TRP	NE1-CE2	8.73	1.48	1.37
1	A	468	TRP	NE1-CE2	8.72	1.48	1.37
1	B	110	TRP	NE1-CE2	8.72	1.48	1.37
1	A	320	TRP	NE1-CE2	8.70	1.48	1.37
1	B	320	TRP	NE1-CE2	8.69	1.48	1.37
1	A	110	TRP	NE1-CE2	8.65	1.48	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	TYR	Sidechain

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	3560	0	3485	372	0
1	B	3560	0	3485	356	0
All	All	7120	0	6970	726	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 52.

All (726) 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:206:PRO:CG	1:A:477:GLY:HA3	1.69	1.21
1:A:206:PRO:HG3	1:A:477:GLY:CA	1.74	1.17
1:B:190:ILE:H	1:B:190:ILE:HD12	1.04	1.14
1:A:162:PRO:HG3	1:A:171:VAL:HG21	1.29	1.10
1:A:475:ALA:HB1	1:A:476:PRO:HD2	1.23	1.07
1:B:475:ALA:HB1	1:B:476:PRO:HD2	1.30	1.07
1:A:195:LYS:HG3	1:A:199:LYS:HA	1.41	1.03
1:B:240:GLY:C	1:B:290:PHE:CE1	2.32	1.03
1:A:192:LEU:HD13	1:A:201:PHE:CZ	1.98	0.98
1:A:280:ARG:HH22	1:A:283:LYS:HB2	1.29	0.97
1:A:236:TYR:HD2	1:A:236:TYR:C	1.68	0.96
1:A:461:GLY:HA3	1:A:465:GLU:HG2	1.48	0.96
1:B:240:GLY:HA3	1:B:290:PHE:CZ	2.02	0.94
1:A:162:PRO:HG3	1:A:171:VAL:CG2	1.99	0.92
1:A:475:ALA:HB1	1:A:476:PRO:CD	1.99	0.92
1:B:475:ALA:HB1	1:B:476:PRO:CD	2.00	0.91
1:A:236:TYR:C	1:A:236:TYR:CD2	2.41	0.90
1:B:400:LEU:H	1:B:400:LEU:HD12	1.35	0.90
1:B:240:GLY:CA	1:B:290:PHE:CE1	2.55	0.90
1:B:109:CYS:SG	1:B:114:VAL:HG11	2.11	0.90
1:B:240:GLY:HA3	1:B:290:PHE:CE1	2.08	0.89
1:A:206:PRO:HG3	1:A:477:GLY:HA3	0.91	0.89
1:A:162:PRO:CG	1:A:171:VAL:HG21	2.02	0.88
1:A:381:PRO:HA	1:A:386:GLU:HG3	1.56	0.87
1:B:190:ILE:HD12	1:B:190:ILE:N	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:HA	1:B:172:GLN:HE21	1.39	0.86
1:B:185:TYR:CD2	1:B:185:TYR:N	2.42	0.86
1:B:185:TYR:HB2	1:B:412:PHE:HB3	1.58	0.86
1:B:287:VAL:HB	1:B:314:LEU:HD23	1.57	0.85
1:B:190:ILE:H	1:B:190:ILE:CD1	1.82	0.85
1:B:180:ILE:HD12	1:B:180:ILE:N	1.90	0.85
1:A:301:SER:HA	1:A:330:TYR:HE2	1.38	0.84
1:A:227:VAL:O	1:A:255:ILE:HG23	1.77	0.84
1:A:301:SER:HA	1:A:330:TYR:CE2	2.13	0.84
1:A:188:THR:HB	1:A:208:ASP:OD1	1.79	0.83
1:A:287:VAL:HB	1:A:314:LEU:HD23	1.60	0.83
1:B:205:VAL:HG23	1:B:206:PRO:HD2	1.60	0.83
1:A:236:TYR:HD2	1:A:236:TYR:O	1.60	0.82
1:B:379:ARG:NH2	1:B:381:PRO:HA	1.95	0.82
1:A:45:VAL:HB	1:A:101:LEU:HD23	1.59	0.81
1:B:192:LEU:HA	1:B:198:TYR:CE2	2.15	0.81
1:A:461:GLY:HA3	1:A:465:GLU:CG	2.09	0.81
1:A:116:LEU:HD23	1:B:177:LEU:HD11	1.62	0.81
1:B:192:LEU:HA	1:B:198:TYR:CD2	2.16	0.81
1:B:261:ILE:HG21	1:B:295:THR:HG23	1.63	0.81
1:B:415:ASN:HD22	1:B:467:VAL:HG21	1.45	0.80
1:B:285:ARG:HG2	1:B:312:PHE:HA	1.63	0.80
1:A:122:PHE:O	1:A:156:ILE:HD11	1.81	0.80
1:A:334:ALA:O	1:A:484:LEU:HD23	1.81	0.80
1:A:383:HIS:CD2	1:A:384:LEU:N	2.50	0.80
1:B:300:LEU:O	1:B:303:MET:HB2	1.82	0.80
1:A:375:ARG:O	1:A:375:ARG:HG3	1.82	0.79
1:A:188:THR:O	1:A:208:ASP:CG	2.20	0.79
1:B:119:SER:HA	1:B:122:PHE:HD2	1.48	0.79
1:B:227:VAL:HG12	1:B:286:VAL:HB	1.64	0.78
1:B:362:ASN:HD21	1:B:365:ASN:HB3	1.45	0.78
1:A:172:GLN:HB2	1:A:182:GLN:OE1	1.83	0.78
1:A:383:HIS:HD2	1:A:384:LEU:N	1.80	0.78
1:B:293:GLY:O	1:B:296:VAL:HB	1.84	0.78
1:B:508:ASP:HB3	1:B:511:LYS:HB3	1.64	0.77
1:A:309:VAL:HG12	1:A:310:GLY:H	1.48	0.77
1:A:236:TYR:CD2	1:A:236:TYR:O	2.36	0.77
1:B:178:PHE:HB2	1:B:180:ILE:HD11	1.65	0.77
1:A:195:LYS:HD2	1:A:472:LYS:O	1.85	0.77
1:A:195:LYS:HE3	1:A:195:LYS:HA	1.67	0.76
1:A:373:GLN:HE22	1:A:386:GLU:HA	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:CYS:SG	1:A:114:VAL:HG11	2.26	0.76
1:A:488:GLU:CD	1:A:488:GLU:H	1.89	0.76
1:B:185:TYR:H	1:B:185:TYR:HD2	1.31	0.75
1:B:270:PHE:CE1	1:B:298:GLY:HA3	2.20	0.75
1:B:185:TYR:CE1	1:B:413:VAL:HG22	2.23	0.74
1:B:185:TYR:N	1:B:185:TYR:HD2	1.80	0.74
1:B:190:ILE:HD11	1:B:239:SER:O	1.87	0.74
1:B:230:VAL:HG11	1:B:273:LEU:HD21	1.69	0.74
1:B:379:ARG:NH1	1:B:379:ARG:HB2	2.01	0.74
1:A:359:LEU:HD21	1:A:380:LEU:HD13	1.70	0.74
1:B:169:ILE:O	1:B:173:ASN:HB2	1.86	0.73
1:A:189:SER:HA	1:A:208:ASP:OD2	1.88	0.73
1:A:270:PHE:O	1:A:273:LEU:HB3	1.88	0.73
1:B:67:CYS:SG	1:B:114:VAL:HG21	2.29	0.73
1:A:156:ILE:HD13	1:A:156:ILE:H	1.53	0.73
1:B:285:ARG:CG	1:B:312:PHE:HA	2.19	0.72
1:A:210:LEU:N	1:A:210:LEU:HD23	2.03	0.72
1:B:357:LEU:HD13	1:B:368:PHE:HZ	1.54	0.72
1:A:500:TRP:HD1	1:A:505:LEU:HD13	1.53	0.72
1:B:172:GLN:HE21	1:B:172:GLN:CA	2.01	0.72
1:B:183:ILE:HA	1:B:202:LEU:O	1.89	0.72
1:A:55:HIS:CD2	1:A:71:ARG:HD2	2.24	0.72
1:B:373:GLN:O	1:B:377:GLN:N	2.22	0.71
1:A:192:LEU:HD23	1:A:198:TYR:CD2	2.26	0.71
1:B:95:LEU:HD11	1:B:96:LEU:HG	1.72	0.71
1:B:231:HIS:CE1	1:B:260:LYS:HG2	2.25	0.71
1:B:85:THR:HG21	1:B:417:ILE:HG21	1.72	0.71
1:A:248:ALA:HB1	1:A:253:LEU:HB3	1.72	0.70
1:B:85:THR:O	1:B:89:ILE:HG13	1.90	0.70
1:A:270:PHE:CE1	1:A:298:GLY:HA3	2.27	0.70
1:B:84:HIS:O	1:B:87:ASP:HB2	1.90	0.70
1:B:483:ASN:OD1	1:B:512:ILE:HG23	1.92	0.70
1:A:507:ILE:HG22	1:A:508:ASP:N	2.05	0.70
1:B:229:ALA:HB1	1:B:241:MET:CE	2.21	0.70
1:B:261:ILE:CG2	1:B:295:THR:HG23	2.21	0.70
1:A:451:LEU:O	1:A:454:LEU:N	2.20	0.70
1:B:375:ARG:HG3	1:B:375:ARG:HH11	1.55	0.69
1:B:274:LEU:HG	1:B:278:ARG:HD2	1.72	0.69
1:B:58:PRO:O	1:B:62:VAL:HG23	1.92	0.69
1:B:301:SER:HA	1:B:330:TYR:HE2	1.57	0.69
1:A:227:VAL:O	1:A:255:ILE:HD12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD22	1:B:201:PHE:CZ	2.28	0.69
1:B:369:PRO:HB2	1:B:385:LEU:HD12	1.75	0.69
1:A:76:ILE:HG13	1:A:371:PHE:CG	2.28	0.69
1:A:376:PHE:CE2	1:A:398:GLU:HB3	2.28	0.69
1:B:112:SER:O	1:B:116:LEU:HB2	1.93	0.69
1:A:475:ALA:CB	1:A:476:PRO:HD2	2.13	0.69
1:A:461:GLY:N	1:A:465:GLU:O	2.26	0.69
1:B:210:LEU:HD11	1:B:500:TRP:HH2	1.58	0.68
1:A:375:ARG:HG2	1:A:376:PHE:CZ	2.29	0.68
1:B:240:GLY:O	1:B:290:PHE:HE1	1.76	0.68
1:A:230:VAL:HA	1:A:259:ASP:O	1.92	0.68
1:A:240:GLY:HA3	1:A:290:PHE:CE2	2.28	0.68
1:A:278:ARG:HB3	1:A:278:ARG:NH1	2.08	0.68
1:A:62:VAL:N	1:A:63:PRO:CD	2.57	0.68
1:A:183:ILE:HA	1:A:202:LEU:O	1.94	0.68
1:B:163:GLY:HA2	1:B:186:SER:OG	1.94	0.68
1:B:304:ARG:HG2	1:B:304:ARG:HH11	1.58	0.68
1:B:119:SER:HA	1:B:122:PHE:CD2	2.29	0.67
1:B:162:PRO:HG3	1:B:167:VAL:HG12	1.76	0.67
1:A:342:LEU:HA	1:A:479:TYR:HB3	1.77	0.67
1:B:275:ARG:O	1:B:279:GLU:HG3	1.95	0.67
1:A:47:ILE:HD13	1:A:420:MET:HG3	1.77	0.67
1:A:280:ARG:HH22	1:A:283:LYS:CB	2.07	0.67
1:B:73:GLN:H	1:B:73:GLN:NE2	1.92	0.67
1:A:110:TRP:CZ2	1:A:164:SER:HB2	2.30	0.67
1:B:172:GLN:HG2	1:B:198:TYR:HB3	1.77	0.67
1:A:164:SER:HB3	1:A:167:VAL:HG23	1.77	0.67
1:A:76:ILE:HG13	1:A:371:PHE:CD1	2.30	0.66
1:B:266:GLY:O	1:B:270:PHE:HB2	1.95	0.66
1:B:301:SER:HA	1:B:330:TYR:CE2	2.31	0.66
1:B:454:LEU:O	1:B:457:SER:HB2	1.95	0.66
1:A:459:PHE:N	1:A:459:PHE:CD2	2.61	0.66
1:B:82:MET:HG2	1:B:105:ILE:HD11	1.77	0.66
1:A:188:THR:O	1:A:208:ASP:OD1	2.14	0.66
1:A:202:LEU:N	1:A:202:LEU:HD23	2.11	0.66
1:A:206:PRO:CB	1:A:477:GLY:HA3	2.25	0.66
1:A:281:LEU:HB3	1:A:282:PRO:HA	1.77	0.66
1:B:342:LEU:HD21	1:B:412:PHE:HE2	1.60	0.66
1:A:290:PHE:CD1	1:A:317:SER:HB3	2.31	0.65
1:A:491:ARG:HD2	1:A:492:TYR:O	1.96	0.65
1:B:48:GLY:H	1:B:156:ILE:HG23	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HG11	1:A:424:LEU:HD11	1.78	0.65
1:B:109:CYS:HB2	1:B:114:VAL:HG11	1.79	0.65
1:B:312:PHE:CD2	1:B:312:PHE:N	2.60	0.65
1:A:62:VAL:N	1:A:63:PRO:HD3	2.12	0.65
1:A:309:VAL:HG12	1:A:310:GLY:N	2.10	0.65
1:A:339:THR:OG1	1:A:482:MET:HB2	1.96	0.65
1:A:491:ARG:NH1	1:A:492:TYR:O	2.28	0.65
1:A:347:VAL:HG12	1:A:350:PHE:H	1.61	0.65
1:B:109:CYS:CB	1:B:114:VAL:HG11	2.25	0.65
1:A:278:ARG:HB3	1:A:278:ARG:HH11	1.58	0.65
1:B:281:LEU:HB3	1:B:282:PRO:HA	1.77	0.65
1:A:483:ASN:HD22	1:A:484:LEU:H	1.45	0.65
1:B:240:GLY:C	1:B:290:PHE:CD1	2.70	0.64
1:A:195:LYS:HE2	1:A:198:TYR:O	1.96	0.64
1:A:54:HIS:HD2	1:A:70:ILE:HD12	1.62	0.64
1:A:270:PHE:CZ	1:A:298:GLY:HA3	2.33	0.64
1:B:202:LEU:HD23	1:B:202:LEU:N	2.11	0.64
1:B:95:LEU:CD1	1:B:96:LEU:HG	2.26	0.64
1:A:327:ILE:HD12	1:A:328:GLU:N	2.12	0.64
1:A:332:VAL:HB	1:A:333:GLU:OE2	1.97	0.64
1:B:216:LEU:O	1:B:216:LEU:HD23	1.98	0.64
1:B:240:GLY:O	1:B:290:PHE:CE1	2.50	0.64
1:A:211:GLN:HG3	1:A:340:ILE:HG21	1.80	0.64
1:A:218:ILE:HD11	1:A:481:ILE:HD12	1.79	0.64
1:A:51:PHE:CD1	1:A:78:ARG:HB3	2.34	0.63
1:B:306:LEU:O	1:B:306:LEU:HD12	1.97	0.63
1:A:210:LEU:HB2	1:A:479:TYR:OH	1.97	0.63
1:B:72:GLU:H	1:B:73:GLN:NE2	1.96	0.63
1:A:169:ILE:O	1:A:173:ASN:HB2	1.99	0.63
1:A:305:ARG:NH1	1:A:305:ARG:HG3	2.14	0.63
1:A:500:TRP:CZ2	1:A:503:GLY:HA2	2.33	0.63
1:B:300:LEU:HD13	1:B:334:ALA:HB2	1.79	0.63
1:A:195:LYS:HE3	1:A:195:LYS:CA	2.24	0.63
1:A:309:VAL:HG11	1:A:333:GLU:HA	1.81	0.63
1:B:362:ASN:ND2	1:B:365:ASN:HB3	2.12	0.63
1:B:382:GLY:N	1:B:386:GLU:OE1	2.32	0.63
1:A:300:LEU:O	1:A:303:MET:HB2	1.99	0.62
1:B:312:PHE:H	1:B:312:PHE:HD2	1.46	0.62
1:B:65:ARG:HG3	1:B:65:ARG:HH11	1.64	0.62
1:B:199:LYS:NZ	1:B:448:ARG:HH12	1.97	0.62
1:B:261:ILE:HD11	1:B:265:ALA:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:HIS:CD2	1:A:383:HIS:C	2.74	0.62
1:B:400:LEU:HD12	1:B:400:LEU:N	2.13	0.62
1:B:508:ASP:HB3	1:B:511:LYS:CB	2.30	0.62
1:B:82:MET:CG	1:B:105:ILE:HD11	2.30	0.62
1:B:85:THR:CG2	1:B:417:ILE:HG21	2.29	0.61
1:A:306:LEU:O	1:A:308:VAL:HG13	2.00	0.61
1:A:483:ASN:HD22	1:A:484:LEU:N	1.98	0.61
1:B:322:ASP:CG	1:B:322:ASP:O	2.38	0.61
1:B:508:ASP:CB	1:B:511:LYS:HB3	2.30	0.61
1:A:71:ARG:O	1:A:76:ILE:HG12	1.99	0.61
1:B:47:ILE:CG2	1:B:420:MET:HG2	2.31	0.61
1:B:195:LYS:HG3	1:B:472:LYS:O	1.99	0.61
1:A:89:ILE:HD11	1:A:418:TYR:CD2	2.35	0.61
1:A:470:ASP:C	1:A:470:ASP:OD2	2.38	0.61
1:A:342:LEU:H	1:A:342:LEU:HD12	1.66	0.61
1:B:50:LEU:HD21	1:B:122:PHE:HE2	1.64	0.61
1:A:275:ARG:HG2	1:A:279:GLU:OE1	2.00	0.61
1:A:60:GLU:CD	1:A:60:GLU:H	2.04	0.61
1:A:232:THR:HG21	1:A:292:GLU:HB2	1.82	0.61
1:A:85:THR:O	1:A:89:ILE:HG13	2.00	0.60
1:A:414:ILE:O	1:A:417:ILE:HB	2.00	0.60
1:A:485:GLN:HE21	1:A:495:VAL:HG21	1.66	0.60
1:B:65:ARG:HG3	1:B:65:ARG:NH1	2.16	0.60
1:B:216:LEU:HD23	1:B:216:LEU:C	2.22	0.60
1:A:82:MET:CG	1:A:105:ILE:HD11	2.31	0.60
1:A:156:ILE:H	1:A:156:ILE:CD1	2.11	0.60
1:A:459:PHE:N	1:A:459:PHE:HD2	1.98	0.60
1:A:497:VAL:O	1:A:507:ILE:HG23	2.01	0.60
1:A:213:ARG:CG	1:A:213:ARG:HH11	2.14	0.60
1:A:89:ILE:CG1	1:A:418:TYR:HE2	2.15	0.60
1:A:226:TYR:HE2	1:A:280:ARG:NH2	1.99	0.60
1:A:471:GLU:HG3	1:A:472:LYS:N	2.17	0.60
1:A:280:ARG:HH21	1:A:284:ALA:HB2	1.66	0.60
1:B:240:GLY:C	1:B:290:PHE:HE1	2.01	0.60
1:B:178:PHE:HB2	1:B:180:ILE:CD1	2.31	0.60
1:B:241:MET:N	1:B:290:PHE:CD1	2.69	0.60
1:B:379:ARG:NH1	1:B:379:ARG:CB	2.65	0.60
1:A:185:TYR:O	1:A:205:VAL:HG11	2.01	0.60
1:A:172:GLN:NE2	1:A:201:PHE:HB2	2.17	0.59
1:A:240:GLY:HA3	1:A:290:PHE:HE2	1.66	0.59
1:B:393:VAL:HG12	1:B:394:CYS:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:O	1:A:219:VAL:HG23	2.03	0.59
1:B:240:GLY:CA	1:B:290:PHE:CZ	2.79	0.59
1:B:330:TYR:N	1:B:330:TYR:CD1	2.70	0.59
1:B:71:ARG:NH2	1:B:74:TYR:CD2	2.69	0.59
1:B:210:LEU:HD11	1:B:500:TRP:CH2	2.37	0.59
1:B:492:TYR:N	1:B:492:TYR:CD2	2.69	0.59
1:A:198:TYR:CD1	1:A:198:TYR:N	2.70	0.59
1:A:227:VAL:HG23	1:A:255:ILE:CD1	2.33	0.59
1:A:54:HIS:CD2	1:A:70:ILE:HD12	2.38	0.58
1:A:327:ILE:HD12	1:A:327:ILE:C	2.23	0.58
1:B:270:PHE:CZ	1:B:298:GLY:HA3	2.37	0.58
1:B:510:TYR:CD1	1:B:510:TYR:C	2.76	0.58
1:A:47:ILE:HD13	1:A:420:MET:CG	2.32	0.58
1:B:60:GLU:HG2	1:B:61:LYS:N	2.16	0.58
1:B:248:ALA:HB1	1:B:253:LEU:HB3	1.86	0.58
1:A:375:ARG:NH2	1:A:402:GLU:O	2.36	0.58
1:B:36:ARG:HD2	1:B:118:GLN:NE2	2.19	0.58
1:B:162:PRO:HG3	1:B:167:VAL:CG1	2.33	0.58
1:A:59:ALA:O	1:A:62:VAL:HG23	2.04	0.58
1:A:488:GLU:HG2	1:A:489:ALA:N	2.19	0.58
1:B:376:PHE:CE1	1:B:398:GLU:HB2	2.38	0.58
1:B:233:GLU:HB3	1:B:262:TYR:CD2	2.38	0.57
1:B:232:THR:HG21	1:B:292:GLU:HG3	1.87	0.57
1:B:379:ARG:HH22	1:B:381:PRO:HA	1.68	0.57
1:A:226:TYR:O	1:A:227:VAL:HG13	2.04	0.57
1:B:47:ILE:HD13	1:B:420:MET:CG	2.33	0.57
1:A:427:MET:O	1:A:430:ALA:N	2.35	0.57
1:A:55:HIS:N	1:A:69:GLU:O	2.35	0.57
1:B:351:ASP:O	1:B:355:LEU:HG	2.03	0.57
1:A:305:ARG:HG3	1:A:305:ARG:HH11	1.70	0.57
1:B:375:ARG:HG3	1:B:375:ARG:NH1	2.19	0.57
1:B:483:ASN:HD22	1:B:484:LEU:H	1.53	0.57
1:A:218:ILE:CD1	1:A:481:ILE:HD12	2.35	0.57
1:B:86:LEU:HA	1:B:89:ILE:HD12	1.86	0.57
1:B:178:PHE:CB	1:B:180:ILE:HD11	2.34	0.56
1:B:192:LEU:HA	1:B:198:TYR:HE2	1.68	0.56
1:A:110:TRP:CE2	1:A:164:SER:HB2	2.40	0.56
1:B:321:ALA:HB3	1:B:323:ARG:HG3	1.87	0.56
1:B:510:TYR:HD1	1:B:510:TYR:O	1.87	0.56
1:A:213:ARG:HG3	1:A:213:ARG:NH1	2.19	0.56
1:A:301:SER:CB	1:A:305:ARG:HH22	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:SER:O	1:A:319:GLY:N	2.37	0.56
1:B:172:GLN:CG	1:B:198:TYR:HB3	2.34	0.56
1:B:379:ARG:CB	1:B:379:ARG:HH11	2.18	0.56
1:A:507:ILE:CG2	1:A:508:ASP:N	2.68	0.56
1:A:211:GLN:N	1:A:479:TYR:OH	2.38	0.56
1:A:451:LEU:O	1:A:452:ASP:C	2.43	0.56
1:B:54:HIS:HD1	1:B:70:ILE:HA	1.69	0.56
1:B:471:GLU:HG3	1:B:472:LYS:H	1.70	0.56
1:A:192:LEU:HD13	1:A:201:PHE:CE2	2.41	0.56
1:A:499:THR:N	1:A:506:ASN:O	2.36	0.56
1:A:214:ALA:O	1:A:218:ILE:HG13	2.06	0.56
1:B:73:GLN:H	1:B:73:GLN:CD	2.09	0.56
1:B:85:THR:HG22	1:B:89:ILE:HD11	1.88	0.56
1:A:54:HIS:HB3	1:A:68:GLY:O	2.05	0.56
1:A:188:THR:O	1:A:208:ASP:OD2	2.24	0.56
1:A:82:MET:HG2	1:A:105:ILE:HD11	1.87	0.55
1:A:451:LEU:O	1:A:454:LEU:HB2	2.05	0.55
1:A:233:GLU:HG2	1:A:260:LYS:HD2	1.88	0.55
1:A:359:LEU:HD21	1:A:380:LEU:CD1	2.37	0.55
1:B:71:ARG:O	1:B:75:GLY:HA3	2.07	0.55
1:B:304:ARG:HG2	1:B:304:ARG:NH1	2.22	0.55
1:B:507:ILE:HG23	1:B:508:ASP:N	2.22	0.55
1:A:167:VAL:O	1:A:171:VAL:HG23	2.06	0.55
1:A:172:GLN:HG3	1:A:172:GLN:O	2.07	0.55
1:A:203:ARG:NE	1:A:474:ASP:OD1	2.39	0.55
1:A:480:ASP:OD1	1:A:499:THR:HG22	2.06	0.55
1:B:48:GLY:O	1:B:159:VAL:HA	2.07	0.55
1:B:206:PRO:HB3	1:B:210:LEU:HD23	1.88	0.55
1:B:427:MET:HB2	1:B:453:PHE:CD2	2.42	0.55
1:A:45:VAL:O	1:A:102:GLY:N	2.36	0.55
1:A:256:ALA:HB1	1:A:280:ARG:HE	1.72	0.55
1:A:351:ASP:O	1:A:355:LEU:HG	2.07	0.55
1:A:498:GLY:HA3	1:A:507:ILE:HA	1.87	0.55
1:B:50:LEU:HD21	1:B:122:PHE:CE2	2.42	0.55
1:A:379:ARG:NH1	1:A:381:PRO:HG3	2.22	0.55
1:A:482:MET:SD	1:A:496:HIS:HA	2.47	0.55
1:B:192:LEU:HA	1:B:198:TYR:HD2	1.70	0.54
1:B:379:ARG:O	1:B:393:VAL:HG13	2.07	0.54
1:B:71:ARG:NH2	1:B:74:TYR:HD2	2.05	0.54
1:B:78:ARG:O	1:B:82:MET:N	2.38	0.54
1:A:210:LEU:N	1:A:210:LEU:CD2	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:O	1:B:195:LYS:HE3	2.08	0.54
1:A:375:ARG:NH2	1:A:400:LEU:O	2.40	0.54
1:B:179:ASP:C	1:B:180:ILE:HD12	2.27	0.54
1:B:97:PRO:HB2	1:B:98:ASN:OD1	2.07	0.54
1:B:47:ILE:HG21	1:B:420:MET:HG2	1.90	0.54
1:A:67:CYS:SG	1:A:114:VAL:HG11	2.48	0.54
1:A:422:HIS:NE2	1:A:459:PHE:CD1	2.76	0.53
1:A:480:ASP:HB3	1:A:496:HIS:NE2	2.23	0.53
1:B:216:LEU:HD21	1:B:220:LYS:HD2	1.89	0.53
1:B:234:GLY:O	1:B:238:GLU:CB	2.56	0.53
1:B:194:ASP:OD2	1:B:194:ASP:C	2.45	0.53
1:B:261:ILE:CG2	1:B:295:THR:CG2	2.87	0.53
1:B:481:ILE:HG12	1:B:498:GLY:O	2.08	0.53
1:A:48:GLY:O	1:A:159:VAL:HA	2.08	0.53
1:B:232:THR:H	1:B:291:CYS:HA	1.73	0.53
1:A:169:ILE:HD12	1:A:192:LEU:HD21	1.89	0.53
1:A:315:ILE:HA	1:A:338:ILE:O	2.08	0.53
1:B:301:SER:O	1:B:305:ARG:HB2	2.07	0.53
1:B:235:ASN:O	1:B:239:SER:HB2	2.08	0.53
1:B:475:ALA:CB	1:B:476:PRO:HD2	2.20	0.53
1:B:467:VAL:HG12	1:B:468:TRP:N	2.24	0.53
1:A:259:ASP:OD1	1:A:260:LYS:N	2.42	0.52
1:B:207:SER:HB2	1:B:474:ASP:OD2	2.09	0.52
1:A:75:GLY:O	1:A:79:VAL:HG23	2.10	0.52
1:A:383:HIS:HD2	1:A:384:LEU:H	1.56	0.52
1:B:412:PHE:O	1:B:413:VAL:C	2.46	0.52
1:B:491:ARG:HG2	1:B:492:TYR:N	2.22	0.52
1:A:461:GLY:CA	1:A:465:GLU:HG2	2.31	0.52
1:B:276:LYS:O	1:B:279:GLU:HB2	2.10	0.52
1:B:320:TRP:CD1	1:B:320:TRP:C	2.80	0.52
1:B:483:ASN:HD22	1:B:484:LEU:N	2.06	0.52
1:A:87:ASP:OD2	1:A:364:ARG:NH1	2.36	0.52
1:B:79:VAL:HG13	1:B:105:ILE:HG21	1.92	0.52
1:A:213:ARG:CG	1:A:213:ARG:NH1	2.67	0.52
1:A:214:ALA:HB2	1:A:500:TRP:CE2	2.45	0.52
1:B:320:TRP:CD1	1:B:321:ALA:O	2.63	0.52
1:A:309:VAL:CG1	1:A:333:GLU:HA	2.39	0.52
1:A:480:ASP:HA	1:A:499:THR:HA	1.92	0.52
1:B:54:HIS:ND1	1:B:70:ILE:HA	2.24	0.52
1:A:45:VAL:O	1:A:46:ILE:HD13	2.09	0.52
1:A:164:SER:OG	1:A:165:SER:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:CYS:HB2	1:B:114:VAL:CG1	2.39	0.52
1:A:79:VAL:HG13	1:A:105:ILE:HG21	1.90	0.52
1:A:281:LEU:CB	1:A:282:PRO:HA	2.37	0.52
1:A:317:SER:C	1:A:319:GLY:N	2.63	0.52
1:A:480:ASP:HB3	1:A:499:THR:HG22	1.92	0.52
1:A:221:ARG:HG3	1:A:222:TYR:CE2	2.45	0.51
1:A:318:ASP:HA	1:A:340:ILE:O	2.09	0.51
1:B:55:HIS:CE1	1:B:71:ARG:NE	2.78	0.51
1:B:345:PRO:HG2	1:B:463:SER:HB3	1.91	0.51
1:B:231:HIS:O	1:B:231:HIS:ND1	2.43	0.51
1:A:383:HIS:CD2	1:A:385:LEU:H	2.28	0.51
1:A:475:ALA:CB	1:A:476:PRO:CD	2.74	0.51
1:B:52:SER:O	1:B:75:GLY:HA2	2.10	0.51
1:B:475:ALA:CB	1:B:476:PRO:CD	2.79	0.51
1:A:301:SER:OG	1:A:305:ARG:NH2	2.40	0.51
1:B:407:ASP:HB3	1:B:410:MET:HE2	1.93	0.51
1:B:197:LEU:C	1:B:198:TYR:CD1	2.84	0.51
1:A:162:PRO:HG3	1:A:167:VAL:HG12	1.92	0.51
1:A:164:SER:HB3	1:A:167:VAL:CG2	2.40	0.51
1:A:270:PHE:CE2	1:A:299:LEU:N	2.78	0.51
1:A:438:LEU:HD11	1:A:442:MET:HG2	1.92	0.51
1:B:261:ILE:HG23	1:B:261:ILE:O	2.11	0.51
1:B:315:ILE:HA	1:B:338:ILE:O	2.11	0.51
1:A:319:GLY:O	1:A:323:ARG:NH1	2.44	0.51
1:B:300:LEU:CD1	1:B:334:ALA:HB2	2.40	0.51
1:B:119:SER:O	1:B:122:PHE:HB2	2.11	0.50
1:A:320:TRP:HZ2	1:A:327:ILE:CG2	2.24	0.50
1:B:399:SER:OG	1:B:401:GLU:HG3	2.10	0.50
1:B:462:VAL:HG22	1:B:462:VAL:O	2.12	0.50
1:A:45:VAL:HG11	1:A:424:LEU:CD1	2.42	0.50
1:A:489:ALA:O	1:A:491:ARG:N	2.44	0.50
1:B:393:VAL:HG12	1:B:394:CYS:H	1.77	0.50
1:A:172:GLN:O	1:A:176:GLN:HG2	2.12	0.50
1:A:227:VAL:HG12	1:A:286:VAL:HB	1.93	0.50
1:B:216:LEU:HD13	1:B:247:LEU:HB3	1.93	0.50
1:A:162:PRO:HG2	1:A:167:VAL:HB	1.94	0.50
1:A:331:GLU:HB3	1:A:492:TYR:CD2	2.46	0.50
1:A:343:GLN:O	1:A:343:GLN:HG2	2.12	0.50
1:B:428:HIS:HB2	1:B:442:MET:SD	2.52	0.50
1:A:44:ASP:OD2	1:A:100:THR:HG23	2.11	0.50
1:A:317:SER:C	1:A:319:GLY:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HG21	1:A:414:ILE:CD1	2.42	0.50
1:B:400:LEU:H	1:B:400:LEU:CD1	2.11	0.50
1:A:347:VAL:HG21	1:A:414:ILE:HD11	1.94	0.50
1:B:36:ARG:CD	1:B:118:GLN:NE2	2.75	0.50
1:B:347:VAL:H	1:B:406:GLN:HE22	1.60	0.50
1:A:393:VAL:HG12	1:A:394:CYS:H	1.77	0.49
1:B:86:LEU:HD23	1:B:89:ILE:HD12	1.94	0.49
1:B:165:SER:O	1:B:166:SER:C	2.50	0.49
1:A:85:THR:OG1	1:A:414:ILE:HG23	2.12	0.49
1:A:241:MET:O	1:A:245:LYS:HG3	2.13	0.49
1:B:229:ALA:HB1	1:B:241:MET:HE1	1.91	0.49
1:A:324:ASP:HA	1:A:327:ILE:HD11	1.94	0.49
1:A:447:GLY:O	1:A:450:LEU:N	2.46	0.49
1:B:47:ILE:HG13	1:B:101:LEU:HD22	1.95	0.49
1:B:78:ARG:HA	1:B:81:ALA:HB3	1.94	0.49
1:B:270:PHE:HZ	1:B:295:THR:HA	1.77	0.49
1:A:106:ARG:HD3	1:A:118:GLN:OE1	2.13	0.49
1:B:369:PRO:HB2	1:B:385:LEU:CD1	2.42	0.49
1:A:407:ASP:HB3	1:A:410:MET:HB2	1.95	0.49
1:A:486:TYR:OH	1:A:490:ASN:ND2	2.45	0.49
1:A:216:LEU:HD13	1:A:247:LEU:HB3	1.93	0.49
1:A:226:TYR:CD2	1:A:283:LYS:HB3	2.47	0.49
1:A:438:LEU:HG	1:A:442:MET:HB3	1.94	0.49
1:A:510:TYR:CE1	1:A:511:LYS:HG3	2.47	0.49
1:B:413:VAL:O	1:B:416:ALA:HB3	2.13	0.49
1:A:280:ARG:HH21	1:A:284:ALA:CB	2.26	0.49
1:A:450:LEU:HD12	1:A:450:LEU:O	2.12	0.49
1:A:322:ASP:HA	1:A:494:TYR:CE2	2.48	0.49
1:B:95:LEU:HD12	1:B:96:LEU:N	2.27	0.48
1:B:208:ASP:HB3	1:B:240:GLY:HA2	1.95	0.48
1:B:484:LEU:HD12	1:B:493:ASP:O	2.13	0.48
1:A:56:GLN:HG3	1:A:57:PRO:O	2.14	0.48
1:A:74:TYR:O	1:A:78:ARG:HD2	2.13	0.48
1:A:156:ILE:HD13	1:A:156:ILE:N	2.26	0.48
1:A:221:ARG:HH12	1:A:507:ILE:HB	1.78	0.48
1:A:266:GLY:C	1:A:268:LYS:N	2.66	0.48
1:A:480:ASP:CB	1:A:499:THR:HG22	2.44	0.48
1:B:453:PHE:O	1:B:457:SER:OG	2.22	0.48
1:A:341:LYS:C	1:A:479:TYR:HB3	2.34	0.48
1:A:491:ARG:HD2	1:A:492:TYR:C	2.33	0.48
1:B:38:VAL:HG21	1:B:106:ARG:NH1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:N	1:A:398:GLU:OE1	2.46	0.48
1:A:256:ALA:HB1	1:A:280:ARG:NE	2.29	0.48
1:B:53:VAL:HG23	1:B:107:ASP:OD2	2.13	0.48
1:A:57:PRO:HB3	1:A:66:LYS:O	2.12	0.48
1:A:225:THR:HA	1:A:253:LEU:CD1	2.44	0.48
1:B:190:ILE:CD1	1:B:239:SER:O	2.58	0.48
1:A:500:TRP:CH2	1:A:503:GLY:N	2.74	0.48
1:B:180:ILE:N	1:B:180:ILE:CD1	2.61	0.48
1:B:383:HIS:CD2	1:B:384:LEU:N	2.82	0.48
1:A:192:LEU:HD23	1:A:198:TYR:HD2	1.73	0.48
1:B:169:ILE:HG13	1:B:198:TYR:CZ	2.49	0.48
1:B:172:GLN:OE1	1:B:201:PHE:HB2	2.13	0.48
1:A:213:ARG:HA	1:A:247:LEU:CD1	2.44	0.47
1:B:233:GLU:HG2	1:B:262:TYR:CE2	2.49	0.47
1:B:47:ILE:HG23	1:B:420:MET:HG2	1.95	0.47
1:B:78:ARG:O	1:B:81:ALA:N	2.46	0.47
1:B:461:GLY:N	1:B:465:GLU:O	2.46	0.47
1:A:362:ASN:HD21	1:A:365:ASN:HB3	1.79	0.47
1:A:393:VAL:HG12	1:A:394:CYS:N	2.28	0.47
1:B:178:PHE:C	1:B:180:ILE:HD12	2.35	0.47
1:A:38:VAL:HG12	1:A:39:ALA:N	2.29	0.47
1:A:320:TRP:NE1	1:A:494:TYR:OH	2.47	0.47
1:A:329:GLY:C	1:A:331:GLU:H	2.17	0.47
1:B:55:HIS:ND1	1:B:71:ARG:HD2	2.29	0.47
1:B:82:MET:HG2	1:B:105:ILE:CD1	2.43	0.47
1:B:199:LYS:HZ1	1:B:448:ARG:HH12	1.63	0.47
1:B:207:SER:O	1:B:210:LEU:HB3	2.14	0.47
1:B:490:ASN:C	1:B:490:ASN:HD22	2.16	0.47
1:A:209:THR:O	1:A:213:ARG:HB2	2.14	0.47
1:A:490:ASN:C	1:A:490:ASN:HD22	2.17	0.47
1:B:281:LEU:HB3	1:B:282:PRO:CA	2.44	0.47
1:A:305:ARG:HH11	1:A:305:ARG:CG	2.26	0.47
1:A:327:ILE:C	1:A:327:ILE:CD1	2.83	0.47
1:A:329:GLY:O	1:A:331:GLU:N	2.46	0.47
1:A:369:PRO:CB	1:A:383:HIS:HE1	2.27	0.47
1:A:379:ARG:O	1:A:381:PRO:HD3	2.15	0.47
1:B:74:TYR:O	1:B:78:ARG:HD2	2.14	0.47
1:B:339:THR:OG1	1:B:482:MET:HB2	2.14	0.47
1:A:216:LEU:HD23	1:A:217:ASP:OD1	2.14	0.47
1:B:38:VAL:HG12	1:B:39:ALA:N	2.29	0.47
1:B:72:GLU:HB2	1:B:371:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:SER:O	1:B:116:LEU:CB	2.63	0.47
1:B:197:LEU:HB3	1:B:198:TYR:CE1	2.50	0.47
1:B:297:ARG:HG3	1:B:326:VAL:O	2.15	0.47
1:B:330:TYR:N	1:B:330:TYR:HD1	2.10	0.47
1:B:459:PHE:CE1	1:B:467:VAL:HB	2.50	0.47
1:A:89:ILE:HG12	1:A:418:TYR:HE2	1.80	0.47
1:A:507:ILE:CG2	1:A:508:ASP:H	2.28	0.47
1:B:234:GLY:O	1:B:238:GLU:HB3	2.15	0.47
1:B:345:PRO:HG2	1:B:463:SER:CB	2.45	0.47
1:A:500:TRP:CZ2	1:A:503:GLY:CA	2.98	0.46
1:B:54:HIS:HA	1:B:69:GLU:O	2.15	0.46
1:B:212:ALA:HB2	1:B:290:PHE:CE1	2.50	0.46
1:B:364:ARG:O	1:B:366:PRO:HD3	2.15	0.46
1:B:379:ARG:HB2	1:B:379:ARG:CZ	2.44	0.46
1:B:415:ASN:ND2	1:B:467:VAL:HG21	2.23	0.46
1:B:446:ASP:OD1	1:B:446:ASP:C	2.52	0.46
1:A:364:ARG:O	1:A:366:PRO:HD3	2.16	0.46
1:A:280:ARG:NH2	1:A:284:ALA:H	2.13	0.46
1:B:294:MET:SD	1:B:294:MET:N	2.89	0.46
1:B:196:THR:OG1	1:B:197:LEU:N	2.48	0.46
1:B:383:HIS:O	1:B:386:GLU:HB2	2.15	0.46
1:B:469:PHE:N	1:B:469:PHE:CD1	2.82	0.46
1:A:47:ILE:CD1	1:A:420:MET:HG3	2.44	0.46
1:B:47:ILE:HD13	1:B:420:MET:HG3	1.97	0.46
1:A:61:LYS:C	1:A:63:PRO:HD2	2.35	0.46
1:B:62:VAL:HB	1:B:63:PRO:HD3	1.97	0.46
1:B:65:ARG:HH11	1:B:65:ARG:CG	2.28	0.46
1:B:70:ILE:HD13	1:B:371:PHE:HA	1.98	0.46
1:B:468:TRP:N	1:B:468:TRP:CD1	2.84	0.46
1:A:264:ASN:N	1:A:264:ASN:OD1	2.48	0.46
1:A:278:ARG:NH2	1:A:311:GLU:OE1	2.34	0.46
1:A:304:ARG:HG2	1:A:304:ARG:HH11	1.80	0.46
1:B:55:HIS:CE1	1:B:71:ARG:HD2	2.50	0.46
1:B:99:ILE:HD13	1:B:438:LEU:CD2	2.46	0.46
1:A:53:VAL:HG23	1:A:107:ASP:OD2	2.16	0.46
1:A:318:ASP:N	1:A:318:ASP:OD1	2.49	0.46
1:A:400:LEU:O	1:A:404:TYR:HB2	2.16	0.46
1:A:415:ASN:O	1:A:418:TYR:HB2	2.16	0.46
1:A:433:PRO:O	1:A:435:HIS:HD2	1.99	0.46
1:B:387:ASN:OD1	1:B:389:ASN:N	2.49	0.46
1:A:272:ARG:HG3	1:A:275:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:PHE:CD1	1:A:469:PHE:N	2.82	0.45
1:B:45:VAL:HB	1:B:101:LEU:HD23	1.97	0.45
1:B:510:TYR:CD1	1:B:510:TYR:O	2.68	0.45
1:A:210:LEU:O	1:A:213:ARG:HB3	2.16	0.45
1:A:221:ARG:HG3	1:A:222:TYR:CD2	2.51	0.45
1:A:450:LEU:O	1:A:454:LEU:HG	2.15	0.45
1:A:507:ILE:HG22	1:A:508:ASP:H	1.76	0.45
1:B:276:LYS:HD3	1:B:279:GLU:OE2	2.16	0.45
1:B:428:HIS:CG	1:B:428:HIS:O	2.68	0.45
1:A:162:PRO:HD2	1:A:168:ALA:HB2	1.98	0.45
1:A:162:PRO:CD	1:A:171:VAL:HG21	2.46	0.45
1:A:172:GLN:C	1:A:174:LEU:N	2.68	0.45
1:B:199:LYS:HZ3	1:B:448:ARG:HH12	1.64	0.45
1:B:201:PHE:C	1:B:202:LEU:HD23	2.37	0.45
1:B:195:LYS:HD3	1:B:198:TYR:O	2.16	0.45
1:B:387:ASN:HD21	1:B:389:ASN:HB2	1.79	0.45
1:B:500:TRP:HA	1:B:504:VAL:O	2.16	0.45
1:A:488:GLU:CG	1:A:489:ALA:N	2.79	0.45
1:B:206:PRO:HB3	1:B:476:PRO:O	2.16	0.45
1:A:278:ARG:HH11	1:A:278:ARG:CB	2.28	0.45
1:A:347:VAL:HG12	1:A:347:VAL:O	2.16	0.45
1:B:471:GLU:HG3	1:B:472:LYS:N	2.31	0.45
1:A:72:GLU:HG3	1:A:371:PHE:CZ	2.52	0.45
1:A:438:LEU:CD1	1:A:442:MET:HG2	2.46	0.45
1:B:234:GLY:O	1:B:238:GLU:HB2	2.17	0.45
1:A:341:LYS:O	1:A:479:TYR:HB3	2.16	0.45
1:A:350:PHE:CE2	1:A:354:PHE:HB2	2.52	0.45
1:B:505:LEU:HD21	1:B:507:ILE:HD13	1.99	0.45
1:A:167:VAL:O	1:A:170:GLN:HB3	2.17	0.45
1:B:96:LEU:N	1:B:97:PRO:HD3	2.32	0.45
1:B:285:ARG:HG3	1:B:312:PHE:HA	1.99	0.45
1:B:481:ILE:HG12	1:B:498:GLY:C	2.37	0.44
1:A:344:SER:HB2	1:A:412:PHE:CE2	2.52	0.44
1:B:301:SER:HB3	1:B:305:ARG:NH2	2.32	0.44
1:A:61:LYS:C	1:A:63:PRO:CD	2.85	0.44
1:A:300:LEU:HD13	1:A:334:ALA:HB2	1.98	0.44
1:A:471:GLU:CG	1:A:472:LYS:N	2.80	0.44
1:B:39:ALA:HB3	1:B:105:ILE:HB	2.00	0.44
1:B:316:GLY:O	1:B:339:THR:HA	2.16	0.44
1:A:300:LEU:CD1	1:A:334:ALA:HB2	2.48	0.44
1:B:61:LYS:O	1:B:64:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ALA:O	1:B:172:GLN:HB3	2.17	0.44
1:B:272:ARG:O	1:B:272:ARG:HG2	2.17	0.44
1:A:201:PHE:C	1:A:202:LEU:HD23	2.37	0.44
1:A:263:SER:HB2	1:A:292:GLU:OE2	2.17	0.44
1:A:447:GLY:O	1:A:448:ARG:C	2.55	0.44
1:B:241:MET:C	1:B:243:ALA:N	2.70	0.44
1:A:78:ARG:NE	1:A:407:ASP:OD1	2.50	0.44
1:A:110:TRP:CD1	1:A:110:TRP:O	2.71	0.44
1:A:232:THR:OG1	1:A:292:GLU:N	2.44	0.44
1:A:342:LEU:CA	1:A:479:TYR:HB3	2.44	0.44
1:A:376:PHE:CD2	1:A:398:GLU:HG2	2.52	0.44
1:B:51:PHE:C	1:B:108:SER:OG	2.56	0.44
1:B:230:VAL:O	1:B:291:CYS:SG	2.76	0.44
1:B:206:PRO:CB	1:B:210:LEU:HD23	2.48	0.44
1:B:414:ILE:O	1:B:417:ILE:HB	2.18	0.44
1:A:89:ILE:HD11	1:A:418:TYR:HD2	1.80	0.44
1:A:306:LEU:O	1:A:306:LEU:HG	2.18	0.44
1:A:327:ILE:HG22	1:A:334:ALA:CB	2.48	0.44
1:B:49:ALA:O	1:B:50:LEU:HD23	2.17	0.44
1:B:281:LEU:CB	1:B:282:PRO:HA	2.43	0.44
1:A:478:ARG:HE	1:A:501:HIS:CE1	2.36	0.43
1:B:70:ILE:HD13	1:B:371:PHE:CA	2.47	0.43
1:A:226:TYR:CE2	1:A:280:ARG:NH2	2.84	0.43
1:B:300:LEU:HA	1:B:303:MET:HG3	2.00	0.43
1:A:39:ALA:HB3	1:A:105:ILE:HB	2.00	0.43
1:A:206:PRO:HB3	1:A:477:GLY:HA3	2.00	0.43
1:B:230:VAL:CG1	1:B:273:LEU:HD21	2.44	0.43
1:A:373:GLN:NE2	1:A:386:GLU:HA	2.23	0.43
1:A:116:LEU:HD23	1:B:177:LEU:CD1	2.40	0.43
1:A:379:ARG:HB2	1:A:386:GLU:OE2	2.18	0.43
1:B:55:HIS:CG	1:B:71:ARG:HD2	2.53	0.43
1:B:76:ILE:HG21	1:B:371:PHE:CE2	2.54	0.43
1:B:176:GLN:HE21	1:B:176:GLN:HB2	1.35	0.43
1:A:51:PHE:CE1	1:A:78:ARG:HB3	2.54	0.43
1:A:304:ARG:HG2	1:A:304:ARG:NH1	2.33	0.43
1:A:488:GLU:CD	1:A:488:GLU:N	2.62	0.43
1:B:57:PRO:HG3	1:B:67:CYS:N	2.34	0.43
1:B:83:PHE:HD2	1:B:83:PHE:HA	1.70	0.43
1:B:164:SER:HB3	1:B:167:VAL:HG23	2.01	0.43
1:B:232:THR:HG21	1:B:292:GLU:CG	2.48	0.43
1:B:357:LEU:HD13	1:B:368:PHE:CZ	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:PHE:CD1	1:B:459:PHE:C	2.91	0.43
1:B:229:ALA:O	1:B:258:SER:HA	2.19	0.43
1:B:387:ASN:ND2	1:B:390:PHE:CZ	2.87	0.43
1:B:423:GLY:HA3	1:B:454:LEU:HD23	2.01	0.43
1:A:90:ASN:OD1	1:A:101:LEU:N	2.41	0.43
1:A:484:LEU:HD12	1:A:493:ASP:O	2.18	0.43
1:B:41:MET:HB3	1:B:103:SER:H	1.84	0.43
1:B:172:GLN:CA	1:B:172:GLN:NE2	2.74	0.43
1:B:365:ASN:OD1	1:B:365:ASN:O	2.36	0.43
1:A:82:MET:HG2	1:A:105:ILE:CD1	2.49	0.43
1:B:56:GLN:HB3	1:B:109:CYS:O	2.19	0.43
1:A:281:LEU:HD21	1:A:284:ALA:O	2.19	0.43
1:A:438:LEU:CG	1:A:442:MET:HG2	2.49	0.43
1:A:211:GLN:CG	1:A:340:ILE:HG21	2.45	0.42
1:B:52:SER:O	1:B:75:GLY:CA	2.66	0.42
1:B:483:ASN:O	1:B:495:VAL:N	2.51	0.42
1:A:488:GLU:HG2	1:A:489:ALA:H	1.84	0.42
1:B:335:ASN:OD1	1:B:485:GLN:HA	2.18	0.42
1:A:74:TYR:N	1:A:74:TYR:CD1	2.88	0.42
1:A:195:LYS:HA	1:A:195:LYS:CE	2.43	0.42
1:B:195:LYS:NZ	1:B:473:GLY:HA3	2.34	0.42
1:B:285:ARG:HG3	1:B:311:GLU:O	2.18	0.42
1:B:507:ILE:CG2	1:B:508:ASP:N	2.82	0.42
1:A:49:ALA:O	1:A:50:LEU:HD23	2.19	0.42
1:A:272:ARG:HH11	1:A:272:ARG:HD3	1.60	0.42
1:A:342:LEU:H	1:A:342:LEU:CD1	2.26	0.42
1:A:406:GLN:O	1:A:407:ASP:C	2.58	0.42
1:B:205:VAL:HG23	1:B:206:PRO:CD	2.41	0.42
1:B:342:LEU:HD21	1:B:412:PHE:CE2	2.46	0.42
1:B:387:ASN:OD1	1:B:387:ASN:C	2.58	0.42
1:A:77:GLN:O	1:A:81:ALA:HB2	2.19	0.42
1:B:261:ILE:HG12	1:B:270:PHE:CE2	2.55	0.42
1:B:427:MET:HG3	1:B:453:PHE:CE2	2.54	0.42
1:A:235:ASN:OD1	1:A:235:ASN:O	2.38	0.42
1:A:368:PHE:HB3	1:A:369:PRO:HD3	2.01	0.42
1:A:510:TYR:CD1	1:A:511:LYS:HG3	2.55	0.42
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.89	0.42
1:A:270:PHE:CE2	1:A:298:GLY:C	2.93	0.42
1:A:394:CYS:HB3	1:A:398:GLU:OE2	2.19	0.42
1:B:44:ASP:N	1:B:100:THR:OG1	2.53	0.42
1:B:202:LEU:N	1:B:202:LEU:CD2	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG21	1:A:106:ARG:NH1	2.34	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.77	0.42
1:B:243:ALA:C	1:B:245:LYS:N	2.73	0.42
1:A:191:ASP:OD2	1:A:235:ASN:OD1	2.38	0.42
1:A:226:TYR:CE2	1:A:283:LYS:HB3	2.54	0.42
1:A:443:LYS:HA	1:A:444:PRO:HA	1.78	0.42
1:B:53:VAL:O	1:B:70:ILE:HA	2.20	0.42
1:B:77:GLN:O	1:B:81:ALA:HB2	2.19	0.42
1:B:379:ARG:NH2	1:B:381:PRO:CA	2.77	0.42
1:A:96:LEU:HB3	1:A:99:ILE:HB	2.02	0.42
1:A:172:GLN:HB2	1:A:172:GLN:HE21	1.49	0.42
1:A:176:GLN:HE21	1:A:176:GLN:HB2	1.49	0.42
1:A:221:ARG:NH1	1:A:507:ILE:HB	2.34	0.42
1:A:231:HIS:CE1	1:A:260:LYS:HB3	2.55	0.42
1:A:296:VAL:O	1:A:300:LEU:HG	2.20	0.42
1:A:452:ASP:C	1:A:454:LEU:H	2.23	0.42
1:B:278:ARG:NH1	1:B:278:ARG:HB3	2.35	0.42
1:A:172:GLN:HE22	1:A:201:PHE:CA	2.33	0.41
1:A:431:LEU:C	1:A:433:PRO:HD3	2.39	0.41
1:B:58:PRO:HB2	1:B:60:GLU:OE1	2.20	0.41
1:B:267:GLU:O	1:B:271:ASP:HB2	2.20	0.41
1:A:77:GLN:O	1:A:81:ALA:CB	2.68	0.41
1:A:202:LEU:N	1:A:202:LEU:CD2	2.79	0.41
1:A:222:TYR:O	1:A:223:ASN:HB2	2.19	0.41
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.91	0.41
1:B:106:ARG:HD3	1:B:118:GLN:OE1	2.20	0.41
1:B:387:ASN:CG	1:B:390:PHE:CE1	2.93	0.41
1:B:393:VAL:CG1	1:B:394:CYS:N	2.81	0.41
1:B:169:ILE:HG22	1:B:170:GLN:N	2.35	0.41
1:B:241:MET:O	1:B:243:ALA:N	2.53	0.41
1:B:317:SER:HA	1:B:340:ILE:HB	2.02	0.41
1:B:378:CYS:HB2	1:B:392:LYS:O	2.21	0.41
1:A:342:LEU:HD11	1:A:409:LYS:HE3	2.03	0.41
1:B:98:ASN:OD1	1:B:98:ASN:N	2.52	0.41
1:B:320:TRP:O	1:B:321:ALA:HB3	2.20	0.41
1:B:368:PHE:HA	1:B:371:PHE:HB3	2.02	0.41
1:B:375:ARG:NH1	1:B:375:ARG:CG	2.81	0.41
1:B:459:PHE:HD1	1:B:460:VAL:O	2.03	0.41
1:A:350:PHE:HD2	1:A:351:ASP:OD2	2.04	0.41
1:B:163:GLY:O	1:B:186:SER:HB2	2.21	0.41
1:B:192:LEU:HD22	1:B:201:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:O	1:B:213:ARG:HB2	2.20	0.41
1:B:328:GLU:HA	1:B:331:GLU:OE2	2.21	0.41
1:A:384:LEU:C	1:A:384:LEU:HD23	2.41	0.41
1:B:70:ILE:HD13	1:B:371:PHE:HB2	2.03	0.41
1:B:70:ILE:CD1	1:B:371:PHE:HB2	2.50	0.41
1:A:89:ILE:CG1	1:A:418:TYR:CE2	3.01	0.41
1:A:185:TYR:CD1	1:A:413:VAL:HG22	2.56	0.41
1:A:189:SER:CA	1:A:208:ASP:OD2	2.65	0.41
1:A:358:ARG:HG2	1:A:359:LEU:N	2.35	0.41
1:A:56:GLN:HG3	1:A:57:PRO:N	2.35	0.41
1:A:335:ASN:C	1:A:337:GLY:H	2.24	0.41
1:B:411:GLY:O	1:B:412:PHE:C	2.57	0.41
1:A:232:THR:HG21	1:A:292:GLU:CB	2.51	0.41
1:A:232:THR:HG21	1:A:292:GLU:CG	2.51	0.41
1:A:294:MET:O	1:A:297:ARG:N	2.54	0.41
1:A:342:LEU:HD12	1:A:342:LEU:N	2.32	0.41
1:A:365:ASN:HA	1:A:366:PRO:HD2	1.90	0.41
1:A:435:HIS:CD2	1:A:435:HIS:N	2.89	0.41
1:B:198:TYR:CD1	1:B:198:TYR:N	2.87	0.41
1:B:205:VAL:CG2	1:B:206:PRO:HD2	2.39	0.41
1:B:355:LEU:C	1:B:357:LEU:H	2.24	0.41
1:B:373:GLN:OE1	1:B:387:ASN:HB3	2.21	0.41
1:A:96:LEU:N	1:A:97:PRO:HD3	2.36	0.41
1:A:261:ILE:HG12	1:A:262:TYR:N	2.36	0.41
1:A:274:LEU:HD11	1:A:312:PHE:CE2	2.56	0.41
1:A:347:VAL:O	1:A:406:GLN:NE2	2.54	0.41
1:B:172:GLN:HB2	1:B:182:GLN:OE1	2.21	0.41
1:B:209:THR:HG22	1:B:243:ALA:CB	2.50	0.40
1:A:421:ALA:O	1:A:424:LEU:HB2	2.22	0.40
1:B:309:VAL:HG22	1:B:333:GLU:HB3	2.01	0.40
1:B:449:LYS:C	1:B:451:LEU:N	2.75	0.40
1:A:122:PHE:HB3	1:A:156:ILE:HG13	2.04	0.40
1:A:320:TRP:O	1:A:321:ALA:HB3	2.21	0.40
1:A:112:SER:HB3	1:A:170:GLN:HE21	1.85	0.40
1:A:166:SER:O	1:A:169:ILE:HB	2.22	0.40
1:A:172:GLN:O	1:A:173:ASN:C	2.59	0.40
1:A:483:ASN:ND2	1:A:484:LEU:N	2.67	0.40
1:A:490:ASN:ND2	1:A:490:ASN:C	2.75	0.40
1:B:72:GLU:OE2	1:B:375:ARG:HD2	2.22	0.40
1:B:320:TRP:C	1:B:320:TRP:HD1	2.24	0.40
1:B:383:HIS:HD2	1:B:384:LEU:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:O	1:A:281:LEU:HG	2.22	0.40
1:B:218:ILE:HD13	1:B:338:ILE:HG21	2.04	0.40
1:B:318:ASP:O	1:B:321:ALA:HB2	2.22	0.40
1:B:323:ARG:HH21	1:B:325:GLU:CD	2.25	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	444/490 (91%)	379 (85%)	58 (13%)	7 (2%)	9 44
1	B	444/490 (91%)	390 (88%)	50 (11%)	4 (1%)	17 55
All	All	888/980 (91%)	769 (87%)	108 (12%)	11 (1%)	13 49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA
1	B	68	GLY
1	A	330	TYR
1	A	490	ASN
1	B	385	LEU
1	A	318	ASP
1	A	453	PHE
1	A	487	THR
1	A	163	GLY
1	B	473	GLY
1	B	475	ALA

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	384/422 (91%)	337 (88%)	47 (12%)	5 23
1	B	384/422 (91%)	345 (90%)	39 (10%)	7 28
All	All	768/844 (91%)	682 (89%)	86 (11%)	6 25

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	86	LEU
1	A	92	ASP
1	A	98	ASN
1	A	156	ILE
1	A	172	GLN
1	A	173	ASN
1	A	176	GLN
1	A	188	THR
1	A	195	LYS
1	A	198	TYR
1	A	202	LEU
1	A	210	LEU
1	A	213	ARG
1	A	216	LEU
1	A	233	GLU
1	A	236	TYR
1	A	238	GLU
1	A	239	SER
1	A	242	ASP
1	A	250	GLN
1	A	270	PHE
1	A	280	ARG
1	A	290	PHE
1	A	312	PHE
1	A	313	SER
1	A	325	GLU

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	344	SER
1	A	368	PHE
1	A	383	HIS
1	A	386	GLU
1	A	408	SER
1	A	438	LEU
1	A	439	CYS
1	A	440	ASP
1	A	452	ASP
1	A	459	PHE
1	A	465	GLU
1	A	478	ARG
1	A	479	TYR
1	A	480	ASP
1	A	483	ASN
1	A	488	GLU
1	A	490	ASN
1	A	491	ARG
1	A	506	ASN
1	B	54	HIS
1	B	95	LEU
1	B	98	ASN
1	B	172	GLN
1	B	173	ASN
1	B	176	GLN
1	B	185	TYR
1	B	186	SER
1	B	190	ILE
1	B	198	TYR
1	B	202	LEU
1	B	205	VAL
1	B	227	VAL
1	B	242	ASP
1	B	259	ASP
1	B	262	TYR
1	B	270	PHE
1	B	289	CYS
1	B	290	PHE
1	B	312	PHE
1	B	318	ASP
1	B	322	ASP

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Mol	Chain	Res	Type
1	B	324	ASP
1	B	326	VAL
1	B	328	GLU
1	B	333	GLU
1	B	360	ASP
1	B	368	PHE
1	B	379	ARG
1	B	390	PHE
1	B	399	SER
1	B	440	ASP
1	B	465	GLU
1	B	474	ASP
1	B	483	ASN
1	B	488	GLU
1	B	490	ASN
1	B	507	ILE
1	B	508	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	173	ASN
1	A	176	GLN
1	A	211	GLN
1	A	231	HIS
1	A	383	HIS
1	A	406	GLN
1	A	426	ASN
1	A	435	HIS
1	A	483	ASN
1	A	485	GLN
1	A	490	ASN
1	B	55	HIS
1	B	73	GLN
1	B	170	GLN
1	B	173	ASN
1	B	176	GLN
1	B	250	GLN
1	B	264	ASN
1	B	362	ASN
1	B	383	HIS

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Mol	Chain	Res	Type
1	B	406	GLN
1	B	415	ASN
1	B	483	ASN
1	B	490	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	448/490 (91%)	-0.52	0	100	100	21, 37, 69, 88	0
1	B	448/490 (91%)	-0.56	0	100	100	17, 30, 51, 67	0
All	All	896/980 (91%)	-0.54	0	100	100	17, 33, 59, 88	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.